BIGSdb Documentation

Release 1.24.0

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Gene-by-gene population annotation and analysis

BIGSdb is software designed to store and analyse sequence data for bacterial isolates. Any number of sequences can be linked to isolate records - these can be small contigs assembled from dideoxy sequencing through to whole genomes (complete or multiple contigs generated from parallel sequencing technologies such as 454 or Illumina).

BIGSdb extends the principle of MLST to genomic data, where large numbers of loci can be defined, with alleles assigned by reference to sequence definition databases (which can also be set up with BIGSdb). Loci can also be grouped into schemes so that types can be defined by combinations of allelic profiles, a concept analagous to MLST.

The software has been released under the GNU General Public Licence version 3. The latest version of this documentation can be found at http://bigsdb.readthedocs.org/.

CHAPTER 1

Concepts and terms

1.1 BIGSdb

BIGSdb is the software platform - not a specific database. There are many instances of BIGSdb databases, so referring to 'the BIGSdb' is meaningless.

1.2 Loci

Loci are regions of the genome that are identified by similarity to a known sequence. They can be defined by DNA or peptide sequence. They are often complete coding sequences (genes), but may represent gene fragments (such as used in MLST), antigenic peptide loops, or indeed any sequence feature.

In versions of BIGSdb prior to 1.8.0, an isolate record could only have one live *allele* designation for a locus (inactive/pending designations could be stored within the database but were unavailable for querying or analysis purposes). Since biology is rarely so clean, and some genomes may contain more than one copy of a gene, later versions of the software allow multiple allele designations for a locus, all of which can be queried and analysed.

Paralogous loci can be difficult to differentiate by sequence similarity alone. Because of this, loci can be further defined by context, where in silico PCR or hybridization reactions can be performed to *filter the genome* to specific regions based on sequence external to the locus.

1.3 Alleles

Alleles are instances of loci. Every unique sequence, either DNA or peptide depending on the locus, is defined as a new allele and these are defined in a sequence definition database, where they are given an allele identifier. These identifiers are usually integers, but can be text strings. Allele identifiers in text format can be constrained by length and formatting.

When a specific allele of a locus is identified within the sequence data of an isolate record, the allele designation, i.e. identifier, is associated with the isolate record. This efficiently stores the sequence variation found within an isolate.

Two isolates with the same allele designation for a locus have identical sequences at that locus. Once the sequence variation within a genome has been reduced to a series of allele designations, genomes can be efficiently compared by identifying which loci vary between them.

It is important to note that allele identifiers are usually arbitrary and are allocated sequentially in the order of discovery. Alleles with adjacent identifiers may vary by a single nucleotide or by many.

1.4 Schemes

Schemes are collections of loci that may be associated with additional field values. At their simplest they just group loci together. Example uses of simple schemes include:

- Antibiotic resistance genes
- · Genes involved in specific biochemical pathways
- Antigens
- Vaccine components
- Whole genome MLST (wgMLST)

When schemes are associated with additional fields, one of these fields must be the primary key, i.e. its value uniquely defines a particular combination of alleles at its member loci. The pre-eminent example of this is MLST - where a sequence type (ST) is the primary key that uniquely defines combinations of alleles that make up the MLST profiles. Additional fields can also then be included. The values for these need not be unique. In the MLST example, a field for clonal complex can be included, and the same value for this can be set for multiple STs.

1.5 Profiles

Profiles are instances of *schemes*. A profile consists of a set of *allele identifiers* for the *loci* that comprise the scheme. If the scheme has a primary key field, e.g. sequence type (ST) in MLST schemes, then the unique combination of alleles in a complete profile can be defined by the value of this field.

1.6 Classification groups

Classification groups are a way to cluster scheme profiles using a specified threshold of pairwise allelic mismatches. Currently, single-linkage clustering is supported whereby each member of a group must have no more than the specified number of allelic differences with at least one other member of the group.

1.7 Sequence tags

Sequence tags record locus position within an isolate record's sequence bin. The process of creating these tags, is known as *tag-scanning*. A sequence tag consists of:

- · sequence bin id this identifies a particular contig
- locus name
- start position
- end position

- flag to indicate if sequence is reversed
- flag to indicate if sequence is complete and does not continue off the end of the contig

1.8 Sets

Sets provide a means to take a large database with multiple loci and/or schemes and present a subset of these as though it was a complete database. The loci and schemes chosen to belong to a set can be renamed when used with this set. The rationale for this is that in a database with disparate isolates and a large number of loci, the naming of these loci may have to be long to specify a species name. For example, you may have a database that contains multiple MLST schemes for different species, but since these schemes may use different fragments of the same genes they may have to be named something like 'Streptococcus_pneumoniae_MLST_aroE' to uniquely specify them. If we define a set for 'Streptococcus pneumoniae' we can then choose to only include S. pneumoniae loci and therefore shorten their names, e.g. to 'aroE'.

Additional metadata fields can also be associated with each set so it is possible to have a database containing genomes from multiple species and a generic set of metadata, then have additional specific metadata fields for particular species or genera. These additional fields only become visible and searchable when the specific set that they belong to has been selected.

CHAPTER 2

BIGSdb dependencies

2.1 Required packages

BIGSdb requires a number of software components to be installed:

2.1.1 Linux packages

- Apache2 web server with mod_perl2
- PostgreSQL database 9.5+
- Perl 5.10+
- BioPerl
- BLAST+
- EMBOSS
 - infoalign use to extract alignment stats in Genome Comparator.
 - sixpack used to translate sequences in multiple reading frames.
 - stretcher used for sequence alignment in allele query.
- Ipcress part of exonerate package used to simulate PCR reactions which can be used to filter the genome to predicted amplification products.
- Xvfb X virtual framebuffer needed to support SplitsTree in command line mode as used in Genome Comparator.

2.1.2 Perl modules

These are included with most Linux distributions.

• Archive::Zip - Used to upload to iTOL.

- Bio::Biblio This used to be part of BioPerl but will need to be installed separately if using BioPerl 1.6.920 or later.
- CGI (version 4.04+) Common Gateway Interface requests and responses (used to be a core module but recently removed).
- Config::Tiny Configuration file handling.
- Crypt::Eksblowfish::Bcrypt Used for password hashing.
- Data::Random
- Data::UUID Globally unique identifer handling for preference storage.
- DBD::Pg PostgreSQL database driver for DBI.
- DBI Database independent interface module used to interact with databases.
- Email::MIME Used to format E-mail messages.
- Email::Sender Used to send E-mail messages by submission system.
- Email::Valid Used to validate E-mails sent by job manager.
- Excel::Writer::XLSX Used to export data in Excel format.
- Exception::Class Exception handing.
- IO::String
- JSON Used to manipulate JSON data.
- List::MoreUtils (version 0.28+).
- Log::Dispatch::File Object for logging to file.
- Log::Log4perl Configurable status and error logging.
- LWP::UserAgent Used to upload via API
- Net::Oauth Required for REST authentication (this needs to be installed even if you are not using REST).
- Parallel::ForkManager Required for multi-threading tools and plugins.
- Time::Duration Used by Job Viewer to display elapsed time in rounded units.
- Try::Tiny
- XML::Parser::PerlSAX part of libxml-perl Used to parse XML configuration files.

2.1.3 Optional packages

Installing these packages will enable extra functionality, but they are not required by the core BIGSdb package.

- ChartDirector (Perl) library used for generating charts. Used by some plugins.
- ImageMagick mogrify used by some plugins.
- MAFFT 6.8+ sequence alignment used by some plugins.
- Muscle sequence alignment used by some plugins.
- Splitstree4 used by GenomeComparator plugin.

CHAPTER 3

Installation and configuration of BIGSdb

3.1 Software installation

BIGSdb consists of two main Perl scripts, bigsdb.pl and bigscurate.pl, that run the query and curator's interfaces respectively. These need to be located somewhere within the web cgi-bin directories. In addition, there are a large number of library files, used by both these scripts, that are installed by default in /usr/local/lib/BIGSdb. Plugin scripts are stored within a 'Plugins' sub-directory of this library directory.

All databases on a system can use the same instance of the scripts, or alternatively any database can specify a particular path for each script, enabling these script directories to be protected by apache htaccess directives.

- Software requirements
- Download from SourceForge.net or GitHub.
- 1. Unpack the distribution package in a temporary directory:

```
gunzip bigsdb_1.x.x.tar.gz
tar xvf bigsdb_1.x.x.tar
```

- 2. Copy the bigsdb.pl and bigscurate.pl scripts to a subdirectory of your web server's cgi-bin directory. Make sure these are readable and executable by the web server daemon.
- Copy the contents of the lib directory to /usr/local/lib/BIGSdb/. Make sure you include the Plugins and Offline directories which are subdirectories of the main lib directory.
- Copy the javascript directory to the root directory of your website, i.e. accessible from http://your_website/ javascript/.
- 5. Copy the css directory to root directory of your website, i.e. accessible from http://your_website/css/.
- Copy the webfonts directory to the root directory of your website, i.e. accessible from http://your_website/ webfonts/.
- 7. Copy the images directory to the root directory of your website, i.e. accessible from http://your_website/images/.
- 8. Copy the contents of the conf directory to /etc/bigsdb/. Check the paths of helper applications and database names in the bigsdb.conf file and modify for your system.

9. Create a PostgreSQL database user called apache - this should not have any special priveleges. First you will need to log in as the postgres user:

sudo su postgres

Then use the createuser command to do this, e.g.

createuser apache

From the psql command line, set the apache user password:

```
psql
ALTER ROLE apache WITH PASSWORD 'remote';
```

10. Create PostgreSQL databases called bigsdb_auth, bigsdb_prefs and bigsdb_refs using the scripts in the sql directory. Create the database using the createdb command and set up the tables using the psql command.

```
createdb bigsdb_auth
psql -f auth.sql bigsdb_auth
createdb bigsdb_prefs
psql -f prefs.sql bigsdb_prefs
createdb bigsdb_refs
psql -f refs.sql bigsdb_refs
```

- 11. Create a writable temporary directory in the root of the web site called tmp, i.e. accessible from http://your_website/tmp.
- 12. Create a log file, bigsdb.log, in /var/log owned by the web server daemon, e.g.

```
touch /var/log/bigsdb.log
chown www-data /var/log/bigsdb.log
```

(substitute www-data for the web daemon user).

3.2 Configuring PostgreSQL

PostgreSQL can be configured in many ways and how you do this will depend on your site requirements.

The following security settings will allow the appropriate users 'apache' and 'bigsdb' to access databases without allowing all logged in users full access. Only the UNIX users 'postgres' and 'webmaster' can log in to the databases as the Postgres user 'postgres'.

You will need to edit the pg_hba.conf and pg_ident.conf files. These are found somewhere like /etc/postgresql/9.1/main/

3.2.1 pg_hba.conf

```
# Database administrative login by UNIX sockets
local all postgres ident map=mymap
# TYPE DATABASE USER CIDR-ADDRESS METHOD
# "local" is for Unix domain socket connections only
local all all ident map=mymap
```

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# IPv4	local c	onnections:			
host	all	all	127.0.0.1/32	md5	
# IPv6	local c	onnections:			
host	all	all	::1/128	md5	

3.2.2 pg_ident.conf

# MAPNAME	SYSTEM-USERNAME	PG-USERNAME
mymap	postgres	postgres
mymap	webmaster	postgres
mymap	www-data	apache
mymap	bigsdb	bigsdb
mymap	bigsdb	apache

You may also need to change some settings in the postgresql.conf file. As an example, a configuration for a machine with 16GB RAM, allowing connections from a separate web server may have the following configuration changes made:

```
listen_addresses = '*'
max_connections = 200
shared_buffers = 1024Mb
work_mem = 8Mb
effective_cache_size = 8192Mb
stats_temp_directory = '/dev/shm'
```

Setting stats_temp_directory to /dev/shm makes use of a ramdisk usually available on Debian or Ubuntu systems for frequently updated working files. This reduces a lot of unneccessary disk access.

See Tuning Your PostgreSQL Server for more details.

Restart PostgreSQL after any changes, e.g.

/etc/init.d/postgresql restart

3.3 Setting global connection parameters

Global database connection parameters can be entered in /etc/bigsdb/db.conf. This allows you to set default values for the host, port, user and password. Default values are as follows:

- · dbhost: localhost
- dbport: 5432
- dbuser: apache
- · dbpassword: remote

These can all be over-ridden in individual *database configuration config.xml files* using the terms host, port, user, and password.

3.4 Site-specific configuration

Site-specific configuration files are located in /etc/bigsdb by default.

- bigsdb.conf main configuration file
- logging.conf error logging settings. See log4perl project website for advanced configuration details.

The dropdown menu can be customized by modifying the menu_header.html file located in /etc/bigsdb. Any HTML in this file will be inserted at the top of the menu. The included file displays the BIGSdb logo hyperlinked to the root of the web site. This file can be edited as you wish, or alternatively menu_header.html can be placed in the root directory of the web site - this will be used in preference to the version in /etc/bigsdb.

3.5 Setting up the offline job manager

To run plugins that require a long time to complete their analyses, an offline job manager has been developed. The plugin will save the parameters of a job to a job database and then provide a link to the job status page. An offline script, run frequently from CRON, will then process the job queue and update status and outputs via the job status page.

1. Create a 'bigsdb' UNIX user, e.g.:

sudo useradd -s /bin/sh bigsdb

2. As the postgres user, create a 'bigsdb' user and create a bigsdb_jobs database using the jobs.sql SQL file, e.g.:

```
createuser bigsdb [no need for special priveleges]
createdb bigsdb_jobs
psql -f jobs.sql bigsdb_jobs
```

From the psql command line, set the bigsdb user password::

```
psql
ALTER ROLE bigsdb WITH PASSWORD 'bigsdb';
```

3. Set up the jobs parameters in the /etc/bigsdb/bigsdb.conf file, e.g.:

```
jobs_db=bigsdb_jobs
max_load=8
```

The jobs script will not process a job if the server's load average (over the last minute) is higher than the max_load parameter. This should be set higher than the number of processor cores or you may find that jobs never run on a busy server. Setting it to double the number of cores is probably a good starting point.

- 4. Copy the job_logging.conf file to the /etc/bigsdb directory.
- 5. Set the script to run frequently (preferably every minute) from CRON.

Copy bigsjobs.pl to /usr/local/bin

You should install xvfb, which is a virtual X server that may be required for third party applications called from plugins. This is required, for example, for calling splitstree4 from the Genome Comparator plugin.

Add the following to /etc/crontab::

* * * * * bigsdb xvfb-run -a /usr/local/bin/bigsjobs.pl

(set to run every minute from the 'bigsdb' user account).

If you'd like to run this more frequently, e.g. every 30 seconds, multiple entries can be added to CRON with an appropriate sleep prior to running, e.g.:

* * * * bigsdb xvfb-run -a /usr/local/bin/bigsjobs.pl * * * * bigsdb sleep 30;xvfb-run -a /usr/local/bin/bigsjobs.pl

6. Create a log file, bigsdb_jobs.log, in /var/log owned by 'bigsdb', e.g.:

```
sudo touch /var/log/bigsdb_jobs.log
sudo chown bigsdb /var/log/bigsdb_jobs.log
```

3.6 Setting up the submission system

The submission system allows users to submit new data to the database for curation. Submissions are placed in a queue for a curator to upload. All communication between submitters and curators can occur via the submission system.

 Create a writable submissions directory in the root of the web site called submissions, i.e. accessible from http: //your_website/submissions. This is used for file uploads. The directory should be writable by the Apache web daemon (user 'www-data' on Debian/Ubuntu systems). If you are running the *RESTful interface* the directory should also be writable by the bigsdb user. To ensure this, make the directory group-writable and add the bigsdb user to the apache group ('www-data' on Debian/Ubuntu systems). If you will be allowing submissions via the RESTful interface, you should also add the apache user ('www-data' on Debian/Ubuntu systems) to the bigsdb group, e.g.

```
sudo usermod -a -G www-data bigsdb
sudo usermod -a -G bigsdb www-data
```

The actual directory can be outside of the web root and made accessible using a symlink provided your Apache configuration allows this, e.g. the default location is /var/submissions symlinked to /var/www/submissions (assuming your web site is located in /var/www), e.g.

```
sudo touch /var/submissions
sudo chown www-data:www-data /var/submissions
sudo chmod 775 /var/submissions
sudo ln -s /var/submissions /var/www
```

- 2. Set the submission_dir location in bigsdb.conf.
- 3. Set the smtp_server in bigsdb.conf to the IP or DNS name of your organisation's SMTP relay. Depending on how your E-mail system is configured, you may be able to use the localhost address (127.0.0.1).
- 4. Make sure the curate_script and query_script values are set in bigsdb.conf. These point to the web-accessible location of the web scripts and are required to allow curators to be directed between the web interfaces as needed.
- 5. Set submissions="yes" in the system tag of the *database config.xml file* of each database for which submissions should be enabled.

3.7 Setting up a site-wide user database

A site-wide user database allows users to register themselves for accounts and associate these with specific databases. It means that a single set of log-in credentials can be used across databases, rather than each database maintaining its own.

Users can access/update their account details by calling the bigsdb.pl script without any additional attributes, e.g. http://website/cgi-bin/bigsdb.pl.

Site admins can access administration features by calling the bigscurate.pl script without any additional attributes.

1. Create a user database, e.g. pubmlst_bigsdb_users:

```
createdb pubmlst_bigsdb_users
psql -f users.sql pubmlst_bigsdb_users
```

Set up sync_user_dbase_users.pl to run every hour as a CRON JOB, e.g. in /etc/crontab, add the following to run this at 5 minutes past each hour

```
05 * * * * bigsdb /usr/local/bin/sync_user_dbase_users.pl --user_database_

ubmlst_bigsdb_users
```

Add the user database details to each database that you want to allow to use it.

You need to add the users database details to each client database that will use it.

2. If you want to allow users to register themselves you need to modify bigsdb.conf.

You can define multiple user databases (as a comma-separated list) but usually you would have just one. Define this using the site_user_dbs attribute. Use a short domain (site) name separated by a pipe (l) and the name of the database, e.g. add the following to /etc/bigsdb.conf:

site_user_dbs=PubMLST|pubmlst_bigsdb_users

Make sure default database connection parameters are set in /etc/bigsdb/db.conf.

3. Set up site admin user in new user database. This has to be done manually - other users will either be able to register themselves or be created by curators from other databases.:

```
psql pubmlst_bigsdb_users
INSERT INTO USERS (user_name,surname,first_name,email,affiliation,
    date_entered,datestamp,status) VALUES ('kjolley','Jolley','Keith',
    'keith.jolley@zoo.ox.ac.uk','University of Oxford, UK','now','now',
    'validated');
```

Set the password for this user using the add_user.pl script (change XXXXXXXX to the password value):

add_user.pl -a -d pubmlst_bigsdb_users -n kjolley -p XXXXXXXX

Add specific permissions that this admin user can have by directly adding the following terms to the permissions table:

- set_site_user_passwords:
 - Allow admin to set user passwords.
- import_dbase_configs:
 - Allow admin to define which database configurations are made available for registration.
- merge_users
 - Allow admin to merge user accounts.
- modify_users
 - Allow admin to edit user details.

e.g.

```
psql pubmlst_bigsdb_users
INSERT INTO permissions (user_name,permission,curator,datestamp) VALUES
  ('kjolley','import_dbase_configs','kjolley','now');
```

- 4. Specific *permissions can be set for curators* in individual databases:
 - import_site_users
 - This allows the curator to import site users in to the database.
 - modify_site_users
 - You may not wish to do this! It allows the curator of any database with this permission to change the details of a user that may be used on other databases on the site.
- 5. HTML header files can be defined for use when bigsdb.pl or bigscurate.pl are called without a database configuration, such as when a user is registering or modifying their user details. These files, site_header.html, site_footer.html, site_curate_header.html and site_curate_footer.html should be placed in the root directory of the web site.

3.8 Periodically delete temporary files

There are two temporary directories (one public, one private) which may accumulate temporary files over time. Some of these are deleted automatically when no longer required but some cannot be cleaned automatically since they are used to display results after clicking a link or to pass the database query between pages of results.

The easiest way to clean the temp directories is to run a cleaning script periodically, e.g. create a root-executable script in /etc/cron.hourly containing the following::

```
#!/bin/sh
#Remove temp BIGSdb files from secure tmp folder older than 1 week.
find /var/tmp/ -name '*BIGSdb_*' -type f -mmin +10080 -exec rm -f {} \; 2>/dev/null
#Remove .jnlp files from web tree older than 1 day
find /var/www/tmp/ -name '*.jnlp' -type f -mmin +1440 -exec rm -f {} \; 2>/dev/null
#Remove other tmp files from web tree older than 1 week
find /var/www/tmp/ -type f -mmin +10080 -exec rm -f {} \; 2>/dev/null
```

3.9 Prevent preference database getting too large

The preferences database stores user preferences for BIGSdb databases running on the site. Every user will have a globally unique identifier (guid) stored in this database along with a datestamp indicating the last access time. On public databases that do not require logging in, this guid is stored as a cookie on the user's computer. Databases that require logging in use a combination of database and username as the identifier. Over time, the preferences database can get quite large since every unique user will result in an entry in the database. Since many of these entries represent casual users, or even web indexing bots, they can be periodically cleaned out based on their last access time. A weekly CRON job can be set up to remove any entries older than a defined period. For example, the following line entered in /etc/crontab will remove the preferences for any user that has not accessed any database in the past 6 months (the script will run at 6pm every Sunday).

3.10 Log file rotation

Set the log file to auto rotate by adding a file called 'bigsdb' with the following contents to /etc/logrotate.d:

```
/var/log/bigsdb.log {
 weekly
 rotate 4
 compress
 copytruncate
 missingok
 notifempty
 create 640 root adm
}
/var/log/bigsdb_jobs.log {
 weekly
 rotate 4
 compress
 copytruncate
 missingok
 notifempty
 create 640 root adm
```

3.11 Upgrading BIGSdb

Major version changes, e.g. 1.7 -> 1.8, indicate that there has been a change to the underlying database structure for one or more of the database types. Scripts to upgrade the database are provided in sql/upgrade and are named by the database type and version number. For example, to upgrade an isolate database (bigsdb_isolates) from version 1.7 to 1.8, log in as the postgres user and type:

psql -f isolatedb_v1.8.sql bigsdb_isolates

Upgrades are sequential, so to upgrade from a version earlier than the last major version you would need to upgrade to the intermediate version first, e.g. to go from $1.6 \rightarrow 1.8$, requires upgrading to 1.7 first.

Minor version changes, e.g. 1.8.0 -> 1.8.1, have no modifications to the database structures. There will be changes to the Perl library modules and possibly to the contents of the Javascript directory, images directory and CSS files.

3.12 Running the BIGSdb RESTful interface

BIGSdb has an Application Programming Interface (API) that allows third-party applications to access the data within the databases. The script that runs this is called bigsrest.pl. This is a Dancer2 application that can be run using a wide range of options, e.g. as a stand-alone script, using Perl webservers with plackup, or from apache. Full documentation for deploying Dancer2 applications can be found online.

The script requires a new database that describes the resources to make available. This is specified in the bigsdb.conf file as the value of the 'rest_db' attribute. By default, the database is named bigsdb_rest.

A SQL file to create this database can be found in the sql directory of the download archive. It is called rest.sql. To create the database, as the postgres user, navigate to the sql directory and type

```
createdb bigsdb_rest
psql -f rest.sql bigsdb_rest
```

This database will need to be populated using psql or any tool that can be used to edit PostgreSQL databases. The database contains three tables that together describe and group the databases resources that will be made available through the API. The tables are:

- resources
 - this contains two fields (both compulsory):
 - * **dbase_config** the name of the database configuration used with the database. This is the same as the name of the directory that contains the config.xml file in the /etc/bigsdb/dbases directory.
 - * description short description of the database.
- groups (used to group related resources together)
 - this contains two fields (compulsory fields shown in bold):
 - * **name** short name of group. This is usually a single word and is also the key that links resources to groups.
 - * **description** short description of group.
 - * long_description fuller description of group.
- group_resources (used to add resources to groups)
 - this contains two fields (both compulsory)
 - * group_name name of group. This must already exist in the groups table.
 - * dbase_config the name of database resource. This must already exist in the resources table.

For example, to describe the PubMLST resources for Neisseria, connect to the bigsdb_rest database using psql,

psql bigsdb_rest

Then enter the following SQL commands. First add the database resources:

```
INSERT INTO resources (dbase_config,description) VALUES
('pubmlst_neisseria_seqdef','Neisseria sequence/profile definitions');
INSERT INTO resources (dbase_config,description) VALUES
('pubmlst_neisseria_isolates','Neisseria isolates');
```

Then create a 'neisseria' group that will contain these resources:

```
INSERT INTO groups (name,description) VALUES
('neisseria','Neisseria spp.');
```

Finally, add the database resources to the group:

```
INSERT INTO group_resources (group_name,dbase_config) VALUES
('neisseria','pubmlst_neisseria_seqdef');
INSERT INTO group_resources (group_name,dbase_config) VALUES
('neisseria','pubmlst_neisseria_isolates');
```

The REST API will need to run on its own network port. By default this is port 3000. To run as a stand-alone script, from the script directory, as the bigsdb user, simply type:

./bigsrest.pl

This will start the API on port 3000. You will be able to check that this is running using a web browser by navigating to http://localhost:3000 on the local machine, or using the server IP address from a remote machine. You may need to modify your server firewall rules to allow connection to this port.

Running as a stand-alone script is useful for testing, but you can achieve much better performance using a Perl webserver with plackup. There are various options to choose. PubMLST uses Starman.

To run the API using Starman, type the following as the bigsdb user:

plackup -a /var/rest/bigsrest.pl -s Starman -E deployment

where the value of -a refers to the location of the bigsrest.pl script. Starman defaults to using port 5000.

Different Linux distributions use different means to control services/daemons. To start the REST interface on system boot on systems using upstart, create a file called bigsdb-rest.conf in /etc/init. The contents of this file should be something like (modify file paths as appropriate):

```
description "Start BIGSdb REST interface"
version "1.0"
author "Keith Jolley"
start on runlevel [12345]
## tell upstart we're creating a daemon
expect fork
script
exec su -s /bin/sh -c 'exec "$0" "$@"' bigsdb -- /usr/local/bin/plackup -a /var/rest/
→bigsrest.pl -s Starman -E deployment
end script
```

The service will then start automatically on boot or can be manually started by calling:

sudo service bigsdb-rest start

For systems using systemd, create a file in /etc/systemd/system called bigsdb-rest.service with the following contents (again, modify file paths as appropriate):

```
[Unit]
Description=BIGSdb REST interface
After=network.target
[Service]
User=bigsdb
ExecStart=/usr/bin/plackup -a /var/rest/bigsrest.pl -s Starman -E deployment
Restart=always
[Install]
WantedBy=multi-user.target
```

To start the service automatically on boot you need to enable it:

sudo systemctl enable bigsdb-rest.service

It can also be manually started by calling:

```
sudo systemctl start bigsdb-rest.service
```

3.12.1 Proxying the API to use a standard web port

Usually you will want your API to be available on the standard web port 80. To do this you will need to set up a virtual host using a different domain name from your web site to proxy the API port. For example, PubMLST has a separate domain 'http://rest.pubmlst.org' for its API. This is set up as a virtual host directive in apache with the following configuration file:

```
<VirtualHost *>
 ServerName rest.pubmlst.org
 DocumentRoot /var/rest
 ServerAdmin keith.jolley@zoo.ox.ac.uk
  <Directory /var/rest>
   AllowOverride None
   Require all granted
 </Directory>
 ProxyPass / http://rest.pubmlst.org:5000/
 ProxyPassReverse / http://rest.pubmlst.org:5000/
 <Proxy *>
     Order allow, deny
     Allow from all
 </Proxy>
 ErrorLog /var/log/apache2/rest.pubmlst.org-error.log
 CustomLog /var/log/apache2/rest.pubmlst.org-access.log common
</VirtualHost>
```

You should also set 'rest_behind_proxy=1' in bigsdb.conf.

CHAPTER 4

Database setup

There are two types of BIGSdb database:

- · sequence definition databases, containing
 - allele sequences and their identifiers
 - scheme data, e.g. MLST profile definitions
- isolate databases, containing
 - isolate provenance metadata
 - genome sequences
 - allele designations for loci defined in sequence definition databases.

These two databases are independent but linked. A single isolate database can communicate with multiple sequence definition databases and vice versa. Different access restrictions can be placed on different databases.

Databases are described in XML files telling BIGSdb everything it needs to know about them. Isolate databases can have any fields defined for the isolate table, allowing customisation of metadata - these fields are described in the XML file (config.xml) and must match the fields defined in the database itself.

4.1 Creating databases

There are templates available for the sequence definition and isolate databases. These are SQL scripts found in the sql directory.

To create a database, you will need to log in as the postgres user and use these templates. For example to create a new sequence definition database called bigsdb_test_sequef, navigate to the sql directory and log in as the postgres user, e.g.

```
sudo su postgres
```

then

createdb bigsdb_test_seqdef
psql -f seqdef.sql bigsdb_test_seqdef

Create an isolate database the same way:

```
createdb bigsdb_test_isolates
psql -f isolatedb.sql bigsdb_test_isolates
```

The standard fields in the isolate table are limited to essential fields required by the system. To add new fields, you need to log in to the database and alter this table. For example, to add fields for country and year, first log in to the newly created isolate database as the postgres user:

```
psql bigsdb_test_isolates
```

and alter the isolate table:

ALTER TABLE isolates ADD country text; ALTER TABLE isolates ADD year int;

Remember that any fields added to the table need to be described in the config.xml file for this database.

4.2 Database-specific configuration

Each BIGSdb database on a system has its own configuration directory, by default in /etc/bigsdb/dbases. The database has a short configuration name used to specify it in a web query and this matches the name of the configuration sub-directory, e.g. http://pubmlst.org/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_neisseria_isolates is the URL of the front page of the PubMLST Neisseria isolate database whose configuration settings are stored in /etc/bigsdb/dbases/pubmlst_neisseria_isolates. This database sub-directory contains a number of files (hyperlinks lead to the files used on the Neisseria database):

- config.xml the database configuration file. Fields defined here correspond to fields in the isolate table of the database.
- banner.html optional file containing text that will appear as a banner within the database index pages. HTML markup can be used within this text.
- header.html HTML markup that is inserted at the top of all pages. This can be used to set up site-specific menubars and logos.
- footer.html HTML markup that is inserted at the bottom of all pages.
- curate_header.html HTML markup that is inserted at the top of all curator's interface pages.
- curate_footer.html HTML markup that is inserted at the bottom of all curator's interface pages.
- profile_submit.html HTML markup for text that is inserted in to the submission interface prior to profile submission finalization. This can be used to add specific instructions such as the requirement to make an isolate submission.
- allele_submit.html HTML markup for text that is inserted in to the submission interface prior to allele submission finalization. This can be used to add specific instructions such as the requirement to attach Sanger trace files.
- registration_success.txt Text file containing message content to be used in an automated E-mail when granting access to a user who has requested access to the database using the site-wide account system (where autoregistration is not enabled).

The header and footer files can alternatively be placed in the root directory of the web site for site-wide use.

There are four additional files, site_header.html, site_footer.html, curate_site_header.html and curate_site_footer.html which are used when either bigsdb.pl or bigscurate.pl are called without a database configuration. These should be placed in the root directory of the web site.

You can also add HTML meta attributes (such as a favicon) by including a file called meta.html in the database configuration directory. For example to set a favicon this file can contain something like the following:

<link rel="shortcut icon" href="/favicon.ico" type="image/ico" />

These attributes will appear in the <head> section of the HTML page.

4.3 XML configuration attributes used in config.xml

The following lists describes the attributes used in the config.xml file that is used to describe databases.

4.3.1 Isolate database XML attributes

Please note that database structure described by the field elements must match the physical structure of the database isolate table. Required attributes are in **bold**:

<db>

Top level element. Contains child elements: system and field.:

<system>

Any value set here can be overridden in a system.overrides file.

- authentication
 - Method of authentication: either 'builtin' or 'apache'. See user authentication.

• db

- Name of database on system.
- dbtype
 - Type of database: either 'isolates' or 'sequences'.
- description
 - Description of database used throughout interface.
- align_limit
 - Overrides the sequence export record alignment limit in the Sequence Export plugin. Default: '200'.
- all_plugins
 - Enable all appropriate plugins for database: either 'yes' or 'no', default 'no'.
- annotation
 - Semi-colon separated list of accession numbers with descriptions (separated by a l), eg. 'AL157959/Z2491;AM421808/FAM18;NC_002946/FA 1090;NC_011035/NCCP11945;NC_014752/020-06'. Currently used only by Genome Comparator plugin.
- BLAST

- Enable Blast plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the Blast plugin can be disabled by setting this attribute to 'no'.
- BURST
 - Enable BURST plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the BURST plugin can be disabled by setting this attribute to 'no'.
- cache_schemes
 - Enable automatic refreshing of scheme field caches when batch adding new isolates: either 'yes' or 'no', default 'no'.
 - See scheme caching.
- CodonUsage
 - Enable Codon Usage plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the Codon Usage plugin can be disabled by setting this attribute to 'no'.
- codon_usage_limit
 - Overrides the record limit for the Codon Usage plugin. Default: '500'.
- contig_analysis_limit
 - Overrides the isolate number limit for the Contig Export plugin. Default: '1000'.
- ContigExport
 - Enable contig export plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the contig export plugin can be disabled by setting this attribute to 'no'.
- curate_config
 - The database configuration that should be used for curation if different from the current configuration. This is used when the submission system is being used so that curation links in the 'Manage submissions' pages for curators load the correct database configuration.
- curate_link
 - URL to curator's interface, which can be relative or absolute. This will be used to create a link in the public interface dropdown menu.
- curate_path_includes
 - Partial path of the bigscurate.pl script used to curate the database. See user authentication.
- curate_script
 - Relative web path to curation script. Default 'bigscurate.pl' (version 1.11+).
 - This is only needed if automated submissions are enabled. If bigscurate.pl is in a different directory from bigsdb.pl, you need to include the whole web path, e.g. /cgi-bin/private/bigsdb/bigscurate.pl.
- curator_home
 - URL of curator's index page, which can be relative or absolute. This will be used to add a link in the dropdown menu.
- curators_only

- Set to 'yes' to prevent ordinary authenticated users having access to database configuration. This is only effective if read_access is set to 'authenticated_users'. This may be useful if you have different configurations for curation and querying with some data hidden in the configuration used by standard users. Default 'no'.
- daily_pending_submissions
 - Overrides the daily limit on pending submissions that a user can submit via the web submission system. Default: '15'.
- daily_rest_submissions_limit
 - Overrides the limit on number of submissions that can be made to the database via the RESTful interface. This is useful to prevent flooding of the submission system by aberrant scripts. Default: '100'.
- default_access
 - The default access to the database configuration, either 'allow' or 'deny'. If 'allow', then specific users can be denied access by creating a file called 'users.deny' containing usernames (one per line) in the configuration directory. If 'deny' then specific users can be allowed by creating a file called 'users.allow' containing usernames (one per line) in the configuration directory. See *default access*.
- default_private_records
 - The default number of private isolate records that a user can upload. The user account must have a status of either 'submitter', 'curator', or 'admin'. This value is used to set the private_quota field when creating a new user record (which can be overridden for individual users). Changing it will not affect the quotas of existing users. Default: '0'.
- default_seqdef_config
 - Isolate databases only: Name of the default seqdef database configuration used with this database. Used to automatically fill in details when adding new loci.
- default_seqdef_dbase
 - Isolate databases only: Name of the default seqdef database used with this database. Used to automatically fill in details when adding new loci.
- default_seqdef_script
 - Isolate databases only: URL of BIGSdb script running the seqdef database (default: '/cgibin/bigsdb/bigsdb.pl').
- disable_updates
 - Set to 'yes' to prevent updates. This is useful when moving databases or temporarily running on a backup server.
- disable_update_message
 - Message shown when updates are disabled.
- eav_fields
 - Name to call sparsely-populated fields. Default: 'phenotypic fields'.
- eav_field_icon
 - Icon from FontAwesome to use on isolate info page for sparsely-populated fields. Default 'fa-microscope'.
- eav_groups
 - Comma-separated list of category names that sparsely-populated fields can be grouped in to. If this value is set, a category drop-down list will appear when adding or updating sparsely-populated fields.

- export_limit
 - Overrides the default allowed number of data points (isolates x columns) to export. Default: '25000000'.
- fast_scan
 - Sets whether fast mode scanning is enabled via the web interface. This will scan all loci together, using exemplar sequences. In cases where multiple loci are being scanned this should be significantly faster than the standard locus-by-locus scan, but it will take longer for the first results to appear. *Allele exemplars* should be defined if you enable this option. Set to 'yes' to enable. Default: 'no'.
- fieldgroup1 fieldgroup10
 - Allows multiple fields to be queried as a group. Value should be the name of the group followed by a colon
 (:) followed by a comma-separated list of fields to group, e.g. identifiers:id,strain,other_name.
- GenomeComparator
 - Enable Genome Comparator plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the Genome Comparator plugin can be disabled by setting this attribute to 'no'.
- genome_comparator_limit
 - Overrides the isolate number limit for the Genome Comparator plugin. Default: '1000'.
- genome_comparator_max_ref_loci
 - Overrides the limit on number of loci allowed in a reference genome. Default: '10000'.
- genome_comparator_threads
 - The number of threads to use for data gathering (BLAST, database queries) to populate data structure for Genome Comparator analysis. You should not set this to less than 2 as this will prevent job cancelling due to the way isolates are queued. Default: '2'.
- hide_unused_schemes
 - Sets whether a scheme is shown in a main results table if none of the isolates on that page have any data for the specific scheme: either 'yes' or 'no', default 'no'.
- host
 - Host name/IP address of machine hosting isolate database, default 'localhost'.
- job_priority
 - Integer with default job priority for offline jobs (default:5).
- job_quota
 - Integer with number of offline jobs that can be queued or currently running for this database.
- kiosk
 - Set to a page name to restrict configuration to always start on this page, rather than an index page. This faciliates running in a cut-down *kiosk mode* that doesn't allow access to all features. *Currently only 'sequenceQuery' is supported*.
- kiosk_allowed_pages
 - Comma-separated list of pages that the configuration is allowed to show, apart from the page set in the 'kiosk' attribute. Example for a sequence query configuration would be 'sequenceTranslate' to allow access to the translated sequence page following a query.
- kiosk_locus

- Restrict sequence query to a specific locus or scheme. Use either the locus primary name or 'SCHEME_X' where X is the scheme number.
- kiosk_no_genbank
 - Set to "yes" to hide the Genbank accesssion form element in kiosk mode.
- kiosk_no_upload
 - Set to "yes" to hide the sequence file upload in kiosk mode.
- kiosk_simple
 - Remove most explanatory text from kiosk page.
- kiosk_text
 - Alternative text to show on kiosk page.
- kiosk_title
 - Title text to use when running in kiosk mode.
- labelfield
 - Field that is used to describe record in isolate info page, default 'isolate'.
- locus_aliases
 - Display locus aliases and use them in dropdown lists by default: must be either 'yes' or 'no', default 'no'. This option can be overridden by a user preference.
- locus_superscript_prefix
 - Superscript the first letter of a locus name if it is immediately following by an underscore, e.g. f_abcZ would be displayed as fabcZ within the interface: must be either 'yes' or 'no', default 'no'. This can be used to designate gene fragments (or any other meaning you like).
- maindisplay_aliases
 - Default setting for whether isolates aliases are displayed in main results tables: either 'yes' or 'no', default 'no'. This setting can be overridden by individual user preferences.
- Microreact
 - Enable Microreact plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the Microreact plugin can be disabled by setting this attribute to 'no'. Note that for the plugin to be active, a country field containing a defined list of allowed values and an integer year field must be defined in the isolates table.
- noshow
 - Comma-separated list of fields not to use in breakdown statistic plugins.
- no_publication_filter
 - Isolate databases only: Switches off display of publication filter in isolate query form by default: either 'yes' or 'no', default 'no'.
- only_sets
 - Don't allow option to view the 'whole database' only list sets that have been defined: either 'yes' or 'no', default 'no'.
- password
 - Password for access to isolates database, default 'remote'.

- pcr_limit
 - Overrides the isolate number limit for the in silico PCR plugin. Default: '10000'.
- PhyloViz
 - Enable third party PhyloViz plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the PhyloViz plugin can be disabled by setting this attribute to 'no'.
- port
 - Port number that the isolate host is listening on, default '5432'.
- privacy
 - Displays E-mail address for sender in isolate information page if set to 'no'. Default 'yes'.
- public_login
 - Optionally allow users to log in to a public database this is useful as any jobs will be associated with the user and their preferences will also be linked to the account. Set to 'no' to disable. Default 'yes'.
- query_script
 - Relative web path to bigsdb script. Default 'bigsdb.pl' (version 1.11+).
 - This is only needed if automated submissions are enabled. If bigsdb.pl is in a different directory from bigscurate.pl, you need to include the whole web path, e.g. /cgi-bin/bigsdb/bigsdb.pl.
- read_access
 - Describes who can view data: either 'public' for everybody or 'authenticated_users' for anybody who has been able to log in. Default 'public'.
- recommended_schemes
 - Comma-separated list of recommended schemes to suggest to Genome Comparator users. If lots of schemes are defined, a user may be tempted to click 'All loci' and this may not be the best option. Populating this attribute, results in an additional list of preferred schemes that can be chosen.
- related_databases
 - Semi-colon separated list of links to related BIGSdb databases on the system. This should be in the form of database configuration name followed by a 'l' and the description, e.g. 'pubmlst_neisseria_seqdeflSequence and profile definitions'. This is used to populate the dropdown menu.
- remote_contigs
 - Optionally allow the use of remote contigs. These are stored in a remote BIGSdb database, accessible via the RESTful API. Set to 'yes' to enable.
- rest_kiosk
 - If 'kiosk' attribute is set, then the REST interface will be disabled for the configuration unless a value is set here. The only supported value currently is 'sequenceQuery' which will enable API routes for querying sequences.
- rMLSTSpecies
 - Enable rMLST Species identifier plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the plugin can be disabled by setting this attribute to 'no'. Note that for the plugin to be active, a country field containing a defined list of allowed values and an integer year field must be defined in the isolates table.
- script_path_includes

- Partial path of the bigsdb.pl script used to access the database. See user authentication.
- · SeqbinBreakdown
 - Enable Sequence bin breakdown plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the plugin can be disabled by setting this attribute to 'no'. Note that for the plugin to be active, a country field containing a defined list of allowed values and an integer year field must be defined in the isolates table.
- seqbin_size_threshold
 - Sets the size values in Mbp to enable for the seqbin filter.
 - Example: seqbin_size_threshold="0.5,1,2,4".
- seq_export_limit
 - Overrides the sequence export limit (records x loci) in the Sequence Export plugin. Default: '1000000'.
- sets
 - Use sets: either 'yes' or 'no', default 'no'.
- set_id
 - Force the use of a specific set when accessing database via this XML configuration: Value is the name of the set.
- start_id
 - Defines the minimum record id to be used when uploading new isolate records. This can be useful when it is anticipated that two databases may be merged and it would be easier to do so if the id numbers in the two databases were different. Default: '1'.
- submissions
 - Enable automated submission system: either 'yes' or 'no', default 'no' (version 1.11+).
 - The curate_script and query_script paths should also be set, either in the bigsdb.conf file (for site-wide configuration) or within the system attribute of config.xml.
- submissions_deleted_days
 - Overrides the default number of days before closed submissions are deleted from the system. Default: '90'.
- TagStatus
 - Enable Tag status plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the plugin can be disabled by setting this attribute to 'no'. Note that for the plugin to be active, a country field containing a defined list of allowed values and an integer year field must be defined in the isolates table.
- tblastx_tagging
 - Sets whether tagging can be performed using TBLASTX: either 'yes' or 'no', default 'no'.
- total_pending_submissions
 - Overrides the total limit on pending submissions that a user can submit via the web submission system. Default: '20'.
- user
 - Username for access to isolates database, default 'apache'.
- user_job_quota

- Integer with number of offline jobs that can be queued or currently running for this database by any specific user - this parameter is only effective if users have to log in.
- user_projects
 - Sets whether authenticated users can create their own projects in order to group isolates: either 'yes' or 'no', default 'no'.
- view
 - Database view containing isolate data, default 'isolates'.
- views
 - Comma-separated list of views of the isolate table defined in the database. This is used to set a view for a set, or to restrict loci or schemes to a subset of isolate data.
- webroot
 - URL of web root, which can be relative or absolute. This is used to provide a hyperlinked item in the dropdown menu. Default '/'.

<field>

Element content: Field name + optional list <optlist> of allowed values, e.g.:

```
<field type="text" required="no" length="40" maindisplay="no"

web="http://somewebsite.com/cgi-bin/script.pl?id=[?]" optlist="yes">epidemiology

<optlist>

<optlist>coption>carrier</optlion>

<optlist>equation>case</optlist>

<optlist>equation>case</optlist>

<optlist>equation>coptlist>

</optlist>

</field>
```

• type

- Data type: int, text, float, bool, or date.
- comments * optional
 - Comments about the field. These will be displayed in the field description plugin and as tooltips within the curation interface.
- curate_only
 - Set to 'yes' to hide field unless logged-in user is a curator or admin.
- default
 - Default value. This will be entered automatically in the web form but can be overridden.
- dropdown
 - Select if you want this field to have its own dropdown filter box on the query page. If the field has an option list it will use the values in it, otherwise all values defined in the database will be included: 'yes' or 'no', default 'no'. This setting can be overridden by individual user preferences.
- length
 - Length of field, default 12.

- maindisplay
 - Sets if field is displayed in the main table after a database search, 'yes' or 'no', default 'yes'. This setting can be overridden by individual user preferences.
- max
 - Maximum value for integer and date types. Special values such as CURRENT_YEAR and CUR-RENT_DATE can be used.
- min
 - Minimum value for integer and date types.
- multiple
 - Sets if field allows multiple values to be set for it, 'yes' or 'no', default 'no'. This is only supported for fields with option lists. If set to 'yes', then the underlying field in the database must be an ARRAY type, e.g. text ARRAY.
- no_curate
 - Setting this will hide the field in the curator interface and prevent it from being manually modified. This is
 useful for fields that are populated by automated scripts or database triggers. Can be 'yes' or 'no', default
 'no'.
- no_submissions
 - Setting this will hide the field in the submission template. The field is still available if it is added back to the template manually.
- optlist
 - Sets if this field has a list of allowed values, default 'no'. Surround each option with an <option> tag.
- regex
 - Regular expression used to constrain field values, e.g. regex="^[A-Z].*\$" forces the first letter of the value to be capitalized.
- required
 - Sets if data is required for this field, 'yes' or 'no', default 'yes'.
- userfield
 - Select if you want this field to have its own dropdown filter box of users (populated from the users table): 'yes' or 'no', default 'no'.
- web
 - URL that will be used to hyperlink field values. If [?] is included in the URL, this will be substituted for the actual field value.

Special values

The following special variables can be used in place of an actual value:

- CURRENT_DATE: current date in yyyy-mm-dd format
- CURRENT_YEAR: the 4 digit value of the current year

4.3.2 Sequence definition database XML attributes

Required attributes are in **bold**.

<db>

Top level element. Contains child element: system.

<system>

Any value set here can be overridden in a system.overrides file.

- authentication
 - Method of authentication: either 'builtin' or 'apache'. See user authentication.
- db
 - Name of database on system.
- dbtype
 - Type of database: either 'isolates' or 'sequences'.
- description
 - Description of database used throughout interface.
- align_limit
 - Overrides the sequence export record alignment limit in the Sequence Export plugin. Default: '200'.
- allele_comments
 - Enable comments on allele sequences: either 'yes' or 'no', default 'no'.
 - This is not enabled by default to discourage the practice of adding isolate information to allele definitions (this sort of information belongs in an isolate database).
- allele_flags
 - Enable flags to be set for alleles: either 'yes' or 'no', default 'no'.
- BURST
 - Enable BURST plugin: either 'yes' or 'no'. If no value is set then the plugin will not be available unless
 the all_plugins attribute is set to 'yes'. If the all_plugins attribute is set to 'yes', the BURST plugin can be
 disabled by setting this attribute to 'no'.
- curate_config
 - The database configuration that should be used for curation if different from the current configuration.
 This is used when the submission system is being used so that curation links in the 'Manage submissions' pages for curators load the correct database configuration.
- curate_path_includes
 - Partial path of the bigscurate.pl script used to curate the database. See user authentication.
- curate_script
 - Relative web path to curation script. Default 'bigscurate.pl' (version 1.11+).
 - This is only needed if automated submissions are enabled. If bigscurate.pl is in a different directory from bigsdb.pl, you need to include the whole web path, e.g. /cgi-bin/private/bigsdb/bigscurate.pl.
- curator_home

- URL of curator's index page, which can be relative or absolute. This will be used to add a link in the dropdown menu.
- curators_only
 - Set to 'yes' to prevent ordinary authenticated users having access to database configuration. This is only effective if read_access is set to 'authenticated_users'. This may be useful if you have different configurations for curation and querying with some data hidden in the configuration used by standard users. Default 'no'.
- daily_pending_submissions
 - Overrides the daily limit on pending submissions that a user can submit via the web submission system. Default: '15'.
- daily_rest_submissions_limit
 - Overrides the limit on number of submissions that can be made to the database via the RESTful interface. This is useful to prevent flooding of the submission system by aberrant scripts. Default: '100'.
- diploid
 - Allow IUPAC 2-nuclotide ambiguity codes in allele definitions for use with diploid typing schemes: either 'yes' or 'no', default 'no'.
- disable_seq_downloads
 - Prevent users or curators from downloading all alleles for a locus (admins always can). 'yes' or 'no', default 'no'.
- exemplars
 - Use exemplar sequences in the BLAST caches used for the sequence query pages. This is useful on larger databases as it speeds up the query significantly. *Exemplar alleles MUST* be defined otherwise sequence queries will fail. 'yes' or 'no', default 'no'.
- isolate_database
 - The config name of the isolate database. This is used to provide a link to isolate submissions. You also need to set isolate_submissions="yes".
- isolate_submissions
 - Set to yes to provide a link to isolate submissions. The isolate_database attribute also needs to be set. Default: 'no'.
- job_priority
 - Integer with default job priority for offline jobs (default:5).
- job_quota
 - Integer with number of offline jobs that can be queued or currently running for this database.
- profile_submissions
 - Enable profile submissions (automated submission system): either 'yes' or 'no', default 'no' (version 1.11+).
 - To enable, you will also need to set submissions="yes". By default, profile submissions are disabled since generally new profiles should be accompanied by representative isolate data, and the profile can be extracted from that.
- public_login

- Optionally allow users to log in to a public database this is useful as any jobs will be associated with the user and their preferences will also be linked to the account. Set to 'no' to disable. Default 'yes'.
- query_script
 - Relative web path to bigsdb script. Default 'bigsdb.pl' (version 1.11+).
 - This is only needed if automated submissions are enabled. If bigsdb.pl is in a different directory from bigscurate.pl, you need to include the whole web path, e.g. /cgi-bin/bigsdb/bigsdb.pl.
- read_access
 - Describes who can view data: either 'public' for everybody, or 'authenticated_users' for anybody who has been able to log in. Default 'public'.
- related_databases
 - Semi-colon separated list of links to related BIGSdb databases on the system. This should be in the form of database configuration name followed by a 'l' and the description, e.g. 'pubmlst_neisseria_isolateslIsolates'. This is used to populate the dropdown menu.
- script_path_includes
 - Partial path of the bigsdb.pl script used to access the database. See user authentication.
- seq_export_limit
 - Overrides the sequence export limit (records x loci) in the Sequence Export plugin. Default: '1000000'.
- sets
 - Use sets: either 'yes' or 'no', default 'no'.
- set_id
 - Force the use of a specific set when accessing database via this XML configuration: Value is the name of the set.
- submissions
 - Enable automated submission system: either 'yes' or 'no', default 'no' (version 1.11+).
 - The curate_script and query_script paths should also be set, either in the bigsdb.conf file (for site-wide configuration) or within the system attribute of config.xml.
- submissions_deleted_days
 - Overrides the default number of days before closed submissions are deleted from the system. Default: '90'.
- total_pending_submissions
 - Overrides the total limit on pending submissions that a user can submit via the web submission system. Default: '20'.
- user_job_quota
 - Integer with number of offline jobs that can be queued or currently running for this database by any specific user - this parameter is only effective if users have to log in.
- webroot
 - URL of web root, which can be relative or absolute. This is used to provide a hyperlinked item in the dropdown menu. Default '/'.

4.4 Over-riding global defaults set in bigsdb.conf

Certain values set in bigsdb.conf can be over-ridden by corresponding values set in a database-specific config.xml file. These can be set within the system tag like other attributes:

- query_script
 - Relative web path to bigsdb script.
- curate_script
 - Relative web path to curation script.
- prefs_db
 - The name of the preferences database.
- auth_db
 - The name of the authentication database.
- tmp_dir
 - Path to the web-accessible temporary directory.
- secure_tmp_dir
 - Path to the web-inaccessible (secure) temporary directory.
- ref_db
 - The name of the references database.

4.5 Over-riding values set in config.xml

Any attribute used in the system tag of the database config.xml file can be over-ridden using a file called **system.overrides**, placed in the same directory as config.xml. This is very useful as it allows you to set up multiple configs for a database, with the config.xml files symlinked so that any changes to one will be seen in each database configuration. An example of why you may wish to do this would be if you create separate public and private views of the isolate table that filters on some attribute. The system.overrides file uses key value pairs separated by = with the values quoted, e.g.

```
view="private"
read_access="authenticated_users"
description="Private view of database"
```

It is also possible to override the required or maindisplay attribute of a particular field using a file called **field.overrides**. The field.overrides file uses the format 'field:attribute="value" on each line, e.g.

date_received:required="yes"

4.6 Setting field validation rules

Sometimes it may be necessary to restrict the allowed values in one isolate field depending on the values submitted for another field. It is possible to do this using field validation rules. These combine one or more conditions which all have to match for validation to fail and an isolate record upload to be rejected.

An example of this may be if you have an age_year and an age_month field but you only want age_month to be populated if the subject is less than one year old. You can do this as follows.

As an admin, on the curator interface, click the 'Field' toggle to show the validation table links. Then click 'Add' on the 'Validation conditions' setting:

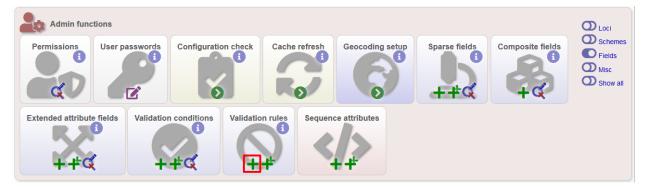
Admin fund	tions							
Permissions	User passwords	Configuration ch	eck Cache	Geocod	ding setup i	Sparse fields	Composite fields	Schemes Fields Misc Show all
Extended attribut	8	val	idation rules	Sequence attribut	les			

Add the following conditions separately:

- $age_year > 0$
- age_month NOT null

PubMLST Database	e home Curator home Contents	
Logged in: Keith Jolley (keith)	y, t∳Log out Change password	Toggle: (1)
Add new valid	lation condition	
Please fill in the fields be	elow - required fields are marked with an exclamation mark (!).	+
Record	Action	
id:! 1	Reset Submit	
field:! age_y		
operator:! >	~	
value: 1 0	 	
curator:! Keith	Jolley (keith)	
datestamp: 2019-0	06-27	

Now add a new 'Validation rule', by clicking 'Add' on the 'Validation rules' setting:



Here you just enter the message that will be returned when the validation fails:

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). 🗘 Log out Change password		Toggle: 🚺 📃
Add new validation rule		
Please fill in the fields below - required fields are marked with an exclamation mark (!). Record id:! 1 message:! age_mth should only be set when age_yr < 1. curator:! Keith Jolley (keith) datestamp:! 2019-06-27	 Action Reset Submit	ľ

Finally add the conditions to the rule by clicking 'Add' on the 'Rule conditions' setting:

Admin functions Permissions i		juration check	che refresh	Geocoding setur	Sparse	5	 Loci Schemes Fields Misc Show all
Extended attribute fiel	ds Composite fields	Validation conditio	6	on rules i t	conditions	Sequence attributes	

Select the rule message and the condition from the dropdown boxes:

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). DeLog out Change password	Toggle: 🚺 📘
Add new rule condition	
Please fill in the fields below - required fields are marked with an exclamation mark (!). Record Action rule id:! 1) age_mth should only be set when age_yr < 1.	ľ

Make sure you do this for each of the conditions that have to match.

Validation checks are performed when adding or updating an isolate record, or when a user submits via the automated submission interface. Currently these checks are not enforced when doing a batch update.

4.6.1 Special condition values

Use the value **null** to indicate that the field is empty, e.g.

• age_month NOT null

Use a field name in square brackets to compare the value in that field, e.g. suppose you have two date fields, 'date_sampled' and 'date_received', and you want to ensure that 'date_received' is not before 'date_sampled'. You can do this with the following condition:

• date_received < [date_sampled]

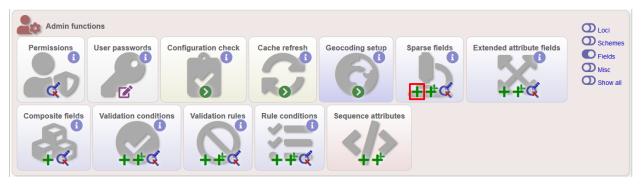
The two fields have to be of the same data type in order to be compared (you cannot compare a text field to an integer field for example).

4.7 Sparsely-populated fields

Commonly used isolate fields should be described in the config.xml file and included as columns within the isolates table. Sometimes, however, you may have a need to record information that is only likely to be found in a minority of records. This can be done more efficiently with the use of sparsely-populated fields. These are stored differently in the database (using an entity-attribute-value [EAV] model) but can still be searched and exported in a similar way to normal fields. There is no limit to the number of such fields that can be defined.

The default name for these fields is 'phenotypic fields' and this is how they will be grouped in the interface. You can change this by setting the 'eav_fields' attribute in the *system tag of config.xml*. It is also possible to group these fields in to categories - these can be defined with a comma-separated list in the 'eav_groups' attribute in the *system tag of config.xml*.

You will need to be an admin to define sparely-populated fields. Make sure that the 'Fields' toggle is selected on the curators' page. Click the add (+) button on the 'Sparse fields' function.



Fill in the form and click 'Submit'.

PubMLST Database home	Curator home Contents			
Logged in: Keith Jolley (keith). 🔂 Log ou	t Change password			Toggle: ()
Add new sparse fie	eld			
Record field:1 value format:1 no submissions:1 curator:1 datestamp:1	O true ● false ● O true ● false ● Keith Jolley (keith)		Action Reset Submit	ľ
length: option list:	\$71;R			
value regex: conditional formatting:		•		
html link text: html message:	0			

Field options are:

- field
 - name of field
- value_format
 - date type either integer, float, text, date or boolean.
- no_curate
 - Set to true to prevent user updates of fieldThis setting could be used if the value is calculated by an external script rather than entered by a curator.
- no_submissions
 - Set to true to prevent the field being listed in the submissions template.
- description
 - Tooltip text that will appear on curator forms.
- length
 - Restrict allowed length of value.
- option_list
 - Semi-colon separated list of allowed values.
- value_regex
 - Regular expression that can constrain allowed values.
- conditional_formatting
 - Semi-colon separated list of values each consisting of the value, followed by a pipe character (l) and HTML to display instead of the value. If you need to include a semi-colon within the HTML, use two semi-colons (;;) otherwise it will be treated as the list separator.'
- html_link_text

- This defines the text that will appear on an information link that will trigger a slide-in message (if defined int the next field). Default is 'info'.
- html_message
 - This message will slide-in on the isolate information page when the field value is populated and the information link is clicked. Full HTML formatting is supported.
- min_value
 - Valid for number fields only.
- max_value
 - Valid for number fields only.
- field_order
 - Integer indicating the order that fields should be displayed. If this is not set they will appear alphabetically.

4.8 Kiosk mode

Kiosk mode allows you to run a cut-down interface that offers a single main functionality. Currently, only a sequence query page is supported. The interface is locked down so that only specified functionality is supported and data cannot be exported.

See the *kiosk_* attributes* in config.xml.

As an example, the following settings are used for the rMLST 'Identify species' tool at https://pubmlst.org/rmlst/. The database usually requires a user to log in, but this tool offers a restricted functionality without logging in.

```
kiosk="sequenceQuery"
kiosk_allowed_pages="sequenceTranslate"
kiosk_title="Identify species"
kiosk_locus="SCHEME_1"
kiosk_simple="yes"
kiosk_no_upload="no"
kiosk_no_genbank="no"
rest_kiosk="sequenceQuery"
```

When you go to this example kiosk page you see only the sequence query page and trying to access any other functionality is prevented.

The rest_kiosk attribute enables queries to also be performed using the *RESTful API* which will be similarly locked down.

PubMLST Database home Contents		
	Help 🛛	Toggle: 🚺
Identify species		
Please paste in your sequence to query against the database.		
Enter query sequence (single or multiple contigs up to whole genome in size)		
Select FASTA file:		
Browse No file selected.		
Reset	Submit	
		_

4.9 User authentication

You can choose whether to allow Apache to handle your authentication or use built-in authentication.

4.9.1 Apache authentication

Using apache to provide your authentication allows a flexible range of methods and back-ends (see the Apache authentication HowTo for a start, or any number of tutorials on the web).

At its simplest, use a .htaccess file in the directory containing the bigscurate.pl (and bigsdb.pl for restriction of readaccess) script or by equivalent protection of the directory in the main Apache server configuration. It is important to note however that, by default, any BIGSdb database can be accessed by any instance of the BIGSdb script (including one which may not be protected by a .htaccess file, allowing public access). To ensure that only a particular instance (protected by a specific htaccess directive) can access the database, the following attributes can be set in the system tag of the database XML description file:

- script_path_includes: the BIGSdb script path must contain the value set.
- curate_path_includes: the BIGSdb curation script path must contain the value set.

For public databases, the 'script_path_includes' attribute need not be set.

To use apache authentication you need to set the authentication attribute in the system tag of the database XML configuration to 'apache'.

4.9.2 Built-in authentication

BIGSdb has its own built-in authentication, using a separate database to store password and session hashes. The advantages of using this over many forms of apache authentication are:

- Users are able to update their own passwords.
- Passwords are not transmitted over the Internet in plain text.

When a user logs in, the server provides a random one-time session variable and the user is prompted to enter their username and password. The password is encrypted within the browser using a Javscript one-way hash algorithm, and

this is combined with the session variable and hashed again. This hash is passed to the server. The server compares this hash with its own calculated hash of the stored encrypted password and session variable that it originally sent to the browser. Implementation is based on perl-md5-login. Stored passwords are salted and hashed using bcrypt.

To use built-in authentication you need to set the authentication attribute in the system tag of the database XML configuration to 'builtin'.

4.10 Setting up the admin user

The first admin user needs to be manually added to the users table of the database. Connect to the database using psql and add the following (changing details to suit the user).:

If you are using built-in authentication, set the password for this user using the *add_user:pl* script. This hashes the password and stores this within the authentication database. Other users can be added by the admin user from the curation interface accessible from http://your_website/cgi-bin/private/bigscurate.pl?db=test_db (or wherever you have located your bigscurate.pl script).

4.11 Retrieving PubMed citations from NCBI

Publications listed in PubMed can be associated with individual isolate records, profiles, loci and sequences. Full citations for these are stored within a local reference database, enabling these to be displayed within isolate records and searching by publication and author. This local database is populated by a script that looks in BIGSdb databases for PubMed records not locally stored and then requests the full citation record from the PubMed database.

The script is called retrieve_pubmed_records.pl and can be found in the scripts/maintenance directory.

Simply run the script either as the 'postgres' user or an account that is allowed to connect as the postgres user.

This should be run periodically from a CRON job, e.g. every hour.

4.12 Configuring access to remote contigs

It is possible for isolate records to have contigs in an external BIGSdb database. These must be accessible via the *RESTful API*. The advantage of this is that it enables multiple isolate databases to use the same genome assemblies without having to duplicate the storage of those assemblies. If access to the external database requires authenticated access, OAuth settings can be set to enable contig retrieval.

To enable remote contigs, set the remote_contigs attribute in the <system> tag of config.xml, i.e.

remote_contigs = "yes"

4.12.1 Setting up authentication

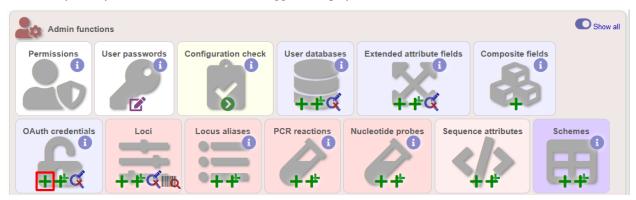
A client key for the BIGSdb remote contig manager needs to be generated. This can be done using the *cre-ate_client_credentials.pl* script, e.g.

```
create_client_credentials.pl --a 'BIGSdb remote contig manager' --insert
```

This will generate a client id (key) and a client secret and add them to the authentication database.

You will then need to obtain an access token and access secret using the client key and secret with the get_oauth_access_token.pl script. You will need to enter the API database URI (e.g. http://rest.pubmlst.org/db/pubmlst_rmlst_isolates) and the web database URL (e.g. https://pubmlst.org/bigsdb?db=pubmlst_rmlst_isolates). You will then be prompted to follow a link and log in to the database with your user credentials. A verification code will be generated. You need to enter this in to the script when prompted. An access token and secret will be returned to you.

From the curators' page, click the oauth credentials add link in the administrator settings. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Populate the OAuth_credentials table with the client key/secret and access token/secret. You should also enter the root REST URI for the database (e.g. http://rest.pubmlst.org/db/pubmlst_rmlst_isolates).

PubMLST Databas	ase home Curator home Contents	
Logged in: Keith Jolley (ke	(keith). @Log out Change password	Toggle: 🚯 🗧
Add new OA	Auth credentials	
Record	ds below - required fields are marked with an exclamation mark (!). 	t i i i i i i i i i i i i i i i i i i i
	y:! RylqmtjBbSAkyyrZ5ZUyHzae	
	t! U6B_^%HJP9N^1Ax2wemPPkmqrt_J%m_rX6pkgkfdho n:! eHTH8jMXsnyhIUvJZFmDF7nji5IZQJsd	
	t! QODGPqKoSgVcGwdlKBejufDsn4B1beX1	
	r.! Keith Jolley (keith) d:! 2017-11-23	
datestamp:!	o:! 2017-11-23	

4.12.2 Processing remote contigs

When remote contigs are first linked to a record, the sequences are downloaded in bulk (without their metadata). This allows the sequence lengths to be recorded as this is needed for various queries and outputs. The curator is then given an option to process the contigs, which involves downloading each contig individually to record metadata including the original designation and the sequence platform used. This may take a while so it may be preferable to perform this

task offline. This can be done using the process_remote_contigs.pl script found in the scripts/automation directory. Options for using this script are shown below:

```
remote_contigs.pl --help
NAME
   process_remote_contigs.pl
   Download, check length and create checksum contigs stored as URIs
SYNOPSIS
   process_remote_contigs.pl --database NAME [options]
OPTIONS
--database NAME
   Database configuration name.
--exclude_isolates LIST
   Comma-separated list of isolate ids to ignore.
--exclude_projects LIST
   Comma-separated list of projects whose isolates will be excluded.
--help
   This help page.
--isolates LIST
   Comma-separated list of isolate ids to scan (ignored {f if} -p used).
--isolate_list_file FILE
   File containing list of isolate ids (ignored if -i or -p used).
--min ID
   Minimum isolate id.
--max ID
   Maximum isolate id.
--projects LIST
   Comma-separated list of project isolates to scan.
--quiet
   Only display errors.
```

CHAPTER 5

Administrator's guide

Please note that links displayed within the curation interface will vary depending on database contents and the permissions of the curator.

5.1 Types of user

There are four types of user in BIGSdb:

- User can view data but never modify it. Users should be created for every submitter of data so that records can be tracked, even if they do not actually use the database.
- Submitter (isolate databases only) can add and modify their own isolate data and data submitted by anybody else that is in the same *user group* as them but not anyone elses. A limited range of *Individual permissions* can be set for each submitter, so their roles can be controlled. A submitter with no specific permissions set has no more power than a standard user.
- Curator can modify data but does not have full control of the database. *Individual permissions* can be set for each curator, so their roles can be controlled. A curator with no specific permissions set has no more power than a standard user.
- Admin has full control of the database, including setting permissions for curators and setting user passwords if built-in authentication is in use.

5.2 User groups

User groups allow submitter accounts to be grouped such that the submitter can edit isolates where the sender is either themselves or any member of a user group to which they belong.

5.3 Curator permissions

Individual permissions can be set for each curator:

- disable_access if set to true, this user is completely barred from access.
- query_users allowed to query and view users registered to the database. This is automatically allowed if permission is set to modify users.
- modify_users allowed to add or modify user records. They can change the status of users, but can not revoke admin privileges from an account. They can also not raise the status of a user to admin level.
- modify_usergroups allowed to add or modify user groups and add users to these groups.
- set_user_passwords allowed to modify other users' passwords (if built-in authentication is in use).
- modify_loci allowed to add or modify loci.
- modify_locus_descriptions allowed to modify the description text and external hyperlinks used. Even with this setting, only loci for which a user is explicitly set as a curator can be modified.
- modify_schemes allowed to add or modify schemes.
- modify_sequences allowed to add sequences to the sequence bin (for isolate databases) or new allele definitions (for sequence definition databases).
- modify_experiments define new experiments that can be used to group contigs uploaded to the sequence bin.
- modify_isolates allowed to add or modify isolate records.
- modify_projects allowed to create projects, modify their descriptions and add or remove isolate records to these.
- modify_composites allowed to add or modify composite fields (fields made up of other fields, including scheme fields defined in external databases). Composite fields involve defining regular expressions that are evaluated by Perl this can be dangerous so this permission should be granted with discretion.
- modify_field_attributes allow user to create or modify secondary field attributes (lookup tables) for isolate record fields.
- modify_value_attributes allow user to add or modify secondary field values for isolate record fields.
- modify_probes allow user to define PCR or hybridization reactions to filter tag scanning.
- tag_sequences allowed to tag sequences with locus information.
- designate_alleles allowed to manually designate allele numbers for isolate records.
- modify_profiles allowed to add or modify scheme profiles (only used in a sequence definitions database).
- import_site_users allowed to import site users in to the database.
- modify_site_users allowed to modify site user details (you may not want to this! The user account can be used by multiple databases on the site and any changes to user details will be seen throughout the site).

Permissions can be set by clicking the Update/delete button in the Permissions box in the admin functions area of the curator's interface:



Choose one or more curators from the list (hold down Ctrl to select multiple values). click 'Select'.

PubMLST Database home Curator	ome Contents	
Logged in: Keith Jolley (keith). Hog out Change pass	vord	Неір 🗗
Set curator permissions		
Select curator(s) Clark, Stephen (SClark) Clemence, Marianne (mclemence) Debech, Nadia (ndebech) Deghmane, Ala-Eddin (deghmane) Diallo, Kanny (kdiallo) Exley, Rachel (rexley) Feavers, Ian (ifeavers) Goodyer-Sait, Lily (Igoodyer)	Action Select	

Click the appropriate checkboxes to modify permissions. There are also 'All/None' buttons to facilitate quicker selection of options. Click 'Update'.

PubMLST Database	home Curator hor	ne Content	S	
Logged in: Keith Jolley (keith).	.œLog out Change passwor	d		Help 🗹
Set curator per	rmissions			
Select curator(s)		Action—		
Clark, Stephen (SClark) Clemence, Marianne (mo		Select		
Debech, Nadia (ndebech)				
Deghmane, Ala-Eddin (d				
Diallo, Kanny (kdiallo) Exley, Rachel (rexley)				
Feavers, Ian (ifeavers)				
Goodyer-Sait, Lily (Igood	yer) 👻			
All Nor	ne			
		s with a status o	f 'submitter	' have a restricted list of allowed permissions that can be selected. Attributes
with a red background add	restrictions.			
				Action
	Curato			Update
Permission	Clemence, Marianne		All/None	opuare
modify users				
modify isolates	V	V		
modify projects		V		
modify sequences		V		
tag sequences		V		
designate alleles		V		
modify usergroups				
set user passwords				
modify loci		V		
modify schemes modify composites				
modify field attributes				
modify value attributes				
modify probes				
modify experiments				
delete all				
import site users				
modify site users				
only private				
disable access				
All/None				

The 'disable access' option provides a quick way to disable access to a curator. This will not be selected by the 'All/None' buttons.

5.4 Locus and scheme permissions (sequence definition database)

To be allowed to define alleles or scheme profiles, curators must be granted specific permission for each locus and scheme by adding their user id number to the 'locus curator' and 'scheme curator' lists.

The easiest way to modify these lists is to use the batch update link next to 'locus curator control list' and 'scheme curator control list':



Select the curator from the list:

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). [+Log out Change password	Ξ
Batch update locus curator access records	
users: Jolley, Keith (keith)	

Then select loci/schemes that the user is allowed to curate in the left hand 'Available' list, and click the right button to move these to the 'Selected' list:

PubMLST Database home Curator home Contents
Logged in: Keith Jolley (keith). [+Log out Change password
Batch update locus curator access records
User: Keith Jolley Select values to enable or disable and then click the appropriate arrow button. Select loci WEIS0004 NEIS0005 NEIS0006 NEIS0007 NEIS0009 NEIS0010 NEIS0012 NEIS0014 NEIS014 Neisono Neisono <tr< th=""></tr<>

If you uncheck the 'Hide curator name from public view' checkbox, the curator name and E-mail address will appear alongside loci in the download table on the website.

5.5 Controlling access

5.5.1 Restricting particular configurations to specific user accounts

Suppose you only wanted specific users to access a database configuration.

In the config.xml, add the following directive:

default_access="deny"

This tells BIGSdb to deny access to anybody unless their account name appears within a file called users.allow within the config directory. The users.allow file should contain one username per line. You can also use a usergroups.allow file. This file should contain the names of user groups, the members of which are allowed access. The file should contain one user group name per line.

Alternatively, you can deny access to specific users, while allowing every other authenticated user. In config.xml, add the following directive:

```
default_access="allow"
```

This tells BIGSdb to allow access to anybody unless their account name appears within a file called users.deny within the config directory. The users.deny file should contain one username per line.

5.6 Setting user passwords

Please note that these instructions only apply if using the built-in BIGSdb authentication system.

If you are an administrator or a curator with specific permission to change other users' passwords, you should see a 'User passwords' box in the admin section of the curator's index page. Click the 'Set passwords' link.

Admin func	tions					O Show all
Permissions	User passwords	Configuration check	Configuration repair	Locus curators	Scheme curators	
¢		6	• •	++\$	+#¢≯	

Select the appropriate user from the drop-down list box and enter the new password twice where prompted.

PubMLST Database	home Curator home	Contents	
Logged in: Keith Jolley (keith). 🍽 Log out Change password		
Set user pass	word		
Passwords must be at lea	ast 8 characters long.		
Passwords			Action
User:	Jolley, Keith (keith)	•	Set password
New password:	•••••		
Retype password:	•••••		

Click 'Set password' and the password will be updated.

5.7 Setting the first user password

To set the first administrator's password for a new database, use the add_user.pl script found in the scripts/maintenance directory:

add_user.pl [-a] -d <dbase> -n <username> -p <password>

The first user account needs to be added to the database *manually*.

5.8 Enabling plugins

Some plugins can be enabled/disabled for specific databases. If you look in the get_attributes function of the specific plugin file and see a value for system_flag, this value can be used in the system tag of the database configuration XML file to enable the plugin.

For example, the get_attributes function of the BURST plugin looks like:

```
sub get_attributes {
       my %att = (
                              => 'BURST',
                 name
                 name => 'BURST',
author => 'Keith Jolley',
                 affiliation => 'University of Oxford, UK',
                 email => 'keith.jolley@zoo.ox.ac.uk',
                 description => 'Perform BURST cluster analysis on query results query_
\leftrightarrow results',
                 category => 'Cluster',
                 buttontext => 'BURST',
                 menutext => 'BURST',
                module => 'BURST',
version => '1.0.0',
dbtype => 'isolates, sequences',
section => 'postquery',
order => 10,
                 system_flag => 'BURST',
                 input => 'query',
                 requires => 'mogrify',
                 min => 2,
                              => 1000
                 max
        );
        return \%att;
}
```

The 'system_flag' attribute is set to 'BURST', so this plugin can be enabled for a database by adding:

BURST="yes"

to the system tag of the database XML file. If the system_flag value is not defined then the plugin is always enabled if it is installed on the system. If the system_flag value is set to 'no' then the plugin will be disabled even if the all_plugins attribute is set to 'yes'.

5.9 Temporarily disabling database updates

There may be instances where it is necessary to temporarily disable database updates. This may be during periods of server or database maintenance, for instance when running on a backup database server.

Updates can be disabled on a global or database-specific level.

5.9.1 Global

In the /etc/bigsdb/bigsdb.conf file, add the following line:

```
disable_updates=yes
```

An optional message can also be displayed by adding a disable_update_message value, e.g.

disable_update_message=The server **is** currently undergoing maintenance.

5.9.2 Database-specific

The same attributes described above for use in the bigsdb.conf file can also be used within the system tag of the database config.xml file, e.g.

```
<system

db="bigsdb_neisseria"

dbtype="isolates"

...

disable_updates="yes"

disable_update_message="The server is currently undergoing maintenance."
```

5.10 Host mapping

During periods of server maintenance, it may be necessary to map a database host to an alternative server. This would allow a backup database server to be used while the primary database server is unavailable. In this scenario, you would probably also want to *disable updates*.

Host mapping can be achieved by editing the /etc/bigsdb/host_mapping.conf file. Each host mapping is placed on a single line, with the current server followed by any amount of whitespace and then the new mapped host, e.g.

#Existing_host	Mapped_host
server1	server2
localhost	server2

[Lines beginning with a hash are comments and are ignored.]

This configuration would use server2 instead of server 1 or localhost wherever they are defined in the database configuration (either host attribute in the database config.xml file, or within the loci or schemes tables).

5.11 Improving performance

5.11.1 Use mod_perl

The single biggest improvement to speed can be obtained by running BIGSdb under mod_perl. There's very little point trying anything else until you have mod_perl set up and running - this can improve start-up performance a hundred-fold since the script isn't compiled on each page access but persists in memory.

5.11.2 Cache scheme definitions within an isolate database

If you have a large number of allelic profiles defined for a scheme, you can cache these definitions within an isolate database to speed up querying of isolates by scheme criteria (e.g. by ST for a MLST scheme).

To do this use the update_scheme_caches.pl script found in the scripts/maintenance directory, e.g. to cache all schemes in the pubmlst_bigsdb_neisseria_isolates database

update_scheme_caches.pl --database pubmlst_bigsdb_neisseria_isolates

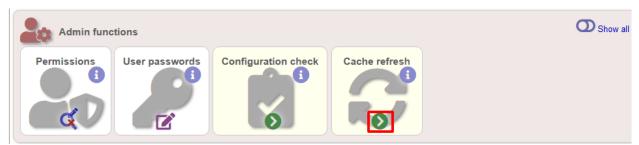
This script creates indexed tables within the isolate database called temp_scheme_X and temp_isolates_scheme_fields_1 (where X is the scheme_id). If these table aren't present, they are created as temporary tables every time a query is performed that requires a join against scheme definition data. This requires

importing all profile definitions from the definitions database and determining scheme field values for all isolates. This may sound like it would be slow but caching only has a noticeable effect once you have >5000 profiles.

You are able to update the cache for a single scheme, or a list of schemes, and choose the method of update. For large schemes, such as cgMLST, a full refresh may take a long time, so you may wish to only perform this infrequently (perhaps once a week) with more regular 'daily' or 'daily_replace' updates. A full list of options available are shown by typing

```
update_scheme_caches.pl --help
NAME
    update_scheme_caches.pl - Update scheme field caches
SYNOPSIS
    update_scheme_caches.pl --database NAME [options]
OPTIONS
--database NAME
   Database configuration name.
--help
   This help page.
--method METHOD
    Update method - the following values are allowed:
    full: Completely recreate caches
    incremental: Only add values for records not in cache.
    daily: Only add values for records not in cache updated today.
    daily_replace: Refresh values only for records updated today.
--quiet
    Don't output progress messages.
--schemes SCHEMES
    Comma-separated list of scheme ids to use.
    If left empty, all schemes will be updated.
```

Note that you will need to run this script periodically as a CRON job to refresh the cache. Admins can also refresh the caches manually from a link on the curators' page. This link is only present if the caches have been previously generated.



You can also set cache_schemes="yes" in the system tag of config.xml to enable automatic refreshing of the caches (using the 'daily' method) when batch adding new isolates (you should still periodically run the update_scheme_caches.pl script via CRON to ensure any changes in the sequence definition database are picked up).

If queries are taking longer than 5 seconds to perform and a cache is not in place, you will see a warning message in bigsdb.log suggesting that the caches be set up. Unless you see this warning regularly, you probably don't need to do this.

5.11.3 Use a ramdisk for the secure temporary directory

If you are running BIGSdb on a large server with lots of RAM, you could use some of this as a ramdisk for temporary files. Debian/Ubuntu systems make available up to half the system RAM as a ramdisk mounted under /run/shm (or /dev/shm) by default. Set the secure_tmp_dir to this RAM disk and you should see significant improvement in operations requiring the writing of lots of temporary files, e.g. tag scanning and the Genome Comparator plugin. This is only likely to be appropriate if you have very large amounts of RAM available. As an example, the server hosting the PubMLST databases is a dedicated machine with 1TB RAM with temporary files rarely using more than 50GB space.

5.12 Dataset partitioning

5.12.1 Sets

Sets provide a means to partition the database in to manageable units that can appear as smaller databases to an end user. Sets can include constrained groups of isolates, loci, and schemes from the complete database.

See also:

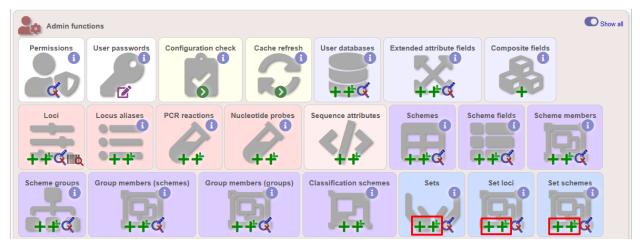
Sets (concept)

5.12.2 Configuration of sets

First sets need to be enabled in the XML configuration file (config.xml) of the database. Add the following attribute to the system tag:

sets="yes"

With this attribute, the curation interface now has options to add sets, and then add loci or schemes to these sets. These functions are normally hidden, so you may need to click the 'Show all' toggle to display it.



The name of a locus or scheme to use within a set can be defined in the set_name field when adding loci or schemes to a set. Common names can also be set for loci - equivalent to the common name used within the loci table.

Now when a user goes to the contents page of the database they will be presented with a dropdown menu of datasets and can choose either the 'whole database' or a specific set. This selection is remembered between sessions.

PubMLST Database home Contents
HØ Log in
Neisseria PubMLST database
The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample.
Datasets
This database contains multiple datasets. You can choose to display a single set or the whole database. Please select: Whole database Choose
Query database Main public projects Option settings Search or browse database Search by combinations of loci (profiles) Main public projects Set general options - including isolate table field handling. Manage submissions General information • Search by combinations of loci (profiles) • Your projects • Set display and query options for locus, schemes or scheme fields. • Manage submissions • Isolates: 46,731 • Update history • Update history • Update history • About BIGSdb
Breakdown Export Analysis Third party tools Single field - Export dateset - Codon usage - Codon usage - Codon usage Unique combinations - Sequences - XMFA / concatenated FASTA formats - Codon usage - Codon usage - Codon usage Scheme and alleles - Sequences - XMFA / concatenated FASTA formats - Codon usage - Codon usage - HyloViz - Visualization of genomic relationships Scheme and alleles - Sequence bin - Miscellaneous - Species identification - HyloViz - Visualization and sharing for genomic epidemiology • Description of database fields - Description of database fields - Hird Party tools - HyloViz - Visualization of genomic relationships

Alternatively, a specific set can be selected within the XML config file so that only a specific set is available when accessed via that configuration. In that case, the user would be unaware that the database contains anything other than the loci and schemes available within the set.

To specify this, add the following attributute to the system tag:

set id="1"

where the value is the name of the set.

Note: If the set_id attribute is set, database configuration settings in the curator's interface are disabled. This is because when the configuration is constrained to a set, only loci and schemes already added to the set are visible, so functionality to edit schemes/loci would become very confusing. To modify these settings, you either need to access the interface from a different configuration, i.e. an alternative config.xml with the set_id attribute not set, or temporarily remove the set_id directive from the current config.xml while making configuration changes.

5.12.3 Set views

Finally the isolate record table can be partitoned using database views and these views associated with a set. Create views using something like the following:

```
CREATE VIEW spneumoniae AS SELECT ★ FROM isolates WHERE species = 'Streptococcus_

→pneumoniae';

GRANT SELECT ON spneumoniae TO apache;
```

Add the available views to the XML file as a comma separated list in the system tag 'views' attribute:

```
<system
.....
sets="yes"
views="spneumoniae,saureus"
```

(continues on next page)

(continued from previous page)

</system>

Set the view to the set by using the 'Add set view' link on the curator's page.

5.12.4 Using only defined sets

The only_sets attribute can be set to 'yes' to disable the option for 'Whole database' so that only sets can be viewed, e.g.

```
<system
.....
sets="yes"
only_sets="yes"
>
</system>
```

5.13 Setting a site-wide users database

On large sites you may wish to employ a site-wide users database so that user details are kept in a single location and the user can log in to any database using the same credentials.

Once a *site-wide user database has been set up*, this can be defined within each client database as follows. From the curators' contents page, click the add (+) user databases link. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Enter the user database details. You only need to enter the full database connection details if these are different from those set in db.conf. Press submit.

PubMLST Database	home Curator ho	ome Contents		
Logged in: Keith Jolley (keith	n). 🕩 Log out Change pas	sword		Toggle: ()
Add new user	database			
Please fill in the fields be — Record	elow - required fields a	re marked with an exclamation mark	c (I).	Action
id:!	1	A V		Reset Submit
name:!	PubMLST	Site/domain name		
dbase name:!	pubmlst_bigsdb_users	s	Name of the database holding user data	
curator:!	Keith Jolley (keith)			
datestamp:!	2016-12-16			
list order:				
auto registration:	🔘 true 🔘 false	Allow user to register themself for databa	ise	
dbase host:			 IP address of database host 	
dbase port:		🗧 🜖 Network port accepting database	connections	
dbase user:			0	
dbase password:			0	

Curators will need *specific permissions* set to be able to modify details in, or import users from a site-wide users database.

5.14 Adding new loci

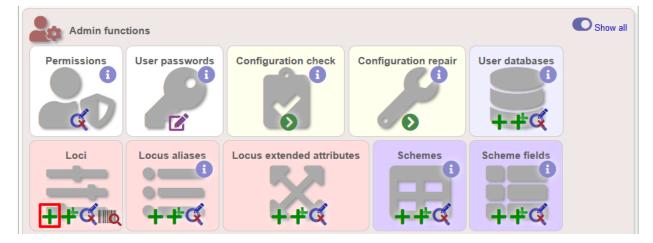
See also:

Loci (concept)

5.14.1 Sequence definition databases

Single locus

Click the add (+) loci link on the curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



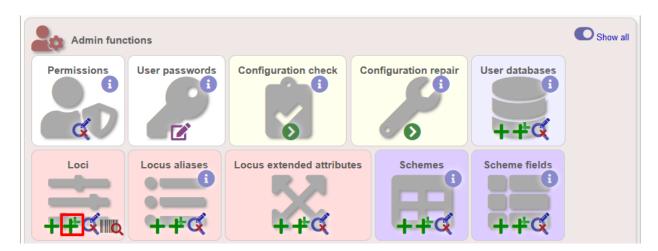
Fill in the web form with appropriate values. Required fields have an exclamation mark (!) next to them:

- id The name of the locus.
 - Allowed: any value starting with a letter, number or underscore.
- data_type Describes whether the locus is defined by nucleotide or peptide sequence.
 - Allowed: DNA/peptide.
- allele_id_format The format for allele identifiers.
 - Allowed: integer/text.
- length_varies Sets whether alleles can vary in length.
 - Allowed: true/false.
- coding_sequence Sets whether the locus codes for a protein.
 - Allowed: true/false.
- formatted_name Name with HTML formatting (optional).
 - This allows you to add formatting such as bold, italic, underline and superscripting to locus names as they
 appear in the web interface.
 - Allowed: valid HTML.
- common_name The common name for the locus (optional).
 - Allowed: any value.
- formatted_common_name Common name with HTML formatting (optional).
 - Allowed: valid HTML.
- allele_id_regex Regular expression to enforce allele id naming (optional).
 - ^: the beginning of the string
 - \$:the end of the string
 - d: digit
 - D: non-digit
 - s: white space character
 - S: non white space character
 - w: alpha-numeric plus '_'
 - .: any character
 - *: 0 or more of previous character
 - +: 1 or more of previous character
 - e.g. ^Fd-d+\$ states that an allele name must begin with a F followed by a single digit, then a dash, then one or more digits, e.g. F1-12
- length Standard length of locus (required if length_varies is set to false.
 - Allowed: any integer.
- min_length Minimum length of locus (optional).
 - Allowed: any integer.
- max_length Maximum length of locus (optional).

- Allowed: any integer (larger than the minimum length).
- orf Open reading frame of locus (optional).
 - 1-3 are the forward reading frame, 4-6 are the reverse reading frames.
 - Allowed: 1-6.
- genome_position The start position of the locus on a reference genome (optional).
 - Allowed: any integer.
- match_longest Specifies whether in a sequence query to only return the longest match (optional).
 - This is useful for some loci that can have some sequences shorter than others, e.g. peptide loci defining antigenic loops. This can lead to instances of one sequence being longer than another but otherwise being identical. In these cases, usually the longer sequence is the one that should be matched.
 - Allowed: true/false.
- full_name Full name of the locus (optional).
 - Allowed: any value.
- product Name of gene product (optional).
 - Allowed: Any value.
- description Description of the locus (optional).
 - Allowed: any value.
- aliases Alternative names for the locus (optional).
 - Enter each alias on a separate line in the text box.
 - Allowed: any value.
- pubmed_ids PubMed ids of publications describing the locus (optional).
 - Enter each PubMed id on a separate line in the text box.
 - Allowed: any integer.
- links Hyperlinks pointing to additional resources to display in the locus description (optional).
 - Enter each link on a separate line in the format with the URL first, followed by a | then the description (URL/description).

Batch adding

Click the batch add (++) loci link on the curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Click the link to download a header line for an Excel spreadsheet:

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). C+Log out Change password		Toggle: 🚯
Batch insert loci		
 This page allows you to upload locus data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish Download tab-delimited header for your spreadsheet - use 'Paste Special Stext' to paste the data. Download submission template (xlsx format) 		ľ
Paste in tab-delimited text (include a field header line).	- Action	
	Reset Subr	mit

Fill in the spreadsheet using the fields described for *adding single loci*.

Fill in the spreadsheet fields using the table above as a guide, then paste the completed table into the web form and press 'Submit query'.

5.14.2 Isolate databases

Single locus

Click the add (+) loci link on the curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

Admin func	tions					Show a
Permissions	User passwords	Configuration check	Cache refresh	User databases	Extended attribute f	ields
Composite fields		Locus aliases	PCR reactions	PCR locus links	Nucleotide probes	

Fill in the web form with appropriate values. Required fields have an exclamation mark (!) next to them:

Logged in: Keith Jolley (keith). 🗭 Log o	out Change password				Toggle: 🜖 📃
Add new locus					Show tools
Please fill in the fields below - re-	quired fields are marke	ed with an exclamation mark (!).			+
id:					
data type:!				Reset Submit	
allele id format!					
	○ true ● false 1				
coding sequence:					
	allele only - 0				
	○ true ● false 1				
	● true ○ false 0				
	● true ○ false 0				
	Keith Jolley (keith)				
date entered:!	2016-07-26				
datestamp:!	2016-07-26				
formatted name:			0		
common name:			0		
formatted common name:			0		
allele id regex:			0		
length:		→ 0			
orf:	- 0				
genome position:		20			
match longest:	🔘 true 🔘 false 🜖				
reference sequence:					
				0	
	🔘 true 🔘 false 🜖	Do NOT set to true unless you define			
	🔘 true 🔘 false 🜖	Do NOT set to true unless you define	probe sequences linked to this locus.		
	pubmlst_bigsdb_neiss	seria_seqdef	Name of the database holding allele sequences		
dbase host:			IP address of database host		
dbase port:		O Network port accepting database			
dbase user:			0		
dbase password:			0		
dbase id:	PUT_LOCUS_NAME_H	HERE	Name of locus in seqdef database		

- id The name of the locus
 - Allowed: any value starting with a letter or underscore.
- data_type Describes whether the locus is defined by nucleotide or peptide sequence.

- Allowed: DNA/peptide.
- allele_id_format The format for allele identifiers.
 - Allowed: integer/text.
- length_varies Sets whether alleles can vary in length.
 - Allowed: true/false.
- coding_sequence Sets whether the locus codes for a protein.
 - Allowed: true/false.
- isolate_display Sets how alleles for this locus are displayed in a detailed isolate record this can be overridden by user preference.
 - Allowed: allele only/sequence/hide.
- main_display Sets whether or not alleles for this locus are displayed in a main results table by default this can be overridden by user preference.
 - Allowed: true/false.
- query_field Sets whether or not alleles for this locus can be used in queries by default this can be overridden by user preference.
 - Allowed: true/false.
- analysis Sets whether or not alleles for this locus can be used in analysis functions by default this can be overridden by user preference.
 - Allowed: true/false.
- formatted_name Name with HTML formatting (optional).
 - This allows you to add formatting such as bold, italic, underline and superscripting to locus names as they
 appear in the web interface.
 - Allowed: valid HTML.
- common_name The common name for the locus (optional).
 - Allowed: any value.
- formatted_common_name Common name with HTML formatting (optional).
 - Allowed: valid HTML.
- allele_id_regex Regular expression to enforce allele id naming.
 - ^: the beginning of the string
 - \$:the end of the string
 - d: digit
 - D: non-digit
 - s: white space character
 - S: non white space character
 - w: alpha-numeric plus '_'
 - .: any character
 - *: 0 or more of previous character
 - +: 1 or more of previous character

- e.g. ^Fd-d+\$ states that an allele name must begin with a F followed by a single digit, then a dash, then one or more digits, e.g. F1-12
- length Standard length of locus (required if length_varies is set to false).
 - Allowed: any integer.
- orf Open reading frame of locus (optional). 1-3 are the forward reading frame, 4-6 are the reverse reading frames.
 - Allowed: 1-6.
- genome_position The start position of the locus on a reference genome.
 - Allowed: any integer.
- match_longest Only select the longest exact match when tagging/querying.
 - This is useful for some loci that can have some sequences shorter than others, e.g. peptide loci defining antigenic loops. This can lead to instances of one sequence being longer than another but otherwise being identical. In these cases, usually the longer sequence is the one that should be matched.
 - Allowed: true/false.
- reference_sequence Sequence used by the automated sequence comparison algorithms to identify sequences matching this locus. This is only used if a sequence definition database has not been set up for this locus.
- pcr_filter Set to true if this locus is further defined by genome filtering using in silico PCR.
 - Allowed: true/false.
- probe_filter Set to true if this locus is further defined by genome filtering using in silico hybdridization.
 - Allowed: true/false.
- introns Set to true if locus may contain introns. This setting will only be available if BLAT is configured in bigsdb.conf.
 - Allowed: true/false.
- dbase_name Name of database (system name).
 - Allowed: any text.
- dbase_host Resolved name of IP address of database host leave blank if running on the same machine as the isolate database.
 - Allowed: network address, e.g. 129.67.26.52 or zoo-oban.zoo.ox.ac.uk
- dbase_port Network port on which the sequence definition database server is listening leave blank unless using a non-standard port (5432).
 - Allowed: integer.
- dbase_user Name of user with permission to access the sequence definition database depending on the database configuration you may be able to leave this blank.
 - Allowed: any text (no spaces).
- dbase_password Password of database user again depending on the database configuration you may be able to leave this blank.
 - Allowed: any text (no spaces).
- dbase_id Name of locus in seqdef database. This is usually the same as the id field.
 - Allowed: any text (no spaces).

- description_url The URL used to hyperlink to locus information in the isolate information page. This can either be a relative (e.g. /cgi-bin/...) or an absolute (containing http://) URL.
 - Allowed: any valid URL.
- url The URL used to hyperlink to information about the allele. This can either be a relative or absolute URL. If [?] (including the square brackets) is included then this will be substituted for the allele value in the resultant URL. To link to the appropriate allele info page on a corresponding seqdef database you would need something like /cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_neisseria_seqdef&page=alleleInfo&locus=abcZ&allele_id=[?].
 - Allowed: any valid URL.
- submission_template Sets whether or not a column for this locus is included in the Excel submission template.
 - Allowed: true/false (default: false)
- view Restrict this scheme to only isolates contained in the specified database view. This option will only appear if the views attribute is set in the system tag. The view needs to have been defined in the database as a subset of the isolate table (usually filtered by the value of one or more of its fields).

Using existing locus definition as a template

When defining a new locus in the isolate database, it is possible to use an existing locus record as a template. To do this, click the 'Show tools' link in the top-right of the screen:

PubMLST Database home	Curator home Contents	
Logged in: Keith Jolley (keith). 🗭 Log of	ut Change password	Toggle: 🚺 📃
Add new locus		Show tools
Please fill in the fields below - requ	ired fields are marked with an exclamation mark (!).	-
Record		
id:!		
data type:!	DNA 👻	
allele id format:!	integer 💌	
	⊖ true ● false	
coding sequence:		
isolate display:!	allele only 💌	
main display:!	⊙ true ● false	
query field:!	● true	
analysis:!	● true ○ false	
curator:!	Keith Jolley (keith)	
date entered:!		
datestamp:!	2018-06-18	
formatted name:		
common name:		
formatted common name:		
allele id regex:		
length:		
	◯ true ◯ false	
orf:	▼	
genome position:		
	◯ true ◯ false	
reference sequence:		

This displays a drop-down box containing existing loci. Select the locus that you wish to use as a template, and click 'Copy'.

PubMLST	Database home	Curator home	Contents			
Logged in: Keit	Logged in: Keith Jolley (keith). [+Log out Change password Toggle: 1]					
Add ne	w locus		Hide tools			
Please fill in — Record-	coding sequence:! isolate display:! main display:!	DNA integer true false false	Copy configuration from NEIS0001 (lpxC) Copy All parameters will be copied except id, common name, reference sequence, genome position and length. The copied locus id will be substituted for 'PUT_LOCUS_NAME_HERE' in fields that include it.			
		● true ○ false Keith Jolley (keith)				
form	orf: genome position: match longest:	2018-06-18 ○ true ○ false ▼				
	reference sequence:					

The configuration will be copied over to the web form, with the exception of name fields. Some fields will require you to change the value 'PUT_LOCUS_NAME_HERE' with the value you enter in the id field. These are usually the dbase_id2_value, description_url and url fields:

allele id regex:		0	
length:	÷ 0	· ·	
orf:			
genome position:	÷ 0		
match longest:			
reference sequence:			
pcr filter:	◯ true ◯ false n	0 lb.	
	○ true ○ false 1		
	pubmlst_bigsdb_neisseria_seqdef	Name of the database holding allele sequences	
dbase host:	publinat_bigadb_nelasena_sequel	IP address of database host	
dbase port:	() Network port accepting database	-	
dbase user:		0	
dbase password:		0	
dbase table:		Database table that holds sequence information for this locus	
dbase id field:		Primary field in sequence database that defines allele, e.g. 'allele_id'	
dbase id2 field:		I Secondary field that defines allele, e.g. 'locus'	
	PUT_LOCUS_NAME_HERE	Secondary field value, e.g. locus name	
dbase seq field:		Field in sequence database containing allele sequence	
	/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_ne locus=PUT_LOCUS_NAME_HERE	· · · · · · · · · · · · · · · · · · ·	
urt:	/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_ne locus=PUT_LOCUS_NAME_HERE&allele_id=[?]		
		(1) It.	
submission template:	C true Include column in isolate submission	template for this locus	
aliases:			
Action			

Complete the form and click 'Submit'.

Batch adding

Click the batch add (++) loci link on the curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

Admin func	tions					Shov
Permissions	User passwords	Configuration check	Cache refresi	User databases ++¢	Extended attribute field	5
Composite fields		Locus aliases	PCR reactions	PCR locus links	Nucleotide probes	

Click the link to download an Excel template:

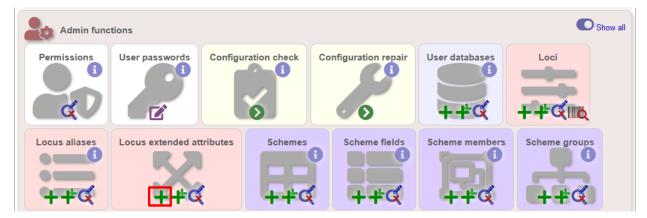
PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). C+Log out Change password		Toggle: 🚯 📃
Batch insert loci		
 This page allows you to upload locus data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. Enter aliases (alternative names) for your locus as a semi-colon (;) separated list. Download tab-delimited header for your spreadsheet - use 'Paste Special S Text' to paste the data. 		Ħ
Download submission template (xlsx format) Paste in tab-delimited text (include a field header line).	Action —	
	Reset Submit	

Fill in the spreadsheet fields using the *table above as a guide*, then paste the completed table into the web form and press 'Submit query'.

5.15 Defining locus extended attributes

You may want to add additional metadata for the allele definitions of some loci. Since these are likely to be specific to each locus, they cannot be defined generically within the standard locus definition. We can, instead, define extended attributes. Examples of these include higher order grouping of antigen sequences, antibody reactivities, identification of important mutations, or cross-referencing of alternative nomenclatures.

To add extended attributes for a locus, click add (+) locus extended attributes in the sequence definition database curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Fill in the web form with appropriate values. Required fields have an exclamation mark (!) next to them:

PubMLST Datat	ase home Curator home Content	ts		
Logged in: Keith Jolley (keith). ➡Log out Change password			Toggle: 🕚
Add new loo	cus extended attribute			
		1		
Please fill in the fields	below - required fields are marked with an exc	clamation mark (!).		
Record				Action
locus:	•			Action Reset Submit
field:				
value format:!	text 🔹			
	🔿 true 🔘 false 🚯			
	🖲 true 🔘 false 🕚			
	Keith Jolley (keith)			
datestamp:!	2018-06-18			
value regex:		0		
description:				
option list:				
url:			.:: () ()	
length:			•	
field order:				
neid ofder.	•			

- locus Select locus from dropdown box.
 - Allowed: existing locus name.
- field Name of extended attributes.
 - Allowed: any value.
- value_format Data type of attribute.
 - Allowed: integer/text/boolean.
- required Specifies whether the attribute value but be defined when adding a new sequence.
 - Allowed: true/false.
- value_regex Regular expression to enforce allele id naming (optional).
 - ^: the beginning of the string
 - \$:the end of the string
 - d: digit
 - D: non-digit
 - s: white space character
 - S: non white space character
 - w: alpha-numeric plus '_'
 - .: any character
 - *: 0 or more of previous character

- +: 1 or more of previous character
- description Description that will appear within the web form when adding new sequences (optional).
 - Allowed: any value.
- option_list Pipe (l) separated list of allowed values (optional).
- length Maximum length of value (optional).
 - Allowed: any integer.
- field_order Integer that sets the position of the field within scheme values in any results (optional).
 - Allowed: any integer.

Once extended attributes have been defined, they will appear in the web form when adding new sequences for that locus. The values are searchable when using a *locus-specific sequence query*, and they will appear within query results and allele information pages.

5.16 Defining schemes

Schemes are collections of loci that may be associated with particular fields - one of these fields can be a primary key, i.e. a field that uniquely defines a particular combination of alleles at the associated loci.

A specific example of a scheme is MLST - see workflow for setting up a MLST scheme.

To set up a new scheme, you need to:

- 1. Add a new scheme description.
- 2. Define loci as 'scheme members'.
- 3. Add 'scheme fields' associated with the scheme.

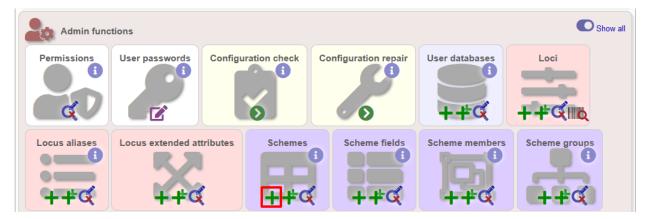
See also:

Schemes (concept)

5.16.1 Sequence definition databases

As with all configuration, tables can be populated using the batch interface (++) or one at a time (+). Details for the latter are described below:

Click the add (+) scheme link on the curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Fill in the scheme description in the web form. The next available scheme id number will be filled in already.

The display_order field accepts an integer that can be used to order the display of schemes in the interface - this can be left blank if you wish.

PubMLST Database I	nome Curator home Contents	
Logged in: Keith Jolley (keith).	Log out Change password	Toggle: 🚯 🗧
Add new scher	ne	
Please fill in the fields below	 required fields are marked with an exclamation mark (!). 	
Record		_
id:!	1 *	
name:!		
curator:!	Keith Jolley (keith)	
datestamp:!		
date entered:	2018-06-18	
description:		
display order:		
allow missing loci:	◯ true ◯ false 1 This is only relevant to schemes with primary key fields, e.g. MLST.	
disable:	☉ true ☉ false Set to true to disable scheme. This can be overridden by user preference settings.	
no submissions:	🗇 true 🗇 false 💫 Set to true to prevent submission of profiles of this scheme via the automated submission syst	em.
flags:	experimental	
	in development	
	please cite	
	unpublished T Use CTRL/SHIFT click to select or deselect values	
PubMed ids:		
links: (Format: URL description)		
(Formal, OREJUESCIPIION)		
-Action		
Reset Submit		

To add loci to the scheme, click the add (+) scheme members link on the curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

Admin fund	tions				Show all
Permissions	User passwords	ifiguration check	Configuration repair	User databases	
Locus aliases	Locus extended attribute	Schemes	Scheme fields	Scheme members	Scheme groups

Select the scheme name and a locus that you wish to add to the scheme from the appropriate drop-down boxes. *Loci need to have already been defined*. The field_order field allows you to set the display order of the locus within a profile - if these are left blank that alphabetical ordering is used.

PubMLST Dat	abase home Curator home Contents	
Logged in: Keith Jolle	((keith). € Log out Change password	Toggle: 🚯 📘
Add new s	cheme member	
	at any modifications to the structure of this scheme will result in the removal of all data from it. This is done to ensure dat t allele designations, but any profiles will have to be reloaded.	a integrity.
Record scheme id:! locus:!	abcZ Keith Jolley (keith)	ŧ
field order:		

To add scheme fields, click the add (+) scheme fields link on the curator's interface contents page.

Admin fund	tions				Show all
Permissions	User passwords	infiguration check	Configuration repair	User databases	
Locus aliases	Locus extended attribut	Schemes	Scheme fields	Scheme members	Scheme groups

Fill in the web form with appropriate values. Required fields have an exclamation mark (!) next to them:

PubMLST Dat	abase home	Curator home	Contents				
Logged in: Keith Jolle	y (keith). 🗭 Log out	Change password					Toggle: 🚯
Add new s	cheme fi	eld					
		ons to the structure ons, but any profiles			noval of all data from it	. This is done to ensure	e data integrity.
Please fill in the fie	lds below - requir	ed fields are marked	with an exclamati	on mark (!).			
					Action		
scheme id:!	MLST		•		Reset Subm	it	
field:	ST						
type:!	integer 👻						
primary key:!	◉ true ☉ false	0					
dropdown:!	🔘 true 🔘 false	0					
curator:	Keith Jolley (ke	eith)					
datestamp:!	2018-06-18						
description:							
field order:	-	×					
	© true © false	0					
value regex:				0			

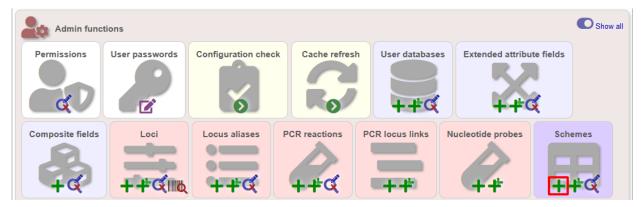
- scheme_id Dropdown box of scheme names.
 - Allowed: selection from list.
- field Field name.
 - Allowed: any value.
- type Format for values.
 - Allowed: text/integer/date.
- primary_key Set to true if field is the primary key. There can only be one primary key for a scheme.
 - Allowed: true/false.
- dropdown Set to true if a dropdown box is displayed in the query interface, by default, for values of this field to be quickly selected. This option can be overridden by user preferences.
 - Allowed: true/false.
- description This field isn't currently used.
- field_order Integer that sets the position of the field within scheme values in any results.
 - Allowed: any integer.
- value_regex Regular expression to enforce field values.
 - ^: the beginning of the string
 - \$:the end of the string
 - d: digit
 - D: non-digit
 - s: white space character

- S: non white space character
- w: alpha-numeric plus '_'
- .: any character
- *: 0 or more of previous character
- +: 1 or more of previous character

5.16.2 Isolate databases

As with all configuration, tables can be populated using the batch interface (++) or one at a time (+). Details for the latter are described below:

Click the add (+) scheme link on the curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Fill in the scheme description in the web form. Required fields have an exclamation mark (!) next to them:

Logged in: Keith Jolley (keith).	Decg out Change password		Toggle: 🚯 🔳
Add new schen	ne		
Record	w - required fields are marked with an exclamation mark (!).	Action	E+
name:! isolate display:! main display:! query field:! query status:! analysis:!		Reset Submit	
	ł.		
dbase name:	0		
dbase host:	0		
dbase port:	÷ 0		
dbase user:	0		
dbase password:	0		
dbase id:			
display order:			
allow missing loci: flags:	Thue This is only relevant to schemes with primary key fields, e.g. MLST. citation required experimental in development unpublished		
PubMed ids:	i.		
links: (Format: URL description)			

- id Index number of scheme the next available number will be entered automatically.
 - Allowed: any positive integer.
- description Short description this is used in tables so make sure it's not too long.
 - Allowed: any text.
- isolate_display Sets whether or not fields for this scheme are displayed in a detailed isolate record this can be overridden by user preference.
 - Allowed: allele only/sequence/hide.
- main_display Sets whether or not fields for this scheme are displayed in a main results table by default this can be overridden by user preference.
 - Allowed: true/false.
- query_field Sets whether or not fields for this scheme can be used in queries by default this can be overridden by user preference.
 - Allowed: true/false.
- query_status Sets whether a dropdown list box should be displayed in the query interface to filter results based on profile completion for this scheme this can be overridden by user preference.
 - Allowed: true/false.

- analysis Sets whether or not alleles for this locus can be used in analysis functions by default this can be overridden by user preference.
 - Allowed: true/false.
- dbase_name Name of seqdef database (system name) containing scheme profiles (optional).
 - Allowed: any text.
- dbase_host Resolved name of IP address of database host leave blank if running on the same machine as the isolate database (optional).
 - Allowed: network address, e.g. 129.67.26.52 or zoo-oban.zoo.ox.ac.uk
- dbase_port Network port on which the sequence definition database server is listening leave blank unless using a non-standard port, 5432 (optional).
 - Allowed: integer.
- dbase_user Name of user with permission to access the sequence definition database depending on the database configuration you may be able to leave this blank (optional).
 - Allowed: any text (no spaces).
- dbase_password Password of database user again depending on the database configuration you may be able to leave this blank (optional).
 - Allowed: any text (no spaces).
- dbase_id Id of scheme in the sequence definition database.
 - Allowed: any integer.
- view Restrict this scheme to only isolates contained in the specified database view. This option will only appear if the views attribute is set in the system tag. The view needs to have been defined in the database as a subset of the isolate table (usually filtered by the value of one or more of its fields).
- display_order Integer reflecting the display position for this scheme within the interface (optional).
 - Allowed: any integer.
- allow_missing_loci Allow profile definitions to contain '0' (locus missing) or 'N' (any allele).

5.17 Organizing schemes into hierarchical groups

Schemes can be organized in to groups, and these groups can in turn be members of other groups. This faciliates hierarchical ordering of loci, but with the flexibility to allow loci and schemes to belong to multiple groups.

This hierarchical structuring can be seen in various places within BIGSdb, for example the allele download page.

				ut Change password							Help 🗹
ownl	oad	allel	e se	equences							
elect loci	by sche	eme Alp	habetic	al list All loci by s	scheme						
	-						of schemes - clicking	a group folder will di	anlay the loci for all	Lechemes within the	group and any subgrou
ick the no					g to seneme	s or groups	or senemes - eliening	a group loider will di	splay the loci for all	r senemes within the	group and any subgrou
										A	
		eplicatio									
		🔋 DNA r									
	L (Nucle	otide e:	cision repair							
Þ	🔊 Ti	ranscripti	ion								
þ.	🛄 Ti	ranslatio	ı							_	
ļ <u>(</u>	Geno	mic islan	ds							=	
	_	qe Scher									
4		•	nes								
P 4	-										
¢ 4	N. goi	norrhoea	e AMR								
k 🛴	Plasn	nids									
- A- 🧸	Typing	9									
	🔊 M	ILST									
										T	
LST											
							h Full name/produc		Last updated		
abcZ adk	*	DNA DNA	879 651	Fixed: 433 bp Fixed: 465 bp	433 465	434 465		O. Harrison, K. Joll O. Harrison, K. Joll			
auk aroE	*	DNA	929	Fixed: 465 bp	405	405		O. Harrison, K. Joll			
umC	1	DNA	976	Fixed: 450 bp	463	465		O. Harrison, K. Joll			
gdh	1	DNA	911	Fixed: 501 bp	501	513		O. Harrison, K. Joll			
odhC	*	DNA	897	Fixed: 480 bp	480	503		O. Harrison, K. Joll			
	*	DNA	932	Fixed: 450 bp	447	450		O. Harrison, K. Joll	ey 2018-06-11		
pgm											

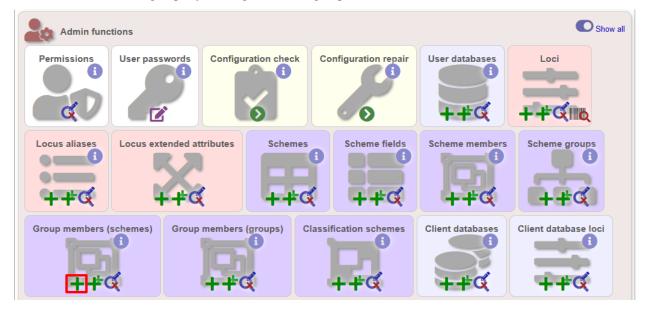
Scheme groups can be added in both the sequence definition and isolate databases. To add a new group, click the add (+) scheme group link on the curator's contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

Admin funct						C Shov
Permissions	User passwords	Configuration check	k Cache refresh	User databases	Extended attribut	
Composite fields		Locus aliases	PCR reactions	PCR locus links	Nucleotide probes	Sequence attributes
Schemes	Scheme fields	Scheme members	Scheme groups	Group members (so	chemes) Group n	nembers (groups)

Enter a short name for the group - this will appear within drop-down list boxes and the hierarchical tree, so it needs to be fairly short.

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). Change password		Toggle: 🜖 📃
Add new scheme group		
Please fill in the fields below - required fields are marked with an exclamation mark (!). Record id:! 1 curator:! Typing curator:! Keith Jolley (keith) datestamp:! 2018-06-18	Action Reset Submit	ľ
description: display order: seq query: O true O false I		

If you are creating a scheme group in the sequence definition database, there is an additional field called 'seq_query'. Set this to true to add the scheme group to the dropdown lists in the *sequence query* page. This enables all loci belonging to schemes within the group to be queried together.



Schemes can be added to groups by clicking the add (+) group members (scheme) link.

Select the scheme and the group to add it to, then click 'Submit'.

PubMLST Database home Curator home Contents	5	
Logged in: Keith Jolley (keith). Cog out Change password		Toggle: 🚯 📒
Add new scheme group scheme me	mber	
Please fill in the fields below - required fields are marked with an excl Record group id:! Typing scheme id:! MLST curator:! Keith Jolley (keith) datestamp:! 2018-06-18	lamation mark (!). Action Reset Submit	ľ

Scheme groups can be added to other scheme groups in the same way by clicking the add (+) scheme group group members link.

5.18 Setting up client databases

Sequence definition databases can have any number of isolate databases that connect as clients. Registering these databases allows the software to perform isolate data searches relevant to results returned by the sequence definition database, for example:

- Determine the number of isolates that a given allele is found in and link to these.
- Determine the number of isolates that a given scheme field, e.g. a sequence type, is found in and link to these.
- Retrieve specific attributes of isolates that have a given allele, e.g. species that have a particular 16S allele, or penicillin resistance given a particular penA allele.

Multiple client databases can be queried simultaneously.

To register a client isolate database for a sequence definition database, click the add (+) client database link on the curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

Permissions User passwords User passwords User databases User databases U	-
.ocus extended attributes	
Schemes Scheme fields Scheme members Scheme groups Group members (scheme	the off
	FX
	es)
<u>++4</u> ++4 ++4 ++4 ++4	
roup members (groups) Classification schemes Client databases Client database loci Client database fields Locus c	urators

Fill in the web form with appropriate values. Required fields have an exclamation mark (!) next to them:

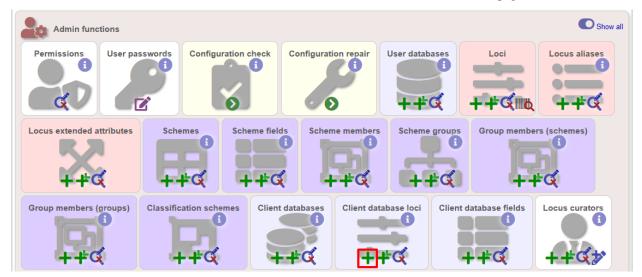
PubMLST Database	e home Curator home Co	ntents	
Logged in: Keith Jolley (keith). 🕩 Log out Change password		Toggle: 🚺 📃
Add new clien	t database		
Please fill in the fields bel	ow - required fields are marked with	an exclamation mark (!).	
		Action	
id:!	1	Reset Submit	
name:!	PubMLST isolates		
description:!	diversity of <u>Neisseria</u> spe database there is at leas	ction of isolates that represent the total known ecies. For every <u>allelic</u> profile in the profiles t one corresponding isolate deposited here. Any to this database and consequently it should be noted t a population sample.	
dbase name:!	pubmlst_bigsdb_neisseria_isolates	Name of the database holding isolate data	
dbase config name:!	pubmlst_neisseria_isolates	Name of the database configuration	
curator:	Keith Jolley (keith)		
datestamp:!	2018-06-19		
dbase host:		IP address of database host	
dbase port:	🕀 🕚 Network	<pre>k port accepting database connections</pre>	
dbase user:		θ	
dbase password:		θ	
dbase view:	isolates	View of isolates table to use	
url:	/cgi-bin/bigsdb/bigsdb.pl	Web URL to database script	

- id Index number of client database. The next available number is entered automatically but can be overridden.
 - Allowed: any positive integer.
- name Short description of database. This is used within the interface result tables so it is better to make it as short as possible.
 - Allowed: any text.
- description Longer description of database.
 - Allowed: any text.
- dbase_name Name of database (system name).
 - Allowed: any text.

- dbase_config_name Name of database configuration this is the text string that appears after the db= part of script URLs.
 - Allowed: any text (no spaces)
- dbase_host Resolved name of IP address of database host (optional).
 - Allowed: Network address, e.g. 129.67.26.52 or zoo-oban.zoo.ox.ac.uk
 - Leave blank if running on the same machine as the sequef database.
- dbase_port Network port on which the client database server is listening (optional).
 - Allowed: integer.
 - Leave blank unless using a non-standard port (5432).
- dbase_user Name of user with permission to access the client database.
 - Allowed: any text (no spaces).
 - Depending on the database configuration you may be able to leave this blank.
- · dbase_password Password of database user
 - Allowed: any text (no spaces).
 - Depending on the database configuration you may be able to leave this blank.
- url URL of client database bigsdb.pl script
 - Allowed: valid script path.
 - This can be relative (e.g. /cgi-bin/bigsdb/bigsdb.pl) if running on the same machine as the seqdef database or absolute (including http://) if on a different machine.

5.18.1 Look up isolates with given allele

To link a locus, click the add (+) client database loci link on the curator's interface contents page.



Link the locus to the appropriate client database using the dropdown list boxes. If the locus is named differently in the client database, fill this name in the locus_alias.

PubMLST Databa	se home Curator ho	me Contents			
Logged in: Keith Jolley (ke	<i>ith).</i> ⇔Log out Change passwo	ord			Toggle: 🚺 📃
Add new loc	us to client da	tabase definit	ion		
Record client dbase id:! locus:!	Keith Jolley (keith)	arked with an exclamation	mark (!).	Action Reset Submit	ť
locus alias:			name that this locus is referred by in client database (if different)		

Now when information on a given allele is shown following a query, the software will list the number of isolates with that allele and link to a search on the database to retrieve these.



5.18.2 Look up isolates with a given scheme primary key

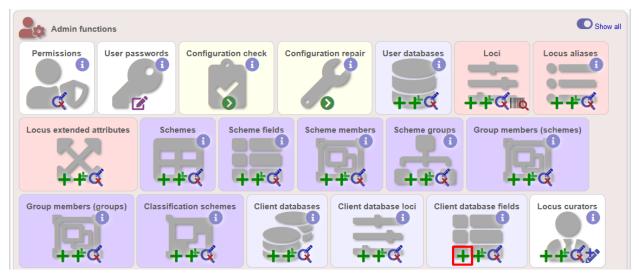
Setting this up is identical to setting up for alleles (see above) except you click on the add (+) client database schemes link and choose the scheme and client databases in the dropdown list boxes.

Now when information on a given scheme profile (e.g. MLST sequence type) is shown following a query, the software will list the number of isolates with that profile and link to a search on the database to retrieve these.

PubMLST Database home Contents		
+9 Log in	Help 🗹	Toggle: 🚯
Profile information for ST-11 (MLST)		
STabcZadkaroEfumCgdhpdhCpgmclonal complex112343846ST-11 complex		
sender: Paula Kriz, Paula Kriz and Keith Jolley		
curator: Keith Jolley, University of Oxford, UK		
date entered: 2001-02-07		
datestamp: 2009-11-11		
Client database		
PubMLST isolates: Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic pro there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequen does not represent a population sample. 5433 isolates		

5.18.3 Look up specific isolate database fields linked to a given allele

To link an allele to an isolate field, click the add (+) 'client database fields linked to loci' link on the curator's interface contents page.



Select the client database and locus from the dropdown lists and enter the isolate database field that you'd like to link. The 'allele_query' field should be set to true.

PubMLST Databa	se home Curator home Contents	
Logged in: Keith Jolley (ke	ith). (+Log out Change password	Toggle: 🜖
Add new loci	us to client database isolate field definition	
Record client dbase id:! locus:! isolate field:! curator.! datestamp:!	1) PubMLST isolates penA penicillin_range Keith Jolley (keith)	ction eset Submit

Now, in the allele record or following a sequence query that identifies an allele, all values for the chosen field from isolates with the corresponding allele are shown.

ged in: Keith Jolley (keith).	Description of the second se	Help 🖪
lele informat	ion - penA: 9	
Provenance/met	a data	
locus:	penA	
allele:	9	
sequence:	GACGGCGTTT IGCTGCCGGT CAGCTTTGAA AAACAGGCGG TIGCGCCGCA AGGCAAACGT ATATTTAAAG CATCGACCGC ACGTCAGGTG CGTGAGTTGA IGGTTTCIGT AACCGAACCT GGCGGTACGG GTACGGCGGG TGCGGTAGAT GGTTTCGACG TCGGCGCAAA AACCGGTACG GCGCGTAAGT IGGTTAACGG TCGTTACGTC GATTACAAAC ACGTTGCCAC TTTCATCGGT TTTGCCCCGG CTAAAAATCC GCGGTGGATT GTGGCGGTAA CCATGACGA CCCGACTGCA AACCGTTACT ACGGCGGCGCT AGTGACAGGT CCGGTCTTCA AACAAGTTAT GGGCGGTAGC CTGAACATCT TGGGCGTTTC TCCGACCAAA CCTCTGACCA AT	
length:	402	
status:	Sanger trace checked	
date entered:	2006-09-04	
datestamp:	2006-09-04	
sender:	Muhamed-Kheir Taha, National Reference Center for Meningococci, Institut Pasteur, France	
curator:	Keith Jolley, University of Oxford, UK	
mutation F504L:	yes	
mutation A510V:	yes	
mutation I515V:	yes	
mutation H541N:	yes	
mutation 1566V:	yes	
Publication (1)		
Heuberger S, Hoffma Stefanelli P, Thulin S	JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enríquez R, Fazio C, Frr ann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczyn S, Tzanakaki G, Unemo M, Vogel U, Zarantonelli ML (2007). Target gene sequencing to characterize the penicillin G susceptibility of Neiss crob Agents Chemother 51:2784-92	iska A,
Isolate database	IS	
PubMLST isolates:	Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profil there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be does not represent a population sample. <u>494 isolates</u>	
Linked data		
	>0.06 - 1 (intermediate) [n=92] PubMLST isolates	

5.19 Rule-based sequence queries

The RuleQuery plugin has been designed to extract information from a pasted-in genome sequence, look up scheme fields and client database fields, and then format the output in a specified manner.

Rules are written in Perl, allowing the full power of this scripting language to be utilised. Helper functions that perform specific actions are available to the script (see example).

Please note that direct access to the database is prevented as are system calls.

5.19.1 Example rule code

An example can be found on the Neisseria sequence database that takes a genome sequence and determines a fine type and antibiotic resistance.

The code for this rule is as follows:

```
#Clinical identification rule
#Update job viewer status
update_status({stage=>'Scanning MLST loci'});
#Scan genome against all scheme 1 (MLST) loci
scan_scheme(1);
#Update job viewer status
update_status({percent_complete=>30, stage=>'Scanning PorA and FetA VRs'});
#Scan genome against the PorA VR and FetA VR loci
scan_locus($_) foreach qw(PorA_VR1 PorA_VR2 FetA_VR);
Add text to main output
append_html("<h1>Strain type</h1>");
#Set variables for the scanned results. These can be found in the
#$results->{'locus'} hashref
my %alleles;
$alleles{$_} = $results->{'locus'}->{$_} // 'ND' foreach qw(PorA_VR1 PorA_VR2);
$alleles{'FetA_VR'} = $results->{'locus'}->{'FetA_VR'} // 'F-ND';
#Scheme field values are automatically determined if a complete
#profile is available. These are stored in the $results->{'scheme'} hashref
my $st = $results->{'scheme'}->{1}->{'ST'} // 'ND';
append_html("P1.$alleles{'PorA_VR1'}, $alleles{'PorA_VR2'}; $alleles{'FetA_VR
→'}; ST-$st ");
#Reformat clonal complex using a regular expression, e.g.
#'ST-11 clonal complex/ET-37 complex' gets rewritten to 'cc11'
my $cc = $results->{'scheme'}->{1}->{'clonal_complex'} // '-';
$cc =~ s/ST-(\S+) complex.*/cc$1/;
append_html("($cc)");
if ($st eq 'ND') {
 append_html("ST not defined. If individual MLST loci have been found "
  . "they will be displayed below:");
 #The get_scheme_html function automatically formats output for a scheme.
 #Select whether to display in a table rather than a list, list all loci, and/or.
\rightarrow list fields.
 append_html(get_scheme_html(1, {table=>1, loci=>1, fields=>0}));
}
#Antibiotic resistance
update_status({percent_complete=>80, stage=>'Scanning penA and rpoB'});
scan_locus($_) foreach qw(penA rpoB);
if (defined $results->{'locus'}->{'penA'} || defined $results->{'locus'}->{'rpoB'} ){
 append_html("<h1>Antibiotic resistance</h1>");
 if (defined $results->{'locus'}->{'penA'}) {
   append_html("<i>penA</i> allele: $results->{'locus'}->{'penA'}");
    #If a client isolate database has been defined and values have been defined in
    #the client_dbase_loci_fields table, the values for a field in the isolate
→database can be
    #retrieved based on isolates that have a particular allele designated.
```

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Rule files

The rule file is placed in a rules directory within the database configuration directory, e.g. /etc/bigsdb/dbase/pubmlst_neisseri_seqdef/rules. Rule files are suffixed with '.rule' and their name should be descriptive since it is used within the interface, i.e. the above rule file is named Clinical_identification.rule (underscores are converted to spaces in the web interface).

Linking to the rule query

Links to the rule query are not automatically placed within the web interface. The above rule query can be called using the following URL:

http://pubmlst.org/perl/bigsdb/bigsdb.pl?db=pubmlst_neisseria_seqdef&page=plugin&name=RuleQuery&ruleset=Clinical_identification

To place a link to this within the database contents page an HTML file called job_query.html can be placed in a contents directory within the database configuration directory, e.g. in /etc/bigsdb/dbases/pubmlst_neisseria_seqdef/contents/job_query.html. This file should contain a list entry (i.e. surrounded with and

Adding descriptive text

Descriptive text for the rule, which will appear on the rule query page, can be placed in a file called description.html in a directory with the same name as the rule within the rule directory, e.g. in /etc/bigsdb/dbases/pubmlst_neisseria_seqdef/rules/Clinical_identification/description.html.

5.20 Workflow for setting up a MLST scheme

The workflow for setting up a MLST scheme is as follows (the example seqdef database is called seqdef_db):

Seqdef database

- 1. Create appropriate loci
- 2. Create new scheme 'MLST'

- 3. Add scheme_field 'ST' with primary_key=TRUE (add clonal_complex if you want; set this with primary_key=FALSE)
- 4. Add each locus as a scheme_member
- 5. You'll then be able to add profiles

Isolate database

- 1. Create the same loci with the following additional parameters (example locus 'atpD')
- dbase_name: seqdef_db
- dbase_id: atpD
- url: something like /cgi-bin/bigsdb/bigsdb.pl?db=seqdef_db&page=alleleInfo&locus=atpD&allele_id=[?]
- 2. Create scheme 'MLST' with:
- dbase_name: seqdef_db
- dbase_id: 1 (or whatever the id of your seqdef scheme is)
- 3. Add scheme_field ST as before
- 4. Add loci as scheme_members

5.21 Automated assignment of scheme profiles

It is not practical to define cgMLST profiles via the web interface. A script is provided in the scripts/automation directory of the BIGSdb package called define_profiles.pl that can be used to scan an isolate database and automatically define cgMLST profiles in the corresponding sequence definition database.

The script is run as follows:

define_profiles.pl --database <name> --scheme <scheme_id>

A full list of options can be found by typing:

```
define_profiles.pl --help
NAME
    define_profiles.pl - Define scheme profiles found in isolate database
SYNOPSIS
    define_profiles.pl --database NAME --scheme SCHEME_ID [options]
OPTIONS
--cache
    Update scheme field cache in isolate database.
--database NAME
    Database configuration name.
--help
    This help page.
--exclude_isolates LIST
    Comma-separated list of isolate ids to ignore.
```

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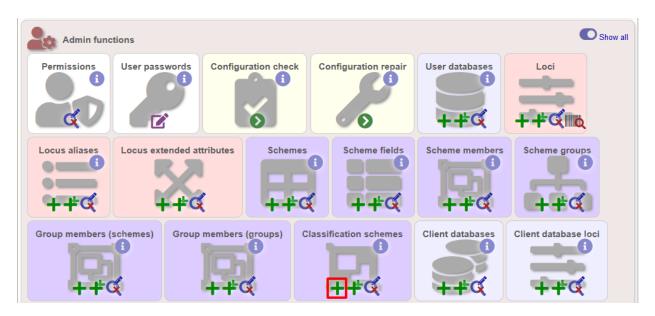
```
--exclude_projects LIST
   Comma-separated list of projects whose isolates will be excluded.
--ignore_multiple_hits
    Set allele designation to 'N' if there are multiple designations set for
    a locus. The default is to use the lowest allele value in the profile
    definition.
--isolates LIST
   Comma-separated list of isolate ids to scan (ignored if -p used).
--isolate_list_file FILE
   File containing list of isolate ids (ignored {\tt if} -i {\tt or} -p used).
--match missing
   Treat missing loci as specific alleles rather than 'any'. This will
   allow profiles for every isolate that has <= threshold of missing alleles
   to be defined but may result {\bf in} some isolates having >1 ST.
--max ID
   Maximum isolate id.
--min TD
   Minimum isolate id.
--min_size SIZE
   Minimum size of seqbin (bp) - limit search to isolates with at least this
   much sequence.
--missing NUMBER
   Set the number of loci that are allowed to be missing in the profile. If
   the remote scheme does not allow missing loci then this number will be set
   to 0. Default=0.
--projects LIST
   Comma-separated list of project isolates to scan.
--scheme SCHEME_ID
   Scheme id number.
```

5.22 Scheme profile clustering - setting up classification schemes

Classification groups are a way to cluster scheme profiles using a specified threshold of pairwise allelic mismatches. Any number of different classification schemes can sit on top of a standard scheme (such as cgMLST), allowing different similarity thresholds to be pre-determined. Currently, single-linkage clustering is supported whereby each member of a group must have no more than the specified number of allelic differences with at least one other member of the group.

5.22.1 Defining classification scheme in sequence definition database

Once a scheme has been defined, add a classification scheme by clicking the add classification schemes (+) link on the curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Select the underlying scheme and enter a name for the classification scheme, the number of mismatches allowed in order to include a scheme profile in a group, and a description. An example name for such a scheme could be 'Nm_cgc_25' indicating that this is a classification scheme for *Neisseria meningitidis* core genome cluster with a threshold of 25 mismatches.

You can additionally choose whether a relative threshold is used to calculate the number of mismatches to account for missing loci in pairwise comparisons. In this case, in order to be grouped, the number of matching alleles must exceed:

```
(number of common loci x (total loci - defined threshold)) / total loci
```

rather than

```
total loci - defined threshold
```

when an absolute threshold is used.

As this threshold has to be calculated for each pairwise comparison, clustering using relative thresholds is slower than using an absolute value, and probably makes little real world difference.

The status can be 'experimental' or 'stable'. The status of a scheme will be shown in the web interface to indicate that any groupings are subject to change and do not form part of the stable nomenclature.

Press 'Submit' to create the classification scheme.

PubMLST Database hom	e Curator home Contents	
Logged in: Keith Jolley (keith). 🗘 Log	out Change password	Toggle: 🚹
Add new classific	cation scheme	
Please fill in the fields below - re	quired fields are marked with an exclamation mark (!).	
Record		
id:!	2	
	N. meningitidis cgMLST v1.0	
	Nm_cgc_25 3	
inclusion threshold:		
use relative threshold:		
	experimental 💌	
	Keith Jolley (keith)	
datestamp:		
description:	Single linkage clustering with each group member having fewer than 25 allelic mismatches to at least one other member of the group. Missing loci are ignored in comparisons.	
display order:	A V	
Action		
Reset Submit		
Sublinit		

5.22.2 Defining classification scheme in isolate database

Duplicate the scheme definition from the sequence definition database. Click the add classification schemes (+) link on the curator's interface contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

Permissions	User passwords	Configuration check	Cache refresh	User databases	Extended attribute fields	Composite fields
	Locus aliases	PCR reactions	PCR locus links	cleotide probes		ichemes
Scheme fields	Scheme members	Scheme groups	Group members (so	hemes) Group n	nembers (groups)	ication schemes

Enter the same details used in the sequence definition database. If a different id number is used in the isolate and sequence definition databases, you can set the sequef id in the sequef_cscheme_id field (the default is to use the same id).

You can also define a display order - this is an integer field on which the ordering of classification schemes is sorted when displayed in the isolate information page.

PubMLST Database hom	e Curator home Contents		
Logged in: Keith Jolley (keith). 🗘 Log	out Change password		Toggle: 🚯 📃
Add new classific	cation scheme		
Please fill in the fields below - re	quired fields are marked with an exclamation mark (!).	Action	ť
id:1	2		
	Z IN. meningitidis cqMLST v1.0 ▼	Reset Submit	
	Nm cgc 25		
inclusion threshold:	- 5 -		
use relative threshold:			
	experimental -		
	Keith Jolley (keith)		
datestamp:!	2018-06-19		
description:	Single linkage clustering with each group member having fewer than 25 <u>allelic</u> mismatches to at least one other member of the group. Missing loci are ignored in comparisons.		
seqdef cscheme id:	2 cscheme_id number defined in seqdef database		
display order:			

It is a good idea to *check the configuration*.

5.22.3 Clustering

Clustering is performed using the cluster.pl script found in the scripts/automation directory of the BIGSdb package. It should be run by the bigsdb user account (or any account with access to the databases).

Currently only single-linkage clustering is supported.

The script is run as follows from the command line:

cluster.pl --database <database configuration> --cscheme <classification scheme id>

A full list of options can be found by typing:

```
cluster.pl --help
NAME
    cluster.pl - Cluster cgMLST profiles using classification groups.
SYNOPSIS
    cluster.pl --database NAME --cscheme_id SCHEME_ID [options]
OPTIONS
--cscheme CLASSIFICATION_SCHEME_ID
    Classification scheme id number.
--database NAME
    Database configuration name.
--help
    This help page.
--reset
    Remove all groups and profiles currently defined for classification group.
```

Note: Note that for classification schemes to be accessible within the isolate database, *scheme cache tables* must be

generated and kept up-to-date.

Where an isolate has been clustered in to a group with other isolates, this information is available in the *isolate information page*.

epidemiolog	se: invasive (unspecilied/other gy: endemic)		otters Bar, UK		
Publications	(2)					
	SJ, Urwin R, Russell JE, Bygr J Clin Microbiol 37:3883-7		B, Maiden MC (199	9). Multilocus sequence typing and a	ntigen gene sequencing in the investigation	n of a meningococcal
	M, Bratcher HB, Harrison OB, F nethods. <i>J Clin Microbiol</i> 50: 30		Aaiden MC (2012). F	Resolution of a meningococcal diseas	e outbreak from whole-genome sequence	data with rapid Web-
Sequence bin						
conti	gs: 259	mean length:	8,245 bp	N90 contig number: 63	N95 length (L9	5): 4,593
total leng	th: 2,135,447 bp	N50 contig number:	18	N90 length (L90): 8,06	6 loci tagge	ed: 2,180
-	th: 130,716 bp	N50 length (L50):	38,364	N95 contig number: 79	detailed breakdow	/n: Display
Similar isolate	th: 130,716 bp es (determined by classi are subject to change and are r	fication schemes)		N99 contig number: 79	detailed breakdov	m: Display
Similar isolate	es (determined by classi are subject to change and are r	fication schemes)	nomenclature.		detailed breakdow	m: Display
Similar isolate	es (determined by classi are subject to change and are r	fication schemes)	nomenclature.			m: Display
Similar isolate xperimental schemes	es (determined by classi are subject to change and are r Underlying scheme N. meningitidis cgMLST v1.0 N. meningitidis cgMLST v1.0	fication schemes) not a stable part of the r Clustering method M	nomenclature.	I Status Group	s)	m: Display
Similar isolate Experimental schemes Classification schemes Nm_cgc_200 Nm_cgc_100 Nm_cgc_50	es (determined by classi are subject to change and are r by Underlying scheme N. meningitidis cgMLST v1.0 N. meningitidis cgMLST v1.0 N. meningitidis cgMLST v1.0	fication schemes) not a stable part of the r Clustering method M Single-linkage Single-linkage Single-linkage	nomenclature. lismatch threshold 200 100 50	Status Group experimental group: 17 (641 isolate experimental group: 38 (568 isolate experimental group: 45 (4 isolates	s) s)	m: Display
Similar isolate Experimental schemes Classification schemes Nm_cgc_200 Nm_cgc_100	es (determined by classi are subject to change and are r Underlying scheme N. meningitidis cgMLST v1.0 N. meningitidis cgMLST v1.0	fication schemes) not a stable part of the r Clustering method M Single-linkage Single-linkage	nomenclature. lismatch threshold 200 100	Status Group experimental group: 17 (841 isolate experimental group: 38 (588 isolate	s) s)	n: Display
Similar isolate Experimental schemes Classification schemes Nm_cgc_200 Nm_cgc_100 Nm_cgc_50	es (determined by classi are subject to change and are r Underlying scheme N. meningitidis cgMLST v1.0 N. meningitidis cgMLST v1.0 N. meningitidis cgMLST v1.0 N. meningitidis cgMLST v1.0 Ioci	fication schemes) not a stable part of the r Clustering method M Single-linkage Single-linkage Single-linkage	nomenclature. Lismatch threshold 200 100 50 25	Status Group experimental group: 17 (841 isolate experimental group: 38 (568 isolate experimental group: 45 (4 isolates experimental group: 45 (4 isolates	s) s)	n: Display

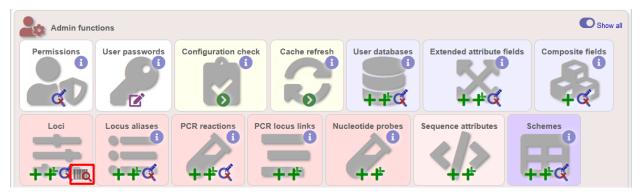
Clicking the hyperlinks will take you to a table containing matching isolates, from where standard analyses can be performed.

ged in: Keith Jolle	y (keith). 🗭 Log o	ut Change	password							пе	lp 🗹 👘	Toggle: 🔇
arch or	browse	Neiss	seria PubN	ILST database	9							
iter search criter	ia or leave blank	to brows	e all records. Modify	form parameters to filter or	enter a list	of values.						
-Isolate provena	ance/phenotype	fields			Allele design	nations/schem	e fields					
id	• =		▼ Enter value	1 1 +	lm_cgc_25 g	roup 👻	- • 4	15	+	6		
-Display/sort o	otions				Action							
Order by:					Reset	Submit						
	25 - records		0	docentaing	Reset	Submit						
-Your projects-			etailed information.									
Your projects]	ie fields ()				MLST	Fine	typing anti	aens	
- Your projects Select project		records]	te fields () species	serogrou	p genogroup	capsule group			typing anti		/R
-Your projects – Select project d isolate al 52 2837 M97/	✓ Add these iases country 252508 UK	records y year 1997 in	Isola disease vasive (unspecified/c	species other) Neisseria meningitidi	s C	p genogroup		ST clonal compl 50 ST-11 comple	ex PorA VR1 ex 5-1	PorA VR2 10-4	PetAV F3-6	
Your projects – Select project d isolate al 52 2837 M97/ 70 2840 M97/	✓ Add these iases country 252508 UK 252535 UK	y year 1997 in 1997 in	Isola disease vasive (unspecified/c vasive (unspecified/c	species other) Neisseria meningitidi other) Neisseria meningitidi	s C s C	p genogroup	C C	ST clonal compl 50 ST-11 comple 50 ST-11 comple	ex PorA VR1 ex 5-1 ex 5-1	I PorA VR2 10-4 10-4	PetA V F3-6 F3-6	
Vour projects – Select project d isolate al 62 2837 M97/ 70 2840 M97/ 71 2844 M97/	 Add these 252508 UK 252535 UK 252781 UK 	y year 1997 in 1997 in 1997 in	Isola disease vasive (unspecified/c vasive (unspecified/c vasive (unspecified/c	species other) Neisseria meningitidi other) Neisseria meningitidi other) Neisseria meningitidi	s C s C s C	p genogroup	C C C	ST clonal compl 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple	ex PorA VR1 ex 5-1 ex 5-1 ex 5-1 ex 5-1	PorA VR2 10-4 10-4 10-4	FetA V F3-6 F3-6 F3-6	
- Your projects - Select project d isolate al 62 2837 M97/ 70 2840 M97/	 Add these 252508 UK 252535 UK 252781 UK 	y year 1997 in 1997 in 1997 in	Isola disease vasive (unspecified/c vasive (unspecified/c vasive (unspecified/c	species other) Neisseria meningitidi other) Neisseria meningitidi	s C s C s C	p genogroup	C C C	ST clonal compl 50 ST-11 comple 50 ST-11 comple	ex PorA VR1 ex 5-1 ex 5-1 ex 5-1 ex 5-1	I PorA VR2 10-4 10-4	PetA V F3-6 F3-6	
Your projects – Select project d isolate al 52 2837 M97, 70 2840 M97, 71 2844 M97, 72 2847 M97,	 Add these iases countr 252508 UK 252781 UK 252943 UK 	y year 1997 in 1997 in 1997 in	Isola disease vasive (unspecified/c vasive (unspecified/c vasive (unspecified/c	species other) Neisseria meningitidi other) Neisseria meningitidi other) Neisseria meningitidi	s C s C s C	p genogroup	C C C	ST clonal compl 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple	ex PorA VR1 ex 5-1 ex 5-1 ex 5-1 ex 5-1	PorA VR2 10-4 10-4 10-4	FetA V F3-6 F3-6 F3-6	
Your projects Select project d isolate al S2 2837 M97. 70 2840 M97. 71 2844 M97. 72 2847 M97.	✓ Add these iases country 252508 UK 252505 UK 252781 UK 252943 UK	y year 1997 in 1997 in 1997 in 1997 in 1997 in	Isola disease vasive (unspecified/c vasive (unspecified/c vasive (unspecified/c	species other) Neisseria meningitidi other) Neisseria meningitidi other) Neisseria meningitidi other) Neisseria meningitidi	s C s C s C s C		C C C	ST clonal compl 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple	ex PorA VR1 ex 5-1 ex 5-1 ex 5-1	PorA VR2 10-4 10-4 10-4	FetA V F3-6 F3-6 F3-6	
Vour projects – Select project d isolate al 62 2837 M97/ 70 2840 M97/ 71 2844 M97/	✓ Add these iases country 252508 UK 252505 UK 252781 UK 252943 UK	records y year 1997 in 1997 in 1997 in 1997 in Field	Isola disease vasive (unspecified/c vasive (unspecified/c vasive (unspecified/c vasive (unspecified/c Combinations Pot	species other) Neisseria meningitidi other) Neisseria meningitidi other) Neisseria meningitidi	s C s C s C s C	p genogroup	C C C	ST clonal compl 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple	ex PorA VR1 ex 5-1 ex 5-1 ex 5-1	PorA VR2 10-4 10-4 10-4	FetA V F3-6 F3-6 F3-6	
Your projects Select project d isolate al S2 2837 M97. 70 2840 M97. 71 2844 M97. 72 2847 M97. alysis tools: Selectors	Add these Add these Sountry S2508 UK 252535 UK 252781 UK 252943 UK Fields Two	records y year 1997 in 1997 in 1997 in 1997 in Field	Isola disease vasive (unspecified/c vasive (unspecified/c vasive (unspecified/c vasive (unspecified/c Combinations Pol	species ther) Neisseria meningitidi ther) Neisseria meningitidi ther) Neisseria meningitidi ymorphic sites Schemes	s C s C s C s C		C C C	ST clonal compl 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple 50 ST-11 comple	ex PorA VR1 ex 5-1 ex 5-1 ex 5-1	PorA VR2 10-4 10-4 10-4	FetA V F3-6 F3-6 F3-6	

5.23 Defining new loci based on annotated reference genome

An annotated reference genome can be used as the basis of defining loci. The 'Databank scan' function will create an upload table suitable for pasting directly in to the batch locus add form of the *sequence definition* or *isolate* databases.

Click 'Database scan' within the 'Loci' group on the curator's contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Enter an EMBL or Genbank accession number for a complete annotated genome and press 'Submit'.

PubMLST Database home Curator home Contents
Logged in: Keith Jolley (keith). 🗣 Log out Change password
Scan EMBL/Genbank record for loci
This function allows you to scan an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci. ——Please enter accession number —— ——Primary identifier ———Action ——
Accession: AM421808

A table of loci will be generated provided a valid accession number is provided.

PubMLST Data	base home Curator home Contents	
Logged in: Keith Jolley	keith). C+Log out Change password	Ξ
Scan EMBL	/Genbank record for loci	
Please enter ac		
Accession: AM42	308 ● locus tag Submit	
Download table: tab-	alimited text Excel format (suitable for batch upload of loci).	
Download alleles: tak	delimited text Excel format (suitable for defining the first allele in the seqdef database).	
Annotation info	nation	
	sion: AM421808	
Ve	sion: 1	
	type: dna	
	ngth: 2194961	
	tion: Neisseria meningitidis serogroup C FAM18 complete genome.	
coding re	ions: 1975	
Coding sequence	25	
Locus Alias	s Product	Length
NMC0001 IpxC	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924
env		004
NMC0002 pilS		291
NMC0003 pilS NMC0004 fbp	truncated pilin peptidyl-prolyl cis-trans isomerase	366
NMC0005	putative membrane protein	219
NMC0006	putative initiaties processing	954
NMC0007 met		2058
NMC0008 glm		1839
NMC0009	putative lipoprotein	519
NMC0010 gna3		1326
NMC0011	putative integral membrane protein	840
NMC0012	putative lipoprotein	1167

Tab-delimited text and Excel format files will be created to be used as the basis for upload files for the sequence definition and isolate databases. Batch sequence files, in text and Excel formats, are also created for defining the first allele once the locus has been set up in the sequence definition database.

PubMLST	Database I	nome Curator home Contents	
Logged in: Keith	Jolley (keith).	Log out Change password	Ξ
Scan EN	//BL/Ge	nbank record for loci	
	nter accession	can an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci. number — Primary identifier – Action —	
		I text Excel format (suitable for batch upload of loci). ed text Excel format (suitable for defining the first allele in the seqdef database). •	
Annotation	informatio	n	
	accession:	AM421808	
	version:	1	
	type:	dna	
	length:	2194961	
	description:	Neisseria meningitidis serogroup C FAM18 complete genome.	
codi	ing regions:	1975	
Coding seq	quences		
Locus	Aliases	Product	Length
NMC0001	IpxC;	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924
	envA		
NMC0002	pilS1	pilin (fragment)	291
NMC0003	pilS2	truncated pilin	366
NMC0004 NMC0005	fbp	peptidyl-prolyl cis-trans isomerase putative membrane protein	330 219
NMC0005 NMC0006		putative memorane protein putative glycerate dehydrogenase	954
NMC0006	metG	putative giycerate denydrogenase methionyl-tRNA synthetase	2058
NMC0007	glmS	glucosaminefructose-6-phosphate aminotransferase [isomerizing]	1839
NMC0009	gino	putative lipoprotein	519
NMC0010	gna33	outer membrane lipoprotein Gna33 1	1326
	gnuos		
NMC0011		putative integral membrane protein	840

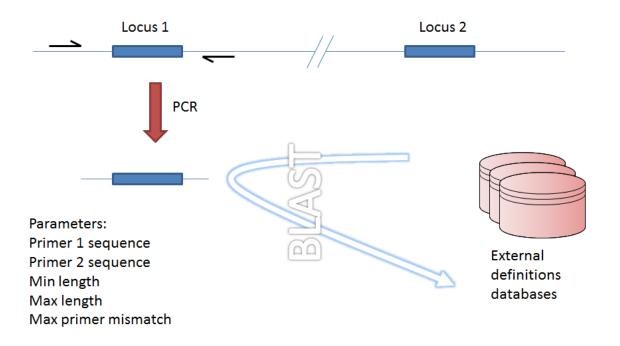
5.24 Genome filtering

Within a genome there may be multiple loci that share allele pools. If an allele sequence is tagged from a genome using only BLAST then there is no way to determine which locus has been identified. It is, however, possible to further define loci by their context, i.e. surrounding sequence.

5.24.1 Filtering by in silico PCR

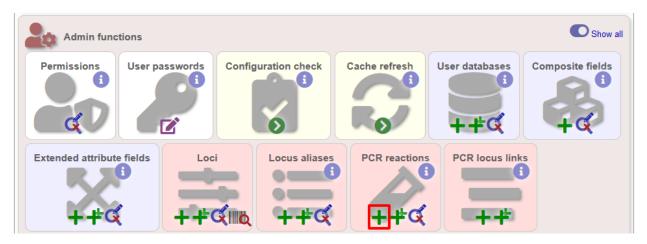
Provided a locus can be predicted to be specifically amplifed by a PCR reaction, the genome can be filtered to only look at regions predicted to fall within amplification products of one or more PCR reactions. Since this is *in silico* we don't need to worry about problems such as sequence secondary structure and primers can be any length.

To define a PCR reaction that can be linked to a locus definition, click the add (+) PCR reaction link on the curator's main page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Locus 1 and locus 2 share allele pool

Fig. 1: Genome filtering by in silico PCR.

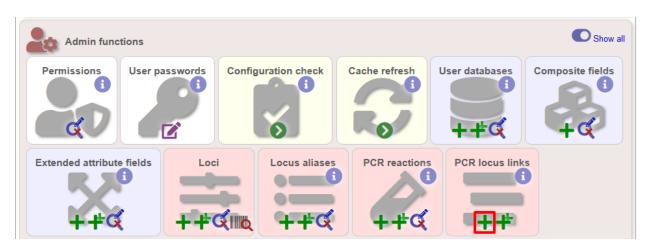


In the resulting web form you can enter values for your two primer sequences (which can be any length), the minimum and maximum lengths of reaction products you wish to consider and a value for the allowed number of mismatches per primer.

PubMLST Database hor	me Curator home Contents	
Logged in: Keith Jolley (keith). 🍽	og out Change password	Toggle: 🚯
Add new PCR re	action	
Please fill in the fields below - n	required fields are marked with an exclamation mark (!).	-
id:	2	
description:		
primer1:!		
primer2:!	i.	
curator:!	Keith Jolley (keith)	
datestamp:!	2018-06-19	
min length:	Minimum length of product to return	
max length:	Maximum length of product to return	
max primer mismatch:	👻 🕚 Maximum sequence mismatch per primer	
Action Reset Submit		

- id PCR reaction identifier number.
 - Allowed: integer.
- description Description of PCR reaction product.
 - Allowed: any text.
- primer1 Primer 1 sequences
 - Allowed: nucleotide sequence (IUPAC ambiguous characters allowed).
- primer2 Primer 2 sequence.
 - Allowed: nucleotide sequence (IUPAC ambiguous characters allowed).
- min_length Minimum length of predicted PCR product.
 - Allowed: integer.
- max_length Maximum length of predicted PCR product.
- max_primer_mismatch Number of mismatches allowed in primer sequence.
 - Allowed: integer.
 - Do not set this too high or the simulation will run slowly.

Associating this with a particular locus is a two step process. First, create a locus link by clicking the add (+) PCR locus link on the curator's main page. This link will only appear once a PCR reaction has been defined.



Select the locus and PCR reaction name from the dropdown lists to create the link. You also need to edit the locus table and set the pcr_filter field to 'true'.

Now when you next perform *tag scanning* there will be an option to use PCR filtering.

5.24.2 Filtering by in silico hybridization

An alternative is to define a locus by proximity to a single probe sequence. This is especially useful if you have multiple contigs and the locus in question may be at the end of a contig so that it doesn't have upstream or downstream sequence available for PCR filtering.

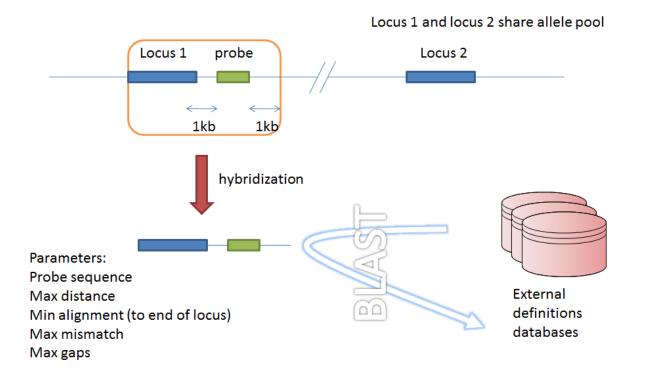
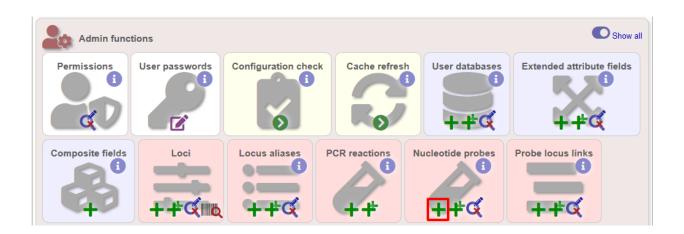
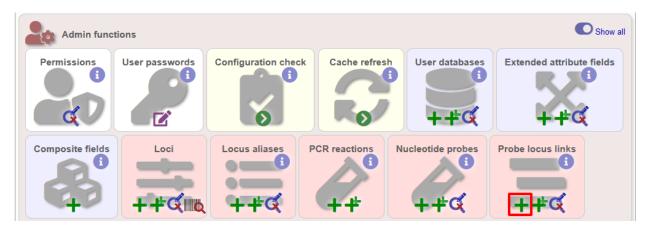


Fig. 2: Filtering by in silico hybridization

The process is very similar to setting up PCR filtering, but this time click the nucleotide probe link on the curator's content page.



Enter the nucleotide sequence and a name for the probe. Next you need to link this to the locus in question. Click the add (+) probe locus links link on the curator's main page. This link will only appear once a probe has been defined.



Fill in the web form with appropriate values. Required fields have an exclamation mark (!) next to them:

- probe_id Dropdown list of probe names.
 - Allowed: selection from list.
- locus Dropdown list of loci.
 - Allowed: selection from list.
- max_distance Minimum distance of probe from end of locus.
 - Allowed: any positive integer.
- min_alignment Minimum length of alignment allowed.
 - Allowed: any positive integer.
- max_mismatch Maximum number of mismatches allowed in alignment.
 - Allowed: any positive integer.
- max_gaps Maximum number of gaps allowed in alignment.
 - Allowed: any positive integer.

Finally edit the locus table and set the probe_filter field for the specified locus to 'true'.

Now when you next perform tag scanning there will be an option to use probe hybridization filtering.

5.25 Setting locus genome positions

The genome position for a locus can be set directly by editing the locus record. To batch update multiple loci based on a tagged genome, however, a much easier way is possible. For this method to work, the reference genome must be represented by a single contig.

From the curator's main page, you need to do a query to find the isolate that you will base your numbering on. Click 'isolate query' to take you to a standard query form.

Curator funct	tions			O Show all
Users ++¢¢+	Isolates ++	Sequence bin	Sequence tags	

Perform your search and click the hyperlinked id number of the record.

PubMLST	Database ho	ome Cu	irator hom	e Contents	5									
Logged in: Keit	h Jolley (keith). 🗭	Log out Cha	nge password								Help	C	Toggle: 🕻	
Isolate	query/up	date												
	criteria or leave t		owse all recor	rds. Modify forn	n parametei	rs to filter (or enter a	list of values						Modify
— Isolate p	provenance/pheno	type fields												form option
isolate	-	=	▼ mc58		+] 🚯								option
— Display/	sort options						-Action	n						
Order	by: id				- ascend	ling 👻	Reset	Submit						
Disp	lay: 25 🔻 reco	ords per pa	ige 🚯											
1 record retur	ned. Click the hy	perlink for a	detailed inform	nation.										
Delete		anning						Your projects						
											_			
Delete A	L Sca	an	Select proj	ect		 Link 	Se	elect project.	Add t	nese record	S			
						lsolate fie					MLST	Fi	netypin	g
Delete Up	late Sequence	New				Isolate fie	elas						ntigens	
	bin	version	id isolate	aliases count	y year di	sease	pecies	serogroup	genogroup	capsule group	ST clonal complex	PorA VR1		FetA VR
×	/ <u>1</u>	+	240 MC58	Z7176 UK	1983	N	eisseria	B			4 ST-32	7		F1-5
							eningitidis				complex		ø	<i>S</i>

In the isolate record, click the sequence bin 'Display' button to bring up details of the isolate contigs.

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). (+Log out Change password		Help 🗹 🛛 Toggle: 🕕 🔤
Full information on isolate MC58 (id:240)		
Delete record - Update record - Sequence bin - New version - Delete Update Update Upload contigs Create	Scan	
Provenance/meta data		
id: 240	serotype:	15
isolate: MC58	sero subtype:	P1.7,16-2
alias: Z7176	comments:	Genome sequenced by TIGR.
strain designation: B: P1.7,16-2: F1-5: ST-74 (cc32) country: UK	sender:	Mumtaz Virji, Dept. Pathology and Microbiology, University of Bristol
continent: Europe year: 1983	curator:	Nina Billows, University of Oxford (E-mail: nina.billows@some.ox.ac.uk)
species: Neisseria meningitidis	update history:	313 updates show details
serogroup: B	date entered:	2001-05-11
capsule group: B	datestamp:	2018-06-04
E Publications (6)		
Z Sequence bin		
contigs: 1		
length: 2272360 bp		
loci tagged: 2,226		
detailed breakdown: Display		

Click the 'Renumber' button:

gged in: Keitl	h Jolley (keith). 🗭	_og out Change pas	sword							Help 🗹	Toggle: 🕚	
equen	ice bin fo	r MC58										
ontig sun	nmary statistic	cs										
	Contigs: 1											
	-	070 000										
	Length: 2,	272,360										
• Downlo	oad sequences (F	ASTA format)										
	bad sequences (F bad sequences wi		MBL form	at)								
- Downie	au sequences wi			acj								
	Coguanaine	Original							EMDI	Artomic	Donumber	
equence	Sequencing method	Original designation	Length	Comments	Locus	Start	End	Direction	EMBL format	Artemis	Renumber	
equence 1		Original designation	Length 2272360	Comments whole	Locus NEIS2139	Start 7	End 498	Direction ←]
	method								format	3	3	J
	method			whole	NEIS2139	7	498	←	format	3	3]
	method			whole	NEIS2139 NEIS2140	7 502	498 897	$\stackrel{\leftarrow}{\leftarrow}$	format	3	3]
	method			whole	NEIS2139 NEIS2140 NEIS2141	7 502 918	498 897 2312	$\begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \\ \leftarrow \end{array}$	format	3	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142	7 502 918 2517	498 897 2312 3161	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	format	3	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143	7 502 918 2517 3158	498 897 2312 3161 3511	↑ ↓ ↓ ↓ ↑ ↓ ↓ ↓	format	3	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2142 NEIS2143 NEIS2144	7 502 918 2517 3158 3635	498 897 2312 3161 3511 4117	$\begin{array}{c} \downarrow \\ \downarrow \\ \downarrow \\ \downarrow \\ \downarrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\$	format	3	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2145	7 502 918 2517 3158 3635 4311	498 897 2312 3161 3511 4117 4961	$\begin{array}{c} \downarrow \\ \downarrow \\ \uparrow \\$	format	3	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2145 NEIS2146 NEIS2147	7 502 918 2517 3158 3635 4311 4958	498 897 2312 3161 3511 4117 4961 5875	$\begin{array}{c} \downarrow \\ \downarrow \\ \downarrow \\ \downarrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\$	format	3	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2144 NEIS2145 NEIS2146	7 502 918 2517 3158 3635 4311 4958 5936	498 897 2312 3161 3511 4117 4961 5875 6214	$\downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \uparrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \uparrow \downarrow \uparrow \downarrow \downarrow$	format	3	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2145 NEIS2146 NEIS2147 NEIS2148 (pgk) NEIS2149	7 502 918 2517 3158 3635 4311 4958 5936 6281 7573	498 897 2312 3161 3511 4117 4961 5875 6214 7492 8826	↓ ↓	format	3	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2145 NEIS2146 NEIS2147 NEIS2147 NEIS2149 tRNA-lys	7 502 918 2517 3158 3635 4311 4958 5936 6281 7573 9197	498 897 2312 3161 3511 4117 4961 5875 6214 7492 8826 9272	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	format	3	3	
Sequence 1	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2145 NEIS2146 NEIS2147 NEIS2148 (pgk) NEIS2149	7 502 918 2517 3158 3635 4311 4958 5936 6281 7573	498 897 2312 3161 3511 4117 4961 5875 6214 7492 8826	↓ ↓	format	3	3	

A final confirmation screen is displayed with the option to remove existing numbering that doesn't appear within the reference genome. Click 'Renumber'.

PubMLST Database home Curate	or home Contents	
Logged in: Keith Jolley (keith). 🕩 Log out Change p	assword	=
Renumber locus genom	e positions based on tagged sequences	
You have selected to renumber the genome p	ositions set in the locus table based on the tagged sequences in sequence id#1.	
Option	Action	
Remove positions for loci not tagged in t	his sequence Renumber	
The following designations will be used as		
The following designations will be made:		
Locus	ne position ♦ New genome position ♦	
NEIS2139	7	
NEIS2140	502	
NEIS2141	918	
NEIS2142	2517	
NEIS2143	3158	
NEIS2144	3635	
NEIS2145	4311	
NEIS2146	4958	
NEIS2147	5936	
NEIS2148	6281	
NEIS2149	7573	
tRNA-lys	9197	
NEIS2150	9346	
NEIS2151	10350	
NEIS2152	10840	
NEIS2153	12174	
NEIS2979	13848	
NEIS0001	15221	
NEIS0210	17229	
NEISp0210	17232	
pilS	18127	

5.26 Defining composite fields

Composite fields are virtual fields that don't themselves exist within the database but are made up of values retrieved from other fields or schemes and formatted in a particular way. They are used for display and analysis purposes only and can not be searched against.

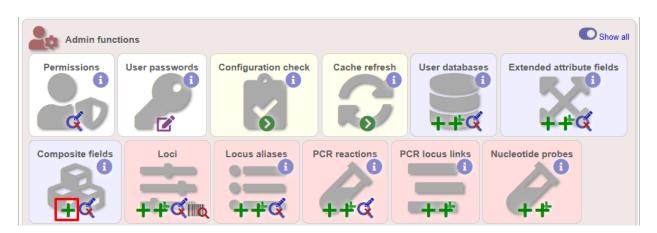
One example of a composite field is used in the Neisseria PubMLST database which has a strain designation composite field made up of serogroup, PorA VR1 and VR2, FetA VR, ST and clonal complex designations in the format:

[serogroup]: P1.[PorA_VR1],[PorA_VR2]: [FetA_VR]: ST-[ST] ([clonal_complex])

e.g. A: P1.5-2,10: F1-5: ST-4 (cc4)

Additionally, the clonal complex field in the above example is converted using a regular expression from 'ST-4 complex/subgroup IV' to 'cc4'.

Composite fields can be added to the database by clicking the add (+) composite fields link on the curator's main page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Initially you just enter a name for the composite field and after which field it should be positioned. You can also set whether or not it should be displayed by default in main results tables following a query - this is overrideable by user preferences.

PubMLST Databa	se home Curato	r home	Contents			
Logged in: Keith Jolley (ke	<i>ith).</i> ເ⇔Log out Change pa	issword				Toggle: 🜖
Add new con	nposite field	d			 	
position after:! main display:!	strain_designation	✓ field	present in the isolate	name of the field as it will appear in t	Action Reset Submit	ľ
datestamp:						

Once the field has been created it needs to be defined. This can be done from query composite field link on the main curator's page.

Admin func	tions					Show all
Permissions	User passwords	Configuration check	Cache refresh	User databases	Extended attribut	0
Composite fields		Locus aliases	PCR reactions	PCR locus links	Nucleotide probes	

Select the composite field from the list and click 'Update'.

PubMLS	T Da	atabase home	Curator ho	me Cont	ents	
Logged in: I	Keith Jol	lley (keith). 🗘 Log out	Change passwo	rd		-
Updat	te or	r delete co	mposit	e field		
1 composi	ite field	defined.				
Delete	Update	field name	position after	main display	definition	missing data
×	ø	strain_designation	isolate	false	[capsule_group]: P1.[PorA_VR1].[PorA_VR2]: [FetA_VR]: ST-[scheme 1:ST] ([scheme 1:clonal_complex])	ND: P1.ND,ND: F-ND: ST- ND (-)
					Contra_comptory	

From this page you can build up your composite field from snippets of text, isolate field, locus and scheme field values. Enter new values in the boxes at the bottom of the page.

odate compos	ite field	l - strain	_designati	on						
-Position/display										
position after: isolate		-								
main display: 🔘 true 🔍 fa	lse									
Update										
field	empty value		regex	curator	datestamp	delete	edit	mo	bve	
apsule_group [isolate field]	ND			Keith Jolley	2017-08-15	×			↓	
: P1.				Keith Jolley	2009-11-12	×			◆	
PorA_VR1 [locus]	ND			Keith Jolley	2009-11-12	×			▶	
				Keith Jolley	2009-11-12	×			↓	
PorA_VR2 [locus]	ND			Keith Jolley	2009-11-12	×			↓	
:				Keith Jolley	2009-11-12	×			↓	
FetA_VR [locus]	F-ND			Keith Jolley	2009-11-12	×			•	
: ST-				Keith Jolley	2009-11-12	×			•	
ST [MLST field]	ND			Keith Jolley	2009-11-12	×			•	
(Keith Jolley	2009-11-12	×			↓	
onal_complex [MLST field]	-	s/ST-(\S+)	complex.*/cc\$1/	Keith Jolley	2009-11-12	×			•	
)				Keith Jolley	2009-11-12	×			•	
Add new field:										
text field:		+								
isolate field:		-+								
locus field:		•	-							

Once a field has been added to the composite field, it can be edited by clicking the 'edit' button next to it to add a regular expression to modify its value by specific rules, e.g. in the clonal complex field above, the regular expression is set as:

s/ST-(\S+) complex.*/cc\$1/

which extracts one or more non-space characters following the 'ST-' in a string that then contains the work 'complex', and appends this to 'cc' to produce the final string.

This will convert 'ST-4 complex/subgroup IV' to 'cc4'.

You can also define text to be used for when the field value is missing, e.g. 'ND'.

5.27 Extended provenance attributes (lookup tables)

Lookup tables can be associated with an isolate database field such that the database can be queried by extended attributes. An example of this is the relationship between continent and country - every country belongs to a continent but you wouldn't want to store the continent with each isolate record (not only could data be entered inconsistently but it's redundant). Instead, each record may have a country field and the continent is then determined from the lookup table, allowing, for example, a search of isolates limited to those from Europe.

To set up such an extended attribute, click the add (+) isolate field extended attributes link on the curator's main page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

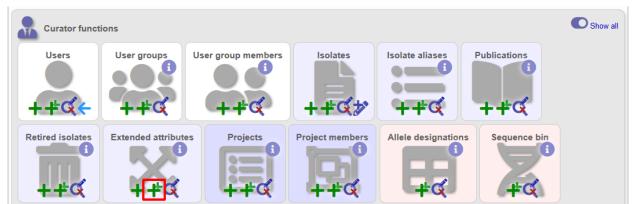


Fill in the web form with appropriate values. Required fields have an exclamation mark (!) next to them:

- isolate_field Dropdown list of isolate fields.
 - Allowed: selection from list.
- attribute Name of extended attribute, e.g. continent.
 - Allowed: any text (no spaces).
- value_format Format for values.
 - Allowed: integer/float/text/date.
- value_regex Regular expression to enforce allele id naming.
 - ^: the beginning of the string
 - \$:the end of the string
 - d: digit
 - D: non-digit
 - s: white space character
 - S: non white space character
 - w: alpha-numeric plus '_'
 - .: any character
 - *: 0 or more of previous character
 - +: 1 or more of previous character
 - e.g. ^Fd-d+\$ states that a value must begin with a F followed by a single digit, then a dash, then one or more digits, e.g. F1-12
- description Long description this isn't currently used but may be in the future.

- Allowed: any text.
- url URL used to hyperlink values in the isolate information page. Instances of [?] within the URL will be substituted with the value.
 - Allowed: any valid URL (either relative or absolute).
- length Maximum length of extended attribute value.
 - Allowed: any positive integer.
- field_order Integer that sets the order of the field following it's parent isolate field.
 - Allowed: any integer.

The easiest way to populate the lookup table is to do a batch update copied from a spreadsheet. Click the batch add (++) isolate field extended attribute values link on the curator's main page (this link will only appear once an extended attribute has been defined). This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Download the Excel template:

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). DLog out Change password	Toggle: ()
Batch insert isolate value extended attributes	
This page allows you to upload isolate field extended attribute value data as tab-delimited text or copied from a spreadsh • Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. • Download tab-delimited header for your spreadsheet - use 'Paste Special S Text' to paste the data. • Download submission template (xlsx format)	heet.
Paste in tab-delimited text (include a field header line).	Action
ī	Reset Submit

Fill in the columns with your values, e.g.

isolate_field	attribute	field_value	value
country	continent	Afghanistan	Asia
country	continent	Albania	Europe
country	continent	Algeria	Africa
country	continent	Andorra	Europe
country	continent	Angola	Africa

Paste from the spreadsheet in to the upload form and click 'Submit'.

5.28 Sequence bin attributes

It is possible that you will want to store extended attributes for sequence bin contigs when you upload them. Examples may be read length, assembler version, etc. Since there are almost infinite possibilities for these fields, and they are likely to change over time, they are not hard-coded within the database. An administrator can, however, create their own attributes for a specific database and these will then be available in the web form when uploading new contig data. The attributes are also searchable.

To set up new attributes, click the add (+) 'sequence attributes' link on the isolate database curator's index page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

Admin func	tions					C Show all
Permissions	User passwords	Configuration check	Cache refresh	User databases	5	te fields
Composite fields			PCR reactions	PCR locus links	Nucleotide probes	Sequence attributes

Enter the name of the attribute as the 'key', select the type of data (text, integer, float, date) and an optional short description. Click 'Submit'.

PubMLST Da	tabase home	Curator home	Contents			
Logged in: Keith Jolle	ey (keith). 🕩 Log out	Change password				Toggle: 🚺
Add new s	sequence	attribute				
Record key: type: curator:	read_length integer → Keith Jolley (ke 2018-06-19	ed fields are marked	with an exclama	ation mark (!). Action Reset Subi	mit	ľ

This new attribute will then be available when uploading contig data.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). (+Log out Change password	Toggle: ()
Batch insert sequences	
This page allows you to upload sequence data for a specified isolate record in FASTA format. If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any or FASTA file. This allows data for multiple isolates to be uploaded. Please note that you can reach this page for a specific isolate by querying isolates and then clicking 'Upload' within t	A
Please fill in the following fields - required fields are marked with an exclamation mark (!).	
- Paste in sequences in FASTA format.	Attributes isolate id: !

5.29 Checking external database configuration settings

Click the 'Configuration check' link on the curator's index page.

Admin function	ns			C	Show all
Permissions	Jser passwords	Configuration check	Cache refresh		

The software will check that required helper applications are installed and executable and, in isolate databases, test every locus and scheme external database to check for connectivity and that data can be retrieved. By default, only loci which have an issue will be displayed but you can click the 'show all loci' link to display them all.

ged in: Keith Jolley	(keith). 🔁 Log out Change password						
onfigurati	on check - Neisseria	a PubM	LST				
elper applicatio	ns.						
Program	Path	Installed E:					
MBOSS infoalign	/usr/bin/infoalign	 ✓ 	 ✓ 				
MBOSS sixpack	/usr/bin/sixpack	 ✓ 	×				
MBOSS stretcher		~	✓				
blastn	/usr/local/ncbi-blast+/bin/blastn	 ✓ 	×				
blastp	/usr/local/ncbi-blast+/bin/blastp	 ✓ 	~				
blastx	/usr/local/ncbi-blast+/bin/blastx	 ✓ 	×				
clustalw	/usr/bin/clustalw	~	~				
ipcress	/usr/bin/ipcress	 ✓ 	✓				
mafft	/usr/bin/mafft	 ✓ 	×				
makeblastdb	/usr/local/ncbi-blast+/bin/makeblastdb	✓	~				
mogrify	/usr/bin/mogrify	 ✓ 	×				
muscle	/usr/bin/muscle	 ✓ 	 ✓ 				
tblastx	/usr/local/ncbi-blast+/bin/tblastx	~	×				
cus database	s (only showing loci with poten Database H				le Sequence que	ry Sequences assi	igned
Locus		ost Port	Id field value D NEIS0895		le Sequence que	ry Sequences assi ×	igned
Locus EIS0895 (parA) p	Database H	ost Port berlour 5432	Id field value D NEIS0895 NEIS0903	atabase accessib			igned
Locus EIS0895 (parA) p EIS0903 (opaD) p NEIS1454 p	Database H ubmlst_bigsdb_neisseria_seqdef zoo-a ubmlst_bigsdb_neisseria_seqdef zoo-a ubmlst_bigsdb_neisseria_seqdef zoo-a	ost Port berlour 5432 berlour 5432 berlour 5432	Id field value D NEIS0895 NEIS0903 NEIS1454	atabase accessib	✓	×××××	igned
Locus EIS0895 (parA) p EIS0903 (opaD) p NEIS1454 p	Database H ubmlst_bigsdb_neisseria_seqdef zoo-a ubmlst_bigsdb_neisseria_seqdef zoo-a	ost Port berlour 5432 berlour 5432 berlour 5432	Id field value D NEIS0895 NEIS0903	atabase accessib	~	××	igned
Locus EIS0895 (parA) p EIS0903 (opaD) p NEIS1454 p EIS1551 (opaC) p	Database H ubmlst_bigsdb_neisseria_seqdef zoo-a ubmlst_bigsdb_neisseria_seqdef zoo-a ubmlst_bigsdb_neisseria_seqdef zoo-a	ost Port berlour 5432 berlour 5432 berlour 5432 berlour 5432	Id field value D NEIS0895 NEIS0903 NEIS1454 NEIS1551	atabase accessib	~	× × × ×	igned
Locus EIS0895 (parA) p EIS0903 (opaD) p NEIS1454 p EIS1551 (opaC) p NEIS2013 p	Database H ubmlst_bigsdb_neisseria_seqdef zoo-a ubmlst_bigsdb_neisseria_seqdef zoo-a ubmlst_bigsdb_neisseria_seqdef zoo-a ubmlst_bigsdb_neisseria_seqdef zoo-a	ost Port berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432	Id field value D NEIS0895 NEIS0903 NEIS1454 NEIS1551 NEIS2013	atabase accessib	* * * *	× × × ×	igned
Locus EIS0895 (parA) p EIS0903 (opaD) p NEIS1454 p EIS1551 (opaC) p NEIS2013 p	Database H ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a	ost Port berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432	Id field value D NEIS0895 NEIS0903 NEIS1454 NEIS1551 NEIS2013	atabase accessib	****	× × × ×	igned
Locus EIS0895 (parA) p EIS0903 (opaD) p NEIS1454 p EIS1551 (opaC) p NEIS2013 p NEIS2538 p	Database H ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a	ost Port berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432	Id field value D NEIS0895 NEIS0903 NEIS1454 NEIS1551 NEIS2013	atabase accessib	****	× × × ×	igned
Locus EIS0895 (parA) p EIS0903 (opaD) p NEIS1454 p EIS1551 (opaC) p NEIS2013 p NEIS2538 p	Database H ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a	ost Port berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432	Id field value D NEIS0895 NEIS0903 NEIS1454 NEIS1551 NEIS2013	atabase accessib	****	× × × ×	igned
Locus EIS0895 (parA) p EIS0903 (opaD) p NEIS1454 p EIS1551 (opaC) p NEIS2013 p NEIS2538 p	Database H ubmist_bigsdb_neissenia_seqdef zoo-a ubmist_bigsdb_neissenia_seqdef zoo-a ubmist_bigsdb_neissenia_seqdef zoo-a ubmist_bigsdb_neissenia_seqdef zoo-a ubmist_bigsdb_neissenia_seqdef zoo-a es	ost Port berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432	Id field value D NEIS0895 NEIS0903 NEIS1454 NEIS1551 NEIS2013 NEIS2538	atabase accessib	****	× × × × × × ×	igned
Locus EIS0895 (parA) p EIS0895 (parA) p NEIS1454 p EIS1551 (pac) p NEIS2013 p NEIS2538 p theme databas	Database H ubmist_bigsdb_neissenia_seqdef zoo-a ubmist_bigsdb_neissenia_seqdef zoo-a ubmist_bigsdb_neissenia_seqdef zoo-a ubmist_bigsdb_neissenia_seqdef zoo-a	ost Port berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432	Id field value D NEIS0895 NEIS0903 NEIS1454 NEIS1551 NEIS2013 NEIS2538	atabase accessib	se accessible Pro	x x x x x x	igned
Locus IEIS0895 (parA) p IEIS0895 (parA) p NEIS1454 p IEIS1541 (papC) p NEIS2013 p NEIS2538 p NEIS2538 p Cheme databas Scheme M	Database H ubmist_bigsdb_neisseria_seqdef zoo-a ubmist_bigsdb_neisseria_seqdef zoo-a	ost Port berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432 berlour 5432	Id field value D NEIS0895 NEIS0903 NEIS1454 NEIS1551 NEIS2013 NEIS2538	Port Id Databa	****	× × × × × × ×	igned

Any problems will be highlighted with a red X.

5.30 Exporting table configurations

Sometimes it is useful to transfer configurations between different databases or to export a configuration for troubleshooting. Data from most of the tables can be exported in tab-delimited text format suitable for batch uploading. For example, to export scheme configuration data, click the query link (Update or delete) next to schemes in the curator's interface. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

Admin fund	tions						C Show
Permissions	User passwords	Configuration check	k Cache refres	User databases	Extended attribute field	s Composite fields	
	Locus aliases	PCR reactions	CR locus links	Nucleotide probes	Sequence attributes	Schemes Sche	eme fields

Expand the filters and select the required scheme in the dropdown box, then press submit.

PubMLST	Database home	Curator home	Contents							
Logged in: Keith .	Jolley (keith). 🕩 Log out	Change password				Toggle: 🕚	Ξ			
Query schemes for Neisseria PubMLST database										
		low (or leave blank ar	nd submit to return all re							
Search cri	teria –	_		Display Order by: id	- ascending					
IU	• =	•	+ 0		records per page	•				
-—⊽ Filter qu	ery by isolate display:	▼ 8		Action						
	main display:	▼ 8		Reset Submit						
	query field:	- C								
	query status:	• 6								
	analysis:	• •								
allo	w missing loci:	▼ 3								
	curator:		▼ 🕄							
	scheme: MLS	Г	▼ 3							

Click the button 'Export configuration/data'.

PubMLST Database home Curator home Cont	ents					
Logged in: Keith Jolley (keith). [+Log out Change password						Toggle: 🚯 📃
Query schemes for Neisseria Pub	MLST da	tabase				
Please enter your search criteria below (or leave blank and subn Search criteria	nit to return all rec					
id • = •	+ 3	Display Order by	r id	▼ ascendir		
		Display		ords per page 3	g ·	
		Action				
isolate display: 💽 💽 🕚		Reset S	ubmit			
query field:						
query field: v 0 query status: v 0						
analysis: 🗨 😗						
allow missing loci: 💽 🔽 👔						
curator: scheme: MLST	€ ▼ 6					
Scheme. MLS1						
1 record returned.						
Delete Database configuration						
Delete ALL Export configuration/data						
Delete Update id name dbase name	lbase dbase dba	ase isolate	main query	query analysis*	display allow	ator datestamp da
	host port i			status	order loci	· ente
X / 1 MLST pubmlst_bigsdb_neisseria_seqdef	1				1 🗌 Ke Jol	
Pefault values are displayed for this field. These may be overridde	n by up or professor					•

The three tables that are used to define a scheme (schemes, scheme_members and scheme_fields) are displayed in a format suitable for copy and pasting.

schemes
<pre>id description dbase_name dbase_host dbase_port dbase_user dbase_password dbase_ →table isolate_display main_display query_field query_status analysis display_ →order allow_missing_loci curator datestamp date_entered 1 MLST pubmlst_bigsdb_neisseria_seqdef mv_scheme_1 1 1 1 1 1 1 → 2 2012-03-22 2009-11-12</pre>
scheme_members
scheme_id locus profile_name field_order curator datestamp 1 abcZ 1 2 2009-11-12 1 adk 2 2 2009-11-12 1 aroE 3 2 2009-11-12 1 fumC 4 2 2009-11-12 1 gdh 5 2 2009-11-12 1 pdhC 6 2 2009-11-12 1 pgm 7 2 2009-11-12
<pre>scheme_fields </pre>

5.31 Authorizing third-party client software to access authenticated resources

If you are running the *RESTful API*, you will need to specifically authorize client software to connect to authenticated resources. This involves creating a client key and a client secret that is used to sign requests coming from the application. The client key and secret should be provided to the application developer.

There is a script to do this in the scripts/maintenance directory of the download archive. The script is called create_client_credentials and should be run by the postgres user. A full list of options can be found by typing:

```
create_client_credentials.pl --help
NAME
    create_client_credentials.pl - Generate and populate
    authentication database with third party application (API client)
    credentials.
SYNOPSIS
    create_client_credentials.pl --application NAME [options]
OPTIONS
-a, --application NAME
    Name of application.
-d, --deny
    Set default permission to 'deny'. Permissions for access to specific
    database configurations will have to be set. If not included, the default
```

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```
permission will allow access to all resources by the client.
-h, --help
This help page.
-i, --insert
Add credentials to authentication database. This will fail if a matching
application version already exists (use --update in this case to overwrite
existing credentials).
-u, --update
Update exisitng credentials in the authentication database.
-v, --version VERSION
Version of application (optional).
```

5.32 BLAST caches

Sequence definition databases cache any BLAST databases that they create in order to perform sequence queries. These caches can be found in subdirectories named with the database name in the temp directory defined by the secure_tmp_dir attribute in bigsdb.conf, e.g. /var/tmp/pubmlst_bigsdb_neisseria_seqdef.

These BLAST databases will be marked stale if new alleles are added to the BIGSdb database for any locus covered by the cache. A cache marked stale will be recreated the next time a matching sequence query needs to use it. BLAST databases will also be marked stale if they are older than the cache_days setting in bigsdb.conf (default = 7 days).

It is possible to also manually create and refresh these caches using the update_blast_caches.pl script found in the scripts/maintenance directory.

A full list of options can be found by typing:

```
update_blast_caches.pl --help
NAME
   update_cached_blast_dbs.pl - Refresh BLAST database caches
SYNOPSIS
   update_cached_blast_dbs.pl --database DB_CONFIG [options]
OPTIONS
--all_loci
   Refresh or create cache for all loci.
--database DATABASE CONFIG
   Database configuration name.
--delete_all
   Remove all cache files.
--delete_old
   Remove cache files older than the cache_days setting in bigsdb.conf or
   that have been marked stale.
--delete_single_locus
   Remove caches containing only one locus. There can be many of these and
```

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(continued from previous page)

```
they can clutter the cache directory. They are generally quick to recreate
when needed.
--help
This help page.
--quiet
Only show errors.
--refresh
Refresh existing caches.
--scheme SCHEME_ID
Refresh or create cache for specified scheme.
```

5.33 Config-specific file downloads

You can make files available on a static website but restrict their access only to users who can authenticate for access to the current database configuration.

This can be done by adding a file called download_files.conf to the database configuration directory within /etc/bigsdb/dbases. This file consists of three columns in tab-delimited format:

- The full path of the file in the file system
- · Label which will be used to hyperlink to the file
- A description of the file
- The file type (docx, html, gif, jpg, pdf, png, tar, tar, xlsx currently supported)

The files can be downloaded directly from a BIGSdb URL: /cgi-bin/bigsdb.pl?db=CONFIG&page=downloadFiles&file=LABEL (where CONFIG is the database config name and LABEL is the label used in the download_files.conf file. These URLs can be used as standard links within a web page.

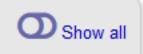
You can also list all available files with the URL: /cgi-bin/bigsdb.pl?db=CONFIG&page=downloadFiles

Navigating to these links will prompt the user to log-in if they are not already (if the database config requires this).

CHAPTER 6

Curator's guide

Please note that links displayed within the curation interface will vary depending on database contents and the permissions of the curator. Some infrequently used links are usually hidden by default. These can be enabled by clicking the 'Show all' toggle switch.



6.1 Adding new sender details

All records within the databases are associated with a sender. Whenever somebody new submits data, they should be added to the users table so that their name appears in the dropdown lists on the data upload forms.

To add a user, click the add users (+) link on the curator's contents page.

PubMLST Databas	se home Curator h	ome Contents	
Logged in: Keith Jolley (kei	th). ເ→Log out Change passv	ord	Toggle: 🚯 🗮
Database cur	rator's interfa	ce - Neisseria profile/sequence defii	nitions
Curator funct	tions		O Show all
Users	Sequences + + Eas CC	MLST profiles	

Enter the user's details in to the form.

PubMLST Database hom	e Curator home Contents		
Logged in: Keith Jolley (keith). 🗭 Log	out Change password	Help 🛃	Toggle: 🜖 📃
Add new user			
Please fill in the fields below - re	quired fields are marked with an exclamation mark (!).		
Record		Action	
id:!	360	Reset Submit	
user name:!	jbloggs		
surname:	Bloggs		
first name:!	Joe		
email:!	joe.bloggs@zoo.ox.ac.uk		
affiliation:!	University of Oxford, UK		
status:	user 🔻		
date entered:	2018-06-07		
datestamp:!	2018-06-07		
curator:	Keith Jolley (keith)		
submission emails:	O true () false () Receive new submission E-mails (curators only)		
account request emails:	O true false Receive new account request E-mails (curators only)		

Normally the status should be set as 'user'. Only admins and curators with special permissions can create users with a status of curator or admin.

If the submission system is in operation there will be an option at the bottom called 'submission_emails'. This is to enable users with a status of 'curator' or 'admin' to receive E-mails on receipt of new submissions. It is not relevant for users with a status of 'user' or 'submitter'.

6.2 Adding new allele sequence definitions

6.2.1 Single allele

To add a single new allele, click the sequences add (+) link on the curator's main page.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). [+Log out Change password	Toggle: 🚯 🗮
Database curator's interface - Neisseria profile/sequence definitions	
Curator functions Users Sequences HLST profiles	Show all

Select the locus from the dropdown list box. The next available allele id will be entered automatically (if the allele id format is set to integer). Paste the sequence in to form, set the status and select the sender name from the dropdown box. If the sender does not appear in the box, you will need to add them to the registered users.

The status reflects the level of curation that the curator has done personally - the curator should not rely on assurances from the submitter. The status can either be:

• Sanger trace checked

- Sequence trace files have been assembled and inspected by the curator.
- WGS: manual extract (BIGSdb)
 - The sequence has been extracted manually from a BIGSdb database *by the curator*. There may be some manual intervention to identify the start and stop sites of the sequence.
- WGS: automated extract (BIGSdb)
 - The sequences have been generated by a BIGSdb tag scanning run and have had no manual inspection or intervention.
- WGS: visually checked
 - Short read data has been inspected visually using an alignment program by the curator.
- WGS: automatically checked
 - The sequences have been checked by an automated algorithm that assesses the quality of the data to ensure it meets specified criteria.
- unchecked
 - If none of the above match, then the sequence should be entered as unchecked.

You can also choose whether to designate the sequence as a type allele or not. Type alleles can be used to constrain the sequence search space when defining new alleles using the *web-based scanner* or *offline auto allele definer*.

PubMLST Database	e home Curator home Contents			
Logged in: Keith Jolley (keith). 🕩 Log out Change password	Help 🗹	Toggle: 🜖	
Add new allele	e sequence			
			_	_
Please fill in the fields bel	ow - required fields are marked with an exclamation mark (!).			
Record				
locus:	abcZ 🔹			
allele id:!				
sequence:!	TTTGATACCGTTGCCGAAGGTTTGGGTAAAATTCGCGATTTATTGCGCCGTTACCACCGCGTCGGTCAT AAACGGTTCGGGTGAGGCTTTGTTGAAAGAACTCAACGAATTACAACTTGAAATCGAAGCGAAGGACGG TGGATGCGGCAGTCAAGCAGACTTGGGCGAAGTCGGTTGGCGGAAAAAAATCGGCAAGCACTT CAGAAAAAGCGTGTCGCCTTGGGCGCAGGCTTGGGTGCAGAACACCG TTTGGATATTGACGCGATTATCTGGTTGGAAAACCTGCTCAGGCCGTTTGAAGGCAGCCAGC	GCTGGAAGO ICCGGCGGT GACCAACCA		
status:!	Sanger trace checked			
sender:!	Jolley, Keith (keith)			
	Keith Jolley (keith)			
date entered:	2018-06-07			
datestamp:!	2018-06-07			
type allele:	\odot true \odot false New allele searches can be constrained to use just type alleles in compariso	ons		
comments:				
Flags:	atypical contains IS element downstream fusion frameshift internal stop codon Use Ctrl click to select/deselect multiple choices			
PubMed ids:				
ENA ids:				
Genbank ids:	ii ii			
Override sequence				
Action				
Reset Submit				

Press submit. By default, the system will test whether your sequence is similar enough to existing alleles defined for that locus. The sequence will be rejected if it isn't considered similar enough. This test can be overridden by checking the 'Override sequence similarity check' checkbox at the bottom. It will also check that the sequence length is within the allowed range for that locus. These checks can also be overridden by checking the 'Override sequence length check' checkbox, allowing the addition of unusual length alleles.

See also:

allele sequence flags

Sequences can also be associated with PubMed, ENA or Genbank id numbers by entering these as lists (one value per line) in the appropriate form box.

6.2.2 Batch adding multiple alleles

There are two methods of batch adding alleles. You can either upload a spreadsheet with all fields in tabular format, or you can upload a FASTA file provided all sequences are for the same locus and have the same status.

Upload using a spreadsheet

Click the batch add (++) sequences link on the curator's main page.

PubMLST	Database home	Curator home	Contents					
Logged in: Keith	h Jolley (keith). 🕩 Log out	t Change password		Toggie: 🜖 📃				
Database curator's interface - Neisseria profile/sequence definitions								
Cura	ator functions			O Show all				
Use + +	Sequence Se	Million Andrew Andr	T profiles					

Download a template Excel file from the following page.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). [+Log out Change password	Help 🗹 🛛 Toggle: 🜖 📃
Batch insert sequences	
 This page allows you to upload allele sequence data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. If the locus uses integer allele ids you can leave the allele_id field blank and the next available number will be u The status defines how the sequence was curated. Allowed values are: 'Sanger trace checked', 'WGS: manual WGS: visually checked', 'WGS: automatically checked', unchecked'. Sequence flags can be added as a semi-colon (;) separated list. Download tab-delimited header for your spreadsheet - use 'Paste Special O Text' to paste the data. Download submission template (xlsx format) Please note, some loci have extended attributes which may be required. For affected loci please use the batch Reload page specific for locus: Select Please select the sender from the list below: 	sed. extract (BIGSdb)', 'WGS: automated extract (BIGSdb)',
Select sender ▼ Value will be overridden if you include a sender field in your past Ignore existing or duplicate sequences Ignore sequences containing non-nucleotide characters Ignore sequences are also ignored. Override sequence similarity check	
Paste in tab-delimited text (include a field header line).	Reset Submit

Fill in the spreadsheet. If the locus uses integer allele identifiers, the allele_id can be left blank and the next available number will be used automatically.

The status can be either: 'Sanger trace checked', 'WGS: manual extract (BIGSdb)', 'WGS: automated extract (BIGSdb)', 'WGS: visually checked', 'WGS: automatically checked' or 'unchecked'. See full explanations for these in the *single allele upload* section.

The 'type_allele' field is boolean (true/false) and specifies if the sequence should be considered as a type allele. These can be used to constrain the sequence search space when defining new alleles using the *web-based scanner* or *offline auto allele definer*.

Paste the entire sheet in to the web form and select the sender from the dropdown box.

Additionally, there are a number of options available. Some of these will ignore sequences if they don't match certain criteria - this is useful when sequence data has been extracted from genomes automatically. Available options are:

- Ignore existing or duplicate sequences.
- Ignore sequences containing non-nucleotide characters.
- Silently reject all sequences that are not complete reading frames these must have a start and in-frame stop codon at the ends and no internal stop codons. Existing sequences are also ignored.
- Override sequence similarity check.

Legged in Kath Julky (ketago ud Dange password Batch insert sequences Batch insert sequences This page allows you to uplead allele sequence data as tab-delimited text or copied from a spreadsheet. • Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. • If the locus uses integer allele ids you can leave the allele_id field blank and the next available number will be used. • The status defines how he sequence was currented. Allowed walkes are: "Sanger trace checked", WOS: manual extract (BIGSdb), WOS: automated extract (BIGSdb). • WOS: washly checkef, WOS: automatically checked, unchecked. • Sequence flags can be added as a sem-coling of list. • Download tab.definited header for your spreadsheet - use Paste Special Text to paste the data. • Download tab.definited header for your spreadsheet - use Paste Special Text to paste the data. • Download tab.definited header for your spreadsheet - use Paste Special Text to paste the data. • Download tab.definited header for your spreadsheet - use Paste Special Text to paste the data. • Download tab.definited header for your spreadsheet - use Paste Special Text to paste the data. • Download tab.definited header for your spreadsheet - use Paste Special Text to paste the data. • Download tab.definited header for your spreadsheet - use Paste Special Text to paste the data. • Download tab.definited header for your spreadsheet will be overridden if you include a sender field in your pasted data. • [Injone existing or duplicate sequences • [Injone existing or duplicate sequences • [Injone existing or duplicate sequences • [Injone assignmenes wind any check Paste in tab.definited text (fictude a field header line) Action Reset Submit Field A status sequences • [Injone assignmenes wind any check Paste in tab.definited text (fittagstb) <	PubMLST Database home Curator home Contents					
This page allows you to upload allele sequence data as tab-delimited text or copied from a spreadsheet.	Logged in: Keith Jolley (keith). E+Log out Change password			Help 🖍	Toggle: 🚯	Ξ
 Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. If the locus uses integer allele ids you can leave the allele id field blank and the next available number will be used. The status defines how the sequence was curated. Allowed values are: 'Sanger trace checked', WGS: manual extract (BIGSdb)', WGS: automated extract (BIGSdb)', Walue will be overridden if you include a sender field in your pasted data. Optione sequences and also ignored. Override sequence: allele_id field beader line). Action Nest Submit Yest automated extract (BIGSdb)', Walue will be available avail	Batch insert sequences					
Please select the sender from the list below: Jolley, Keith (keith) Value will be overridden if you include a sender field in your pasted data. Ignore existing or duplicate sequences Ignore existing or duplicate sequences Ignore existing on duplicate sequences Silently reject all sequences that are not complete reading frames - these must have a start and in-frame stop codon at the ends and no internal stop codons. Existing sequences are also ignored. Override sequence similarity check Paste in tab-delimited text (include a field header line). Action Reset Submit Reset	 Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. If the locus uses integer allele ids you can leave the allele_id field blank and the next available number will be u The status defines how the sequence was curated. Allowed values are: 'Sanger trace checked', 'WGS: manual 'WGS: visually checked', WGS: automatically checked', 'unchecked'. Sequence flags can be added as a semi-colon (;) separated list. Download tab-delimited header for your spreadsheet - use 'Paste Special O Text' to paste the data. Download submission template (xlsx format) Please note, some loci have extended attributes which may be required. For affected loci please use the batch 	ised. extract (BIGS)			t (BIGSdb)',	F
Jolley, Keith (keith) Value will be overridden if you include a sender field in your pasted data. Ignore existing or duplicate sequences Ignore sequences containing non-nucleotide characters Ignore sequences that are not complete reading frames - these must have a start and in-frame stop codon at the ends and no internal stop codons. Existing sequences are also ignored. Override sequence similarity check Paste in tab-delimited text (include a field header line). Action Icous allele_id status sequence status sequence Ignore existing or duplicate extract (BISSdb) Reset Submit THERACCETARGEGAARTICEGGARTITISCEGCERTITISTEGECGARTITICATCCATEGEAGACAGEGEGEGEGAACTICGARGEGETAR Reset Submit						
Ignore existing or duplicate sequences Ignore sequences containing non-nucleotide characters Ignore sequences that are not complete reading frames - these must have a start and in-frame stop codon at the ends and no internal stop codons. Existing sequences are also ignored. Override sequence similarity check Paste in tab-delimited text (include a field header line). Incrus allele_id status sequence abc2 WSS: automated extract (BIGSdb) ITTEGATACTETECCAAAGETITEGECGAAATICCAACTTACCAACCGCCGAAGEAACGEGGAAGACGEGETEGAAACTEGATCGAACTGAACT		ted data				
locus allele_id status sequence abc2 WGS: automated extract (BIGSdb) Reset Submit ITIGATACIGTICSCCGAAGGTIGGCGAATICCGCGATTATIGCGCCGTIATCATCCACCACTGAGGTIGGAAAATG Reset Submit ITIGATACIGTICSCCGAAGGTIGGCGAATICCGCGATTATIGCGCCGTIATCATCCACGACGACGGCCGGAAAATGGAATGG	 Ignore sequences containing non-nucleotide characters Silently reject all sequences that are not complete reading frames - these must have a start and in-frame st sequences are also ignored. Override sequence similarity check 		e ends and no	internal stop c	odons. Exist	ting
abc2 WGS: automated extract (BIGSdb) TTTGATACTGTTCCCGAAGGGTTGGCGGAATTCGCGATTATTGCGCCGTTATCATCATCATGCACCAGGAGGTGGAAATG GTTCCAGTGAGGCTTTGGCGGAAATTCGCGATTTATGCGCCGCTATCGAAGGAGGCGCTGGAAACTGGATGCGGCG GTCCAGCGAGGCTTGGCGGAAATCGAAATGCGAACGACCGCCGAGGAGGACGCCGGGAAACTGGATGCGGCG GCCTTGGCGCAGGCTTGGTGGAGGAGCGCGCTGGACGACCGAC		Action				
	abc2 WGS: automated extract (BIGSdb) TITGATACIGTIGCCGAAGGTIIGGCGAAATICGCGATITATIGCCCCGTIATCATCATGTAGGCAAGGTIGGAAAATGGTIGCGAAGGCGAAGGCGAGGCG	Reset	Submit			

Press submit. You will be presented with a page indicating what data will be uploaded. This gives you a chance to back out of the upload. Click 'Import data'.

PubMLS	ST D	atabase home)	Curator home	Contents									
Logged in:	Keith Jo	olley (keith). 🗭 Log out	Change password								Help 🗹	Toggle: 🕚	Ξ
Batcl	n ins	sert seque	nces										
Import	status												
Sender: F	Ceith Jo	lley											
No obviou	is probl	ems identified so far											
-Actio	n												
Impo	rt data	1											
		-											
Data to	be in	nported											
The follo	wing tal	ble shows your data	. Any field with red to	ext has a problem and ne	eds to be checked.	Note: valid sequ	ence flags are	e display	ed with a	red backgrour	id not red text.		
locus a	illele_i	d	sequence		statu	s	type_allele	sender	curator	date_entered	datestamp com	nents flags	
abcZ	878	TTTGATACTGTTG	CCGAAGG GC	GAATTGTCGAACTTGACC	WGS: automated e	xtract (BIGSdb)		2	2	2018-06-07	2018-06-07		
abcZ	879	TTTGATACCGTTC	CCGAAGG GC	GGATTGTCGAACTTGACC	WGS: automated e	xtract (BIGSdb)		2	2	2018-06-07	2018-06-07		

If there are any problems with the submission, these should be indicated at this stage, e.g.:

PubML	ST D	atabase home	Curator ho	me C	ontents												
Logged in	Logged in: Keith Jolley (keith). 🗘 Log out Change password Help 🗹 Toggle: 🕕																
Batc	h ins	sert seque	nces														
Impor	t status	5															
	Primary	kev		Problem	(s)												
	<i>.</i>	ele_id: 878 Sequen				characte	rs.										
Data t	o be im	ported															
The foll	owing tab	ole shows your data.	Any field with	red text h	nas a problei	m and nee	eds to be check	ked. <i>Note: v</i>	alid seque	ence flags a	re displa	yed with a	a red backgrou	nd not red tex	t.		
locus	allele i	d	seque	nce			9	status		type allele	sende	r curator	date entere	d datestamp	comm	ents flag	s
abcZ	878	TTTGATACTGTTG			TTGTCGAAC	TTGACC	WGS: automat	ted extract (<i>// _</i>	2	2	2018-06-07	2018-06-07			
abcZ	879	TTTGATACCGTTG	CCGAAGG	GCGGA	TTGTCGAAC	TTGACC	WGS: automat	ted extract (BIGSdb)		2	2	2018-06-07	2018-06-07			

Upload using a FASTA file

Uploading new alleles from a FASTA file is usually more straightforward than generating an Excel sheet.

Click 'FASTA' upload on the curator's contents page.

PubMLST Database home Curator home Contents							
Logged in: Keith Jolley (Keith). (+Log out Change password Toggle: 3							
Database curator's interface - Neisseria profile/sequence definitions							
Curator functions Users ++++CCC ++++CCC	Show all						

Select the locus, status and sender from the dropdown boxes and paste in the new sequences in FASTA format.

PubMLST	Database home Curator home Contents		
Logged in: Keith .	Jolley (keith). [+Log out Change password	Help 🗗	Toggle: 🚺 📃
Batch in	sert sequences		
next available i	ws you to upload allele sequence data in FASTA format. The identifiers in the FASTA file will be used unl id (loci with integer ids only). Do not include the locus name in the identifier in the FASTA file.	ess you select the optio	n to use the
	at you can not use this page to upload sequences for loci with extended attributes.		
Enter para			
locus:!	abcZ 👻		
status:!	Sanger trace checked 🔹		
sender:!	Jolley, Keith (keith) 🔻		
(FASTA):!	<pre>>isolate1 TTIGATACTGTTGCCGAAGGTTTGGGCGAAATTCGCGATTTATTGCGCCGTTATCATCAT GTCAGCCATCGAGTGGAAAAAGGTTGGGGCGAAGGCTTGGTGGAAACAACTCAACCAAC</pre>		
codons. Exi	Ill sequences that are not complete reading frames - these must have a start and in-frame stop codon at isting sequences are also ignored. sequence similarity check tt available id (only for loci with integer ids)	the ends and no interna	l stop
Action Reset	Check		

For loci with integer ids, the next available id number will be used by default (and the identifier in the FASTA file will be ignored). Alternatively, you can indicate the allele identifier within the FASTA file (do not include the locus name in this identifier).

As with the spreadsheet upload, you can select options to ignore selected sequences if they don't match specific criteria.

Click 'Check'.

The sequences will be checked. You will be presented with a page indicating what data will be uploaded. This gives you a chance to back out of the upload. Click 'Upload valid sequences'.

PubMLST	Databas	se home	Curate	or home	Contents							
Logged in: Keit	th Jolley (kei	<i>th).</i> ເ€Log o	ut Change p	assword					Help 🗹	Toggle:	0	Ξ
Batch i	nsert a	sequ	ences									
Sequence	check											
Locus: abc2	2											
Original d	esignation	Allele id	Status	-Action-								
isola		878	OK	Upload v	alid sequences							
isola	ate2	879	OK									

Any invalid sequences will be indicated in this confirmation page and these will not be uploaded (you can still upload the others), e.g.

PubMLST	Databas	se home	Curator home	Contents				
Logged in: Keit	h Jolley (kei	th). 🕩 Log ol	ut Change password				Help 🗹	Toggle: 🚯 📒
Batch i	nsert :	seque	ences					
Sequence	check							
Locus: abcZ	:							
Original de	esignation	Allele id		Status	- 1	Action		
isola	ate1	878		OK		Upload valid sequences)	
isola	ate2	879	Sequence contains no	on nucleotide (A C G T) charact	ters.	opioud valid sequences	J	

6.3 Updating and deleting allele sequence definitions

Note: You cannot update the sequence of an allele definition. This is for reasons of data integrity since an allele may form part of a scheme profile and be referred to in multiple databases. If you really need to change a sequence, you will have to remove the allele definition and then re-add it. If the allele is a member of a scheme profile, you will also have to remove that profile first, then re-create it after deleting and re-adding the allele.

In order to update or delete an allele, first you must select it. Click the update/delete sequences link.

PubMLST Databas	se home Curator home Contents							
Logged in: Keith Jolley (keith). 🗘 Log out Change password Toggle: 🚯 📃								
Database curator's interface - Neisseria profile/sequence definitions								
Curator funct	tions	O Show all						
Users ++¢¢+	Sequences + + MLST profiles + + + C							

Either search for specific attributes in the search form, or leave it blank and click 'Submit' to return all alleles. For a specific allele, select the locus in the filter (click the small arrow next to 'Filter query by' to expand the filter) and enter the allele number in the allele_id field.

PubMLST Database home Curator home Contents
Logged in: Keith Jolley (keith). (>Log out Change password Help [27] Toggle: ()
Query sequences for Neisseria profile/sequence definitions database
Some loci have additional fields which are not searchable from this general page. Search for these at the locus-specific query page. Use this page also for access to the sequence analysis or export plugins. Also note that some loci in this database have allele ids defined as text strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter your search to a locus that uses integer allele ids using the drop-down list. Please enter your search criteria below (or leave blank and submit to return all records).
Search criteria
allele id • = • 4 + 6 Order by: locus • ascending •
Display: 25 👻 records per page 3
Filter query by Action
locus: abcZ
status:
type allele:
sender:
allele flag:

Click the appropriate link to either update the allele attributes or to delete it. If you have appropriate permissions, there may also be a link to 'Delete ALL'. This allows you to quickly delete all alleles returned from a search.

PubMLST Database home Curator home Contents	;								
Logged in: Keith Jolley (keith). HLog out Change password							Help 🗹	Toggle: 🜖	
Query sequences for Neisseria prof	ile/sequ	ence de	finitio	ns dat	abase				
Some loci have additional fields which are not searchable from this ge analysis or export plugins. Also note that some loci in this database have allele ids defined as te your search to a locus that uses integer allele ids using the drop-dow	ext strings. Que n list.	ries using the '<		· ·					
Please enter your search criteria below (or leave blank and submit to — Search criteria	return all record	us). — Display — — —							
allele id v = v 4	+ 3	Order by:	locus	√ a	scending 👻				
		Display:	25 - reco	ords per pa	ge 🕕				
──── Filter query by									
locus: abcZ	•	Reset Subi	nit						
status:									
type allele:									
curator:	_ 0								
allele flag:									
1 record returned.									
Delete ALL Export configuration/data Batch set	1								
Delete ALL Export conliguration/data Eaten set	J								
									5
Delete Update locus allele id sequence	sequence length	status	type allele	sender	curator	date entered	datestamp co	omments flag	S
abcZ 4 TTTGATACCGTTGCC TTGTCGAACTCGATC	433	Sanger trace checked		Keith Jolley	Man-Suen Chan	2001-02-07	2009-11-11		

If you choose to delete, you will be presented with a final confirmation screen. To go ahead, click 'Delete!'. Deletion will not be possible if the allele is part of a scheme profile - if it is you will need to delete any profiles that it is a member of first. You can also choose to delete and retire the allele identifier. If you do this, the allele identifier will not be re-used.

PubMLST Database	home Curator home Contents						
Logged in: Keith Jolley (keith).	GeLog out Change password						
Delete allele se	Delete allele sequence						
You have chosen to delete the following record. Select 'Delete and Retire' to prevent the identifier being reused.							
locus:	abcZ						
allele id:	4						
sequence:	TITGATACCG TIGCCGAAGG TITIGGGCGAA ATICGIGAIT TAITGCGCCG TIAICAICAI GICAGCCAIG AGITGGAAAA IGGIICGAGI GAGGCIIIGI						
	TGAAAGAACT CAACGAATTG CAACTTGAAA TCGAAGCGAA GGACGGCTGG AAACTGGATG CGGCAGTCAA GCAGACTTTG GGGGAACTCG GTTTGCCCGGA						
	ANATGANANA ATCGGCAACC TTTCCGGCGG TCAGANANAG CGCGTCGCCT TGGCTCAGCC TGGGTGCAA AAGCCCGACG TATTGCTGCT GGACGAGCCG						
	ACCAACCATT TGGATATCGA CGCGATTATT TGGCTGGAAA ATCTGCTCAA AGCGTTTGAA GGCAGCTTGG TTGTGATTAC CCACGACCGC CGTTTTTTGG ACAATATCGC CACGCGGATT GTCGAACTCG ATC						
status:	Sanger trace checked						
type allele:							
	Keith Jolley						
	Man-Suen Chan						
date entered:	2001-02-07						
datestamp:	2009-11-11						
comments:							
Action							
Delete Delete and	Retire						

If instead you clicked 'Update', you will be able to modify attributes of the sequence, or link PubMed, ENA or Genbank records to it. You will not be able to modify the sequence itself.

). €+Log out Change password	Toggle:
date allele	sequence	
se fill in the fields bel	ow - required fields are marked with an exclamation mark (!).	
Record		— — Action — C
locus:	abcZ	Reset Submit
allele id:	4	
sequence:!	TITGATACCG TTGCCGAAGG TTTGGGCGAA ATTCGTGATT TATTGCGCCG TTATCATCAT GCAGCCATG AGTTGGAAAA TGGTTCGAGT GAGGCTTTGT TGAAAGAACT CAACGAATTG CAACTTGAAA TCGAACGGAA GGACGGCTGG AAACTGGATG CGGCAGTCAA GCAGCCTGG GGGGAACTCG GTTTGCCGGA AAATGAAAAA	
status:!	Sanger trace checked	
sender:!	Jolley, Keith (keith)	
	Keith Jolley (keith)	
date entered:!	2001-02-07	
datestamp:!	2018-06-07	
type allele:	\odot true \odot false New allele searches can be constrained to use just type alleles in comparisons	
comments:		
comments: Flags:	atypical contains IS element downstream fusion frameshift internal stop codon	
	contains IS element downstream fusion frameshift internal stop codon - Use Ctrl click to select/deselect multiple choices	
Flags:	contains IS element downstream fusion frameshift internal stop codon v Use Ctrl click to select/deselect multiple choices	
Flags: PubMed ids:	contains IS element downstream fusion frameshift internal stop codon - Use Ctrl click to select/deselect multiple choices	

Note: Adding flags and comments to an allele record requires that this feature is enabled in the *database configuration*.

6.4 Retiring allele identifiers

Sometimes there is a requirement to prevent the automated assignment of a particular allele identifier - an allele with that identifier may have been commonly used and has since been removed. Reassignment of the identifier to a new sequence may lead to confusion, so in this instance, it would be better to prevent this.

You can retire an allele identifier by clicking the 'Add' retired allele ids link on the sequence database curators' page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

PubMLST Database home Curator home Contents							
Logged in: Keith Jolley (keit	th). ເ ⇔Log out Change passwo	ord				Toggle: 🜖 📃	
Database cur	ator's interfac	e - Neisseria pr	ofile/sequence o	definitions			
Curator funct	tions				(Show all	
Users ++¢¢+	User groups	User group members	Locus descriptions	Locus links	Sequences + + RAS		
Retired alleles	Allele accessions	Allele publications	Bexsero Antigen Sequ	ence Typing (BAST)	profiles		

Select the locus from the dropdown list box and enter the allele id. Click 'Submit'.

PubMLST Datab	ase home Curator home	Contents	
Logged in: Keith Jolley (k	eith). ⇔Log out Change password		Toggle: 🕚
Add new ret	ired allele id		
Record locus:! NEIS allele id:! 67	n Jolley (keith)	d with an exclamation mark (!). Action Reset Sub	mit

You cannot retire an allele that already exists, so you must delete it before retiring it. Once an identifier is retired, you will not be able to create a new allele with that name.

You can also retire an allele identifier when you delete an allele.

6.5 Updating locus descriptions

Loci in the sequence definitions database can have a description associated with them. This may contain information about the gene product, the biochemical reaction it catalyzes, or publications providing more detailed information etc. This description is accessible from various pages within the interface such as an *allele information page* or from the *allele download page*.

Note: In recent versions of BIGSdb, a blank description record is created when a new locus is defined. The following

instructions assume that this is the case. It is possible for this record to be deleted or it may never have existed if the locus was created using an old version of BIGSdb. If the record does not exist, it can be added by clicking the Add (+) button in the 'locus descriptions' box. Fill in the fields in the same way as described below.

To edit a locus description, first you need to find it. Click the update/delete button in the 'locus descriptions' box on the sequence database curator's page (depending on the permissions set for your user account not all the links shown here may be displayed). This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

PubMLST [Database home	Curator home	Contents			
Logged in: Keith J	olley (keith). 🗭 Log ou	t Change password				Toggle: 🜖 📃
Databas	e curator's	interface	- Neisseria pr	ofile/sequence d	definitions	
Curate	or functions					Show all
Users	User	groups U:	ser group members	Locus descriptions	Locus links +++C	

Either enter the name of the locus in the query box:

PubMLST	Database home	Curator home	Contents						
Logged in: Keith	h Jolley (keith). ເ⇒Log out	Change password						Toggle: 🚯	Ξ
Query I	ocus descri	ptions for	Neisseria pr	ofile/sequ	ience	definition	s data	base	
Please enter	your search criteria be	low (or leave blank ar	nd submit to return all r	ecords).					
Search o	criteria			— — Display —					
locus	- =	NEIS0620	+ (Order by:	locus	 ascending 	•		
				Display:	25 - I	records per page 🕄			
—⊳ Filter o	uery by	Action							
		Reset Sub	mit						
									_

or expand the filter list and select it from the dropdown box:

PubMLST Database home	Curator home Conter	nts						
Logged in: Keith Jolley (keith). 🗭 Log out	Change password							Toggle: 🚺
Query locus descri	otions for Neiss	seria proi	file/sequ	ence	e def	inition	s d	latabase
Please enter your search criteria bel	ow (or leave blank and submit	to return all reco	rds).					
Search criteria			— Display —					
locus 👻 =	▼	+ 🚯	Order by:	locus	▼ ;	ascending	•	
			Display:	25 🔻	records	per page 🚯		
			Action					
locus: NEIS	0620 (maeA)	• 8	Reset Sub	omit				
curator:		v 3						
common name:		3						

Click 'Submit'.

If the locus description exists, click the 'Update' link (if it doesn't, see the note above).

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). [+Log out Change password	Toggle: 🚯 📃
Query locus descriptions for Neisseria profile/sequence definitions database	
Please enter your search criteria below (or leave blank and submit to return all records).	
Search criteria Display locus v = v + 1 Order by: locus v scending	
Display: 25 v records per page 0	
Filter query by Action locus: NEIS0620 (maeA) curator: common name:	
1 record returned.	
— Delete — — Database configuration —	
Delete ALL Export configuration/data	
Delete Update locus full name product description curator datestamp X Image: Construction of the state of the	

Fill in the form as needed:

PubMLST Database h	nome Curator home Contents	
Logged in: Keith Jolley (keith).	Dog out Change password	Toggle: 🚯 📕
Update locus d	lescription	
Please fill in the fields below	r - required fields are marked with an exclamation mark (!).	
curator:!	NEIS0620 Keith Jolley (keith)	
datestamp:! full name:	2018-06-07	
tai name.		
product:	malate oxidoreductase (EC 1.1.1.38)	
description:	Final step in TCA cycle producing oxaloacetate.	
aliases:	NG00240 A NMA0870 C NMB0671	
PubMed ids:	14917678 	
links: (Format: URL description)	http://www.enzyme-database.org /query.php?ec=1.1.1.38 EC 1.1.1.38	
Action Reset Submit		

• full_name

The full name of the locus - often this can be left blank as it may be the same as the locus name. An example of where it is appropriately used is where the locus name is an abbreviation, e.g. PorA_VR1 - here we could enter 'PorA variable region 1'. This should not be used for the 'common name' of the locus (which is defined within the locus record itself) or the gene product.

• product

The name of the protein product of a coding sequence locus.

• description

This can be as full a description as possible. It can include the specific part of the biochemical pathway the gene product catalyses or may provide background information, as appropriate.

aliases

These are alternative names for the locus as perhaps found in different genome annotations. Don't duplicate the locus name or common name defined in the locus record. Enter each alias on a separate line.

• Pubmed_ids

Enter the PubMed id of any paper that specifically describes the locus. Enter each id on a separate line. The software will retrieve the full citation from PubMed (this happens periodically so it may not be available for display immediately).

• Links

Enter links to additional web-based resources. Enter the URL first followed by a pipe symbol (I) and then the description.

Click 'Submit' when finished.

6.6 Adding new scheme profile definitions

Provided a scheme has been set up with at least one locus and a scheme field set as a primary key, there will be links on the curator's main page to add profiles for that scheme.

To add a single profile you can click the add (+) profiles link in the box named after the scheme name (e.g. MLST):



A form will be displayed with the next available primary key number already entered (provided integers are used for the primary key format). Enter the new profile, associated scheme fields, and the sender, then click 'Submit'. The new profile will be added provided the primary key or the profile has not previously been entered.

PubMLST Databa	ase home Curator h	ome Contents			
Logged in: Keith Jolley (k	eith). 🗭 Log out Change pass	vord		Help 🗹	Toggle: 🚯 📕
Add new ML	ST profile				
Please fill in the fields	below - required fields are	marked with an exclamation	mark (!).		
ST:	3015				
abcZ:					
adk:					
aroE:	! 4 🚔				
fumC:					
gdh:					
pdhC:					
pgm:			_		
	[!] Jolley, Keith (keith)		•		
clonal_complex					
	! Keith Jolley (keith)				
date_entered:					
datestamp: PubMed ids	2018-06-07				
Publivied las					
Action					
Reset Subr	nit				
Julia					

More usually, profiles are added in a batch mode. It is often easier to do this even for a single profile since it allows copying and pasting data from a spreadsheet.

Click the batch add (++) profiles link next to the scheme name:

PubMLST Databa	se home Curator home Contents	
Logged in: Keith Jolley (kei	ith). 🕩 Log out Change password	Toggle: 🚯 📃
Database cui	rator's interface - Neisseria proi	ile/sequence definitions
Curator func Users	Sequences + + FAS C MLST profiles + + FAS C	Show all

Click the 'Download submission template (xlsx format)' link to download an Excel submission template.

PubMLST Database home Curator home Contents			
Logged in: Keith Jolley (keith). 🕒 Log out Change password	Help 🗹	Toggle: 🚯	
Batch insert MLST profiles			
 This page allows you to upload profiles as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. You can choose whether or not to include a ST field - if it is omitted, the next available ST will be used automatically. If however, y then you must also provide it for each profile record. 	you include it in	the header lin	ne,
Download tab-delimited header for your spreadsheet - use Paste Special S Text to paste the data. Download submission template (xlsx format) Please paste in tab-delimited text (include a field header line)			

Fill in the spreadsheet using the copied template, then copy and paste the whole spreadsheet in to the large form on the upload page. If the primary key has an integer format, you can exclude this column and the next available number will be used automatically. If the column is included, however, a value must be set. Select the sender from the dropdown list box and then click 'Submit'.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). I Log out Change password	Help 🔀 Toggle: 🜖 📃
Batch insert MLST profiles	
 then you must also provide it for each profile record. Download tab-delimited header for your spreadsheet - use Paste Special Download submission template (xlsx format) 	al fields can be omitted if you wish. available ST will be used automatically. If however, you include it in the header line,
Please paste in tab-delimited text (include a field header line) aboz adk axak func gdh pdhC pgm clo	onal complex
Parameters Action	
Sender: Jolley, Keith (keith) Value will be overridden if you include a sender field in your pasted data.	Submit
 Ignore previously defined profiles Ignore duplicate profiles 	

You will be given a final confirmation page stating what will be uploaded. If you wish to proceed with the submission, click 'Import data'.



6.7 Updating and deleting scheme profile definitions

In order to update or delete a scheme profile, first you must select it. Click the update/delete profiles link in the scheme profiles box named after the scheme (e.g. MLST):

PubMLST I	Database home	Curator home	Contents		
Logged in: Keith J	olley (keith). 🗭 Log ou	it Change password			Toggle: 🚺 📃
Databas	e curator's	interface -	· Neisseri	a profile/sequence definitions	
Curat	or functions				O Show all
Users	s Sequences	uences M F FAS CC +	LST profiles		

Search for your profile by entering search criteria (alternatively you can use the browse or list query functions).

PubMLST	Database h	nome C	urator home	Contents								
Logged in: Keit	h Jolley (keith). 🖲	➡Log out Ch	ange password								Help 🗹	Toggle: 🚺
Query/	u <mark>pd</mark> ate p	orofile	s - Neiss	eria profil	le/seq	uence a	lefi	nitions				
Schemes												Modi form
Please sele	ct the scheme y	ou would lil	ke to query:									optio
MLST			✓ Select									_
	n criteria or leave cheme fields –	e blank to b	rowse all records ▼ 4563	. Modify form parar	meters to fi + 3	— Display/sort Order by:	option ST	15	ascending er page ()	•	Action Reset	Submit
1 record retur — Delete — Delete Al												
Delete Up	date ST abci 4563 2	Z <mark>adk</mark> aro 76	E <mark>fumC gdh pd</mark> 13 9 1	hC pgm clonal co 8 8 ST-167 c								

To delete the profile, click the 'Delete' link next to the profile. Alternatively, if your account has permission, you may be able to 'Delete ALL' records retrieved from the search.

For deletion of a single record, the full record will be displayed. Confirm deletion by clicking 'Delete'. You can also choose to delete and retire the profile identifier. If you do this, the profile identifier will not be re-used.

ogged in: Keith Jolley (keith).	CPLog out Change password
elete profile	
You have chosen to delete t	the following record. Select 'Delete and Retire' to prevent the identifier being reused.
scheme id:	1) MLST 4563
ST:	4563
abcZ :	2
adk :	7
aroE :	6
fumC :	13
gdh :	9
pdhC :	18
pgm :	8
clonal_complex :	ST-167 complex
sender:	Ana-Belen Ibarz-Pavon
curator:	Keith Jolley
date entered:	2005-03-03
datestamp:	2009-11-11
Action	
Delete Delete and	

To modify the profile, click the 'Update' link next to the profile following the query. A form will be displayed - make any changes and then click 'Update'.

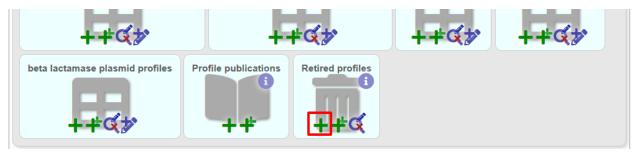
PubMLST Databa	se home Curator home Contents			
Logged in: Keith Jolley (keith). (>Log out Change password			Help 🖍	Toggle: 🜖 📃
Update profil	le			
Record		Action		
Update your record as	s required - required fields are marked with an exclamation mark (!):	Reset Submit		_0
ST: !	4563			
abcZ: !	2			
adk: !	7			
aroE: !	6			
fumC: !	13			
gdh: !				
pdhC: !				
pgm: !	8			
clonal_complex:	ST-167 complex			
sender: !	Ibarz-Pavon, Ana-Belen (aibarz)			
curator: !	Keith Jolley (keith)			
date_entered: !	2005-03-03			
datestamp: !	2018-06-07			
PubMed ids:	h.			

6.8 Retiring scheme profile definitions

Sometimes there is a requirement to prevent the automated assignment of a particular profile identifier (e.g. ST) - a profile with that identifier may have been commonly used and has since been removed. Reassignment of the identifier

to a new profile may lead to confusion, so in this instance, it would be better to prevent this.

You can retire a profile identifier by clicking the 'Add' link in the 'Retired profiles' box on the sequence database curators' page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Select the scheme from the dropdown list box and enter the profile id. Click 'Submit'.

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). Co Log out Change password		Toggle: 🜖
Add new retired profile		
Please fill in the fields below - required fields are marked with an exclamation Record scheme id:1 MLST (id 1) profile id:1 57232 curator:! Keith Jolley (keith) datestamp:! 2018-06-07	Action Reset Submit	ľ

You cannot retire a profile identifier that already exists, so you must delete it before retiring it. Once an identifier is retired, you will not be able to create a new profile with that name.

You can also retire a profile definition when you *delete a profile*.

6.9 Adding isolate records

To add a single record, click the add (+) isolates link on the curator's index page.

PubMLST Databas	se home Curator ho	me Contents		
Logged in: Keith Jolley (kei	i th). ເ €Log out Change passwo	rd		Toggle: 🜖 📃
Database cui	rat <mark>or's inter</mark> fac	e - Neisseria	a PubMLST	
Curator func	tions			O Show all
Users	Isolates	Sequence bin	Sequence tags	

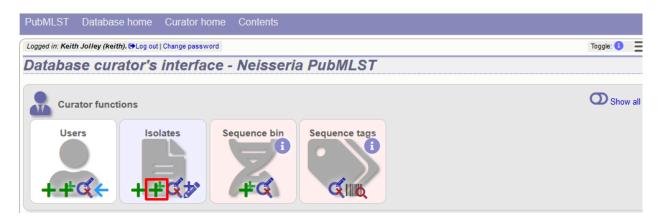
The next available id will be filled in automatically but you are free to change this. Fill in the individual fields. Required fields are listed first and are marked with an exclamation mark (!). Some fields may have drop-down list boxes of allowed values. You can also enter allele designations for any loci that have been defined.

PubMLST Database ho	ome Curator home Co	ontents							
Logged in: Keith Jolley (keith). 🕩	Logged in: Keith Jolley (keith). 🗘 Log out Change password Toggle: 🚯 📃								
Add new isolate									
Please fill in the fields below -	required fields are marked with	an excla	mation mark	(!).					
Isolate fields					- — Allele design	ations			
id:!	60465 😫 🕄								
isolate:	_	6			abcZ	adk	MLST aroE	fumC	
country:!	UK 🔫 (8			abcz	auk	aroe	iume	
species:!	Neisseria meningitidis		- 0		qdh	pdhC	pgm		
sender:!	Jolley, Keith (keith)			- 3	gun	punc	Pan		
	Keith Jolley (keith) 🕚								
	2018-06-07 🕚						ing antigens		
	2018-06-07 🕚				PorA VR1	PorA VR2	PorA VR3	FetA VR	
region:		0							
	2014 🗧 🕄				-Action				
epidemiological year:					Reset	Submit			
age yr:									
age mth:									
sex:									
disease:	meningitis	-	8						
source:	CSF 🔻 🕄								
epidemiology:	•								
serogroup:	B 🔻 🚯								
genogroup:	• •								
MLEE designation:	-								
serotype:									
sero subtype:									
ET no:									
penicillin:	0								
penicillin range:	•	6							

Press submit when finished.

More usually, isolate records are added in batch mode, even when only a single record is added, since the submission can be prepared in a spreadsheet and copied and pasted.

Select batch add (++) isolates link on the curator's index page.



Download a submission template in Excel format from the link.

PubMLST Database home Curator home	Contents	
Logged in: Keith Jolley (keith). GLog out Change password		Toggle: ()
Batch insert isolates		
 Enter aliases (alternative names) for your isolates Enter references for your isolates as a semi-color You can also upload allele fields along with the of template for locus names). These will be added with the other of the second secon	can be in any order. Optional fields can be omitted if you wish. s as a semi-colon (;) separated list. n (;) separated list of PubMed ids (non-integer ids will be ignore ther isolate data - simply create a new column with the locus n vith a confirmed status and method set as 'manual'. umber field - if it is omitted, the next available id will be used a	ame (see the 'allowed_loci' tab in the Excel
Select sender	Value will be overridden if you include a sender field in your paste	ed data.
Paste in tab-delimited text (include a field header	r line).	Action
		Reset Submit

Prepare your data in the spreadsheet - the column headings must match the database fields. In databases with large numbers of loci, there won't be columns for each of these. You can, however, manually add locus columns.

Pick a sender from the drop-down list box and paste the data from your spreadsheet in to the web form. The next available isolate id number will be used automatically (this can be overridden if you manually add an id column).

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). 🗘 Log out Change password	Toggle: 🚯 🗮
Batch insert isolates	
 This page allows you to upload isolate data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish Enter aliases (alternative names) for your isolates as a semi-colon (;) separated list. Enter references for your isolates as a semi-colon (;) separated list of PubMed ids (non-integer ids will be igno You can also upload allele fields along with the other isolate data - simply create a new column with the locus for locus names). These will be added with a confirmed status and method set as 'manual'. You can choose whether or not to include an id number field - if it is omitted, the next available id will be used at bownload tab-delimited header for your spreadsheet - use 'Paste Special Text' to paste the data. Download submission template (xlsx format) 	red). name (see the 'allowed_loci' tab in the Excel template
Jolley, Keith (keith) Value will be overridden if you include a sender field in your pas	sted data.
Paste in tab-delimited text (include a field header line).	Action
<pre>isolate aliases references country region year epidemiological_year age_yr age_mth sex disease source epidemiology species serogroup genogroup MLEE_designation serotype sero_subtype ET_no penicillin penicillin_range amoxicillin sulphonamide ceftriaxone ceftriaxone_range chloramphenicol chloramphenicol range cefotaxime cefotaxime_range pending_assembly assembly_status ENA_accession private_project comments abc2 adk aroE fumC gdh pdhC pgm PorA_VR1 PorA_VR2 FetA_VR gyrA penA rpoB J323_2 UK 2014 meningitis CSF Neisseria meningitidis B</pre>	Reset Submit

Press submit. Data are checked for consistency and if there are no problems you can then confirm the submission.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). (+Log out Change password	gle: 🚯 📃
Batch insert isolates	
Import status	
Sender: Keith Jolley	
No obvious problems identified so far.	
Action	
Import data	
Data to be imported	
The following table shows your data. Any field with red text has a problem and needs to be checked.	
id isolate aliases references country region year epidemiological_year age_yr age_mth sex disease source epidemiology species ser	group ge
60465 J323_2 UK 2014 meningitis CSF Neisseria	B
meningitidis	+

Any problems with the data will be listed and highlighted within the table. Fix the data and resubmit if this happens.

PubMLST Database home Curator	home Contents		
Logged in: Keith Jolley (keith). 🗭 Log out Change pas	sword		Toggle: 🚺
Batch insert isolates			
Import status			
Primary key	Problem(s)		
id: 60465 species "Neisseria mengitidis" i	s not on the list of allowed values for th	is field.	
Data to be imported			
The following table shows your data. Any field	vith red text has a problem and needs t	o be checked.	
id isolate aliases references country			epidemiology species serogroup gene
60465 J323_2 UK	2014	meningitis CSF	Neisseria B mengitidis
•			۱. ۲

6.10 Updating and deleting single isolate records

First you need to locate the isolate record. You can either browse or use a search or list query.

PubMLST Dat	abase home Curator h	ome Contents		
Logged in: Keith Jolle	y (keith). ເ⇒Log out Change passw	rord		Toggie: 🜖 📃
Database o	curator's interfa	ce - Neisseri	a PubMLST	
Curator f	unctions			O Show all
Users ++	++	Sequence bin	Sequence tags	

The query interface is the same as the *public query interface*. Following a query, a results table of isolates will be displayed. There will be delete and update links for each record.

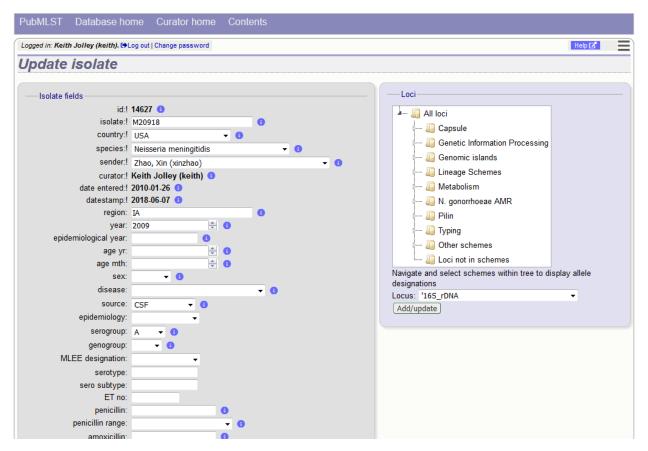
PubMLS	ST Da	atabase h	ome (Curato	r home	Contents									
Logged in:	Keith Jol	ley (keith). 🖨	Log out C	hange pa	ssword								Help 🗹	Toggle:	• =
Isolat	te qu	ery/up	odate												
Enter se	arch crite	eria or leave	blank to l	browse a	all records. N	Aodify form pa	arameters	to filte	er or enter a list of va	alues.					Modify
Isola	ate prove	nance/pheno	otype field	s											
Combi	ne with:	AND -													
coun	try	•	=	-	USA		+	8							_
year		•	=	•	2009										
Disc	olay/sort	options —							- Action						
	rder by:	·				-	ascendin	q 🔻		ubmit					
	Display:		cords per	page 🚯			abacitati	9	Reset	ubmit					
				3											
		1.44 OF 1					e								
30 record	s returne	d (1 - 25 dis	played). (Click the	e hyperlinks	for detailed in	formation								
Delet	e	– — Tag s	canning-	-Pr	ojects —										
Delet	e ALL	Sc	an	Sele	ect project		•	Lir	nk						
_								-							
Page: 1	20	Last													
		Sequence	New						lsolate fields 🚯					Seqbin	
Delete	Update	bin	version	id	isolate	aliases	country	year	disease	species	serogroup	genogroup	capsule group	size (bp)	Conti
×	ø	1	+	12674	M18700		USA	2009		Neisseria	В		В	0	0
		•	-	12675	M18701		USA	2009		meningitidis Neisseria	В		В	0	0
×		1	+	12075	1110701		USA	2009		meningitidis	D		D	U	U
×	ø	1	+	12676	M18725		USA	2009		Neisseria meningitidis	В		В	0	0
×	ø	1	+	13090	M19024	PA09015	USA	2009	meningitis	Neisseria	В		В	0	0
_										meningitidis					
×	ø	1	+	14627	M20918		USA	2009		Neisseria meningitidis	A		A	1717803	204(
×		1	+	14998	M21319		USA	2009	invasive	Neisseria	В		В	0	0
									(unspecified/other)	meningitidis					
×		+	+	15000	M21323		USA	2009	invasive	Neisseria	B		B	0	0

Clicking the 'Delete' link takes you to a page displaying the full isolate record.

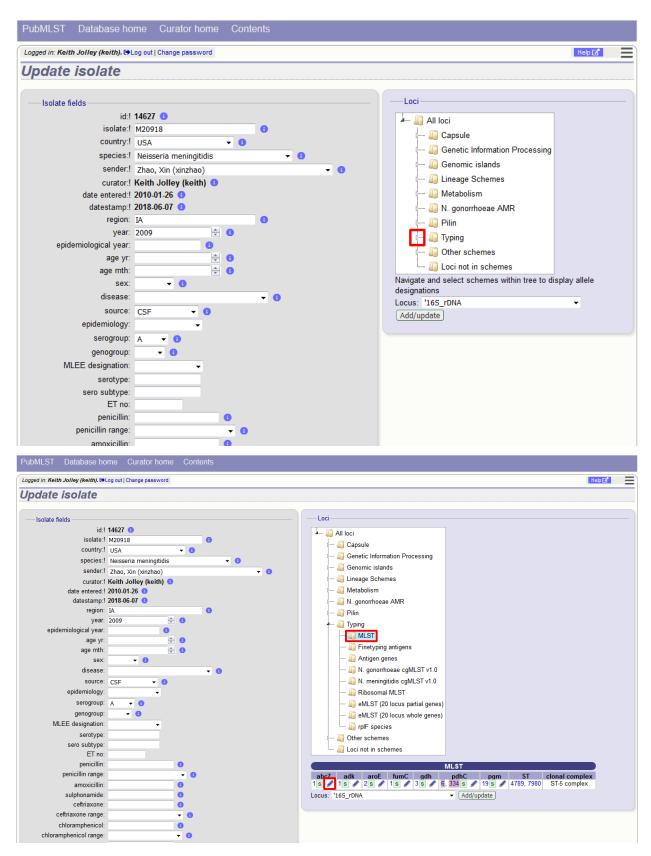
id: 14627 region: IA sender: Xin Zhao, Novartis (forme at US CDC) isolate: M20918 year: 2009 at US CDC) strain designation: A: P120,9: F3-1: source: CSF curator: Auto Tagger country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A datestamp: 2018-01-31	elete isolate	Log out Change password				Help 🗹
id: 14627 region: IA sender: Xin Zhao, Novartis (forme at US CDC) isolate: M20918 year: 2009 curator: Auto Tagger Strain designation: A: P120,9: F3-1: source: CSF curator: Auto Tagger country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A date stamp: 2018-01-31 Publication (1) Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display <th>elete isolate</th> <th></th> <th></th> <th></th> <th></th> <th></th>	elete isolate					
id: 14627 region: IA sender: Xin Zhao, Novartis (forme at US CDC) isolate: M20918 year: 2009 curator: Auto Tagger Strain designation: A: P120,9: F3-1: source: CSF curator: Auto Tagger country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A date stamp: 2018-01-31 Publication (1) Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display <th></th> <th>-</th> <th>elete and Retire' to prevent t</th> <th>he isolate id being reused.</th> <th></th> <th></th>		-	elete and Retire' to prevent t	he isolate id being reused.		
isolate: M20918 year: 2009 at US CDC) strain designation: A: P1.20.9: F3-1: source: CSF curator: Auto Tagger ST-4789,7980 (cc5) species: Neisseria meningitidis update history: 63 updates show details country: USA serogroup: A date entered: 2010-01-26 continent: Noth America capsule group: A datestamp: 2018-01-31 Publication (1) - - datestamp: 2018-01-31 Publication (1) - - - datestamp: 2018-01-31 Sequence bin - - - - - - Contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display	Provenance/met	a data				
strain designation: A: P1.20,9; F3.1: source: CSF curator: Auto Tagger strain designation: A: P1.20,9; F3.1: source: CSF update history: @3 updates show details country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A datestamp: 2018-01-31 Publication (1) . . Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90); 456 detailed breakdown: Display	id:	14627	region:	IA	sender:	Xin Zhao, Novartis (forme
Start 789,7980 (cc5) species: Neisseria meningitidis update history: (B3 updates show details country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A date entered: 2018-01-31 Publication (1) • Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display	isolate:	M20918	year:	2009		at US CDC)
country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A datestamp: 2018-01-31 Publication (1) • Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display	strain designation:	A: P1.20,9: F3-1:	source:	CSF	curator:	Auto Tagger
continent: North America capsule group: A datestamp: 2018-01-31 Publication (1) • Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display		ST-4789,7980 (cc5)	species:	Neisseria meningitidis	update history:	63 updates show details
Publication (1) • Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hare BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display	country:	USA	serogroup:	Α	date entered:	2010-01-26
 Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. <i>Bioinformatics</i> 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display 	continent:	North America	capsule group:	A	datestamp:	2018-01-31
 Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. <i>Bioinformatics</i> 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display 	Publication (1)					
BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display		Amount C. Hanna MC. Cau	alau AR, Jawasanan D, Malali		A Cavil D Mais DD T	HI I/M Tandalla MI Llass
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mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display	contigs:				0	1 - Contract - Contrac
	contigs: total length:	1,717,803 bp	N50 length (L50):	1,155	N95 length (L95):	324
Action	contigs: total length: max length:	1,717,803 bp 5,436 bp	N50 length (L50): N90 contig number:	1,155 1,414	N95 length (L95): loci tagged:	324 1,518
	contigs: total length: max length:	1,717,803 bp 5,436 bp	N50 length (L50): N90 contig number:	1,155 1,414	N95 length (L95): loci tagged:	324 1,518

Pressing 'Delete' from this record page confirms the deletion.

Clicking the 'Update' link for an isolate takes you to an update form. Make the required changes and click 'Update'.



Allele designations can also be updated by clicking within the scheme tree and selecting the 'Add' or 'Update' link next to a displayed locus.



Schemes will only appear in the tree if data for at least one of the loci within the scheme has been added. You can additionally add or update allelic designations for a locus by choosing a locus in the drop-down list box and clicking

'Add/update'.

PubMLST Database hom	ne Curator home Conte	nts	
Logged in: Keith Jolley (keith). 🗘 Log	g out Change password		Help 🗹
Update isolate			
isolate:! M country:! (JSA 🔻 🕄	0	Loci
sender:! z		• 0 • 0	Generic islands Genomic islands Genomic islands Genomic islands Genomic islands Generic islands G
epidemiological year: 2 epidemiological year: age yr: age mth:	A	0	Wind Point Point Wind Point
sex: disease: source: c epidemiology: serogroup: genogroup: MLEE designation:	CSF • •	• 0	Navigate and select schemes within tree to display allele designations Locus: abcZ
serotype: sero subtype:			

The allele designation update page allows you to modify an existing designation, or alternatively add additional designations. The sender, status (confirmed/provisional) and method (manual/automatic) needs to be set for each designation (all pending designations have a provisional status). The method is used to differentiate designations that have been determined manually from those determined by an automated algorithm.

PubMLST Database I	nome Curator home	Contents
Logged in: Keith Jolley (keith).	Log out Change password	
Update abcZ al	lele for isolate	14627
Provenance/met	a data	Locus: abcZ
id:	14627	Add new allele designation
strain designation: country: region: year: source: species serogroup: capsule group: sender: curator: update history: date entered: date stamp: Update other loci: Locus: abcZ	IA 2009 CSF Neisseria meningitidis A A Xin Zhao Auto Tagger C3 updates show details 2010-01-26	Record isolate id: 14627 locus: abcZ allele id: 5 sender: Jolley, Keith (keith) status: confirmed method: manual curator: Keith Jolley (keith) datestamp: 2018-06-07 comments: Action Reset Submit Existing designations
Add/update		Update Delete allele id sender status method comments Image: I

6.11 Batch updating multiple isolate records

Select 'batch update' isolates link on the curator's index page.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). De Log out Change password	Toggle: 🚯 📃
Database curator's interface - Neisseria PubMLST	
Curator functions Users ++++CC+ +++CC+ Curator functions Sequence bin ++++CC+ Curator functions	Show all

Prepare your update data in 3 columns in a spreadsheet:

- 1. Unique identifier field
- 2. Field to be updated
- 3. New value for field

You should also include a header line at the top - this isn't used so can contain anything but it should be present.

Columns must be tab-delimited which they will be if you copy and paste directly from the spreadsheet.

So, to update isolate id-100 and id-101 to serogroup B you would prepare the following:

```
id field value
100 serogroup B
101 serogroup B
```

Select the field you are using as a unique identifier, in this case id, from the drop-down list box, and paste in the data. If the fields already have values set, you should also check the 'Update existing values' checkbox. Press 'submit'.

PubMLST Database home Curator home Co	ntents	
Logged in: Keith Jolley (keith). 🗘 Log out Change password		Help 🗗
Batch isolate update		
combination of primary and secondary fields are unique	ed. d that you are selecting isolates on). If a secondary selection e), this should be entered in the second column. Ind then the final column should contain the value to be enter columns will be ignored.	red, e.g.
value(s) used. Usually the database id will be used.	Ontines	Allele designations
Please paste in your data below:	Options Primary selection field: id	 Allele designations Add additional new designation
100 serogroup B 101 serogroup B	Optional selection field: <none></none>	Replace existing designations
	✓ Update existing values	Action Reset Submit
		Reset

A confirmation page will be displayed if there are no problems. If there are problems, these will be listed. Press 'Upload' to upload the changes.

PubMLST	Dat	abase ho	ome Cur	ator home	Contents									
.ogged in: Keith	Jolle	y (keith). 🕩	Log out Chan	ge password								Hel	p 🗹 👘	
Bat <mark>ch</mark> is	sola	ate up	odate											
changes, pres	ss yo	ur browser'	s back butto	n.		s is what you intend and t	then p	oress 'U	Jpload'.	lf you do	o not wis	h to make	e these	
Transaction	_			Value(s) curi	rently in database									
1		serogroup			С	update field with new va								
2	101	serogroup	В		С	update field with new va	alue							
Action -														
Upload														

You can also use a secondary selection field such that a combination of two fields uniquely defines the isolate, for

example using country and isolate name.

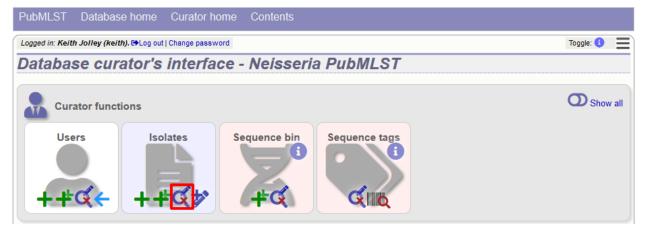
So, for example, to update the serogroups of isolates CN100 and CN103, both from the UK, select the appropriate primary and secondary fields and prepare the data as follows:

isolate	country	field	value
CN100	UK	serogroup	В
CN103	UK	serogroup	В

6.12 Deleting multiple isolate records

Note: Please note that standard curator accounts may not have permission to delete multiple isolates. Administrator accounts are always able to do this.

Before you can delete multiple records, you need to search for them. From the curator's main page, click the update/delete isolates link:



Enter search criteria that specifically return the isolates you wish to delete. Click 'Delete ALL'.

PubMLS	ST Data	abase ho	ome Curato	r home Contents			
ogged in:	Keith Jolley	y (keith). 🕩	Log out Change pa	ssword		Нер [2"	Toggle: 🚯
solat	te que	ery/up	date				
— Isola	ate provena	ance/pheno		all records. Modify form pa	rameters to filt	Iter or enter a list of values. Display/sort options	Mo form
Combir	ne with: A	ND 🔻				Order by: id 🔹 ascending 👻	opu
date	entered	-		2014-03-18	+ 🕚	Display: 25 👻 records per page 🕄	
curat	tor (surnam	ne) 🔻	= •	Jolley		Action	
						Reset Submit	
records	returned (Click the h	vperlinks for deta	ailed information			
			· ·	ojects			
Delet	10			1			
					▼ 11	Link	
Delet	te ALL	Sc	an See	ect project	· · · ·		
Delet	te ALL	Sc	an Sele	et projett	•		
					•		ntigens
			bin New versio			Isolate fields ① Finetyping a	
						Isolate fields ① Finetyping a	R2 FetA VR
Delete		Sequence	bin New versio	n id isolate aliases	s country yea	Isolate fields ① Finetyping a ar disease species serogroup genogroup capsule group PorA VR1 PorA V	R2 FetA VR + +

PubMLST	Database home Curator home Contents
Logged in: Keith J	Jolley (keith). 🗘 Log out Change password
Delete m	nultiple isolate records
Warning	If you proceed, you will delete 3 isolate records. Please confirm that this is your intention.

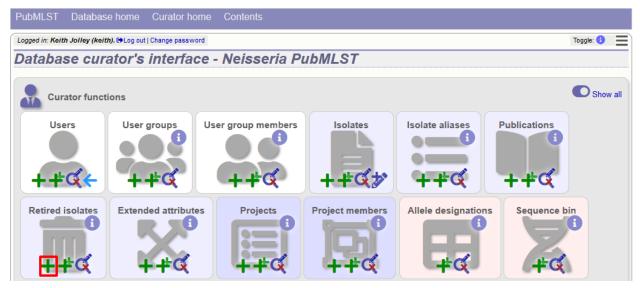
You will have a final chance to change your mind:

Click 'Confirm deletion!'.

6.13 Retiring isolate identifiers

Sometimes there is a requirement to prevent the automated assignment of a particular isolate identifier number - an isolate with that identifier may have been commonly referred to and has since been removed. Reassignment of the identifier to a new isolate record may lead to confusion, so in this instance, it would be better to prevent this.

You can retire an isolate identifier by clicking the 'Add' retired isolates link on the isolates database curators' page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Enter the isolate id to retire and click 'Submit'.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). I+Log out Change password	Toggle: 🚺 📃
Add new retired isolate id	
Please fill in the fields below - required fields are marked with an exclamation mark (!).	
Record Action isolate id:1 46262 curator:1 Keith Jolley (keith) datestamp:1 2016-12-21	Ē

You cannot retire an isolate identifier that already exists, so you must delete it before retiring it. Once an identifier is retired, you will not be able to create a new isolate record using that identifier.

You can also retire an isolate identifier when you delete an isolate record.

6.14 Setting alternative names for isolates (aliases)

Isolates can have any number of alternative names that they are known by. These isolate aliases can be set when isolates are first added to the database or batch uploaded later. When querying by isolate names, the aliases are also searched automatically.

If adding isolates singly, add the aliases in to the aliases box (one alias per line):

If batch adding isolates, they can be entered as a semi-colon (;) separated list in the aliases column.

As stated above, aliases can also be batch added. To do this, click the batch add (++) isolate aliases link on the curator's index page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

PubMLST D	atabase home Curator	home Contents				
Logged in: Keith Jo	ley (keith). 🍽 Log out Change pas	sword				Toggle: 🚯 📃
Database	curator's interf	ace - Neisseria Pu	IbMLST			
Curato	functions					Show all
Users	User groups	User group members	Isolates	Isolate aliases	Publications	
+#6	<mark>< + +</mark> ⊄	+ # ¢	++&>	+₽€	+#¢	

Prepare a list in a spreadsheet using the provided template. This consists of two columns: isolate_id and alias. For example, to add the aliases 'JHS212' and 'NM11' to isolate id 5473, the values to paste in look like:

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). @Log out Change password	Toggle: 🚯 📃
Batch insert isolate aliases	
This page allows you to upload isolate alias data as tab-delimited text or copied from a spreadsheet. • Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. • Download tab-delimited header for your spreadsheet - use 'Paste Special I Text' to paste the data. • Download submission template (dsx format) Paste in tab-delimited text (include a field header line). Isolate_idalias St73MN11 #	Action Reset Submit
Back	

A confirmation page will be displayed.

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). @Log out Change password	Toggle: 🚯	Ξ
Batch insert isolate aliases		
Import status		
No obvious problems identified so far.		
Action Import data		
Data to be imported		
The following table shows your data. Any field with red text has a problem and needs to be checked.		
isolate_id alias datestamp curator		
5473 JHS212 2016-12-16 2 5473 MN11 2016-12-16 2		
3473 MINTI 2010-12-10 2		

Click 'import data'.

6.15 Linking isolate records to publications

Isolates can be associated with publications by adding PubMed id(s) to the record. This can be done when *adding the isolate*, where lists of PubMed ids can be entered in to the web form.

They can also be associated in batch after the upload of isolate records. Click the PubMed batch add (++) link on the curator's main page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

PubMLST Databas	e home Curator he	ome Contents				
Logged in: Keith Jolley (keit	h). ເ⇔Log out Change passw	rord				Toggle: 🚯 📃
Database cura	ator's interfa	ce - Neisseria Pu	bMLST			
Curator funct	User groups	User group members	Isolates	Isolate aliases	Publications i	Show all

Open the Excel template by clicking the link.

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). [+Log out Change password		Toggle: 🜖 📃
Batch insert refs		
This page allows you to upload PubMed link data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. Download tab-delimited header for your spreadsheet - use 'Paste Special Text' to paste the data. Download submission template (xlsx format) Paste in tab-delimited text (include a field header line).	Action Reset Submit	ľ

The Excel template has two columns, isolate_id and pubmed_id. Simply fill this in with a line for each record and then paste the entire spreadsheet in to the web form and press submit.

PubMLST Data	abase home	Curator home	Contents							
Logged in: Keith Jolley	r (keith). ເ≯Log out C	change password						Тод	gle: 🚯	
Batch inse	rt refs									
 Field header Download tal Download su 	names must be in b-delimited header ibmission template limited text (inclu- pubmed_id 7841 7841	cluded and fields of for your spreadshe (xlsx format)	an be in any order. eet - use 'Paste Spe	opied from a spreads Optional fields can l ecial	be omitted if you wish.	Action Reset	Submit			Ī

To ensure that publication information is stored locally and available for searching, the references database needs to be *updated regularly*.

6.16 Uploading sequence contigs linked to an isolate record

6.16.1 Select isolate from drop-down list

To upload sequence data, click the sequences add (+) sequence bin link on the curator's main page.



Select the isolate that you wish to link the sequence to from the dropdown list box (or if the database is large and there are too many isolates to list, enter the id in the text box). You also need to enter the person who sent the data. Optionally, you can add the sequencing method used.

Paste sequence contigs in FASTA format in to the form.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). [+Log out Change password	Toggle: 🕦
Upload sequences	
This page allows you to upload sequence data for a specified isolate record in FASTA format. If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any ot FASTA file. This allows data for multiple isolates to be uploaded. <i>Please note that you can reach this page for a specific isolate by querying isolates and then clicking 'Upload' within th</i> Please fill in the following fields - required fields are marked with an exclamation mark (I).	A
Paste in sequences in FASTA format: ACCGTCARAATCGGTCGGCATCGATGAATCGATACCGCGCGAAAACAAATTTCTTGGATT TCGCCGTGGTCGTTGTCGTGATGAAGCGGTGAAGGCGGACGAGTGGTTTTAAACAGG CCGGAAGGGCGTGGAAGAATGAAATCCTTCTGTCGAATACACGAATCACAGAGG GGAATGCGCCACAAAATCGCGGCCGTTTCTGTCGAATACACGAATCACGAATGAGG GAAATCCGCACCAAAATCGGGCATCACCGAACACGGAAGACGCCCGGCGTGTGGGCGC CGCCGGCGCGACAGCGATTGGGGCCGGTTCTCCCCGACGCCCCGCTGTGGGCCCT CGTCAAGGAAAGCCAACAAATCGCGCCGCTTCCCCGCCGTTGTCGCGCCTTT CGTCAACGGAAGCCAACGGCGTTCCCCCCCCGCCGTGTGCGCCCCTTT CGCATCGCGGCGGAGAGCGGCCGTTCCCCCCGCCGTTCGCCGCGCCTTTCCGGCCCCTTT CGCATCGCGGCGCGGAGACGAGCCGCCCTCTCCCGGACGCCCCGACGCCCTT CGACTGCGGCGCGGCACGACGCCCCCGGACCGCCCCGGACCGCCTT CGACTGCGGCGCTGTGCCTCCCGCATCCCCGGCGGCGGCGGCGGCCGGC	Attributes isolate id: ! 2 isoley, Keth (keth) method: run id: assembly id: Options Options Options Attributes Alternatively upload FASTA file or enter Genbank accession Select FASTA file: Browse No file selected. Action Reset Submit

Click 'Submit'. A summary of the number of isolates and their lengths will be displayed. To confirm upload, click 'Upload'.

ed in: Keith Jolley (keith). 🗭 Log out Change password			Toggle: 🕄
load sequences			
The following sequences will be entered.		SummaryAction	
Original designation	Sequence length Comments	Number of contigs: 364 Upload	
180062 NODE_116_length_5370_cov_18.338547	5408	Minimum length: 100	
180063 NODE_267_length_64_cov_54.562500	102	Maximum length: 50093	
180064 NODE_1024_length_456_cov_16.434210	494	Total length: 2069108	
180065 NODE_367_length_3545_cov_22.858955	3583	Mean length: 5684	
180066 NODE_361_length_87_cov_17.862068	125	N50 contig number: 44	
180067 NODE_1617_length_297_cov_11.111111	335	N50 contig length (L50): 15404	
180068 NODE_909_length_95_cov_9.073684	133	N90 contig number: 146	
180069 NODE_699_length_98_cov_110.918365	136	N90 contig length (L50): 3907	
180070 NODE_553_length_84_cov_47.964287	122	N95 contig number: 180	
180071 NODE_182_length_6772_cov_19.882162	6810	N95 contig length (L50): 2305	
180072 NODE_928_length_347_cov_35.201729	385	1495 contig length (LSU). 2305	
180073 NODE_19_length_12542_cov_19.259449	12580		
180074 NODE_60_length_5125_cov_18.960781	5163		
180075 NODE_168_length_7439_cov_17.615808	7477		
180076 NODE_1041_length_109_cov_27.752293	147		
180077 NODE_71_length_2120_cov_19.594339	2158		
180078 NODE_318_length_1827_cov_15.821566	1865		
180079 NODE_207_length_6398_cov_19.577681	6436		
80080 NODE_162_length_13775_cov_18.618221	13813		
180081 NODE_664_length_160_cov_35.068748	198		
180082 NODE_56_length_9475_cov_20.244328	9513		
180083 NODE_356_length_297_cov_41.383839	335		
180084 NODE_778_length_582_cov_42.140892	620		
180085 NODE_137_length_10168_cov_16.055567	10206		
180086 NODE_1102_length_82_cov_43.329269	120		

6.16.2 Select from isolate query

As an alternative to selecting the isolate from a dropdown list (or entering the id on large databases), it is also possible to upload sequence data following an isolate query.

Click the isolate update/delete link from the curator's main page.



Enter your search criteria. From the list of isolates displayed, click the 'Upload' link in the sequence bin column of the appropriate isolate record.

PubMLST Database home Curator ho	ne Contents			
Logged in: Keith Jolley (keith). [+Log out] Change passw	d		ŀ	ielp 🗹 🛛 Toggle: 🜖
Isolate query/update				
Enter search criteria or leave blank to browse all re	ords. Modify form parameters to filter or enter a list of values			Modify
Isolate provenance/phenotype fields	Display/sort options		Action	form option
isolate 🔹 = 💌 fa	· · · · · · · · · · · · · · · · · · ·	✓ ascending	 Reset 	Submit
	Display: 25 👻	records per page 🚯		
1 record returned. Click the hyperlink for detailed in	rmation.			
	3			
Delete ALL Scan Select p	oject Link			
Delete Undete Sequence New	Isolate fields			Finetyping antigens
Delete Update bin version id is	late aliases country year disease	species serogroup genogroup group		PorA PorA FetA VR1 VR2 VR
🗙 🥒 🤽 🕂 698 F.	M18 NIBSC_3076; USA 1983 invasive	Neisseria C C		5 🖋 2 🖋 F1-30
	Z4259 (unspecified/other)	meningitidis	complex	ø

The same upload form as detailed above is shown. Instead of a dropdown list for isolate selection, however, the chosen isolate will be pre-selected.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). De Log out Change password	Toggle: ()
Upload sequences	
This page allows you to upload sequence data for a specified isolate record in FASTA format. If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any of FASTA file. This allows data for multiple isolates to be uploaded.	A
Please note that you can reach this page for a specific isolate by querying isolates and then clicking 'Upload' within	the isolate table.
Please fill in the following fields - required fields are marked with an exclamation mark (!).	
Paste in sequences in FASTA format:	Attributes isolate id: 698) FAM18 sender: Select sender method: run id: assembly id: Options Options Options Don't insert sequences shorter than 25 bps. Link to experiment: Atternatively upload FASTA file or enter Genbank accession Select FASTA file: Browse No file selected. Action Reset Submit

6.16.3 Upload options

On the upload form, you can select to filter out short sequences from your contig list.

If your database has experiments defined (experiments are used for grouping sequences and can be used to filter the sequences used in *tag scanning*), you can also choose to upload your contigs as part of an experiment. To do this, select the experiment from the dropdown list box.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). 🗘 Log out Change password	Toggle: ()
Upload sequences	
This page allows you to upload sequence data for a specified isolate record in FASTA format. If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any of FASTA file. This allows data for multiple isolates to be uploaded. Please note that you can reach this page for a specific isolate by querying isolates and then clicking 'Upload' within the Please fill in the following fields - required fields are marked with an exclamation mark (I).	A
Paste in sequences in FASTA format:	Attributes isolate id: 1 698) FAM18 sender: ! Select sender • method: • method: • assembly id: • Ontions Ontions Don't insert sequences shorter than 25 • bps. Link to experiment: • Alternatively upload FASTA file • or enter Genbank accession - Select FASTA file: • Browse No file selected. • Reset Submit

6.17 Batch uploading sequence contigs linked to multiple isolate records

To upload contigs for multiple isolates, click the batch add (++) sequence bin link on the curator's main page.

PubMLST Database	home Curator h	nome Contents		
Logged in: Keith Jolley (keith).	. 🔁 Log out Change pass	word		Toggle: 🚺
Database cura	tor's interfa	ace - Neisseri	a PubMLST	
Curator function	Isolates	Sequence bin	Sequence tags	O Show all

The first step is to upload the name of the contig file that will be linked to each isolate record. This can be done by pasting two columns in tab-delimited text format (e.g. from a spreadsheet) - the first column contains the isolate identifier, the second contains the filename of the contigs file, which should be in FASTA format.

You can choose which field to use for identifying the isolates, e.g. id (database id) or isolate (name of isolate). The value provided for this field needs to uniquely identify the isolate in the database - please note that only id is guaranteed to be unique.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). C+Log out Change password	Toggle: 🚯 📃
Batch upload sequence assemblies to multiple isolate records	
This function allows you to upload assembly contig files for multiple records together. The first step in the upload process is to state which assembly contig FASTA file should be linked to each isolate record. You can use any provenance metad uniquely identifies an isolate. You can upload up to 100 genomes at a time. Identifying field name Field: isolate Filenames Paste in tab-delimited text, e.g. copied from a spreadsheet, consisting of two columns. The first column should be the value for the isolate identifier field (sp and the second should be the filename that you are going to upload. You need to ensure that you use the full filename, including any suffix such as .fas or .: may be hidden by your operating system.	ecified above),
MB_21293 MB_21293.fasta MB_21294 JB_21294.fasta Action Reset Submit Submit	

Click Submit. The system will check to make sure that the isolate records are uniquely identified (if not, you will see an error message informing you of this and you will need to use the database id as the identifier). You will then see a file upload form.

aed in: Ke	ith Jolley	v (keith). 🍽	og out I Char	nge password			Toggle: (1
-							
atch	uplo	ad se	quen	ce assen	iblies to n	nultiple i	isolate records
ease uplo	ad the a	assembly c	ontig files f	for each isolate re	ecord.		
remove			current se	equence bin sta	te a		
row	id	isolate	contigs	total size (bp		upload status	
	61222	JB_21292	-	-	JB_21292.fasta	×	
		JB_21293		-	JB_21293.fasta		
	61224	JB_21294	-	-	JB_21294.fasta	×	
Remove							
		o upload.					
- Contig	assemb	ly files —	blies with t	he filenames as v	/ou specified (indic	ated in the table	e). Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go
—Contig Please up	assemb bload co	ly files ntig asseml			you specified (indic size of the upload		e). Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go
— Contig Please up	assemb bload co	ly files ntig asseml					e). Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go
—Contig Please up	assemb bload co	ly files ntig asseml					e). Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go
— Contig Please up	assemb bload co	ly files ntig asseml					e). Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go
— Contig Please up	assemb bload co	ly files ntig asseml		so that the total	size of the upload	can be larger.	
— Contig Please up	assemb bload co	ly files ntig asseml		so that the total	size of the upload	can be larger.	e). Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go
— Contig Please up	assemb bload co	ly files ntig asseml		so that the total	size of the upload	can be larger.	
— Contig Please up	assemb bload co	ly files ntig asseml		so that the total	size of the upload	can be larger.	
— Contig Please up	assemb bload co	ly files ntig asseml		so that the total	size of the upload	can be larger.	
—Contig Please up	assemb bload co	ly files ntig asseml		so that the total	size of the upload	can be larger.	

Drag and drop your FASTA format contig files in to the dotted drop area. Provided the filenames exactly match the filename you stated, these will be uploaded to a staging area.

Click 'Validate' to check that these files are valid FASTA format.

PubMLS	T Dat	abase ho	ome Cu	irator home C	ontents		
Logged in: K	eith Jolle	y (keith). 🕩	Log out Cha	nge password			Toggle: 🜖
Batch	uplo	oad se	quen	ce asseml	blies to n	nultiple	isolate records
				for each isolate reco			et -
remove row	id	isolate	current so	equence bin state total size (bp)	filename	upload status	
	61222	JB_21292	-	-	JB_21292.fasta	 ✓ 	
	61223	JB_21293	-	-	JB_21293.fasta	~	
	61224	JB_21294	-	-	JB_21294.fasta	~	
All files up All files up Valida	oloaded. 1 n	The sequen	ces have n	ot yet been validate	d. This needs to	be done before	they can be added to the database.

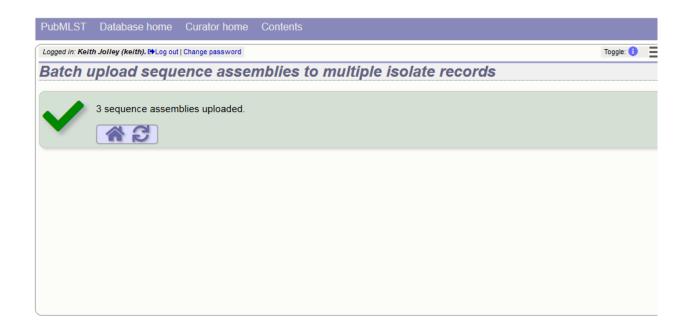
The files will be checked and a table will be displayed showing the total sequence size and number of contigs found. Select the data sender and, optionally the sequencing method from the dropdown lists. Then click 'Upload validated contigs'.

PubMLST Database home Curator h	ome	Contents			
Logged in: Keith Jolley (keith). 🗭 Log out Change passw	vord			Toggle: 🕚	Ξ
Batch upload sequence as	sser	nblies	to multiple isolate records		
Validation					
id isolate filename valid FASTA 61222 JB 21292 JB 21292.fasta ✓	contige 364	2,069,108			
61223 JB_21293 JB_21293.fasta	1	2,194,961			
61224 JB_21294 JB_21294.fasta	1	2,272,360			
You can upload 3 records.					
Attributes			Options		
sender: ! Jolley, Keith (keith)			▼ Don't insert sequences shorter than 25 ▼ bps.		
method: Illumina 🗸			Action		
			Upload validated contigs		

You can also choose to filter out short contigs from the upload by selecting the checkbox and choosing the minimum length from the dropdown box in the options settings.

PubMLST Database home Curator h	ome Contents	
Logged in: Keith Jolley (keith). 🗭 Log out Change passw	vord	Toggle: 🜖 📃
Batch upload sequence as	ssemblies	to multiple isolate records
Validation		
id isolate filename valid FASTA	contigs total size	
61222 JB_21292 JB_21292.fasta 🗸	364 2,069,108	
61223 JB_21293 JB_21293.fasta 🗸	1 2,194,961	
61224 JB_21294 JB_21294.fasta	1 2,272,360	
You can upload 3 records.		
Attributes		Options
sender: ! Jolley, Keith (keith)		✓ Don't insert sequences shorter than 100 bps.
method: Illumina 👻		
		Upload validated contigs

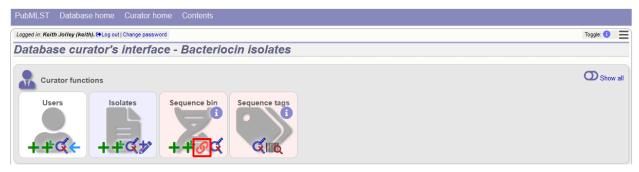
A confirmation message will be displayed after clicking the Upload button.



6.18 Linking remote contigs to isolate records

If *remote contigs have been enabled*, isolates can be linked to contigs stored in an external BIGSdb database, rather than directly uploaded. These well then be loaded when needed, for example during scanning or data export. This will be marginally slower than hosting contigs within the same database, but minimises duplication of sequence data and associated storage. Contigs need to be accessible via the BIGSdb *RESTful API*.

Click the sequences link icon on the curator's main page.



Either select the isolate id from the dropdown list, or enter it manually (list is disabled if there are >1000 records in the database). Enter the URI for the RESTful API of the parent isolate record, e.g. http://rest.pubmlst.org/db/pubmlst_rmlst_isolates/933. This URI can require authentication if credentials have been *set up*.

Press submit.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). (ALog out Change password	Toggle: 🚯 🚍
Add remote contigs	
This page allows you to link contigs stored in a remote BIGSdb database to an isolate record. Access to these contig Valid URIs are in the form 'http://rest.pubmlst.org/db/{database_config}/isolates/(isolate_id)'. — Enter details isolate id: ! 1 isolate record URI: ! http://rest.pubmlst.org/db/pubmlst_rmlst_isolates/isolates/933	s is via the BIGSdb RESTful API which must be running on the remote database. - Action Reset Submit

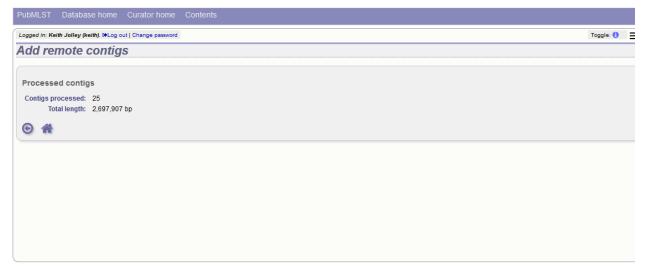
Summary information about the number of contigs and their total length will be downloaded from the remote isolate record. You will then be prompted to upload this information to the database, by clicking the 'Upload' button.



The contigs will be downloaded in bulk in order to determine their lengths. This information is stored within the local database as it is required for various outputs. Full metadata is not stored at this stage.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). 🖗 Log out Change password) =
Add remote contigs	
25 remote contigs added.	
Please note that so far only links to the contig records have been added to the database. The contigs themselves have not been downloaded and checked. Processing records the length of each conting stores a checksum within the database so that it is possible to tell if the sequence ever changes. You can either do this now or it can be performed offline by a scheduled task. Total contigs: 25 Remote contigs: 25 (25 unprocessed) Total length: 2,697,907 Action Process contigs now	tig

This is all that is required for the contigs to be used as normal. In order to get the full metadata about the contigs (sequencing platform used, sender and datestamp information), you can choose to process the contigs by clicking the 'Process contigs now' button. This will download each contig in turn, and store its provenance metadata locally.

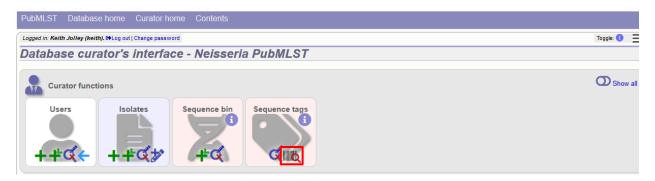


Alternatively, this step can be *performed offline automatically*.

6.19 Automated web-based sequence tagging

Sequence tagging, or tag-scanning, is the process of identifying alleles by scanning the sequence bin linked to an isolate record. Defined loci can either have a single reference sequence, that is defined in the locus table, or they can be linked to an external database that contains the sequences for known alleles. The tagging function uses BLAST to identify sequences and will tag the specific sequence region with locus information and an allele designation if a matching allele is identified by reference to an external database.

Select 'scan' sequence tags on the curator's index page.



Next, select the isolates whose sequences you wish to scan against. Multiple isolates can be selected by holding down the Ctrl key. All isolates can be selected by clicking the 'All' button under the isolate selection list.

Select either individual loci or schemes (collections of loci) to scan against. Again, multiple selections can be made.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). @Log out Change password	Help 🗹 Toggle: 🚯 💻
Logged in: Keith Jolicy (Keith), I9Log out Change password Sequence tag scan Please select the required isolate ids and loci for sequence scanning - use Ctrl or Shift to make multiple selections. In addition to selecting individual loc the appropriate scheme description. By default, loci are only scanned for an isolate when no allele designation has been made or sequence tagged. You selecting the appropriate options. Isolates Loci Schemes 19/ 53131 10 165_rRNA (SSU_rRNA) Intege Schemes 23/ 26 23/ 26 abc2 (NEIS1015) abc2 (NEIS1015) 30/ 14 30/ 14 30/ 20 abc2 (NEIS1015) abc2 (NEIS1027) 35/ 26 abc2 (NEIS1027) abc4 (NEIS1727) abc4 (NEIS1727) abc7 (NEIS1727) 31/ 10 10/ 255 [old version] abc7 (NEIS1727) abc7 (NEIS1727) abc7 (NEIS1727) 36/ 27 39/ 36 abc7 (NEIS1727) abc7 (NEIS1727) abc7 (NEIS1727) abc7 (NEIS1727) 36/ 39/ 39/ 30 abc7 (NEIS17427) abc7 (NEIS17427) abc7 (NEIS17427) abc7 (NEIS17427) 37/ 30/ 30 abc7 (NEIS17427) abc7 (NEIS17427) abc7 (NEIS17427) abc7 (NEIS17427) 38/ 40/ 39/ 39/ 30 abc7 (NEIS17427) abc7 (NEIS17427) abc7 (NEIS	H, you can choose to include all loci defined in schemes by selecting
Action Reset Scan	

Choose your scan parameters. Lowering the value for BLASTN word size will increase the sensitivity of the search at the expense of time. Using TBLASTX is more sensitive but also much slower. TBLASTX can only be used to identify the sequence region rather than a specific allele (since it will only match the translated sequence and there may be multiple alleles that encode a particular peptide sequence).

By default, for each isolate only loci that have not had either an allele designation made or a sequence region scanned will be scanned again. To rescan in these cases, select either or both the following:

- · Rescan even if allele designations are already set
- Rescan even if allele sequences are tagged

You can select to only use type alleles to identify the locus. This will constrain the search space so that allele definitions don't become more variable over time. If a partial match is found to a type allele then a full database lookup will be performed to identify any known alleles. An allele can be given a status of type allele when *defining*.

If fast scanning is enabled, there will also be an option to 'Scan selected loci together'. This can be significantly quicker than a locus-by-locus search against all alleles but is not enabled by default as it can use more memory on the server and requires *exemplar alleles* to be defined.

Options can be returned to their default setting by clicking the 'Defaults' button.

PUDMLS1 Database nome Curator nome Contents	
Logged in: Keith Jolley (keith). (HLog out Change password	Help 🕼 Toggle: 🚯 💻
Sequence tag scan	
Please select the required isolate ids and loci for sequence scanning - use Cht or Shift to make multiple selections. In addition to selecting individual loci, yo the appropriate options. Isolates Loci 19) \$3131 1 23) 24 165_CNNA 30) 14 235_RNA 30) 14 abc2 33) 26 Exercise All R - in 46) 255 (Jold version] acce (NEIS1229) 3642 (NEIS12727) acnA (NEIS1727) acnA (NEIS1280) ath (None Paste list	

Press 'Scan'. The system takes approximately 1-2 seconds to identify each sequence (depending on machine speed and size of definitions databases). Alternatively, if 'Scan selected loci together' is available and selected, it may take longer to return initial results but total time should be less (e.g. a 2000 loci cgMLST scheme may be returned in 1-2 minutes). Any identified sequences will be listed in a table, with checkboxes indicating whether allele sequences or sequence regions are to be tagged.

olate I	latch	Locus	Allele	% identity	Alignment length	Allele lengt	E-value	Sequence bin id	Start End	Predicted star	t Predicted end	Orientation	Designate allele		Flag 🚯	
4) 20			1	100.00	433	433	0.0	182791	7064 7496		7496 extract -	←			nug O	-
) 20	exact	adk	3	100.00	465	465	0.0	182750	1392 1856	1392	1856 extract →	\rightarrow	V			•
4) 20	exact	aroE	1	100.00	490	490	0.0	182731	32577 3306	6 32577	33066 extract -	~	V	V		•
) 20	exact	fumC	1	100.00	465	465	0.0	182815	19783 2024	7 19783	20247 extract -	\rightarrow	V			•
) 20	exact	gdh	1	100.00	501	501	0.0	182852	7516 8016	7516	8016 extract -	\rightarrow	V			-
4) 20	exact	pdhC	1	100.00	480	480	0.0	182819	13868 1434	7 13868	14347 extract -	\rightarrow	V	V		-
4) 20	exact	pgm	3	100.00	450	450	0.0	182831	24559 2500	8 24559	25008 extract -	\rightarrow	V			-
Actior Tag a		sequen	ces										All None	All None		

Individual sequences can be extracted for inspection by clicking the 'extract \rightarrow ' link. The sequence (along with flanking regions) will be opened in another browser window or tab.

Checkboxes are enabled against any new sequence region or allele designation. You can also set a flag for a particular sequence to mark an attribute. These will be set automatically if these have been defined within the sequence definition database for an identified allele.

See also:

Sequence tag flags

Ensure any sequences you want to tag are selected, then press 'Tag alleles/sequences'.

If any new alleles are found, a link at the bottom will display these in a format suitable for automatic allele assignment

by batch uploading to sequence definition database.

See also:

Offline curation tools

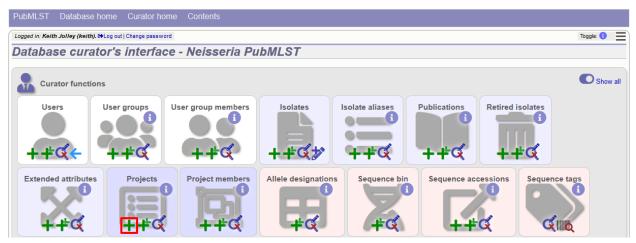
Automated offline sequence tagging

6.20 Projects

6.20.1 Creating the project

The first step in grouping by project is to set up a project.

Click the add (+) project link on the curator's main page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Enter a short description for the project. This is used in drop-down list boxes within the query interfaces, so make sure it is not too long.

You can also enter a full description. If this is added, the project description can displayed at the top of an isolate information page (but see 'isolate_display' flag below). The full description can include HTML formatting, including image links.

There are additionally two flags that affect how projects are listed:

- isolate_display Setting this is required for the project and its description to be listed at the top of an isolate record (default: false).
- list Setting this is required for the project to be listed in a page of projects linked from the main contents page.

There are a further two option flags:

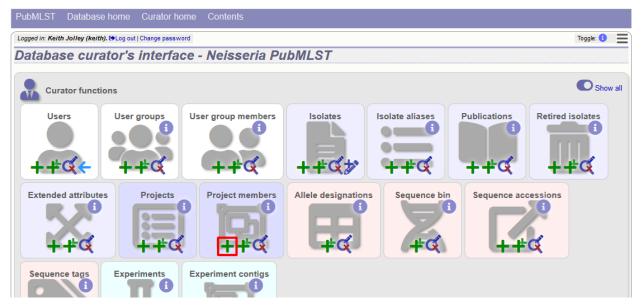
- private Setting this makes the project a private *user project*. You will be set as the project owner and will be the only user able to access it by default. You can add additional users or user groups who will be able to access and update the project data later.
- no_quota If set, isolates added to this project will not count against a user's quota of *private records* (only relevant to private projects).

Click 'Submit'.

ogged in: Keith Jolley (keith). E+Log out Change password			Toggle: 🕚
dd new proje	ect description			
Please fill in the fields bel	ow - required fields are marked with an exclamation mark (!).			
Record		-Action-		
id:!	3	Reset	Submit	
short description:!	MRF Meningococcus Genome Library 3			
isolate display:!	🖲 true 🔿 false 🚯			
list:!	e true ○ false ①			
private:	🔿 true 🔘 false 🚯			
no quota:!	🖲 true 🔿 false 🕄			
curator:!	Keith Jolley (keith)			
datestamp:!	2018-06-08			
full description:	<pre><div style="float:right; padding: 0 2em"></div> <div>>the MRF Meningococcus Genome Library is a collaboration between Public Health England, the Scottish Haemophilus, Legionella, Meningococcus and Pneumococcus Reference (SHLMFB) Laboratory, The Wellcome Trust Sanger Institute and the University of Oxford, funded by the Meningitis Research</div></pre>			

6.20.2 Explicitly adding isolates to a project

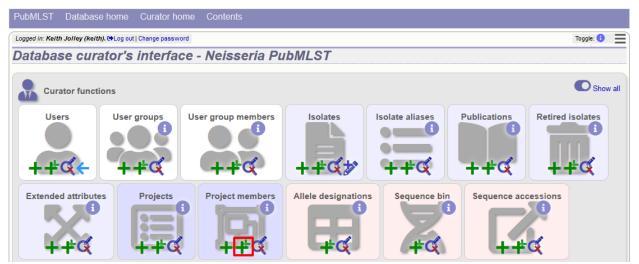
Explicitly adding isolates to the project can be done individually or in batch mode. To add individually, click the add (+) project member link on the curator's main page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



Select the project from the dropdown list box and enter the id of the isolate that you wish to add to the project. Click 'Submit'.

PubMLST Data	abase home Curator home	Contents	
Logged in: Keith Jolley	/ (keith). ➡Log out Change password		Toggle: 🚯 📃
Add new p	roject member		
Record project id:! isolate id:!	Keith Jolley (keith)	Action	ľ

To add isolates in batch mode. Click the batch add (++) project members link on the curator's main page.



Download an Excel submission template:

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). (+Log out Change password		Toggle: 🜖 📃
Batch insert project members		
 This page allows you to upload project member data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. Download tab-delimited header for your spreadsheet - use 'Paste Special ⁽²⁾ Text' to paste the data. Download submission template (xlsx format) 		ľ
Paste in tab-delimited text (include a field header line).	Action	
	Reset Submit	

You will need to know the id number of the project - this is the id that was used when you created the project. Fill in the spreadsheet, listing the project and isolate ids. Copy and paste this to the web upload form. Press 'Submit'.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). 🗘 Log out Change password	Toggle: 🜖 📃
Batch insert project members	
This page allows you to upload project member data as tab-delimited text or copied from a spreadsheet. • Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. • Download tab-delimited header for your spreadsheet - use 'Paste Special Text' to paste the data. • Download submission template (xlsx format) Paste in tab-delimited text (include a field header line). project_idisolate_id 3	Action Reset Submit

6.21 Isolate record versioning

Versioning enables multiple versions of genomes to be uploaded to the database and be analysed separately. When a new version is created, a copy of the provenance metadata, and publication links are created in a new isolate record. The sequence bin and allele designations are not copied.

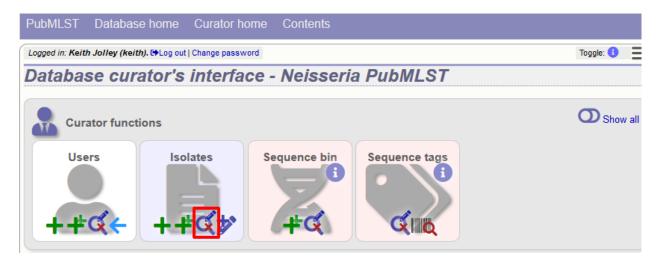
By default, old versions of the record are not returned from queries. Most query pages have a checkbox to 'Include old record versions' to override this.

Links to different versions are displayed within an isolate record:

ged in: Keith Jolley (keith).	€Log out Change password		Help 🗹	Toggle: 🚯
Ill informatio	n on isolate M17	661 (id:19377)		
Provenance/me	ta data			
id:	19377	species:	Neisseria meningitidis	
	M17661	serogroup:		
	W: P1.5-1,10-8: F-ND: ST-11 (c	0 1		
country:		,	Keith Jolley, University	of Oxford, UK
	North America		Auto Tagger	
region:	MI	update history:	51 updates show detail	s
year:	2008	date entered:	2012-06-27	
disease:	invasive (unspecified/other)	datestamp:	2018-01-31	
Versions	is isolate record exist.			
Newer versions:	40500			
Publication (1)				
RD, Tatti KM, Tonde		AB, Jayaraman P, Nelakuditi V, Hun lordan IK (2010). A computational ge isolates		
Sequence bin				
		ig number: 591	N95 contig number:	2,006
contigs:	2,511 N50 cont	ig nambori oo i		
		ngth (L50): 1,011	N95 length (L95):	267
	1,805,445 bp N50 le		N95 length (L95): loci tagged:	

The different versions will also be listed in analysis plugins, with old versions identified with an [old version] designation after their name.

To create a new version of an isolate record, query or browse for the isolate:

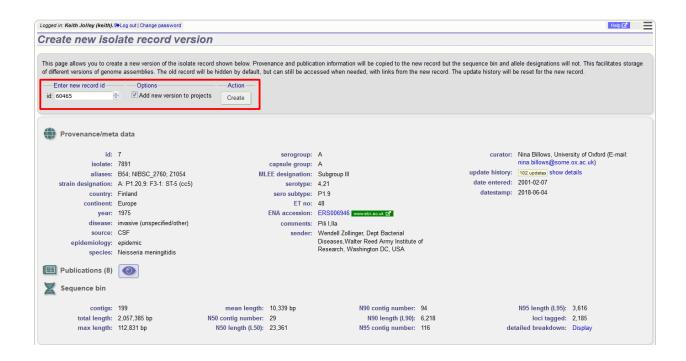


Click the 'create' new version link next to the isolate record:

ed in: Keith Joll	l ey (keith). 🕒 Log o	out Change passv	ord										н	elp 🛃	Toggle: 🕚
late qu	iery/upda	ate													
r search crite	eria or leave blank	k to browse all r	ecords. Modify	form parameters to filter or	enter a list of valu	es.									
leolate prover	nance/phenotype	fielde		· · · · · · · · · · · · · · · · · · ·	Display/sort option					Action					
d					Order by: id	15									
3	▼ =	• E	nter value	+ 0		_			ing 🝷 🛛 F	Reset Submit					
					Display: 25	- reco	ords per page 🕄								
1 records retu	turned (1 - 25 disp	played). Click th	e hyperlinks fo	or detailed information.											
elete	- Tag scanni	iing Proje	te		- Private rec	ords -									
	, č	· · ·				0100									
elete ALL	Scan	Select	project	 Link 	Publish										
			Last												
e: <mark>1 2 3</mark>	456	789>	Last												
					,,		Inclusio Califa					ALL CT	Floret		•
				alianan		uoos	Isolate fields ()	encelos			a ST	MLST		/ping ant	
ete Update	Sequence bin	New version	d isolate	aliases B1: NIRSC 2803: 71001		year	disease	species Neisseria manianitidis		enogroup capsule grou		clonal complex	PorA VR1	PorA VR	2 FetA \
ete Update		New version i		B1; NIBSC_2803; Z1001	USA	1937 i	disease invasive (unspecified/other)	Neisseria meningitidis	A	enogroup capsule grou A A	p ST 4	clonal complex ST-4 complex	PorA VR1 5-2 🖋	PorA VR 10 🖋	2 FetA V F1-5
ete Update	Sequence bin	New version + +	d isolate 1 A4/M1027	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	USA Pakistan	1937 i 1967 n	disease invasive (unspecified/other) meningitis and septicaemia	Neisseria meningitidis Neisseria meningitidis	A	A		clonal complex	PorA VR1	PorA VR	2 FetA V F1-5
ete Update	Sequence bin	New version + + +	d isolate 1 A4/M1027 2 120M	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	USA Pakistan UK	1937 i 1967 n 2000 i	disease invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B	A	4	clonal complex ST-4 complex	PorA VR1 5-2 / 5-2 /	PorA VR: 10 🖋 10 🖋	2 FetA \ F1-5 / F5-1 /
ete Update	Sequence bin 1 1 1	New version -	d isolate 1 A4/M1027 2 120M 3 M00242905	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	USA Pakistan UK USA	1937 i 1967 n 2000 i 1937 i	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B	A A B	4 1 1099	clonal complex ST-4 complex ST-1 complex	PorA VR1 5-2 / 5-2 / 19 /	PorA VR: 10 /	2 FetA V F1-5 4 F5-1 4
ete Update	Sequence bin 1 1 2 1 2 1 1	New version -	d isolate 1 A4/M1027 2 120M 3 M00242905 4 M1027	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	USA Pakistan UK USA UK	1937 i 1967 n 2000 i 1937 i 2000 i	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B	A A B A	4 1 1099 4	Clonal complex ST-4 complex ST-1 complex ST-4 complex	PorA VR1 5-2 / 5-2 / 19 / +	PorA VR 10 / 10 / 15 / +	2 FetA F1-5 / F5-1 / +
ete Update	Sequence bin 1 1 1 1 1 1 1 1 1 1 1 1 1	New version	d isolate 1 A4/M1027 2 120M 3 M00242905 4 M1027 5 M00240227	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	USA Pakistan UK USA UK UK	1937 i 1967 n 2000 i 1937 i 2000 i 2000 i	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B	A A B A B	4 1099 4 1100	Clonal complex ST-4 complex ST-1 complex ST-4 complex ST-32 complex	PorA VR1 5-2 / 5-2 / 19 / + 7 /	PorA VR: 10 / 10 / 15 / + 16 /	2 FetA \ F1-5 / F5-1 / + + +
ete Update	Sequence bin 1 1 1 1 1 1 1 1 1 1 1 1 1	New version	d isolate 1 A4/M1027 2 120M 3 M00242905 4 M1027 5 M00240227 6 M00282207	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	USA Pakistan UK USA UK UK Finland	1937 i 1967 n 2000 i 1937 i 2000 i 2000 i 1975 i	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B W	A B A B W	4 1099 4 1100 1101 5	ST-4 complex ST-1 complex ST-4 complex ST-4 complex ST-32 complex ST-22 complex	PorA VR1 5-2 / 5-2 / 19 / + 7 / +	PorA VR: 10 / 10 / 15 / + 16 / +	2 FetA \ F1-5 / F5-1 / + + +
ete Update	Sequence bin 1 1 2 1 2 1 1	New version + + + + + + + + + +	d isolate 1 A4/M1027 2 120M 3 M00242905 4 M1027 5 M00240227 5 M00240227 7 7891	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	USA Pakistan UK USA UK UK Finland UK	1937 i 1967 n 2000 i 1937 i 2000 i 2000 i 1975 i 2000 i	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A	A B A B W A	4 1099 4 1100 1101 5 1102	Clonal complex ST-4 complex ST-1 complex ST-4 complex ST-32 complex ST-22 complex ST-5 complex	PorA VR1 5-2 / 5-2 / 19 / + 7 / 20 /	PorA VR: 10 / 10 / 15 / + 16 / 9 /	2 FetA V F1-5 4 F5-1 4 + + + F3-1 4
ete Update	Sequence bin 1 1 1 1 1 1 1 1 1 1 1 1 1	New version + + + + + + + + + + + + +	d isolate 1 A4/M1027 2 120M 3 M00242905 4 M1027 5 M00242207 6 M00282207 7 7891 8 M00242007	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	USA Pakistan UK USA UK UK Finland UK Czech Republic	1937 i 1967 n 2000 i 1937 i 2000 i 2000 i 1975 i 2000 i 1984 i	disease imasive (unspecified/other) meningitis and septicaemia imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A B	A A B A W A B	4 1099 4 1100 1101 5 1102	Clonal complex ST-4 complex ST-1 complex ST-32 complex ST-32 complex ST-22 complex ST-53 complex ST-18 complex	PorA VR1 5-2 / 5-2 / 19 / + 7 / + 20 / +	PorA VR: 10 / 10 / 15 / + 16 / + 9 / 14 /	2 FetA V F1-5 4 F5-1 4 + + F3-1 4 F3-1 4 +
lete Update K 🧳	Sequence bin 1 1 1 1 1 1 1 1 1 1 1 1 1	New version + + + + + + + + + + + + +	d isolate 1 A4/M1027 2 120M 3 M00242905 4 M1027 5 M00240227 5 M00240227 7 7891 8 M00242007 9 0021/84	B1: NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054	USA Pakistan UK USA UK UK Finland UK Czech Republic Canada	1937 i 1967 n 2000 i 1937 i 2000 i 2000 i 1975 i 2000 i 1984 i 1971 i	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A	A B W A B W	4 1099 4 1100 1101 5 1102	Clonal complex ST-4 complex ST-1 complex ST-32 complex ST-32 complex ST-52 complex ST-518 complex ST-18 complex ST-22 complex	PorA VR1 5-2 / 5-2 / 19 / + 7 / + 20 / + + +	PorA VR 10 / 10 / 15 / + 16 / + 9 / 14 / +	2 FetA V F1-5 a F5-1 a + + F3-1 a F3-1 a + F3-1 a F5-1 a
lete Update × 🧪	Sequence bin 1 1 1 1 1 1 1 1 1 1 1 1 1	New version + + + + + + + + + + + + + + + + + + +	d isolate 1 A4/M1027 2 120M 3 M00242905 4 M1027 5 M00240227 6 M00282207 7 7891 8 M00242007 9 0021/84 0 6748	B1: NIBSC_2803; 21001 B35; NIBSC_2822; 21035 B43; NIBSC_3076; 21043 B54; NIBSC_2760; 21054 B73; NIBSC_2784; 21073	USA Pakistan UK USA UK UK Finland UK Czech Republic Canada Germany	1937 i 1967 n 2000 i 1937 i 2000 i 2000 i 1975 i 2000 i 1975 i 1984 i 1971 i 1964 i	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis	A B B W A B W A A A	A A B A B W A B W A A	4 1099 4 1100 1101 5 1102 114 1 1	Clonal complex ST-4 complex ST-1 complex ST-32 complex ST-32 complex ST-22 complex ST-5 complex ST-18 complex ST-22 complex ST-21 complex	PorA VR1 5-2 / 5-2 / 19 / + 7 / + 20 / + + 18-1 /	PorA VR 10 / 10 / 15 / + 16 / + 9 / 14 / + 3 /	2 FetA V F1-5 a F5-1 a + + F3-1 a F3-1 a + F3-1 a F5-1 a
	Sequence bin ± ± ± ± ± ± ± ± ± ± ± ± ±	New version + + + + + + + + + + + + + + + + + + +	d isolate 1 A4/M1027 2 120M 3 M00242905 4 M1027 5 M00240227 6 M00242007 7 7891 8 M00242007 9 0021/84 1 129E	B1: NIBSC_2803; 21001 B35; NIBSC_2822; 21035 B43; NIBSC_3076; 21043 B54; NIBSC_2760; 21054 B73; NIBSC_2784; 21073	USA Pakistan UK USA UK VK Finland UK Czech Republic Canada Germany Czech Republic	1937 i 1967 n 2000 i 1937 i 2000 i 2000 i 1975 i 2000 i 1975 i 1984 i 1971 i 1964 i	disease imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis	A B B W A B W A A A	A A B A B W A B W A A	4 1099 4 1100 1101 5 1102 114 1 1	Clonal complex ST-4 complex ST-1 complex ST-32 complex ST-32 complex ST-52 complex ST-18 complex ST-18 complex ST-12 complex ST-1 complex ST-1 complex	PorA VR1 5-2 / 19 / + 7 / + 20 / + + 18-1 / 5-2 /	PorA VR 10 / 10 / 15 / + 16 / + 9 / 14 / + 3 / 10 /	2 FetA V F1-5 / F5-1 / + + F3-1 / F3-1 / + F5-1 / F3-6 / F3-6 /
lete Update × 🧪	Sequence bin 1 1 1 1 1 1 1 1 1 1 1 1 1	New version + + + + + + + + + + + + + + + + + + +	d isolate 1 A4/M1027 2 120M 3 M00242905 4 M1027 5 M00240227 6 M00240227 5 M00240227 7 7891 8 M00242007 9 0021/84 0 6748 1 129E 2 0090/89	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073 B92; NIBSC_2828; Z1092	USA Pakistan UK USA UK VK Finland UK Czech Republic Canada Germany Czech Republic Philippines	1937 i 1967 n 2000 i 1937 i 2000 i 2000 i 1975 i 2000 i 1975 i 1984 i 1984 i 1964 i 1989 i	disease imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other) imasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis	A B B W A B W A A B B W	A A B W A B W A A B B	4 1099 4 1100 1101 5 1102 114 1 1 1015	clonal complex ST-4 complex ST-1 complex ST-2 complex ST-22 complex ST-52 complex ST-52 complex ST-12 complex ST-12 complex ST-11 complex ST-11 complex ST-12 complex	PorA VR1 5-2 / 5-2 / 19 / + 7 / + 20 / + + 18-1 / 5-2 / 7 /	PorA VR 10 / 10 / 15 / + 16 / + 9 / 14 / + 3 / 10 / 16 /	2 FetA V F1-5 4 F5-1 4 + + F3-1 4 F3-1 4 + F5-1 4 F5-1 6

The isolate record will be displayed. The suggested id number for the new record will be displayed - you can change this. By default, the new record will also be added to any projects that the old record is a member of. Uncheck the 'Add new version to projects' checkbox to prevent this.

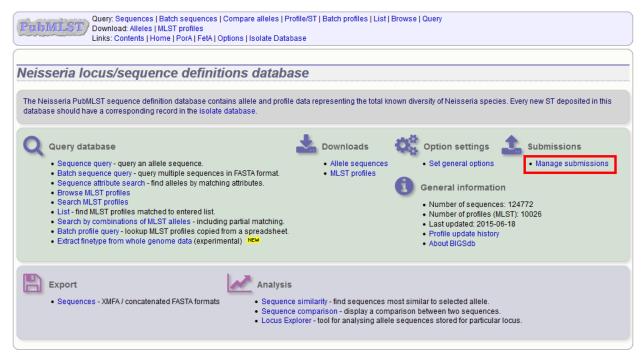
Click the 'Create' button.



CHAPTER 7

Curating data submitted via the automated submission system

Data may be submitted by users using the automated submission system if it has been enabled for a specific database. As a curator, you will be notified of pending submissions when you log in to the curator's interface or if you access the 'Manage submissions' links from the standard contents page. Additionally, if your user account has the 'submission_emails' flag set in the users' table you will also receive E-mail notification of new submissions for which you have sufficient privileges to curate.



Any submissions for which you have sufficient privileges to curate will be shown.

.ogged in: Keith Jolley (keith). 🍽 Lo	g out Change password		
lanage submiss	ions		
Submit new data			
Data submitted here will go in	to a queue for handling by a curator or by an autom	ated script. You will be abl	e to track the status of any submission.
Submission type:			
 alleles 			
 MLST profiles 			
New allele sequence su	bmissions waiting for curation		
Your account is authorized to h	andle the following submissions:		
Submission id	Submitted Updated Submitter	Locus Sequences	
BIGSdb_20150623074942_3	1862_84622 2015-06-23 2015-06-23 Joe Bloggs	NEIS0001 3	
Return to index page			

7.1 Alleles

Click the link to the appropriate submission on the 'Manage submissions' page.

PTDMLST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
Logged in: Keith Jolley (keith). I#Log out Change password Hel	р 🗗
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
alleles MLST profiles	
New allele sequence submissions waiting for curation	
Your account is authorized to handle the following submissions:	
Submission id Submitted Updated Submitter Locus Sequences BIGSdb_20150709132553_20864_89729 2015-07-09 2015-07-09 Joe Bloggs NEIS0001 (lpxC) 3	
Return to index page	

You will see a summary section that describes details about how the sequences were obtained. There should also be link here to download all the sequences in FASTA format.

Download: Alleles MLST profiles Links: Contents Home PorA FetA O	tions Isolate Databa	ISE			Help G
urate submission	729				
Summary type: alleles submitter: Joe Bloggs, University of Oxford, UK datestamp: 2015-07-09 status: pending locus: NEIS0001 (lpxC) sequences: 3 ps technology: Illumina read length: 100-199 coverage: 20-49x assembly: de novo assembly: software: Velvet	Sequences Identifier Length UK322 924 UK323 924 UK347 924 Batch curate Messages Message: Appe	ATGCTGCAAAGAACTTCGGC ACATCAGAAATTGTGGATAA ATGCTGCAAAGAACTTTGGC ACATCAGAACTTGTGGATAA ATGCTGCAAAGAACTTTGGC ACATCAGAAATTGTGGATAA ATGCTGCAAAGAACTTTGGC ACATCAGAAATTGTGGATAA Archive Archive Archive Download	Complete CDS	Status pending pending pending	Curate

There will also be a table summarizing the sequences in the submission and their current submission status.

Query: Sequences Batch sequences Con Download: Alleles MLST profiles Links: Contents Home PorA FetA Option	mpare alleles Profile/ST Batch profiles List Browse Query		
Logged in: Keith Jolley (keith). I Log out Change password			Help 🗗
Curate submission			
Submission: BIGSdb_20150709132553_20864_8972	19 Sequences		
type: alleles submitter: Joe Bloggs, University of Oxford, UK datestamp: 2015-07-09 status: pending locus: NEIS0001 (IpxC) sequences: 3 technology: Illumina read length: 100-199 coverage: 20-49x	Identifier Length Sequence UK322 924 ATECTECAAAGAACTTCGEC ACATCAGAAATTGTGGATAA UK323 924 ATECTECAAAGAACTTTGEC ACATCAGAAATTGTGGATAA UK347 924 ATECTECAAAGAACTTTGEC ACATCAGAAATTGTGGATAA Batch curate	 Status pending • pending • pending •	Assigned allele Curate Curate Update

7.1.1 Individual allele curation

Individual sequences can be curated singly by clicking the 'Curate' links next to the sequence in the table. If you have supporting data attached to the submission, e.g. Sanger trace files then you may need to assess the submission based on the policy of the database.

gged in: Keith Jolley (keith). HLog out Change password						н
urate submission						
ubmission: BIGSdb_20150709132553_20864_897	29					
	Identifier Lengt	h	Sequence	Complete CDS	Status	Assigned allele
type: alleles	UK322 924	ATGCTGCAAAGAACT	CCGC ACATCAGAAATTGTGGATAA	~	pending 👻	Curate 3
submitter: Joe Bloggs, University of Oxford, UK	UK323 924	ATGCTGCAAAGAACT?	TTGGC ACATCAGAACTTGTGGATAA	~	pending 👻	Curate
datestamp: 2015-07-09	UK347 924	ATGCTGCAAAGAACT:	TTGGC ACATCAGAAATTGTGGATAA	~	pending 👻	Curate
status: pending	Batch curate					Update
locus: NEIS0001 (lpxC)	Daton carato					opullo
sequences: 3 FAS	— Messages —		Archive			
technology: Illumina			Archive of submission and any supp	orting files:		
read length: 100-199			Deverland			
coverage: 20-49x			Download TAR			
assembly: de novo	Message: Appe	end Send now				

Clicking this link takes you to the curation interface *single sequence upload page*. The upload form will be filled with details from the submission. You may wish to manually change the status from the dropdown list of values.

PubMLST Use	abase: Species home Curator's page (species) Curator's page (database) ers: Add Query/update i: Add ST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith	h). @Log out Change password Help E	🚹 Toggle: 🚺
Add new allele	e sequence	
Please fill in the fields be	elow - required fields are marked with an exclamation mark (!).	
	NEIS0001 -	
allele id:	210	
sequence:	ATGCTGCAAAGAACTTCGGCGAAATCCATCAGCGTTACCGGAGTCGGCCTGCATTCCGGCGAACGGGTCGC ACCCTGCACCCCGCGCCTGAAAACAGCGGGATTTCCTTCC	LACAA CCGTC = CACCC LAAAG CGCCG +
status:!	unchecked 👻	
sender:!	Bloggs, Joe (jbloggs)	
	Keith Jolley (keith)	
date entered:!		
datestamp:! comments:	2015-07-09	
comments:		
Flags:	atypical contains IS element downstream fusion	

Clicking 'Submit' from this form will define the new allele and add it to the database. A link on the confirmation page will take you back to the submission management page.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). B+Log out Change password	Help 🗗	Toggle: 🚺
Add new allele sequence		
Sequence NEIS0001 (IpxC): 210 added!		
Add another Return to submission Back to main page		

You will find that the status of the newly assigned sequence has changed in the summary table. The assigned value and status are determined on display and should always reflect the live database values.

	h). HLog out Change password						Hel
ırate submi	ssion						
	b_20150709132553_20864_8972						
- Summary		Sequences					
submitter: datestamp:		Identifier Leng UK322 924 UK323 924 UK347 924	4 ATGCTGCAAAGAACT	Sequence ICGGC ACATCAGAAATTGTGGATAA ITGGC ACATCAGAACTTGTGGATAA ITGGC ACATCAGAAATTGTGGATAA	Complete CDS	Status assigned pending v pending v	Assigned allele 210 Curate
	pending NEIS0001 (IpxC) 3 TAS	Batch curate Messages		Archive			Update
technology: read length: coverage:	100-199			Archive of submission and any supp Download TAR	orting files:		
and a second block	de novo	Message: Ap	pend Send now				

7.1.2 Batch allele curation

Often, you will want to batch upload submitted sequences. This can be done by clicking the 'Batch curate' button.

Note: Batch curation is only available for loci that do not have extended attributes defined. Entries for these loci

require additional values set for these additional fields and so need to be handled individually.

PubMLST / Dov	ery: Sequences Batch sequences Co wnload: Alleles MLST profiles ks: Contents Home PorA FetA Optic			List Browse Query			
ogged in: Keith Jolley (keit	h). HLog out Change password						Help 🗹
Curate submi	ssion						
	b_20150709132553_20864_897						
Summary		Sequences					
type:	alleles	Identifier Lengtl UK322 924		Sequence	Complete CDS	Status assigned	Assigned allele 210
submitter:	Joe Bloggs, University of Oxford, UK	UK323 924		TGGC ACATCAGAAATTGTGGATAA	- ×	pending +	Curate
datestamp:	2015-07-09	UK347 924	ATGCTGCAAAGAACTT	TIGGC ACATCAGAAATTGTGGATAA		pending +	Curate
status:	pending	Batch curate				ponding	Update
locus:	NEIS0001 (IpxC)	Batch curate					Opdate
sequences:	3 PAS	Messages —		Archive			
technology:	Illumina			Archive of submission and any supp	orting files:		
read length:	100-199			Download			
coverage:	20-49x			Download TAR			
assembly:	de novo	Message: Appe	end Send now				
assembly software:	Velvet						

This takes you to the batch FASTA upload page in the curators' interface.

The upload form will be filled with details from the submission. You may wish to manually change the status from the dropdown list of values.

PubML	Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith	Jolley (keith). @Log out Change password Help C	Toggle: 🚯
Batch in	sert sequences	
only). Do not i	ows you to upload allele sequence data in FASTA format. The identifiers in the FASTA file will be used unless you select the option to use the next available id (loci with in nclude the locus name in the identifier in the FASTA file. nat you can not use this page to upload sequences for loci with extended attributes. ameters	teger ids
locus:!	NEIS0001 (IpxC) -	
status:!	unchecked •	
sender:!	Bloggs, Joe (jbloggs) 🗸	
☑ Reject : ignored. ☑ Overrid	>UK323 ATGCTGCAAAGAACTTGGCGAATCGATCAGGGTTACCGGAGTCGGGGCTGCATTCGGGGC GAACGGCTGCAACGACCGGCGCGCGCGCGCGCGCGGCACGATCGCTTCCGCCGCT ACCCGATTTGGACGGCGACGAACAAACGGCGCGCGCGCGC	also
Action		
Reset	Check	

Click 'Check' on this form will perform some standard checks before allowing you to upload the sequences.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). @Log out Change password	elp 🗗 🛛 Togg	gle: 🚯
Batch insert sequences		
Sequence check Original designation Allele id UK323 211 UK347 212 OK OK		

A link on the confirmation page will take you back to the submission management page.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loc: Add MLST profiles: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). (+Log out Change password	Help 🖉	Toggle: 🚯
Batch insert sequences		
Upload succeeded. Return to submission Upload more Back to main page		

The status of the sequences should reflect their newly assigned status.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
Logged in: Keith Jolley (keith).	Delog out Change password		Help 🖾								
Curate submise	sion										
Summary	_20150709132553_20864_897	29 Sequences Identifier Length Sequence CDS Status Assigned allele									
type: al		UK322 924 ATGCTGCAAAGAACTTCGGC ACATCAGAAATTGTGGATAA 🖌 assigned 210									
	oe Bloggs, University of Oxford, UK	UK323 924 ATGCTGCAAAGAACTTTGGC ACATCAGAACTTGTGGATAA 🗸 assigned 211									
datestamp: 20		UK347 924 ATGCTGCAAAGAACTTTGGC ACATCAGAAATTGTGGATAA 🖌 assigned 212									
status: pe	-	Messages Archive Action									
	IEIS0001 (IpxC)	Archive of submission and any supporting files: Close submission									
sequences: 3 technology: III read length: 10 coverage: 20 assembly: dr assembly software: Ve	umina 00-199 0-49x e novo	Message: Append Send now									

7.1.3 Rejecting sequences

Sometimes you may need to reject all, or some of, the sequences in a submission. You can do this by changing the value in the status dropdown box next to each sequence. Click 'Update' to make the change.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
Logged in: Keith Jolley (keith). @Log out Change password Help [2											
Curate submission											
Summary type: submitter: datestamp: status: outcome:	db_20150709132553_20864_897 alleles Joe Bloggs, University of Oxford, UK 2015-07-09 pending accepted - data uploaded NEIS0001 (IpxC) 3 [x]	29 Sequences Identifier Lengt UK322 924 UK323 924 UK347 924 Batch curate Messages	ATGCTGCAAAGAACT ATGCTGCAAAGAACT	Sequence TCGGC ACATCAGAAATTGTGGATAA TTGGC ACATCAGAACTTGTGGATAA TTGGC ACATCAGAAATTGTGGATAA - Achive Archive	Complete CDS	Status rejected ← rejected ← rejected ←	Assigned allele Curate Curate Curate Update				
technology: read length: coverage: assembly: assembly software:	100-199 20-49x de novo	Message: App	end Send now	Download TAR							

7.1.4 Requesting additonal information

You can send a message to the submitter by entering it in the Messages box and clicking 'Send now'. This will append a message to the submission and send an update to the submitter so that they can respond.

7.1.5 Closing the submission

You can add a message to the submitter by entering it in the message box and clicking 'Append'. Once sequences have all been either assigned or rejected, the 'Close submission' button will be displayed. Click this to close the submission. The submitter will be notified of their submission status.

PubMLST Do	ery: Sequences Batch sequences Co wnload: Alleles MLST profiles ks: Contents Home PorA FetA Optic				es List Brov	vse Query					
Logged in: Keith Jolley (kei	h). Houg out Change password										Help 🖓
Curate submi	ssion										
Submission: BIGSo	lb_20150709132553_20864_8972	29 — Sequence									
- Summary		Identifier Le			Sequen	20		Complete CDS	Status	Assigned alle	
type:	alleles			ATGCTGCAAAGAACI					rejected		
	Joe Bloggs, University of Oxford, UK	UK323	924	ATGCTGCAAAGAACT	TTTGGC	ACATCAGAACTTGT	GGATAA	4	rejected		
datestamp:		UK347	924	ATGCTGCAAAGAACT	TTTGGC	ACATCAGAAATTGT	GGATAA	~	rejected	•	
	pending									Update	
	NEIS0001 (IpxC)										
sequences:	3 FAS	Messages	s					Arch			
technology:	Illumina		estamp			Message			e of submi	ission and any sup	porting files:
read length:	100-199	2015-07-09	9 12:39	:35+00 Keith Jolley	These sequ	ences are not NEI	IS0001 a	lleles Downl	oad TAR		
coverage:											
assembly:								Acti	on		
assembly software:	Velvet				Mess	age: Append	Send		se submis	sion	

7.2 Profiles

Click the appropriate submission on the 'Manage submissions' page.

Ouery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
Logged in: Keith Jolley (keith). (Hog out Change password	elp 🗗
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
alleles MLST profiles	
New allelic profile submissions waiting for curation	
Your account is authorized to handle the following submissions:	
Submission id Submitted Updated Submitter Scheme Profiles BIGSdb_20150709134405_4219_35535 2015-07-09 2015-07-09 Joe Bloggs MLST 3	
Return to index page	

You will see a table summarizing the profiles in the submission and their current status.

PubMLST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
Logged in: Keith Jolley (keith). (DLog out Change password Help 12											
Curate submission											
Submission: BIGSdb_20150709134405_4219_35538 —Summary type: profiles submitter: Joe Bloggs, University of Oxford, UK datestamp: 2015-07-09 status: pending —Archive Archive of submission and any supporting files: Download	Identifier adk abcZ aroE fumC gdh pdhC pgm UK32 43 2 12 32 32 3 2 1 UK33 7 56 4 3 2 12 12 12	Status Assigned ST pending Curate pending Curate pending Curate Update Message: Append Send now									

7.2.1 Individual profile curation

Individual profiles can be curated singly by clicking the 'Curate' links next to the profile in the table.

Prrfst/LST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database														
Logged in: Keith Jolley (Keith). @Log out Change password Help 2													Help 🗗	
Curate submission														
Submission: BIG Sdb_20150709134405_4219_35535 Summary Type: profiles submitter: Joe Bloggs, University of Oxford, UK datestamp: 2015-07-09 status: pending														
Messages Archive Archive of submissi Message: Append Send now	on and any		orting	files:						Update				

Clicking this link takes you to the curation interface *single profile upload page*. The upload form will be filled with details from the submission.

Prrisivits V Loc: Add Query/update Batch insert										
Logged in: Keith Jolley (kei	th). 🕩 Log out Change passw	ord		Help 🖉	Toggle: 🚺					
Add new MLST profile										
~										
Please fill in the fields t	oelow - required fields are	marked with an exclamati	on mark (!).							
ST: !	10056									
adk: !										
abcZ: !										
aroE: !	12 ≑									
fumC: !	32 🗘									
gdh: !										
pdhC: !										
pgm: !	2									
sender: !	Bloggs, Joe (jbloggs)	•								
clonal_complex:										
curator: ! I	Keith Jolley (keith)									
date_entered: ! 2										
datestamp: ! 2	2015-07-09									
PubMed ids:										
Action										
Reset Subm	it									

Clicking 'Submit' from this form will define the new profile and add it to the database. A link on the confirmation page will take you back to the submission management page.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). II-Log out Change password	Help 🖉	Toggle: 🜖
Add new MLST profile		
ST-10056 added! Return to submission Add another Back to main page		

You will find that the status of the newly assigned profile has changed in the summary table. The assigned value and status are determined on display and should always reflect the live database values.

PrrfsT/TLST Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
Logged in: Keith Jolley (keith). @Log out Change password Help 0											
Curate submission											
Submission: BIGSdb_20150709134405_4219_3553 — Summary type: profiles submitter: Joe Bloggs, University of Oxford, UK datestamp: 2015-07-09 status: pending	5 Profiles Identifier UK32 UK33 UK34 Batch c	adk 43 7 76	abcZ 2 56 3	aroE 12 4 5	fumC 32 3 3	gdh 32 2 87	pdhC 3 12 43	pgm 2 12 34	Status assigned pending v pending v	Assigned ST 10056 Curate Curate Update	
Messages Append Send now	on and any	suppo	orting	files:							

7.2.2 Batch profile curation

Often, you will want to batch upload submitted profiles. This can be done by clicking the 'Batch curate' button.

PTTDMLST Ownload: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database												
Logged in: Keith Jolley (keith). @Log out Change password Help												Help 🖉
Curate submi	ssion											
— Summary type: submitter: datestamp:	Ib_20150709134405_4219_3553 profiles Joe Bloggs, University of Oxford, UK 2015-07-09 pending	5 Profiles Identifier UK32 UK33 UK34 Batch co	adk 43 7 76	abcZ 2 56 3	aroE 12 4 5	fumC 32 3 3	gdh 32 2 87	pdhC 3 12 43	pgm 2 12 34	Status assigne pending pending	Curate	1
	Archive of submissi	ion and any	suppo	orting	iles:							
Message: Append	Send now											

This takes you to the *batch profile upload page* in the curators' interface.

The upload form will be filled with details from the submission.

PubM		sers: Add (ci: Add	ecies home Query/updat :: Add Quer	e		ies) Curator's page (database)	
Logged in: K	eith Jolley (kei	i th). ເ∌ Log ou	t Change pa	ssword				Help 🖉 Toggle: ()
Batch	insert l	MLST	profile	S				
• Fie • Yo it fi	eld header na u can choose or each profile	mes must whether or e record. lelimited he	be included r not to inclu ader for you	and fields (de a ST fiel Ir spreadsh	can be in an d - if it is om		can be omitted if you wish. ST will be used automatical	y. If however, you include it in the header line, then you must also provide
Pleas	e paste in tat	o-delimited	text (include	e a field hea	ider line) —			Parameters
adk 7 76	abc2 56 3	aroE 4 5	fumC 3 3	gdh 2 87	pdhC 12 43	pgm 12 34		Sender: Bloggs, Joe (jbloggs) Value will be overridden if you include a sender field in your pasted data. Ignore duplicate profiles Action Reset Submit
Back								

After upload, a link on the confirmation page leads back to the submission management page.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). @Log out Change password Help (🛂 Toggle: 🚯
Batch insert MLST profiles	
Database updated ok	
Return to submission Back to main page	

The status of the profiles should reflect their newly assigned status.

(PubMLST) Do	ery: Sequences Batch sequences Co wnload: Alleles MLST profiles ks: Contents Home PorA FetA Optic				ST B	atch pi	rofiles	s List	t Bro	wse Query			
Logged in: Keith Jolley (keit	th). @Log out Change password											Help 🗹	
Curate submi	ssion												
— Summary type: submitter: datestamp:	Ib_20150709134405_4219_35533 profiles Joe Bloggs, University of Oxford, UK 2015-07-09 pending	Profiles	adk 43 7 76 ges	abcZ 2 56 3	12 4 5	fumC 32 3 3	32 2 87	3 12 43 Arct Dov	2 12 34 archive nive o wnloa	Status A assigned assigned assigned f submission d tas submission	10056 10057 10058		5:

7.2.3 Rejecting profiles

Sometimes you may need to reject all, or some of, the profiles in the submission. This may be because isolate data had not been made available, against the policy of the database. You can do this by changing the value in the status dropdown box next to each profile. Click 'Update' to make the change.

PubMLST Do	ery: Sequences Batch sequences Co wnload: Alleles MLST profiles ks: Contents Home PorA FetA Opti		1			atch p	rofiles	s List	Bro	wse Quei	ŋ			
Logged in: Keith Jolley (keit	h). I Log out Change password													Help 🗹
Curate submi	ssion													
— Summary — type: submitter: datestamp: status:	Ib_20150709134405_4219_35533 profiles Joe Bloggs, University of Oxford, UK 2015-07-09 pending accepted - data uploaded	5 Profiles Identifier UK32 UK33 UK34 Batch c Message	adk 43 7 76 urate ges	abcZ 2 56 3	12 4 5	fumC 32 3 3 3	32 2 87	3 12 43 — A Arct	2 12 34 rchive	rejected rejected rejected	* * *	Assigned ST Curate Curate Curate Update	ing files:	

7.2.4 Requesting additonal information

You can send a message to the submitter by entering it in the Messages box and clicking 'Send now'. This will append a message to the submission and send an update to the submitter so that they can respond.

7.2.5 Closing the submission

You can add a message to the submitter by entering it in the message box and clicking 'Append'. Once profiles have all been either assigned or rejected, the 'Close submission' button will be displayed. Click this to close the submission. The submitter will be notified of their submission status.

Query: Sequences Batch sequences Co Download: Alleles MLST profiles Links: Contents Home PorA FetA Option				ST B	atch p	orofile	s Lis	t Brov	wse Query			
Logged in: Keith Jolley (keith). HLog out Change password												Help 🖉
Curate submission												
Submission: BIGSdb_20150709134405_4219_35538	5 — Profiles											
type: profiles	Identifier	adk	abcZ	aroE	fumC	gdh	pdhC	pgm	Status	Assigned ST	1	
submitter: Joe Bloggs, University of Oxford, UK	UK32	43	2	12	32	32	3	2	rejected 👻			
datestamp: 2015-07-09	UK33	7	56	4	3	2	12	12	rejected 👻			
status: pending	UK34	76	3	5	3	87	43	34	rejected 👻			
oration ponding										Update		
Messages									Archive			
Timestamp User	M	essad	е						Archive of s	ubmission an	d any supporting files:	
2015-07-09 12:55:23+00 Keith Jolley You need to submit so	me represe	entativ	e isol	ates o	lata fo	rthes	e prot	iles.				
									Download	TAR		
									-Action			
				_		~				_		
		Mes	sage:	Ap	pend	S	end n	ow	Close su	bmission		

7.3 Isolates

Clicking the appropriate submission on the 'Manage submissions' page.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). @Log out Change password	Help 🖉
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
isolates	
Pending submissions	
You have submitted the following submissions that are pending curation:	
Submission id Submitted Updated Type Details BIGSdb_20150709121747_1342_99624 2015-07-09 2015-07-09 isolates 2	
Return to index page	

You will see a table summarizing the submission.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publication: Links: Contents Home Options Profiles/sequences of	ons Database submissions
Logged in: Keith Jolley (keith). (+Log out Change password	Help 🖾
Curate submission	
Submission: BIGSdb 20150709121747 1342 99624	
type: isolates	
submitter: Joe Bloggs, University of Oxford, UK datestamp: 2015-07-09	
status: pending	
Isolates	
isolate country disease source species	erogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2
UK322 UK meningitis and septicaemia blood Neisseria meningiti UK325 UK septicaemia CSF Neisseria meningiti	B 2 3 4 3 8 4 6 F1-5 5 2 B 2 3 4 3 18 4 6 F1-5 5-1 2
Batch curate	Record status: pending - Update
Messages Archive	
Messages Archive Archi	no files:
_	ig mos.
Download Tar	
Message: Append Send now	

Click the 'Batch curate' button.

(PtrbMILST) Breakdown: Isolate	owse Profile/ST List e fields Scheme/alleles Publications Home Options Profiles/sequences defir	nitions Databas	e submissions				
Logged in: Keith Jolley (keith). DLog out Ch	ange password						Help 🖉
Curate submission							
Submission: BIGSdb_20150709 — Summary—	121747_1342_99624						
type: isolates							
submitter: Joe Bloggs, U	niversity of Oxford, UK						
datestamp: 2015-07-09							
status: pending							
Isolates							
isolate country disease	source species	sorogroup abo	7 adk aroE fum	CadhadhCaa	m FotA VR Dor	A_VR1 PorA_VR2	
	ticaemia blood Neisseria meningitidis		3 4 3		F1-5	5 2	
UK325 UK septicaemia	a CSF Neisseria meningitidis	B 2	3 4 3	18 4 6	F1-5	5-1 2	
Batch curate				Recor	d status: pendir	ng 👻 Update	
Messages	- Archive						
	Archive of submission and any suppo	orting files:					
	_	-					
	Download TAR						
Message: Append Send now							

This will take you to the *batch isolate upload page* in the curators' interface.

The upload form will be filled with details from the submission.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). @Log out Change password	Toggle: 🜖
Batch insert isolates	
 This page allows you to upload isolate data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. Enter aliases (alternative names) for your isolates as a semi-colon (;) separated list. Enter references for your isolates as a semi-colon (;) separated list of PubMed ids (non-integer ids will be ignored). You can also upload allele fields along with the other isolate data - simply create a new column with the locus name (see locus names). These will be added with a confirmed status and method set as 'manual'. You can choose whether or not to include an id number field - if it is omitted, the next available id will be used automatic Download tab-delimited header for your spreadsheet - use 'Paste Special O Text to paste the data. Download submission template (xlsx format) Please select the sender from the list below: Bloggs, Joe (jbloggs) Value will be overridden if you include a sender field in your pasted data. 	
Paste in tab-delimited text (include a field header line)	Action
isolate country year disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2 UK233 UK 2015 meningitis and septicaemia CSF Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2 UK322 UK 2014 meningitis blood Neisseria meningitidis B 2 3 17 3 8 4 6 F1-5 5 2-1	Reset Submit
Back	

Click submit to check and then import if there are no errors.

After upload, a link on the confirmation page leads back to the submission management page.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). In Log out Change password	Toggle: 🚯
Batch insert isolates	
Database updated ok Return to submission Back to main page	

Note: Depending on the database policy, definitions of new scheme profiles, e.g. for MLST, may require submission

of representative isolate records. Where this is the case, the curator will need to extract the new profile from the submitted record. The tab-delimited isolate text file can be downloaded from the archive of supporting files linked to the submission and used directly for *batch adding new profiles*. Alternatively, the curator could use the *Export functionality* of the database to generate the file required for batch profile definition after upload of the isolate data.

7.3.1 Requesting additonal information

You can send a message to the submitter by entering it in the Messages box and clicking 'Send now'. This will append a message to the submission and send an update to the submitter so that they can respond.

7.3.2 Closing the submission

You can add a message to the submitter by entering it in the message box and clicking 'Append'. Change the record status to either 'accepted' or 'rejected' depending on whether you have accepted the submission. Click 'Update'.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). In Log out Change password	Help 🖉
Curate submission	
Submission: BIGSdb 20150709121747 1342 99624	
Summary	
type: isolates	
submitter: Joe Bloggs, University of Oxford, UK	
datestamp: 2015-07-09	
status: pending	
- Isolates	
isolate country disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2	
UK322 UK meningitis and septicaemia bloot Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2	
UK325 UK septicaemia CSF Neisseria meningitidis B 2 3 4 3 18 <u>4 6 F1-5 5-1 2</u>	
Batch curate Record status: accepted VDpdate	
Messages Archive	
Archive of submission and any supporting files:	
Download R	
Message: Append Send now	

The 'Close submission' button will now appear. Click this to close the submission. The submitter will be notified of their submission status.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). (&Log out Change password	Help 🖉
Curate submission	
Submission: BIGSdb 20150709121747 1342 99624	
Summary	
type: isolates	
submitter: Joe Bloggs, University of Oxford, UK	
datestamp: 2015-07-09	
status: pending	
- Isolates	
isolate country disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_	
UK322 UK meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2	
UK325 UK septicaemia CSF Neisseria meningitidis B 2 3 4 3 18 4 6 F1-5 5-1 2	2
Record status: accepted 🗸 Upd	Jate
Messages Archive Action	
a Download 🔤	
Message: Append Send now	

CHAPTER 8

Offline curation tools

8.1 Automated offline sequence tagging

Sequence tagging is the process of identifying alleles by scanning the sequence bin linked to an isolate record. Loci need to be defined in an external sequence definition database that contains the sequences for known alleles. The tagging function uses BLAST to identify sequences and will tag the specific sequence region with locus information and an allele designation if a matching allele is identified by reference to an external database.

There is a script called 'autotag.pl' in the BIGSdb package. This can be used to tag genome sequences from the command line.

Before autotag.pl can be run for the first time, a log file needs to be created. This can be created if it doesn't already exist with the following:

```
sudo touch /var/log/bigsdb_scripts.log
sudo chown bigsdb /var/log/bigsdb_scripts.log
```

The autotag.pl script should be installed in /usr/local/bin. It is run as follows:

autotag.pl --database <database configuration>

where <database configuration> is the name used for the argument 'db' when using the BIGSdb application.

If you have multiple processor cores available, use the –threads option to set the number of jobs to run in parallel. Isolates for scanning will be split among the threads.

The script must be run by a user that can both write to the log file and access the databases, e.g. the 'bigsdb' user (see 'Setting up the offline job manager').

A full list of options can be found by typing:

```
autotag.pl --help
NAME
autotag.pl - BIGSdb automated allele tagger
```

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```
SYNOPSIS
   autotag.pl -- database NAME [options]
OPTIONS
-0, --missing
   Marks missing loci as provisional allele 0. Sets default word size to 15.
-d, --database NAME
   Database configuration name.
-e, --exemplar
   Only use alleles with the 'exemplar' flag set in BLAST searches to identify
   locus within genome. Specific allele is then identified using a database
   lookup. This may be quicker than using all alleles for the BLAST search,
   but will be at the expense of sensitivity. If no exemplar alleles are set
   for a locus then all alleles will be used. Sets default word size to 15.
-f --fast
    Perform single BLAST query against all selected loci together. This will
   take longer to return any results but the overall scan should finish
   quicker. This method will also use more memory - this can be used with
    --exemplar to mitigate against this.
-h, --help
   This help page.
-i, --isolates LIST
   Comma-separated list of isolate ids to scan (ignored if -p used).
--isolate_list_file FILE
   File containing list of isolate ids (ignored if -i or -p used).
-I, --exclude_isolates LIST
   Comma-separated list of isolate ids to ignore.
-l, --loci LIST
   Comma-separated list of loci to scan (ignored if -s used).
-L, --exclude_loci LIST
   Comma-separated list of loci to exclude
-m, --min_size SIZE
   Minimum size of seqbin (bp) - limit search to isolates with at least this
   much sequence.
-n, --new_only
   New (previously untagged) isolates only. Combine with --new_max_alleles
   if required.
--new_max_alleles ALLELES
   Set the maximum number of alleles that can be designated or sequences
   tagged before an isolate is not considered new when using the --new_only
   option.
-o, --order
   Order so that isolates last tagged the longest time ago get scanned first
```

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```
(ignored if -r used).
--only_already_tagged
   Only check loci that already have a tag present (but no allele designation).
   This must be combined with the --already_tagged option or no loci will
   match. This option is used to perform a catch-up scan where a curator has
   previously tagged sequence regions prior to alleles being defined, without
   the need to scan all missing loci.
-p, --projects LIST
   Comma-separated list of project isolates to scan.
-P, --exclude_projects LIST
   Comma-separated list of projects whose isolates will be excluded.
-q, --quiet
   Only error messages displayed.
-r, --random
   Shuffle order of isolate ids to scan.
--reuse blast
   Reuse the BLAST database for every isolate (when running -- fast option).
   All loci will be scanned rather than just those missing from an isolate.
   Consequently, this may be slower if isolates have already been scanned,
   and for the first isolate scanned by a thread. On larger schemes, such as
   wgMLST, or when isolates have not been previously scanned, setting up the
   BLAST database can take a significant amount of time, so this may be
   quicker. This option is always selected if --new_only is used.
-R, --locus_regex REGEX
   Regex for locus names.
-s, --schemes LIST
   Comma-separated list of scheme loci to scan.
-t, --time MINS
   Stop after t minutes.
--threads THREADS
   Maximum number of threads to use.
-T, --already_tagged
   Scan even when sequence tagged (no designation).
-v, --view VIEW
    Isolate database view (overrides value set in config.xml).
-w, --word_size SIZE
   BLASTN word size.
-x, --min ID
   Minimum isolate id.
-y, --max ID
   Maximum isolate id.
```

8.2 Defining exemplar alleles

Exemplar alleles are a subset of the total number of alleles defined for a locus that encompass the known diversity within a specified identity threshold. They can be used to speed up *autotagging* as the BLAST queries are performed against exemplars to identify the locus region in the genome followed by a direct database lookup of the sequence found to identify the exact allele found. This is usually combined with the autotagger –fast option.

Once exemplars have been defined you may also wish to set the fast_scan="yes" option in the config.xml file. This enables their use for scanning within the web curators' interface.

There is a script called 'find_exemplars.pl' in the BIGSdb scripts/maintenance directory.

A full list of options can be found by typing:

```
find_exemplars.pl --help
NAME
    find_exemplars.pl - Identify and mark exemplar alleles for use
   by tagging functions
SYNOPSIS
   find_exemplars.pl --database NAME [options]
OPTIONS
--database NAME
   Database configuration name.
--datatype DNA|peptide
   Only define exemplars for specified data type (DNA or peptide)
--exclude_loci LIST
    Comma-separated list of loci to exclude
--help
   This help page.
--loci LIST
   Comma-separated list of loci to scan (ignored {f if} -s used).
--locus_regex REGEX
   Regex for locus names.
--schemes LIST
   Comma-separated list of scheme loci to scan.
--update
   Update exemplar flags in database.
--variation DISSIMILARITY
   Value for percentage identity variation that exemplar alleles
    cover (smaller value will result in more exemplars). Default: 10.
```

8.3 Automated offline allele definition

There is a script called 'scannew.pl' in the BIGSdb scripts/automation directory. This can be used to identify new alleles from the command line. This can (optionally) upload these to a sequence definition database.

Before scannew.pl can be run for the first time, a log file needs to be created. This can be created if it doesn't already exist with the following:

```
sudo touch /var/log/bigsdb_scripts.log
sudo chown bigsdb /var/log/bigsdb_scripts.log
```

The autotag.pl script should be installed in /usr/local/bin. It is run as follows:

```
scannew.pl --database <database configuration>
```

where <database configuration> is the name used for the argument 'db' when using the BIGSdb application.

If you have multiple processor cores available, use the –threads option to set the number of jobs to run in parallel. Loci for scanning will be split among the threads.

The script must be run by a user that can both write to the log file and access the databases, e.g. the 'bigsdb' user (see 'Setting up the offline job manager').

A full list of options can be found by typing:

```
scannew.pl --help
NAME
 scannew.pl - BIGSdb automated allele definer
SYNOPSIS
 scannew.pl --database NAME [options]
OPTIONS
-a, --assign
   Assign new alleles in definitions database.
--allow_frameshift
   Allow sequences to contain a frameshift so that the length is not a
   multiple of 3, or an internal stop codon. To be used with
    --coding_sequences option to allow automated curation of pseudogenes.
   New alleles assigned will be flagged either 'frameshift' or 'internal stop
   codon' if appropriate. Essentially, combining these two options only
   checks that the sequence starts with a start codon and ends with a stop
   codon.
--allow_subsequences
   Allow definition of sub- or super-sequences. By default these will not
   be assigned.
-A, --alignment INT
   Percentage alignment (default: 100).
-B, --identity INT
   Percentage identity (default: 99).
-c, --coding_sequences
   Only return complete coding sequences.
```

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```
-d, --database NAME
   Database configuration name.
-h, --help
   This help page.
-i, --isolates LIST
   Comma-separated list of isolate ids to scan (ignored if -p used).
--isolate_list_file FILE
   File containing list of isolate ids (ignored if -i or -p used).
-I, --exclude_isolates LIST
   Comma-separated list of isolate ids to ignore.
-l, --loci LIST
   Comma-separated list of loci to scan (ignored if -s used).
-L, --exclude_loci LIST
   Comma-separated list of loci to exclude.
-m, --min_size SIZE
   Minimum size of seqbin (bp) - limit search to isolates with at least this
   much sequence.
-n, --new_only
   New (previously untagged) isolates only.
-o, --order
   Order so that isolates last tagged the longest time ago get scanned first
    (ignored if -r used).
-p, --projects LIST
   Comma-separated list of project isolates to scan.
-P, --exclude_projects LIST
   Comma-separated list of projects whose isolates will be excluded.
-r, --random
   Shuffle order of isolate ids to scan.
-R, --locus_regex REGEX
   Regex for locus names.
-s, --schemes LIST
   Comma-separated list of scheme loci to scan.
-t, --time MINS
   Stop after t minutes.
--threads THREADS
   Maximum number of threads to use.
--type_alleles
   Only use alleles with the 'type_allele' flag set to identify locus.
   If a partial match is found then a full database lookup will be performed
```

```
(continues on next page)
```

(continued from previous page)

```
to identify any known alleles. Using this option will constrain the search
space so that allele definitions don't become more variable over time. Note
that you must have at least one allele defined as a type allele for a locus
if you use this option otherwise you will not find any matches!
-T, --already_tagged
Scan even when sequence tagged (no designation).
-v, --view VIEW
Isolate database view (overrides value set in config.xml).
-w, --word_size SIZE
BLASTN word size.
-x, --min ID
Minimum isolate id.
-y, --max ID
Maximum isolate id.
```

8.4 Cleanly interrupting offline curation

Sometimes you may wish to stop running autotagger or allele autodefiner jobs as they can be run for a long time and as CRON jobs. If these are running in single threaded mode, the easiest way is to simply send a kill signal to the process, i.e. identify the process id using 'top', e.g. 23232 and then

```
kill 23232
```

The scripts should respond to this signal within a couple of seconds, clean up all their temporary files and write the history log (where appropriate). Do not use 'kill -9' as this will terminate the processes immediately and not allow them to clean up.

If these scripts are running using multiple threads, then you need to cleanly kill each of these. The simplest way to terminate all autotagger jobs is to type

pkill autotag

The parent process will wait for all forked processes to cleanly terminate and then exit itself.

Similarly, to terminate all allele autodefiner jobs, type

pkill scannew

8.5 Uploading contigs from the command line

There is a script called upload_contigs.pl in the BIGSdb scripts/maintenance directory. This can be used to upload contigs from a local FASTA file for a specified isolate record.

The upload_contigs.pl script should be installed in /usr/local/bin. It is run as follows:

```
upload_contigs.pl --database <NAME> --isolate <ID> --file <FILE>
--curator <ID> --sender <ID>
```

The script must be run by a user who has the appropriate database permissions and the local configuration settings should be modified to match the database user account to be used. The default setting uses the 'apache' user which is used by the BIGSdb web interface.

A full list of options can be found by typing:

```
upload_contigs.pl --help
NAME
    upload_contigs.pl - Upload contigs to BIGSdb isolate database
SYNOPSIS
   upload_contigs.pl --database NAME --isolate ID --file FILE
         --curator ID --sender ID [options]
OPTIONS
-a, --append
   Upload contigs even {\tt if} isolate already has sequences {\tt in} the bin.
-c, --curator ID
   Curator id number.
-d, --database NAME
   Database configuration name.
-f, --file FILE
   Full path and filename of contig file.
-h, --help
   This help page.
-i, --isolate ID
    Isolate id of record to upload to.
-m, --method METHOD
   Method, e.g. 'Illumina', default 'unknown'.
--min_length LENGTH
   Exclude contigs with length less than value.
-s, --sender ID
    Sender id number.
```

CHAPTER 9

Definition downloads

The sequence definition database defines alleles, i.e. links an allele identifier to a sequence. It also defines scheme, e.g. MLST, profiles.

9.1 Allele sequence definitions

Click the 'Allele sequences' link in the 'Downloads' section. Depending on the database, you may see either a hierarchical scheme tree or a table of loci. You can choose to display links either by scheme using the scheme tree, as an alphabetical list or a page of all schemes, by selecting the appropriate link at the top of the page.

9.1.1 Scheme tree



You can drill down through the tree by clicking branch nodes. Clicking the labels of internal nodes will display tables of all schemes belonging to that scheme group. Clicking the labels of terminal nodes will display that single scheme table.

sugal.	and a			<i></i>							Help 🗹
ownie	oad a	allele	e se	quences							
elect loci	by scher	me Alph	nabetic	cal list All loci by scheme	e						
				ails of loci belonging to s band/collapse.	chemes or groups of sche	mes - clicking a gro	up folder will dis	play the loci for	all schemes with	in the group and	d any
	Genomio Metaboli Typing	Informat c islands ism		ocessing							
	🧾 eMLS	yping an species en gene ST (20 lo ST (20 lo eningitid chemes	s cus pa cus wh is cgM	ırtial genes) nole genes) LST v1.0							
LST	Finet, rpIF s Antig eMLS eMLS M eMLS N. m Other sc Loci not	typing an species len gene ST (20 lo 3T (20 lo eningitid chemes in scher	s cus pa cus wh is cgM nes	uttial genes) nole genes) LST v1.0							
LST Locus [Gownload	typing an species en gene ST (20 lo ST (20 lo eningitid chemes in scher d Type	s cus pa cus wh is cgM nes Alleles	utial genes) nole genes) LST v1.0	e/product Curator(s)						
LST .ocus [] bc2 6	Finet rpIF s Antig eMLS eMLS N. me Other sc Loci not	yping an species en gene ST (20 lo ST (20 lo eningitid chemes in scher d Type DNA	s cus pa cus wh is cgM nes Alleles 728	ntial genes) nole genes) LST v1.0 <u>Length</u> Full name Fixed: 433 bp	O. Harrison, K.	lolley 2015-06-22					
LST occus C bcZ 0 adk 0	Finet, rpIF s Antig eMLS eMLS N. me Other sc Loci not	yping an species en gene ST (20 lo ST (20 lo eningitid chemes in scher DNA DNA	s cus pa cus wh is cgM nes Alleles 728 501	rtial genes) tole genes) LST v1.0 Fixed: 433 bp Fixed: 435 bp	O. Harrison, K. O. Harrison, K.	lolley 2015-06-22 lolley 2015-06-08					
LST ocus E bcZ 0 adk 0 roE 0	Finet prplF s Antig eMLS eMLS N. me Other sc Loci not	yping an species en gene ST (20 lo ST (20 lo eningitid chemes in scher DNA DNA DNA	s cus pa cus wh is cgM nes Alleles 728 501 775	Irtial genes) nole genes) LST v1.0 Fixed: 433 bp Fixed: 465 bp Fixed: 455 bp	O. Harrison, K. O. Harrison, K. O. Harrison, K.	Jolley2015-06-22Jolley2015-06-08Jolley2015-06-22					
LST LST LSC LSC LSC LSC LSC LSC LSC LSC LSC LSC	Finet profession	yping an species en gene ST (20 lo ST (20 lo eningitid themes in scher DNA DNA DNA DNA	s cus pa cus wh is cgM nes 728 501 775 732	Itial genes) hole genes) LST v1.0 Fixed: 433 bp Fixed: 435 bp Fixed: 465 bp Fixed: 465 bp	O. Harrison, K. O. Harrison, K. O. Harrison, K. O. Harrison, K.	Jolley 2015-06-22 Jolley 2015-06-08 Jolley 2015-06-22 Jolley 2015-06-02					
LST	Finet prplF s Antig eMLS eMLS N. me Other sc Loci not	yping an species len gene ST (20 lo ST (20 lo eningitid themes in scher DNA DNA DNA DNA DNA	s cus pa cus wh is cgM nes 728 501 775 732 732	Irtial genes) nole genes) LST v1.0 Fixed: 433 bp Fixed: 465 bp Fixed: 455 bp	O. Harrison, K. O. Harrison, K. O. Harrison, K. O. Harrison, K. O. Harrison, K.	Jolley2015-06-22Jolley2015-06-08Jolley2015-06-22					

Click the download link for the required locus

Locus	Download	Туре	Alleles	Length	Full name/product	Curator(s)	Last updated
abcZ 🚺	*	DNA	728	Fixed: 433 bp		O. Harrison, K. Jolley	2015-06-22
adk 🕦	<u>له</u>	DNA	501	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-08
aroE 🕕	<u>ئە</u>	DNA	775	Fixed: 490 bp		O. Harrison, K. Jolley	2015-06-22
fumC 🚺	*	DNA	732	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-02
gdh 🚺	*	DNA	732	Fixed: 501 bp		O. Harrison, K. Jolley	2015-06-11
pdhC 🚺	*	DNA	747	Fixed: 480 bp		O. Harrison, K. Jolley	2015-06-25
pgm 🕕	*	DNA	749	Fixed: 450 bp		O. Harrison, K. Jolley	2015-06-22

Alleles will be downloaded in FASTA format, e.g.

>fumC_1

(continues on next page)

	(continued from previous page)
ACCATCGGTATGGCGGGCGCGCCGGGGCAATTTCGAGCTGAACGTCTATATGCCCGTCATC	
GCCTACAACCTCTTGCAATCCATCCGCCTGTTGGGCGACGCGTGCAACAGCTTCAACGAA	
CACTGCGCCGTCGGCATTGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC	
CTGATGCTCGTTACCGCGTTAAACCGCAAAATCGGTTACGAAAAC	
>fumC_2	
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG	
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGG	
TTGGGCGAAATCAAAATCCCCCGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC	
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT	
ACCATCGGCATGGCGGGCGCGCGGGGCAATTTCGAGCTGAACGTCTATATGCCCGTTATC	
GCCTACAACCTCTTGCAATCCATCCGCCTCTTGGGCGACGCGTGCAACAGCTTCAACGAA	
CACTGCGCCATCGGCATCGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC	
CTGATGCTCGTTACCGCGTTAAACCGCAAAATCGGTTACGAAAAC	
>fumC_3	
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG	
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGG	
TTGGGCGAAATCAAAATCCCCGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC	
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT	
ACCATCGGCATGGCGGGCGCGCGGGGCAATTTCGAGCTGAACGTCTATATGCCCGTTATC	
GCCTACAACCTCTTGCAATCCATCCGCCTGTTGGGCGACGCGTGCAACAGCTTCAACGAA	
CACTGCGCCGTCGGCATCGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC	
CTGATGCTGGTTACTGCGTTAAAACCGTAAAATCGGCTACGAAAAC	

9.1.2 Alphabetical list

Loci can be displayed in an alphabetical list. Loci will be grouped in to tables by initial letter. If common names are set for loci, they will be listed by both primary and common names.

							Help
ownload al	lele se	eque	ence	25			
Select loci by scheme	Alphabet	ical list	All loo	i by scheme			
			· .				
1							
Locus	Download	Туре	Alleles	Length	Full name/product	Curator(s)	Last updated
ArsR [NEIS1769] 🕕	*	DNA	70	Variable: No limits set	ArsR family transcriptional regulator		2015-03-18
AsnC [NEIS1566] 🕕	±	DNA	160	Variable: No limits set	transcription regulator AsnC		2015-05-20
abcZ 🕕	±	DNA	728	Fixed: 433 bp		O. Harrison, K. Jolley	2015-06-22
abcZ [NEIS1015] 🕕	٤.	DNA	493	Variable: No limits set	ABC transporter ATP-binding protein		2015-05-19
aceF [NEIS1279] 🕕	٠.	DNA	477	Variable: (1563 min; 1641 max)	dihydrolipoamide acetyltransferase (EC 2.3.1.12)		2015-05-19
ackA2 [NEIS1727] 🕕	<u>*</u>	DNA	408	Variable: No limits set	acetate kinase		2015-05-20
acnA [NEIS1729] ()	±	DNA	527	Variable: No limits set	aconitate hydratase 1 (EC 4.2.1.3)		2015-05-20
acnB [NEIS1492] ()	<u>*</u>	DNA	476	Variable: No limits set	aconitate hydratase 2 (EC 4.2.1.3)		2015-05-19
adhA [NEIS0486] ()	±	DNA	614	Variable: No limits set	alcohol dehydrogenase		2015-05-17
adhC [NEIS1241] ()	±	DNA	239	Variable: No limits set	alcohol dehydrogenase		2015-05-20
adk 🕕	±	DNA	501	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-08
adk [NEIS0767] ()	<u>*</u>	DNA	208	Variable: No limits set	adenylate kinase		2015-05-18
aldA [NEIS1942] ()	±	DNA	447	Variable: No limits set	aldehyde dehydrogenase		2015-05-20
aniA [NEIS1549] 🕕		DNA	0	Variable: No limits set	nitrite reductase, major outer membrane copper-containing protein		
anmK [NEIS1788] ()	*	DNA	480	Variable: No limits set	anhydro-N-acetylmuramic acid kinase	A. Jamet	2015-05-20
apaH [NEIS0610] 🕦	±	DNA	116	Variable: No limits set	diadenosine tetraphosphatase		2015-05-17
argH [NEIS0580] 🕕	±	DNA	433	Variable: No limits set	argininosuccinate lyase		2015-05-18
aroE ()	±	DNA	775	Fixed: 490 bp		O. Harrison, K. Jolley	2015-06-22
aroE [NEIS1810] 🕕	*	DNA	305	Variable: No limits set	shikimate dehydrogenase		2015-05-21
aspA 🕕	±	DNA	189	Fixed: 432 bp		K. Jolley	2015-04-21
aspA [NEIS1185] ()	*	DNA	501	Variable: No limits set	aspartate ammonia-lyase		2015-05-20
atIA [NEIS2274] ()	*	DNA	18	Variable: No limits set	atlA / peptidoglycan transglycosylase	O. Harrison	2014-12-10
autA [NEIS1859] ()	±	DNA	242	Variable: No limits set	autotransporter A		2015-05-20

Click the download links for the required locus.

9.1.3 All loci by scheme

Loci can also be displayed by scheme with all schemes displayed.

												Help 🗹
ownload	allold	0.000	mon	000								
willoau	allele	: sey	luell	Les								
elect loci by sch	ame (Alph	abetical	.i list Ali	loci by scheme								
LST												
ocus Downlo	ad Type		Leng	th Full name	Inroduct	Curator(s)	Last up	dated				
bcZ 🚺 🎿	DNA		Fixed: 43			. Harrison, K. Jolle						
dko 🕹			Fixed: 46			. Harrison, K. Jolle						
roE 🚺 🕹	DNA		Fixed: 49	•		Harrison, K. Jolle						
mC 🚯 🛓	DNA	732 F	Fixed: 46	35 bp	0	Harrison, K. Jolle	y 2015-0	06-02				
dh 🚯 👎 📩	DNA	732 F	Fixed: 50	01 bp	0	Harrison, K. Jolle	y 2015-0	06-11				
dhC 🚯 🛛 📥	DNA	747 F	Fixed: 48	30 bp	0	. Harrison, K. Jolle	y 2015-0	06-25				
gm 🚯 📩	DNA	749 F	Fixed: 45	50 bp	0	. Harrison, K. Jolle	y 2015-0	06-22				
Locus Dov		ype Al	lleles	Length	Full	name/product C	urator(s)	Last updated				
						ariable region 1		2015-06-16				
						ariable region 2		2015-06-16				
etA VR 🕕	📩 pe	ptide !	581 Va	ariable: No limit	s set	I.	. Feavers	2015-06-26				
IF species												
ir species												
ocus Downloa	l Type Al	leles	Length	n Ful	l name/prod	luct Curat	or(s) Las	t updated				
olF 🚯 🛛 📩	DNA 1	123 Fi	ixed: 413	3 bp 50S riboso	mal protein	L6 (partial) E. Wa	tkins 201	15-01-30				
D Is a sector of a	plosynti	lesis										
P-heptose	Dow	nload Ty	ype Alle	eles Ler	ath		Full nam	e/product	Aliases	Curator(s)	Last updated	
P-heptose				44 Variable: N		D-beta-D		7-phosphate kinase	NMB0825; NMC0769; rfaE		2015-05-18	
Locus		🛓 D									0045 05 47	
Locus NEIS0769 (hIdA) 🔂 🕹		DNA 31		o limits set	ADP-D-	·beta-D he	eptose epimerase	NMB0828; NMC0773	C. Kahler	2015-05-17	
Locus NEIS0769 (hldA NEIS0773 (hldD) 🔂 🕹	Ł D		11 Variable: N				eptose epimerase / bisphosphate phosphatase	NMB0828; NMC0773 NMB2033; NMC2014	C. Kahler C. Kahler		
DP-heptose Locus NEIS0769 (hidA NEIS0773 (hidD JEIS2014 (gmhE NEIS2055 (hidC) ()) () 3) ()	b D	DNA 31	11 Variable: N 16 Variable: N		D-alpha,beta,D-He	eptose 1,7			C. Kahler		

Click the green download links for the required locus.

9.1.4 Download locus table

The locus table can be downloaded in tab-delimited text or Excel formats by clicking the links following table display.

	Genomi Metaboli Typing MLS ^T Finet Finet Control Antig Control MLS Control MLS Control N. m Other sc	c islands ism typing an species ien gene ST (20 lo ST (20 lo eningitid	tigens s cus pa cus wi is cgM	artial genes) hole genes) ILST v1.0						
MLST	ownloa	d Type	Allolos	Length	Full name/product Curator(s)	Last updated				
abcZ (1)	<u>.</u>	DNA	728	Fixed: 433 bp	O. Harrison, K. Jolley					
adk 🕕	±	DNA	501	Fixed: 465 bp	O. Harrison, K. Jolley					
aroE 🕕	±	DNA	775	Fixed: 490 bp	O. Harrison, K. Jolley					
fumC 🕕	*	DNA	732	Fixed: 465 bp	O. Harrison, K. Jolley	2015-06-02				
gdh 🕕	*	DNA	732	Fixed: 501 bp	O. Harrison, K. Jolley	2015-06-11				
pdhC 🕕	*	DNA	747	Fixed: 480 bp	O. Harrison, K. Jolley	2015-06-25				
pgm 🕦	*	DNA	749	Fixed: 450 bp	O. Harrison, K. Jolley	2015-06-22				
Download	table ta	b-delimi	ted tex	t Excel format]					

9.2 Scheme profile definitions

Scheme profiles, e.g. those for MLST, can be downloaded by clicking the appropriate link on the contents page.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Download: Alleles MLST profiles Links: Contents Home Options PubMLST.org Isolate Database	e Query
Campylobacter locus/sequence definitions database	
The Campylobacter PubMLST sequence definition database contains allele and profile data representing the total kno database should have a corresponding record in the isolate database.	wn diversity of C. jejuni and C. coli. Every new ST deposited in this
Query database Sequence query - query an allele sequence. Batch profile query - query multiple sequences in FASTA format. Search by combinations of MLST profiles copied from a spreadsheet. 	Option settings Submissions • Set general options • Manage submissions General information • Number of sequences: 412175 • Number of profiles (MLST): 7841 • Last updated: 2015-06-17 • Profile update history • About BIGSdb
Export Sequences - XMFA / concatenated FASTA formats Analysis Sequence similarity - find sequences most sin Sequence comparison - display a comparison Locus Explorer - tool for analysing allele sequence 	n between two sequences.

If multiple schemes are available, you will need to select the scheme in the dropdown box and click 'Download profiles'

Profit/UST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Toggle: ()
Neisseria locus/sequence definitions database
The Neisseria PubMLST sequence definition database contains allele and profile data representing the total known diversity of Neisseria species. Every new ST deposited in this database should have a corresponding record in the isolate database.
 Query database Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Batch sequence atribute search - find alleles by matching attributes. Browse profiles Search profiles Search profile matched to entered list. Search profile query - lookup profiles copied from a spreadsheat. Extract finetype from whole genome data
 Export Sequences - XMFA / concatenated FASTA formats Analysis Sequence similarity - find sequences most similar to selected allele. Sequence comparison - display a comparison between two sequences. Locus Explorer - tool for analysing allele sequences stored for particular locus.

Profiles will be downloaded in tab-delimited format, e.g.

ST	abcZ	adk	aroE	fumC	gdh	pdhC	pgm	clonal_complex
1	1	3	1	1	1	1	3	ST-1 complex/subgroup I/
⇔II								
2	1	3	4	7	1	1	3	ST-1 complex/subgroup I/
∽II								
3	1	3	1	1	1	23	13	ST-1 complex/subgroup I/
⇔II			_				_	
4	1	3	3	1	4	2	3	ST-4 complex/subgroup IV
5	1	1	2	1	3	2	3	ST-5 complex/subgroup_
⇔III	-							
6	1	1	2	1	3	2	11	ST-5 complex/subgroup_
∽III	-							
7	1	1	2	1	3	2	19	ST-5 complex/subgroup_
∽III	-							
8	2	3	7	2	8	5	2	ST-8 complex/Cluster A4
9	2	3	8	10	8	5	2	ST-8 complex/Cluster A4
10	2	3	4	2	8	15	2	ST-8 complex/Cluster A4
11	2	3	4	3	8	4	6	ST-11 complex/ET-37
⇔con	nplex							
12	4	3	2	16	8	11	20	
13	4	10	15	7	8	11	1	ST-269 complex
14	4	1	15	7	8	11	1	ST-269 complex

CHAPTER 10

Data records

Record pages for different types of data can be accessed following a query by clicking appropriate hyperlinks.

10.1 Isolate records

An Isolate record page displays everything known about an isolate.

Full information	n on isol	ate M10 240474						
-								
This isolate is a member of the following projects:								
			ngococcus Genome Library					
The MRF Meningococcus Genome Library is a collaboration between Public Health England, The Wellcome Trust Sanger Institute and the University of Oxford, funded by the Meningitis Research Foundation.								
Use of the MRF Genome Lib	Use of the MRF Genome Library data must be cited in any publication or presentation making use of it.							
					Research Foundation			
			899_MRF					
MRF-MGL isolates epi years	s 2010/2011 to 20	011/2012 excluding Northern Ireland						
		E&W	_genogroup_B_MRF					
All MRF Meningococcus Ge	enome Library ge	nogroup B isolates from England and Wa	les in 2010/11 and 2011/12					
	_		MRF_no_NI					
All MRF genomes excluding	Northern Ireland	1						
Provenance/meta data	I.							
id: 1896				Neisseria meningitidis				
isolate: M10 strain designation: B: P		-9: ST-269 (cc269)	serogroup: ENA accession:	B ERR086224 → www.ebi.ac.uk				
country: UK	1.10-1,10-11.10	-3. 51-203 (00203)		Dorothea Hill				
continent: Euro	ope		curator:	Dorothea Hill, University of Oxford, UK	(E-mail:			
region: Sou			un data biatanu	dorothea.hill@zoo.ox.ac.uk)				
year: 2010 epidemiological year: 07/2			date entered:	103 updates show details				
	sive (unspecifie	d/other)	datestamp:					
Sequence bin								
contigs: 275		NOO	6405					
total length: 219								
max length: 1098			1611					
mean length: 7982		detailed breakdown:	Display					
N50: 3430	08							
Schemes and loci								
		Novigate and a cleat a share a with 's tage	to diaplay allolo designations					
All loci		Navigate and select schemes within tree	to display allele designations					
Genetic Informatio	on Processing							
⊳ 📗 Metabolism								
i Chen								
Pilin								
 Image: Image of the sector of t								

Each record will have some or all of the following sections:

10.1.1 Projects

Projects This isolate is a member of the following projects:	
MRF Meningococcus Genome Library	
The MRF Meningococcus Genome Library is a collaboration between Public Health England, The Wellcome Trust Sanger Institute and the University of Oxford, funded by the Meningitis Research Foundation. Use of the MRF Genome Library data must be cited in any publication or presentation making use of it.	Meningitis 2 Research Foundation

This displays a list of projects that the isolate is a member of. Only projects that have a full description will be displayed.

10.1.2 Provenance metadata

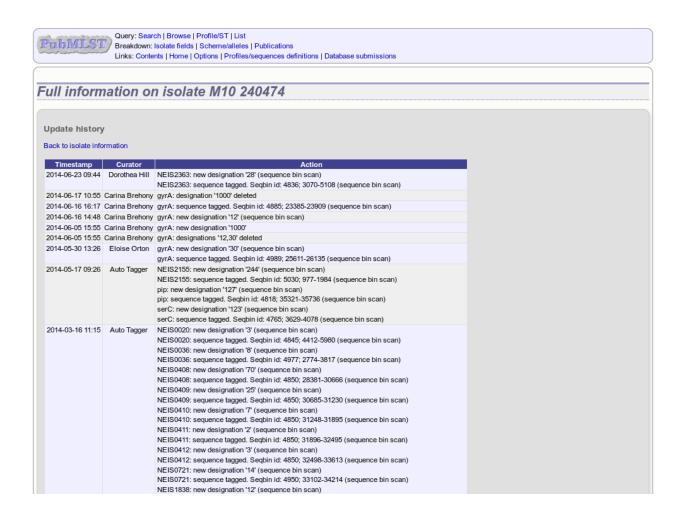
```
id: 18968
                                                                                               species: Neisseria meningitidis
            isolate: M10 240474
                                                                                             serogroup: B
                                                                                        ENA accession: ERR086224 → www.ebi.ac.uk
  strain designation: B: P1.19-1,15-11: F3-9: ST-269 (cc269)
           country: UK
                                                                                               sender: Dorothea Hill
          continent: Europe
                                                                                               curator: Dorothea Hill, University of Oxford, UK (E-mail:
                                                                                                       dorothea.hill@zoo.ox.ac.uk)
            region: South East
             year: 2010
                                                                                         update history: 103 updates show details
epidemiological year: 07/2010-06/2011
                                                                                          date entered: 2012-02-15
                                                                                            datestamp: 2014-06-23
           disease: invasive (unspecified/other)
```

This section includes:

Provenance/meta data

- provenance fields
- · housekeeping data
 - who sent the isolate
 - who last curated
 - record creation times
 - last update times
 - links to update history

The update link displays page with exact times of who and when updated the record.



10.1.3 Publications

Publications (8) show/hide

- Bennett JS, Jolley KA, Sparling PF, Saunders NJ, Hart CA, Feavers IM, Maiden MC (2007). Species status of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from multilocus sequence typing. BMC Biol 5:35 576 isolates
- Didelot X, Urwin R, Maiden MC, Falush D (2009). Genealogical typing of Neisseria meningitidis. Microbiology 155:3176-86 [93 isolates]
- Jolley KA, Sun L, Moxon ER, Maiden MC (2004). Dam inactivation in Neisseria meningitidis: prevalence among diverse hyperinvasive lineages. BMC Microbiol 4:34 [34 isolates]
- Jolley KA, Wilson DJ, Kriz P, McVean G, Maiden MC (2005). The influence of mutation, recombination, population history, and selection on patterns of genetic diversity in Neisseria meningitidis. Mol Biol Evol 22:562-9 [378 isolates]
- Maiden MC, Bygraves JA, Feil E, Morelli G, Russell JE, Urwin R, Zhang Q, Zhou J, Zurth K, Caugant DA, Feavers IM, Achtman M, Spratt BG (1998). Multilocus sequence typing: a portable approach to the identification of clones within populations of pathogenic microorganisms. Proc Natl Acad Sci U S A 95:3140-5 107 isolates
- Thompson EA, Feavers IM, Maiden MC (2003). Antigenic diversity of meningococcal enterobactin receptor FetA, a vaccine component. Microbiology 149:1849-58 [107 isolates]
- Urwin R, Russell JE, Thompson EA, Holmes EC, Feavers IM, Maiden MC (2004). Distribution of surface protein variants among hyperinvasive meningococci: implications for vaccine design. Infect Immun 72:5955-62 [78 isolates]
- Wang JF, Caugant DA, Li X, Hu X, Poolman JT, Crowe BA, Achtman M (1992). Clonal and antigenic analysis of serogroup A Neisseria meningitidis with particular reference to epidemiological features of epidemic meningitis in the People's Republic of China. Infect Immun 60:5267-82 [47] isolates]

This section includes full citation for papers linked to the isolate record. Each citation has a button that will return a dataset of all isolates linked to the paper.

If there are five or more references they will be hidden by default to avoid cluttering the page too much. Click the 'Show/hide' button to display them in this case.

10.1.4 Sequence bin summary

Sequence bin			
contigs:	275	N90:	6405
total length:	2195045 bp	N95:	3513
max length:	109859 bp	loci tagged:	1611
mean length:	7982 bp	detailed breakdown:	Display
N50:	34308		

This section contains basic statistics describing the sequence bin. Clicking the 'Display' button navigates to the *sequence bin record*.

10.1.5 Scheme and locus data

A hierarchical tree displays available schemes. Click within internal nodes to expand them.

Schemes and loci	
ä. 🛄 All loci	Navigate and select schemes within tree to display allele designations
🗁 🌆 Capsule	
- 📗 Genetic Information Processing	
🗁 🌆 Metabolism	
🗁 🌆 Pilin	
🗁 🌆 Typing	
Other schemes	
🕼 Loci not in schemes	

Clicking any terminal node will display data available for a scheme or group of schemes.

Schemes and loci									
Genetic Information Processing					М	LST			
Pilin Typing MLST 	abcZ 4 S	adk 10 S	aroE 15 S	fumC 9S	gdh 8 S	pdhC 11 S	9S	ST 269	clonal complex ST-269 complex

Click an allele number within the scheme profile, will display the appropriate *allele definition record*. Clicking the green 'S' link will display the appropriate *sequence tag record*.

10.2 Allele definition records

An allele definition record displays information about a defined allele in a sequence definition database.



If the allele is a member of a scheme profile, e.g. MLST, this will be listed. In this case, there will be a button to display all profiles of that scheme that contain the allele.

Similarly, if a *client database* has been setup for the database and the allele has been identified in an isolate, there will be a button to display all isolates that have that allele.

10.3 Sequence tag records

EIS0346 alle	ele sequen	ice: id-1	8968										
ontig position													
sequence bin id:	4956				length:	744							
contig length:	22993			огі	ientation:	forward							
start:	13864			с	omplete:	yes							
end:	14607				method:	Illumina							
equence													
ACTGTACGC GGCGCAC	GGC TTCAGCATTG	CGGGCAGGCG	GAAAAACTAT	TACCGTACAG	CCGACGGI	TAA AACCGAAGA	GCCGTCTTAA	TGGAGAAAAT	ATGTTAAGCG	CGCGCTACCT	CCACCTGCAC	GAAGCCTTGG 0	GTTTGGGCCC
ATGTGGTTG AAGCGGGG	GAG CCGTCGTCCT	GCCGTCCGCA	ACATTGCCGG	AAAGCCCGAC	ACAAATCO		AAACCGTCCT	CAGCATTCCG	CAGCGTCCGT	CCGAACAGCA	TACCGGTCAG	GCACGGCTCA #	
STGTTGGAA ACAACCG						000 0000144410							
		CAAACCCGCG	CCTGAAACCG		GICCGGC	GTT TCAGACGGC	A TCGCCCCCGT						
ATGGTTTAC GGGCAAC	TGT TCCACGGAAA	CAAACCCGCG AGCGGGTGTC	CCTGAAACCG CTGCTCGACA	ATATACTCAA	GTCCGGCC	GTT TCAGACGGC. GGG CTCGATGCC	A TCGCCCCCGT G CCTATGTCCA	CAAAACCTGT	TGGGTGAAAA	CCGCCGCCGT	CGGCAACCCG	ATGCCGTCTG #	AAGCGGCAAT
GCAAATGCG CTGGAAC	CTGT TCCACGGAAA	CAAACCCGCG AGCGGGTGTC ACTCGACGGC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC	ATATACTCAA CCGCCGTCCT	GTCCGGCC AGCCGTAC GTTCCTCC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA	CAAAACCTGT ACGGCAGGCG	TGGGTGAAAA ATGATTGAAA	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
	CTGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC	ATATACTCAA CCGCCGTCCT	GTCCGGCC AGCCGTAC GTTCCTCC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA	CAAAACCTGT ACGGCAGGCG	TGGGTGAAAA ATGATTGAAA	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAAATGCG CTGGAAC SCCCGGCTG TTGCGCC CAAAATGAC CGATTTC	CTGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC	ATATACTCAA CCGCCGTCCT	GTCCGGCC AGCCGTAC GTTCCTCC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA	CAAAACCTGT ACGGCAGGCG	TGGGTGAAAA ATGATTGAAA	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAAATGCG CTGGAACA	CTGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC	ATATACTCAA CCGCCGTCCT	GTCCGGCC AGCCGTAC GTTCCTCC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA	CAAAACCTGT ACGGCAGGCG	TGGGTGAAAA ATGATTGAAA	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAAATGCG CTGGAAC SCCCGGCTG TTGCGCC CAAAATGAC CGATTTC	CTGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC	ATATACTCAA CCGCCGTCCT	GTCCGGCC AGCCGTAC GTTCCTCC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA	CAAAACCTGT ACGGCAGGCG	TGGGTGAAAA ATGATTGAAA	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAAATGCG CTGGAAC SCCCGGCTG TTGCGCC CAAAATGAC CGATTTC ranslation	TGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA CCGC CAAGATTTCC	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC TTAAATTCTC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC CCTC	ATATACTCAA CCGCCGTCCT TCAAGCAGCT	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT GTC TTGGCGCAA	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA G GCGGCGGCAG	CAAAACCTGT ACGGCAGGCG TTGAAGCGCG	TGGGTGAAAA ATGATTGAAA CCGCACGGGG	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
ECAAATGCG CTGGAAC SCCCGGCTG TTGCGCC CAAAATGAC CGATTCC ranslation H C T	R R T A S	A L R A	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC CCTC	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC	GTT TCAGACGGC GGG CTCGATGCO GGA CAGGCGTTT GTC TTGGCGCAA	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA G GCGGCGGCAG M P S *	W R K	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAAATGCG CTGGAAC SCCCGGCTG TTGCCCC CAAAATGAC CGATTCC Tanslation H C T T V R	TGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA CCGC CAAGATTTCC	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC TTAAATTCTC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC CCTC	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P	GTCCGGCG AGCCGTAG GTTCCTCC CAAACGTC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT GTC TTGGCGCAA T V K P K R X N R 1	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA G GCGGCGGCAG M P S R C R L	WRK NGEN	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAAATGCG CTGGAAC CCCGGCTG TTGGGCCI CAAATGAC CGATTCC ranslation H C T T V R L Y J 1 CACTGTAC	TGT TCCACGGAAA CCGCCCGCGA CAAC CCGAACTCAA CCGC CAAGATTTCC R R T A S & G A R L (A A H G F CCGCGCCACGCTT(CAAACCCGCG AGCGGGTETC ACTCGACGGC AGCCGCGCC TIAAATICTC A L R J Q H C G S I A G CAGCATIGCGGG	CCTGAAACCG CTGCTCGACA TGCCGCGCGAC TGGCAGACGC CCTC A G G K Q A E K R R K 1 5CAGGCGGAAAJ	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATTACCG	GTCCGGCG AGCCGTAG GTTCCTCC CAAACGTC CAAACGTC Y S R T A D TACAGCCGJ	STT TCAGACGEC GGG CTCGATGCC GGA CAGGCGTTT STC TTGGCGCAA I V K P K R M R I G K T E ACGGTAAAACCGA	A TCGCCCCGT G CTATATGTCA G TCAAACCGGA G CGGCGGGAG M P S R C R L D A V L D A V L	CAAAACCIGI ACGGCAGGGG IIGAAGCGCG W R K N G E N M E K I AAIGGAGAAAA	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 I 100	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAAATGCG CTGGAAC CCCGGCTG TTGGGCCI CAAATGAC CGATTCC ranslation H C T T V R L Y J 1 CACTGTAC	TGT TCCACGGAAA CAAA CCGCCGCGA CAAC CCGAAACTCAA CCGC CAAGATTTCC R R T A S & G A R L (A A H G F	CAAACCCGCG AGCGGGTETC ACTCGACGGC AGCCGCGCC TIAAATICTC A L R J Q H C G S I A G CAGCATIGCGGG	CCTGAAACCG CTGCTCGACA TGCCGCGCGAC TGGCAGACGC CCTC A G G K Q A E K R R K 1 5CAGGCGGAAAJ	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATTACCG	GTCCGGCG AGCCGTAG GTTCCTCC CAAACGTC CAAACGTC Y S R T A D TACAGCCGJ	STT TCAGACGEC GGG CTCGATGCC GGA CAGGCGTTT STC TTGGCGCAA I V K P K R M R I G K T E ACGGTAAAACCGA	A TCGCCCCGT G CTATATGTCA G TCAAACCGGA G CGGCGGGAG M P S R C R L D A V L D A V L	CAAAACCIGI ACGGCAGGGG IIGAAGCGCG W R K N G E N M E K I AAIGGAGAAAA	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 I 100	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAAATGCG CTGGAAC SCCCGGCTG TTGCGCCC SAAATGAC CGATTCC ranslation H C T T V R L Y J 1 CACTGTAC 	TGT TCCACGGAAA CAAA COGCCCCCA AAC CCGAACATCAA CCGC CAAGATTCC R R T A S & G A R L (A A H G F GCGGCGCCACGCCTT 	CAAACCCGCG AGCGGGTGTC AGCCGCGCGCC TIAAATICTC A L R J Q H C G S I A G CAGCATTGCGGG	CCTGAAACCG CTGCTCGACA TGCCCCGCAC TGGCAGACGC CCTC A G G K Q A E K R R K 1 SCAGGCGGAAA 	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATTACCG :!:	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC Y S R T A D TACAGCCGJ	STT TCAGACGEC SGG CTCGATGCC GGA CAGGCGCTT STC TIGGCGCAA I V K P K R N R I G K T E ACGGTAAAACCGA -:!	A TCGCCCCCGT 5 CTATATCCA 5 CCAACCGGA 5 GCGGCGGCAG 6 CCGCCGGCAG 8 C R L D A V L 4 GATGCCGTCTT 	CAAAACCIGI ACGGCAGGGG TIGAAGCGCG N G K N M E K I AAIGGAGAAAA 	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 I 100 I	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAATEGC CTGEAAC SCCCEGECTS TIECCCCC CAAATEGC CEATTCC Tanslation H C T T V R L Y 1 1 CACTETAC 	TGT TCCACGGAAA CCGCCCGCGA CAAC CCGAACTCAA CCGC CAAGATTTCC R R T A S & G A R L (A A H G F CCGCGCCACGCTT(CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCGCGCC TTAAATTCTC A L R J Q H C G S I A G S I A G S I A G P A R S	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGCCGCGCAC CCTC A G G K Q A E K R R K 1 SCAGGCGGAAAA : L G F (ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATTACCG ::: S P D V	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC Y S R T A D TACAGCCG7 V E A	STT TCAGACGEC SGG CTCGATGCC SGC CAGCGCTT STC TIGGCGCAA I V K P K R N R 1 G K T E G S R R	M P S M P S CCBACGGCGGCAG M P S CCBCCGCGCGCAG A V L D A V L D A V L P A V R	CAAAACCTGT ACGGCAGGGG TTGAAGCGCG N G E N M E K I AATGGAGAAAA : N I A G	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 I 100 F1	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAATEGC CTGEAALC SCCGGCTG TIGCCCCC SAAATGC CATTCC ranslation H C T T V R L Y J 1 CACTGTAC 	TIGT ICCACGGAAA CAA COGGCCGCGA AAC COGACACTCAA COGC CAAGAITICC R R T A S R G A R L (A A H G F COGGCGCACGCGGCTT 	CAAACCCGCG AGCGGGTGTC AGTCGACGGC AGCCGCGCGC TTAATTCTC A L R J Q H C G S I A G CAGCATTGCGGC CAGCATTGCGGC CAGCATTGCGGC L H E J	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC CCTC A G G K Q A E K R R K 1 5CAGGCGGAAA L G F (A L G L	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y R AACTATTACCG ::: 3 P D V G P M W	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC Y S R T A D TACAGCCGJ V E A L K H	TI TCAGAGGGC GGG CTCGATGCO GGA CAGGCGTTI GTC TIGGCGCAA R R K R K R R R R R R R R R R R R R R	A TCGCCCCCGT G CTATATCCCA G TCAAACCGA G CGGCGGCAG A V R AGAIGCCGTCTT P A V R L P S A	CAAAACCTGT ACGGCAGGGG TTGAAGCGCG M R K N G E N M E K I AATGGAGAAA 	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 I 100 F1	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAATEGC CTGEAAC SECCEGETG TIECECCC TANSIATECC CEATTCC TANSIATION H C T T V R L Y U 1 CACTGTACC V K H M L S C & A 101 ATGTTAAC	TRET TCCAGGGAAA CAA CCGACCGGA AC CCGAAGTCAA CCGC CAAGATTCC CGC CAAGATTCC CGC CAAGATTCC A A H G F GCGCCGCCACGCCACGCCTC 	CAAACCCECG AGCGGGTGTC ACTCGACGGC AGCCGCGCCC TITAATICTC A L R J Q H C G S I A G C AGCATTGCGGG C CAGCATTGCGGG L H E J I C T K ACCTGCACGGAAC	CCTGALACCE CTGCTCGACA TGGCCGCACA TGGCCGCACA TGGCAGAACGC CCTC A G G K Q A E K R R K 1 CCAGCGGAALA :L G F (A L G L P W V W SCCTTGGGTTT	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATACA G P M W A R C GGCCCGATGT	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC Y S R T A D TACAGCCGJ V E A L K H G * S GGTGAAGC	TI V K P K GG CICGAIGCO GG CACGCGITI SIC TIGGCGCAA C K P K C K R K C K R K C C K R C C R C R C	A TORECCECTET S CCTAIGICCA S TCAAACCGAA S CCACCGACAG A C R L D A V L AGAIGCCGICTI P A V R L P S A S C R P L P S A C R P C R C C C R C C C R C	CANAACCIGT ACGGCAGGGG TIGAAGGGGG N G E N M E K I AATGGAGAAA 	TGGGTGAAAA ATGATGAAA CCCCACGGGG Y F1 F2 F3 T 100 I F1 E F2 F3 G 200	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAATEGC CTGEAAC SECCEGETG TIECECCC TANSIATECC CEATTCC TANSIATION H C T T V R L Y U 1 CACTGTACC V K H M L S C & A 101 ATGTTAAC	THET TECACEGANA TARA COSCOCEGEA TAC COSACACTERA COSC CARGATTERA R R T A S R G A R L (A A H G F GCGGGCCCACEGCTT 	CAAACCCECG AGCGGGTGTC ACTCGACGGC AGCCGCGCCC TITAATICTC A L R J Q H C G S I A G C AGCATTGCGGG C CAGCATTGCGGG L H E J I C T K ACCTGCACGGAAC	CCTGALACCE CTGCTCGACA TGGCCGCACA TGGCCGCACA TGGCAGAACGC CCTC A G G K Q A E K R R K 1 CCAGCGGAALA :L G F (A L G L P W V W SCCTTGGGTTT	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATACA G P M W A R C GGCCCGATGT	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC Y S R T A D TACAGCCGJ V E A L K H G * S GGTGAAGC	TI V K P K GG CICGAIGCO GG CACGCGITI SIC TIGGCGCAA C K P K C K R K C K R K C C K R C C R C R C	A TORECCECTET S CCTAIGICCA S TCAAACCGAA S CCACCGACAG A C R L D A V L AGAIGCCGICTI P A V R L P S A S C R P L P S A C R P C R C C C R C C C R C	CANAACCIGT ACGGCAGGGG TIGAAGGGGG N G E N M E K I AATGGAGAAA 	TGGGTGAAAA ATGATGAAA CCCCACGGGG Y F1 F2 F3 T 100 I F1 E F2 F3 G 200	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAATEGC CTGEAAC CCCCCCCT TECCCCC CAAATEGC CATTCC TANATEGC CATTCC T V R L Y J 1 CACTETAC V K I M L S C A 101 ATETTACC	TIGT ICCACGGAAA CAA COGGACGCAA AC COGACACTCAA COGC CAAGAITICC R A T A S R G A R L (A A H G F CGGGGCGCACGGCTT R A L P P A R A T S : CGGGGGCACCTCCC 	CAACCOGGS AGCGGGTGTC AGCCGGGGC AGCCCGGGCC TTAAATTCTC Q H C G S I A G CAGCATTCCGGC P A R S L H E J T C T K ACCTGCAGGARG	CCTGAAACGC CTGCTCGACA TGCCCGCACA TGCCCGCACA CCTC A G G K Q A E K R R K 1 CCGCCGCAAA CCGCCGAAAA CCGCCGCAAAA CCGCCGCGAAA CCGCCGCGAAA CCGCCGGAAA CCGCCGGAAA CCGCCGGGAAA CCGCCGGGAAA CCGCCGGGAAA CCGCCGGGAAA CCGCCGGGAAA CCGCCGGGAAA CCGCCGGGAAA CCGCCGGGAAA CCGCCGGGAAA CCGCCCCCCCC	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T L L P N Y Y R AACTATTACCG S P D V G P M W 3GGCCCGATGT :	GTCCGGCC AGCCGTA GTCCTCC CAAACGTC Y S R T A D TACAGCCG V E A G S GGTGAAGC 	I V K P K G C A CAGCGTIT STC TIGGCGCAA I V K P K R N R I G K T E CGGTAAAACCGA CGGTAAAACCGA G E P S CGGGGGAGCCGTCG I I I	M P S CCRIGCCCCGT CCRAGCCGA CCRCGCGCGCGCA CCRCGCGCGCGCA ACCRL D A V L MARIGCCGTCT P A V R L P S A C R L P A V R L P S A C R L CCRCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGCG	CAAAACCIGT ACGGCAGGCG ITGAAGCGCG N G E N M E K I AAATGGGAAAA N I A G T L P CAACATIGCCG	TGGGTGAJAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 T 100 I F1 E F2 F3 S 200 I	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAATEGE CTGEAAC CCCGECTG TIECECCC ANATEGE CEATTCC Tanslation H C T T V R L Y J 1 CACTGTAC 	TRET TCCAGGGAAA CAA CCGACCGGA AC CCGAAGTCAA CCGC CAAGATTCC CGC CAAGATTCC CGC CAAGATTCC A A H G F GCGCCGCCACGCCACGCCTC 	CAACCOSCG AGCOGGTGTC AGCCOGGCC THAATTCTC AGCCCGCGCC THAATTCTC A L R J Q H C G S I A G S I A G CACCATTCCCGG -:	CCTGALACCE CTGCTGGCA TGGCCGGACA TGGCCGGACA TGGCAGACGC CCTC A G G K K R R K 1 CCASCGGALA :	I I I V L L P V L L P N Y Y R ARCTATIACG G P M W A R C S A A	GTCCGGCC AGCCGTAC GTTCCTCC AAACGTC Y S R T A D TACAGCCGS V E A G S G S S V R	T V K P K G C C G A C G C G C C G A C G C G C G C	A TOBOCCOCOT S CCTAIGTOCA S CCTAIGTOCA S TCAAACCOBA S CC R L D A V L BARICCOGTCIT P A V R L P S A S C R P COCTECCOTCOC 	CAAAACCIGT ACGGCAGGCG IIGAAGCGCG N G E N M E K I AAIGGAGAAAA 	TGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 T 100 I F1 F1 F1 F1	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC

A sequence tag record displays information about the location within a contig of a region associated with a locus. The nucleotide sequence will be displayed along with upstream and downstream flanking sequence. The length of these flanking sequences can be modified within the *general options*.

If the tag is for a DNA locus and it is marked as a coding sequence, the three-frame translation will also be displayed.

10.4 Profile records

(PubMLST) D	uery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query ownload: Alleles MLST profiles inks: Contents Home PorA FetA Options Isolate Database
Profile inform	nation for ST-11 (MLST)
ST abcZ adk at 11 2 3 3	aroE fumC gdh pdhC pgm clonal complex 4 3 8 4 6 ST-11 complex/ET-37 complex
sender:	Paula Kriz, Paula Kriz and Keith Jolley
curator:	Keith Jolley, University of Oxford, UK (E-mail: keith.jolley@zoo.ox.ac.uk)
date entered:	2001-02-07
datestamp:	2009-11-11
Client database	
PubMLST isolates:	Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample. 2809 isolates

A profile record displays information about a scheme, e.g. MLST, profile. Each allele number within the profile will be hyperlinked. Clicking these will take you to the appropriate *allele definition record*.

If a *client database* has been setup for the database and an isolate has the profile, there will be a button to display all isolates that have the profile.

10.5 Sequence bin records

Profit Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions										
										Toggle
Sequence	e bin for N	110 240474								
Contig summ	ary statistics	Contig size	e distribution	Cumulative con	itig lengt	h				
 Total leng Minimum Maximum Mean leng σ length: N50: 3430 N90: 6403 N95: 3513 Download 	l length: 109859 gth: 7982 16244 08 5 3 d sequences (FAS	Click to enlar	ge load lengths			,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,				
Sequence Seq	uencing method	Original designation	Length Comments	Locus	Start	End	Direction	EMBL format	Artemis i	
4869	Illumina	NODE_90_length_109787_cov_40.983086	109859	NEIS1151	488	1144	←	EMBL	Artemis	
				NEIS1150	1141	2913	←			
				NEIS1149	3155	3733	\rightarrow			
				NEIS1148	3896	4513	\rightarrow			
				NEIS1147	4521	5384	\rightarrow			
				NEIS1146	5397	5831	-			
				NEIS1145	6141	6869	\rightarrow			
				NEIS1144	6892	7923	÷.			
				NEIS1143	8005	8313	÷			
				NEIS1142	9288	10541	÷			
				NEIS1140	10613		÷			
				NEIS1139		12744	\rightarrow			
				NEIS1138		14362	\rightarrow			
				NEIS1137		15046	\rightarrow			
				NEIS1136		15392	é			
				NEIS1135	15585	16832	\rightarrow			
				NEIS1134		17520	\rightarrow			

A sequence bin record contains information about that contigs associated with an isolate record. This includes:

- Number of contigs
- Total length
- Minimum length
- · Maximum length
- N50, N90 and N95 values
- Size distribution charts

There are also links to download the contigs in FASTA or EMBL format.

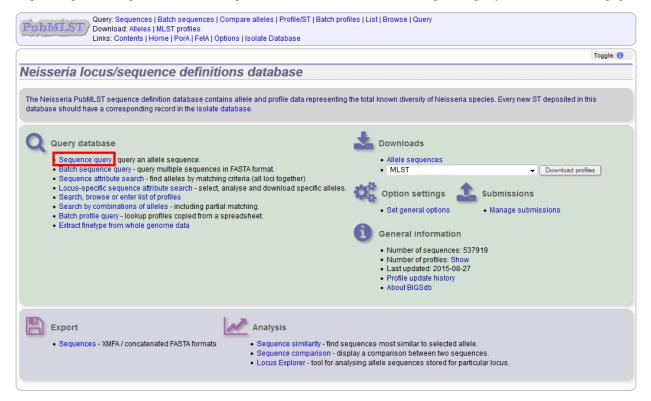
Finally there is a table that shows the loci that are tagged on each contig. Individual contigs can also be downloaded in EMBL format.

CHAPTER 11

Querying data

11.1 Querying sequences to determine allele identity

Sequence queries are performed in the sequence definition database. Click 'Sequence query' from the contents page.



Paste your sequence in to the box - there is no need to trim. Normally, you can leave the locus setting on 'All loci' - the software should identify the correct locus based on your sequence. Sometimes, it may be quicker, however, to

select the specific locus or scheme (e.g. MLST) that a locus belongs to.

Note: If the locus you are querying is a shorter version of another, e.g. an MLST fragment of a gene where the full length gene is also defined, you will need to select the specific locus or the scheme from the dropdown box. Leaving the selection on 'All loci' will return a match to the longer sequence in preference to the shorter one.

Click 'Submit'.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles L Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	ist Browse Query
Sequence query - Neisseria locus/sequence definitions	
Please paste in your sequence to query against the database. Query sequences will be checked first for an partial matches will be identified if an exact match is not found. You can query using either DNA or peptide s	
GACGCGGTGCGCGATGAAAAAGTCAAAGTCATCAAGTCATGAAGCCGCTGAACGCGTCGAA TCTGTCAATGAAAATGTCGTGCGCGGGACAATATACCGCCGCCGAAAGGCATGAACGGCTAT CTTGAAGGAAATCAACTATCGGTTGSCCAACGACATCACGCAGTCAAAAACATTGCCAT TGAGSGCAAAACCATTTGCTTTGGCGGGGGGGGGGGGGGG	Select FASTA file: Reset Submit Browse_ No file selected.

If an exact match is found, this will be indicated along with the start position of the locus within your sequence.

Cuery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database						
Sequence query - Neisseria locus/sequence definitions						
Please paste in your sequence to query against the database. Query sequences will be checked first for an exa partial matches will be identified if an exact match is not found. You can query using either DNA or peptide sequences partial matches will be identified if an exact match is not found. You can query using either DNA or peptide sequences must be added to the sequence of the sequence is the sequence of th						
1 exact match found.						
Translate query Allele Length Start position Flags Comments						
aroE: 8 490 136 625						

If only a partial match is found, the most similar allele is identified along with any nucleotide differences. The varying nucleotide positions are numbered both relative to the pasted in sequence and to the reference sequence. The start position of the locus within your sequence is also indicated.

Cuery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database						
Sequence query - Neisseria locus/sequence definitions						
Please paste in your sequence to query against the database. Query sequences will be checked first for an exact match against the chosen (or all) loci - they do not need to be trimmed. The nearest partial matches will be identified if an exact match is not found. You can query using either DNA or peptide sequences.						
Please select locus/scheme Order results by -						
MLST v locus v						
Enter query sequence (single or multiple contigs up to whole genome in size) Alternatively upload FASTA file	Action					
SACGCGGTGCGCGATGAAAAAGTCAAAGTCATCAAGTCATTGAAGCCGCTGACCGTCGAA Select FASTA file:	Reset Submit					
TCTGTCAATGAAAAATGTCGTGCCCGGGACAATATATGCGCCGSCCAAAGCGATGAACGGCTAT CTTGAAGAAAATGTCGTGCGCGGGGCGACGGCGCGGCG						
Translate query Closest match: aroE: 8						
Show alignment						
Differences						
2 differences found.						
269 _{T →} 393 _A 333 _A → 408 _G						
The locus start point is at position 136 of your query sequence.						

As an alternative to pasting a sequence in to the box, you can also choose to upload sequences in FASTA format by clicking the file browse button.

(PTIDMLST) Download: Alleles	Batch sequences Compare alleles Profile/ST Batch MLST profiles ime PorA FetA Options Isolate Database	profiles List Browse Query				
Sequence query - Neisseria locus/sequence definitions Please paste in your sequence to query against the database. Query sequences will be checked first for an exact match against the chosen (or all) loci - they do not need to be trimmed. The nearest						
partial matches will be identified if an exa Please select locus/scheme All loci	gainst the database. Query sequences will be checked ct match is not found. You can query using either DNA o		- they do not need to be trimmed. The nearest			

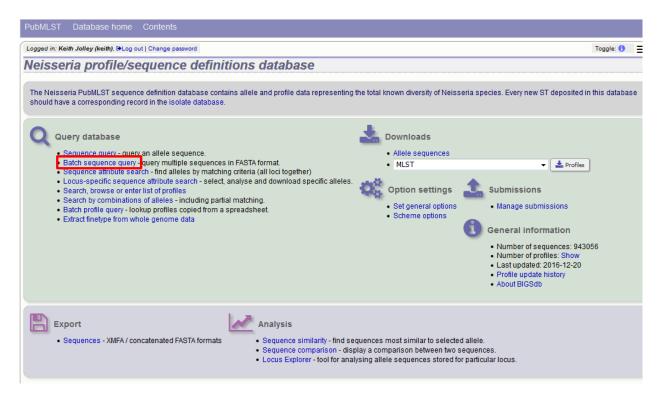
11.1.1 Querying whole genome data

The sequence query is not limited to single genes. You can also paste or upload whole genomes - these can be in multiple contigs. If you select a specific scheme from the dropdown box, all loci belonging to that scheme will be checked (although only exact matches are reported for a locus if one of the other loci has an exact match). If all loci are matched, scheme fields will also be returned if these are defined. This, for example, enables you to identify the MLST sequence type of a genome in one step.

PubM	LST	Download: A	lleles MLST p	rofiles	are alleles Profile/ST Bati Isolate Database	ch profiles List	Browse Query	
Seauer	ice (auerv - I	Veisseri	a locus/se	quence definit	ions		
					ry sequences will be check can query using either DN/			ci - they do not need to be trimmed. The nearest
Please	select	ocus/scheme		Order r	esults by-			
MLST				✓ locus	•			
— Enter q	uery se	quence (single	e or multiple co	ntigs up to whole g	enome in size)			Action
>4758 1	NODE :	192 length	1326 cov	47.828808			Select FASTA file:	Reset Submit
					CTAGATICCCGCIIIC GACAAAAGCCIGCCAI		Browse No file selected.	
CTCAAA	TAGCC	JTCGGATTCG	AGAATCCGAC	TGCCAAACCGGG	CGCGGACGCTCCGGCC			
					ATTCGGATTTTCCAAT TGACAAAAATATAGTG			
					AGATAGTACGGTAAGG	· ·		
7 exact mate	aboo fou	nd						
7 exact mate	ales lou	nu.						
				lags Comments				
abcZ: 4 adk: 10	433 465	203051 938327	203483 938791					
aroE: 15	490	1775325	1775814					
fumC: 9	465	1134240	1134704					
gdh: 8	501	961439	961939					
pdhC: 11	480	1341678	1342157					
pgm: 9	450	1416246	1416695					
MLST								
ST	2	59						
		7-269 complex						

11.2 Querying multiple sequences to identify allele identities

You can also query mutiple sequences together. These should be in FASTA format. Click 'Batch sequence query' from the contents page.



Paste your sequences (FASTA format) in to the box. Select a specific locus, scheme or 'All loci'.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). (HLog out Change password	=
Batch sequence query - Neisseria profile/sequence definition	ons
Please paste in your sequences to query against the database. Query sequences will be checked first for an a trimmed. The nearest partial matches will be identified if an exact match is not found. You can query using eith Please select locus/scheme Order results by	

The best match will be displayed for each sequence in your file. If this isn't an exact match, the differences will be listed.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). [+Log out Change password
Batch sequence query - Neisseria profile/sequence definitions
Please paste in your sequences to query against the database. Query sequences will be checked first for an exact match against the chosen (or all) loci - they do not need to be trimmed. The nearest partial matches will be identified if an exact match is not found. You can query using either DNA or peptide sequences. Please select locus/schemeOrder results by
Sequence Results UIW_3 Exact match found; adk: 2 UEY_1 Partial match found; adk: 2: 2 differences found. ¹⁰⁸ T → ¹⁰⁸ A; ¹⁰⁷ T → ¹⁰⁷ A
DSH_1 Partial match found: adk: 10: 1 difference found. 286 G → 286 T
Text format. list table

11.3 Searching for specific allele definitions

There are two query pages available that allow searching for specific allele definitions. The first allows querying of all loci together by criteria that are common to all. The second is a locus-specific attribute query that can search on any extended attributes that may be defined for a locus. This locus- specific query also allows you to paste in lists of alleles for download or analysis.

11.3.1 General (all loci) sequence attribute search

To retrieve specific allele designations, click 'Sequence attribute search' on a sequence definition database contents page.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	iles List Browse Query
	Toggle: 🚯
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing database should have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in this
Query database • Sequence query - query multiple sequences in FASTA format. • Batch sequence query - query multiple sequences in FASTA format. • Sequence attribute search • Industry and alleles by matching criteria (all loci together) • Locus-specific sequence attribute search - select, analyse and download specific alleles. • Search, browse or enter list of profiles • Search by combinations of alleles - including partial matching. • Batch profile query - lookup profiles copied from a spreadsheet. • Extract finetype from whole genome data	 Downloads Allele sequences MLST Download profiles Option settings Submissions Set general options Manage submissions General information Number of profiles: 537919 Number of profiles: Show Last updated: 2015-08-27 Profile update history
Sequence comparison - disp	About BIGSdb quences most similar to selected allele. play a comparison between two sequences. ysing allele sequences stored for particular locus.

Enter your query using the dropdown search box - additional terms can be added by clicking the '+' button.

Designations can be queried using standard operators.

PULST Download: Al	nces Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query leles MLST profiles ts Home PorA FetA Options Isolate Database
	Toggle: i
Query sequences f	or Neisseria locus/sequence definitions database
Some loci have additional fields w plugins.	hich are not searchable from this general page. Search for these at the locus-specific query page. Use this page also for access to the sequence analysis or export
Also note that some loci in this dat locus that uses integer allele ids u	abase have allele ids defined as text strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter your search to a ising the drop-down list.
Please enter your search criteria b	elow (or leave blank and submit to return all records). Matching sequences will be returned and you will then be able to update their display and query settings.
Search criteria	Display
locus 🗸 =	abcZ + i Order by: locus accending picelar: 25 usurds accending
	Display: 25 🔻 records per page 👔
> Filter query by	Action
	Reset Submit

Click submit.

PubMLST / Dow	ry: Sequences Batch sequences /nload: Alleles MLST profiles s: Contents Home PorA FetA C	Compare alleles Profile/ST Batch	profiles List Browse Query	
LIIK	s. Contents [Home] ForA [FeA] C	pitons fisolate Database		
				Toggle: i
Query sequen	ces for Neisseria lo	ocus/sequence defi	nitions database	
Some loci have additiona plugins.	I fields which are not searchable fr	om this general page. Search for th	ese at the <u>locus-specific query</u> page. Us	e this page also for access to the sequence analysis or export
	in this database have allele ids def llele ids using the drop-down list.	ined as text strings. Queries using t	ne '<' or '>' modifiers will work alphabetic	ally rather than numerically unless you filter your search to a
Please enter your search	criteria below (or leave blank and	submit to return all records). Matchir	g sequences will be returned and you w	vill then be able to update their display and query settings.
Search criteria		Display		
Combine searches with	n: AND 👻	Order b	Clocus - ascending -	•
locus	= → abcZ	+ i Displa	25 v records per page i	
allele id 🔹	• = • 5			
Filter query by	Action Reset Submit	Ī		
1 record returned. Click the	e hyperlink for detailed information			
locus allele id	sequence	sequence length comments fia	as	
	ACCGTTGCC TCGTCGAACTCGA			

Click the hyperlinked results to display allele records.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Toggle: [i]
Query sequences for Neisseria locus/sequence definitions database
Some loci have additional fields which are not searchable from this general page. Search for these at the locus-specific query page. Use this page also for access to the sequence analysis or export plugins.
Also note that some loci in this database have allele ids defined as text strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter your search to a locus that uses integer allele ids using the drop-down list.
Please enter your search criteria below (or leave blank and submit to return all records). Matching sequences will be returned and you will then be able to update their display and query settings.
- Search criteria - Display -
Combine searches with: AND - Order by: locus - ascending -
locus • = • abcZ + I Display: 25 • records per page [
allele id • = • 5
Filter query by Action Reset Submit
1 record returned. Click the hyperlink for detailed information.
locus allele id sequence sequence length comments flags abc2 5 TITGATACCGTTGCC TCGTCGAACTCGATC 433

llele inform	ation - abcZ: 5
Provenance/meta	data
locus:	abcZ i
allele:	5
sequences:	ITIGATACCG TIGCCGAAGG TITGGGCGAA ATTCGCCGATI TAITGCGCCG ITAITCATCAI GICAGCCAIG AGTIGGAAAA TGGTICGAGT GAGGCTITGI TGAAAGAGCI TAACGAATIG CAACIGAAA TCGAAGCGAA GGACGGCIGG AAGCIGGAIG CGGCAGICAA GCAGACITIG GGIGGAACIIG GITIGCCAGA AAACGAAAAA ACCGGCAACC TCTCCCGGCG ACAGAAAAAG CGGIGIIGCCC TAGGGCAGGC TIGGGIGCG AAGCIGGAIG TAITCGCCG GACGAACCG ACCAACCAII GGACAIGA CGCGAITAII IGGCIGGAAA AICIGCITAA AGCGIIGAA GGCAGCCIGG TIGIGAITAC CCACGACCGC CGITITIIGG ACAATAICGC CACGCCAIC GICGAACCG AIC
length:	433
status:	Sanger trace checked
date entered:	2001-02-07
datestamp:	2009-11-11
sender:	Keith Jolley, University of Oxford, UK
curator:	Man-Suen Chan, University of Oxford (E-mail: man-suen.chan@paediatrics.ox.ac.uk)
Profiles containin	g this allele
MLST:	183 profiles
solate databases	
PubMLST isolates:	Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample.

Various search criteria can also be selected by combining with filters. Click the filter heading to display these.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Toggle: []
Query sequences for Neisseria locus/sequence definitions database
Some loci have additional fields which are not searchable from this general page. Search for these at the locus-specific query page. Use this page also for access to the sequence analysis or export plugins.
Also note that some loci in this database have allele ids defined as text strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter your search to a locus that uses integer allele ids using the drop-down list.
Please enter your search criteria below (or leave blank and submit to return all records). Matching sequences will be returned and you will then be able to update their display and query settings.
- Search criteria - Display
allele id • < • 10 + I Order by: locus • ascending •
Display: 25
- Filter query by Action
locus: abcZ Reset Submit
status:
sender. 💌 🛛
curator:
allele flag:
9 records returned. Click the hyperlinks for detailed information.
locus allele id sequence sequence length comments flags
abcZ 1 TITGATACTGTIGCC TIGTCGBACTCGATC 433
abcZ 2 TITGATACCGTTGCC TITGCGAACTCGATC 433 abcZ 3 TITGATACCGTTGCC TITGTGAACTTGACC 433
abc2 4 TITGRATCOTTECC TIETCEAACTCEATC 433
abcz 4 Indianacontoc Tercegantcanto 433
abc2 6 TITGRARCOFTECC TETECEARCTCATC 433
abcz 7 ITIGATACTGITGCC TIGTCGAACTCGATC 433
abcz 8 ITTGATACCGITGCC ITGTCGAACTTGACC 433
abcz 9 TITGATACCGITGCC TIGTCGAACTCGAIC 433

11.3.2 Locus-specific sequence attribute search

Some loci have *extended attribute fields*. To query these, click 'Locus-specific sequence attribute search' on a sequence definition database contents page.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profile Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	iles List Browse Query
	Toggle: 🜖
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing database should have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in this
 Query database Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching criteria (all loci together) Locus-specific sequence attribute search. search, prove or enter rist or promes Search by combinations of alleles - including partial matching. Batch profile query - locup profiles copied from a spreadsheet. Extract finetype from whole genome data 	 Downloads Allele sequences MLST Download profiles Option settings Set general options Set general options Manage submissions Number of sequences: 537919 Number of profiles: Show Last updated: 2015-08-27 Profile update history About BIGSdb
Sequence comparison - dis	quences most similar to selected allele. play a comparison between two sequences. ysing allele sequences stored for particular locus.

Pick the required locus from the dropdown box.

PTTTTILLST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
Help 🗹	Toggle: 🚺
Query PorA VR2 sequences - Neisseria locus/sequence definitions database	
Locus PorA_VR2 Page will reload when changed • Further information is available for this locus. Please enter your search criteria below (or leave blank and submit to return all records).	Modify form options
Allele fields Display Action allele id • • Display: 25 • records per page •	

The fields specific for that locus will be added to the dropdown query boxes.

ित्तिय	LST)	Query: Sequences Batch se Download: Alleles MLST pr Links: Contents Home Po	ofiles		Batch pro	ofiles L	_ist Browse	Query				
											Help 🖉	Toggle: 🕄
Query	PorA	VR2 sequences	s - Neisseria	a locus/se	quen	ce d	efinitio	ons data	base			
Locus: Po	rA_VR2			when changed								Modi
• Furt	her inforr	mation is available for this loc	cus.									form
Please ent	er vour se	earch criteria below (or leave	blank and submit to re	eturn all records)								opuo
Allele fi	ields —			— Dis					Action			
family				+ 0 0	order by:	allele io	- I	 ascending 	 Reset 	Sut	omit	
					Display:	25 👻	records pe	r page 🕕				
Page: 1	2 3	1 - 25 displayed). Click the hy										
	allele id	sequence	sequence length	comments	_	variant	l old name		-		mAb2 reactivity f	lags
PorA VR2	2	HFVQQTPKSQPTLVP	15		2			MN16C13F4	+	AF202	-	
PorA VR2	2-1	HFVQQPPKSQPTLVP	15		2	1	2b	MN16C13F4	-	AF202	+	
PorA VR2	2-10	HFVQQAPQSQSTLVP	15		2	10						
PorA VR2	2-11	HFVLQTPQSQPTLVP	15		2	11						
PorA VR2	2-12	HEVQQIPKSQPTLVP	15		2	12						
PorA VR2	2-13	YFVQQTPQSQPTLVP	15		2	13		MN16C13F4	+			
PorA VR2	2-14											
		HFVQQKLASKPTLVP	15		2	14	33					
PorA VR2		HFVQQKLASKPILVP	15		2	14 15	33 33a (33-1)					
PorA VR2 PorA VR2												

The query form can be modified by clicking the 'Modify form options' tab:

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
	Help 🗹	Toggle: 🚺									
Query abcZ sequence	es - Neisseria locus/sequence definitions database										
Locus: abcZ • Further information is available to Please enter your search criteria below	Page will reload when changed for this locus. r (or leave blank and submit to return all records).	Modify form options									
Allele fields allele id 👻 =	Order by: allele id vascending v Reset Submit Display: 25 v records per page 6										

A list box can be added by clicking the 'Show' button for 'Allele id list box'.

PubMLST	Download: Alleles Links: Contents H	MLST profiles Iome PorA FetA O	Compare alleles Profile/ ptions Isolate Database a profile/sequ			s database	Help C	Toggle: (1)
	nation is available f arch criteria below	for this locus.	will reload when changed submit to return all records	Display Order by:	allele id 25	 ✓ ascending ascending 	 Modify form parameters Click to add or remove additional que Allele fields Allele id list box Filters 	Modify form options

Close the form modification tab and you can now enter a list of allele ids for retrieval.

PUDMLST / Dow	nload: Alleles MLST p	equences Compare alleles Pr ofiles rA FetA Options Isolate Datat		List Browse Query	
				Help 🖉	Toggle: 🚯
Query abcZ se	quences - N	eisseria locus/sec	quence defini	tions database	
Locus: abcZ	n is available for this lo	 Page will reload when change 	ed		Modify
		blank and submit to return all re	aarda)		options
Allele fields			Allele id list	Display Order by: allele id ascending Tecords per page ● Action Reset Submit	

Various analysis and export options will be available for use on the retrieved sequences. These include FASTA output and *Locus Explorer* analysis.

Further information is available for this locus.												
Please	Please enter your search criteria below (or leave blank and submit to return all records).											
Allel	le field	S		— Allele id list — —	– — Display———							
allel	e id	• = •	+ 0	1	Order by: allele id 🚽 ascending 🚽							
			0	2	Display: 25 🗸 records per page 🜖							
				3								
				5								
					Reset Submit							
5 records	roturn	ed. Click the hyperlinks for detailed information										
Jiecolus	return	ied. Olick the hyperninks for detailed mormation										
locus a	allele io	sequence	sequence length	comments flags								
abcZ	1	TTTGATACTGTTGCC TTGTCGAACTCGATC	433									
abcZ	2	TTTGATACCGTTGCC TTGTCGAACTCGATC	433									
abcZ	3	TTTGATACCGTTGCC TTGTTGAACTTGACC	433									
abcZ abcZ	4	TTTGATACCGTTGCC TTGTCGAACTCGATC TTTGATACCGTTGCC TCGTCGAACTCGATC	433 433									
aucz	5	TITGATACCOTTOCC TOUTCOAACTOGATC	433									
Analys	is too	ols:										
Expor	t FA	STA Table										
Analysis		cus Explorer										
)						

11.4 Browsing scheme profile definitions

If a sequence definition database has schemes defined that include a primary key field, i.e. collections of loci that together create profiles, e.g. for MLST, these can be browsed by clicking the link to 'Search, browse or enter list of profiles'.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch prof Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	iles List Browse Query
	Toggle: 🕄
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in this database should
Query database Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching criteria (all loci together) Louis spacific sequence attribute search - select, analyse and download specific alleles. Search, browse or enter list of profiles Search by combinations of alleles - including partial matching. Batch profile query - lookup profiles copied from a spreadsheet. Extract finetype from whole genome data	 Downloads Allele sequences MLST Download profiles Option settings Submissions Set general options Manage submissions General information Number of sequences: 537919 Number of sequences: 537919 Submissions Last updated: 2015-08-27 Profile update history About BIGSdb
Sequence comparison - disp	quences most similar to selected allele. Day a comparison between two sequences. Iysing allele sequences stored for particular locus.

Leave query form fields blank (the display of these may vary depending on modification options set by the user). Choose the field to order the results by, the number of results per page to display, and click 'Submit'.

Pul	Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database									
	Toggle: 🚯									
Sea	Search or browse profiles - Neisseria locus/sequence definitions									
						P . C				
Enter	rsea	arch c	riteria	orlea	ve bla	nk to b	rows	e all records. Modify form param	meters to filter or enter a list of values.	
			eme f							
S		sisui	entei		1			C.		
3				•	=		•		Reset Sublinit	
									Display: 25 🗸 records per page 🚺	
Brows	sing	all red	cords.							
40050					05 48		-	inte de la compania dan dan dan dan dan dari		
10050	brec	oras i	returni	ea (1 -	25 QI	spiaye	a). Ci	ick the hyperlinks for detailed in	niormauon.	
Page	: 1	2	3	4	5	6 7	8	9 > Last		
	_		_	_						
ST	adk	abcZ	aroE	fumC	adh	pdhC	pam	clonal complex		
1	3	1	1	1	1	1	3	ST-1 complex/subgroup I/II		
2	3	1	4	7	1	1	3	ST-1 complex/subgroup I/II		
3	3	1	1	1	1	23	13	ST-1 complex/subgroup I/II		
4	3	1	3	1	4	2	3	ST-4 complex/subgroup IV		
5	1	1	2	1	3	2	3	ST-5 complex/subgroup III		
6	1	1	2	1	3	2	11	ST-5 complex/subgroup III		
7	1	1	2	1	3	2	19	ST-5 complex/subgroup III		
8	3	2	7	2	8	5	2	ST-8 complex/Cluster A4		
9	3	2	8	10	8	5	2	ST-8 complex/Cluster A4		
10	3	2	4	2	8	15	2	ST-8 complex/Cluster A4		
11	3	2	4	3	8	4	6	ST-11 complex/ET-37 complex	X	
12	3	4	2	16	8	11	20			
10	10	4	15	7	0	44	4	ST 260 complex		

Clicking the hyperlink for any profile will display full information about the profile.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Help 02
Profile information for ST-11 (MLST)
ST adk abcZ aroE fumC gdh pdhC pgm clonal complex 11 3 2 4 3 8 4 6 ST-11 complex/ET-37 complex
sender: Paula Kriz, Paula Kriz and Keith Jolley
curator: Keith Jolley, University of Oxford, UK (E-mail: keith.jolley@zoo.ox.ac.uk)
update history: 2 updates show details
date entered: 2001-02-07
datestamp: 2013-04-27
Client database
PubMLST isolates: Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample. 1133 isolates

11.5 Querying scheme profile definitions

Click the link to 'Search, browse of enter list of profiles'.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profile Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	files List Browse Query
	Toggle: 🜖
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in this database should
Query database • Sequence query - query an allele sequence. • Batch sequence query - query multiple sequences in FASTA format. • Sequence attribute search - find alleles by matching criteria (all loci together) • Locus spacific sequence attribute search - select, analyse and download specific alleles. • Search by combinations of alleles - including partial matching. • Batch profile query - lookup profiles copied from a spreadsheet. • Extract finetype from whole genome data	 Downloads Allele sequences MLST Download profiles Option settings Submissions Set general options Manage submissions General information Number of sequences: 537919 Number of profiles: Show Satu update(2015-08-27) Profile update history About BIGSdb
Sequence comparison - disp	quences most similar to selected allele. play a comparison between two sequences. lysing allele sequences stored for particular locus.

Enter the search criteria you wish to search on. You can add search criteria by clicking the '+' button in the 'Locus/scheme fields' section. These can be combined using 'AND' or 'OR'.

Pub	Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
										Toggle: 🚯		
Soor	Search or browse profiles - Neisseria locus/sequence definitions											
Enter search criteria or leave blank to browse all records. Modify form parameters to filter or enter a list of values.												
Enters	earc	ch crite	ina or	leave	Diank	to pro	wsea	all records. Modify form paramet	ers to filter or enter a list of values.	Modify		
Lo	cus/	schen	ne field	ds —					— Display/sort options — Action — Action	- form		
Com	bine	searc	hes w	ith: Al	ND .	-			Order by: ST 🗸 ascending 🗸 Reset Submit	options		
dat	e en	itered		• >	>		-	2013-02-01 +	O Display: 25			
ser	nder	(surna	ime)	• =	•		•	Jolley				
5051 re	cord	ls retu	med (*	1 - 25 (displa	aved). (Click	the hyperlinks for detailed inforn	nation.			
	_											
Page:	1	2	3 4	5	6][7]	8	9 > Last				
						pdhC		cional complex				
5001	-	12	12	352	9	18	9	OT 14/14				
5002 5003	5 5	2	9	9 143	9 5	6 119	8 18	ST-41/44 complex/Lineage 3				
5003	8	9	185	26	10	1	16	ST-18 complex				
5005	8	7	10	19	10	351	16	ST-18 complex				
5006	8	13	10	19	10	1	9	ST-18 complex				
5007	8	7	10	3	9	15	20	er to complex				
5008	7	12	381	91	5	21	16					
5009	8	187	10	116	10	15	20					
5010	8	7	10	17	10	1	9	ST-18 complex				
5011	3	7	72	26	10	1	16					

Each field can be queried using standard operators.

Clicking the hyperlink for any profile will display full information about the profile.

PTDI/JIST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database														
														Toggle: 🚯
Search	n or	bro	ws	e n	rofi	iles	- Neisseria lo	cus/s	equence	definitio	ns			
- cui oi							Increase and a second real second real second secon	040/0	oquonoc	dominuo				
Enter sear	rch crit	eria or	leave	blank	to bro	wse a	all records. Modify form par	ameters to	filter or enter a	listofvalues				
				Jun			in records, modify form par							Modify
Locus	/scher	ne fiel	ds —						— Display/sor	t options			Action	form options
Combine	e sear	ches w	ith: A	ND -	•			_	Order by:	ST	 ascending 	-	Reset Submit	opuons
date er	ntered		•	>		-	2013-02-01	+ 0	Display:	25 - records	per page 🜖			
sender	r (surn	ame)	•	-		-	Jolley							
5051 record						Click 1	he hyperlinks for detailed i	information	I.					
				_										
ST adk	abcī		fumC	adb	ndhC	nam	clonal complex							
5001 6	12	12	352	9	18	9	cional complex	-						
5002 5	2	9	9	9	6	8	ST-41/44 complex/Lineag	e 3						
5003 5	9	6	143	5	119	18								
5004 8	7	185	26	10	1	16	ST-18 complex							
5005 8	7	10	19	10	351	16	ST-18 complex							
5006 8	13	10	19	10	1	9	ST-18 complex							
5007 8	7	10	3	9	15	20								

Other query options are available by clicking the 'Modify form options' tab.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database									
									Toggle: 📵
Search or brows	se profiles	s - Neisseria locu	is/se	quence	definition	าร			
Estave and activity of the					list studies				
Enter search criteria or leave blank to browse all records. Modify form parameters to filter or enter a list of values. — Locus/scheme fields — Display/sort options — Action									
ST +	= •	+	0	Order by:		→ ascending →		Submit	_ form options
		_		Display:	25 👻 records	per page 🕕			

For example, you can enter a list of attributes to query on by clicking the 'Show' button next to 'Attribute values list'.

Public Miles Query: Sequences Batch sequences Compare alleles Profile/ST [] Batch profiles Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database										
Logged in: Keith Jolley (keith).	Log out Change password			Help 🗹	Toggle: 🚯					
Search or brow	se profiles - Neiss	eria profile/sequen	ce definitions							
Enter search criteria or leav	ve blank to browse all records. Mo	dify form parameters to filter or ente	a list of values.		Modify					
			ort options	×	form					
ST 🗸	= •	+ 0 Order	y: ST 👻 ascen	Modify form parameters	options					
		Displ	y: 25 ▼ records per page	Click to add or remove additional que • O Locus/scheme field va • O Attribute values list • O Filters						

A list box will appear within the page. Hide the form modification tab by clicking the 'X' in the corner or the purple tab again. Now you can choose the attribute to search on along with a list of values.

Pu	<u>1d</u>	TL S	\mathbf{T}	Down	load:	Alleles	(ML)	ch sequences Compare alleles Profile/ 3T profiles PorA FetA Options Isolate Database	ST Batch profiles List Browse	Query	
											Toggle: 🚯
Sea	arc	h o	r bi	row	se	pro	file	s - Neisseria locus/seo	quence definition	S	
Ente	erse	arch c	riteria	or lea	ve bla	ink to b	rows	e all records. Modify form parameters to fill	ter or enter a list of values.		Modify
	Loci ST	is/sch	eme f		=		,		Attribute values list	Display/sort options Order by: ST ← ascending ←	form
								1 2 3 4	łı.	Display: 25 - records per page () Action Reset Submit	
4 rec	ords	return	ed. C	lick th	e hyp	erlinks	for de	tailed information.			
ST	_	abcZ	aroE	fumO	gdh	pdhC		clonal complex			
1	3	1	1	1	1	1	3	ST-1 complex/subgroup I/II			
2	3	1	4	1	1	1	3	ST-1 complex/subgroup I/II			
3	3	1	3	1	4	23 2	13 3	ST-1 complex/subgroup I/II ST-4 complex/subgroup IV			
Ana Ana	alysi	s too : BU : Se	ols:)	4	2	J	or a complex subgroup iv			

List values will be combined with any other attributes entered in the query form allowing complex queries can be constructed.

You can also add filters to the form by again clicking the 'Modify form options' tab and selecting 'Filters'.

Query: Sequences Batch sequences Compare a Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Iso			Help IZ Toggle: 8
			neipter Toggie.
Search or browse profiles - Neisseria p	profile/sequence definitions		
Enter search criteria or leave blank to browse all records. Modify form particular search criteria or leave blank to browse all records. Modify form particular search criteria search criteri	Arameters to filter or enter a list of values. Attribute values list Field: ST 1 2 3 4 	• 🕒 Locus/s	Additional query terms: cheme field values values list

Available filters will vary depending on the database. These will be combined with other query criteria or lists of attributes.

Query: Sequences Batch sequences Co Download: Alleles MLST profiles Links: Contents Home PorA FetA Opti	ompare alleles Profile/ST Batch profiles List Browse ions Isolate Database	Query
		Toggle: 🕄
Search or browse profiles - Neisse	eria locus/sequence definitions	\$
Enter search criteria or leave blank to browse all records. Modil Locus/scheme fields ST	fy form parameters to filter or enter a list of values. Attribute values list Field: ST I 2 3 4	Filters Modify form options Clonal complex: ST-4 complex/subgroup IV ● Display/sort options Action Order by: ST ◆ ascending ♥ Display: 25 ▼ records per page ●
1 record returned. Click the hyperlink for detailed information. ST adk abcZ aroE fumC gdh pdhC pgm clonal comp 4 3 1 3 1 4 2 3 ST-4 complex/sub Analysis tools: Export: Sequences Sequences Sequences		

11.6 Identifying allelic profile definitions

For schemes such as MLST you can query allelic combinations to identify the sequence type (or more generically, the primary key of the profile).

Click the 'Search by combinations of alleles' link from the sequence definition contents page.

PubMLST Database home Contents		
+8 Log in	Toggh	e: 🚯 🗧
Neisseria profile/sequence definitions database		
The Neisseria PubMLST sequence definition database contains allele and profile data representing the to corresponding record in the isolate database.	tal known diversity of Neisseria species. Every new ST deposited in this database should have a	
Q Query database	Downloads Option settings	
Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching criteria (all loci together)	Allele sequences MLST Scheme options	3
 Locus-specific sequence attribute search - select, analyse and download specific alleles. Search, browse or enter list of profiles 		
Search by combinations of alleles - including partial matching. • Batch profile query - lookup profiles copied from a spreadsheet.	Manage submissio	ons
Extract finetype from whole genome data	General information	
	Number of sequences: 943149 Number of profiles: Show	
	Last updated: 2016-12-20 Profile update history	
	About BIGSdb	
	ces most similar to selected allele. I comparison between two sequences. J allele sequences stored for particular locus.	

If multiple schemes are defined in the database you should select the scheme you wish to check.

PubMLST Database home Contents			
40 Log in	Help 🖉	Toggle: 🜖	Ξ
Search Neisseria profile/sequence definitions database by combinations of loci			
Schemes			
Please select the scheme you would like to query:			
MLST Select			
Please enter your allelic profile below. Blank loci will be ignored. Autofill profile			
abcZ adk aroE fumC gdh pdhC pgm ST: Autofil			
Options Display/sort options Action			
Search: Exact or nearest match 👻 Order by: ST 💌 ascending 💌 Reset Submit			
Display: 25 👻 records per page 🛈			
			-

Enter a combination of allelic values (you can enter a partial profile if you wish).

PubMLST Database home Contents		
+8 Log in	Help 🗗	Toggle: 🚯 📃
Search Neisseria profile/sequence definitions database by combinations of loci		
Schemes		
Please select the scheme you would like to query:		
MLST Select		
Please enter your allelic profile below. Blank loci will be ignored. Autofill profile		
abc/ ack arot rum gon pont pgm SI: Autofill 2 3 4 3 8 4 6 6		
Options — Display/sort options — Action —		
Search: Exact or nearest match 🔹 Order by: ST 🔹 ascending 👻 Reset Submit		
Display: 25 👻 records per page 🖲		

Alternatively, you can automatically populate a profile by entering a value for the scheme primary key field (e.g. ST) and clicking 'Autofill'.

PubMLST Database home Contents			
Logged in: Keith Jolley (keith). (+Log out Change password	Help 🖉	Toggle: 🚯	Ξ
Search Neisseria profile/sequence definitions database by combinations of loci			
Schemes			
Please select the scheme you would like to query:			
MLST Select			
Please enter your allelic profile below. Blank loci will be ignored. Autofill profile abcZ adk aroE fumC gdh pdhC pgm ST. 11 Autofill Options Display/sort options Action Action Reset Submit Search: Exact or nearest match + Order by: ST + ascending + Reset Submit			
Propios. 23 V records per page U			

To find the closest or exact match, leave the search box on 'Exact or nearest match' and click 'Submit'. The best match will be displayed.

PubMLST Database home Contents		
Logged in: Keith Jolley (keith). @Log out Change password	Help 🖉	Toggle: 🚯 🗧
Search Neisseria profile/sequence definitions database by combinations of loci		
Schemes		
Please select the scheme you would like to query:		
MLST - Select		
abcZ adk aroE fumC gdh pdhC pgm ST: 11 Autofill		
2 3 4 3 8 4 6 Options Display/sort options Action Search: Exact or nearest match + Order by: ST ascending + Display: 25 records per page 1 Submit		
Exact matches found (7 loci).		
1 record returned. Click the hyperlink for detailed information.		
ST abcZ adk aroE fumC gdh pdhC pgm clonal complex 11 2 3 4 6 ST-11 complex/ET-37 complex Analysis tools: Analysis tools: Analysis tools: Analysis tools:		
Export Sequences		

Alternatively, if you wish to find all profiles that match the query profile by at least a set number of loci, select the appropriate value in the search dropdown box, e.g. '4 or more matches' will show related profiles that share at least 4 alleles with the query.

ogged ir	n: Kei	ith Jo	lley (ke	eith). 🕩	Log ou	ut Cha	nge p	assword	Help 🗗	Toggle: 🚯
ear	ch	Ne	eiss	eri	a p	rofi	le/	sequence definitions database by combinations of loci		
Scher	mes									
lease	sele	ectin	e sche	eme yo	bu wo	uld lik	e to q	uery.		
MLST								▼ Select		
Ple	ease	ente	r your	allelic	profil	e belo	w. Bl	ank loci will be ignored Autofill profile		
ab	bcZ		adk		aroE	1	fumC	gdh pdhC pgm ST: 11 Autofill		
:	2		3		4		3	8 4 6		
0	otions							Display/sort options Action		
	Sear	_	4 or n	nore m	aatichu	20	Ţ			
```	ocu	<b>.</b>	4 01 11	lore II	accin	35	_	Treset Sublinit		
								Display: 25 👻 records per page 🕄		
9 reco	ords	retur	ned (1	1 - 25 (	displa	ved), (	Click	he hyperlinks for detailed information.		
	_									
ige:	1	2	3	4_5		7	8	9 > Last		
						pdhC				
	2	3	4	2	8	15	2	ST-8 complex/Cluster A4 ST-11 complex/ET-37 complex		
	2	3	4 19	3	8	4	6	ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex		
	2	3	4	23	8	6	6	ST-11 complex/ET-37 complex		
	7	3	4	3	8	4	6	ST-11 complex/ET-37 complex		
	2	3	4	24	8	4	6	ST-11 complex/ET-37 complex		
65	2	3	4	48	8	4	6	ST-11 complex/ET-37 complex		
66	2	3	6	3	3	58	6	ST-11 complex/ET-37 complex		
11	2	3	4	8	8	4	6	ST-11 complex/ET-37 complex		
14	2	3	4	3	48	4	6	ST-11 complex/ET-37 complex		
7 5	2	3	4	5	8 51	4	6	ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex		

# 11.7 Batch profile queries

To lookup scheme definitions, e.g. the sequence type for multiple profiles, click 'Batch profile query' from the sequence definition contents page.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). (HLog out   Change password Neisseria profile/sequence definitions database	Taggle: ()
The Neisseria PubMLST sequence definition database contains allele and profile data representing should have a corresponding record in the isolate database.	Downloads
<ul> <li>Sequence query - query an allele sequence.</li> <li>Batch sequence query - query multiple sequences in FASTA format.</li> <li>Sequence attribute search - find alleles by matching criteria (all loci together)</li> <li>Locus-specific sequence attribute search - select, analyse and download specific alleles.</li> <li>Search, browse or enter list of profiles</li> <li>Search by combinations of alleles - including partial matching.</li> <li>Batch profile query - lookup profiles copied from a spreadsheet.</li> <li>Extract finetype from whole genome data</li> </ul>	<ul> <li>Allele sequences</li> <li>MLST         <ul> <li>MLST</li></ul></li></ul>
Sequence comparison - display the s	equences most similar to selected allele. play a comparison between two sequences. lysing allele sequences stored for particular locus.

If multiple schemes are defined in the database you should select the scheme you wish to check.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). Hog out   Change password	3
Batch profile query - Neisseria profile/sequence definitions	
Schemes	
Please select the scheme you would like to query:	
MLST   Select	
Enter allelic profiles below in tab-delimited text format using copy and paste (for example directly from a spreadsheet). G whitespace. The first column should be an isolate identifier and the remaining columns should comprise the allele nur data. Non-numerical characters will be stripped out of the query. Paste in profiles	

Copy and paste data from a spreadsheet. The first column is the record identifier, and the remaining columns are the alleles for each locus in the standard locus order defined for the scheme. There are links to the column order which can be used as a header line for your spreadsheet and to example data.

Click submit after pasting in the data.

ged in: Keith Jolley	keith). ເ∳Log o	ut   Change p	assword							
tch profil	e query	/ - Neis	sseria j	profile	/seque	ence de	efinitions			
hemes										
nemes										
ease select the so	heme you wo	ould like to q	uery:							
				-						
LST			<ul> <li>Select</li> </ul>	J						
201										
251										
	below in tab-	delimited te	xt format usi		t naste (for e	example dire	octiv from a sprea	idsheet) Colum	ins can be separated by any amount of wh	tesnace
ter allelic profiles									ins can be separated by any amount of wh	
ter allelic profiles	uld be an iso	late identifie							ins can be separated by any amount of wh in order). Click here for example data. Non	
ter allelic profiles e first column sho aracters will be st	uld be an iso ripped out of	late identifie							nn order). Click here for example data. Non	
ter allelic profiles e first column sho	uld be an iso ripped out of	late identifie								
ter allelic profiles e first column sho aracters will be st	uld be an iso ripped out of	late identifie							nn order). Click here for example data. Non	
ter allelic profiles e first column sho aracters will be st – Paste in profiles	uld be an iso ripped out of	olate identifie the query.	er and the re	maining co	lumns shou	ld comprise	the allele numbe		nn order). Click here for example data. Non	
ter allelic profiles e first column sho aracters will be st — Paste in profiles 1solate_6	uld be an iso ripped out of 3	olate identifie the query. 6	er and the re 9	maining col	lumns shou	ld comprise	the allele numbe		nn order). Click here for example data. Non	
ter allelic profiles e first column sho aracters will be st — Paste in profiles i solate_6 i solate_7	uld be an isc ripped out of 3 6 4 2	olate identifie the query. 6 6	er and the re 9 365	5 55	lumns shou 8 72	ld comprise	9 20		nn order). Click here for example data. Non	
ter allelic profiles e first column sho aracters will be st —Paste in profiles isolate_6 isolate_7 isolate_8	uld be an isc ripped out of 3 6 4	olate identifie the query. 6 6 3	9 365 5	5 55 4	8 72 315	ld comprise	9 20 8		nn order). Click here for example data. Non	
ter allelic profiles e first column sho aracters will be st - Paste in profiles isolate_6 isolate_7 isolate_8 isolate_9	uld be an isc ripped out of 3 6 4 2	olate identifie the query. 6 6 3 273	9 365 5 19	5 55 4 3	8 72 315 8	ld comprise 6 6 21 4	9 20 8 6		nn order). Click here for example data. Non	
ter allelic profiles e first column sho aracters will be st - Paste in profiles isolate_6 isolate_7 isolate_8 isolate_9 isolate_10	uld be an isc ripped out of 3 6 4 2 2	olate identifie the query. 6 6 3 273 7	9 365 5 19 159	5 55 4 3 92	8 72 315 8 93	6 6 21 4 6	9 20 8 6 2		nn order). Click here for example data. Non	
ter allelic profiles e first column sho aracters will be st —Paste in profiles isolate_7 isolate_7 isolate_9 isolate_9 isolate_10 isolate_11	uld be an isc ripped out of 3 6 4 2 2 2 2	olate identifie the query. 6 6 3 273 7 5	9 365 5 19 159 12	5 55 4 3 92 143	8 72 315 8 93 29	6 6 21 4 6 285	9 20 8 6 2 7		nn order). Click here for example data. Non	
ter allelic profiles e first column sho aracters will be st - Paste in profiles isolate_6 isolate_7 isolate_8 isolate_10 isolate_11 isolate_12	uld be an isc ripped out of 3 6 4 2 2 2 2 6	olate identifie the query. 6 6 3 273 7 5 7	9 365 5 19 159 12 9	5 55 4 3 92 143 56	8 72 315 8 93 29 26	6 6 21 4 6 285 18	9 20 8 6 2 7 8		nn order). Click here for example data. Non	

#### A results table will be displayed.

gged m. Ken	th Jolle	ey (kei	ith). 🕩 L	.og out	Cha	nge pas	sword				
atch p	rof	ïle	au	erv	- N	leis	ser	ia pl	rofile/sequence d	finitions	
			-								
Inclute	-1-7			6	- db			OT			
		_			gan	pdhC			clonal complex		
isolate_1	8	3	5	4	0	3	8	290	ST-32 complex/ET-5 complex		
isolate_2	2	3	4	86	8	110	118		ST-11 complex/ET-37 complex		
isolate_3	4	26 5	15	9	8	11 130	18	8381 942	ST-269 complex		
isolate_4	20		144	35	8		123		OT (4)(4) as malaulting as a		
isolate_5			13	5	9	6	9		ST-41/44 complex/Lineage 3		
isolate_6		6	9	5	8	6	9	485	ST-41/44 complex/Lineage 3		
isolate_7			365	55	72	6	20	4053			
isolate_8	4	3	5	4	315	21	8	3770	ST-32 complex/ET-5 complex		
isolate_9		273		3	8	4	6		ST-11 complex/ET-37 complex		
solate_10		7		92	93	6	2	10908			
isolate_11		5	12	143	29	285	7	4658			
solate_12		7		56	26	18		10620	ST-175 complex		
solate_13	11	5	18	5	9	24	3	10202	ST-22 complex		
solate_14	222	231	406	12	161	2	16	8927			
solate_15	9	4	9	17	5	3	2	8977	ST-103 complex		

# 11.8 Investigating allele differences

#### 11.8.1 Sequence similarity

To find sequences most similar to a selected allele within a sequence definition database, click 'Sequence similarity' on the contents page.

Query: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profile Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database	iles   List   Browse   Query
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing this database should have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in
Query database           • Sequence query - query an allele sequence.           • Batch sequence query - query multiple sequences in FASTA format.           • Sequence attribute search - find alleles by matching criteria (all locit together)           • Locus-specific sequence attribute search - select, analyse and download specific alleles.           • Search browse or enter list of MLST profiles           • Search by combinations of MLST alleles - including partial matching.           • Batch profile query - lookup MLST profiles copied from a spreadsheet.           • Extract finetype from whole genome data	<ul> <li>Downloads         <ul> <li>Allele sequences</li> <li>MLST profiles</li> <li>Set general options</li> <li>Set general options</li> <li>Manage submissions</li> </ul> </li> <li>General information         <ul> <li>Number of sequences: 124770</li> <li>Number of profiles (MLST): 10058</li> <li>Last updated: 2015-08-19</li> <li>Profile update history</li> <li>About BIGSdb</li> </ul> </li> </ul>
Sequence comparison - disp	quences most similar to selected allele. vlay a comparison between two sequences. ysing allele sequences stored for particular locus.

Enter the locus and allele identifier of the sequence to investigate and the number of nearest matches you'd like to see, then press submit.

Query:         Sequences         Batch sequences         Compare alleles         Profile/ST         Batch profiles         List         Browse         Query           Download:         Alleles         MLST profiles         Links:         Contents         Horn         Port Alleles         Port Alleles<
Find most similar alleles - Neisseria locus/sequence definitions
This page allows you to find the most similar sequences to a selected allele using BLAST.
Select parameters     Action       Locus: abcZ     Allele: 5       Allele: 5     Submit       Number of results: 10 -     Image: Second

A list of nearest alleles will be displayed, along with the percentage identity and number of gaps between the se-

quences.

	LST/D	ownload: Al	leles   I	MLST profiles	ences   Compare alleles   Profile/ST []] Batch profiles   Query s FetA   Options   Isolate Database
Logged in: Ke	eith Jolley (ke	eith). 🗭Log ou	it   Chan	ge password	Help 🗗
Find m	ost sii	nilar a	llele	es - Nei	isseria profile/sequence definitions
This page	allows you t	o find the m	ost sim	nilar sequend	ces to a selected allele using BLAST.
	parameters				Action
	·	s: abcZ		•	Reset Submit
	Allel	e: 5			
Numb	per of result	s: 10 👻			
abcZ-5					
	% Identity	Nismatches	Gaps	Alianment	Compare
	% Identity   99.77	Aismatches 1	Gaps 0	Alignment 433/433	
Allele					4
Allele abcZ: 453	99.77	1	0	433/433	
Allele abcZ: 453 abcZ: 405	99.77 99.77	1 1	0	433/433 433/433	4호           4호           4호
Allele abcZ: 453 abcZ: 405 abcZ: 404	99.77 99.77 99.77	1 1 1	0 0 0	433/433 433/433 433/433	[ 4월 ] [ 4월 ]
Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213	99.77 99.77 99.77 99.77	1 1 1 1	0 0 0 0	433/433 433/433 433/433 433/433	4월       4월       4월       4월       4월
Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166	99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1	0 0 0 0	433/433 433/433 433/433 433/433 433/433	42       42       42       42       42       43       44       44       44
Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166 abcZ: 114	99.77 99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1 1 1	0 0 0 0 0 0 0	433/433 433/433 433/433 433/433 433/433 433/433	4월       4월       4월       4월       4월
Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166 abcZ: 114 abcZ: 103	99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1 1 1 1	0 0 0 0 0 0 0 0 0	433/433 433/433 433/433 433/433 433/433 433/433 433/433	4월 4월 4월 4월 4월 4월

Click the appropriate 'Compare' button to display a list of nucleotide differences and/or a sequence alignment.

Query: Sequences   Batch sequences   Compare alleles   Pro Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Databa	
Allele sequence comparison - Neisseria locu	s/sequence definitions
This tool allows you to select two alleles and highlight the nucleotide differences be	etween them.
Select parameters	
Locus: abcZ  Allele #1: 5 Submit	
Allele #1: 5 Allele #2: 453	
Nucleotide differences between abcZ: 5 and abcZ: 453	
Identity: 99.77 %	
Show alignment	
Differences: 1	
$300: \mathbf{G} \rightarrow \mathbf{A}$	

#### 11.8.2 Sequence comparison

To directly compare two sequences click 'Sequence comparison' from the contents page of a sequence definition database.

Query: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profile: Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database	s   List   Browse   Query
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing the this database should have a corresponding record in the isolate database.	e total known diversity of Neisseria species. Every new ST deposited in
Query database           • Sequence query - query an allele sequence.           • Batch sequence query - query multiple sequences in FASTA format.           • Sequence attribute search - find alleles by matching criteria (all loci together)           • Locus-specific sequence attribute search - select, analyse and download specific alleles.           • Search, browse or enter list of MLST profiles           • Search by combinations of MLST alleles - including partial matching.           • Batch profile query - lookup MLST profiles copied from a spreadsheet.           • Extract finetype from whole genome data	<ul> <li>Downloads         <ul> <li>Allele sequences</li> <li>MLST profiles</li> </ul> <ul> <li>Set general options</li> <li>Set general options</li> <li>Munications</li> </ul> </li> <li>Submissions</li> <li>Manage submissions</li> </ul> 3 3 3 4 5 5 5 5 5 6 6 7 7 7 8 9 9 9 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10<
Sequence comparison displa	ences most similar to selected allele. y a comparison between two sequences. ing allele sequences stored for particular locus.

Enter the locus and two allele identifiers to compare. Press submit.

PubMLST / Download: Alleles	Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query MLST profiles me   PorA   FetA   Options   Isolate Database
Allele sequence comp	arison - Neisseria locus/sequence definitions
This tool allows you to select two alleles	and highlight the nucleotide differences between them.
Select parameters Locus: abcZ Allele #1: 5 Allele #2: 8	Action Submit

A list of nucleotide differences and/or an alignment will be displayed.

Prin MLST / Download: Alleles	Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query   MLST profiles Iome   PorA   FetA   Options   Isolate Database
Allele sequence comp	arison - Neisseria locus/sequence definitions
This tool allows you to select two alleles	s and highlight the nucleotide differences between them.
Select parameters Locus: abcZ Allele #1: 5 Allele #2: 8	
Nucleotide differences between	n abcZ: 5 and abcZ: 8
Show alignment	
Differences: 41 $72: G \rightarrow T$ $78: A \rightarrow G$ $79: A \rightarrow C$ $81: T \rightarrow C$ $82: G \rightarrow A$ $83: G \rightarrow A$	
$87: G \rightarrow A$ $88: A \rightarrow G$ $89: G \rightarrow A$ $90: T \rightarrow C$ $93: G \rightarrow C$ $95: C \rightarrow T$	
90. $C \rightarrow I$ 99: $G \rightarrow A$ 102: $G \rightarrow A$ 102: $G \rightarrow A$	

#### See also:

Locus explorer plugin.

# 11.9 Browsing isolate data

Isolate records can be browsed by clicking the link to 'Search or browse database'.

Cuery: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species profiles/sequence definition database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this of that it does not represent a population sample.	
Query database       Search or browse database         • Search by combinations of loci (profiles)       • Set general options - including isolate table field handling.         • Projects - main projects defined in database.       • Set display and query options for locus, schemes or scheme fields.	Submissions Manage submissions Manage submissions General information Isolates: 35423 Last updated: 2015-08-27 Update history About BIGSdb
Breakdown       Export       Analysis         • Single field       • Export dataset       • Contigs         • Unique combinations       • Sequences - XMFA / concatenated FASTA formats       • Codon usage         • Publications       • Sequence bin       • Miscellaneous         • Description of database fields       • Description of database fields	oci

Leave query form fields blank (the display of these may vary depending on modification options set by the user). Choose the field to order the results by, the number of results per page to display, and click 'Submit'.

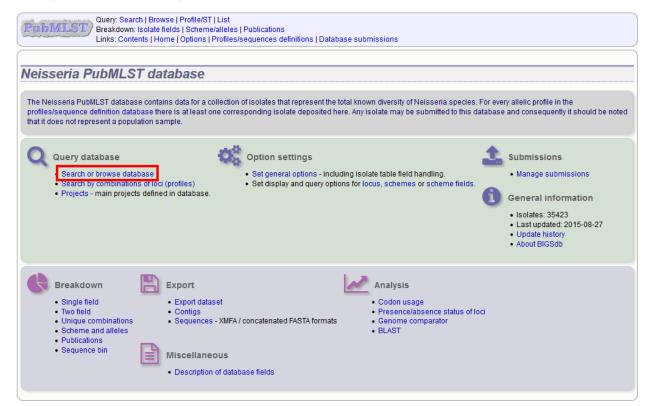
							Help 🗗	Toggle	e 🚯 Field help: id			
2	arch or	browse Neisse	eria PubM	LS	r database							
nte	r search crite	ria or leave blank to browse	all records.									
	Isolate prove	nance/phenotype fields			Display/so	ort options				— — Act	ion	
	d		Enter value		+ Order by				+ ascending +			
	u	•	Entor value		Display				• ascending	Re	set Su	bmit
					Display	y: 25 🗸 records per	page 🕖				_	
					elds ()				MLST		typing antig	
id	isolate	aliases	country	year	disease	species	serogroup		clonal complex	PorA VR1	PorA VR2	FetA VR
1	A4/M1027	B1; NIBSC_2803; Z1001	country USA	year 1937	disease invasive (unspecified/other)	Neisseria meningitidis	A	4	clonal complex ST-4 complex/subgroup IV	PorA VR1 5-2	PorA VR2 10	FetA VR F1-5
1 2	A4/M1027 120M		country USA Pakistan	year 1937 1967	disease invasive (unspecified/other) meningitis and septicaemia	Neisseria meningitidis Neisseria meningitidis	A A	4 1	clonal complex	PorA VR1 5-2 5-2	PorA VR2 10 10	FetA VR
1 2	A4/M1027 120M M00242905	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	Country USA Pakistan UK	year 1937 1967 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B	4	cional complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II	PorA VR1 5-2	PorA VR2 10	FetA VR F1-5
1 2 3 4	A4/M1027 120M M00242905 M1027	B1; NIBSC_2803; Z1001	Country USA Pakistan UK USA	year 1937 1967 2000 1937	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A	4 1 1099 4	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-4 complex/subgroup IV	PorA VR1 5-2 5-2 19	PorA VR2 10 10 15	FetA VR F1-5
1 2 3 4 5	A4/M1027 120M M00242905 M1027 M00240227	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	Country USA Pakistan UK USA UK	year 1937 1967 2000 1937 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B	4 1099 4 1100	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-4 complex/subgroup IV ST-32 complex/ET-5 complex	PorA VR1 5-2 5-2 19	PorA VR2 10 10	FetA VR F1-5
1 2 3 4 5	A4/M1027 120M M00242905 M1027 M00240227 M00282207	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	Country USA Pakistan UK USA UK UK	year 1937 1967 2000 1937 2000 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W	4 1 1099 4	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-32 complex/ET-5 complex ST-22 complex	PorA VR1 5-2 5-2 19	PorA VR2 10 10 15	FetA VR F1-5 F5-1
1 2 3 4 5 6 7	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	Country USA Pakistan UK USA UK UK Finland	year 1937 1967 2000 1937 2000 2000 1975	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A	4 1099 4 1100 1101 5	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-32 complex/ET-5 complex ST-22 complex ST-5 complex/subgroup III	PorA VR1 5-2 5-2 19	PorA VR2 10 10 15 16 9	FetA VR F1-5
1 2 3 4 5 6 7	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	Country USA Pakistan UK USA UK UK Finland	year 1937 1967 2000 1937 2000 2000 1975	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A	4 1099 4 1100 1101	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-32 complex/ET-5 complex ST-22 complex	PorA VR1 5-2 5-2 19 7	PorA VR2 10 10 15 16	FetA VR F1-5 F5-1
1 2 3 4 5 6 7	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	Country USA Pakistan UK USA UK UK Finland UK	year 1937 1967 2000 1937 2000 2000 1975 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A B	4 1099 4 1100 1101 5	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-32 complex/ET-5 complex ST-22 complex ST-5 complex/subgroup III	PorA VR1 5-2 5-2 19 7	PorA VR2 10 10 15 16 9	FetA VR F1-5 F5-1
1 2 3 4 5 6 7 8	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	country USA Pakistan UK USA UK UK Finland UK Czech Republic	year 1937 1967 2000 1937 2000 2000 1975 2000 1984	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A B W	4 1099 4 1100 1101 5 1102	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-32 complex/subgroup IV ST-32 complex/ET-5 complex ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-1 complex/subgroup I/II	PorA VR1 5-2 5-2 19 7	PorA VR2 10 10 15 16 9	FetA VR F1-5 F5-1
1 2 3 4 5 6 7 8 9	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748 129E	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054	country USA Pakistan UK USA UK Finland UK Czech Republic Canada	year 1937 1967 2000 1937 2000 2000 1975 2000 1984 1971	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A B W A	4 1099 4 1100 1101 5 1102 114	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IVI ST-4 complex/subgroup IVI ST-32 complex/ET-5 complex ST-22 complex/ST-22 complex ST-5 complex/subgroup III ST-18 complex ST-22 complex	PorA VR1 5-2 5-2 19 7 20	PorA VR2 10 10 15 16 9 14	FetA VR F1-5 F5-1 F3-1
1 2 3 4 5 6 7 8 9 10	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748 129E 0090/89	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073	country USA Pakistan UK USA UK Finland UK Czech Republic Canada Germany Czech Republic	year 1937 1967 2000 1937 2000 2000 1975 2000 1975 2000 1984 1971 1964 1989	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A A	4 1099 4 1100 1101 5 1102 114 1 1	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-32 complex/subgroup IV ST-32 complex/ET-5 complex ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-1 complex/subgroup I/II	PorA VR1 5-2 5-2 19 7 20 18-1 5-2 7	PorA VR2 10 10 15 16 9 14 3	FetA VR F1-5 F5-1 F3-1 F5-1
1 2 3 4 5 6 7 8 9 10 11	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748 129E	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073	country USA Pakistan UK USA UK Finland UK Czech Republic Canada Germany Czech Republic	year 1937 1967 2000 1937 2000 2000 1975 2000 1984 1971 1964	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A A B	4 1099 4 1100 1101 5 1102 114 1 1	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-32 complex/ET-5 complex ST-22 complex/SU5 ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-2 complex/subgroup I/II ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	PorA VR1 5-2 19 7 20 18-1 5-2	PorA VR2 10 10 15 16 9 14 3 10	FetA VR F1-5 F5-1 F3-1 F5-1
1 2 3 4 5 6 7 8 9 10 11 12	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748 129E 0090/89	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2764; Z1073 B92; NIBSC_2828; Z1092	country USA Pakistan UK USA UK Finland UK Czech Republic Canada Germany Czech Republic Philippines	year 1937 1967 2000 1937 2000 2000 1975 2000 1975 2000 1984 1971 1964 1989 1968	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A A B A A	4 1099 4 1100 1101 5 1102 114 1 1 1015	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IVI ST-4 complex/subgroup IVI ST-3c complex/ET-5 complex ST-2c complex/subgroup III ST-18 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-32 complex/ET-5 complex	PorA VR1 5-2 5-2 19 7 20 18-1 5-2 7	PorA VR2 10 10 15 16 9 9 14 3 10 16	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6
1 2 3 4 5 6 7 8 9 10 11 12 13	A4/M1027 120M M00242905 M1027 M0028207 7891 M00282207 0021/84 6748 129E 0090/89 139M	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2764; Z1073 B92; NIBSC_2828; Z1092	country USA Pakistan UK UK VK Finland UK Czech Republic Canada Germany Czech Republic Philippines Czech Republic	year 1937 1967 2000 1937 2000 2000 1975 2000 1975 2000 1984 1971 1964 1989 1968	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A B A A X	4 1099 4 1100 1101 5 1102 114 1 1 1015 1	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IVI ST-4 complex/subgroup IVI ST-3c complex/ET-5 complex ST-2c complex/subgroup III ST-18 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-32 complex/ET-5 complex	PorA VR1 5-2 5-2 19 7 20 18-1 5-2 7	PorA VR2 10 10 15 16 9 9 14 3 10 16 10	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6
1 2 3 4 5 6 7 8 9 10 11 12 13 14	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748 129E 0090/89 139M 0120/95	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2764; Z1073 B92; NIBSC_2828; Z1092	country USA Pakistan UK UK VK Finland UK Czech Republic Canada Germany Czech Republic Philippines Czech Republic	year 1937 1967 2000 1937 2000 2000 1975 2000 1975 2000 1984 1971 1964 1989 1968 1995	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A B A A X	4 1099 4 1100 1101 5 1102 114 1 1015 1 117	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IVI ST-4 complex/subgroup IVI ST-3c complex/ET-5 complex ST-2c complex/subgroup III ST-18 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-32 complex/ET-5 complex	PorA VR1 5-2 5-2 19 7 20 18-1 5-2 7	PorA VR2 10 10 15 16 9 9 14 3 10 16 10	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6

Clicking the hyperlink for any record will display full information about the profile.

							Help 🖉	Tooole	Field help: id			
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ea	arcn or	prowse weisse	eria Pupini	LJ	i dalabase							
Ente	er search crite	ria or leave blank to browse	all records									
		nance/phenotype fields			Display/so	ort options				— — Act	ion	
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					Display	7: 25 • records per	page 🕦					
					elds ()				MLST		typing antig	
id	isolate	aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1	PorA VR2	FetA VR
1	A4/M1027	B1; NIBSC_2803; Z1001	country USA	year 1937	disease invasive (unspecified/other)	Neisseria meningitidis	A	4	cional complex ST-4 complex/subgroup IV	PorA VR1 5-2	PorA VR2 10	FetA VR F1-5
1 2	A4/M1027 120M		country USA Pakistan	year 1937 1967	disease invasive (unspecified/other) meningitis and septicaemia	Neisseria meningitidis Neisseria meningitidis	A A	4 1	clonal complex	PorA VR1 5-2 5-2	PorA VR2 10 10	FetA VR
1 2	A4/M1027 120M M00242905	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	Country USA Pakistan UK	year 1937 1967 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B	4 1 1099	cional complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II	PorA VR1 5-2	PorA VR2 10	FetA VR F1-5
1 2 3 4	A4/M1027 120M M00242905 M1027	B1; NIBSC_2803; Z1001	Country USA Pakistan UK USA	year 1937 1967 2000 1937	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A	4 1 1099 4	Cional complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-4 complex/subgroup IV	PorA VR1 5-2 5-2 19	PorA VR2 10 10 15	FetA VR F1-5
1 2 3 4 5	A4/M1027 120M M00242905	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	Country USA Pakistan UK	year 1937 1967 2000 1937 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B	4 1 1099 4	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-4 complex/subgroup IV ST-32 complex/ET-5 complex	PorA VR1 5-2 5-2	PorA VR2 10 10	FetA VR F1-5
1 2 3 4 5	A4/M1027 120M M00242905 M1027 M00240227	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	Country USA Pakistan UK USA UK UK	year 1937 1967 2000 1937 2000 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B W	4 1099 4 1100	Cional complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-4 complex/subgroup IV	PorA VR1 5-2 5-2 19	PorA VR2 10 10 15	FetA VR F1-5
1 2 3 4 5 6 7	A4/M1027 120M M00242905 M1027 M00240227 M00282207	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	Country USA Pakistan UK USA UK UK Finland	year 1937 1967 2000 1937 2000 2000 1975	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A	4 1099 4 1100 1101	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-4 complex/subgroup I/I ST-32 complex/ET-5 complex ST-22 complex	PorA VR1 5-2 5-2 19 7	PorA VR2 10 10 15 16	FetA VR F1-5 F5-1
1 2 3 4 5 6 7	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	country USA Pakistan UK USA UK UK Finland UK	year 1937 1967 2000 1937 2000 2000 1975 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A B	4 1099 4 1100 1101 5	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-32 complex/ET-5 complex ST-22 complex ST-5 complex/subgroup III	PorA VR1 5-2 5-2 19 7	PorA VR2 10 10 15 16 9	FetA VR F1-5 F5-1
1 2 3 4 5 6 7 8	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	country USA Pakistan UK USA UK UK Finland UK	year 1937 2000 1937 2000 2000 1975 2000 1975 2000 1984	disease Invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A B W W	4 1099 4 1100 1101 5 1102	clonal complex ST-4 complex/subgroup I/V ST-1 complex/subgroup I/I ST-4 complex/subgroup I/V ST-32 complex/ET-5 complex ST-52 complex ST-5 complex/subgroup III ST-18 complex	PorA VR1 5-2 5-2 19 7	PorA VR2 10 10 15 16 9	FetA VR F1-5 F5-1
1 2 3 4 5 6 7 8 9	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054	country USA Pakistan UK USA UK Finland UK Czech Republic	year 1937 1967 2000 1937 2000 2000 1975 2000 1984 1971	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A B W A	4 1099 4 1100 1101 5 1102 114	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-4 complex/subgroup IV ST-32 complex/ET-5 complex ST-22 complex/ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-22 complex	PorA VR1 5-2 5-2 19 7 20	PorA VR2 10 10 15 16 9 14	FetA VR F1-5 F5-1 F3-1
1 2 3 4 5 6 7 8 9 10	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073	country USA Pakistan UK USA UK Finland UK Czech Republic Canada Germany	year 1937 1967 2000 1937 2000 2000 1975 2000 1984 1971 1964	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A A	4 1099 4 1100 1101 5 1102 114 1 1	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IVI ST-4 complex/subgroup IVI ST-32 complex/ET-5 complex ST-5 complex/subgroup III ST-16 complex ST-22 complex ST-1 complex/subgroup I/II	PorA VR1 5-2 5-2 19 7 20 18-1	PorA VR2 10 10 15 16 9 14 3	FetA VR F1-5 F5-1 F3-1 F5-1
1 2 3 4 5 6 7 8 9 10 11	A4/M1027 120M M00242905 M1027 M0028207 7891 M00282207 0021/84 6748 129E 0090/89 139M	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073	country USA Pakistan UK USA UK Finland UK Czech Republic Canada Germany Czech Republic Philippines	year 1937 1967 2000 1937 2000 2000 1975 2000 1984 1971 1964 1989 1968	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis	A B B W A B W A A B C A A A	4 1099 4 1100 1101 5 1102 114 1 1 1015 1	clonal complex ST-4 complex/subgroup I/V ST-1 complex/subgroup I/V ST-4 complex/subgroup I/V ST-22 complex/ET-5 complex ST-52 complex/subgroup I/I ST-16 complex ST-22 complex ST-22 complex ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I	PorA VR1 5-2 5-2 19 7 20 18-1 5-2	PorA VR2 10 10 15 16 9 14 3 10	FetA VR F1-5 F5-1 F3-1 F5-1
1 2 3 4 5 6 7 8 9 10 11 12	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748 129E 0090/89	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2764; Z1073 B92; NIBSC_2828; Z1092	country USA Pakistan UK USA UK Finland UK Czech Republic Canada Germany Czech Republic Philippines	year 1937 1967 2000 1937 2000 2000 1975 2000 1984 1971 1964 1989 1968	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis	A B B W A B W A A B C A A A	4 1099 4 1100 1101 5 1102 114 1 1 1015	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IVI ST-4 complex/subgroup IVI ST-32 complex/ET-5 complex ST-22 complex/subgroup III ST-18 complex ST-22 complex ST-12 complex/subgroup I/II ST-1 complex/subgroup I/II ST-32 complex/subgroup I/II ST-32 complex/ET-5 complex	PorA VR1 5-2 5-2 19 7 20 18-1 5-2 7	PorA VR2 10 10 15 16 9 14 3 10 16	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748 129E 0090/89 139M 0120/95 1	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2764; Z1073 B92; NIBSC_2828; Z1092	country USA Pakistan UK UK VK Finland UK Czech Republic Canada Germany Czech Republic Philippines Czech Republic	year 1937 1967 2000 1937 2000 2000 1975 2000 1984 1971 1964 1989 1968	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis	A B W A B W A A B A A A A E	4 1099 4 1100 1101 5 1102 114 1 1015 1 1015 1 117 864	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IVI ST-4 complex/subgroup IVI ST-32 complex/ET-5 complex ST-22 complex/subgroup III ST-18 complex ST-22 complex ST-12 complex/subgroup I/II ST-1 complex/subgroup I/II ST-32 complex/subgroup I/II ST-32 complex/ET-5 complex	PorA VR1 5-2 5-2 19 7 20 18-1 5-2 7	PorA VR2 10 10 15 16 9 14 3 10 16 10	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6
1 2 3 4 5 6 7 8 9 10 11 12 13 14	A4/M1027 120M M00242905 M1027 M00240227 7891 M00242007 0021/84 6748 129E 0090/89 139M 0120/95	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2764; Z1073 B92; NIBSC_2828; Z1092	country USA Pakistan UK UK VK Finland UK Czech Republic Canada Germany Czech Republic Philippines Czech Republic	year 1937 1967 2000 1937 2000 2000 1975 2000 1975 2000 1984 1971 1964 1989 1968 1995	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningittidis Neisseria meningittidis	A B B W A B W A A B A A A E	4 1099 4 1100 1101 5 1102 114 1 1015 1 1015 1 117	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IVI ST-4 complex/subgroup IVI ST-32 complex/ET-5 complex ST-22 complex/subgroup III ST-18 complex ST-22 complex ST-12 complex/subgroup I/II ST-1 complex/subgroup I/II ST-32 complex/subgroup I/II ST-32 complex/ET-5 complex	PorA VR1 5-2 5-2 19 7 20 18-1 5-2 7	PorA VR2 10 10 15 16 9 14 3 10 16 10	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6

# 11.10 Querying isolate data

The 'Search or browse database' page of an isolate database allows you to also search by combinations of provenance criteria, scheme and locus data, and more.



To start with, only one provenance field search box is displayed but more can be added by clicking the '+' button (highlighted). These can be linked together by 'and' or 'or'.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definition	ns   Database submissions		
		Toggle: <i>i</i> Field help: id	→ Go
Search Neisseria PubMLST database			
Isolate provenance/phenotype fields         Combine with: AND ↓         country ↓ = ↓ USA + ↓         year ↓ > ↓         Action         Reset       Submit	Display/sort options Order by: id Display: 25    records per page []		Modify form options

After the search has been submitted, the results will be displayed in a table.

Pub	MLST/ E	Breakdo	wn: Isola	te field	Profile/ST   List  s   Scheme/alleles   Publicati   Options   Profiles/sequence		e submissio	ns					
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id	isolate	aliases	country	vear	disease	species	serogroup	ST	clonal complex		PorA VR2 Fe		
341	M7085		USA		invasive (unspecified/other)				ST-11 complex/ET-37 complex				
499	MDL01A0601		USA	2001	meningitis	Neisseria meningitidis		1378					
500	MDL01A2447		USA	2001	invasive (unspecified/other)	Neisseria meningitidis	Y	1379	ST-23 complex/Cluster A3				
866	MD01227		USA	2001		Neisseria meningitidis	1	1624	ST-167 complex				
867	MDO1056		USA	2001		Neisseria meningitidis	1	1625	ST-23 complex/Cluster A3				
868	MDO1066		USA	2001		Neisseria meningitidis	1	1626	ST-269 complex				
2281	M7089		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex	5	2		
2299	M7257		USA		invasive (unspecified/other)				ST-11 complex/ET-37 complex	5	2		
2316	M7086		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	22	ST-22 complex	6	3		
2317	M7084		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	22	ST-22 complex	6	3		
2322	M7092		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1065	ST-22 complex	6	3		
2323	M7100		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1286	ST-22 complex	6	3		
2324	M7259		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1066	ST-22 complex	6	3		

Each field can be queried using standard operators.

More search features are available by clicking the 'Modify form options' tab on the right-hand side of the screen.

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id isolate 341 M708 499 MDL01A0 500 MDL01A2 866 MD012 867 MD010 281 M708 299 M725 316 M708 317 M708 322 M709	3 4 2 aliase 5 6 6 0 1 4 47 27 5 6 6 6 9 7 3 4 4 2	B Country USA USA USA USA USA USA USA USA USA	year 2000 2001 2001 2001 2001 2000 2000 200	Isolate fields [] disease invasive (unspecified/other) meningitis invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi	s Y s Y s Y s W s W s W s W	11 1378 1379 1624 1625 1626 11 11 22 22 1065	cional complex ST-11 complex/ET-37 complex ST-23 complex/Cluster A3 ST-23 complex/Cluster A3 ST-167 complex ST-23 complex/Cluster A3 ST-269 complex ST-211 complex/ET-37 complex ST-11 complex/ET-37 complex ST-22 complex ST-22 complex ST-22 complex ST-22 complex	PorA VR1	PorA VR2 Fe		
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A tab will be displayed. Different options will be available here depending on the database. Queries will be combined from the values entered in all form sections. Possible options are:

- · Provenance fields
  - Search by combination of provenance field values, e.g. country, year, sender.
- · Allele designations/scheme field values
  - Search by combination of allele designations and/or scheme fields e.g. ST, clonal complex information.
- Allele designation status
  - Search by whether allele designation status is confirmed or provisional.
- · Tagged sequence status
  - Search by whether tagged sequence data is available for a locus. You can also search by sequence flags.
- · Attribute values list
  - Enter a list of values for any provenance field, locus, or scheme field.
- Filters
  - Various filters may be available, including
    - * Publications
    - * Projects
    - * MLST profile completion status
    - * Clonal complex
    - * Sequence bin size
    - * Inclusion/exclusion of old versions

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If the interface is modified, a button to save options becomes available within the tab. If this is clicked, the modified form will be displayed the next time you go to the query page.

## 11.10.1 Query by allele designation/scheme field

Queries can be combined with allele designation/scheme field values.

Make sure that the allele designation/scheme field values fieldset is displayed by selecting it in the 'Modify form options' tab.

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Designations can be queried using standard operators.

Additional search terms can be combined using the '+' button.

Add your search terms and click 'Submit'. Allele designation/scheme field queries will be combined with terms entered in other sections.

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## 11.10.2 Query by allele designation count

Queries can be combined with counts of the total number of designations or for individual loci.

Make sure that the allele designation counts fieldset is displayed by selecting it in the 'Modify form options' tab.

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	<ul> <li>Tagged sequence status</li> </ul>										
	Attribute values list										
	Filters										

For example, to find all isolates that have designations at >1000 loci, select 'total designations > 1000', then click 'Submit'.

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id	isolate	aliases	country	year	disease	species	serogroup	(bp)		ST	cional complex	VR1	VR2	VR
1	A4/M1027	B1; NIBSC_2803; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	2069108	364	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; NIBSC_2822; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	2059411	359	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
7	7891	B54; NIBSC_2760; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	2057385	199	5	ST-5 complex/subgroup III	20	9	F3-1
10	6748	B73; NIBSC_2784; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	4241338	652	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129E	B92; NIBSC_2828; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	2072690	272	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
10	120M	D00- NIDSC 2705-	Philippinoc	1069		Noicearia	٨	01/1711	202	1	QT 1	5.2	10	E5 1

You can also search for isolates where any isolate has a particular number of designations. Use the term 'any locus' to do this.

Finally, you can search for isolates with a specific number of designations at a specific locus.

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Additional search terms can be combined using the '+' button. Designation count queries will be combined with terms entered in other sections.

**Note:** Searches for 'all loci' with counts that include zero, e.g. 'count of any locus = 0' or with a '<' operator are not supported. This is because such searches have to identify every isolate for which one or more loci are missing. In databases with thousands of loci this can be a very expensive database query.

## 11.10.3 Query by allele designation status

Allele designations can be queried based on their status, i.e. whether they are confirmed or provisional. Queries will be combined from the values entered in all form sections.

Make sure that the allele designation staus fieldset is displayed by selecting it in the 'Modify form options' tab.

Query: Search   Profile/ST           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions											
Help:     Toggle:     Field help:     id     • Go											
Enter search criteria or leave blank to browse all records. Modify form para Isolate provenance/phenotype fields id • • = • Enter value	meters to filter or enter a list of values.  Display/sort options  Order by: id	X Modify form parameters Modify form									
	Display: 25    records per page ❶	Click to add or remove additional query terms:									

Select a locus from the dropdown box and either 'provisional' or 'confirmed'. Additional query fields can be displayed by clicking the '+' button. Click 'Submit'.

PubMLST Break		eme/alleles   Publications	initions   Database submissions		
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Analysis: Codons			AST		
Export: Dataset	Contigs Sequences				
		_			

Provisional allele designations are marked within the results tables with a pink background. Any scheme field designations that depend on the allele in question, e.g. a MLST ST, will also be marked as provisional.

# 11.10.4 Query by sequence tag count

Queries can be combined with counts of the total number of tags or for individual loci.

Make sure that the tagged sequence counts fieldset is displayed by selecting it in the 'Modify form options' tab.

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Enter search criteria or leave blank to browse all records. Modify form parameters to filter or enter a list of values.  Isolate provenance/phenotype fields  Id  I  Display/sort options  Order by: Id  Display: 25  records per p  Action  Reset Submit	<ul> <li>Modify form parameters</li> <li>Modify form options</li> <li>Click to add or remove additional query terms:</li> <li>Provenance fields</li> <li>Allele designation s/scheme field values</li> <li>Allele designation counts</li> <li>Allele designation status</li> <li>Tagged sequence counts</li> <li>Tagged sequence status</li> <li>Attribute values list</li> <li>Filters</li> </ul>

For example, to find all isolates that have sequence tags at >1000 loci, select 'total tags > 1000', then click 'Submit'.

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1	A4/M1027	B1; NIBSC_2803; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	2069108	364	4	ST-4 complex/subgroup IV	5-2	10	F1-8
2	120M	B35; NIBSC_2822; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	2059411	359	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
7	7891	B54; NIBSC_2760; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	2057385	199	5	ST-5 complex/subgroup III	20	9	F3-1
10	6748	B73; NIBSC_2784; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	4241338	652	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129E	B92; NIBSC_2828; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	2072690	272	1	ST-1 complex/subgroup I/II	5-2	10	F3-6

You can also search for isolates where any isolate has a particular number of sequence tags. Use the term 'any locus' to do this.

Finally, you can search for isolates with a specific number of tags at a specific locus.

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ige id	: 1 2 isolate	3 4 5 6 aliases B1; NIBSC_2803; Z1001 B73;	789 Isol	iate fie year	Lest disease invasive (unspecified/other) invasive	species Neisseria meningitidis Neisseria		size (bp)		51	clonal complex ST-4 complex/subgroup IV ST-1	PorA VR1	PorA VR2	Fet VF F1-
ige id 1	: 1 2 isolate A4/M1027	3 4 5 6 aliases B1; NIBSC_2803; Z1001	789 Isol country USA	late fie year 1937	Lest ids ① disease invasive (unspecified/other)	species Neisseria meningitidis	A	size (bp) 2069108	364	4	clonal complex ST-4 complex/subgroup IV	PorA VR1 5-2	PorA VR2 10	Fet VF F1-
ige id 1	isolate A4/M1027 6748	3 4 5 6 aliases B1; NIBSC_2803; Z1001 B73; NIBSC_2784; Z1073 NIBSC_2731;	789 Isol country USA	ate fie year 1937 1971	Lest disease invasive (unspecified/other) invasive	species Neisseria meningitidis Neisseria meningitidis Neisseria	A	size (bp) 2069108	364	4	Clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-5	PorA VR1 5-2	PorA VR2 10	Fet VF
id	isolate A4/M1027 6748	3 4 5 6 aliases B1; NIBSC_2803; Z1001 B73; NIBSC_2784; Z1073	7 8 9 Isof Country USA Canada	ate fie year 1937 1971	Lest disease invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis	A	size (bp) 2069108 4241338	364 652	4 1 5	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II	PorA VR1 5-2 18-1	PorA VR2 10 3	Fet VF F1-

Additional search terms can be combined using the '+' button. Sequence tag count queries will be combined with terms entered in other sections.

**Note:** Searches for 'all loci' with counts that include zero, e.g. 'count of any locus = 0' or with a '<' operator are not supported. This is because such searches have to identify every isolate for which one or more loci are not tagged. In databases with thousands of loci this can be a very expensive database query.

## 11.10.5 Query by tagged sequence status

Sequence tags identify the region of a contig within an isolate's sequence bin entries that correspond to a particular locus. The presence or absence of these tags can be queried as can whether or not the sequence has an a flag associated with. These flags designate specific characteristics of the sequences. Queries will be combined from the values entered in all form sections.

Make sure that the tagged sequences status fieldset is displayed by selecting it in the 'Modify form options' tab.

Purin/1057 Breakdown: Isolate fields   Scheme/alleles   Pu Links: Contents   Home   Options   Profiles/seq		
Search or browse Neisseria PubMLS	· · · · · · · · · · · · · · · · · · ·	Field help: id • Go
Enter search criteria or leave blank to browse all records. Modify form Isolate provenance/phenotype fields id	n parameters to filter or enter a list of values. Display/sort options + 0 Order by: id	Modify form parameters Modify
	Display: 25    records per page ●	Click to add or remove additional query terms: • • Provenance fields • • Allele designations/scheme field values • • Allele designation counts • • Allele designation status • • Tagged sequence counts • • Tagged sequence status • • Attribute values list • • Filters

Select a specific locus in the dropdown box (or alternatively 'any locus') and a status. Available status values are:

- untagged
  - The locus has not been tagged within the sequence bin.
- tagged
  - The locus has been tagged within the sequence bin.
- complete
  - The locus sequence is complete.
- incomplete
  - The locus sequence is incomplete normally because it continues beyond the end of a contig.
- flagged: any
  - The sequence for the locus has a flag set.
- flagged: none
  - The sequence for the locus does not have a flag set.
- flagged: <specific flag>
  - The sequence for the locus has the specific flag chosen.

Ouer:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/Sequences definitions   Database submissions	
Help[2] Toggle: () Field help: id	Go
Search or browse Neisseria PubMLST database	
Enter search criteria or leave blank to browse all records.	Modify
Isolate provenance/phenotype fields     Tagged sequence status	form
id v = v Enter value + () NEIS0001 (lpxC) v is flagged: internal stop codon v + ()	options
- Display/sort options - Action -	
Order by: id • ascending • Reset Submit	
Display: 25 v records per page 0	
1 record returned. Click the hyperlink for detailed information.	
Isolate fields <b>o</b> MLST Finetyping antigens	
id isolate aliases country year disease species serogroup ST clonal complex PorA VR2 FetA VR	
2077 153 alpha153 Germany 1999 carrier Neisseria meningitidis E 60 ST-60 complex 5 2 F1-7	
Analysis tools:	
Breakdown: Fields Two Field Polymorphic sites Combinations Schemes/alleles Publications Sequence bin Tag status	
Analysis: Codons Presence/Absence Genome Comparator BLAST Export: Dataset Contigs Sequences	
Export Dataset Contigs Sequences	

#### See also:

Sequence tag flags

## 11.10.6 Query by list of attributes

The query form can be modified with a list box in to which a list of values for a chosen attribute can be entered - this could be a list of ids, isolate names, alleles or scheme fields. This list will be combined with any other criteria or filter used on the page.

If the list box is not shown, add it by selecting it in the 'Modify form options' tab.

Help C	Toggle: () Field help: id • Go
Search or browse Neisseria PubMLST database	
Enter search criteria or leave blank to browse all records. Modify form parameters to filter or enter a list of values.  Isolate provenance/phenotype fields Id  Enter value  Order by: Id	Modify form parameters options
Display: 25 → records per pag	Click to add or remove additional query terms:

Select the attribute to query and enter a list of values.

Image: I	ProbMLST         Query: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions							
Enter search ortleria or leave blank to browse all records.  Isolate provenance/phenotype fields id	Help C	Toggle: 🚯 Field help: id 🗸 🗸 Go						
Isolate provenance/phenotype fields       Attroute values IIST         id       • Entervalue       •         Id       1       1         2       3       4         5       -       -         Order by:       id       •       •         Display/soft options       -       Action       -         Order by:       id       •       •       ascending       Reset       Submit         5       records returned. Click the hyperlinks for detailed information.       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -	Search or browse Neisseria PubMLST database							
Isolate provenance/phenotype fields       Attribute values list         id       • Entervalue       •         12       3         3       4         5       5         Display/soft options       -         Order by: id       •       •         Display: 25 • records per page •       •         5       •       •         6       •       •         1       •       •         0       •       •         0       •       •         0       •       •         0       •       •         0       •       •         0       •       •         0       •       •         0       •       •         1       •       •         4       •       •         5       •       •         6       •       •         1       •       •         1       •       •         1       •       •         2       10001       •         1       •       •         1       • <td></td> <td></td>								
Isolate provenance/phenotype fields       Attribute values list         id <ul> <li>Enter value</li> <li>Field: id</li> <li>id</li> <li>a</li> <li>a</li> <li>a</li> <li>a</li> <li>a</li> <li>b</li> <li>c</li> <li>c</li> <li>a</li> <li>c</li> <lic< li=""> <li>c</li> <li>c</li></lic<></ul>	Enter search criteria or leave blank to browse all records.	Modif						
id       • • Enter value       • • PieldC id         1       1       1         2       3       4         5       5       5         Order by:       id       • • ascending       Reset         Display/sort options       • • ascending       Reset       Submit         Display:       25       • records per page       • • • • • • • • • • • • • • • • • • •								
2       3         9       5         Display/soft options       Action         Order by: id       id         Display: 25 records per page •         5         S records returned. Click the hyperlinks for detailed information.         Image: Solate fields •	id							
3       4         5	1							
4         5               Order by:       id         0 isplay/sort options         Stream								
Display/soft options       Action         Order by:       id       ascending       Reset       Submit         Display:       25 records per page       Submit         5 records returned. Click the hyperlinks for detailed information.         1       AdM1027       B1; NIBSC_2803; Z1001       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       5-2       10       F1-5         2       120M       B35; NIBSC_2822; Z103F       Pakistan       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       5-2       10       F1-5         2       120M       B35; NIBSC_2822; Z103F       Pakistan       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       5-2       10       F1-5         3       M00242905       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       5-2       10       F5-1         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/s	4							
Order by: id       seconds per page         Display: 25 • records per page         5 records returned. Click the hyperlinks for detailed information.         Isolate fields O       ML ST       Finetyping antigens         AdMIN027 B1: NIBSC_2003; Z1001       USA       Display: 25 • records returned. Click the hyperlinks for detailed information.         Isolate fields O       ML ST       Finetyping antigens         AdMIN027 B1: NIBSC_2003; Z1001       USA       Display: 25 • records returned. Click the hyperlinks for detailed information.         Isolate fields O       ML ST       Finetyping antigens         AdMIN027 B1: NIBSC_2003; Z1001       USA       PorA VR1 PorA VR2 FetA VR         2       200M B35; NIBSC_2023; Z1001       USA       10 F1-5         UK 2000 invasive (unspecified/other) Neisseria meningitidis       A 1 ST-1 complex/subgroup IVI       5         UK 2000 invasive (unspecified/other) Neisseria meningitidis       B 1009       T-1 complex/subgroup IVI       5         M10242095       UK 2000 invasive (unspecified/other) Neisseria meningitidis <t< td=""><td>5</td><td></td></t<>	5							
Order by: id       seconds per page         Display: 25 • records per page         5 records returned. Click the hyperlinks for detailed information.         Isolate fields O       ML ST       Finetyping antigens         AdMIN027 B1: NIBSC_2003; Z1001       USA       Display: 25 • records returned. Click the hyperlinks for detailed information.         Isolate fields O       ML ST       Finetyping antigens         AdMIN027 B1: NIBSC_2003; Z1001       USA       Display: 25 • records returned. Click the hyperlinks for detailed information.         Isolate fields O       ML ST       Finetyping antigens         AdMIN027 B1: NIBSC_2003; Z1001       USA       PorA VR1 PorA VR2 FetA VR         2       200M B35; NIBSC_2023; Z1001       USA       10 F1-5         UK 2000 invasive (unspecified/other) Neisseria meningitidis       A 1 ST-1 complex/subgroup IVI       5         UK 2000 invasive (unspecified/other) Neisseria meningitidis       B 1009       T-1 complex/subgroup IVI       5         M10242095       UK 2000 invasive (unspecified/other) Neisseria meningitidis <t< td=""><td></td><td></td></t<>								
Order by: id       Bascending       Reset       Submit         Display: 25 • records per page •         5 records returned. Click the hyperlinks for detailed information.         Isolate fields •       MLST       Finetyping antigens         AdMIN027       B1: NIBSC_2003; 21001       USA       T clonal complex       PorA VR1 PorA VR2 FetA VR         AdMIN027       B1: NIBSC_2003; 21001       USA       T clonal complex       PorA VR1 PorA VR2 FetA VR         2       100M       B35; NIBSC_2003; 21001       USA       200 invasive (unspecified/other) Neisseria meningitidis       A 1 ST-1 complex/subgroup IV       5-2       10       F1-5         2 120M       B35; NIBSC_2023; 21035       Paiseria meningitidis       A 1 ST-1 complex/subgroup IV       5-2       10       F1-5         A M00242905       UK 2000 invasive (unspecified/other) Neisseria meningitidis       A 1 ST-4 complex/subgroup IV       5         M00240227       UK 2000 invasive (unspecified/other) Neisseria meningitidis <td colsp<="" td=""><td>Diselevited editors</td><td>201 </td></td>	<td>Diselevited editors</td> <td>201 </td>	Diselevited editors	201 					
Display:       25 • records per page •         5 records returned. Click the hyperlinks for detailed information.         id       isolate       finite         1       A4/M1027       B1; NIBSC_2803; Z1001       USA         1       A4/M1027       B1; NIBSC_2803; Z1001       USA         2       120M       B35; NIBSC_2822; Z1035       Pakistan 1967         3       M00242905       UK       2000 invasive (unspecified/other) Neisseria meningitidis       A         4       M1027       B43; NIBSC_2822; Z1035       Pakistan 1967       meningitidis       B       1099         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other) Neisseria meningitidis       B       1099         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other) Neisseria meningitidis       B       1009       15       19       15         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other) Neisseria meningitidis       B       1100 ST-32 complex/ET-5 complex       7       16         Invasive tools:         Breakdown: Fields Two Field Combinations Polymorphic sites Schemes/alleles Publications Sequence bin Tag status <tr< td=""><td></td><td></td></tr<>								
5 records returned. Click the hyperlinks for detailed information.           Isolate         Isolate fields O         MLST         Finetyping antigens           1         A4/M1027         B11, NIBSC, 2803; 21001         USA         1937         invasive (unspecified/other) Neisseria meningitidis         A         4         ST-4 complex/subgroup IV         5-2         10         F1-5           2         120M         B35; NIBSC_2822; 21035         Pakistan 1967 meningitis and septicaemia Neisseria meningitidis         A         4         ST-4 complex/subgroup IV         5-2         10         F1-5           3         M00242905         UK         2000 invasive (unspecified/other) Neisseria meningitidis         B         1099         19         15           4         M1027         B43; NIBSC_3076; Z1043         USA         1937         invasive (unspecified/other) Neisseria meningitidis         B         1009         19         15           4         M1027         B43; NIBSC_3076; Z1043         USA         1937         invasive (unspecified/other) Neisseria meningitidis         B         1100         ST-4 complex/subgroup IV         5           5         M00240227         UK         2000         invasive (unspecified/other) Neisseria meningitidis         B         1100         ST-32 complex/ET-5 complex         7         16 <td></td> <td></td>								
Isolate fields 0       MLST       Finetyping antigens         id isolate       aliases       country year       disease       species       serogroup       ST       clonal complex       PorA VR1       PorA VR2       FetA VR         1       A4MN1027       B1; NIBSC_2803; Z1001       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4       complex/subgroup IVI       5-2       10       F5-1         2       120M       B35; NIBSC_282; Z1035       Pakistan 1967       mexisseria       meningitidis       B       1099       19       15         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       B       1100       ST-32       complex/ET-5       complex/       7       16         Analysis tools:         Breakdown:       Field       Two Field </td <td>Display. 25 - Tecolds per page •</td> <td></td>	Display. 25 - Tecolds per page •							
Isolate fields 0       MLST       Finetyping antigens         id isolate       aliases       country year       disease       species       serogroup       ST       clonal complex       PorA VR1 PorA VR2 FetA VR         1       A4/M1027       B1; NIBSC_2803; Z1001       USA       1937       invasive (unspecified/other) Neisseria meningitidis       A       4       ST-4       complex/subgroup IV       5-2       10       F1-5         2       120M       B35; NIBSC_282; Z1035       Pakistan 1967       meningitidis       A       4       ST-4       complex/subgroup IV       5-2       10       F1-5         3       M00242905       UK       2000       invasive (unspecified/other) Neisseria meningitidis       B       1099       19       15         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other) Neisseria meningitidis       B       1100       ST-4       complex/subgroup IV       5         5       M00240227       UK       2000       invasive (unspecified/other) Neisseria meningitidis       B       1100       ST-4       complex/ET-5       complex/ET-5       complex/ET-5       complex/ET-5 <td< td=""><td></td><td></td></td<>								
id       isolate       aliases       country       year       disease       species       serogroup       ST       clonal complex       PorA VR1       PorA VR2       FetA VR         1       A4/M1027       B1; NIBSC_203; 21001       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       5-2       10       F1-5         2       1200       B35; NIBSC_2822; 21035       Pakistan 1967       meningitidis       A       1       ST-1 complex/subgroup IV       5-2       10       F1-5         3       M00242905       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1099       19       15         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       B       1009       19       15         5       M00240227       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1100       ST-4 complex/subgroup IV       5         6       M00240227       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1100       ST-4 complex/subgroup IV       16	5 records returned. Click the hyperlinks for detailed information.							
id       isolate       aliases       country       year       disease       species       serogroup       ST       clonal complex       PorA VR1       PorA VR2       FetA VR         1       A4/M1027       B1; NIBSC_203; 21001       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       5-2       10       F1-5         2       1200       B35; NIBSC_2822; 21035       Pakistan 1967       meningitidis       A       1       ST-1 complex/subgroup IV       5-2       10       F1-5         3       M00242905       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1099       19       15         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       B       1009       19       15         5       M00240227       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1100       ST-4 complex/subgroup IV       5         6       M00240227       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1100       ST-4 complex/subgroup IV       16								
id       isolate       aliases       country       year       disease       species       serogroup       ST       clonal complex       PorA VR1       PorA VR2       FetA VR         1       A4/M1027       B1; NIBSC_2803; Z1001       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       5-2       10       F1-5         2       1200       B35; NIBSC_2822; Z1035       Pakistan 1967       meningitidis       A       1       ST-1 complex/subgroup IV       5-2       10       F1-5         3       M00242905       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1099       19       15         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       B       1009       19       15         5       M00240227       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1100       ST-4 complex/subgroup IV       16         5       M00240227       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1100       ST-4 complex/subgroup IV       16	Isolate fields <b>f</b>	MLST Finetyping antigens						
2       120M       B35; NIBSC_2822; Z1035       Pakistan       1967       meningitis and septicaemia       Neisseria meningitidis       A       1       ST-1 complex/subgroup I/II       5-2       10       F5-1         3       M00242905       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1099       19       15         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup I/I       5         5       M00240227       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1100       ST-32 complex/ET-5 complex       7       16         Analysis tools:         Breakdown: Fields Two Field Combinations Polymorphic sites Schemes/alleles Publications Sequence bin Tag status         Analysis:       BURST       Codons       Presence/Absence Genome Comparator       BLAST								
3       M00242905       UK       2000 invasive (unspecified/other) Neisseria meningitidis       B       1099       19       15         4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other) Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       19       15         5       M00240227       UK       2000 invasive (unspecified/other) Neisseria meningitidis       B       1100 ST-32 complex/ET-5 complex       7       16         Analysis tools:         Breakdown: Fields Two Field Combinations Polymorphic sites Schemes/alleles Publications Sequence bin Tag status         Analysis:       BURST       Codons       Presence/Absence       Genome Comparator       BLAST	1 A4/M1027 B1; NIBSC_2803; Z1001 USA 1937 invasive (unspecified/other) Neisseria meningitidis A							
4       M1027       B43; NIBSC_3076; Z1043       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV         5       M00240227       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1100       ST-32 complex/ET-5 complex       7       16         Analysis tools:       Breakdown:       Fields       Two Field       Combinations       Polymorphic sites       Schemes/alleles       Publications       Sequence bin       Tag status         Analysis:       BURST       Codons       Presence/Absence       Genome Comparator       BLAST								
5 M00240227       UK 2000 invasive (unspecified/other) Neisseria meningitidis       B       1100 ST-32 complex/ET-5 complex       7       16         Analysis tools:       Breakdown: Fields       Two Field       Combinations       Polymorphic sites       Schemes/alleles       Publications       Sequence bin       Tag status         Analysis:       BURST       Codons       Presence/Absence       Genome Comparator       BLAST								
Analysis tools:         Breakdown: Fields Two Field Combinations Polymorphic sites Schemes/alleles Publications Sequence bin Tag status         Analysis: BURST Codons Presence/Absence Genome Comparator BLAST								
Breakdown:         Fields         Two Field         Combinations         Polymorphic sites         Schemes/alleles         Publications         Sequence bin         Tag status           Analysis:         BURST         Codons         Presence/Absence         Genome Comparator         BLAST	5 W00240227	1100 ST-S2 complex 1-5 complex 7 To						
Analysis: BURST Codons Presence/Absence Genome Comparator BLAST	Analysis tools:							
Analysis: BURST Codons Presence/Absence Genome Comparator BLAST	Breakdown: Fields Two Field Combinations Polymorphic sites Schemes/alleles Publications Sequ	uence bin Tag status						
Evnor: Dataset Contras Sequences	Export: Dataset Contigs Sequences							

## 11.10.7 Query filters

There are various filters that can additionally be applied to queries, or the filters can be applied solely on their own so that they filter the entire database.

Make sure that the filters fieldset is displayed by selecting it in the 'Modify form options' tab.

Query: Search   Profile/ST Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definition	s	
	Help 🗹 🛛 Toggle: 🚯 🖡	Field help: id 🔹 🖌 😡
Search or browse Neisseria PubMLST databas	e	
Enter search criteria or leave blank to browse all records. Modify form parameters to f	ilter or enter a list of values.	Modify
	Display/sort options	form
id → = → Enter value + 0	Order by: id	Modify form parameters options
	Display: 25 👻 records per page 🜖	Click to add or remove additional query terms:
		Provenance fields
		Allele designations/scheme field values
		Allele designation counts
		Allele designation status
		Co Tagged sequence counts
		<ul> <li>Tagged sequence status</li> </ul>
		Attribute values list
		Filters

The filters displayed will depend on the database and what has been defined within it. Common filters are:

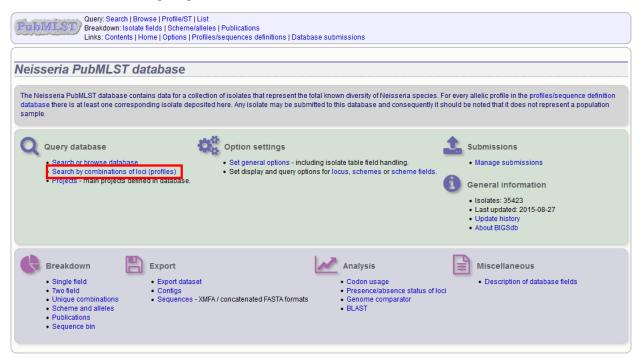
• Publication - Select one or more publication that has been linked to isolate records.

- Project Select one or more project that isolates belong to.
- Profile completion This is commonly displayed for MLST schemes. Available options are:
  - complete All loci of the scheme have alleles designated.
  - incomplete One or more loci have not yet been designated.
  - partial The scheme is incomplete, but at least one locus has an allele designated.
  - started At least one locus has an allele designated. The scheme mat be complete or partial.
  - not started The scheme has no loci with alleles designated.
  - Sequence bin Specify whether any sequence data has been associated with a record. Specific threshold values may be selected if these have been *set up for the database*.
  - Provenance fields Dropdown list boxes of values for specific provenance fields may be present if set for the database. Users can choose to *add additional filters*.
  - Old record versions Checkbox which, if selected, will include all record versions in a query.

# 11.11 Querying by allelic profile

If a scheme, such as MLST, has been defined for an isolate database it is possible to query the database against complete or partial allelic profiles. Even if no scheme is defined, queries can be made against all loci.

On the index page, click 'Search by combinations of loci (profiles)' for any defined scheme. Enter either a partial (any combination of loci) or complete profile.



If multiple schemes are defined, you may have to select the scheme you wish to query in the 'Schemes' dropdown box and click 'Select'.

Outp://www.search.jprofile/ST.jclist           Breakdown: Isolate fields.jScheme/alleles.jPublications           Links: Contents.jHome.jOptions.jProfiles/sequences definitions.jDatabase submiss	sions
	Toggle: i
Search Neisseria PubMLST database by combinations of	loci
Schemes	
Please select the scheme you would like to query:	
MLSI - Select	
-Please enter your allelic profile below. Blank loci will be ignored	searching remote database ——
abcZ adk aroE fumC gdh pdhC pgm ST:	Autofil
	Display/sort options
Project:  vi Search: Exact or nearest match	
Include old record versions	Display: 25 🗸 records per page 👔
Action	
Reset Submit	

Enter the combination of alleles that you want to query for. Fields can be left blank.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: i
Search Neisseria PubMLST database by combinations of loci	
Schemes	
Please select the scheme you would like to query:	
MLST - Select	
<u></u>	
Please enter your allelic profile below. Blank loci will be ignored. — Autofill profile by searching remote database —	
abcZ     adk     aroE     fumC     gdh     pdhC     pgm     ST:     Autofill       2     3     4     3     8     4     Autofill     Autofill	
Filters Options Display/sort options	
	scending 👻
Include old record versions     Display: 25      records per page	
Action	
Reset Submit	

Alternatively, for scheme profiles, you can enter a primary key value (e.g. ST) and select 'Autofill' to automatically fill in the associated profile.

Ouery:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: i
Search Neisseria PubMLST database by combinations of loci	
Schemes	
Please select the scheme you would like to query:	
MLST	
abcZ     adk     aroE     fumC     gdh     pdhC     pgm     ST:     44     Autofill       9     6     9     9     6     9	
- Filters - Display/sort options	
Project: • Search: Exact or nearest match • Order by: id • ascending •	
□ Include old record versions Display: 25  v records per page i	
Action	
Reset Submit	

Select the number of loci that you'd like to match in the options dropdown box. Available options are:

- Exact or nearest match
- · Exact match only
- x or more matches
- y or more matches
- z or more matches

Where x,y, and z will range from n-1 to 1 where n is the number of loci in the scheme.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: i
Search Neisseria PubMLST database by combinations of loci	
Schemes	
Please select the scheme you would like to query:	
MLST v Select	
Please enter your allelic profile below. Blank loci will be ignored. — Autofill profile by searching remote database —	
abcZ adk aroE fumC gdh pdhC pgm ST: 44 Autofill	
- Filters - Display/sort options - Display/so	
Project.	
Include old record versions Display: 25 🚽 records per page 👔	
Action	
Reset Submit	

Click 'Submit'.

			ts   Home   Option:		undere da entre en activita entre l						
											Toggle
	oh Noic	oorio D	UDMI CT d	oto	haaa hu aamhir	actions of los					
ar	cri neis	seria P	IDIMEST O	ala	base by combir		1				
ho	mes										
ne	lies										
ease	select the so	heme you wou	Id like to query:								
				0.1	-						
ILST				Selec	*						
-Ple	ease enter yo	ur allelic profile	below. Blank loci	will be	ignored. — — —	-Autofill profile by searc	hing remote o	database ——			
al	ocZ ad	k aroE	fumC g	idh	pdhC pgm	ST: 44		Autofill			
	96	9	9	9	6 9						
- Cill	ters				Options		Display/c	sort options			
	Project										
					i Search: Exact	t or nearest match 👻	Order b		•	ascend	ing 👻
	nclude old re	cord versions							-		
-Ac	tion						Displa	ay: 25 👻 records per page [	i		
	set Subr	nit					Displa	ay: 25 → records per page[	Ĩ		
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Re		_					Displa	ay: 25 ় records per page [	Ī		
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# 11.12 Retrieving isolates by linked publication

Click 'Publications' in the Breakdown section of the contents page.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
Neisseria PubMLST database	
The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it s sample.	
Query database <ul> <li>Search or browse database</li> <li>Search by combinations of loci (profiles)</li> <li>Projects - main projects defined in database.</li> </ul> <ul> <li>Set display and query options for locus, schemes or scheme fields.</li> </ul>	Submissions • Manage submissions General information • Isolates: 35423 • Last updated: 2015-08-27 • Update history • About BIGSdb
Breakdown     Single field     Won field     Unique combinations     Scheme and alleles     Publications     Sequence bin	Miscellaneous     Description of database fields

A list of publications linked by isolates within the database will be displayed.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions					
Publicati	on breakdown of dataset				
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	All authors    Order by: number of isolates   descending	Submit			
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PubMed id Yea	r Citation	Title	Isolates in database		
17517841 20	7 Taha MK, Vázquez JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enríquez R, Fazio C, Frosch M, Heuberger S, Hoffmann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczynska A, Stefanelli P, Thulin S, Tzanakaki G, Unemo M, Vogel U, Zarantonelli ML (2007) Antimicrob Agents Chemother 51: 2784-92	Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis.	1670 isolates		
18815379 200	18 Buckee CO, Jolley KA, Recker M, Penman B, Kriz P, Gupta S, Maiden MC (2008) Proc Natl Acad Sci U S A 105: 15082-7	Role of selection in the emergence of lineages and the evolution of virulence in Neisseria meningitidis.	1054 isolates		
15776372 20	15 Claus H, Maiden MC, Wilson DJ, McCarthy ND, Jolley KA, Urwin R, Hessler F, Frosch M, Vogel U (2005) J Infect Dis 191: 1263-71	Genetic analysis of meningococci carried by children and young adults.	822 isolates		
15528708 200	4 Yazdankhah SP, Kriz P, Tzanakaki G, Kremastinou J, Kalmusova J, Musilek M, Alvestad T, Jolley KA, Wilson DJ, McCarthy ND, Caugant DA, Maiden MC (2004) J Clin Microbiol 42: 5146-53	Distribution of serogroups and genotypes among disease- associated and carried isolates of Neisseria meningitidis from the Czech Republic, Greece, and Norway.	667 isolates		
17825091 200	17 Bennett JS, Jolley KA, Sparling PF, Saunders NJ, Hart CA, Feavers IM, Maiden MC (2007) BMC Biol 5: 35	Species status of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from multilocus sequence typing.	576 isolates		
15537808 200	5 Jolley KA, Wilson DJ, Kriz P, McVean G, Maiden MC (2005) Mol Biol Evol 22: 562-9	The influence of mutation, recombination, population history, and selection on patterns of genetic diversity in Neisseria meningitidis.	378 isolates		
18375809 20	8 Russell JE. Urwin R. Grav SJ. Fox AJ. Feavers IM. Maiden MC (2008) Microbiology 154:	Molecular epidemiology of meningococcal disease in England and	323 isolates		

These can be filtered by author and/or year, and the sort order changed.

INIICa	ntio	n breakdown of dataset		
	hor:	Jolley KA		
records re PubMed	eturne	d. Click the hyperlinks for detailed information.		Isolates in
id	Year	Citation	Title	database
7517841	2007	Taha MK, Vázquez JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enríquez R, Fazio C, Frosch M, Heuberger S, Hoffmann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczynska A, Stefanelli P, Thulin S, Tzanakai G, Unemo M, Vogel U, Zarantonelli ML (2007) Antimicrob Agents Chemother 51: 2784-92	Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis.	1670 isolates
8815379	2008	Buckee CO, Jolley KA, Recker M, Penman B, Kriz P, Gupta S, Maiden MC (2008) Proc Natl Acad Sci U S A 105: 15082-7	Role of selection in the emergence of lineages and the evolution of virulence in Neisseria meningitidis.	1054 isolates
5776372	2005	Claus H, Maiden MC, Wilson DJ, McCarthy ND, Jolley KA, Urwin R, Hessler F, Frosch M, Vogel U (2005) J Infect Dis <b>191:</b> 1263-71	Genetic analysis of meningococci carried by children and young adults.	822 isolates
5528708	2004	Yazdankhah SP, Kriz P, Tzanakaki G, Kremastinou J, Kalmusova J, Musilek M, Alvestad T, Jolley KA, Wilson DJ, McCarthy ND, Caugant DA, Maiden MC (2004) J Clin Microbiol <b>42:</b> 5146-53	Distribution of serogroups and genotypes among disease-associated and carried isolates of Neisseria meningitidis from the Czech Republic, Greece, and Norway.	667 isolates
7825091	2007	Bennett JS, Jolley KA, Sparling PF, Saunders NJ, Hart CA, Feavers IM, Maiden MC (2007) BMC Biol 5: 35	Species status of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from	576 isolates
			multilocus sequence typing.	

To display the isolate records for any of the displayed publications, click the button to the right of the citation.

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17517841 2007	Taha MK, Vázquez JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enríquez R, Fazio C, Frosch M, Heuberger S, Hoffmann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczynska A, Stefanelli P, Thulin S, Tzanakai G, Unemo M, Vogel U, Zarantonelli ML (2007) Antimicrob Agents Chemother 51: 2784-92	Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis.	1670 isolates
18815379 2008	Buckee CO, Jolley KA, Recker M, Penman B, Kriz P, Gupta S, Maiden MC (2008) Proc Natl Acad Sci U S A 105: 15082-7	Role of selection in the emergence of lineages and the evolution of virulence in Neisseria meningitidis.	1054 isolates
15776372 2005	Claus H, Maiden MC, Wilson DJ, McCarthy ND, Jolley KA, Urwin R, Hessler F, Frosch M, Vogel U (2005) J Infect Dis <b>191:</b> 1263-71	Genetic analysis of meningococci carried by children and young adults.	822 isolates
15528708 2004	Yazdankhah SP, Kriz P, Tzanakaki G, Kremastinou J, Kalmusova J, Musilek M, Alvestad T, Jolley KA, Wilson DJ, McCarthy ND, Caugant DA, Maiden MC (2004) J Clin Microbiol <b>42:</b> 5146-53	Distribution of serogroups and genotypes among disease-associated and carried isolates of Neisseria meningitidis from the Czech Republic, Greece, and Norway.	667 isolates
17825091 2007	Bennett JS, Jolley KA, Sparling PF, Saunders NJ, Hart CA, Feavers IM, Maiden MC (2007) BMC Biol 5: 35	Species status of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from multilocus sequence typing.	576 isolates
15537808 2005	Jolley KA, Wilson DJ, Kriz P, McVean G, Maiden MC (2005) Mol Biol Evol 22: 562-9	The influence of mutation, recombination, population history, and selection on patterns of genetic diversity in Neisseria meningitidis.	378 isolates
15784588 2005	Bennett JS, Griffiths DT, McCarthy ND, Sleeman KL, Jolley KA, Crook DW, Maiden MC (2005) Infect Immun 73: 2424-32	Genetic diversity and carriage dynamics of Neisseria lactamica in infants.	271 isolates
11101585 2000	Iolley KA, Kalmusova I, Feil F I, Gunta S, Musilek M, Kriz P, Maiden MC (2000) J Clin Microbiol 38: 4492-8	Carried meningococci in the Czech Republic: a	[]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]]

The abstract of the paper will be displayed (if available), along with all isolates linked to it.

net JS, Jolley KA, Sparling PF, Saunders NJ, Hart CA, Feavers IM, Maiden MC (2007) <i>BMC Biol</i> 5:35 cies status of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from multilocus sequence typing. seven lock hisseria MLST scheme was readily adapted to N. gonorrhoeae isolates, providing a highly discriminatory typing method. In addition, these data permitted phyl ulation genetic inferences to be made, including direct comparisons with N. meningitidis and N. lactamica. Examination of these data demonstrated that alleles were rarefe e species. Analysis of variation at a single locus, gdh, provided a rapid means of identifying misclassified isolates and determining whether mixed cultures were present. ecords returned (1 - 25 displayed). Click the hyperlinks for detailed information. termination of the second sec	ior					sseria PubMLS	T database						
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Isolate fields [2]         ML ST         Finetyping antiger           Id         isolate fields [2]         Species         serogroup         ST         clonal complex         PorA VR1         PorA VR2         f           1         A4/M1027         B1, Z1001         USA         1937         invasive (unspecified/other)         Neisseria meningitidis         A         ST-4         complex/subgroup IV         5-2         10           2         120M         B35, Z1035         Pakistan         1967         mingitis and septicarmia         Neisseria meningitidis         A         ST-1         complex/subgroup IV         5-2         10           7         7891         B54; Z1034         Finland         1975         invasive (unspecified/other)         Neisseria meningitidis         A         ST-1         complex/subgroup IVI         5-2         10           10         6748         B73; Z1073         Canada         1971         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1         complex/subgroup IVI         5-2         10           13         1308         B99; Z1092         Germany         1964         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1         complex/subgroup IV	cor	ds retur	ned (1 - 25 dis	played). Click	the hy	perlinks for detailed informat	ion.						
Isolate fields [2]         ML ST         Finetyping antiger           Id         isolate fields [2]         Species         serogroup         ST         clonal complex         PorA VR1         PorA VR2         f           1         A4/M1027         B1, Z1001         USA         1937         invasive (unspecified/other)         Neisseria meningitidis         A         ST-4         complex/subgroup IV         5-2         10           2         120M         B35, Z1035         Pakistan         1967         mingitis and septicarmia         Neisseria meningitidis         A         ST-1         complex/subgroup IV         5-2         10           7         7891         B54; Z1034         Finland         1975         invasive (unspecified/other)         Neisseria meningitidis         A         ST-1         complex/subgroup IVI         5-2         10           10         6748         B73; Z1073         Canada         1971         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1         complex/subgroup IVI         5-2         10           13         1308         B99; Z1092         Germany         1964         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1         complex/subgroup IV	_	_											
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1       A4/M1027       B1; Z1001       USA       1937       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       5-2       10         2       120M       B35; Z1035       Pakistan       1967       meningitidis       A       1       ST-1 complex/subgroup IV       5-2       10         7       7891       B54; Z1054       Finland       1975       invasive (unspecified/other)       Neisseria meningitidis       A       1       ST-1 complex/subgroup IV       5-2       10         0       6748       B73; Z1073       Canada       1971       invasive (unspecified/other)       Neisseria meningitidis       A       1       ST-1 complex/subgroup IVI       18-1       3         11       129       B92; Z1092       Germany       1964       invasive (unspecified/other)       Neisseria meningitidis       A       1       ST-1 complex/subgroup IVI       5-2       10         13       139M       B92; Z1092       Philippines       1968       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IVI       7       13-1         24       S4355       B227; Z127       Denmark       1974       invasive (unspecified/other)       Ne										MLSI			
2       120M       B35; Z1035       Pakistan       1967       meningitis and septicaemia Neisseria meningitidis       A       1       ST-1 complex/subgroup /II       5-2       10         7       7891       B54; Z1054       Finland       1975       invasive (unspecified/other)       Neisseria meningitidis       A       5       ST-5 complex/subgroup /II       20       9         0       6748       B73; Z1073       Canada       1971       invasive (unspecified/other)       Neisseria meningitidis       A       5       ST-5 complex/subgroup /II       10-1       3         11       129       B92; Z1092       Germany       1964       invasive (unspecified/other)       Neisseria meningitidis       A       1       ST-1 complex/subgroup /II       5-2       10         13       139M       B93; Z1099       Philippines       1968       Neisseria meningitidis       A       1       ST-1 complex/subgroup /II       5-2       10         19       S3131       B213; Z1213       Ghana       1973       invasive (unspecified/other)       Neisseria meningitidis       A       5       ST-5 complex/subgroup /II       5-1       9         24       S4355       B227; Z1227       Denmark       1974       invasive (unspecified/other)       Neisse				,			SDECIES I						
7         7891         B54; Z1054         Finland         1975         invasive (unspecified/other)         Neisseria meningitidis         A         5         ST-5 complex/subgroup III         20         9           10         6748         B73; Z1073         Canada         1971         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1 complex/subgroup III         20         9           11         129         B92; Z1092         Germany         1964         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1 complex/subgroup III         5-2         10           13         139M         B99; Z1092         Fhilippines         1968         Neisseria meningitidis         A         1         ST-1 complex/subgroup IVI         5-2         10           19         S3131         B213; Z1213         Ghana         1973         invasive (unspecified/other)         Neisseria meningitidis         A         5         ST-5 complex/subgroup IVI         7         13-1           24         S4355         B227; Z127         Nemark         1963         invasive (unspecified/other)         Neisseria meningitidis         A         5         ST-4 complex/subgroup IVI         7         13-1           24										•	PorA VR1	PorA VR2	FetA VR
10         6748         B73; Z1073         Canada         1971         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1 complex/subgroup //II         18-1         3           11         129         B92; Z1092         Germany         1964         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1 complex/subgroup //II         5-2         10           13         139M         B92; Z1092         Germany         1964         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1 complex/subgroup //II         5-2         10           13         139M         B93; Z1099         Philippines         1968         Neisseria meningitidis         A         1         ST-1 complex/subgroup //I         5-2         10           14         S4355         B227; Z123         Ghana         1973 invasive (unspecified/other)         Neisseria meningitidis         A         5         ST-5 complex/subgroup //I         7         13-1           24         S4355         B227; Z1275         Niger         1963 invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup //I         5-2         20         B275; Z1275         Niger         19		120M					Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	PorA VR1 5-2	PorA VR2 10	FetA VR F1-5
11         129         B92; Z1092         Germany         1964         Invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1 complex/subgroup VII         5-2         10           13         139M         B99; Z1099         Philippines         1964         Invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1 complex/subgroup VII         5-2         10           19         S3131         B213; Z1213         Ghana         1973         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup VII         7         13-1           24         S4355         B227; Z1227         Denmark         1974         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup VI         7         13-1           34         20         B257; Z1267         Niger         1963         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup VI         7         13-1           34         20         B275; Z1275         Niger         1963         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup VI         7         13-1				Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis Neisseria meningitidis	A A	4 1	ST-4 complex/subgroup IV ST-1 complex/subgroup I/II	PorA VR1 5-2 5-2	PorA VR2 10 10	FetA VR F1-5 F5-1
13       139M       B99; Z1099       Philippines       1968       Neisseria meningitidis       A       1       ST-1 complex/subgroup I/I       5-2       10         19       S3131       B213; Z1213       Ghana       1973 invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup I/I       7       13-1         24       S4355       B227; Z1227       Denmark       1974 invasive (unspecified/other)       Neisseria meningitidis       A       5       ST-5 complex/subgroup I/I       7       13-1         24       S4355       B227; Z1227       Burkina Faso       1963 invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup I/I       7       13-1         34       20       B275; Z1275       Niger       1963 invasive (unspecified/other)       Neisseria meningitidis       A       1       ST-4 complex/subgroup I/I       7       13-1         35       26       B278; Z1278       Niger       1963 invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup I/I       7       13         46       255       B318; Z1318       Burkina Faso       1966       Neisseria meningitidis       A       4       ST-4 complex/subgroup I/I		7891	B54; Z1054	Pakistan Finland	1967 1975	meningitis and septicaemia invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A	4 1 5	ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-5 complex/subgroup III	PorA VR1 5-2 5-2 20	PorA VR2 10 10 9	FetA VR F1-5 F5-1 F3-1
19       S3131       B213; Z1213       Ghana       1973       Invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7       13-1         24       S4355       B227; Z1227       Denmark       1974       invasive (unspecified/other)       Neisseria meningitidis       A       5       ST-5 complex/subgroup IV       7       13-1         24       S4355       B227; Z1227       Denmark       1963       invasive (unspecified/other)       Neisseria meningitidis       A       5       ST-4 complex/subgroup IV       7       13-1         26       B275; Z1275       Niger       1963       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7       13-1         26       B278; Z1276       Niger       1963       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7       13         26       B278; Z1276       Niger       1963       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7       13         26       B278; Z1276       Niger       1963       invasive (unspecified/other)       Neisseria meningitidis	6	7891 6748	B54; Z1054 B73; Z1073	Pakistan Finland Canada	1967 1975 1971	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A	4 1 5 1	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup III ST-1 complex/subgroup I/I	PorA VR1 5-2 5-2 20 18-1	PorA VR2 10 10 9 3	FetA VR F1-5 F5-1 F3-1 F5-1
24       S4355       B227; Z1227       Denmark       1974       invasive (unspecified/other)       Neisseria meningitidis       A       5       ST-5 complex/subgroup III       5-1       9         21       10       B269; Z1269       Burkina Faso       1963       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup III       5-1       9         24       20       B275; Z1275       Niger       1963       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup III       5-2       10         35       26       B278; Z1278       Niger       1963       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7       13         36       255       B318; Z1318       Burkina Faso       1966       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7-2       13-1         362       Z1362       Cameroon       1966       nexiseria meningitidis       A       4       ST-4 complex/subgroup IV       7-2       13-1         31       393       B392; Z1392       Greece       1966       carrier       Neisseria meningitidis	e	7891 6748 129	B54; Z1054 B73; Z1073 B92; Z1092	Pakistan Finland Canada Germany	1967 1975 1971 1964	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A	4 1 5 1	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup III ST-1 complex/subgroup I/I	PorA VR1 5-2 5-2 20 18-1 5-2	PorA VR2 10 10 9 3	FetA VR F1-5 F5-1 F3-1
31       10       B269, Z1269       Burkina Faso       1963       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7       13-1         34       20       B275, Z1275       Niger       1963       invasive (unspecified/other)       Neisseria meningitidis       A       1       ST-4 complex/subgroup IV       7       13-1         35       26       B278, Z1278       Niger       1963       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7       13         46       255       B318, Z1318       Burkina Faso       1966       invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7-2       13-1         26       255       B318, Z1318       Burkina Faso       1966       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7-2       13-1         26       243       B362, Z1362       Cameroon       1966       Neisseria meningitidis       A       4       ST-4 complex/subgroup IV       7       13-1         51       393       B392, Z1392       Greece       1968       carrier       Neisseria meningitidis       A	e	7891 6748 129	B54; Z1054 B73; Z1073 B92; Z1092	Pakistan Finland Canada Germany	1967 1975 1971 1964	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A	4 1 5 1 1	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup III ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I	PorA VR1 5-2 5-2 20 18-1 5-2	PorA VR2 10 10 9 3 10	FetA VR F1-5 F5-1 F3-1 F5-1
34         20         B275; Z1275         Niger         1963         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1 complex/subgroup I/I         5-2         10           35         26         B278; Z1278         Niger         1963         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup I/I         7         13           46         255         B318; Z1318         Burkina Faso         1966         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup I/I         7         13-1           46         255         B318; Z1318         Burkina Faso         1966         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup I/V         7         13-1           41         393         B362; Z1362         Cameroon         1966         Neisseria meningitidis         A         4         ST-4 complex/subgroup I/V         7         13           41         393         B392; Z1392         Greece         1968         carrier         Neisseria meningitidis         A         1         ST-1 complex/subgroup I/V         7-2         10	6	7891 6748 129 139M	B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099	Pakistan Finland Canada Germany Philippines	1967 1975 1971 1964 1968	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A	4 1 5 1 1 1	ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-5 complex/subgroup I/II ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	PorA VR1 5-2 5-2 20 18-1 5-2 5-2 5-2	PorA VR2 10 10 9 3 10 10	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6
34         20         B275; Z1275         Niger         1963         invasive (unspecified/other)         Neisseria meningitidis         A         1         ST-1 complex/subgroup I/I         5-2         10           35         26         B278; Z1278         Niger         1963         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup I/I         7         13           46         255         B318; Z1318         Burkina Faso         1966         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup I/I         7         13-1           46         255         B318; Z1318         Burkina Faso         1966         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup I/V         7         13-1           41         393         B362; Z1362         Cameroon         1966         Neisseria meningitidis         A         4         ST-4 complex/subgroup I/V         7         13           41         393         B392; Z1392         Greece         1968         carrier         Neisseria meningitidis         A         1         ST-1 complex/subgroup I/V         7-2         10	6 1 S	7891 6748 129 139M 3131	B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213	Pakistan Finland Canada Germany Philippines Ghana	1967 1975 1971 1964 1968 1973	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A A	4 1 5 1 1 1 4	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup IV	PorA VR1 5-2 20 18-1 5-2 5-2 5-2 7	PorA VR2 10 10 9 3 10 10 10 13-1	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1
35         26         B278; Z1278         Niger         1963         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup IV         7         13           46         255         B318; Z1318         Burkina Faso         1966         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup IV         7-2         13-1           26         243         B362; Z1362         Cameroon         1966         nesseria meningitidis         A         4         ST-4 complex/subgroup IV         7-2         13-1           31         B392; Z1392         Greece         1966         carrier         Neisseria meningitidis         A         1         ST-1 complex/subgroup IV         7-2         13	6 1 S S	7891 5748 129 139M 3131 4355	B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227	Pakistan Finland Canada Germany Philippines Ghana Denmark	1967 1975 1971 1964 1968 1973 1974	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A	4 1 5 1 1 1 4 5	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/II ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-5 complex/subgroup II	PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1	PorA VR2 10 10 9 3 10 10 13-1 9	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1 F1-5
46         255         B318, Z1318         Burkina Faso         1966         invasive (unspecified/other)         Neisseria meningitidis         A         4         ST-4 complex/subgroup IV         7-2         13-1           52         243         B362, Z1362         Cameroon         1966         Neisseria meningitidis         A         4         ST-4 complex/subgroup IV         7         13           51         393         B392, Z1392         Greece         1968         carrier         Neisseria meningitidis         A         1         ST-1 complex/subgroup IVI         5-2         10	6 1 S S	7891 5748 129 139M 3131 4355 10	B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269	Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso	1967 1975 1971 1964 1968 1973 1974 1963	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A	4 1 5 1 1 1 4 5 4	ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-5 complex/subgroup I/II ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-4 complex/subgroup I/II ST-5 complex/subgroup III ST-4 complex/subgroup I/I	PorA VR1 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1 7	PorA VR2 10 10 9 3 10 10 13-1 9 13-1	FetA VR F1-5 F5-1 F3-1 F5-1 F5-1 F5-1 F5-1 F1-5 F3-1
52         243         B362, Z1362         Cameroon         1966         Neisseria meningitidis         A         4         ST-4 complex/subgroup IV         7         13           51         393         B392, Z1392         Greece         1968         carrier         Neisseria meningitidis         A         1         ST-1 complex/subgroup IVI         5-2         10	e 1 S	7891 5748 129 139M 33131 4355 10 20	B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B275; Z1275	Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger	1967 1975 1971 1964 1968 1973 1974 1963 1963	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A A A	4 1 5 1 1 1 4 5 4 1	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-5 complex/subgroup IV ST-5 complex/subgroup III ST-4 complex/subgroup III ST-4 complex/subgroup I/I	PorA VR1 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1 7 5-1 7 5-2	PorA VR2 10 10 9 3 10 10 13-1 9 13-1 10	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F3-6 F5-1 F1-5 F3-1 F1-5
51         393         B392; Z1392         Greece         1968         carrier         Neisseria meningitidis         A         1         ST-1 complex/subgroup //II         5-2         10	6 1 S S	7891 5748 129 139M 3131 4355 10 20 26	B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B275; Z1275 B278; Z1278	Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger	1967 1975 1971 1964 1968 1973 1973 1963 1963	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A A A A	4 1 5 1 1 4 5 4 1 4	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup IV ST-5 complex/subgroup IV ST-5 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I	PorA VR1 5-2 20 18-1 5-2 5-2 7 5-1 7 5-1 7 5-2 7	PorA VR2 10 10 9 3 10 10 13-1 9 13-1 10 13	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F1-5 F3-1 F1-5 F3-1 F1-5 F1-7
	e 1 S S	7891 5748 129 139M 33131 4355 10 20 26 255	B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B275; Z1275 B278; Z1278 B318; Z1318	Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso	1967 1975 1971 1964 1968 1973 1974 1963 1963 1963 1965	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A A A A A	4 1 5 1 1 1 4 5 4 1 4 4 4	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-5 complex/subgroup III ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup IV	PorA VR1 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1 7 5-1 7 5-2 7 7 7-2	PorA VR2 10 10 9 3 10 10 13-1 9 13-1 10 13-1 10 13 13-1	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F1-5 F3-1 F1-5 F3-1 F1-5 F1-7 F1-5 F1-5
64 254 B439; Z1439 Diibouti 1966 invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup I/II 5-2 10	e 1 S	7891 5748 129 139M 3131 3131 44355 10 20 26 255 243	854; Z1054 873; Z1073 892; Z1092 899; Z1099 8213; Z1213 8227; Z1227 8269; Z1269 8275; Z1275 8278; Z1278 8318; Z1318 8362; Z1362	Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso Cameroon	1967 1975 1971 1964 1968 1973 1973 1963 1963 1963 1966 1966	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A A A A A A A	4 1 5 1 1 4 5 4 1 4 4 4 4 4	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-5 complex/subgroup I/I ST-4 complex/subgroup I/I	PorA VR1 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1 7 5-2 7 5-2 7 7-2 7	PorA VR2 10 10 9 3 10 10 13-1 13-1 10 13-1 13-1 13-1 13	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F3-6 F5-1 F1-5 F1-5 F1-7 F1-5 F1-5 F1-5 F1-5
	e 1 S S	7891 5748 129 139M 3131 4355 10 20 26 255 243 393	854; Z1054 873; Z1073 892; Z1092 899; Z1099 8213; Z1213 8227; Z1227 8269; Z1269 8275; Z1275 8278; Z1278 8318; Z1318 8362; Z1362 8392; Z1392	Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso Cameroon Greece	1967 1975 1971 1964 1968 1973 1973 1963 1963 1966 1966 1968	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A A A A A	4 1 5 1 1 4 5 4 1 4 4 4 4 1	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-5 complex/subgroup I/I ST-4 complex/subgroup I/I	PorA VR1 5-2 5-2 200 18-1 5-2 5-2 7 5-1 7 5-2 7 7-2 7 7-2 7 5-2	PorA VR2 10 10 9 3 10 10 13-1 9 13-1 10 13 13-1 13 13-1 13 10	FetA VR F1-5 F5-1 F3-1 F3-1 F5-1 F3-6 F5-1 F1-5 F3-1 F1-5 F1-5 F1-5 F1-5 F1-5 F1-5 F1-5 F5-1
22 11-004 B503 21505 Australia 1971 invasive (unspecified/other) Neisseria meningilulas A 5 51-5 complexisubgroup III 20 9	e 1 S S	7891 5748 129 139M 3131 4355 10 20 26 255 243 393 254	854; Z1054 873; Z1073 892; Z1092 899; Z1099 8213; Z1213 8227; Z1227 8269; Z1269 8275; Z1275 8278; Z1278 8318; Z1318 8362; Z1362 8392; Z1392 8439; Z1439	Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso Cameroon Greece Djibouti	1967 1975 1971 1964 1968 1973 1974 1963 1963 1966 1966 1968 1966	meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A A A A A A A A	4 1 5 1 1 4 5 4 1 4 4 4 4 1 1 1	ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-5 complex/subgroup IV ST-5 complex/subgroup IV ST-1 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I	PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-1 7 5-2 7 7 5-2 7 7 5-2 7 5-2 5-2	PorA VR2 10 10 3 10 10 13-1 13-1 10 13-1 13-1 13	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F3-6 F5-1 F1-5 F1-5 F1-7 F1-5 F1-5 F1-5 F1-5

# 11.13 User-configurable options

The BIGSdb user interface is configurable in a number of ways. Choices made are remembered between sessions. If the database requires you to log on, the options are associated with your user account, whereas if it is a public database, that you haven't logged in to, the options are associated with a browser cookie so they will be remembered if you connect from the same computer (using the same browser).

Most options are set by clicking the 'Set general options' link on the database contents page. Most of the available options are visible for isolate databases, whereas sequence definition databases have fewer available.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it sample. Query database • Search or browse database • Search by combinations of loci (profiles) • Projects - main projects defined in database. • Set display and query options for locus, schemes or scheme fields.	
Breakdown       Export       Analysis         • Single field       • Export dataset       • Codon usage         • Unique combinations       • Scheme and alleles       • Sequences - XMFA / concatenated FASTA formats       • Codon usage         • Publications       • Sequence bin       • Sequence - XMFA / concatenated FASTA formats       • Codon usage	Miscellaneous     • Description of database fields

## 11.13.1 General options

The general options tab is displayed by default. If another tab is being shown, click the 'General options' header.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
et database options	
" iere you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear t then you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.	o set
✓ General options	
Display 25 • records per page. Page bar position: top and bottom • Display 100 • nucleotides per line in sequence alignments. Display 100 • nucleotides of flanking sequence (where available). Ø Display locus aliases if set Ø Enable tooltips (beginner's mode). Set options	
▶ Main results table	
▶ Isolate record display	
Provenance field display	
Query filters	
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences. Reset all to defaults	

The general tab allows the following options to be modified:

• Records per page

- Page bar position
- Nucleotides per line Some analyses display sequence alignments. This option allows you to set the width of these alignments so suit your display.
- Flanking sequence length This sets the length of flanking sequence upstream and downstream of a particular locus that is included whenever a sequence is displayed. Flanking sequences are displayed fainter that the locus sequence.
- Locus aliases Loci can have multiple names (aliases). Setting this option will display all alternative names in results tables.
- Tooltips (beginner's mode) Most query forms have help available in the form of information tooltips. These can be switched on/off here. They can also be toggled off by clicking the Toggle: 'i' button at the top-right of the display of some pages.

Click 'Set options' to remember any changes you make.

### 11.13.2 Main results table

The 'main results table' tab contains options for the display of paged results following a query.

Click the 'Main results table' header to display the tab.

Query:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/sequences definitions   Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
General options
Display 25 • records per page. Page bar position: top and bottom • Display 100 • nucleotides per line in sequence alignments. Display 100 • nucleotides of flanking sequence (where available). Ø Display locus aliases if set. Ø Enable tooltips (beginner's mode). Set options
► Main results table
▹ Isolate record display
Provenance field display
Query filters
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences. Reset all to defaults

The 'main results table' tab will scroll up.

Query: Search   Browse   Profile/ST   List         Breakdown: Isolate fields   Scheme/alleles   Publications         Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions
Нер 2
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
General options
✓ Main results table
Hyperlink allele designations where possible.  Jifferentiate provisional allele designations.  Display information about sequence bin records tagged with locus information (tooltip).  Display sequence bin size.  Display contig count.  Display publications.  Set options
▶ Isolate record display
Provenance field display
Query filters
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences. Reset all to defaults

This tab allows the following options to be modified:

- Hyperlink allele designations Hyperlinks point to an information page about the particular allele definition. Depending on the locus, these may exist on a different website.
- Differentiate provisional allele designations Allele designations can be set as confirmed or provisional, usually depending on the method of assignment. Selecting this option will display provisional designations in a different colour to confirmed designations.
- Information about sequence bin records Creates a tooltip that displays details about sequence tags corresponding to a locus.
- Sequence bin records Displays a tooltip linking to the sequence tag if available.
- Sequence bin size Displays the size of the sum of all contigs associated with each isolate record.
- Contig count Displays the number of contigs associated with each isolate record.
- Publications Displays citations with links to PubMed for each record.

#### 11.13.3 Isolate record display

The 'isolate record display' tab contains options for the display of a full isolate record.

Click the 'Isolate record display' tab to display the tab.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
- General options
Display 25 • records per page. Page bar position: top and bottom • Display 100 • nucleotides per line in sequence alignments. Display 100 • nucleotides of flanking sequence (where available). Ø Display locus aliases if set. Ø Enable tooltips (beginner's mode). Set options
Main results table
► Isolate record display
Provenance field display
Query filters
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences. Reset all to defaults

The 'Isolate record display' tab will scroll up.

Query: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
General options
► Main results table
✓ Isolate record display
<ul> <li>Differentiate provisional allele designations.</li> <li>Display sender, curator and last updated details for allele designations (tooltip).</li> <li>Display information about sequence bin records tagged with locus information (tooltip).</li> <li>Display information about whether alleles have flags defined in sequence definition database (shown in sequence detail tooltip).</li> <li>Display full information about sample records (tooltip).</li> <li>Set options</li> </ul>
Provenance field display
Query filters
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences. Reset all to defaults

This tab allows the following options to be modified:

• Differentiate provisional allele designations - Allele designations can be set as confirmed or provisional, usually depending on the method of assignment. Selecting this option will display provisional designations in a different colour to confirmed designations.

- Display sender, curator and last updated records Displays a tooltip containing sender information next to each allele designation.
- Sequence bin information Displays a tooltip with information about the position of the sequence if tagged within the sequence bin.
- Allele flags Displays information about whether alleles have flags defined in sequence definition databases.

## 11.13.4 Provenance field display

The 'provenance field display' tab contains checkboxes for fields to display in the main results table.

Click the 'Provenance field display' tab to display the tab.

Ouery:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/sequences definitions   Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
← General options
Display 25  records per page.
Page bar position: top and bottom
Display 100 - nucleotides of flanking sequence (where available).
✓ Display locus aliases if set ✓ Enable tooltips (beginner's mode).
Set options
► Main results table
► Isolate record display
► Provenance field display
Query filters
Reset
Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences.
Reset all to defaults

The 'Provenance field display' tab will scroll up.

	se   Profile/ST   List elds   Scheme/alleles   Publications me   Options   Profiles/sequences definitions   I	Database submissions	
Set database options			
	e website. Options are remembered between s hing the page (Shift + Refresh) as some page		a PubMLST) only. If some of the options don't appear to set
▶ General options			
▶ Main results table			
Isolate record display			
<ul> <li>Provenance field display</li> </ul>			
	and then selecting the 'Customize' option.	table following a query. Settings for displaying loc amoxicillin sulphonamide ceftriaxone chiramphenicol chiramphenicol chiramphenicol chiramphenicol cfotaxime cefotaxime cefotaxime rifampicin iffampicin_range ciprofloxacin	us and scheme data can be made by performing a ciprofloxacin_range pending_assembly assembly_status PhA_accession private_project comments sender curator date_entered datestamp
Query filters  Reset  Click the reset button to remove all user s  Reset all to defaults	ettings for this database - this includes locus a	nd scheme field preferences.	

Some fields will be checked by default - these are defined during *database setup* (maindisplay option).

Check any fields that you wish to be displayed and then click 'Set options'. You can return to the default selection by clicking 'Default' followed by 'Set options'.

## 11.13.5 Query filters

The 'query filters' tab contains checkboxes for provenance fields and scheme completion status. Checking these results in drop-down list box filters appearing in the query page *filters fieldset*.

Click the 'Query filters' tab to display the tab.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications
Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions
database options
you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
General options
Display 25 - records per page.
Page bar position: top and bottom 👻
Display 100 v nucleotides per line in sequence alignments. Display 100 v nucleotides of flanking sequence (where available).
Display nou   in including sequence (where available).  Display nou   including seque
Z Enable tooltips (beginner's mode).
Set options
Main results table
Isolate record display
Provenance field display
Query filters
et
the reset button to remove all user settings for this database - this includes locus and scheme field preferences.
sset all to defaults

## The 'Query filters' tab will scroll up.

Provenance field display Query filters Select the fields for which you would like dropdown lists ( isolate country	containing known values on which to filter query results. These wil	
Select the fields for which you would like dropdown lists a		
isolate		
continent         region         year         epidemiological_year         age_yr         age_yr         age_mth         sex         disease         source         epidemiology         species         serotype         ET_no         penicillin         subphonamide         ceftriaxone_range         chloramphenicol_range         chloramphenicol_range         rifampicin         rifampicin         rifampicin         infermine         ciprofloxacin         ciprofloxacin         ciprofloxacin_range	ENA_accession private_project comments sender curator date_entered datestamp VMLST profile completion Finetyping antigens profile completion ADP-heptose biosynthesis profile completion Antibiotic resistance profile completion Antibiotic resistance profile completion Antibiotic resistance profile completion Capsule Region A - Serogroup A profile completion Capsule Region A - Serogroup D profile completion Capsule Region A - Serogroup Y profile completion Capsule Region D and D' profile completion Capsule Region D and D' profile completion Capsule Region C profile completion Capsule Region D and D' profile completion Capsule Region D and D' profile completion Capsule Region Profile completion Capsule Region D profile completion Capsule Region D and D' profile completion Capsule Region D and D' profile completion Capsule Region Profil	I be available in the filters section of the query interface. LOS alpha chain transferases profile completion LOS inner core transferases profile completion LOS transport/export profile completion Lipid A biosynthesis: other profile completion N. meninglidis profile completion Nucleotide excision repair profile completion Protein glycosylation profile completion Protein glycosylation profile completion Protein glycosylation profile completion Prini dine metabolism profile completion Primidine metabolism profile completion RNA polymerase profile completion Small regulatory RNAs profile completion UDP-GlcNAc synthesis profile completion UDP-GlcNAc synthesis profile completion ViriB TASS profile completion WiriB TASS profile completion WiriB TASS profile completion Profile completion ViriB TASS profile completion MLST (20 locus partial genes) profile completion MLST (20 locus partial genes) profile completion Pulsition Pulsitions Publications

A list of possible filters appears. Click any checkbox for a filter you would like to make available. Click 'Set options' when done. You can return to the default selection by clicking 'Default' followed by 'Set options'.

## 11.13.6 Modifying locus and scheme display options

Whether or not loci, schemes or scheme fields are displayed in result tables, isolate records, or within query dropdown boxes can all be set with default options when first defined. These attributes can, however, be overridden by a user, and these selections will be remembered between sessions.

The procedure to modify these attributes is the same for locus, schemes or scheme fields, so the steps for loci will be demonstrated only.

Click the appropriate link on the isolate contents page.

Ouery: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions
Neisseria PubMLST database
The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample.
Query database • Search or browse database • Search by combinations of loci (profiles) • Projects - main projects defined in database. • Define settings • Set display and query options for locus, schemes or scheme fields. • Set display and query options for locus, schemes or scheme fields. • Set display and query options for locus, schemes or scheme fields. • Locus, schemes or sc
Breakdown       Export       Analysis       Miscellaneous         • Single field       • Export dataset       • Contigs       • Codon usage       • Description of database fields         • Two field       • Unique combinations       • Sequences - XMFA / concatenated FASTA formats       • Codon usage       • Description of database fields         • Publications       • Sequence bin       • Sequence bin       • BLAST       • Description of database fields

Either select the locus id by querying for it directly.

Ouery: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: i
Query loci for Neisseria PubMLST database	
Please enter your search criteria below (or leave blank and submit to return all records). Matching loci will be returned and you will then be able to update their display and query s	settings.
- Search criteria - Display -	
id v = v abcZ + i Order by: id v ascending v	
Display: 25 👻 records per page 👔	
Reset Submit	
1 record returned. Click the hyperlink for detailed information.	
locus options	
id  data type allele id format length  ength varies coding sequence  orf genome position isolate display* main display* query field* analysis*	
abc2 DNA integer 433 false true 1 1176340 allele only false true true	
* Default values are displayed for this field. These may be overridden by user preference.	

Designations can be queried using standard operators.

Alternatively, you can search by filtering loci by schemes. Click the 'Filter query by' header and select the scheme in the dropdown box.

Publ	MLST	Breakdown	: Isolate fie		e/alleles   Public		initions   Data	base submissions					
													Toggle: i
Quer	y loci	for Neis	sseria	PubM	LST data	bas	e						
Please	enter your	search criteria	a below (or	leave blank	and submit to re	turn all	records). Matc	hing loci will be retur	ned and you w	ill then be ab	le to update	their display and query settings.	
— Sea	arch criteria	a					— — Displa	ıy					
id				•		+ [	i Ord	er by: id	•	<ul> <li>ascending</li> </ul>	9 👻		
							Dis	play: 25 🗸 recor	ds per page 👔				
—⊽ F	ilter query	by-					Action						
		data type:	•				Reset S	ubmit					
		id format:											
		gth varies: sequence:	<b>• i</b>										
	county :		• •										
	mato	ch longest:	• • i										
		pcr filter:	- i										
	p	orobe filter:	▼ 1										
		flag table:	▼ i										
		te display:		•									
		in display:	▼ 1										
	C	query field:	<b>•</b> <u>i</u>										
		analysis: curator:	▼ 1		ī								
	<u> </u>	scheme: M	LST	•		i							
		outerne. M	201										
7			- Northeastern										
/ record:	s returned.	. Click the hype	eninks for o	setalled infor	mation.								
Cus	tomize												
locus	options												
id	data type	allele id forma	at length l	ength varies	coding sequer	ice orf	genome posi	tion isolate display*	main display*	* query field'	* analysis*		
abcZ	DNA	integer	433	false	true	1	1176340	allele only	false	true	true		
adk aroE	DNA DNA	integer integer	465 490	false false	true	1	991951 2079469	allele only allele only	false false	true	true true		
fumC	DNA	integer	465	false	true	1	1592943	allele only	false	true	true		
gdh	DNA	integer	501	false	true	1	1514394	allele only	false	true	true		
pdhC pgm	DNA DNA	integer integer	480 450	false false	true	1	1453970 965481	allele only allele only	false false	true	true		
		-			ridden by user pr			anele offiy	alse	aue	ude		

7 records returned. Click the hyperlinks for detailed information. Customize locus options id data type ele id fori at length length varies coding sequence orf ge olate display* uery field* analysis* ome posit in display* abc7 DNA integer 433 false true 1176340 allele only false true true adk DNA integer 465 false true 1 991951 allele only false true true aroE DNA 490 2 2079469 allele only false true integer false true true allele only fumC DNA integer 465 false true 1 1592943 false true true gdh DNA integer 501 false true 1514394 allele only false true true pdhC 1453970 DNA 480 allele only integer false false true true true integer DNA 450 false true 965481 allele only false true true pgm * Default values an field. These played for this nay be preference

Once loci have been selected, click Customize 'locus options'.

You can then choose to add or remove individual loci from the selection by clicking the appropriate checkboxes. At the bottom of the page are a number of attributes that you can change - clicking 'Change' will affect all selected loci.

Possible options for loci are:

- isolate_display Sets how the locus is displayed within an isolate record:
  - allele only display only identifier
  - sequence display the full sequence
  - hide don't show at all
- main_display Sets whether the locus is displayed in the main results table following a query.
- query_field Sets whether the locus appears in dropdown list boxes to be used within queries.
- analysis Sets whether the locus can be used in data analysis functions.

**Note:** Settings for loci can be overridden by those set for schemes that they are members of. For example, if you set a locus to be displayed within a main results table, but that locus is a member of a scheme and you set that scheme not to be displayed, then the locus will not be shown. Conversely, if you set a scheme to be displayed, but set its member locus not to be shown, then that locus will not be displayed (but other loci and scheme fields may be, depending on their independent settings).

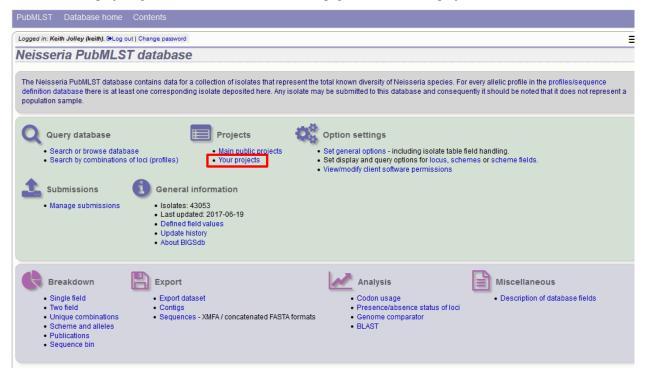
# CHAPTER 12

# User projects

If user projects are enabled, authenticated users are able to set up their own projects in order to group isolates for analysis. If private data and user quotas are enabled, these projects can include private records that can then be shared with other user accounts. Note, that simply adding a record to a user project does not make the record itself private.

**Note:** User projects can be enabled by an administrator by setting 'user_projects="yes" in the *config.xml* file for the database.

To create a new project, go to the isolate database contents page and click 'Your projects'.



Enter the name of your project (this must be unique on the system - you will be told if the name is already used). You can optionally include a description - if you do this, this will appear within *isolate records* when accessed from your account. Click 'Create'.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). (DLog out   Change password
User projects
New private projects Projects allow you to group isolates so that you can analyse them easily together. Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an
isolate record page (only you and users you give access will see this).
New project
Name: UK group W ST-11 2016 Create
Description: Group W ST-11 isolates from the UK in 2016.
Existing projects
You do not own or are a member of any projects.
*

You can either add isolates to your project directly following a query or by manually editing a list of ids.

# 12.1 Adding isolates to a user project following a query

Perform an isolate database query. If you have set up a project, there will be a link in the results header box. Select your project and click 'Add these records'.

gged in	Keith Joll	ey (keith). 🕩Lo	g out	Chang	ge password													He	elp 🖉	Toggl	le: 🚯
eard	ch or	brows	e N	eis	seria PubM	LST a	databas	9													
inter se	earch crite	ria or leave t	lankt	to brov	vse all records. Modif	fy form pa	rameters to filt	er or enter a l	list of value:	s.											Мо
-Isol	ate prover	nance/pheno	type f	fields -				Allele desigr	nations/sch	eme field	s										for
	ine with:							ST (MLST)	-	=		<b>v</b> 11	L			-	- 0				op
cour	ntry	•			▼ UK		+ 0											Actio			
sero	group	•	-		▼ W			Display/sort Order by:													5
year	•	•	=		✓ 2016			Display:		aarda nav		•					centui	ng 🔻 Res	et	Submit	
								Dispidy.	23 <b>v</b> re	cords per	page	0									
Your JK gro	projects -	-11 2016 🗸		dd the	se records	detailed i	nformation.														
-Your JK gro	projects - oup W ST-	-11 2016 🗸	Ac	dd thes	se records	detailed i	nformation.								ML	ST			Finet	yping a	ntige
- Your UK gro	projects - oup W ST-	-11 2016 🗸	6 (	dd thes	se records	source	nformation. species	serogroup	Seqbin size (bp)	Contigs	abcZ	adk a	aroE fi	umC g		ST hC pgn	n ST	cional complex	Finet PorA VR1		Fet
- Your JK gro ge: <b>[</b> id	projects - bup W ST 1 2 3 isolate M16	-11 2016 ↓ 4 5 aliases cou	Ac 6)	dd thes	se records		species Neisseria	serogroup W		Contigs 257	abcZ 2	adk a	aroE fi 4			hC pgn	n ST 11	ST-11	PorA	PorA	Fet Vi
- Your JK gro ge: <b>[</b> id	projects - oup W ST- 1 2 3 isolate	-11 2016 ↓ 4 5 aliases cou	Ac 6)	dd thes 7 ) ≥ year	se records	source	species		size (bp)		abcz				dh pd	hC pgn		ST-11 complex/ET-37	PorA VR1	PorA VR2	Fet Vi
- Your JK gro ge: <b>(</b> id 2451	projects - bup W ST 1 2 3 isolate M16	-11 2016 + 4 5 aliases cou	Ac 6) Intry	dd thes 7 ) ≥ year	se records	source	species Neisseria		size (bp)		abcz			3	dh pd	hC pgn 6		ST-11	PorA VR1	PorA VR2	Fet VI F1
- Your UK gro Ige: 1 id 2451	projects – oup W ST- i 2 3 isolate M16 240077	-11 2016 + 4 5 aliases cou	Ac 6) Intry	dd thes 7 > year 2016	se records   Last  Isolate fields   disease	source	species Neisseria meningitidis	W	size (bp) 2111799	257	2 2	3	4	3	idh pd 8 4	hC pgn 6	11	ST-11 complex/ET-37 complex	PorA VR1 5	PorA VR2 2	Fet VF F1-
- Your UK gra Ige: 1 id 2451 2475	projects - oup W ST- i 2 3 isolate M16 240077 M16 240003 M16	-11 2016 + 4 5 aliases cou	Ac e Intry JK	dd thes 7 > year 2016	se records Last Isolate fields ① disease invasive (unspecified/other) invasive	source	species Neisseria meningitidis Neisseria meningitidis Neisseria	W	size (bp) 2111799	257	2 2	3	4	3	idh pd 8 4	hC pgn 6 6	11	ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex/ET-37 sT-11	PorA VR1 5	PorA VR2 2	Fet VF F1-
- Your UK gra Ige: 1 id 2451 2475	projects - bup W ST- i 2 3 isolate M16 240077 M16 240003	-11 2016 + 4 5 aliases cou	Ac e Intry JK	dd the: 7 > year 2016 2016	invasive (unspecified/other)	source	species Neisseria meningitidis Neisseria meningitidis	W	size (bp) 2111799 2098168	257 222	2 2	3	4	3	idh pd 8 2 8 2	hC pgn 6 6	11	ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex	PorA VR1 5	PorA VR2 2 2	Fet VI F1-
- Your UK gro age: <b>F</b>	projects - oup W ST- i 2 3 isolate M16 240077 M16 240003 M16	aliases co	Action of the second se	dd the: 7 > year 2016 2016	se records Last Isolate fields ① disease invasive (unspecified/other) invasive	source	species Neisseria meningitidis Neisseria meningitidis Neisseria	W	size (bp) 2111799 2098168	257 222	2 2	3	4	3 3 3	idh pd 8 2 8 2	hC pgn I 6 I 6	11	ST-11 complex/ET-37 complex/ ST-11 complex/ET-37 complex/ ST-11 complex/ET-37	PorA VR1 5	PorA VR2 2 2	

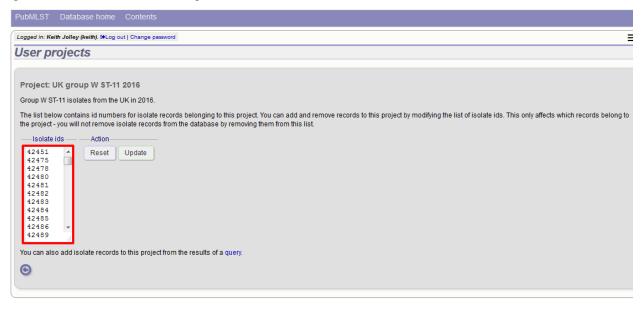
The records will be added to the project. Please note that it doesn't matter whether any of the records have been previously added.

# 12.2 Adding or removing isolates belonging to a user project by editing a list

From the user projects page, click the 'Add/remove records' link for the project that you wish to modify.

PUDMLST Database nome Contents
Logged in: Keith Jolley (keith). @Log out   Change password
User projects
New private projects
Projects allow you to group isolates so that you can analyse them easily together.
Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an isolate record page (only you and users you give access will see this).
Name: Create
Description:
Your projects
Delete  Add/remove records  Modify users  Project   Description  Administrator Isolates  Browse
🗶 🥒 👑 UK group W ST-11 2016 Group W ST-11 isolates from the UK in 2016. 🕝 163 👔
You can also add isolates to projects from the results of a query.
Note that deleting a project will not delete its member isolates.
*

Edit the list of ids of records belonging to the list. You can copy and paste this list if you wish to prepare it in a spreadsheet or text editor. Click 'Update' when finished.



# 12.3 Accessing project isolates

To browse isolate records belonging to a project, go to the user projects page and click the 'Browse' link for the project.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). @Log out   Change password
User projects
New private projects
Projects allow you to group isolates so that you can analyse them easily together.
Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an isolate record page (only you and users you give access will see this).
New project     Action       Name:     Create       Description:
Your projects         Delete Add/remove records       Modify users       Project       Description       Administrator       Isolates       Browse         Image: Comparison of the second

Alternatively, you can select the project from the *projects filter* on the isolate query page. This would enable you to combine the project with additional search criteria

PubMLS	si Data	base h	ome	Conte	nts																
Logged in	: Keith Jolley	/ (keith).	€+Log out	Chang	e password														Help 🖉	Toggle	: <b>0</b> =
Searc	ch or b	orow	se N	eiss	seria PubN	ILST d	latabase														
Enter se	earch criteri	a or lea	ve blank	to brov	vse all records. Moo	lify form par	ameters to filte	r or enter a lis	st of values.												Modify
Isol	late provena	ance/ph	enotype	fields -			F	Filters													form
id		•	- =		- Enter value		+ 0	P	ublication:									¢	D		options
									Project:	1 selecte	ed				¢	0					
									T profiles:	✓ Chec				all	C	3					
								Clonal compl		Irish N				nome	Libra ⁴						
								exsero OMV p		MRF											
							R	bosomal MLS		NI_E>											
								Sequ Include old	uence bin:	penA						1					
							Ľ			C rpoB											
	play/sort op							- Action		UK gr				Ibrary							
	Order by: id					•	ascending	Rese	t Subr	UK &	<u> </u>			11-20	3/14	-					
	Display: 2	5 <del>v</del> r	ecords (	oer pag	e 🕕					•					۴						
163 reco	ords returne	d (1 - 25	5 display	ed). Cli	ck the hyperlinks fo	r detailed in	formation.														
-Your	r projects —																				
Select	t project		- A	dd thes	e records																
				-																	
Page:	1 2 3	46			Last																
					Isolate fields ()										MLS	T			Finet	/ping an	tigens
14	in alata da	lianan					anasian		Seqbin	Contigs	aba7								PorA		FetA
id		mases	country		disease	source	species	serogroup					roE fum		1			clonal complex	VR1	VR2	VR
42451	M16		UK	2016		sputum	Neisseria	W	2111799	257	2	3	4 3	8	4	6	11	ST-11	5	2	F1-1

Please note that you will only see your project in the filter list if you are logged in. As a private project, only you will see it.

# 12.4 Allowing other users to share your project

You can share a project that you own with any other user. In order to do this, you must know the username that they use to log in with. They will see the project in their own list of private projects and in the query interface projects filter.

From the user projects page, click the 'Modify users' link for the specified project:

PubMLST Database home Contents
Logged in: Keith Jolley (keith). @Log out   Change password
User projects
New private projects
Projects allow you to group isolates so that you can analyse them easily together.
Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an isolate record page (only you and users you give access will see this).
New project
Name: Create
Your projects
Delete Add/remove records Modify users Project Description Administrator Isolates Browse
W group W ST-11 2016 Group W ST-11 isolates from the UK in 2016.     You can also add isolates to projects from the results of a query.
Note that deleting a project will not delete its member isolates.
n

Enter the username of the person you wish to share with and click 'Add user':

PubMLST Database home Contents
Logged in: Keith Jolley (keith). @Log out   Change password
User projects
Project: UK group W ST-11 2016
Users
The following users have permission to access the project (either explicitly or through membership of a user group).
Users     Action       User     Iddiremove records       Jolley, Keith (keith)     Image: Control of the sers
Enter username hbratcher You need to know me username or any user you wish to add.
$\odot$

If user groups are in use, you can also share your project with all members of a user group from the same page.

Once a user has been added, you can give them permission to administer (add other users, modify the description or delete) or add/remove records to the project:

PubMLST Database home Contents
Logged in: Keith Jolley (keith). @Log out   Change password
User projects
Project: UK group W ST-11 2016 Users
The following users have permission to access the project (either explicitly or through membership of a user group).
Users     Admin Add/Remove records       Remove     User       Bratcher, Holly (hbratcher)     Update users       Jolley, Keith (Keith)     Image: Construction of the second sec
Add user Addion Enter username: hbratcher You need to know the username of any user you wish to add. Add user
$\odot$

# 12.5 Deleting a user project

You can delete a project from the user projects page by clicking the 'Delete' link next to the project in question.

PubmLS1 Database nome Contents
Logged in: Keith Jolley (keith). @Log out   Change password
User projects
New private projects
Projects allow you to group isolates so that you can analyse them easily together.
Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an isolate record page (only you and users you give access will see this).
New project Action Orreate Create
Your projects
Delete     Add/remove records     Modify users     Project     Description     Administrator     Isolates     Browse       X     V     W group W ST-11 2016     Group W ST-11 isolates from the UK in 2016.     Iso     Iso     Iso       You can also add isolates to projects from the results of a query.     Iso     Iso     Iso     Iso
Note that deleting a project will not delete its member isolates.
*

If the project contains any isolates you will be asked for confirmation. Click the 'Delete project' button.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). @Log out   Change password
User projects
This project contains 163 isolates. Please confirm that you wish to remove the project (the isolates in the project will not be deleted).
× Delete project
New private projects
Projects allow you to group isolates so that you can analyse them easily together.
Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an isolate record page (only you and users you give access will see this).
New project
Name: Create
Your projects
Delete         Add/remove records         Modify users         Project         Description         Administrator         Isolates         Browse           *         *         W group W ST-11 2016         Group W ST-11 isolates from the UK in 2016.         Group M ST-11         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163         163
You can also add isolates to projects from the results of a query.
Note that deleting a project will not delete its member isolates.
*

If the project contains no isolates, the confirmation page is skipped and the project is removed immediately.

**Note:** Removing a project does not delete the isolate records belonging to it. A project is simply a means of grouping records.

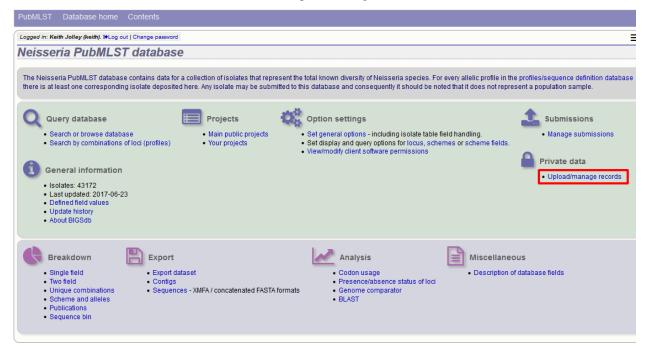
# CHAPTER 13

## Private records

Users with a status of 'submitter', 'curator', or 'admin' can upload private isolate records that will be hidden from public view. A quota needs to be set for the user by an admin before they are able to do this.

## 13.1 Uploading private records

In order to upload private records, you need to make sure that you are logged in. If your account has a quota, there will be a menu item called 'Private data'. Click the 'Upload/manage records' link.



You will see an overview of your quota and links to upload and edit your records. Click the 'Upload private isolate records' link (assuming you have quota available).

PubMLST Database home Contents
Logged in: Keith Jolley (keith). @Log out   Change password
Private records
Limits Accounts have a quota for the number of private records that they can upload. Uploading of private data to some registered projects may not count against your quota.
Records (total): 0 Records (guota): 0
Quota: 100
You can upload: 100
Upload Upload private isolate records
Update private records Curator's interface

You will then be taken to a curator page that allows you to upload data copy and pasted from a spreadsheet. There is a link to an Excel template that you will need to use to prepare your data - this is the same template used if you were to submit your data to a curator.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). DeLog out   Change password	Toggle: 🜖 📃
Batch insert isolates	
Private data upload These isolates will count against your quota of private data. Quota available: 100	ľ
<ul> <li>This page allows you to upload isolate data as tab-delimited text or copied from a spreadsheet.</li> <li>Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish.</li> <li>Enter aliases (alternative names) for your isolates as a semi-colon (;) separated list.</li> <li>Enter references for your isolates as a semi-colon (;) separated list of PubMed ids (non-integer ids will be ignored).</li> <li>You can also upload allele fields along with the other isolate data - simply create a new column with the locus name (see for locus names). These will be added with a confirmed status and method set as 'manual'.</li> <li>You can choose whether or not to include an id number field - if it is omitted, the next available id will be used automaticate.</li> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special C Text' to paste the data.</li> <li>Download submission template (xlsx format)</li> </ul>	
Paste in tab-delimited text (include a field header line).	Action

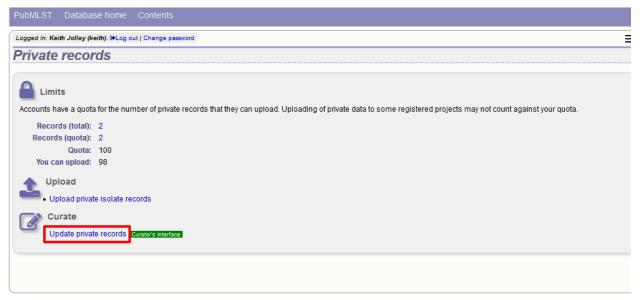
See batch adding isolate records for details of the upload process.

## 13.2 Modifying private records

Click the 'Upload/manage records' link on the contents page.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). 19Log out   Change password Neisseria PubMLST database	Ξ
	esent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition database itited to this database and consequently it should be noted that it does not represent a population sample.
Query database       • Main public projects         • Search or browse database       • Main public projects         • Search by combinations of loci (profiles)       • Main public projects         • Ceneral information       • Your projects         • Isolates: 43172       • Last updated: 2017-06-23         • Defined field values       • Update history         • About BIGSdb       • Main public projects	Option settings       Set general options - including isolate table field handling.       Set display and query options for locus, schemes or scheme fields.       Manage submissions         View/modify client software permissions       Private data         Upload/manage records
Breakdown       Export         Single field       Export dataset         Two field       Contigs         Unique combinations       Scheme and alleles         Publications       Sequences - XMFA / concatenated FASTA	Analysis Codon usage Presence/absence status of loci Genome comparator BLAST Miscellaneous - Description of database fields

Now click the 'Update private records' link. You will be taken to the *curators' interface*, where you will be able to use the standard curator tools.



Use the curators' interface to make any changes to your isolate records, including uploading genome data.

## 13.3 Sharing access to private records

If *user projects* are enabled on the database, you can share access to your private isolates by adding them in to a user project and then sharing this.

See user projects for more details.

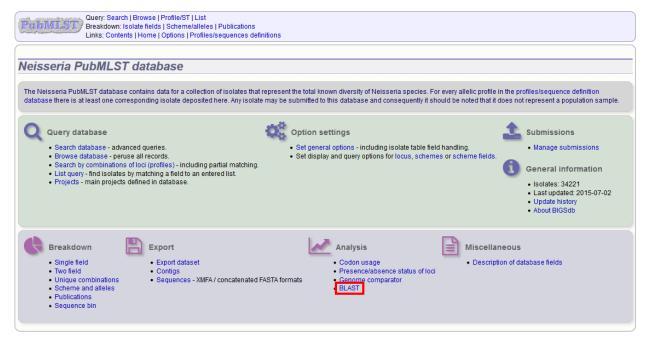
# CHAPTER 14

## Data analysis plugins

## 14.1 **BLAST**

The BLAST plugin enables you to BLAST a sequence against any of the genomes in the database, displaying a table of matches and extracting matching sequences.

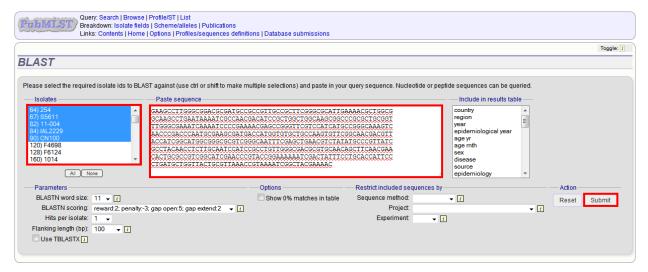
The function can be accessed by selecting the 'BLAST' link on the Analysis section of the main contents page.



Alternatively, it can be accessed following a query by clicking the 'BLAST' button in the Analysis list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

	7 B54; Z1054	UK		invasive (unspecified/other) invasive (unspecified/other)		-	В		ST-32 complex/ET-5 complex	7	16	
7 7891 8 M0024200	B54; Z1054						w	1101	ST-22 complex			
8 M0024200		Finland	1975	invasive (unspecified/other)		-	A	5	ST-5 complex/subgroup III	20	9	F3-1
	7	UK		invasive (unspecified/other)			в	1102	ST-18 complex	20	14	
				invasive (unspecified/other)		-	w	114	ST-22 complex			
10 6748	B73: Z1073	Canada		invasive (unspecified/other)			A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11 129	B92: Z1092	Germany		invasive (unspecified/other)			A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12 0090/89				invasive (unspecified/other)		-	В	1015	ST-32 complex/ET-5 complex	7	16	
13 139M	B99: Z1099	Philippines	1968	, , , , , , , , , , , , , , , , , , , ,	Neisseria m	eningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14 0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria m	eningitidis	Х	117			14	
15 1		Germany	1999	carrier	Neisseria m	eningitidis	E	864				
16 2		Germany	1999	carrier	Neisseria m	eningitidis	В	854	ST-18 complex			
17 3		Germany	1999	carrier	Neisseria m	eningitidis	W	174	ST-174 complex			
18 4		Germany	1999	carrier	Neisseria m	eningitidis	В	19	ST-18 complex			
19 S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria m	eningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20 5		Germany	1999	carrier	Neisseria m	eningitidis	NG	198	ST-198 complex			
21 6		Germany	1999	carrier	Neisseria m	eningitidis	NG	198	ST-198 complex			
22 7		Germany	1999	carrier	Neisseria m	eningitidis	E	60	ST-60 complex			
23 8		Germany	1999	carrier	Neisseria m	eningitidis	в	32	ST-32 complex/ET-5 complex			
24 S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria m	eningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25 9		Germany	1999	carrier	Neisseria m	eningitidis	в	930	ST-334 complex			
Analysis:	Fields Two Fi	ence/Absence	Benome	Combinations Comparator BLAST	Schemes/all	eles Publi	ications	Sequer	nce bin Tag status			

Select the isolate records to analyse - these will be pre-selected if you accessed the plugin following a query. Paste in a sequence to query - this be either a DNA or peptide sequence.



Click submit.

A table of BLAST results will be displayed.

															Togg
45	Т														
se se	elect the reau	uired isolate i	ids to BLAST ad	ainst (use ctr	l or shi	it to make m	nultiple se	lections) and paste	in your qu	erv seque	nce. Nucleotide (	or peptide sequences can b	e queried.		
Isolat			-	aste sequend				,,				Include in result			
	11027					SCGATGCC	GCCGTTG	CCGCTTCGGGCGC	ATTGAAA	ACGCTG	30G	country			
1201								GCTGGCTGGCAAG				region			
7891 ) 674								CGGGTTCGTCCAT				year epidemiological ye			
) 129								TGTGCTGCCAAGT TCGAGCTGAACGT				age yr			
) 139								TGGGCGACGCGTG				age mth			
) S31 ) S41	131 255							AAAAAATCGACTA				sex disease			
9040			СТО	GATGCTGGT	TACTG	CGTTAAAC	CGTAAAA	TCGGCTACGAAAA	C			source			
	(AIL)	None										epidemiology	-		
Para	neters						Optio	ns		Restrict in	cluded sequenc	es by		Action	
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			; penalty:-3; gap	open:5; gap	extend	2 🔻 🚺					Project:		<b>▼</b> [		
н	its per isolat	e: 1 🚽								EX	kperiment:	▼ 1			
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ate id 1 2 7 10 11 13 19 24 30 31 34 35 46 552	ng length (bp e TBLASTX [ A4/M1027 120M 7891 6748 129 139M S3131 S4355 14 10 20 26 255	Sidentity         A           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49           98.49         98.49	ignment length 465 465 465 465 465 465 465 465 465 465	7 7 7 7 7 7 7 12 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	180177 180583 180965 181186 181867 182004 182318 215673 8 182380 182815 182880 183179	19444 4782 19869 19181 35889 36775 19090 4534 1363524 5559 19783 18879 4982	19908 extract _ 5246 extract _ 20333 extract _ 19645 extract _ 37239 extract _ 37239 extract _ 19554 extract _ 4998 extract _ 1363988 extract _ 20247 extract _ 19343 extract _ 5446 extract _	1 1 1 1 1 1 1 1 1 1 1 1	n E-value 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.	807 807 807 807 807 807 807 807 785 807 807 807 807				
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ate id 1 Us 7 10 11 13 19 24 80 31 34 35 52 51 54	ng length (bp e TBLASTX [ A4/M1027 120M 7891 129M 7891 129 139M S3131 S4355 14 10 20 26 255 243 393	):         100         •           100         •         100         •           98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49         98.49	ignment length 465 465 465 465 465 465 465 465 465 465	7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	180177 180583 180965 181186 181867 182004 182318 215673 8 182380 182815 182880 182815 182880 183179 183381	19444 4782 19869 19181 35889 36775 19090 4534 1363524 5559 19783 18879 4982 4532 7217	19908 satract	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	E-value           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0	807 807 807 807 807 807 807 807 807 807				
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ankii Us 1 2 7 10 11 13 19 24 30 31 34 35 46 52 51 54 57 32	I Isolate A4/M1027 120M 7891 6748 129 139M 33131 84355 14 10 20 26 255 243 393 254 43 55611	);         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •         100         •           (100)         •<	ignment length 465 465 465 465 465 465 465 465 465 465	7 7 7 7 7 7 7 12 7 7 7 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	180177 180583 180965 181186 181867 182004 182318 215673 8 182380 182815 182880 183179 183381 183648 183818 183818 183818	19444 4782 19869 19181 35889 36775 19090 4534 1363524 5559 19783 18879 4982 4532 7217 4716 4804	19908 satract _ 5246 satract _ 20338 satract _ 36355 satract _ 37239 satract _ 19656 satract _ 4998 satract _ 1363988 satract _ 19548 satract _ 19548 satract _ 19548 satract _ 19548 satract _ 7681 satract _ 7681 satract _ 7681 satract _ 7681 satract _	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	n E-value 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.	807 807 807 807 807 807 807 807 807 807				
lanki Us ate id	ng length (bp e TBLASTX [ A4M1027 120M 7891 67891 83131 84365 14 10 20 26 255 243 393 254 85611 11-004	100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100         100           100	Ignment length 465 465 465 465 465 465 465 465 465 465	7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7		180177 180583 180965 181186 181867 182004 182318 215673 8 182380 182815 182880 182815 182881 183818 183648 183818 184143 1844297	19444 4782 19869 19181 35889 36775 19090 4534 1363524 5559 19783 18879 4982 4532 7217 4716 4804 19518	19908 extract _ 5246 extract _ 2033 extract _ 19845 extract _ 36355 extract _ 37239 extract _ 19854 extract _ 19858 extract _ 19858 extract _ 20247 extract _ 19448 extract _ 5446 extract _ 5446 extract _ 5468 extract _ 5588 extract _ 5288	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	n E-value 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.	807 807 807 807 807 807 807 807 807 807				

Clicking any of the 'extract' buttons will display the matched sequence along with a translated sequence and flanking sequences.

181867	35889	36353 extract>	$\rightarrow$	0.0	807
182004	36775	37239 extract	$\rightarrow$	0.0	807
182318	19090	19554 extract	$\rightarrow$	0.0	807
215673	4534	4998 extract ->	$\leftarrow$	0.0	807
8	1363524	1363988 extract ->	$\rightarrow$	0.0	785
182380	5559	6023 extract ->	$\rightarrow$	0.0	807
182815	19783	20247 extract ->	$\rightarrow$	0.0	807

acted c	uence: Segbin id#:182318 (19090-19554)	
cieu si	Juence. Sequinia#.102510 (19090-19554)	
	9	equence bin id#182318
		CGA ATTGICCGGC ITGCCGITIG ICAGCGCGCC GAACAAATII GAAGCCIIGG GCGGACGCGA IGCCGCCGII GCCGCIICG
lod		IGG CAAGCGGCCC GCGCTGCGGT TTGGGCGAAA TCAAAATCCC CGAAAACGAG CCGGGTTCGT CCATCATGCC GGGCAAAGT
		FIT ACCATCGGTA TGGCGGGCGC GTCGGGCAAT TTCGAGCTGA ACGTCTATAT GCCCGTCATC GCCTACAACC TCTTGCAAT IGA ACCCGTACCG GAAAAAATCG ACTATTTCCT GCACCATTCC CTGATGCTCG TTACCGCGTT AAACCGCAAA ATCGGTTAC
d 19554 th 465	AAACGCCGC CAAAGTCGCC AAAACCGCCT ACAAAAACAA CAAATCGTTG CGCGAAA	
ation $\rightarrow$		
ation		
	RHGFEQPSRIRRKSRRQTRR	IVRLAVCORAEQI 🖌 F1
	GTGLNSHPEYAEKAAAKLAI	LSGLPFVSAPNKF F2
	A R V 🎽 T A I P N T P K K P P P N S P	NCPACRLSARRTNL F3
	1 CGGCACGGGTTTGAACAGCCATCCCGAATACGCCGAAAAAGCCGCCGCCAAACTCGCC	
	:	- : : :
	S L G R T R C R R C R F G R I E N A G	GKPE K N R O R H P L A G F1
	EALGGRDAAVAASGALKTLA	
	K P W A D A M P P L P L R A H 🞽 K R W 1	
	01 GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGG	
	:	- : : :
	K R P A L R F G R N Q N P R K R A G F '	7 H H A G O S O P D P M R S F1
	SGPRCGLGEIKIPENEPGS	
	Q A A R A A V W A K S K S P K T S R V R	PSCRAKSTRPNAKR F3
	01 CAAGCGGCCCGCGCTGCGGTTTGGGCGAAATCAAAATCCCCCGAAAACGAGCCGGGTTC	
	:	- ; ; ;
	D D H G V L P S V R Q R R Y H R Y G G R	VGOFRAERLYARHR F1
	M T M V C C Q V F G N D V T I G M A G I	-
	* P W C A A K C S A T T L P S V W R A	RRAISS 🛃 TSICPSS F3
	01 GATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTTACCATCGGTATGGCGGGC	
	:	

At the bottom of the results table are links to export the matching sequences in FASTA format, (optionall) including flanking sequences. You can also export the table in tab-delimited text or Excel formats.

07	00011	50.45	405	1	v	104143	4004	J200 extract →	<del>-</del>	0.0	007
82	11-004	98.49	465	7	0	184297	19518	19982 extract -	$\rightarrow$	0.0	807
84	IAL2229	98.49	465	7	0	184635	4530	4994 extract -	←	0.0	807
90	CN100	98.49	465	7	0	184814	5350	5814 extract -	←	0.0	807

#### 14.1.1 Include in results table fieldset

This selection box allows you to choose which isolate provenance fields will be included in the results table.

<ul> <li>Include in results table</li> </ul>	
country	
region	
year	-
epidemiological year	
age yr	
age mth	
sex	
disease	
source	
epidemiology	Ŧ

Multiple values can be selected by clicking while holding down Ctrl.

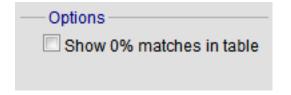
#### 14.1.2 Parameters fieldset

This section allows you to modify BLAST parameters. This affects sensitivity and speed.

Parameters		
BLASTN word size:	11 👻 🧵	
BLASTN scoring:	reward:2; penalty:-3; gap open:5; gap extend:2	<b>▼</b> [i
Hits per isolate:	1 👻	
Flanking length (bp):	100 👻 🧵	
🔲 Use TBLASTX 👔		

- BLASTN word size This is the length of the initial identical match that BLAST requires before extending a match (default: 11). Increasing this value improves speed at the expense of sensitivity.
- BLASTN scoring This is a dropdown box of combinations of identical base rewards; mismatch penalties; and gap open and extension penalties. BLASTN has a constrained list of allowed values which reflects the available options in the list.
- Hits per isolate By default, only the best match is shown. Increase this value to the number of hits you'd like to see per isolate.
- Flanking length Set the size of the upstream and downstream flanking sequences that you'd like to include.
- Use TBLASTX This compares the six-frame translation of your nucleotide query sequence against the six-frame translation of the contig sequences. This is significantly slower than using BLASTN.

#### 14.1.3 No matches



Click this option to create a row in the table indicating that a match was not found. This can be useful when screening a large number of isolates.

#### 14.1.4 Filter fieldset

This section allows you to further filter your collection of isolates and the contig sequences to include.

-Restrict included sec	nuences by	
restrict moldaded set	ductions by	
Sequence method:	▼ i	
Project:		<b>√</b> [i]
Experiment:	▼ i	

Available options are:

- Sequence method Choose to only analyse contigs that have been generated using a particular method. This depends on the method being set when the contigs were uploaded.
- Project Only include isolates belonging to the chosen project. This enables you to select all isolates and filter to a project.
- Experiment Contig files can belong to an experiment. How this is used can vary between databases, but this enables you to only include contigs from a particular experiment.

## **14.2 BURST**

BURST is an algorithm used to group MLST-type data based on a count of the number of profiles that match each other at specified numbers of loci. The analysis is available for both sequence definition database and isolate database schemes that have primary key fields set. The algorithm has to be *specifically enabled* by an administrator. Analysis is limited to 1000 or fewer records.

The plugin can be accessed following a query by clicking the 'BURST' button in the Analysis list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

6 1	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland		invasive (unspecified/other)	-	A	5	ST-5 complex/subgroup III	20	9	F3-1
8 1	M00242007		UK		invasive (unspecified/other)		В	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	В	930	ST-334 complex			
Brea Ai	nalysis: Bu Export: Da	elds Two Fi JRST Prese ataset Conti	noe/Absence	3enome	norphic sites Combinations a Comparator BLAST	Schemes/alleles Pub	lications	Seque	nce bin Tag status			

If there multiple schemes that can be analysed, these can then be selected along with the group definition.

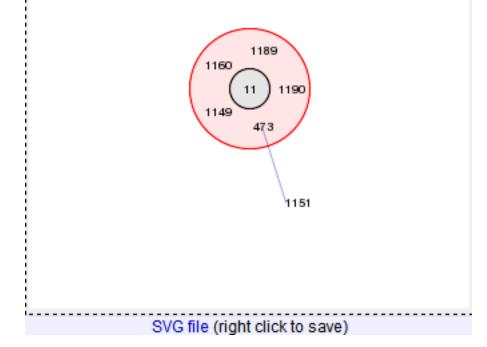
Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/Sequences definitions   Database submissions	
BURST analysis	
This is the original BURST algorithm, developed by Ed Feil, first implemented by Man-Suen Chan. This version h BURST analysis can be used to:	as been adapted for use as a plugin for the BIGSdb database software by Keith Jolley.
Divide strains into groups according to their allelic profiles.     Count the number of Single Locus Variants (SLV), Double Locus Variants (DLV) and Satellites (SAT) for ea     Identify the potential Ancestral Type (AT). These are shown with an asterisk next to their names in the resu	
Graphic representations of BURST groups can be saved in SVG format. This is a vector image format that can be	manipulated and scaled in drawing packages, including the freely available Inkscape.
Options	Action
Select scheme: MLST	Submit
Group definition: profiles match at n-2 v loci to any other member of the group (n = number of loci in scheme).	
✓ Shade variant rings ✓ Hide variant names (useful for overview if names start to overlap)	

Modifying the group definition affects the size of groups and how they link together. By default, the definition is n-2 (where n is the number of loci), so for example on a 7 locus MLST scheme groups contain STs that match at 5 or more loci to any other member of the group.

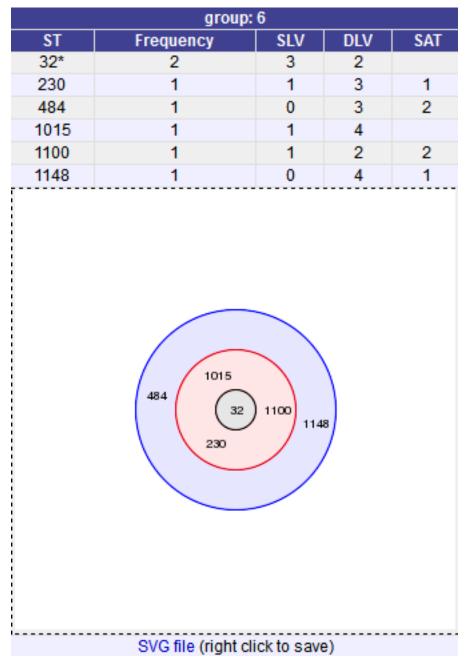
Click Submit.

A series of tables will be displayed indicating the groups of profiles. Where one profile can be identified as a central genotype, i.e. the profile that has the greatest number of other profiles that are single locus variants (SLV), double locus variants (DLV) and so on, a graphical representation will be displayed. The central profile is indicated with an asterisk.

	group:	2		
ST	Frequency	SLV	DLV	SAT
11*	37	5		1
473	1	2	4	
1149	19	1	4	1
1151	1	0	1	5
1160	1	2	3	1
1189	1	1	4	1
1190	1	1	4	1

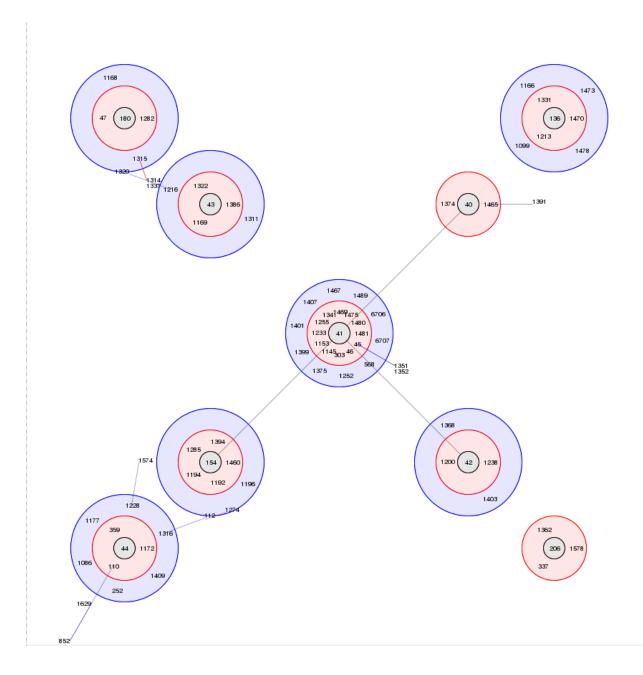


SLV profiles that match the central profile are shown within a red circle surrounding the central profile. Most distant profiles (triple locus variants) may be linked with a line. Larger groups may additionally have DLV profiles. These are



shown in a blue circle.

Groups can get very large, where linked profiles form sub-groups and an attempt is made to depict these.



## 14.3 Codon usage

The codon usage plugin for isolate databases calculates the absolute and relative synonymous codon usage by isolate and by locus.

The function can be selected by clicking the 'Codon usage' link in the Analysis section of the main contents page.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences defin	tions
	epresent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition may be submitted to this database and consequently it should be noted that it does not represent a population sample.
Query database Search database - advanced queries. Browse database - peruse all records. Search by combinations of loci (profiles) - including partial matching. List query - find isolates by matching a field to an entered list. Projects - main projects defined in database.	Option settings Set general options - including isolate table field handling. Set display and query options for locus, schemes or scheme fields.  Submissions General information Isolates: 34221 Last updated: 2015-07-02 Update history About BIGSdb
Breakdown       Export         • Single field       • Export dataset         • Unique combinations       • Contigs         • Scheme and alleles       • Sequences - XMFA / concatenated FA         • Sequence bin       • Sequences - XMFA / concatenated FA	Analysis Codon usage • Presence/absence status of loci • Genome comparator • BLAST

Alternatively, it can be accessed following a query by clicking the 'Codons' button in the Analysis list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

							-			-		
	M00240227		UK		invasive (unspecified/other)		В		ST-32 complex/ET-5 complex	7	16	
	M00282207		UK		invasive (unspecified/other)		W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland		invasive (unspecified/other)		A	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK		invasive (unspecified/other)		В	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada		invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	в	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	В	930	ST-334 complex			
Ana	lysis tools	8: elds Two Fi			Combinations Schemes		Sequence		Tag status			
Dice						AST						
	nalysis: Bu	JRST Code	ons Presence/A	bsence	Genome Comparator BL	AST						

Enter the ids of the isolate records to analyse - these will be already entered if you accessed the plugin following a query. Select the loci you would like to analyse, either from the dropdown loci list, and/or by selecting one or more schemes.

Prrhi/ILST Breakdown: Isolate fields   Scheme/alleles   Publication Links: Contents   Home   Options   Profiles/sequences		
		Toggle: i
Codon usage analysis		
		atabase containing sequences, or with sequences tagged, can be included. It is important to note that ng frame 1). Partial sequnces from the sequence bin will not be analysed. Please check the loci that you
	Loci	
Paste in list of ids to include, start a new line for each. Leave blank to include all ids. 1 2 3 4 5 6	A TISS_rDNA A TISS_rRNA (SSU_rRNA) 23S_rRNA abcZ abcZ (NEIS1015) acd2 (NEIS1279) acd4 (NEIS1727) Al None Pastelist	C Interest Information Proce
Sequence retrieval	Codons	Action
If both allele designations and tagged sequences	Select codon order:	Submit
exist for a locus, choose how you want these handled: i	eliphabetical	
Use sequences tagged from the bin Use allele sequence retrieved from external database	C or G ending codons first	
Do not include sequences with problem flagged (defined alleles will st	ill be used)	

Click submit. The job will be submitted to the queue and will start running shortly. Click the link to follow the job progress and view the output.

Ouery: Search   Browse   Profile/ST  List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: i
Codon usage analysis	
This analysis has been submitted to the job queue.	
Please be aware that this job may take some time depending on the number of sequences to analyse and how busy the server is.	
Follow the progress of this job and view the output.	

Four tab-delimited text files will be created.

- Absolute frequency of codon usage by isolate
- Absolute frequency of codon usage by locus
- Relative synonymous codon usage by isolate
- Relative synonymous codon usage by locus

Cuery: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   P Links: Contents   Home   Options   Profiles/se	
Job status viewer	
Status           Job id: BiGSdb_13269_1405586315_76138           Submit time: 2014-07-17 09:38:35           Status: finished           Start time: 2014-07-17 09:38:39           Progress: 100%           Stop time: 2014-07-17 09:38:05           Total time: 26 seconds	
Absolute frequency of codon usage by isolate     Absolute frequency of codon usage by locus     Relative synonymous codon usage (RSCU) by isolate     Relative synonymous codon usage (RSCU) by locus     Tar file containing output files	
Please note that job results will remain on the server for 7 days.	

## 14.4 Field breakdown

The field breakdown plugin for isolate databases displays the frequency of each value for fields, alleles and schemes.

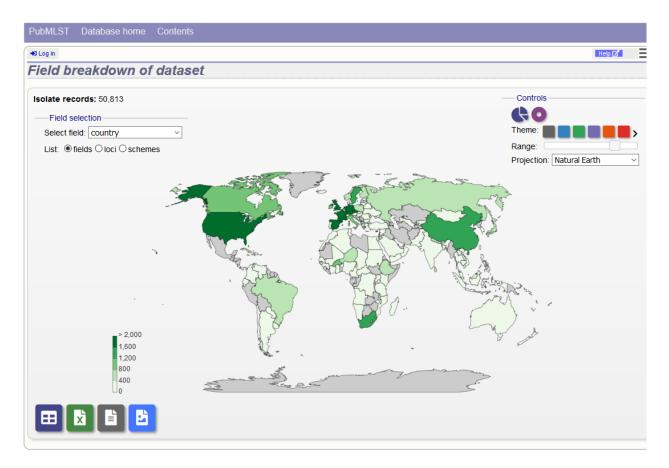
The breakdown function can be selected for the whole database by clicking the 'Single field' link in the Breakdown section of the main contents page.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it is	
Query database     Search database - advanced queries.     Browse database - peruse all records.     Search by combinations of loci (profiles) - including partial matching.     List query - find isolates by matching a field to an entered list.     Projects - main projects defined in database.	
Breakdown       Export       Analysis         Single field       - Export dataset       - Contigs       - Contigs       - Odd usage         • Unique combinations       - Sequences - XMFA / concatenated FASTA formats       - Odd usage       - Presence/absence status of to         • Publications       - Sequence bin       - Sequence - XMFA / concatenated FASTA formats       - Odd usage       - BLAST	Miscellaneous     Description of database fields

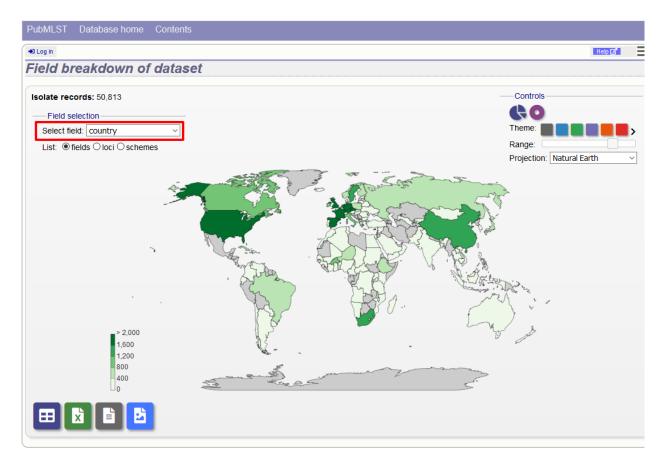
Alternatively, a breakdown can be displayed of the dataset returned from a query by clicking the 'Fields' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

15			Republic		(unspecified/other)	meningitidis								
15	1		Germany	1999	carrier	Neisseria meningitidis	E	0	0	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	0	0	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	0	0	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	0	0	19	ST-18 complex			
19	S3131	B213; NIBSC_2813; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	2061338	173	4	ST-4 complex	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	0	0	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	0	0	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	0	0	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	В	0	0	32	ST-32 complex			
24	S4355	B227; NIBSC_2806; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	A	2071992	198	5	ST-5 complex	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	В	0	0	930	ST-334 complex			

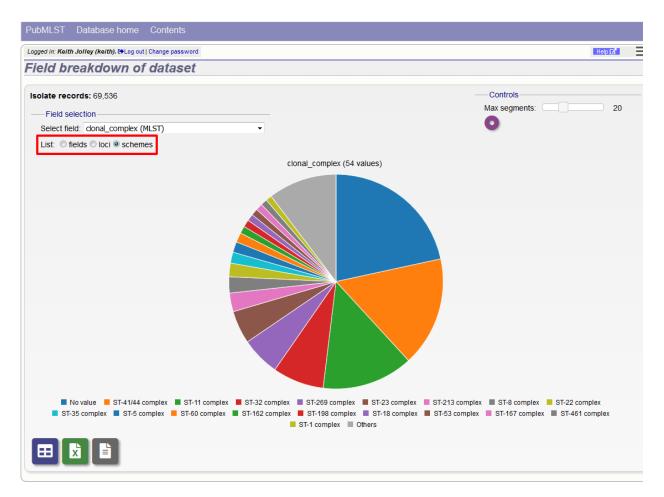
A chart will be displayed for the first field. Depending on the field type, this may be either a world map (for country or continent fields), pie chart, or bar chart.



Other fields can be chosen by selecting them in the dropdown list box.



You can also breakdown loci and schemes by clicking the appropriate button. This will re-populate the dropdown list.

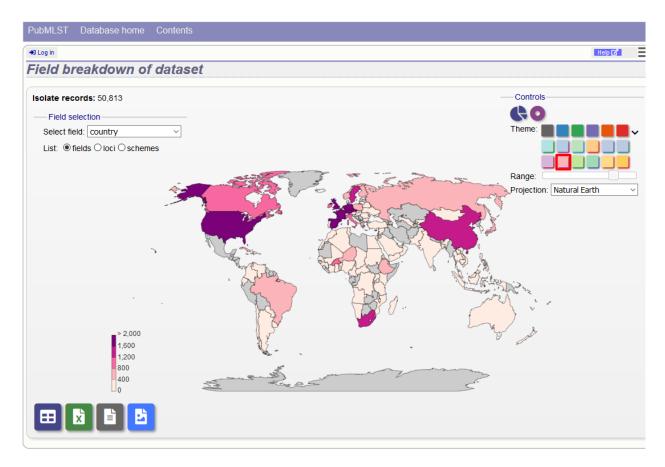


The charts are dynamic and you can manipulate some aspects of them using controls shown on the screen.

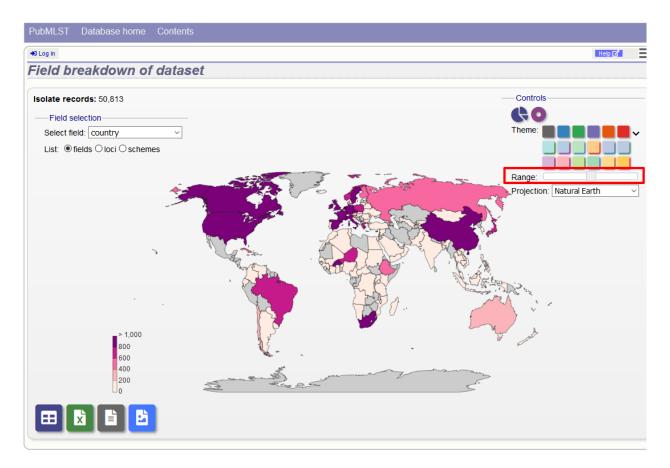
#### 14.4.1 Maps

World maps are shown for country and continent fields (provided standardized country names are used in the database). The maps can be modified in a number of ways.

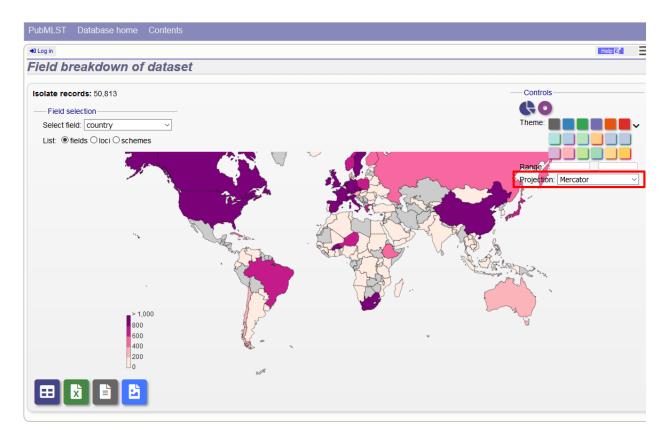
The colour theme can be changed by clicked the appropriate coloured square. Additional themes are available by clicking the '>' link.



The range that is used to decide the colour boundaries can be changed by using the range slider.



Finally the map projection can be changed. The default 'Natural Earth' provides a reasonable display for most latitudes but you may prefer others such as 'Mercator'.

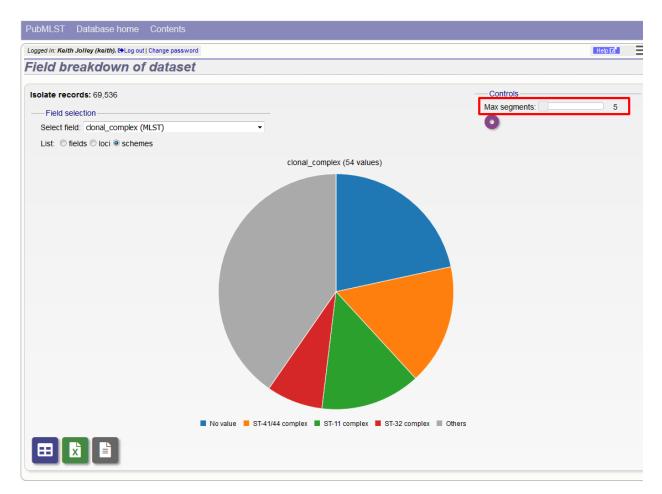


To see the same data as a pie chart, click the 'Pie' or 'Donut' icons.

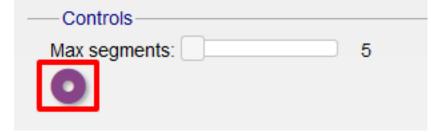


#### 14.4.2 Pie charts

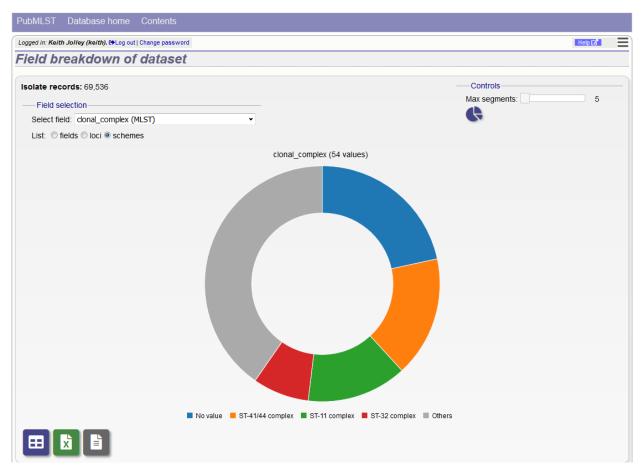
The maximum number of segments shown can be modified by sliding the 'Max segments' control. Low frequency values will be grouped in to a segment called 'Others'.



The chart can be transformed in to a donut chart by clicking the donut icon.



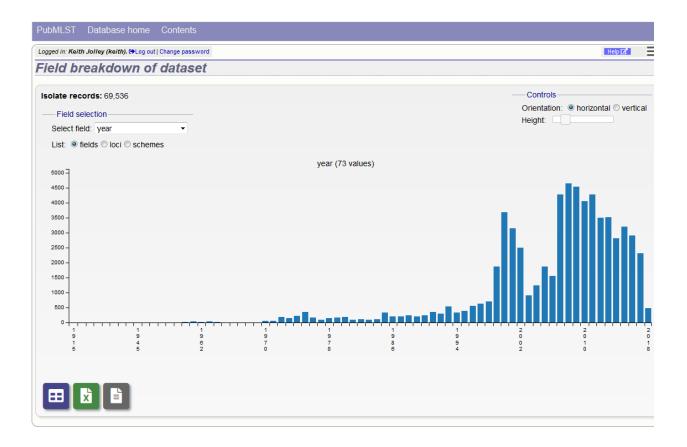
The icon changes to a pie chart image (clicking this will return to the pie chart).



Values can also be removed from the analysis by clicking their label in the legend below the chart. The percentages of the other values will be recalculated. Clicking the label again will re-add the value.

## 14.4.3 Bar charts

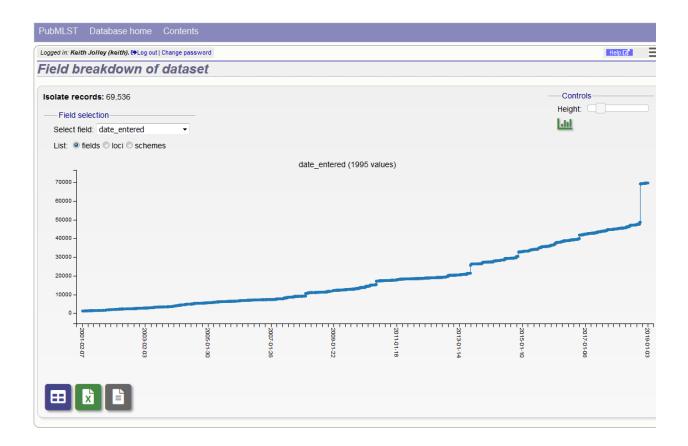
Integer fields will be displayed as a bar chart.



You can modify the height and the orientation of the chart using the controls.

#### 14.4.4 Line charts

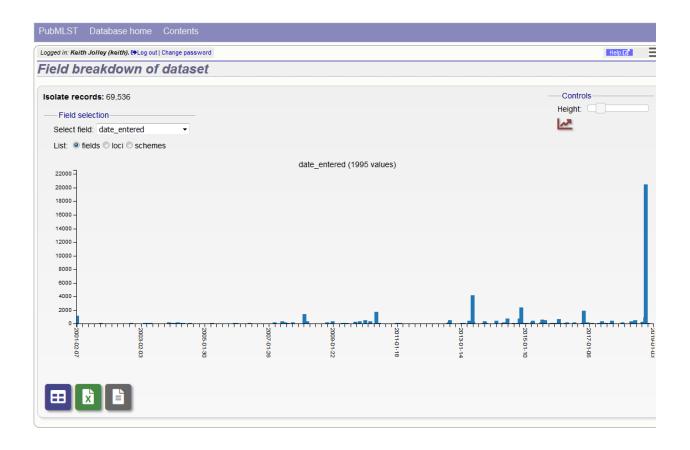
Date fields will be displayed as a line chart. By default this shows the cumulative values.



The chart can be converted in to a bar chart showing discrete values by clicking the bar chart icon.

Controls	
Height:	
<u>Lui</u>	

The icon changes to a line chart image (clicking this will return to the line chart).



#### 14.4.5 Summary tables

The field breakdown can be displayed as a summary table containing values and percentages of all values. This can be selected by clicking the table icon below the displayed chart.



The table can be re-ordered by clicking any of the headings.

in: Keith Jolley (keith)	. 🗭 Log out   Change	password
eakdown by	country	
I values.		
country ¢	Frequency +	Percentage +
UK	20460	29.42
Germany	5390	7.75
France	4744	6.82
Spain	3680	5.29
Czech Republic	3497	5.03
Poland	2897	4.17
The Netherlands	2665	3.83
USA	2618	3.76
Sweden	1730	2.49
Italy	1693	2.43
China	1457	2.10
South Africa	1300	1.87
Ireland	1283	1.85
New Zealand	1110	1.60
Norway	1033	1.49
Belgium	964	1.39
Canada	922	1.33
Greece	850	1.22
Austria	737	1.06
Brazil	651	0.94
Japan	604	0.87
Unknown	596	0.86
Finland	591	0.85
Portugal	590	0.85
Niger	580	0.83
Burkina Faso	570	0.82
Denmark	530	0.76
Russia	497	0.71
Cuba	432	0.62
Slovenia	388	0.56
Australia	321	0.46

The same table can be exported as an Excel file by clicking the Excel icon.

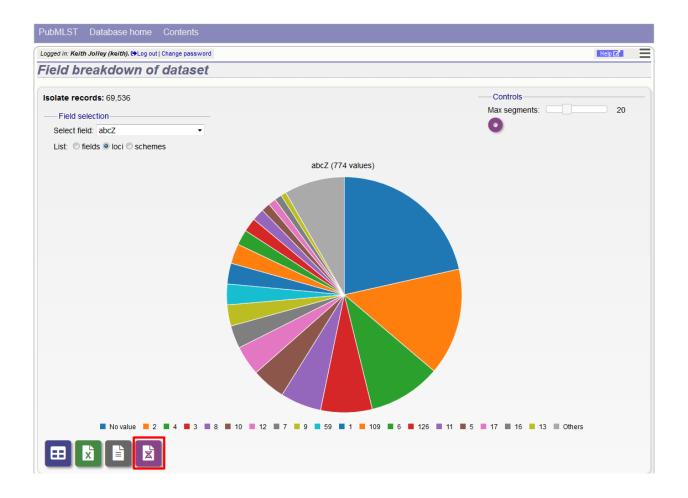


Alternatively, it can be exported as a tab-delimited text file by clicking the text file icon.



## 14.4.6 Exporting allele sequences

If a locus breakdown is being display, you can choose to export the allele sequences in FASTA format by clicking the FASTA file icon.



## 14.5 Gene Presence

The Gene Presence analysis tool will determine whether loci are present or absent, incomplete, have alleles designated, or sequence regions tagged for selected isolates and loci. If a genome is present and a locus designation not set in the database, then the presence and completion status are determined by scanning the genomes. The results can be displayed as interactive pivot tables or a heatmap. The analysis is limited to 500,000 data points (locus x isolates).

The Gene Presence tool can be accessed from the contents page by clicking the 'Gene Presence' link.

PubMLST Database home Contents	
+Ð Log in	=
Neisseria PubMLST database	
The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profil definition database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be n population sample.	
Q Query database 📰 Projects 🗱 Option settings	Submissions
Search or browse database     Search by combinations of loci (profiles)     Search by combinations     Search by combinations     Search by combinations     Search by combinations     Search by combina	Manage submissions
	General
	Isolates: 48,296
	Last updated:
	2019-01-28  • Defined field values
	<ul><li>Update history</li><li>About BIGSdb</li></ul>
Breakdown B Export Analysis Third party tools	
	on of genomic relationships
Two field     Contigs     Gene presence     ITOL - Phylogenetic tree	
	and phylogenetic inference visualization and sharing for
Sequence bin     Miscellaneous	visualization and snaring for
Description of database fields	

Alternatively, it can be accessed following a query by clicking the 'Gene Presence' button at the bottom of the results table. Isolates returned from the query will be automatically selected within the plugin interface.

	0120/85		020011	1990	IIIVGSIVE	Neissenia	~				14	
			Republic		(unspecified/other)	meningitidis						
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19	S3131	B213; NIBSC_2813; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex			
24	S4355	B227; NIBSC_2806; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	В	930	ST-334 complex			

Select the isolates to include. Analysis can be performed on any selection of loci, or more conveniently, you can select a scheme in the scheme selector to include all loci belonging to that scheme.

The parameters of the BLAST query used to determine presence or absence can be modified, but in most cases the

og in				Toggle: 🔇
ene Presen	nce - Neisseria PubMLS	ST		
			tions in list boxes. In addition to selecting individual loci, you can cl	hoose to include
i defined in schem	es by selecting the appropriate scheme	description.		
eractive analysis is	limited to 500,000 data points (isolates	x loci). If you select more than this then output	ut will be restricted to static tables.	
-Isolates		Loci	Recommended schemes	
	Optionally include data not in the	'16S_rDNA	<ul> <li>Select one or more schemes</li> </ul>	
1 <b>^</b>	database.	16S_rRNA (SSU_rRNA)	below or use the full schemes list.	
3	Upload assembly FASTA file	23S_rRNA abcZ	MLST	
5	(or zip file containing multiple	abcz abcz (NEIS1015)	Ribosomal MLST	
5 7 <del>v</del>	FASTA files - one per genome): 1	aceF (NEIS1279)	N. meningitidis cgMLST v1.0	
B		ackA2 (NEIS1727) acnA (NEIS1729)	N. gonorrhoeae cgMLST v1.0	
Clear List all	Browse No file selected.	acha (NEIS1729)	Ψ Ψ	
		All None Paste list	Clear	
Schemes	Paramete	rs / options		
- 💷 🦾	eMLST (20 locus whc * Min	% identity: 70 👻 🚯		
💷 🔎	N. gonorrhoeae cgMI Min %	alignment: 50 👻 🜖		
- <mark>- 😪 🕼</mark>	N. meningitidis cgML BLASTN	word size: 20 - (1)		
	OMV peptide typing			
	Ribosomal MLST			
	rpIF species =			
	ner schemes			
<hr/>				
	,			
-Action				
Reset Subm	nit			

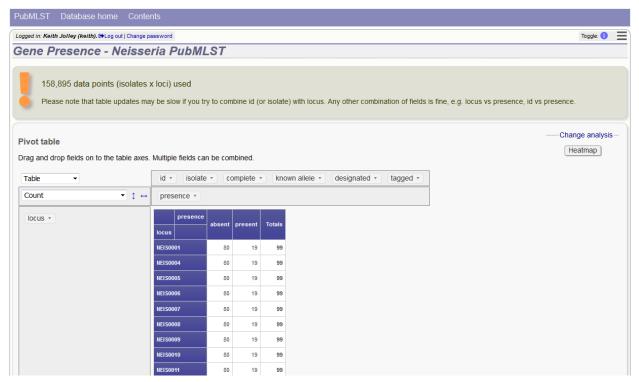
default options should work well. Click 'Submit' to start the analysis.

The job will be sent to the job queue. When it has finished, you will have two options to display the output: 'Pivot Table' or 'Heatmap'.

PubMLST Database ho	me Contents
Logged in: Keith Jolley (keith). 🗭	.og out   Change password
Job status view	er
Status	
Job id:	BIGSdb_194879_1548675927_08172
	2019-01-28 11:45:27
Status:	finished
Start time:	2019-01-28 11:45:43
Progress:	100%
Stop time:	2019-01-28 11:46:38
Total time:	54 seconds
Output Pivot Table H Files Presence/abse	Ieatmap
Please note that job results	will remain on the server for 7 days.

## 14.5.1 Pivot Table

Clicking the 'Pivot Table' button will display an interactive pivot table. The default display shows the number of isolates for which each locus is present or absent.



You can break down any combination of fields by dragging them from the field area at the top of the table to either of the axes. For example, to show how many isolates have alleles designated and sequence regions tagged for each locus, drag the 'designated' and 'tagged' fields to the x-axis selector.

PubMLST Database home Cont					
Logged in: Keith Jolley (keith). 🗘 Log out   Change	password				Toggle: 🜖
Gene Presence - Neiss	eria PubMLST				
158,895 data points (isolate: Please note that table updates n		nbine id (c	or isolate)	h locus. Any other combination of fields is	fine, e.g. locus vs presence, id vs presence.
Pivot table Drag and drop fields on to the table axe	s. Multiple fields can be co	mbined.			Change analysis [Heatmap]
Table 🔻	id • isolate • c	omplete 🔻	know	llele • designated • tagged •	
Count • 🕇 🗧	presence •	+			
locus *	presence locus absent	present	Totals		
	NEIS0001 80	19	99		
	NEIS0004 80		99		
	NEIS0005 80 NEIS0006 80		99		
	NEIS0007 80		99		
	NEIS0008 80		99		
	NEIS0009 80	19	99		
	NEIS0010 80	19	99		
	NEIS0011 80	19	99		

The table will be re-drawn including these fields.

ivot table rag and drop fields on to the table axes.	Multiple	e fields can	be com	bined.							
Table 👻	id •	id • isolate • complete • known allele •									
Count	pres	presence   designated  tagged									
locus *		presence	al	bsent		present					
		designated	not de	esignated	des	ignated	not de	signated	Totals		
		tagged	tagged	untagged	tagged	untagged	tagged	untagged	Totals		
	locus										
	NEIS0001			80	19 19				99		
	NEISOO			80	19				99		
	NEISOO	006		80	19				99		
	NEIS0007			80	19				99		
	NEIS0008			80	19				99		
	NEISOO			80	19				99		
	NEIS00			80	19 18				99		
	NEISOO			80	18		1		99		
	NEISOO			80	19				99		
	NEISOO	)14		80	19				99		
	NEISOO	)15		80	19				99		
	NELSOO	116		80	17		2		99		

**Note:** If your dataset has more than 100,000 data points (locus x isolates), then be aware that combining both id (or isolate) and locus within the table will result in sluggish performace. Any other combination of fields should be fine.

## 14.5.2 Heatmap

Clicking the 'Heatmap' button will display an interactive heatmap. By default the display shows the presence or absence of a locus for each isolate.

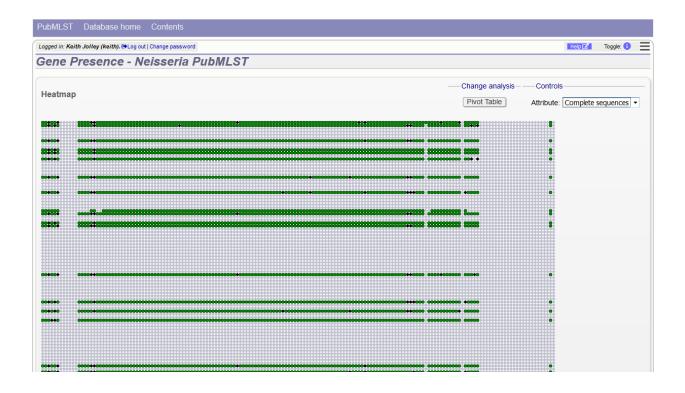
Hovering the mouse cursor or touching a region will identify the isolate and locus in a tooltip.

PubMLST Database home Contents		
Logged in: Keith Jolley (keith). [+Log out   Change password		Toggle: 🜖 📃
Gene Presence - Neisseria PubMLST		
Heatmap	Change analysis - Controls - Controls - Pivol Table Attribute: Presence	•
	id:35; 26 locus:NEIS0379 present	
•		Þ

Change the attribute that is displayed by changing the selection in the attribute dropdown box:

PubMLST Database home Contents		
Logged in: Keith Jolley (keith). HoLog out [ Change password		Toggle: 🚯
Gene Presence - Neisseria PubMLST		
Heatmap	Change analysis Pivot Table	Controls Attribute Complete sequences
۰		Þ

The heatmap does scale to the number of records required to be displayed. If you find individual points to be too small, then choose a smaller subset of data to display:



## 14.6 Genome comparator

Genome Comparator is an optional plugin that can be enabled for specific databases. It is used to compare whole genome data of isolates within the database using either the database defined loci or the coding sequences of an annotated genome as the comparator.

Output is equivalent to a whole genome MLST profile, a distance matrix calculated based on allelic differences and a NeighborNet graph generated from this distance matrix.

Genome Comparator can be accessed on databases where it is enabled from the contents page by clicking the 'Genome Comparator' link.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in th database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it doe	
<ul> <li>Query database</li> <li>Search database - advanced queries.</li> <li>Browse database - peruse all records.</li> <li>Search by combinations of loci (profiles) - including partial matching.</li> <li>List query - find isolates by matching a field to an entered list.</li> <li>Projects - main projects defined in database.</li> </ul>	Submissions Manage submissions General information I losiates: 34221 Last updated: 2015-07-02 Update history About BIGSdb
Breakdown       Export       Analysis       Miscellaned         • Single field       • Export dataset       • Codon usage       • Description         • Two field       • Onligs       • Sequences - XMFA / concatenated FASTA formats       • Codon usage       • Description         • Publications       • Sequence bin       • Sequence bin       • BLASI       • BLASI       • BLASI	ous of database fields

Alternatively, it can be accessed following a query by clicking the 'Genome Comparator' button at the bottom of the results table. Isolates with sequence data returned in the query will be automatically selected within the Genome Comparator interface.

19025 M10 240481	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	1831		22	9	F3-3
19026 M10 240482	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	3754	ST-41/44 complex/Lineage 3	7-2	4	F5-1
19027 M10 240484	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	1097	ST-41/44 complex/Lineage 3	17-1	23	F1-5
19028 M10 240485	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	275	ST-269 complex	22	9	F5-12
19029 M10 240487	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	1049	ST-269 complex	19-1	15-11	F5-1
19030 M10 240489	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	461	ST-461 complex	19-2	13-1	F3-9
19031 M10 240490	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	1161	ST-269 complex	22	9	F5-12
19032 M10 240498	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	41	ST-41/44 complex/Lineage 3	7-2	4	F1-5
19958 M10 240476	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	9812	ST-213 complex	22	14	F5-5
19959 M10 240499	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	275	ST-269 complex	22	9	F5-12
19960 M10 240500	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	41	ST-41/44 complex/Lineage 3	7-2	4	F1-5
19961 M10 240502	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	340	ST-41/44 complex/Lineage 3	7-2	4	F1-5
19962 M10 240503	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	23	ST-23 complex/Cluster A3	5-1	2-2	F1-96
19963 M10 240505	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	1655	ST-23 complex/Cluster A3	5-1	10-10	F4-1
19964 M10 240507	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	183	ST-23 complex/Cluster A3	21	16-5	deleted
19965 M10 240508	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	1575		7-2	13-1	F1-7
19966 M10 240511	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	4713		22	9	F5-12
19967 M10 240512	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	41	ST-41/44 complex/Lineage 3	7-1	1	F1-5
19968 M10 240514	UK	2010 invasive (unspecified/other) Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex	5	2	F1-1
19969 M10 240515	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	269	ST-269 complex	5-1	2-2	F5-1
19970 M10 240520	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	1655	ST-23 complex/Cluster A3	5-1	10-1	F4-1
Analysis tools: Breakdown: Fields Two f Analysis: Presence/Absenc Export: Dataset Con	œ Ge	Codons Polymorphic sites Combinations Schemes/alleles nome Comparator BLAST Sequences	Publ	lications	Sequence bin			

## 14.6.1 Analysis using defined loci

Select the isolate genomes that you wish to analyse. These will either be in a dropdown list or, if there are too many in the database, a text input where a list can be entered. You can also upload your own genomes for analysis - these should be either a single file in FASTA format (if you have just one genome), or a zip file containing multiple FASTA files. Select either the loci from the list or a set of schemes. Press submit.

	y (keith). @Log out   Change password Comparator - Neisseria Pu	MI ST					Help 🖓	Toggle:
ease select the re	equired isolate ids and loci for comparison - neme description. Alternatively, you can enter User genomes	ISE CTRL or SHIF		enome and			o include all loci defined in schemes t Schemes	by sele
662 663 664 665	Optionally include data not in the database. Upload FASTA file (or zip file containing multiple FASTA files - one per genome): • Browse No file selected.	'16S_rDNA 16S_rRNA (S _235_rRNA abcZ abcZ (NEIS1 aceF (NEIS1 ackA2 (NEIS acnA (NEIS1	015) 279) 1727)	isolate countr region year epiden age yr age m sex disease source	y niological year th a		▲— 🗑 🧾 Typing — 💌 🛄 MLST — 🔲 🛄 Finetyping antige	Ш
Reference geno	ome ——————————————————Parameters / o	tions ———	-Distance matrix calculation-		Alignments	Core ge	nome analysis ———	
nter accession n tr choose annotat r upload Genban Browse No f	ted genome: Min % alignn BLASTN word nk/EMBL/FASTA file:	ntity: 70 v 0 eent 50 v 0 size: 20 v 0	With incomplete loci: Completely exclude from a Treat as distinct allele Ignore in pairwise compari		Produce alignments  Include ref sequences in alignment Include ref sequences in alignment Include ref sequences in alignment Aligner: MAFFT		shold (%): 90   ▼  0 late mean distances 6	
Filter by Sequence mett Pro Experim	oject:	Action Reset	Submit					

The job will be submitted to the job queue and will start running shortly. Click the link to follow the job progress and view the output.

Description         Output         Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications         Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: i
Genome Comparator - Neisseria PubMLST	Show options
This analysis has been submitted to the job queue. Please be aware that this job may take a long time depending on the number of comparisons and how busy the server is.	
Follow the progress of this job and view the output.	

There will be a series of tables displaying variable loci, colour-coded to indicate allelic differences. Finally, there will be links to a distance matrix which can be loaded in to SplitsTree for further analysis and to a NeighborNet chart showing relatedness of isolates. Due to processing constraints on the web server, this NeighborNet is only calculated if 200 or fewer genomes are selected for analysis, but this can be generated in the stand-alone version of SplitsTree using the distance matrix if required.

Status           St	Breakdown: Isolate	ise   Profile/ST   List leids   Scheme/alleles   Publications me   Options   Profiles/sequences definitions   Database subr	missions	
	ob status viewer			
	Status			
	Submit time: 2014-07-15 08:41:03 Status: finished Start time: 2014-07-15 08:41:05 Progress: 100%	63_94241		
	Total time: 17 seconds			
		e been defined otherwise sequences will be marked as 'Ney	w#1 'New#2' etc. Missing alleles are ma	arked as 'X' Truncated alleles (located at end of contio) are marked as 'T'
	adk         3         3           aroE         4         19           fumC         3         3           gdh         8         8           pdhC         4         4	3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3	3         3         3         3           4         19         19         19           3         3         3         3           4         8         8         8           4         4         4         4	4 3 8 4
construction       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2 <t< td=""><td></td><th></th><td></td><th>0</th></t<>				0
are before       4       19       4       4       4       4       4       19       19       19       4         c and and and c and c and c and and and c and c and		(2839) 664 (2838) 665 (2845) 666 (2843) 667 (2842) 669 (2	2846) 670 (2840) 671 (2844) 672 (284	7) 698 (FAM18)
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Anique strains : 5 <b>Strain 1 Strain 2 Strain 3 Strain 4 Strain 5</b> St4 (L394289) 662 (2837) 666 (2843) 669 (2845) 669 (2844) 670 (2844) 671 (2844) • Text output file • Distance matrix (Nexus format) - Suitable for loading in to SplitSTree. Distances between taxa are calculated as the number of loci with different allele sequences • Splits graph (Neighbour-net, PNC format) • Splits graph (Neighbour-net, SVG format) - This can be edited in Inkscape or other vector graphics editors • Locus presence frequency • Locus presence frequency • Culck to enlarge) • Locus presence frequency • Culck to enlarge) • Tartile containing output files				
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344 (1934/280) 662 (2337) 666 (2843) 665 (2845) 669 (2846) 659 (2846) 659 (2847) 659 (2847) • Text output file • Text output file • Splits graph (Neighbour-net, PNG format) • Tar file containing output files • Tar file containing output file	Jnique strains: 5			
<ul> <li>Excel format</li> <li>Distance matrix (Neus format) - Suitable for loading in to SplitsTree. Distances between taxa are calculated as the number of loci with different allele sequences</li> <li>Splits graph (Neighbour-net_PNC format)</li> <li>(click to enlarge)</li> <li>(click to enlarge)</li> <li>(click to enlarge)</li> <li>(click to enlarge)</li> <li>Locus presence frequency chart (PNG format)</li> <li>(click to enlarge)</li> </ul>	644 (L93/4286) 662 (2837) 666 (2843) 6 663 (2839) 670 (2840) 667 (2842)			
<ul> <li>(dick to enlarge)</li> <li>Splits graph (Neighbour-net, SVG format) - This can be edited in Inkscape or other vector graphics editors</li> <li>Locus presence frequency</li> <li>Locus presence frequency (click to enlarge)</li> <li>(click to enlarge)</li> <li>Tar file containing output files</li> </ul>	Excel format     Distance matrix (Nexus format) -		re calculated as the number of loci with (	different allele sequences
Splits graph (Neighbour-net, SVG format) - This can be edited in Inkscape or other vector graphics editors     Locus presence frequency     Locus presence f	In the second			
Tar file containing output files	<ul> <li>Splits graph (Neighbour-net; SVC</li> <li>Locus presence frequency</li> </ul>	format) - This can be edited in Inkscape or other vector graphi	cs editors	
Tar file containing output files	- - - 	(dick to enlarge)		
ease note that inh results will remain on the server for 7 days	L			
	lease note that inb results will remain a	the server for 7 days		

## 14.6.2 Analysis using annotated reference genome

Select the isolate genomes that you wish to analyse and then either enter a Genbank accession number for the reference genome, or select from the list of reference genomes (this list will only be present if the administrator has *set it up*). Selecting reference genomes will hide the locus and scheme selection forms.

PubMLST Datab	ase home Contents		
Logged in: Keith Jolley	(keith). DLog out   Change password		Help 🗹 Toggle: 🚯 🚍
Genome Co	mparator - Neisseria Pub	ILST	
		TRL or SHIFT to make multiple selections in list boxes. In addition to selecting individual loci, you cession number for an annotated reference genome and compare using the loci defined in that.	can choose to include all loci defined in schemes by selecting
Isolates		Include in identifiers	
662	Optionally include data not in the	solate	
663	database.	country	
664 665	Upload FASTA file	region /ear	
	(or zip file containing multiple FASTA files - one per genome): 1	epidemiological year	
		age yr age mth	
	Browse No file selected.	Sex	
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	me Parameters / option	Distance matrix calculation Alignments	Core genome analysis
Enter accession n	umber: Min % identity		Core threshold (%): 90 👻 🖲
or choose annotat	ed genome: Min % alignment		Calculate mean distances ()
FAM18 (Nm)	BLASTN word size	20 - 0 Align all loci (not only variable)	
or upload Genban		Kclude paralogous loci	
Browse No f	ile selected. 0		
Ellis hu			
Filter by Sequence meth	and:	Action	
Sequence metro Proj		Reset Submit	
Experim			
Experim	ent. 👻 😈		

Output is similar to when comparing against defined loci, but this time every coding sequence in the annotated reference will be BLASTed against the selected genomes. Because allele designations are not defined, the allele found in the reference genome is designated allele 1, the next different sequence is allele 2 etc.

b stat	us viewer															
atus																
lob id	BIGSdb_21911_1405410488_8452															
	2014-07-15 08:48:08															
	finished															
Start time:	2014-07-15 08:48:34															
Progress:																
	2014-07-15 09:12:58															
Total time:	24 minutes and 24 seconds															
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olusia bu	reference genome															
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version	1															
type	dna															
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length lescription ding regio loci	2194961 Neisseria meningitidis serogroup C FAM18 complete genome. ns 1975	K' Truncated	alleles (loc	ated at end o	f contig) are	marked :	as T									
length lescription ding regio loci	2194961 Neisseria meningitidis serogroup C FAM18 complete genome.															
length lescription ding regio loci	2194961 Neisseria meningitidis serogroup C FAM18 complete genome. ns 1975	Sequence		Reference	644	662	663	664 (2838)	665 (2845)	666 (2843)	667 (2842)	669 (2846)	670 (2840)	671 (2844)	672 (2847)	
length lescription ding regio loci ch unique a Locus	2194961 Neisseria meningilidis serogroup C FAM18 complete genome. ns 1975 allele is defined a number starting at 1. Missing alleles are marked as ?		Genome			662	663			666 (2843) 1					672 (2847) 1	
length lescription ding regio loci ch unique : Locus xC   envA   IMC0001	2194961 Neisseria meningilidis serogroup C FAM18 complete genome. Is 1975 allele is defined a number starting at 1. Missing alleles are marked as 7 Product UDP-3-0-[3-hydroxynyristoyi] N-acetylglucosmine deacetylase	Sequence length 924	Genome position 1261	Reference genome 1	644 (L93/4286) 1	662 (2837) 1	663	(2838) 1	(2845) 1	(2843) 1	(2842) 1	(2846) 1	(2840) 1	(2844) 1	(2847) 1	
length lescription ding regio loci ch unique : Locus kC   envA   IMC0001 pilS1	2194961 Neisseria meningilidis serogroup C FAM18 complete genome. ns 1975 allele is defined a number starting at 1. Missing alleles are marked as 3 Product	Sequence length	Genome position	Reference genome	644	662 (2837)	663		(2845)							
length lescription ding regio loci ch unique : Locus xC   envA   IMC0001 pilS1   IMC0002	2194961 Neisseria meningilidis serogroup C FAM18 complete genome. 1975 allele is defined a number starting at 1. Missing alleles are marked as 7 Product UDP-3-O-[3-hydroxymyristoy] N-acetylglucosmine deacetylase pilin (fragment)	Sequence length 924 291	Genome position 1261 3341	Reference genome 1 1	644 (L93/4286) 1 1	662 (2837) 1 1	663 (2839) 1 1	(2838) 1 1	(2845) 1 1	(2843) 1 1	(2842) 1 1	(2846) 1 1	(2840) 1 1	(2844) 1 1	(2847) 1 1	(FAN
length lescription ding regio loci ch unique a ch unique a Locus xC   envA   IMC0001 pilS1   IMC0002 pilS2	2194961 Neisseria meningilidis serogroup C FAM18 complete genome. Is 1975 allele is defined a number starting at 1. Missing alleles are marked as 7 Product UDP-3-0-[3-hydroxymyristoyi] N-acetylglucosmine deacetylase	Sequence length 924	Genome position 1261	Reference genome 1	644 (L93/4286) 1	662 (2837) 1	663	(2838) 1	(2845) 1	(2843) 1	(2842) 1	(2846) 1	(2840) 1	(2844) 1	(2847) 1	(FAN
length lescription ding regio loci ch unique a ch unique a Locus xC   envA   IMC0001 pilS1   IMC0002 pilS2	2194961 Neisseria meningilidis serogroup C FAM18 complete genome. 1975 allele is defined a number starting at 1. Missing alleles are marked as 7 Product UDP-3-O-[3-hydroxymyristoy] N-acetylglucosmine deacetylase pilin (fragment)	Sequence length 924 291	Genome position 1261 3341	Reference genome 1 1	644 (L93/4286) 1 1	662 (2837) 1 1	663 (2839) 1 1	(2838) 1 1	(2845) 1 1	(2843) 1 1	(2842) 1 1	(2846) 1 1	(2840) 1 1	(2844) 1 1	(2847) 1 1	(FAN
length lescription ding regio loci ch unique : Locus xC   envA   MIC0001 pilS1   IMC0002 pilS2   IMC0003 fbp   JMC0004	2194961 Neisseria meningilidis serogroup C FAM18 complete genome. 1975 allele is defined a number starting at 1. Missing alleles are marked as 3 Product UDP-3-O-[3-hydroxymyristoy] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin peptidyl-protyl cis-trans isomerase	Sequence length 924 291 366 330	Genome position           1261           3341           3675           4069	Reference genome 1 1 1 1 1	644 (L93/4286) 1 2 2	662 (2837) 1 1 2 2 2	663 (2839) 1 1 2 2	(2838) 1 2 2	(2845) 1 2 2	(2843) 1 2 2	(2842) 1 1 2 2	(2846) 1 2 T	(2840) 1 2 2	(2844) 1 2 2	(2847) 1 2 2	(FAN 1 1 1
length Jescription ding regio loci ch unique a th uniq	2194961 Neisseria meningilidis serogroup C FAM18 complete genome. Is 1975 allele is defined a number starting at 1. Missing alleles are marked as 7 Product UDP-3-O-[3-hydroxymyristoy] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin peptidyl-prolyl cis-trans isomerase putative membrane protein	Sequence length 924 291 366 330 219	Genome position           1261           3341           3675           4069           4476	Reference genome 1 1 1 1 1 1	644 (L93/4286) 1 2 2 2	662 (2837) 1 2 2 3	663 (2839) 1 2 2 3	(2838) 1 2 2 3	(2845) 1 2 2 3	(2843) 1 2 2 3	(2842) 1 2 2 3	(2846) 1 2 T 4	(2840) 1 2 2 3	(2844) 1 2 2 5	(2847) 1 2 2 3	(FAN 1 1 1
length Jescription ding regio loci ch unique : Locus xC   envA   IMC0001 pilS1   IMC0002 pilS2   IMC0003 fbp   IMC0004 IMC0004 IMC0006	2194961 Neisseria meningilidis serogroup C FAM18 complete genome. 1975 allele is defined a number starting at 1. Missing alleles are marked as 7 Product UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase pillin (fragment) truncated pillin peptidyl-prolyl cis-trans isomerase putative membrane protein putative glycerate dehydrogenase	Sequence length 924 291 366 330 219 954	Genome position           1261           3341           3675           4069           4476           4816	Reference genome 1 1 1 1 1 1 1 1	644 (L93/4286) 1 2 2 2 2 2	662 (2837) 1 2 2 3 2	663 (2839) 1 2 2 3 2	(2838) 1 2 2 3 2	(2845) 1 2 2 3 2	(2843) 1 2 2 3 2 3 2 3 2 3 3 3 3 3 3 3 3 3 3 3	(2842) 1 2 2 3 2	(2846) 1 2 7 4 2	(2840) 1 2 2 3 2 2	(2844) 1 2 2 5 2	(2847) 1 2 2 3 2 2	(FAN
length description ding regio loci ch unique a Locus xC   envA   VMC0001 pilS1   VMC0002 pilS2   VMC0003	2194961 Neisseria meningilidis serogroup C FAM18 complete genome. Is 1975 allele is defined a number starting at 1. Missing alleles are marked as 7 Product UDP-3-O-[3-hydroxymyristoy] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin peptidyl-prolyl cis-trans isomerase putative membrane protein	Sequence length 924 291 366 330 219	Genome position           1261           3341           3675           4069           4476	Reference genome 1 1 1 1 1 1	644 (L93/4286) 1 2 2 2	662 (2837) 1 2 2 3	663 (2839) 1 2 2 3	(2838) 1 2 2 3	(2845) 1 2 2 3	(2843) 1 2 2 3	(2842) 1 2 2 3	(2846) 1 2 T 4	(2840) 1 2 2 3	(2844) 1 2 2 5	(2847) 1 2 2 3	69 (FAM 1 1 1 1 1 1

## 14.6.3 Include in identifiers fieldset

This selection box allows you to choose which isolate provenance fields will be included in the results table. This does not affect the output of the alignments as taxa names are limited in length by the alignment programs.

-Include in identifiers	
isolate	
country	
region	=
year	
epidemiological year	
age yr	
age mth	
sex	
disease	
source	-

Multiple values can be selected by clicking while holding down Ctrl.

## 14.6.4 Reference genome fieldset

This section allows you to choose a reference genome to use as the source of comparator sequences.

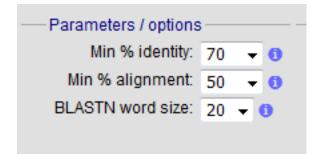
Reference genome Enter accession number: İ or choose annotated genome: FAM18 (Nm) or upload Genbank/EMBL/FASTA file: No file selected. Browse... i

There are three possibilities here:

- 1. Enter accession number Enter a Genbank accession number of an annotated reference and Genome Comparator will automatically retrieve this from Genbank.
- 2. Select from list The administrator may have selected some genomes to offer for comparison. If these are present, simply select from the list.
- 3. Upload genome Click 'Browse' and upload your own reference. This can either be in Genbank, EMBL or FASTA format. Ensure that the filename ends in the appropriate file extension (.gb, .embl, .fas) so that it is recognized.

## 14.6.5 Parameters/options fieldset

This section allows you to modify BLAST parameters. This affects sensitivity and speed.



- Min % identity This sets the threshold identity that a matching sequence has to be in order to be considered (default: 70%). Only the best match is used.
- Min % alignment This sets the percentage of the length of reference allele sequence that the alignment has to cover in order to be considered (default: 50%).
- BLASTN word size This is the length of the initial identical match that BLAST requires before extending a match (default: 20). Increasing this value improves speed at the expense of sensitivity. The default value gives good results in most cases. The default setting used to be 15 but the new default of 20 is almost as good (there was 1 difference among 2000 loci in a test run) but the analysis runs twice as fast.

## 14.6.6 Distance matrix calculation fieldset

This section provides options for the treatment of incomplete and paralogous loci when generating the distance matrix.

<ul> <li>Distance matrix calculation ————————————————————————————————————</li></ul>
With incomplete loci:
Completely exclude from analysis
Treat as distinct allele
Ignore in pairwise comparison
Exclude paralogous loci

For incomplete loci, i.e. those that continue beyond the end of a contig so are incomplete you can:

- Completely exclude from analysis Any locus that is incomplete in at least one isolate will be removed from the analysis completely. Using this option means that if there is one bad genome with a lot of incomplete sequences in your analysis, a large proportion of the loci may not be used to calculate distances.
- Treat as a distinct allele This treats all incomplete sequences as a specific allele 'I'. This varies from any other allele, but all incomplete sequences will be treated as though they were identical.
- Ignore in pairwise comparison (default) This is probably the best option. In this case, incomplete alleles are only excluded from the analysis when comparing the particular isolate that has it. Other isolates with different alleles will be properly included. The effect of this option will be to shorten the distances of isolates with poorly sequenced genomes with the others.

Paralogous loci, i.e. those with multiple good matches, can be excluded from the analysis (default). This is the safest option since there is no guarantee that differences seen between isolates at paralogous loci are real if the alternative matches are equally good. NB: Loci are also only classed as paralogous when the alternative matches identify different sequences, otherwise multiple contigs of the same sequence region would result in false positives.

## 14.6.7 Alignments fieldset

This section enables you to choose to produce alignments of the sequences identified.

- Alignments						
Alginnents						
Produce alignments i						
✓ Include ref sequences in alignment						
Align all loci (not only variable)						
Aligner: MAFFT 🚽						

Available options are:

- Produce alignments Selecting this will produce the alignment files, as well as XMFA and FASTA outputs of aligned sequences. This will result in the analysis taking longer to run.
- Include ref sequences in alignment When doing analysis using an annotated reference, selecting this will include the reference sequence in the alignment files.
- Align all loci By default, only loci that vary among the isolates are aligned. You may however wish to align all if you would like the resultant XMFA and FASTA files to include all coding sequences.
- · Aligner There are currently two choices of alignment algorithm (provided they have both been installed)
  - MAFFT (default) This is the preferred option as it is significantly quicker than MUSCLE, uses less memory, and produces comparable results.
  - MUSCLE This was originally the only choice. It is still included to enable previous analyses to be re-run
    and compared but it is recommended that MAFFT is used otherwise.

#### 14.6.8 Core genome analysis fieldset

This section enables you to modify the inclusion threshold used to calculate whether or not a locus is part of the core genome (of the dataset).

— Core genome analysis — — —
Core threshold (%): 90 👻 👔
🗖 Calculate mean distances 👔

The default setting of 90% means that a locus is counted as core if it appears within 90% or more of the genomes in the dataset.

There is also an option to calculate the mean distance among sequences of the loci. Selecting this will also select the option to produce alignments.

## 14.6.9 Filter fieldset

This section allows you to further filter your collection of isolates and the contigs to include.

Sequence method:	<b>√</b> i	
Project:		<b>√</b> [i]
Experiment:	▼ į	

Available options are:

- Sequence method Choose to only analyse contigs that have been generated using a particular method. This depends on the method being set when the contigs were uploaded.
- Project Only include isolates belonging to the chosen project. This enables you to select all isolates and filter to a project.
- Experiment Contig files can belong to an experiment. How this is used can vary between databases, but this enables you to only include contigs from a particular experiment.

## 14.6.10 Understanding the output

#### **Distance matrix**

The distance matrix is simply a count of the number of loci that differ between each pair of isolates. It is generated in NEXUS format which can be used as the input file for SplitsTree. This can be used to generate NeighborNet, Split decomposition graphs and trees offline. If 200 isolates or fewer are included in the analysis, a Neighbor network is automatically generated from this distance matrix.

#### **Unique strains**

The table of unique strains is a list of isolates that are identical at every locus. Every isolate is likely to be classed as unique if a whole genome analysis is performed, but with a constrained set of loci, such as those for MLST, this will group isolates that are indistinguishable at that level of resolution. nce matrix calculated based on allelic differences and a NeighborNet graph generated from this distance matrix.

Genome Comparator can be accessed on databases where it is enabled from the contents page by clicking the 'Genome Comparator' link.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in th database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it doe	
<ul> <li>Query database</li> <li>Search database - advanced queries.</li> <li>Browse database - peruse all records.</li> <li>Search by combinations of loci (profiles) - including partial matching.</li> <li>List query - find isolates by matching a field to an entered list.</li> <li>Projects - main projects defined in database.</li> </ul>	Submissions Manage submissions General information I losiates: 34221 Last updated: 2015-07-02 Update history About BIGSdb
Breakdown       Export       Analysis       Miscellaned         • Single field       • Export dataset       • Codon usage       • Description         • Two field       • Onligs       • Sequences - XMFA / concatenated FASTA formats       • Codon usage       • Description         • Publications       • Sequence bin       • Sequence bin       • BLASI       • BLASI       • BLASI	ous of database fields

Alternatively, it can be accessed following a query by clicking the 'Genome Comparator' button at the bottom of the results table. Isolates with sequence data returned in the query will be automatically selected within the Genome Comparator interface.

19025 M10 240481	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	1831		22	9	F3-3
19026 M10 240482	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	3754	ST-41/44 complex/Lineage 3	7-2	4	F5-1
19027 M10 240484	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	1097	ST-41/44 complex/Lineage 3	17-1	23	F1-5
19028 M10 240485	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	275	ST-269 complex	22	9	F5-12
19029 M10 240487	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	1049	ST-269 complex	19-1	15-11	F5-1
19030 M10 240489	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	461	ST-461 complex	19-2	13-1	F3-9
19031 M10 240490	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	1161	ST-269 complex	22	9	F5-12
19032 M10 240498	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	41	ST-41/44 complex/Lineage 3	7-2	4	F1-5
19958 M10 240476	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	9812	ST-213 complex	22	14	F5-5
19959 M10 240499	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	275	ST-269 complex	22	9	F5-12
19960 M10 240500	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	41	ST-41/44 complex/Lineage 3	7-2	4	F1-5
19961 M10 240502	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	340	ST-41/44 complex/Lineage 3	7-2	4	F1-5
19962 M10 240503	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	23	ST-23 complex/Cluster A3	5-1	2-2	F1-96
19963 M10 240505	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	1655	ST-23 complex/Cluster A3	5-1	10-10	F4-1
19964 M10 240507	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	183	ST-23 complex/Cluster A3	21	16-5	deleted
19965 M10 240508	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	1575		7-2	13-1	F1-7
19966 M10 240511	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	4713		22	9	F5-12
19967 M10 240512	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	41	ST-41/44 complex/Lineage 3	7-1	1	F1-5
19968 M10 240514	UK	2010 invasive (unspecified/other) Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex	5	2	F1-1
19969 M10 240515	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	269	ST-269 complex	5-1	2-2	F5-1
19970 M10 240520	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	1655	ST-23 complex/Cluster A3	5-1	10-1	F4-1
Analysis tools: Breakdown: Fields Two Analysis: Presence/Absen Export: Dataset Cor	ice Ge	Codons Polymorphic sites Combinations Schemes/alleles anome Comparator BLAST Sequences	Publ	lications	Sequence bin			

## 14.6.11 Analysis using defined loci

Select the isolate genomes that you wish to analyse. These will either be in a dropdown list or, if there are too many in the database, a text input where a list can be entered. You can also upload your own genomes for analysis - these should be either a single file in FASTA format (if you have just one genome), or a zip file containing multiple FASTA files. Select either the loci from the list or a set of schemes. Press submit.

	y (keith). @Log out   Change password Comparator - Neisseria Pu	MI ST					Help 🖓	Toggle:
ease select the re	equired isolate ids and loci for comparison - neme description. Alternatively, you can enter User genomes	ISE CTRL or SHIF		enome and			o include all loci defined in schemes t Schemes	by sele
662 663 664 665	Optionally include data not in the database. Upload FASTA file (or zip file containing multiple FASTA files - one per genome): • Browse No file selected.	'16S_rDNA 16S_rRNA (S _235_rRNA abcZ abcZ (NEIS1 aceF (NEIS1 ackA2 (NEIS acnA (NEIS1	015) 279) 1727)	isolate countr region year epiden age yr age m sex disease source	y niological year th a		▲— 🗑 🧾 Typing — 💌 🛄 MLST — 🔲 🛄 Finetyping antige	Ш
Reference geno	ome ————————————————————Parameters / oj	tions ———	-Distance matrix calculation-		Alignments	Core ge	nome analysis ———	
nter accession n tr choose annotat r upload Genban Browse No f	ted genome: Min % alignn BLASTN word nk/EMBL/FASTA file:	ntity: 70 v 0 eent 50 v 0 size: 20 v 0	With incomplete loci: Completely exclude from a Treat as distinct allele Ignore in pairwise compari		Produce alignments  Include ref sequences in alignment Include ref sequences in align		shold (%): 90   ▼  0 late mean distances 6	
Filter by Sequence mett Pro Experim	oject:	Action Reset	Submit					

The job will be submitted to the job queue and will start running shortly. Click the link to follow the job progress and view the output.

Description         Output         Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications         Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: i
Genome Comparator - Neisseria PubMLST	Show options
This analysis has been submitted to the job queue. Please be aware that this job may take a long time depending on the number of comparisons and how busy the server is.	
Follow the progress of this job and view the output.	

There will be a series of tables displaying variable loci, colour-coded to indicate allelic differences. Finally, there will be links to a distance matrix which can be loaded in to SplitsTree for further analysis and to a NeighborNet chart showing relatedness of isolates. Due to processing constraints on the web server, this NeighborNet is only calculated if 200 or fewer genomes are selected for analysis, but this can be generated in the stand-alone version of SplitsTree using the distance matrix if required.

Status           St	Breakdown: Isolate	ise   Profile/ST   List leids   Scheme/alleles   Publications me   Options   Profiles/sequences definitions   Database subr	missions	
	ob status viewer			
	Status			
	Submit time: 2014-07-15 08:41:03 Status: finished Start time: 2014-07-15 08:41:05 Progress: 100%	63_94241		
	Total time: 17 seconds			
		e been defined otherwise sequences will be marked as 'Ney	w#1 'New#2' etc. Missing alleles are ma	arked as 'X' Truncated alleles (located at end of contio) are marked as 'T'
	adk         3         3           aroE         4         19           fumC         3         3           gdh         8         8           pdhC         4         4	3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3	3         3         3         3           4         19         19         19           3         3         3         3           4         8         8         8           4         4         4         4	4 3 8 4
construction       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2 <t< td=""><td></td><th></th><td></td><th>0</th></t<>				0
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344 (1934/280) 662 (2337) 666 (2843) 665 (2845) 669 (2846) 659 (2846) 659 (2847) 659 (2847) • Text output file • Text output file • Splits graph (Neighbour-net, PNG format) • Tar file containing output files • Tar file containing output file	Jnique strains: 5			
<ul> <li>Excel format</li> <li>Distance matrix (Neus format) - Suitable for loading in to SplitsTree. Distances between taxa are calculated as the number of loci with different allele sequences</li> <li>Splits graph (Neighbour-net_PNC format)</li> <li>(click to enlarge)</li> <li>(click to enlarge)</li> <li>(click to enlarge)</li> <li>(click to enlarge)</li> <li>Locus presence frequency chart (PNG format)</li> <li>(click to enlarge)</li> </ul>	644 (L93/4286) 662 (2837) 666 (2843) 6 663 (2839) 670 (2840) 667 (2842)			
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Tar file containing output files	<ul> <li>Splits graph (Neighbour-net; SVC</li> <li>Locus presence frequency</li> </ul>	format) - This can be edited in Inkscape or other vector graphi	cs editors	
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ease note that inh results will remain on the server for 7 days	L			
	lease note that inb results will remain a	the server for 7 days		

## 14.6.12 Analysis using annotated reference genome

Select the isolate genomes that you wish to analyse and then either enter a Genbank accession number for the reference genome, or select from the list of reference genomes (this list will only be present if the administrator has *set it up*). Selecting reference genomes will hide the locus and scheme selection forms.

PubMLST Databas	se home Contents				
Logged in: Keith Jolley (k	eith). 🔁 Log out   Change password		Help 🗹	Toggle: 🚯	Ξ
Genome Con	nparator - Neisseria Pub	MLST			
		CTRL or SHIFT to make multiple selections in list boxes. In addition to selecting individual loci, you can choose to include all loci defined ccession number for an annotated reference genome and compare using the loci defined in that.	in scheme	s by selectir	ng
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662 663 664 665	Optionally include data not in the database. Upload FASTA file (or zip file containing multiple FASTA files - one per genome): Browse No file selected.	Bolate     A       Country     E       region     E       year     epidemiological year       age mth     sex       dsease     e       source     T			
	ne ————————————————————————————————————				
Enter accession nur					
or choose annotated FAM18 (Nm) or upload Genbank/t Browse No file	BLASTN word size EMBL/FASTA file:	Trast as distinct allele			
Filter by Sequence metho Projec Experimer	ct:	Action Submit			

Output is similar to when comparing against defined loci, but this time every coding sequence in the annotated reference will be BLASTed against the selected genomes. Because allele designations are not defined, the allele found in the reference genome is designated allele 1, the next different sequence is allele 2 etc.

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atus																
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lescription ding regio loci ch unique : Locus xC   envA   MC0001	Neisseria meningitidis serogroup C FAM18 complete genome. ns 1975 allele is defined a number starting at 1. Missing alleles are marked as ' Product UDP-3-O-(3-hydroxymyristoyi) N-acetylglucosmine deacetylase	Sequence length 924	Genome position 1261	Reference genome	644 (L93/4286)	662 (2837) 1	663				(2842) 1			(2844) 1		(FAM 1
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description ding regio loci ch unique : ch unique : xC   envA   vMC0001 pilS1   vMC0002 pilS2   vMC0003 fbp   vMC0005	Neisseria meningitidis serogroup C FAM18 complete genome. 1975 allele is defined a number starting at 1. Missing alleles are marked as ' Product UDP-3-O-[3-hydroxymyristoy] N-acety/glucosmine deacety(ase pilin (tragment) truncated pilin peptidyI-prolyl cis-trans isomerase putative membrane protein	Sequence length 924 291 366 330 219	Genome position           1261           3341           3675           4069           4476	Reference genome 1 1 1 1 1 1	644 (L93/4286) 1 2 2 2	662 (2837) 1 2 2 3	663 (2839) 1 2 2 3	(2838) 1 2 2 3	(2845) 1 2 2 3	(2843) 1 2 2 3	(2842) 1 2 2 3	(2846) 1 2 7 7 4	(2840) 1 2 2 3	(2844) 1 2 2 5	(2847) 1 2 2 3	(FAM 1 1 1 1
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## 14.6.13 Include in identifiers fieldset

This selection box allows you to choose which isolate provenance fields will be included in the results table. This does not affect the output of the alignments as taxa names are limited in length by the alignment programs.

isolate	
country	
region	-
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disease	
source	Ŧ

Multiple values can be selected by clicking while holding down Ctrl.

## 14.6.14 Reference genome fieldset

This section allows you to choose a reference genome to use as the source of comparator sequences.

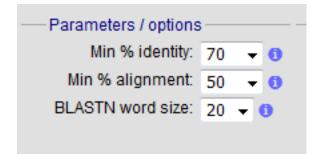
Reference genome Enter accession number: İ or choose annotated genome: FAM18 (Nm) or upload Genbank/EMBL/FASTA file: No file selected. Browse... i

There are three possibilities here:

- 1. Enter accession number Enter a Genbank accession number of an annotated reference and Genome Comparator will automatically retrieve this from Genbank.
- 2. Select from list The administrator may have selected some genomes to offer for comparison. If these are present, simply select from the list.
- 3. Upload genome Click 'Browse' and upload your own reference. This can either be in Genbank, EMBL or FASTA format. Ensure that the filename ends in the appropriate file extension (.gb, .embl, .fas) so that it is recognized.

## 14.6.15 Parameters/options fieldset

This section allows you to modify BLAST parameters. This affects sensitivity and speed.



- Min % identity This sets the threshold identity that a matching sequence has to be in order to be considered (default: 70%). Only the best match is used.
- Min % alignment This sets the percentage of the length of reference allele sequence that the alignment has to cover in order to be considered (default: 50%).
- BLASTN word size This is the length of the initial identical match that BLAST requires before extending a match (default: 20). Increasing this value improves speed at the expense of sensitivity. The default value gives good results in most cases. The default setting used to be 15 but the new default of 20 is almost as good (there was 1 difference among 2000 loci in a test run) but the analysis runs twice as fast.

#### 14.6.16 Distance matrix calculation fieldset

This section provides options for the treatment of incomplete and paralogous loci when generating the distance matrix.

<ul> <li>Distance matrix calculation ————————————————————————————————————</li></ul>
With incomplete loci:
Completely exclude from analysis
Treat as distinct allele
Ignore in pairwise comparison
Exclude paralogous loci

For incomplete loci, i.e. those that continue beyond the end of a contig so are incomplete you can:

- Completely exclude from analysis Any locus that is incomplete in at least one isolate will be removed from the analysis completely. Using this option means that if there is one bad genome with a lot of incomplete sequences in your analysis, a large proportion of the loci may not be used to calculate distances.
- Treat as a distinct allele This treats all incomplete sequences as a specific allele 'I'. This varies from any other allele, but all incomplete sequences will be treated as though they were identical.
- Ignore in pairwise comparison (default) This is probably the best option. In this case, incomplete alleles are only excluded from the analysis when comparing the particular isolate that has it. Other isolates with different alleles will be properly included. The effect of this option will be to shorten the distances of isolates with poorly sequenced genomes with the others.

Paralogous loci, i.e. those with multiple good matches, can be excluded from the analysis (default). This is the safest option since there is no guarantee that differences seen between isolates at paralogous loci are real if the alternative matches are equally good. NB: Loci are also only classed as paralogous when the alternative matches identify different sequences, otherwise multiple contigs of the same sequence region would result in false positives.

## 14.6.17 Alignments fieldset

This section enables you to choose to produce alignments of the sequences identified.

- Alignments
Aigintenta
Produce alignments i
✓ Include ref sequences in alignment
Align all loci (not only variable)
Aligner: MAFFT 🚽

Available options are:

- Produce alignments Selecting this will produce the alignment files, as well as XMFA and FASTA outputs of aligned sequences. This will result in the analysis taking longer to run.
- Include ref sequences in alignment When doing analysis using an annotated reference, selecting this will include the reference sequence in the alignment files.
- Align all loci By default, only loci that vary among the isolates are aligned. You may however wish to align all if you would like the resultant XMFA and FASTA files to include all coding sequences.
- · Aligner There are currently two choices of alignment algorithm (provided they have both been installed)
  - MAFFT (default) This is the preferred option as it is significantly quicker than MUSCLE, uses less memory, and produces comparable results.
  - MUSCLE This was originally the only choice. It is still included to enable previous analyses to be re-run and compared but it is recommended that MAFFT is used otherwise.

#### 14.6.18 Core genome analysis fieldset

This section enables you to modify the inclusion threshold used to calculate whether or not a locus is part of the core genome (of the dataset).

— Core genome analysis — — —
Core threshold (%): 90 👻 👔
🗖 Calculate mean distances 👔

The default setting of 90% means that a locus is counted as core if it appears within 90% or more of the genomes in the dataset.

There is also an option to calculate the mean distance among sequences of the loci. Selecting this will also select the option to produce alignments.

## 14.6.19 Filter fieldset

This section allows you to further filter your collection of isolates and the contigs to include.

Sequence method:	<b>▼</b> [	
Project:		▼ i
Experiment:	<b>▼</b> [	

Available options are:

- Sequence method Choose to only analyse contigs that have been generated using a particular method. This depends on the method being set when the contigs were uploaded.
- Project Only include isolates belonging to the chosen project. This enables you to select all isolates and filter to a project.
- Experiment Contig files can belong to an experiment. How this is used can vary between databases, but this enables you to only include contigs from a particular experiment.

## 14.6.20 Understanding the output

#### **Distance matrix**

The distance matrix is simply a count of the number of loci that differ between each pair of isolates. It is generated in NEXUS format which can be used as the input file for SplitsTree. This can be used to generate NeighborNet, Split decomposition graphs and trees offline. If 200 isolates or fewer are included in the analysis, a Neighbor network is automatically generated from this distance matrix.

#### **Unique strains**

The table of unique strains is a list of isolates that are identical at every locus. Every isolate is likely to be classed as unique if a whole genome analysis is performed, but with a constrained set of loci, such as those for MLST, this will group isolates that are indistinguishable at that level of resolution.

# 14.7 GrapeTree

GrapeTree is a tool for generating and visualising minimum spanning trees. It has been developed to handle large datasets (in the region of 1000s of genomes) and works with 1000s of loci as used in cgMLST. It uses an improved minimum spanning algorithm that is better able to handle missing data than alternative algorithms and is able to produce publication quality outputs. Datasets can include metadata which allows nodes in the resultant tree to be coloured interactively.

GrapeTree can be accessed from the contents page by clicking the 'GrapeTree' link.

leisseria PubMLST	database					
				al known diversity of Neisseria species quently it should be noted that it does n		e profiles/sequence definition database there is at lea imple.
Query database	E	Projects	0	ption settings		1 Submissions
<ul> <li>Search or browse databas</li> <li>Search by combinations or</li> </ul>		<ul> <li>Main public projects</li> <li>Your projects</li> </ul>		et general options - including isolate ta et display and query options for locus, s		Manage submissions
						General information
						<ul> <li>Isolates: 44,865</li> <li>Last updated: 2018-02-20</li> <li>Defined field values</li> <li>Update history</li> <li>About BIGSdb</li> </ul>
Breakdown	Export			Analysis	Third party	tools
<ul> <li>Single field</li> <li>Two field</li> <li>Unique combinations</li> <li>Scheme and alleles</li> </ul>	<ul> <li>Export datase</li> <li>Contigs</li> <li>Sequences - &gt;</li> </ul>	t KMFA / concatenated FASTA	. formats	Codon usage     Presence/absence status of it     Genome comparator     BLAST	oci • 11OL - Phylog • PhyloViz - Vis	/isualization of genomic relationships ienetic trees with data overlays ualization and phylogenetic inference iyen data visualization and sharing for genomic
Publications				Species identification	epidemiolog	
<ul> <li>Sequence bin</li> </ul>						

Alternatively, it can be accessed following a query by clicking the 'GrapeTree' button at the bottom of the results table. Isolates returned from the query will be automatically selected within the GrapeTree interface.

9024 M10 240480 9025 M10 240481			пенаасна пеннуши		2110015	214	1101 01-208 0011		9	1.512
	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2267206	267	1194 ST-41/44 cor	nplex 7-2	4	F1-5
0000 1140 040400	UK	2010 invasive (unspecified/other)	Neisseria meningitid		2194837	274	1831	22	9	F3-3
9026 M10 240482	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2184823	263	3754 ST-41/44 cor	nplex 7-2	4	F5-1
9027 M10 240484	UK	2010 invasive (unspecified/other)	Neisseria meningitid		2168050	253	1097 ST-41/44 cor	nplex 17-1	23	F1-5
9028 M10 240485	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2193457	294	275 ST-269 com	plex 22	9	F5-12
9029 M10 240487	UK	2010 invasive (unspecified/other)	Neisseria meningitid		2188678	241	1049 ST-269 com	plex 19-1	15-11	F5-1
9030 M10 240489	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2218969	275	461 ST-461 com	plex 19-2	13-1	F3-9
9031 M10 240490	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2175692	293	1161 ST-269 com	plex 22	9	F5-12
9032 M10 240498	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2154070	235	41 ST-41/44 cor	nplex 7-2	4	F1-5
9958 M10 240476	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2242902	284	9812 ST-213 com	plex 22	14	F5-5
9959 M10 240499	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2189734	198	275 ST-269 com	plex 22	9	F5-12
9960 M10 240500	UK	2010 invasive (unspecified/other)	Neisseria meningitid		2197545	223	41 ST-41/44 cor	nplex 7-2	4	F1-5
9961 M10 240502	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2173298	188	340 ST-41/44 cor	nplex 7-2	4	F1-5
9962 M10 240503	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is Y	2101043	197	23 ST-23 com	plex 5-1	2-2	F1-96
9963 M10 240505	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is Y	2090713	189	1655 ST-23 com	olex 5-1	10-10	F4-1
9964 M10 240507	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is Y	2108738	170	183 ST-23 com	olex 21	16-5	deleted
9965 M10 240508	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2233910	196	1575	7-2	13-1	F1-7
9966 M10 240511	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2174583	219	4713	22	9	F5-12
9967 M10 240512	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2203751	205	41 ST-41/44 cor	nplex 7-1	1	F1-5
9968 M10 240514	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is W	2110464	160	11 ST-11 com	olex 5	2	F1-1
9969 M10 240515	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is B	2181841	205	269 ST-269 com	plex 5-1	2-2	F5-1
9970 M10 240520	UK	2010 invasive (unspecified/other)	Neisseria meningitid	is Y	2095486	190	1655 ST-23 com	plex 5-1	10-1	F4-1

Select the isolates to include. The tree can be generated from allelic profiles of any selection of loci, or more conveniently, you can select a scheme in the scheme selector to include all loci belonging to that scheme.

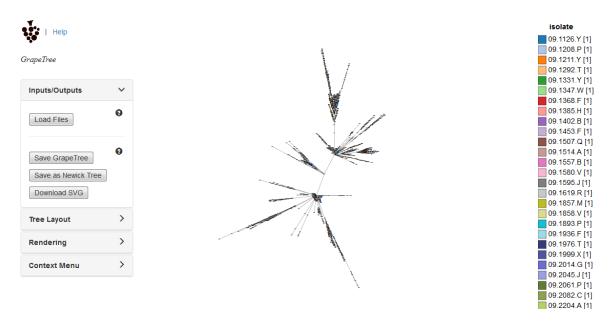
Additional fields can be selected to be included as metadata for use in colouring nodes - select any fields you wish to include. Multiple selections can be made by holding down shift or ctrl while selecting. Click 'Submit' to start the analysis.

	t   Change password			loggle: 😈
rapeTree: Visualiz	ation of genomic rela	ationships - Neisseria PubMLST		
	This plugin gen	ierates a minimum-spanning tree and visualizes within Grape	Tree:	
	GrapeTree: \	Visualization of core genomic relationships		
	GrapeTree is de			
	- Zhemin Nabil-Fa Martin J. Nina Lut Cátta Va; Alexandr	Zhou (1) areed Alikhan (1) Sergeant (1) hmann (1) tz (2.5) re P. Francisco (2.4) dré Carriço (3)		
S.	2. Instituto 3. Universit 4. Instituto 5. ADEETC	K Medical School, University of Warwick, UK de Engenharia de Sistemas e Computadores: Investigação e idade de Lisboa, Faculdade de Medicina, Instituto de Microbiol Superior Técnico, Universidade de Lisboa, Lisboa, Portugal 2, Instituto Superior de Engenharia de Lisboa, Instituto Politéci pu at al. (2017) GrapeTree: Visualization of core genomic relati	ogia and Instituto de Medicina Molecular, Lisboa, Portugal	
'his tool will generate minimum si		. Please check the loci that you would like to include. Alternativ	ely select one or more schemes to include all loci that are mer	nbers of the scheme.
analysis is limited to 50,000 record		Cabamaa	Include fields	Action
nalysis is limited to 50,000 record 	NA a	- Schemes	Include fields Select additional fields to include in GrapeTree metadata.	

The job will be sent to the job queue. When it has finished, click the button marked 'Launch GrapeTree'.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). (HLog out   Change password
Job status viewer
Status
Job id: BIGSdb_141866_1519311802_19416
Submit time: 2018-02-22 15:03:22
Status: finished
Start time: 2018-02-22 15:03:42
Progress: 100%
Stop time: 2018-02-22 15:07:38
Total time: 3 minutes and 55 seconds
Output Launch GrapeTree Profiles (TSV format) (14.2 MB) MS Tree (Newick format) Netadata (TSV format) Netadata (TSV format) Tar file containing output files (only files <10MB included - download larger files separately)
Please note that job results will remain on the server for 7 days.

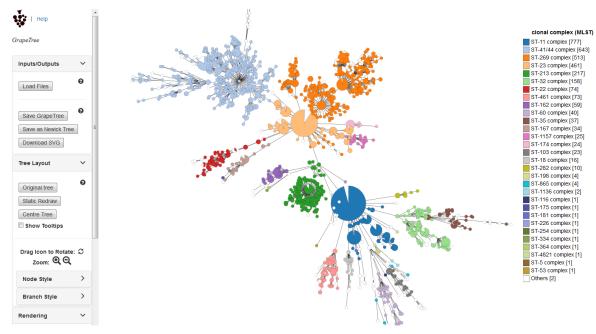
The generated tree will be rendered in the GrapeTree application page.



The image can be manipulated in various ways. These include modifying the tree layout, customising node labels and size, modifying branch lengths and collapsing branches. The image can be saved in SVG format which can be further edited in image publishing software such as Inkscape.

As an example, the default cgMLST tree (above) has been modified (below) as follows:

- Nodes coloured by clonal complex
- · Labels removed
- Branches collapsed where <=100 loci different
- Node size set to 200%
- Kurtosis (node size relative to number of isolates) set to 75%
- Dynamic rendering allowed to run to fan out nodes



Full details can be found in the GrapeTree manual.

Note: GrapeTree has been described in the following publication:

Z Zhou, NF Alikhan, MJ Sergeant, N Luhmann, C Vaz, AP Francisco, JA Carrico, M Achtman (2018) GrapeTree: Visualization of core genomic relationships among 100,000 bacterial pathogens. Genome Res 28:1395-1404.

# 14.8 In silico PCR

This is a tool that can be used to simulate PCR reactions run against genomes stored in the database. This is useful for designing and testing primers. The plugin uses the exonerate ipcress program to perform its simulation.

The tool can be accessed from the contents page of an isolates database by clicking the 'In silico PCR' link.



Alternatively, it can be accessed following a query by clicking the 'PCR' button at the bottom of the results table. Isolates returned from the query will be automatically selected within the analysis interface.

91 B54 48 B73	5; NIBSC_ 4; NIBSC_	2822; 2				invasive (u	inspecilied/other)	weissena meningiliuis	A	4	S1-4 complex	0-2	10	F1-0
48 B73	-		21035	Pakistan	1967	meningitis	and septicaemia	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
		2760; Z	Z1054	Finland	1975	invasive (u	inspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	20	9	F3-1
	B; NIBSC	2784; Z	21073	Canada	1971	invasive (u	inspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	18-1	3	F5-1
9E B92	2; NIBSC_	2828; Z	21092	Germany	1964	invasive (u	inspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F3-6
M B99	; NIBSC_	2795; Z	Z1099	Philippines	1968			Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
31 B21	3; NIBSC	2813;	Z1213	Ghana	1973	invasive (u	inspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13-1	F1-5
55 B22	7; NIBSC	_2806; 2	Z1227	Denmark	1974	invasive (u	inspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	5-1	9	F3-1
4 alp	ha14; Be	nnettTr	ee10	Germany	1999		carrier	Neisseria meningitidis	cnl	53	ST-53 complex	7	30-3	F5-5
D B26	9; NIBSC	_2825; 3	Z1269	Burkina Faso	1963	invasive (u	inspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13-1	F1-5
) B27	5; NIBSC	_2767; 3	Z1275	Niger	1963	invasive (u	inspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F1-7
6 B27	8; NIBSC	_2764; 2	Z1278	Niger	1963	invasive (u	inspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13	F1-5
3 B36	2; NIBSC	_2779; 3	Z1362	Cameroon	1966			Neisseria meningitidis	Α	4	ST-4 complex	7	13	F1-5
3 B39	2; NIBSC	_2823; 3	Z1392	Greece	1968		carrier	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
4 B43	9; NIBSC	_2812; 3	Z1439	Djibouti	1966	invasive (u	inspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F1-7
11 B46	6; NIBSC	_2765;	Z1466	Australia	1977	invasive (u	inspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
004 B50	3; NIBSC	2826;	Z1503	China	1984	invasive (u	inspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	20	9	F3-8
229 B50	6; NIBSC	_2816;	Z1506	Brazil	1976			Neisseria meningitidis	Α	5	ST-5 complex	20	9	F2-1
00 B53	4; NIBSC	2768;	Z1534	UK	1941	invasive (u	inspecified/other)	Neisseria meningitidis	Α	21		5-2	10	F3-9
	31         B21:3           55         B22:3           alp         B26:3           B27:3         B27:3           B27:3         B26:3           B27:3         B36:3           B3         B39:3           H         B43:3           H         B46:0           D4         B50:3           229         B50:0	31         B213; NIBSC           35         B227; NIBSC           alpha14; Be         B269; NIBSC           B275; NIBSC         B275; NIBSC           B275; NIBSC         B362; NIBSC           B3832; NIBSC         B439; NIBSC           B466; NIBSC         B466; NIBSC           29         B506; NIBSC	<ul> <li>B213; NIBSC_2813;</li> <li>B227; NIBSC_2806; alpha14; BennettTr</li> <li>B229; NIBSC_2280;</li> <li>B1985C_2825;</li> <li>B275; NIBSC_2767;</li> <li>B278; NIBSC_2764;</li> <li>B392; NIBSC_2812;</li> <li>B469; NIBSC_2812;</li> <li>B466; NIBSC_2812;</li> <li>B466; NIBSC_2812;</li> <li>B506; NIBSC_2816;</li> <li>29 B506; NIBSC_2816;</li> </ul>	B213; NIBSC_2813; Z1213           B227; NIBSC_2806; Z1227           alpha14; BennettTree10           B269; NIBSC_2825; Z1269           B275; NIBSC_2767; Z1275           B278; NIBSC_2764; Z1278           B B362; NIBSC_2779; Z1362           B B362; NIBSC_2823; Z1392           B B469; NIBSC_2812; Z1439           B466; NIBSC_2765; Z1526           B B56; NIBSC_2765; Z1530           B B56; NIBSC_2812; Z1439	B213; NIBSC_2813; Z1213         Ghana           B227; NIBSC_2806; Z1227         Denmark           alpha14; BennettTree10         Germany           B269; NIBSC_2825; Z1269         Burkina Faso           B275; NIBSC_2767; Z1275         Niger           B278; NIBSC_2764; Z1278         Niger           B 256; NIBSC_2764; Z1278         Niger           B 362; NIBSC_2764; Z1278         Cameroon           B 3892; NIBSC_2823; Z1392         Greece           H 3499; NIBSC_2821; Z1439         Dilbouti           B466; NIBSC_2765; Z1466         Australia           B 506; NIBSC_28216; Z1500         China           29         B506; NIBSC_2816; Z1506         Brazil	B213; NIBSC_2813; Z1213         Ghana         1973           B227; NIBSC_2806; Z1227         Denmark         1974           alpha14; BennettTree10         Germany         1999           B259; NIBSC_2825; Z1259         Burkina Faso         1963           B275; NIBSC_2767; Z1275         Niger         1963           B276; NIBSC_2764; Z1278         Niger         1963           B 256; NIBSC_2779; Z1362         Cameroon         1966           B 8392; NIBSC_283; Z1392         Greece         1968           B 439; NIBSC_283; Z1392         Greece         1968           B 439; NIBSC_283; Z1392         Dibouti         1966           B 449; NIBSC_2862; Z1503         China         1944           B 503; NIBSC_2862; Z1503         China         1944           B 503; NIBSC_2862; Z1503         Greece         1968           B 503; NIBSC_2862; Z1503         Grina         1944           29         B506; NIBSC_2816; Z1503         Brazil         1976	81         B213; NIBSC_2813; Z1213         Ghana         1973 invasive (u           95         B227; NIBSC_2806; Z1227         Denmark         1974 invasive (u           alpha14; BennettTreol0         Germany         1999           B269; NIBSC_2825; Z1269         Burkina Faso         1963 invasive (u           B278; NIBSC_2767; Z1275         Niger         1963 invasive (u           B278; NIBSC_2764; Z1278         Niger         1963 invasive (u           B382; NIBSC_2764; Z1278         Cameroon         1966           B382; NIBSC_2823; Z1392         Greece         1968           B439; NIBSC_2823; Z1392         Greece         1968           B466; NIBSC_2765; Z1466         Australia         1977 invasive (u           B466; NIBSC_2765; Z1466         Australia         1976 invasive (u           29         B506; NIBSC_2816; Z1506         Brazil         1976	B213; NIBSC_2813; Z1213         Ghana         1973 invasive (unspecified/other)           B227; NIBSC_2806; Z1227         Denmark         1974 invasive (unspecified/other)           alpha14; BennetTree10         Germany         1999         carrier           B269; NIBSC_2825; Z1259         Burkina Faso         1963 invasive (unspecified/other)           B275; NIBSC_2767; Z1275         Niger         1963 invasive (unspecified/other)           B278; NIBSC_2764; Z1278         Niger         1963 invasive (unspecified/other)           B362; NIBSC_2779; Z1362         Cameroon         1966           B392; NIBSC_2823; Z1392         Greece         1966         carrier           B439; NIBSC_2826; Z1539         Djibouti         1966 invasive (unspecified/other)           B466; NIBSC_2765; Z1466         Australia         1977 invasive (unspecified/other)           B503; NIBSC_2826; Z1503         China         1946 invasive (unspecified/other)           B503; NIBSC_2826; Z1503         Brazil         1976	B213; NIBSC_2813; Z1213     Ghana     1973 invasive (unspecified/other)     Neisseria meningitidis       B255     B227; NIBSC_2806; Z1227     Denmark     1974 invasive (unspecified/other)     Neisseria meningitidis       alpha14; BennettTree10     Germany     1999     carrier     Neisseria meningitidis       B256; NIBSC_2825; Z1269     Burkina Faso     1963 invasive (unspecified/other)     Neisseria meningitidis       B276; NIBSC_2767; Z1275     Niger     1963 invasive (unspecified/other)     Neisseria meningitidis       B278; NIBSC_2764; Z1278     Niger     1963 invasive (unspecified/other)     Neisseria meningitidis       B362; NIBSC_2764; Z1278     Niger     1963 invasive (unspecified/other)     Neisseria meningitidis       B389; NIBSC_2823; Z1392     Greece     1966     carrier     Neisseria meningitidis       B399; NIBSC_2823; Z1392     Greece     1966 invasive (unspecified/other)     Neisseria meningitidis       B466; NIBSC_2823; Z1392     Greece     1966 invasive (unspecified/other)     Neisseria meningitidis       B466; NIBSC_2826; Z1466     Australia     1977 invasive (unspecified/other)     Neisseria meningitidis       B466; NIBSC_2826; Z1503     China     1984 invasive (unspecified/other)     Neisseria meningitidis       B460; NIBSC_2826; Z1503     China     1976     Neisseria meningitidis       B450; NIBSC_2826; Z1503	B213; NIBSC_2813; Z1213       Ghana       1973 invasive (unspecified/other) Neisseria meningitidis       A         S5       B227; NIBSC_2806; Z1227       Denmark       1974 invasive (unspecified/other) Neisseria meningitidis       A         alpha14; BennetTrree10       Germany       1999       carrier       Neisseria meningitidis       A         B269; NIBSC_2825; Z1259       Burkina Faso       1963 invasive (unspecified/other) Neisseria meningitidis       A         B275; NIBSC_2767; Z1275       Niger       1963 invasive (unspecified/other) Neisseria meningitidis       A         B275; NIBSC_2764; Z1278       Niger       1963 invasive (unspecified/other) Neisseria meningitidis       A         B 362; NIBSC_2779; Z1362       Cameroon       1966       Neisseria meningitidis       A         B 3892; NIBSC_2823; Z1392       Greece       1968       carrier       Neisseria meningitidis       A         B 439; NIBSC_2826; Z1459       Dijbouti       1966       invasive (unspecified/other) Neisseria meningitidis       A         B 446; NIBSC_2826; Z1459       Dijbouti       1966       invasive (unspecified/other) Neisseria meningitidis       A         B 4503; NIBSC_2826; Z1503       China       1974       invasive (unspecified/other) Neisseria meningitidis       A         B 4504; NIBSC_2826; Z1503       China       1976	B213; NIBSC_2813; Z1213       Ghana       1973 invasive (unspecified/other) Neisseria meningitidis       A       4         55       B227; NIBSC_2806; Z1227       Denmark       1974 invasive (unspecified/other) Neisseria meningitidis       A       5         alpha14; BennettTree10       Germany       1999       carrier       Neisseria meningitidis       A       4         B269; NIBSC_2826; Z1259       Burkina Faso       1963 invasive (unspecified/other) Neisseria meningitidis       A       4         B275; NIBSC_2767; Z1275       Niger       1963 invasive (unspecified/other) Neisseria meningitidis       A       4         B276; NIBSC_2764; Z1278       Niger       1963 invasive (unspecified/other) Neisseria meningitidis       A       4         B 3620; NIBSC_2779; Z1326       Carrier       Neisseria meningitidis       A       4         B 3892; NIBSC_2823; Z1392       Greece       1968 invasive (unspecified/other) Neisseria meningitidis       A       1         H 3439; NIBSC_2872; Z1439       Dijbouti       1966 invasive (unspecified/other) Neisseria meningitidis       A       1         H 466; NIBSC_2876; Z1466       Australia       1977 invasive (unspecified/other) Neisseria meningitidis       A       1         H 5039; NIBSC_2826; Z1503       China       1984 invasive (unspecified/other) Neisseria meningitidis       A	B213; NIBSC_2813; Z1213       Ghana       1973 invasive (unspecified/other) Neisseria meningitidis       A       4       ST-4 complex         S5       B227; NIBSC_2806; Z1227       Denmark       1974 invasive (unspecified/other) Neisseria meningitidis       A       5       ST-5 complex         alpha14; BennettTree10       Germany       1999       carrier       Neisseria meningitidis       A       4       ST-4 complex         B269; NIBSC_2825; Z1269       Burkina Faso       1963 invasive (unspecified/other) Neisseria meningitidis       A       4       ST-4 complex         B275; NIBSC_2767; Z1275       Niger       1963 invasive (unspecified/other) Neisseria meningitidis       A       4       ST-4 complex         B278; NIBSC_2764; Z1278       Niger       1963 invasive (unspecified/other) Neisseria meningitidis       A       4       ST-4 complex         B382; NIBSC_2779; Z132       Greece       1968 carrier       Neisseria meningitidis       A       4       ST-4 complex         B389; NIBSC_2872; Z1439       Dijbouti       1966 invasive (unspecified/other) Neisseria meningitidis       A       1       ST-1 complex         B439; NIBSC_2872; Z1439       Dijbouti       1966 invasive (unspecified/other) Neisseria meningitidis       A       1       ST-1 complex         B466; NIBSC_2876; Z1466       Australia       <	B213; NIBSC_2813; Z1213       Ghana       1973 invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex       7         S5       B227; NIBSC_2806; Z1227       Denmark       1974 invasive (unspecified/other)       Neisseria meningitidis       A       5       ST-5 complex       5-1         alpha14; BennettTree10       German 1999       carrier       Neisseria meningitidis       Cnl       53       ST-53 complex       7         B259; NIBSC_2825; Z1269       Burkina Faso       1963 invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex       7         B275; NIBSC_2764; Z1275       Niger       1963 invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex       7         B362; NIBSC_2764; Z1276       Niger       1963 invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex       7         B382; NIBSC_2823; Z1392       Greece       1968       carrier       Neisseria meningitidis       A       1       ST-1 complex       5-2         B439; NIBSC_2826; Z1429       Dijbouti       1968       carrier       Neisseria meningitidis       A       1       ST-1 complex       5-2         B44       B439; NIBSC_2826; Z1439	B213; NIBSC_2813; Z1213         Gnana         1973 invasive (unspecified/other) Neisseria meningitidis         A         4         ST-4 complex         7         13-1           56         B227; NIBSC_2806; Z1227         Denmark         1974 invasive (unspecified/other) Neisseria meningitidis         A         5         ST-5 complex         5-1         9           alpha14; BennettTree10         Germany         1999         carrier         Neisseria meningitidis         A         4         ST-4 complex         7         13-1           B269; NIBSC_2826; Z1269         Burkina Faso         1963 invasive (unspecified/other) Neisseria meningitidis         A         4         ST-4 complex         7         13-3           B275; NIBSC_2767; Z1275         Niger         1963 invasive (unspecified/other) Neisseria meningitidis         A         4         ST-4 complex         7         13-1           B275; NIBSC_2764; Z1278         Niger         1963 invasive (unspecified/other) Neisseria meningitidis         A         4         ST-4 complex         7         13-1           B276; NIBSC_2764; Z1278         Niger         1963 invasive (unspecified/other) Neisseria meningitidis         A         4         ST-4 complex         7         13           B3852; NIBSC_2872; Z1392         Greece         1968         carrier         Neisseri

Select the isolates to include. These will be pre-populated if you arrive here following a search.

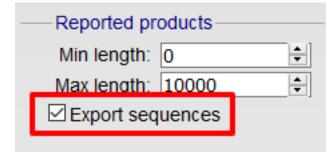
Enter your forward and reverse primer sequences in the appropriate boxes. These may contain wobble bases if necessary. You can also specify how many mismatches are allowed for each primer. Finally, you can restrict the reported length to only those products that fall between a minimum and maximum length range.

PubMLST Database	e home Contents			
+D Log in				Toggle: 🚺
In silico PCR				
ipcress program written	by Guy Slater.		seful for designing and testing primer	s. The plugin is a wrapper for the exonerate
Isolates	Primer 1	Primer 2 GAGAACGAGCCGGGATAGGA : Allowed mismatches: 0 ~	Reported products Min length: 0 + Max length: 10000 + Export sequences	Action

Click 'Submit'. The job will be sent to the job queue. The output will be a table of predicted products, showing the number of products and their positions within a contig. A summary of this table is also available to download in tabdelimited text of Excel formats.

			-	contig		start	end	description
2	A4/M1027	~	1	180126	516	6820	7335	reverse
	120M	~	1	180675	516	1942	2457	forward
7	7891	~	1	180795	516	6818	7333	reverse
10	6748	~	2	181299	516	1948	2463	forward
				181505	516	1957	2472	forward
11	129E	~	1	181720	516	1954	2469	forward
13	139M	~	1	182116	516	6838	7353	reverse
19	S3131	~	1	182225	516	1954	2469	forward
24	S4355	~	1	215556	516	6822	7337	reverse
30 31	14 10	~	1	8 182398	516 516	983478 1954	2469	reverse
			1					forward
34	20	~	1	182791	516	7030	7545 2762	reverse
35 52		~	1	182948 183322	516 516	2247 1958	2473	forward forward
52 61	393	~	1	183655	516	6815	7330	reverse
64	254	ž	1	183761	516	1950	2465	forward
67	S5611	~	1	184197	516	1953	2468	forward
82		÷.	1	184337	516	2245	2466	forward
84	IAL2229	÷.	1	184525	516	6818	7333	reverse
90		- 2	1	184677	516	7256	7771	reverse

It is also possible to export the predicted product sequence. You can do this by selecting the 'Export sequences' checkbox on the options form.



**Note:** The exported sequences will include the primer regions. It is important to note that, unlike a real PCR reaction, these sequences represent the sequence within this region in the genome. In a real PCR reaction, the primers are themseleves incorporated in to the product, so even if there was a mismatch in the primer region, the product sequence would include the primer sequence.

# 14.9 Interactive Tree of Life (iTOL)

The ITOL plugin allows you to generate and visualise phylogenetic trees calculated from concatenated sequence alignments of selected loci (or the loci belonging to a particular scheme). Currently, only Neighbour-joining trees are supported. Datasets can include metadata which allows nodes in the resultant tree to be coloured.

ITOL can be accessed from the contents page by clicking the 'iTOL' link.

sseria PubMLST	database				
oocha i abiiiLoi	ultubube				
			total known diversity of Neisseria s ibase and consequently it should l		the profiles/sequence definition database at a population sample.
Query database	Proj	ects	option settings		1 Submissions
<ul> <li>Search or browse databas</li> <li>Search by combinations of</li> </ul>			general options - including isolate display and query options for locu		Manage submissions
					General information
					<ul> <li>Isolates: 51,555</li> </ul>
					<ul> <li>Last updated: 2019-07-04</li> </ul>
					<ul> <li>Defined field values</li> </ul>
					Update history
					About BIGSdb
Breakdown	Export		Analysis	Third party tools	
Single field	Export dataset		Codon usage	<ul> <li>GrapeTree - Visualization of</li> </ul>	at denomic relationships
Two field	Contigs		Gene presence	iTOL Phylogenetic trees v	
Unique combinations	<ul> <li>Sequences - XMFA / con</li> </ul>	atenated FASTA formats	Genome comparator	<ul> <li>PhyloViz - Visualization and</li> </ul>	
Publications			BLAST		ualization and sharing for genomic
Sequence bin	Miscellaneous		<ul><li>Species identification</li><li>In silico PCR</li></ul>	epidemiology	5 5
	Description of database				

Alternatively, it can be accessed following a query by clicking the 'iTOL' button at the bottom of the results table. Isolates returned from the query will be automatically selected within the iTOL interface.

	A4/M1027	B1; NIBSC_2803; Z1001	USA	1937 invasive	(unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	5-2	10	F1-5
2	120M	B35; NIBSC_2822; Z1035	Pakistan	1967 meningit	is and septicaemia	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
3	M00242905		UK	2000 invasive	(unspecified/other)	Neisseria meningitidis	В	1099		19	15	
4	M1027	B43; NIBSC_3076; Z1043	USA	1937 invasive	(unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex			
5	M00240227		UK	2000 invasive	(unspecified/other)	Neisseria meningitidis	В	1100	ST-32 complex	7	16	
6	M00282207		UK	2000 invasive	(unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; NIBSC_2760; Z1054	Finland	1975 invasive	(unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	20	9	F3-1
8	M00242007		UK	2000 invasive	(unspecified/other)	Neisseria meningitidis	В	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984 invasive	(unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; NIBSC_2784; Z1073	Canada	1971 invasive	(unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	18-1	3	F5-1
11	129E	B92; NIBSC_2828; Z1092	Germany	1964 invasive	(unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F3-6
12			Czech Republic		(unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex	7	16	
13		B99; NIBSC_2795; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex	5-2	10	F5-1
14			Czech Republic	1995 invasive	(unspecified/other)	Neisseria meningitidis	Х	117			14	
15			Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17			Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19	S3131	B213; NIBSC_2813; Z1213	Ghana	1973 invasive	(unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13-1	F1-5
20			Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG		ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex			
24		B227; NIBSC_2806; Z1227	Denmark		(unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			

Select the isolates to include. The tree can be generated from concatenated sequences of any selection of loci, or more conveniently, you can select a scheme in the scheme selector to include all loci belonging to that scheme.

Additional fields can be selected to be included as metadata for use in colouring nodes - select any fields you wish to include in the 'iTOL datasets' list. Multiple selections can be made by holding down Shift or Ctrl while selecting. You can also choose how nodes are labeled by metadata - either by colouring the labels or using coloured strips.

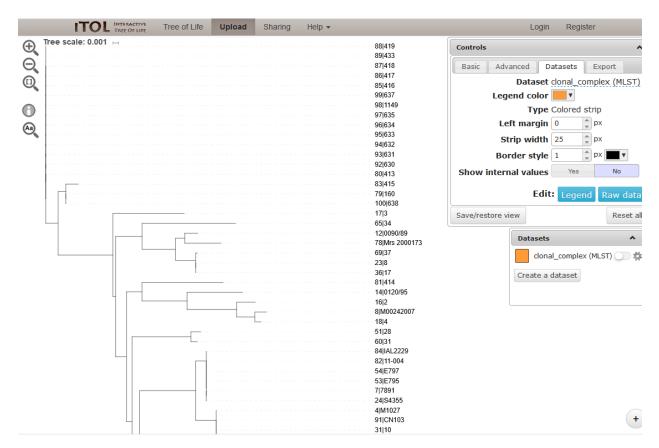
Click 'Submit' to start the analysis.

PubMLST Database hon					
Logged in: Keith Jolley (keith). 🔂 Lo	g out   Change password				Toggle: ()
iTOL - Interactive	Tree of Life - Neisse	eria PubMLST			
	4. Department of Bioinformatic Web site: https://itol.embl.de/ Publication: Letunic & Bork (2016)	sis within the Interactive Tree of Life online : an online tool for the display and thestr 142, 69126 Heidelberg, Germany Laboratory, Meyerhofstrasse 1, 69117 Hei lecular Medicine, 13125 Berlin, Germany s, Biocenter, University of Würzburg, 97074 Interactive tree of life (ITOL) v3: an online d other trees. <i>Nucleic Acids Res</i> 44(W1):W	annotation of phylogenetic and ot delberg, Germany Würzburg, Germany looi for the display	ther trees	
Please check the loci that you Analysis is limited to 2,000 re		elect one or more schemes to include all lo		allele sequence identifiers, or DNA and peptide loci with genom	e sequences, can be included.
2 data 3 Upic 5 (or z 7 V FAS 8 d	ionally include data not in the base. bad assembly FASTA file pp file containing multiple TA files - one per genome): • owsse No file selected.	"165_rDNA 165_rRNA (SSU_rRNA) 235_rRNA abcZ abcZ (NEIS1015) aceF (NEIS1279) acAc2 (NEIS1727) acnA (NEIS1727) acnA (NEIS1729) Al None Paste let	Image: Second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second seco	ST (MLST) clonal complex (MLST) pST (beta lactamase plasmid) BAST (Bexsero Antigen Sequence Typing (BAST)) pST (Conjugative Plasmid)	Otext tabels Coloured strips — Include in identifier— Elisotate name — Action— Submit

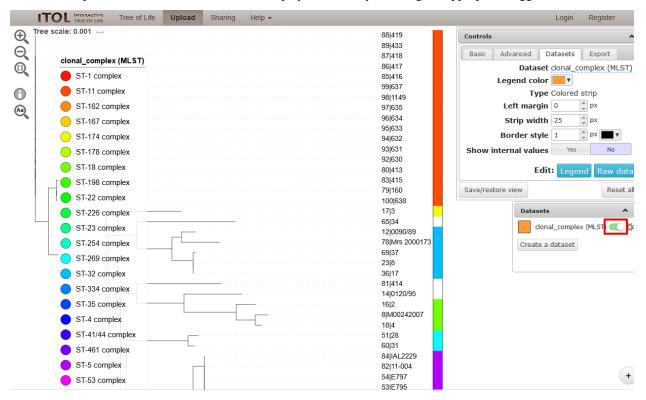
The job will be sent to the job queue. When it has finished, the generated tree and associated metadata will be uploaded to the Interactive Tree of Life website (https://itol.embl.de/). Click the button marked 'Launch iTOL'.

ubMLST Database home Contents	
ogged in: Keith Jolley (keith). (+Log out   Change password	=
ob status viewer	
Status	
Job id: BIGSdb_190460_1562236303_79711	
Submit time: 2019-07-04 11:31:43	
Status: finished	
Start time: 2019-07-04 11:32:03	
Progress: 100%	
Stop time: 2019-07-04 11:32:31	
Total time: 28 seconds	
Output	
Output	
Launch iTOL	
Files	
Concatenated FASTA	
Nease note that job results will remain on the server for 7 days.	

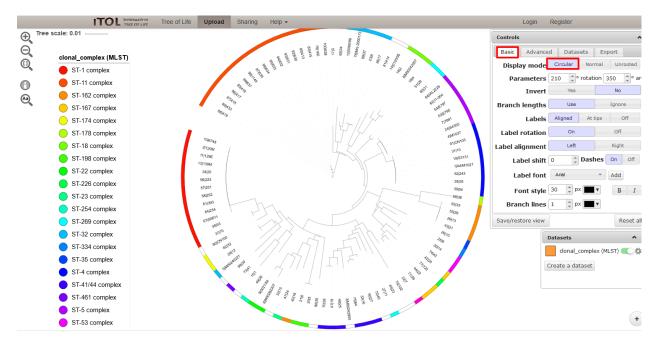
Your browser will open the iTOL website with your tree.



You can manipulate the tree in the browser, and display metadata by selecting the appropriate toggle.



The tree layout can be changed by clicking the 'Basic tab' and, for example, selecting a circular display mode.

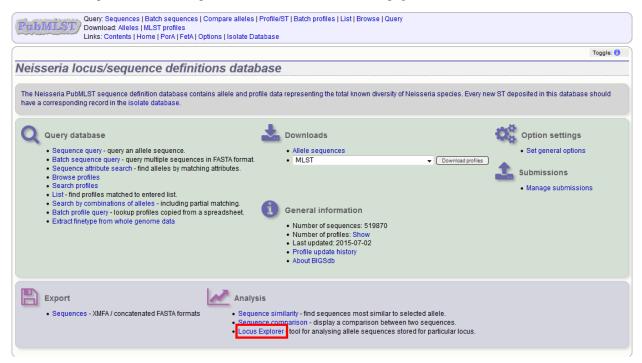


See the detailed documentation on the iTOL website for more information about manipulating and exporting trees.

# 14.10 Locus explorer

The locus explorer is a sequence definition database plugin. It can create schematics showing the polymorphic sites within a locus, calculate the GC content and generate aligned translated sequences.

Click 'Locus Explorer' from the sequence definition database contents page.



## 14.10.1 Polymorphic site analysis

Select the locus you would like to analyse in the Locus dropdown box. The page will reload.

PubMLST / Downloa	sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse ad: Alleles   MLST profiles contents   Home   PorA   FetA   Options   Isolate Database	
		Help 🗹
Locus Explorer -	Neisseria locus/sequence definitions	
Please select locus for analy	sis:	
Locus adk	➡ Page will reload when changed	
Select sequences — -		Action
1 All None	<ul> <li>Polymorphic Sites - Display polymorphic site frequencies and sequence schematic</li> <li>Codon - Calculate G+C content and codon usage</li> <li>Translate - Translate DNA to peptide sequences</li> </ul>	Submit

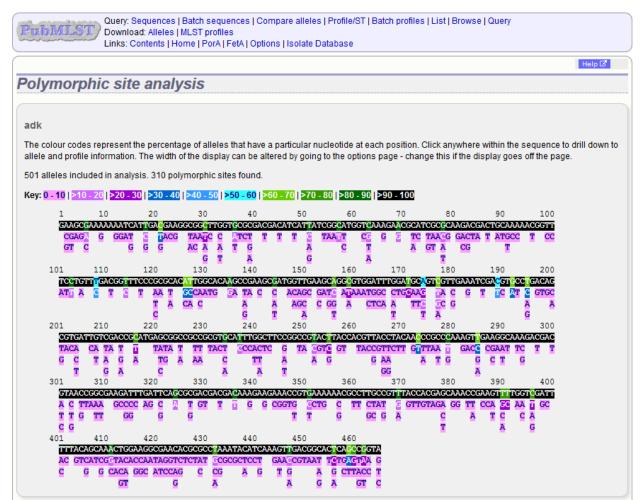
Select the alleles that you would like to include in the analysis. Variable length loci are limited to 2000 sequences or fewer since these need to be aligned. Select 'Polymorphic Sites' in the Analysis selection and click 'Submit'.

PubMLST Down	y: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query nload: Alleles   MLST profiles :: Contents   Home   PorA   FetA   Options   Isolate Database	
[		Help 🖉
Locus Explorer	r - Neisseria locus/sequence definitions	
Please select locus for ana	alysis:	
Locus: adk		
Select sequences	Select analysis     Action     Polymorphic Sites     Display polymorphic site frequencies and sequence schematic     Submit     Codon - Calculate G+C content and codon usage     Translate - Translate DNA to peptide sequences	

If an alignment is necessary, the job will be submitted to the job queue and the analysis performed. If no alignment is

necessary, then the analysis is shown immediately.

The first part of the page shows the schematic.



Clicking any of the sequence bases will calculate the exact frequencies of the different nucleotides at that position.

>40	- 5	0 >	• <b>50</b> -	60	>6	0 - 1	70	>70	- 80	>80	- 90	>9
3	80			40			5	0		60	)	
GCGC	<b>iC</b> T	TGG	TGC	GCG	ACG	ACA	TCA	TTA	TCGG	CATC	(GTCA	AA(
TAA	VTC	С	AT	СТ	Т	Т	Т	С	TAA	TT	CG	G
AC	А	А	т	G				Α		С	Т	
	G	Т		A				G			A	

	voloror			 	Help 🗹
2 E)	xplorer			 	
k pos	ition 51				
l allele	s included in anal	ysis.			
se Nu	mber of alleles P	ercentage of alle	les MLST profiles		
Г	401	80.04	11130 / 11407		
2	98	19.56	(97.57%) 275 / 11407		
			(2.41%)		
A	1 (adk-351)	0.20	1 / 11407 (0.01%)		
3	1 (adk-413)	0.20	1 / 11407 (0.01%)		
	(dair (10)		(0.0170)		

The second part of the page shows a table listing nucleotide frequencies at each of the variable positions.

C	G															Т		A	C	
401		410		42			30	44		45			60							
						ACACGC														
C			ACA			GTCTCT	C CG			T G		GC								
•			GT	000	AIU	G	A	*	9	A	_	A		r c						
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ition 🗢				<b>_</b>		lucleot														
		C≑		T ¢	_	%A ≑			%I≑	‰- ≑										
2	499	1	1	0	0		0.20													
3	498	0	2	1	0	99.40			0.20											
4	1	0	500		0	0.20		99.80												
5	0	500	1	0	0		99.80													
6	53	8	440		0		1.60													
9	499	0	2	0	0	99.60		0.40												
12	500	0	1	0	0			0.20												
13	500	0	1	0	0	99.80		0.20												
14	1	0	0	500		0.20			99.80											
15	0	488	1	12				0.20												
18	0	86	8	407				1.60												
21	0	315	1	185			62.87	0.20	36.93											
22	9	0	492	0	0	1.80		98.20												
23	500	1	0	0	0	99.80	0.20													
24	500	0	1	0	0	99.80		0.20												
27	3	488	0	10	0		97.41		2.00											
28	2	2	497		0		0.40													
29	2	0	499	0	0	0.40		99.60												
30	3	367	2	129		0.60	73.25	0.40												
31	0	11	0	490	0		2.20		97.80											
	2	5	492	2	0	0.40	1.00	98.20	0.40											
33		0	445	3	0	10.58		88.82	0.60											
33 36	53	•																		

#### See also:

- Investigating allele differences.
- Polymorphism analysis following isolate query.

## 14.10.2 Codon usage

Select the alleles that you would like to include in the analysis. Again, variable length loci are limited to 200 sequences or fewer since these need to be aligned. Click 'Codon'.

Query: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query           Download: Alleles   MLST profiles           Links: Contents   Home   PorA   FetA   Options   Isolate Database
Locus Explorer - Neisseria locus/sequence definitions
Please select locus for analysis:
Locus: adk   Page will reload when changed
Select sequences       Analysis functions         459       460         461       Codon Calculate G+C content and codon usage         463       Translate DNA to peptide sequences

The GC content of the alleles will be determined and a table of the codon frequencies displayed.

		wnload: Allele	s   MLST profil	les	pare alleles   Profile/ST   Batch profiles   List   Browse   Query s   Isolate Database
odon	Usage				
dk					
RF used: 1	1				
34 alleles i	included in a	nalysis.			
C conten	at .				
oding: GC					
st letter: GO	C 65.31% C 31.73%				
rd letter: G					
odons					
				g its redunda	
requency: l odon 🗢 🗛	Usage of give	en codon per 1 Fraction ¢	1000 codons. Frequency ¢	-	
requency: l odon 🔶 A GCA	Usage of give tmino acid \$ A	Fraction \$	1000 codons. Frequency ¢ 17.353	Number \$	
equency: ( odon ¢ A GCA GCC	Usage of give Imino acid \$ A A	rn codon per 1 Fraction \$ 0.262 0.246	1000 codons. Frequency ¢ 17.353 16.254	Number ¢ 1248 1169	
equency: l odon ¢ A GCA GCC GCG	Usage of give mino acid \$ A A A A	rn codon per 1 Fraction ↓ 0.262 0.246 0.389	1000 codons. Frequency ♦ 17.353 16.254 25.751	Number ¢ 1248 1169 1852	
equency: U odon 🔶 A GCA GCC GCG GCT	Usage of give Imino acid \$ A A A A A A	rn codon per 1 Fraction 0.262 0.246 0.389 0.103	1000 codons. Frequency ¢ 17.353 16.254 25.751 6.813	Number ¢ 1248 1169 1852 490	
equency: ( odon \$ A GCA GCC GCC GCG GCT TGC	Usage of give xmino acid \$ A A A A A C	rn codon per 1 Fraction ♦ 0.262 0.246 0.389 0.103 0.987	1000 codons. Frequency ↓ 17.353 16.254 25.751 6.813 6.452	Number 1248 1169 1852 490 464	
equency: ( odon \$ A GCA GCC GCG GCT TGC TGT	Usage of give mino acid \$ A A A A A C C C	rn codon per 1 Fraction ♦ 0.262 0.246 0.389 0.103 0.987 0.013	1000 codons. Frequency ↓ 17.353 16.254 25.751 6.813 6.452 0.083	Number ↓ 1248 1169 1852 490 464 6	
equency: ( odon \$ A GCA GCC GCC GCT TGC TGT GAC	Usage of give mino acid \$ A A A A C C C D	r codon per 1 Fraction ◆ 0.262 0.246 0.389 0.103 0.987 0.013 0.747	1000 codons. Frequency ¢ 17.353 16.254 25.751 6.813 6.452 0.083 91.073	Number 1248 1169 1852 490 464 6 6550	
equency: 0 odon \$ A GCA GCC GCG GCT TGC TGT GAC GAT	Usage of give A A A C C C D D	r codon per 1 Fraction + 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812	Number ♦ 1248 1169 1852 490 464 6 6550 2216	
equency: l odon  A GCA GCC GCG GCT TGC TGT GAC GAT GAA	Usage of give A A A A C C D D E	r codon per 1 Fraction ♦ 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397	Number ♦ 1248 1169 1852 490 464 6 6550 2216 5926	
don ♦ A GCA GCC GCC GCG GCT TGC TGT GAC GAT GAA GAG	Usage of give mino acid A A A C C D D E E	r codon per 1 Fraction ♦ 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.084	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564	Number ♦ 1248 1169 1852 490 464 6 5550 2216 5926 544	
equency: l GCA GCC GCC GCT TGC TGT GAC GAT GAA GAA GAG TTC	Usage of give mino acid A A A C C D D E E F	r codon per 1 Fraction ↓ 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.084 0.594	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295	Number ◆ 1248 1169 1852 490 464 6 6550 2216 5926 544 1100	
equency: l odon	Usage of give mino acid A A A A C C D D E E F F	r codon per 1 Fraction ↓ 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.084 0.594 0.406	1000 codons. Frequency ◆ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470	Number ♦ 1248 1169 1852 490 464 6 6550 2216 5926 5926 544 1100 753	
requency: I       odon €       A       GCA       GCC       GCG       GCT       TGC       TGT       GAC       GAT       GAA       GAA       GAG       TTC       TTC       TTT       GGA	Usage of give mino acid A A A C C C D D E E F F G	r codon per 1 Fraction ♦ 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.084 0.594 0.406 0.007	1000 codons. Frequency ◆ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.542	Number ◆           1248           1169           1852           490           464           6           6550           2216           5926           544           1100           753           39	
equency: l odon $\blacklozenge$ A GCA GCC GCG GCT TGC GAC GAC GAC GAA GAA GAA GAG TTC TTT GGA GGA	Usage of give A A A A C C C D D E E F F F G G	raction ≠ 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.084 0.594 0.406 0.007 0.765	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.542 59.497	Number ◆           1248           1169           1852           490           464           6           6550           2216           5926           544           1100           753           39           4279	
equency: l odon ♦ A GCA GCC GCC GCT TGC TGC TGC TGC GAC GAC GAA GAA GAG TTC TTT GGA GGC GGC	Usage of give mino acid + A A A A C C D D D C D D E F F G G G	n codon per 1 Fraction € 0.262 0.246 0.389 0.103 0.987 0.013 0.987 0.013 0.747 0.253 0.916 0.894 0.594 0.406 0.007 0.765 0.001	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.542 59.497 0.042	Number ¢ 1248 1169 1852 490 464 6 6550 2216 5926 544 1100 753 39 4279 3	
equency: l odon ¢ A GCA GCC GCC GCT TGC TGT GAC GAC GAC GAA TTC TTT GGA GGG GGG GGG	Usage of give mino acid A A A A A C C C D D D D C C D D C C C C C C C C C C C C C	n codon per 1 Fraction ♦ 0.262 0.246 0.289 0.103 0.987 0.013 0.747 0.253 0.916 0.084 0.994 0.084 0.994 0.406 0.007 0.765 0.001 0.227	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.542 59.497 0.042 17.659	Number ♦ 1248 1169 1852 490 464 6 6550 2216 5926 544 1100 753 39 4279 3 1270	
equency: 1 odon $\diamond$ A GCA GCC GCG GCG GCT TGC TGC TGT GAC GAT GAA GAG TTT GGA GGG GGG GGT CAC	Usage of give imino acid e A A A A A A A C C C C D D D D E F F G G G G H	n codon per 1 Fraction ◆ 0.262 0.246 0.389 0.103 0.987 0.013 0.987 0.013 0.747 0.253 0.916 0.984 0.594 0.594 0.406 0.070 0.765 0.001 0.227 0.749	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.470 0.59.497 0.042 17.659 19.258	Number ◆ 1248 1169 1852 490 485 490 485 5926 544 1100 753 39 4279 3 1270 1385	
equency: l odon ¢ A GCA GCC GCC GCT TGC TGT GAC GAC GAC GAA TTC TTT GGA GGG GGG GGG	Usage of give mino acid A A A A A C C C D D D D C C D D C C C C C C C C C C C C C	n codon per 1 Fraction ♦ 0.262 0.246 0.289 0.103 0.987 0.013 0.747 0.253 0.916 0.084 0.994 0.084 0.994 0.406 0.007 0.765 0.001 0.227	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.542 59.497 0.042 17.659	Number ♦ 1248 1169 1852 490 464 6 6550 2216 5926 544 1100 753 39 4279 3 1270	

## 14.10.3 Aligned translations

If a DNA coding sequence locus is selected, an aligned translation can be produced.

Select the alleles that you would like to include in the analysis. Again, variable length loci are limited to 200 sequences or fewer since these need to be aligned. Click 'Translate'.

Query: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query           Download: Alleles   MLST profiles           Links: Contents   Home   PorA   FetA   Options   Isolate Database
Locus Explorer - Neisseria locus/sequence definitions
Please select locus for analysis:
Locus: adk       Page will reload when changed         Select sequences       Analysis functions         459       Codon         461       Codon         462       Codon         483       Translate         All Nore       Nore

An aligned amino acid sequence will be displayed.

933 1	
434 1	L
435_1	Т
436 1	
437_1	
438 1	
439_1	
440_1	К.
441_1	
442_1	
443_1	I.
444_1	
445_1	
446_1	
447_1	
448_1	
449_1	
450_1	
451_1	
452_1	кт.
453_1	
454_1	
455_1	
456_1	
457_1	G
458_1	
459_1	
460_1	s.
461_1	
462_1	
463 1	
464 1	I
Consensus	EAKKIIDEGGLVRDDIIIGMVKERIAQDDCKNGFLFDGFPRTLAQAEAMVEAGVDLDAVVEIDVPDSVIVDRMSGRRVHLASGRTYHVTYNPPKVEGKDD
	110 120 130 140 150
	:
1_1	
2 1	
3 1	
2_1 3_1 4_1	
5_1	
6_1	
7_1	
8 1	

If there appear to be a lot of stop codons in the translation, it is possible that the orf value in the *locus definition* is not set correctly.

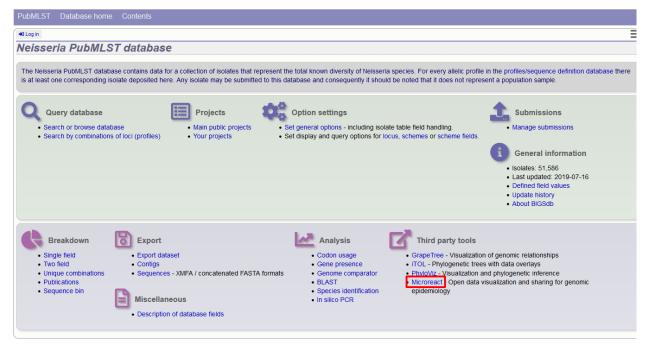
# 14.11 Microreact

Microreact is a tool for visualising genomic epidemiology and phylogeography. Individual nodes on a displayed tree are linked to nodes on a geographical map and/or timeline, making any spatial and temporal relationships between isolates apparent.

The Microreact plugin generates Neighbour-joining trees from concatenated sequences for any selection of loci or schemes and uploads these, together with country and year field values to the Microreact website for display.

**Note:** While Microreact itself is able to display isolates using GPS coordinates, the BIGSdb plugin is currently limited to the level of country.

Microreact can be accessed from the contents page by clicking the 'Microreact' link.



Alternatively, it can be accessed following a query by clicking the 'Microreact' button at the bottom of the results table. Isolates returned from the query will be automatically selected within the Microreact plugin interface.

11	129E	B92; NIBSC_2828; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	А	1	SI-1 complex	5-2	10	F3-6
13	139M	B99; NIBSC_2795; Z1099	Philippines	1968		Neisseria meningitidis	А	1	ST-1 complex	5-2	10	F5-1
19	S3131	B213; NIBSC_2813; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	А	4	ST-4 complex	7	13-1	F1-5
24	S4355	B227; NIBSC_2806; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	А	5	ST-5 complex	5-1	9	F3-1
31	10	B269; NIBSC_2825; Z1269	Burkina Faso	1963	invasive (unspecified/other)	Neisseria meningitidis	А	4	ST-4 complex	7	13-1	F1-5
34	20	B275; NIBSC_2767; Z1275	Niger	1963	invasive (unspecified/other)	Neisseria meningitidis	А	1	ST-1 complex	5-2	10	F1-7
35	26	B278; NIBSC_2764; Z1278	Niger	1963	invasive (unspecified/other)	Neisseria meningitidis	А	4	ST-4 complex	7	13	F1-5
52	243	B362; NIBSC_2779; Z1362	Cameroon	1966		Neisseria meningitidis	А	4	ST-4 complex	7	13	F1-5
61	393	B392; NIBSC_2823; Z1392	Greece	1968	carrier	Neisseria meningitidis	А	1	ST-1 complex	5-2	10	F5-1
64	254	B439; NIBSC_2812; Z1439	Djibouti	1966	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F1-7
67	S5611	B466; NIBSC_2765; Z1466	Australia	1977	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
82	11-004	B503; NIBSC_2826; Z1503	China	1984	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	20	9	F3-8
84	IAL2229	B506; NIBSC_2816; Z1506	Brazil	1976		Neisseria meningitidis	Α	5	ST-5 complex	20	9	F2-1
90	CN100	B534; NIBSC_2768; Z1534	UK	1941	invasive (unspecified/other)	Neisseria meningitidis	Α	21		5-2	10	F3-9
120	F4698	NIBSC_2731; Z3515	Saudi Arabia	1987	carrier	Neisseria meningitidis	А	5	ST-5 complex	20	9	F3-1
128	F6124	NIBSC_2730; Z3524	Chad	1988	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	20	9	F3-1
160	1014	NIBSC_2821; Z3667	Sudan	1985	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13-1	F1-5
210	H1964	NIBSC_2796; Z3771	UK	1987	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	20	9	F3-1
237	H44/76	44/76-3; NIBSC_2724; Z3842	Norway	1976	invasive (unspecified/other)	Neisseria meningitidis	В	32	ST-32 complex	7	16	F3-3
238	153	NIBSC_2733; Z3905	China	1966	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	20	9	F3-1
239	154	NIBSC_2766; Z3906	China	1966	invasive (unspecified/other)	Neisseria meningitidis	Α	6	ST-5 complex	20	9	F3-1
G	Breakdown	Fields Two Field Comb	pinations Pol	lymorp	ohic sites Publications Se	equence bin						
2	🛃 Analysis	BURST Codons Gene	Presence G	enome	Comparator BLAST rM	ILST species id PCR						
	Export											
-2	Export Third party			at 1								

Select the isolates to include. The tree can be generated from allelic profiles of any selection of loci, or more conveniently, you can select a scheme in the scheme selector to include all loci belonging to that scheme.

Additional fields can be selected to be included as metadata for use in colouring nodes - select any fields you wish

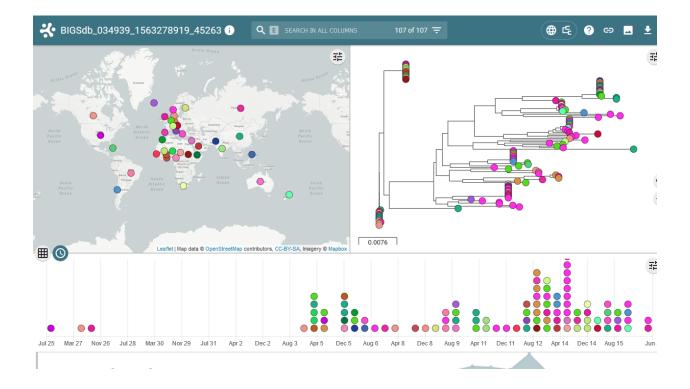
to include. Multiple selections can be made by holding down shift or ctrl while selecting. Click 'Submit' to start the analysis.

11 ···································	
Artemij Fedosejev	
Jyothish NT	
Stephano	
• Stephano	
in the Aanensen Research Group at Imperial College London and The Centre for Genomic F	Pathogen Surveillance.
Web site: https://microreact.org	
Publication: Argimón at al. (2016) Microreact: visualizing and sharing data for genomic epide	miology and phylogeography. Microb Genom 2:e000093.
<u></u>	
This tool will generate neighbor-joining trees from concatenated nucleotide sequences. Only	DNA loci that have a corresponding database containing allele sequence identifiers, or DNA and
peptide loci with genome sequences, can be included. Please check the loci that you would	ike to include. Alternatively select one or more schemes to include all loci that are members of the
scheme.	
scheme.	
Analysis is limited to 2,000 records or 100,000 sequences (records x loci).	
Analysis is infinited to 2,000 records or 100,000 sequences (records x loci).	
1 165_rDNA ^	~
	ismids
7 235_rRNA 4- 🖬 💭 Ty	bing
10 abc7	
11 abcZ (NEIS1015)	MLST
13	Finetyping antigens
24 ackA2 (NEIS1727) acnA (NEIS1729)	16S
	Antigen genes
Clear List all All None Paste list	Bexsero Antigen Seg Y
	Bexsero Antigen Seq *
Descriptions	-Include fieldsAction
Modify the values below - these will be displayed within the created Microreact project.	Select additional fields to include in Microreact data table Submit
	(isolate, country and year are always included).
Title:	version in the second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second
Description: Neisseria PubMLST	continent
Description. Relabella Publica	region
	date received
li.	date sampled
	non culture
	epidemiological year 🗸

The job will be sent to the job queue. When it has finished, click the button marked 'Launch Microreact'.

+D Log in		Ξ
Job status view	rer	
Status		
Job id:	BIGSdb_034939_1563278919_45263	
Submit time:	2019-07-16 13:08:39	
Status:	finished	
Start time:	2019-07-16 13:08:42	
Progress:	100%	
Stop time:	2019-07-16 13:09:13	
Total time:	30 seconds	
Output Launch Microrea Files Concatenated		

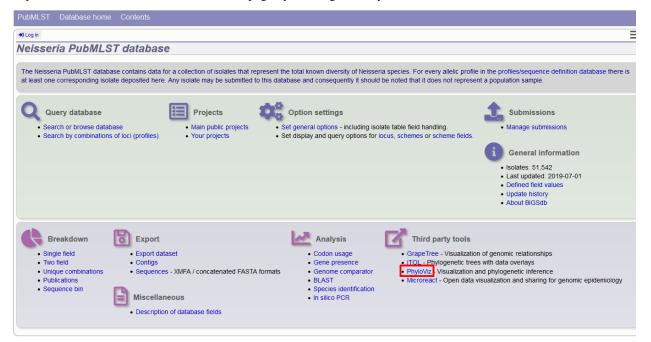
The generated tree will be uploaded to the Microreact website and displayed. Clicking any node will show its position(s) within the tree, map and timeline. A node on the map may correspond to multiple nodes in the tree or timeline.



# 14.12 PhyloViz

PhyloViz Online is a tool for generating and visualising minimum-spanning trees. Datasets can include metadata which allows nodes in the resultant tree to be coloured interactively.

PhyloViz can be accessed from the contents page by clicking the 'PhyloViz' link.

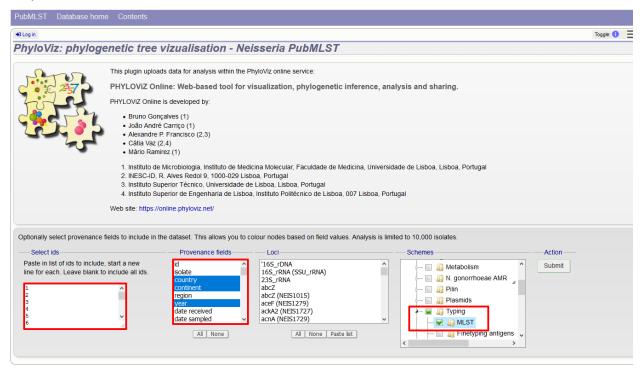


Alternatively, it can be accessed following a query by clicking the 'PhyloViz' button at the bottom of the results table. Isolates returned from the query will be automatically selected within the PhyloViz interface.

13 14 (	129E 0090/89	B92; NIBSC_2828; Z1092	Germany	1964 invasive (	unepocified/othor)	A factor and a second a subfattor						
13 14 (					unspecifieu/ourier)	Neisseria meningitidis	A	1	ST-1 complex	5-2	10	F3-6
14 (			Czech Republic	1989 invasive (	unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex	7	16	
	139M	B99; NIBSC_2795; Z1099	Philippines	1968		Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
	0120/95		Czech Republic	1995 invasive (	unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19	S3131	B213; NIBSC_2813; Z1213	Ghana	1973 invasive (	unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex			
24	S4355	B227; NIBSC_2806; Z1227	Denmark	1974 invasive (	unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	В	930	ST-334 complex			
24 25	S4355		Denmark	1974 invasive (	unspecified/other)	Neisseria meningitidis	А	5	ST-5 complex	5-1	9	
B	Breakdown	Fields Two Field Cor	nbinations Pol	lymorphic sites	Publications Se	quence bin						
12	Analysis	BURST Codons Ger	e Presence G	enome Comparat	tor BLAST rM	LST species id PCR						
	Export											
	C Export	Dataset Contigs Se	quences									
<b>N</b>	Third party	GrapeTree ITOL Phy	/loViz Microrea	act								

Select the isolates to include. The tree can be generated from allelic profiles of any selection of loci, or more conveniently, you can select a scheme in the scheme selector to include all loci belong to that scheme.

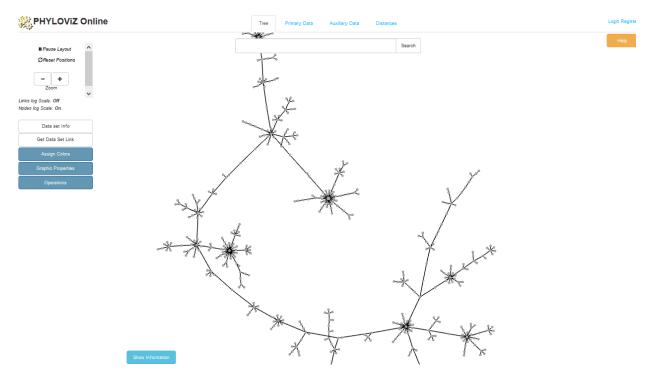
Provenance fields can be selected to be included as metadata for use in colouring nodes - select any fields you wish to include. Multiple selections can be made by holding down Shift or Ctrl while selecting. Click 'Submit' to start the analysis.



The necessary files will be generated immediately. When this has finished, click the button launch 'Launch PhyloViz'.

	ase home Contents	
+3 Log in		Toggle: ()
PhyloViz: ph	nylogenetic tree vizualisation - Neisseria PubMLST	
Shor	This plugin uploads data for analysis within the PhyloViz online service:	
235	PHYLOViZ Online: Web-based tool for visualization, phylogenetic inference, analysis and sharing.	
hill	PHYLOVIZ Online is developed by:	
	Bruno Gonçalves (1)     João André Carriço (1)     Alexandre P. Francisco (2,3)     Cátia Vaz (2,4)     Mário Ramirez (1)	
	1. Instituto de Microbiologia, Instituto de Medicina Molecular, Faculdade de Medicina, Universidade de Lisboa, Lisboa, Portugal 2. INESC-ID, R. Alves Redol 9, 1000-029 Lisboa, Portugal 3. Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal 4. Instituto Superior de Engenharia de Lisboa, Instituto Politécnico de Lisboa, 007 Lisboa, Portugal	
	Web site: https://online.phyloviz.net/	
	essing to finish (do not refresh page). essed and sent to PhyloViz Online.	
Generating profile da	ata file 🗸	
Generating auxiliary	file ✔	
Sending data to Phy	loViz online ✔	
Launch Phyl	loViz	

The tree will be sent to and rendered within the PhyloViz website.



See more information about manipulating the tree on the PhyloViz website.

# 14.13 Polymorphisms

The Polymorphisms plugin generates a *Locus Explorer* polymorphic site analysis on the alleles designated in an isolate dataset following a query.

The analysis is accessed by clicking the 'Polymorphic sites' button in the Breakdown list at the bottom of a results table following a query.

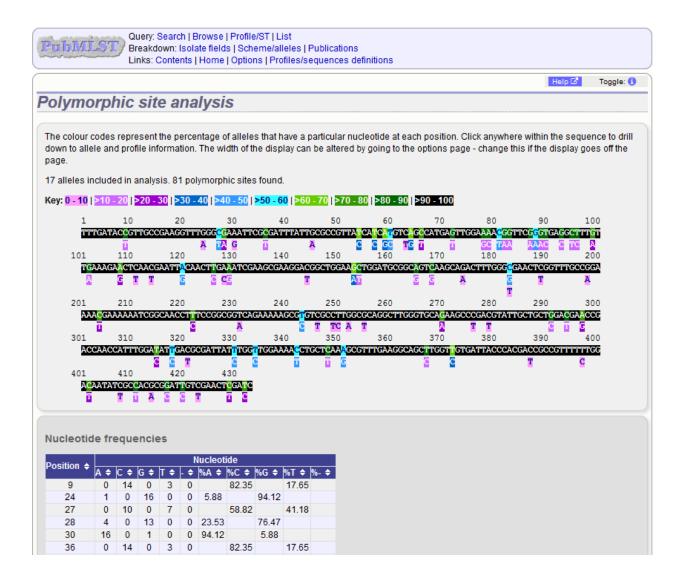
10       6748       673;21073       Canada       1971       invasive (unspecified/other)       Neisseria meningilidis       A       1       ST-1 complex/subgroup I/II       18-1       3       F5-1         11       129       B92;21092       Germany       1964       invasive (unspecified/other)       Neisseria meningilidis       A       1       ST-1 complex/subgroup I/II       5-2       100       F3-6         12       0990%       Czech Republic       1989       invasive (unspecified/other)       Neisseria meningilidis       A       1       ST-1 complex/subgroup I/II       5-2       100       F3-6         13       139M       B99;21099       Philippines       1986       Neisseria meningilidis       X       11       ST-1 complex/subgroup I/II       5-2       100       F5-1         14       012095       Czech Republic       1995       invasive (unspecified/other)       Neisseria meningilidis       X       117       14       14         16       2       Germany       1999       carrier       Neisseria meningilidis       B       854       ST-18 complex       117       14         18       4       Germany       1999       carrier       Neisseria meningilidis       B       19       ST-14 complex							-						
12         0900/09         Czech Republic         1989 invasive (unspecified/other)         Neisseria meningitidis         B         1015         ST-32 complex/ET-5 complex         7         16           13         139M         B99; 21099         Philippines         1988         Neisseria meningitidis         A         1         ST-1000000000000000000000000000000000000	10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
13       139M       B99, Z1099       Philippines       1988       Neisseria meningitidis       A       1       ST-1 complex/subgroup I/II       5-2       10       F5-1         14       0120/95       Czech Republic       1995       invasive (unspecified/other)       Neisseria meningitidis       X       117       17       14       14         15       1       Germany       1999       carrier       Neisseria meningitidis       E       864       ST-18 complex       14       14         16       2       Germany       1999       carrier       Neisseria meningitidis       B       854       ST-18 complex       14       14         17       3       Germany       1999       carrier       Neisseria meningitidis       W       174       ST-14 complex       14       14         18       4       Germany       1999       carrier       Neisseria meningitidis       W       174       ST-14 complex       14       15-1       15-1       15       15       15       15       16       15-1       16       16       16       16       16       16       16       16       16       16       16       16       16       174       ST-14 complex       1	11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
14       0120/95       Czech Republic       195 invasive (unspecified/other)       Neisseria meningitidis       X       117       11       14         15       1       Germany       1999       carrier       Neisseria meningitidis       E       864       14         16       2       Germany       1999       carrier       Neisseria meningitidis       E       864       14         17       3       Germany       1999       carrier       Neisseria meningitidis       B       854       ST-18 complex       14         18       4       Germany       1999       carrier       Neisseria meningitidis       B       19       ST-18 complex       14         19       S3131       B213; Z1213       Ghana       1973 invasive (unspecified/other)       Neisseria meningitidis       A       4       ST-4 complex       14         20       5       Germany       1999       carrier       Neisseria meningitidis       NG       198       ST-198 complex       14         21       6       Germany       1999       carrier       Neisseria meningitidis       NG       198       ST-198 complex       14         23       8       Germany       1999       carrier       Ne	12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
15       1       Germany       1999       carrier       Neisseria meningitidis       E       864       0       0       0       0         16       2       Germany       1999       carrier       Neisseria meningitidis       B       854       ST-18 complex       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0       0<	13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
16       2       Germany       1999       carrier       Neisseria meningitidis       B       854       ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-18 complex       Image: ST-1	14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
17       3       Germany       1999       carrier       Neisseria meningitidis       W       174       ST-174 complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Complex       Image: Com	15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
18     4     Germany     1999     carrier     Neisseria meningitidis     B     19     ST-18 complex       19     S3131     B213, Z1213     Ghana     1973     invasive (unspecified/other) Neisseria meningitidis     A     4     ST-4 complex/subgroup IV     7     13-1     F1-5       20     5     Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex     2       21     6     Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex     2       22     7     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex     2       23     8     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex     2       24     \$4355     B227,Z1227     Denmark     1974     invasive (unspecified/other) Neisseria meningitidis     A     5     ST-5 complex/subgroup III     5-1     9       25     9     Germany     1999     carrier     Neisseria meningitidis     B     930     ST-334 complex	16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
19       \$3131       B213;Z1213       Ghana       1973 invasive (unspecified/other) Neisseria meningitidis       A       4       \$T-4 complex/subgroup IV       7       13-1       F1-5         20       5       Germany       1999       carrier       Neisseria meningitidis       NG       198       \$T-198 complex/subgroup IV       7       13-1       F1-5         21       6       Germany       1999       carrier       Neisseria meningitidis       NG       198       \$T-198 complex       192         22       7       Germany       1999       carrier       Neisseria meningitidis       E       60       \$T-506 complex       198       \$T-198 complex/subgroup IV       7       13-1       F1-5         23       8       Germany       1999       carrier       Neisseria meningitidis       E       60       \$T-506 complex       198       \$T-198 complex/subgroup IV       7       13-1       F1-5         24       \$84355       B227; Z1227       Denmark       1974 invasive (unspecified/other)       Neisseria meningitidis       A       5       \$T-500 complex/subgroup IV       5-1       9       \$T-314       9       \$T-314       \$T-314       \$T-314       \$T-314       \$T-314       \$T-314       \$T-314       \$T-32	17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
20     5     Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex       21     6     Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex       22     7     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-50 complex       23     8     Germany     1999     carrier     Neisseria meningitidis     E     32     ST-32 complex/ET-5 complex       24     S4355     B227,Z1227     Denmark     1974     invasive (unspecified/other)     Neisseria meningitidis     A     5     ST-50 complex/SUbgroup III     5-1     9       25     9     Germany     1999     carrier     Neisseria meningitidis     B     930     ST-34 complex	18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
21       6       Germany       1999       carrier       Neisseria meningitidis       NG       198       ST-198 complex       198       Carrier       Neisseria meningitidis       E       60       ST-198 complex       198       Carrier       Neisseria meningitidis       E       60       ST-198 complex       198       Carrier       Neisseria meningitidis       E       60       ST-320 complex/F-5 complex       198       Carrier       Neisseria meningitidis       B       32       ST-320 complex/F-5 complex       198       24       S4355       B227, Z1227       Denmark       1974       invasive (unspecified/other) Neisseria meningitidis       A       5       ST-5 complex       9       F3-1       9       F3-1         25       9       Germany       1999       carrier       Neisseria meningitidis       B       930       ST-334 complex       5       ST-334 complex	19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex/subgroup IV	7	13-1	F1-5
22     7     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex     6       23     8     Germany     1999     carrier     Neisseria meningitidis     B     32     ST-32 complex/ET-5 complex     6       24     S4355     B227, Z1227     Denmark     1974     invasive (unspecified/other)     Neisseria meningitidis     A     5     ST-6 complex/subgroup III     5-1     9     F3-1       25     9     Germany     1999     carrier     Neisseria meningitidis     B     930     ST-334 complex     5	20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
23     8     Germany     1999     carrier     Neisseria meningitidis     B     32     ST-32 complex/ET-5 complex/       24     S4355     B227, Z1227     Denmark     1974     invasive (unspecified/other)     Neisseria meningitidis     A     5     ST-5 complex/subgroup III     5-1     9     F3-1       25     9     Germany     1999     carrier     Neisseria meningitidis     B     930     ST-334 complex	21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
24     \$4355     B227; Z1227     Denmark     1974     invasive (unspecified/other) Neisseria meningitidis     A     5     \$T-5 complex/subgroup III     5-1     9     F3-1       25     9     Germany     1999     carrier     Neisseria meningitidis     B     930     \$T-334 complex     5     \$T-334 complex	22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
25 9 Germany 1999 carrier Neisseria meningitidis B 930 ST-334 complex	23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex			
	24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
Analysis tools:	25	9		Germany	1999	carrier	Neisseria meningitidis	В	930	ST-334 complex			
Breakdown: Fields Two Field Polymorphic sites Combinations Schemes/alleles Publications Sequence bin Tag status Analysis: BURST Codons Presence/Absence Genome Comparator BLAST Export Dataset Contigs Sequences	Brea Ar	kdown: F nalysis: B	ields Two Fi	ns Presence/Al	bsence			Sequence t	oin 🗌	Tag status			

Select the locus that you would like to analyse from the list.

PubliALSTD Breakel Profile/STI List Breakfown: Solate fields   Schemelalleles   Publications Links: Contents   Home   Options   Profiles/Sequences definitions   Database submissions	
	Toggle: i
Polymorphic site analysis	
This tool will analyse the polymorphic sites in the selected locus for the current isolate dataset.	
If more than 50 sequences have been selected, the job will be run by the offline job manager which may take a few minutes (or longer depending on the queue). This is because sequences may have gaps in them and consequently need to be aligned which is a processor- and memory- intensive operation.	
Loci       Options       Action         '165_rDNA       If both allele designations and tagged sequences       Analyse         185_rRNA (SSU rRNA)       Image: State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State	

Click 'Analyse'.

A schematic of the locus is generated showing the polymorphic sites. A full description of this can be found in the *Locus Explorer polymorphic site analysis* section.



# 14.14 Species identification

The species identification tool extracts ribosomal MLST alleles from genomes and determines the species based on the count of alleles that are uniquely found within a single species (or higher taxonomic rank if alleles unique to a species are not found). This is done by making a query to the rMLST genome database.

The tool can be accessed from the front page of an isolate database.

PubMLST Database hom				
+) Log in				
Neisseria PubML	ST database			
	base contains data for a collection of isolates that represent the posited here. Any isolate may be submitted to this database a			
Q Query database	Projects	Option settings		1 Submissions
<ul> <li>Search or browse dat</li> <li>Search by combination</li> </ul>		Set general options - including isola Set display and query options for lo		Manage submissions
			(	General information
				<ul> <li>Isolates: 51,574</li> <li>Last updated: 2019-07-12</li> </ul>
				Defined field values
				Update history
				About BIGSdb
Breakdown	Export	Analysis	Third party tools	
<ul> <li>Single field</li> </ul>	Export dataset	<ul> <li>Codon usage</li> </ul>	<ul> <li>GrapeTree - Visualization or</li> </ul>	
Two field	Contigs	Gene presence	<ul> <li>iTOL - Phylogenetic trees w</li> </ul>	
<ul> <li>Unique combinations</li> <li>Publications</li> </ul>	Sequences - XMFA / concatenated FASTA formats	<ul> <li>Genome comparator</li> <li>BLAST</li> </ul>	<ul> <li>PhyloViz - Visualization and</li> <li>Microreact Open data visu</li> </ul>	phylogenetic inference alization and sharing for genomic epidemiology
Sequence bin		<ul> <li>Species identification</li> </ul>	- meroreaut - Open data visu	anzaton and sharing to genomic epidemiology
	Miscellaneous	<ul> <li>In silico PCR</li> </ul>		
	Description of database fields			
	•			

Alternatively, it can be accessed following a query by clicking the 'rMLST species id' button at the bottom of the results table. Isolates returned from the query will be automatically selected within the species id interface (note that only isolates with a genome assembly will be able to be checked).

Display/sort options Order by: Id ✓ ascending ✓ Display: 25 ✓ records per page 0	MLST pro Clonal complex (ML N. gonorrhoeae cgM OMV peplide typing Cluster (OMV pepli Ribosomal MLST pro Sequence Include oid record Action Reset Submit	ST):	♥ 0 ♥ 0 ♥ 0 ♥ 0 ♥ 0 ₩ 0 ₩ 1 ₩ 1 ₩ 1 ₩ 1 ₩ 1 ₩ 1 ₩ 1 ₩ 1 ₩ 1 ₩ 1	0								
records returned. Click the hyperlinks for detailed information.  Isolate fields ① MLST Finetyping antigens												
			MIST	Eine	typing antig							
	species	capsule group	MLST ST clonal complex									
id isolate aliases country year disease	species ) Neisseria meningitidis		ST clonal complex	PorA_VR1	1 PorA_VR2	FetA_VR						
Id         isolate         allases         country         year         disease           1         A4/M1027         B1; NIBSC_2803; Z1001         USA         1937 invasive (unspecified/other	) Neisseria meningitidis	A	ST clonal complex 4 ST-4 complex	PorA_VR1 5-2	1 PorA_VR2 10	FetA_VR F1-5						
Id         isolate         allases         country         year         disease           1         A4/M1027         B1; NIBSC_2803; Z1001         USA         1937 invasive (unspecified/other	) Neisseria meningitidis Neisseria meningitidis	A A	ST cional complex 4 ST-4 complex	PorA_VR1	1 PorA_VR2	FetA_VR						
Id         Isolate         aliases         country         year         disease           1         A4/M1027         B1; NIBSC_2803; Z1001         USA         1937         invasive (unspecified/other)           2         120M         B35; NIBSC_2822; Z1035         Pakistan         1967         meningitis and septicaemia	<ul> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> </ul>	A A A	ST clonal complex           4         ST-4 complex           1         ST-1 complex	PorA_VR1 5-2 5-2	1 PorA_VR2 10 10	FetA_VR F1-5 F5-1						
Id         Isolate         alliases         country         year         disease           1         A4/M1027         B1; NIBSC_2803; Z1001         USA         1937         invasive (unspecified/other           2         120M         B35; NIBSC_2823; Z1005         Pakistan         1967         menagitis and septicaemii           7         7881         B54; NIBSC_2760; Z1054         Finland         1975         invasive (unspecified/other	<ul> <li>) Neisseria meningitidis</li> <li>a Neisseria meningitidis</li> <li>) Neisseria meningitidis</li> <li>) Neisseria meningitidis</li> </ul>	A A A A	ST         clonal complex           4         ST-4 complex           1         ST-1 complex           5         ST-5 complex	PorA_VR1 5-2 5-2 20	1 PorA_VR2 10 10 9	FetA_VR F1-5 F5-1 F3-1						
Id         Isolate         aliases         country         year         disease           1         A4/M1027         B1; NIBSC_2803; Z1001         USA         1937         invasive (unspecified/other           2         120M         B35; NIBSC_2822; Z1035         Pakistan         1967         meningtits and septicaemia           7         7891         B54; NIBSC_2760; Z1054         Finland         1975         invasive (unspecified/other           0         6748         B73; NIBSC_2784; Z1073         Canada         1971         invasive (unspecified/other	<ul> <li>) Neisseria meningitidis</li> <li>a Neisseria meningitidis</li> <li>) Neisseria meningitidis</li> <li>) Neisseria meningitidis</li> </ul>	A A A A A	ST clonal complex           4         ST-4 complex           1         ST-1 complex           5         ST-5 complex           1         ST-1 complex	PorA_VR1 5-2 5-2 20 18-1	I PorA_VR2 10 10 9 3	FetA_VR F1-5 F5-1 F3-1 F5-1						
Id         Isolate         allasse         country         year         disease           1         A4/M1027         B1; NIBSC_2803, Z1001         USA         1937         Invasive (unspecified/other           2         120M         B35; NIBSC_2822, Z1035         Pakistan         1967         meningitis and septicaemic           7         7891         B54; NIBSC_2760, Z1054         Finland         1975         invasive (unspecified/other           10         6748         B73; NIBSC_2762, Z1035         Canada         1971         invasive (unspecified/other           11         120E         B92; NIBSC_2828, Z1029         Germany         1964         invasive (unspecified/other	<ul> <li>) Neisseria meningitidis</li> <li>a Neisseria meningitidis</li> <li>) Neisseria meningitidis</li> <li>) Neisseria meningitidis</li> <li>) Neisseria meningitidis</li> <li>) Neisseria meningitidis</li> <li>Neisseria meningitidis</li> </ul>	A A A A A A A	ST     clonal complex       4     ST-4 complex       1     ST-1 complex       5     ST-5 complex       1     ST-1 complex       1     ST-1 complex       1     ST-1 complex       1     ST-1 complex	PorA_VR1 5-2 5-2 20 18-1 5-2	I PorA_VR2 10 10 9 3 10	FetA_VR F1-5 F5-1 F3-1 F5-1 F3-6						

Finally, the analysis is also possible directly from an isolate record, if the isolate has a genome assembly associated with it.

		biley KA, Sparling Biol 5:35 576 isola		Feavers IM, Maio	den MC (2007). Species st	atus of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from multilocus sequence							
			A, Parkhill J, Maiden MC (2 nomics 15:1138 108 isolat		-gene population genomic	s platform: de novo assembly, annotation and genealogical analysis of 108 representative Neisseria							
	• Didelot X, Urw	rin R, Maiden MC,	Falush D (2009). Genealo	gical typing of Ne	isseria meningitidis. Micro	biology 155:3176-86 93 isolates							
Z	Sequence bin												
	contigs:	364	N50 contig number:	44	N95 contig number:	180							
	total length:	2,069,108 bp	N50 length (L50):	15,404	N95 length (L95):	2,305							
	max length:	50,093 bp	N90 contig number:	146	loci tagged:	2,182							
	mean length:	5,685 bp	N90 length (L90):	3,907	detailed breakdown:	Display							
	Schemes and lo	ci											
à 🧸	All loci		Navigate and select sche	emes within tree t	o display allele designatio	ns							
	- 🏭 Capsule												
	- 🔊 Genetic Inform	-											
	- 🏭 Genomic island												
	- Ineage Scher	nes											
	🚑 Metabolism 🚑 Pilin												
	🏭 Pilin 🏭 Typing												
	- 🛺 Other schemes												
	- In Loci not in sch												
<u>m</u>	Tools												
	Analysis: rMLST	species id PCR	)										

The tool interface is simply a list of isolate ids to check. This will be pre-populated if accessed following a query or directly from an isolate record. Click 'Submit'.

PubMLST Database home Contents	
40 Log in T	oggle: 🚺
rMLST species identification - Neisseria PubMLST	
This analysis attempts to identify exact matching rMLST alleles within selected isolate sequence record(s). A predicted taxon will be shown where identified alleles have been linke validated genomes in the rMLST database.	d to
Please select the required isolate ids to run the species identification for. These isolate records must include genome sequences.	
IsolatesAction	
1 Submit	
13 19	
Clear List all	

The job will be sent to the job queue.

Results will be displayed in a table as they are generated. The table will display the highest taxonomic rank that can be reliably identified, e.g. species, the taxon and its full taxonomy. An indication of the confidence for the result will also be displayed - this is based on the proportion of alleles found that are unique to a taxon.

u	tput			Prediction from identified rMLST alleles linked to genomes			dentified rSTs
id	isolate	Rank	Taxon	Taxonomy	Support Matches		Species
1	A4/M1027	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2504	Neisseria meningitidis
2	120M	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2532	Neisseria meningitidis
7	7891	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2434	Neisseria meningitidis
10	6748	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2530	Neisseria meningitidis
11	129E	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2528	Neisseria meningitidis
13	139M	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2433	Neisseria meningitidis
19	S3131	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2285	Neisseria meningitidis
ile	s						

Clicking the '+' icon on any row will display further details about the matches.

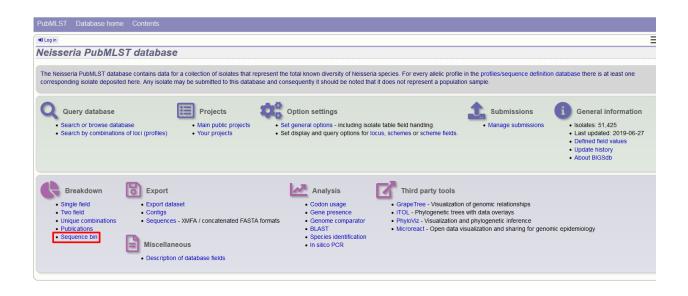
id	isolate					Predi	ction from identified rMLST alleles linked to genomes				Identified rSTs		
	isolate	F	lank	Ta	xon		Taxonomy	Support	Matches	rST	Species		
1	A4/M1027					Proteobacte Neisseria me		100%	0	2504	Neisseria meningitid		
2	120M	SP	ECIES	Neisseria	meningitidis		Proteobacteria > Betaproteobacteria > Nelsseriales > Nelsseriaceae > Nelsseria > 100%						
7	7891	SP	ECIES	Neisseria		Proteobacte Neisseria me	2434 Neisseria meningitid						
10 6748 SPECIES Neisseria meningitidis				Proteobacte Neisseria me	ria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > ningitidis	•	2530	Neisseria meningitio					
53 lo	oci matche	ed (rM	LST use	s 53 in to	otal)								
	Locus	Allele	Length	Contig	Start position	End position	Linked data values						
BAC	CT000001	174	1680	181603	32429	34108	species: Neisseria meningitidis [n=1759]						
BAC	CT000002	9	729	181098	6971	7699	species: Neisseria meningitidis [n=674]						
BAC	CT000003	1	693	181315	13840	14532	species: Neisseria meningitidis [n=1701]						
BAC	CT000003	1	693	181474	5814	6506	species: Neisseria meningitidis [n=1701]						
BAC	CT000004	2	621	181315	5569	6189	species: Neisseria meningitidis [n=7346]; Neisseria sp. [n=1]						
BAC	CT000005	1	519	181315	9345	9863	species: Neisseria meningitidis [n=15997]; Neisseria sp. [n=1]						
BAC	CT000005	1	519	181474	10483	11001	species: Neisseria meningitidis [n=15997]; Neisseria sp. [n=1]						
BAC	CT000006	5	369	181603	53216	53584	species: Neisseria meningitidis [n=1945]; Neisseria sp. [n=1]						
BAC	CT000007	1	471	181145	2253	2723	species: Neisseria meningitidis [n=13786]; Neisseria sp. [n=1]						
BAC	CT000007	1	471	181374	2271	2741	species: Neisseria meningitidis [n=13786]; Neisseria sp. [n=1]						
BAC	CT000008	2	393	181315	10796	11188	species: Neisseria meningitidis [n=6991]						
BAC	CT000009	1	393	181193	16935	17327	species: Neisseria meningitidis [n=2942]						
BAC	CT000009	1	393	181591	20941	21333	species: Neisseria meningitidis [n=2942]						
BAC	CT000010	1	312	181315	19833	20144	0144 species: Neisseria meningitidis [n=898]						
BAC	CT000010	1	312	181474	202	513	species: Neisseria meningitidis [n=898]						
BAC	CT000011	2	396	181315	6209	6604	species: Neisseria gonorrhoeae [n=9494]; Neisseria meningitidis [n=6718]; N	leisseria sp	[n=1]				

**Note:** Ribosomal MLST was first described in Jolley et al. 2012. Ribosomal multilocus sequence typing: universal characterization of bacteria from domain to strain. *Microbiology* 158:1005-15

# 14.15 Sequence bin breakdown

The sequence bin breakdown plugin calculates statistics based on the number and length of contigs in the sequence bin as well as the number of loci tagged for an isolate record.

The function can be selected by clicking the 'Sequence bin' link on the Breakdown section of the main contents page.



Alternatively, it can be accessed following a query by clicking the 'Sequence bin' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

	120M	B35; NIBSC_2822; Z1035	Pakistan	1967 meningiti	s and septicaemia	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
3 N	100242905		UK	2000 invasive	unspecified/other)	Neisseria meningitidis	В	1099		19	15	
4	M1027	B43; NIBSC_3076; Z1043	USA	1937 invasive	unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex			
5 N	100240227		UK	2000 invasive	unspecified/other)	Neisseria meningitidis	В	1100	ST-32 complex	7	16	
6 N	100282207		UK	2000 invasive	unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; NIBSC_2760; Z1054	Finland	1975 invasive	unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	20	9	F3-1
8 N	100242007		UK	2000 invasive	unspecified/other)	Neisseria meningitidis	В	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984 invasive	unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; NIBSC_2784; Z1073	Canada	1971 invasive	unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	18-1	3	F5-1
11	129E	B92; NIBSC_2828; Z1092	Germany	1964 invasive	unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F3-6
12	0090/89		Czech Republic	1989 invasive	unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex	7	16	
13	139M	B99; NIBSC_2795; Z1099	Philippines	1968		Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
14	0120/95		Czech Republic	1995 invasive	unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19	S3131	B213; NIBSC_2813; Z1213	Ghana	1973 invasive	unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex			
24	S4355	B227; NIBSC_2806; Z1227	Denmark	1974 invasive	unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	В	930	ST-334 complex			

Select the isolate records to analyse - these will be pre-selected if you accessed the plugin following a query. You can also select loci and/or schemes which will be used to calculate the totals and percentages of loci designated and tagged. This may be useful as a guide to assembly quality if you use a scheme of core loci where a good assembly would be expected to include all member loci. To determine the total of all loci designated or tagged, click 'All loci' in the scheme tree.

There is also an option to determine the mean G+C content and various assembly stats of the sequence bin of each isolate. Note that selecting these will make the analysis run much slower since each contig needs to be examined.

Click submit.

PubMLST Database	home Contents			
+D Log in				Help 🔀
Breakdown of	sequence bin contig p	properties		
Please select the requir	ed isolate ids for comparison - use Ctrl o	r Shift to make multiple selections. Select loci/schemes	to use for calculating percentage of alleles designated or tagged.	
Isolates	Loci	Schemes	Options	
93 ^	'16S_rDNA	All loci	Contig analysis (min, max, N50 etc.)	
94	16S_rRNA (SSU_rRNA)	- Capsule	Calculate %GC	
95 96 97	23S_rRNA abcZ		Filter by	
97 98	abcZ (NEIS1015)		Sequence method:	
98 99 ¥ 100 .:	aceF (NEIS1279) ackA2 (NEIS1727)	— 😪 🎧 Lineage Schemes	Project:	
100	acnA (NEIS1729)	🗸 🖂 🔛 Metabolism	Experiment:	
Clear List all	All None Paste list	👻 🎣 N. gonorrhoeae AMR	Action	
		< >		
			Reset Submit	

If there are fewer than 100 isolates selected, the table will be generated immediately. Otherwise it will be submitted to the job queue.

A table of sequence bin stats will be generated.

PubMLST	Database	nome C	ontents								
+) Log in										Help 🛛	Ξ
				use Ctrl or Shift to	o make multiple selections. S	elect loci/scheme	s to use for calculat	ing percentage of allel	es designated or tagged.		
Isolates	s	Loci		Schemes		Options					
1 2 3 4 5 6 7 8 Clear	1         ^           2         '16S_rRNA (SSU_rRNA)           3         23S_rRNA           4         abcZ           5         abcZ (NEIS1015)           6         aceF (NEIS1279)           8		Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Image: Construction     Image: Construction       Imag								
Loci selecte		<b>•</b> • • • • •									
Isolate id	Isolate + A4/M1027	contigs ¢ 364	Total length \$ / 2069108	Alleles designate 2077	d ¢ % Alleles designated 68.1	Loci tagged + 2182	% Loci tagged ≑ 71.5	Sequence bin ¢ Display →			
2	120M	359	2059108	2067	67.8	2182	71.7	Display →			
7	7891	199	2057385	2165	71.0	2213	72.6	Display →			
10	6748	652	4241338	2164	71.0	2193	71.9	Display →			

You can choose to export the data in tab-delimited text or Excel formats by clicking the appropriate link at the bottom of the table.

67	20011	194	2084213	2139	70.1	2198	72.1	Uisplay →		
82	11-004	258	2055227	2134	70.0	2210	72.5	Display →		
84	IAL2229	188	2051679	2154	70.6	2212	72.5	Display →		
90	CN100	236	2118544	2175	71.3	2244	73.6	Display →		
Click on the following charts to enlarge										
Number o	Number of contigs Total length									
Overall mea	n: 254.3; σ: 12									
Overall mean: 254.3; 0: 123.7         Overall mean: 2188922.1; 0: 497829.9           Image: State of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of the state of th										

Sequence bin records can also be accessed by clicking the 'Display' button for each row of the table.

Clear (		acnA (NEIS	1729) All None Pa	v stelst (		sule Region / sule Region /	Experi Action Reset Sub	
solate id 🕯	+ Isolate +	Contigs ¢	Total length 🗧	Alleles designated +	% Alleles designated a	Loci tagged 🗢	% Loci tagged 🗢	Sequence bin ¢
1	A4/M1027	364	2069108	2077	68.1	2182	71.5	Display →
2	120M	359	2059411	2067	67.8	2186	71.7	Display →
7	7891	199	2057385	2165	71.0	2213	72.6	Display →
10	6748	652	4241338	2164	71.0	2193	71.9	Display →
11	129E	272	2072690	2111	69.2	2180	71.5	Display →
13	139M	293	2141711	2139	70.1	2196	72.0	Display →
19	S3131	173	2061338	2141	70.2	2190	71.8	Display →
24	S4355	198	2071992	2154	70.6	2202	72.2	Display →
30	14	1	2145295	2077	68.1	2062	67.6	Display →
31	10	275	2059146	2122	69.6	2191	71.8	Display →
34	20	213	2067373	2132	69.9	2186	71.7	Display →

## 14.16 Two field breakdown

The two field breakdown plugin displays a table breaking down one field against another, e.g. breakdown of serogroup by year.

The analysis can be selected for the whole database by clicking the 'Two field breakdown' link on the main contents page.

Query:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/sequences definitions									
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does									
<ul> <li>Query database</li> <li>Search database - advanced queries.</li> <li>Browse database - peruse all records.</li> <li>Search by combinations of loci (profiles) - including partial matching.</li> <li>List query - find isolates by matching a field to an entered list.</li> <li>Projects - main projects defined in database.</li> </ul>	Submissions • Manage submissions General information • Isolates: 34221 • Last updated: 2015-07-02 • Update history • About BIGSdb								
Breakdown       Export       Analysis       Miscellaneou         • Sincle field       • Export dataset       • Contigs       • Contigs       • Contigs         • Unique combinations       • Scheme and alleles       • Sequences - XMFA / concatenated FASTA formats       • Codon usage       • Description of         • Publications       • Sequence bin       • Sequence and alleles       • Description of       • Description of	us If database fields								

Alternatively, a two field breakdown can be displayed of the dataset returned from a query by clicking the 'Two field' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

6	M00282207		UK	2000				1101	S1-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A A	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	B	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A I	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A I	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	в	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	X	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	в	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W I	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	в	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	в	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	A I	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			
Analysis tools: Breakdown: Field Codons Polymorphicsites Combinations Schemes/alleles Publications Sequence bin Tag status Analysis: BURST Presence/Absence Genome Comparator BLAST Export: Dataset Contigs Sequences												

Select the two fields you wish to breakdown and how you would like the values displayed (percentage/absolute values and totaling options).

ProDATIST Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions									
Two field breakdown of dataset Show options									
Here you can create a table breaking down one field by another, e.g. breakdown Select fields Field 1: clonal complex (MLST) Field 2: serogroup Field 2: serogroup Field 2: serogroup Field 3: serogroup Fie	Calculate percentages by - Action @ dataset Reset Submit								

Click submit. The breakdown will be displayed as a table. Bar charts will also be displayed provided the number of returned values for both fields are fewer than 30.

Links: Con	wn						_		
Breakdown of clonal_co		1 0	f da	_					
Breakdown of clonal_co				itas	set				
_	nple								
_	nnle								
Selected options: Display value	inpre	∍x (N	NLST	) by	sero	grou	p:		
	s onl	ly.							
Reverse Values and	nerr	centa	nes						
	pere	Jointa	geo						
						ogroup			
clonal_complex (MLST) \$	4 ÷ 1	в <del>÷</del> 3	C 🗧 1	E 🗧 I 1	NG ≑ 4	vv ≑	X ≑ 1	Y ≑ Z	
	13	3		-	4				13
ST-11 complex/ET-37 complex			16						16
ST-162 complex		5							5
ST-167 complex					1			2	3
ST-174 complex				1	1	1			3
ST-178 complex ST-18 complex		3			1				3
ST-198 complex		5			2				2
ST-22 complex						2			2
ST-226 complex		1							1
ST-23 complex/Cluster A3								1	1
ST-254 complex					1				1
ST-269 complex		2			1				3
ST-32 complex/ET-5 complex ST-334 complex		6 1							6
ST-35 complex		-			1				1
ST-4 complex/subgroup IV	8				1				8
ST-41/44 complex/Lineage 3		5			1				6
ST-461 complex		1							1
ST-5 complex/subgroup III	6								6
ST-53 complex					2				2
ST-60 complex Total	28	27	17	1	15	2	1	2	1 1 98
Total	20	21	11/	•	10	3		3	90

The table values can be exported in a format suitable for copying in to a spreadsheet by clicking 'Download as tabdelimited text' underneath the table.

**Note:** The job will be submitted to the offline job queue if the query returns 10,000 or more isolates. In this case, the buttons to reverse the axes or to change whether values or percentages are shown will not be available.

## 14.17 Unique combinations

The Unique Combinations plugin calculates the frequencies of unique file combinations within an isolate dataset. Provenance fields, composite fields, allele designations and scheme fields can be combined.

The function can be selected by clicking the 'Unique combinations' link in the Breakdown section of the main contents page. This will run the analysis on the entire database.

PubMLST Database hom	e Contents				
+D Log in					=
Neisseria PubML	ST database				
			ent the total known diversity of Neisseria plate may be submitted to this database a		
Q Query database	[	Projects	Option settings		1 Submissions
<ul> <li>Search or browse data</li> <li>Search by combination</li> </ul>		<ul> <li>Main public projects</li> <li>Your projects</li> </ul>	<ul> <li>Set general options - including isolat</li> <li>Set display and query options for loc</li> </ul>	0	Manage     submissions
General informati	on				
• Isolates: 51,359					
<ul> <li>Last updated: 2019-06</li> <li>Defined field values</li> </ul>	5-19				
Update history					
About BIGSdb					
Breakdown	Export		Analysis	Third party tools	
<ul> <li>Single field</li> </ul>	<ul> <li>Export datase</li> </ul>	et	Codon usage	<ul> <li>GrapeTree - Visualization of</li> </ul>	
Two field	<ul> <li>Contigs</li> </ul>		<ul> <li>Gene presence</li> </ul>	<ul> <li>iTOL - Phylogenetic trees w</li> </ul>	
Unique combinations	<ul> <li>Sequences -</li> </ul>	XMFA / concatenated FASTA forr		PhyloViz - Visualization and	
Publications	_		BLAST	<ul> <li>Microreact - Open data visu</li> </ul>	alization and sharing for
<ul> <li>Sequence bin</li> </ul>	Miscellaned		<ul> <li>Species identification</li> <li>In silico PCR</li> </ul>	genomic epidemiology	
			• IT SILCO FOR		
	<ul> <li>Description or</li> </ul>	f database fields			

Alternatively, it can be accessed following a query by clicking the 'Combinations' button in the Breakdown list at the bottom of the results table. This will run the analysis on the dataset returned from the query. Please note that the list of functions here may vary depending on the setup of the database.

	M00240227		UK	0000	invasive (unspecified/other)	Materia and	a la alti di a		4400	ST-32 complex/ET-5 complex	7	40	
								B			1	16	
6	M00282207	DC 4: 74054	UK		invasive (unspecified/other)			w	1101	ST-22 complex	00	0	50.4
1	7891	B54; Z1054	Finland		invasive (unspecified/other)			A	5	ST-5 complex/subgroup III	20	9	F3-1
	M00242007		UK		invasive (unspecified/other)			В	1102	ST-18 complex		14	
9	0021/84				invasive (unspecified/other)			W	114	ST-22 complex			
10	6748	B73; Z1073	Canada		invasive (unspecified/other)			A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany		invasive (unspecified/other)			A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89				invasive (unspecified/other)			В		ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria me		A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95				invasive (unspecified/other)		-	Х	117			14	
15	1		Germany	1999	carrier	Neisseria me		E	864				
16	2		Germany	1999	carrier	Neisseria me		В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria me	ningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria me		В	19	ST-18 complex			
19		B213; Z1213	Ghana		invasive (unspecified/other)			Α	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria me	ningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria me	ningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria me	ningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria me	ningitidis	В	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria me	ningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria me	ningitidis	в	930	ST-334 complex			
	25     9     Germany     1999     carrier     Neisseria meningitidis     B     930     ST-334 complex       nalysis tools:     reakdown:     Fields     Two Field     Polymorphicistles     Combinations     Schemes/alleles     Publications     Sequence bin     Tag status												
Brea	akdown.		Analysis: BURST Codons Presence/Absence Genome Comparator BLAST										
			ons Presence/Al	bsence	Genome Comparator BL	AST							
	nalysis: B			_	Genome Comparator BL	AST							

Select the combination of fields to analyse, e.g. serogroup and finetyping antigens.

PubMLST Database home Contents	
HD Log in	Help 🛃 🛛 Toggle: 🜖 📃
Frequencies of field combinations	
Here you can determine the frequencies of unique field combinations in the dataset. Please so one or more schemes to include all loci (and/or fields) from a scheme.	ite fields 0 Loci
Schemes All None All None Action	All None
Pilin Submit	
← ■ 🛺 Typing	
<ul> <li>MLST</li> <li>Finetyping antigens</li> <li>16S</li> <li>Antigen genes</li> </ul>	
⊡Include all fields from selected schemes ⊡Include all loci from selected schemes	

Click submit. The job will be submitted to the job queue. Once analysis has completed, you will be able to download the results in tab-delimited text or Excel formats.

PubMLST Database home Contents	
+D Log in	Ξ
Job status viewer	
Status	
Job id: BIGSdb_091597_1560952265_74679	
Submit time: 2019-06-19 14:51:05	
Status: finished	
Start time: 2019-06-19 14:51:22	
Progress: 100%	
Stop time: 2019-06-19 14:51:33	
Total time: 11 seconds	
Output         Number of unique combinations: 650         The percentages may add up to more than 100% if you have selected loci or scheme fields with multiple values for an isolate.         Files         Combinations table (text)         Image: Combinations table (text)	
Please note that job results will remain on the server for 7 days.	

# CHAPTER 15

# Data export plugins

# 15.1 Contig export

The contig export plugin can be accessed by clicking the 'Contigs' link in the Export section of the contents page of isolate databases.

Query: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions									
Neisseria PubMLST database									
	ent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition e submitted to this database and consequently it should be noted that it does not represent a population								
Query database       Image: Constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of the constraint of th	Option settings       Submissions         • Set general options - including isolate table field handling.       • Manage submissions         • Set display and query options for locus, schemes or scheme fields.       • Manage submissions         • General information       • Isolates: 34218         • Last updated: 2015-06-30       • Update history         • About BIGSdb       • Manage submissions								
Breakdown     Single field     Two field     Unique combinations     Scheme and alleles     Publications     Sequence bin	ormats Analysis - Codon usage - Presence/absence status of loci - Genome comparator - BLAST - Miscellaneous - Description of database fields								

Alternatively, it can be accessed following a query by clicking the 'Contigs' button in the Export section at the bottom of the results table.

282207 891 B54; Z10 242007 21/84 748 B73; Z10 29 B92: Z10	UK Czech Republic	1975 2000	invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)		meningitidis	w					
242007 21/84 748 B73; Z10	UK Czech Republic	2000		Neisseria		**	1101	ST-22 complex			
21/84 748 B73; Z10	Czech Republic		invasive (unspecified/other)		meningitidis	A	5	ST-5 complex/subgroup III	20	9	F3-1
748 B73; Z10		109/	intradire (andpeenrearourer)	Neisseria	meningitidis	В	1102	ST-18 complex		14	
	73 Conodo	1304	invasive (unspecified/other)	Neisseria	meningitidis	W	114	ST-22 complex			
DO DO: 710	o o o o o o o o o o o o o o o o o o o	1971	invasive (unspecified/other)	Neisseria	meningitidis	A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
29 092,210	92 Germany	1964	invasive (unspecified/other)	Neisseria	meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
90/89	Czech Republic	1989	invasive (unspecified/other)	Neisseria	meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
39M B99; Z10	99 Philippines	1968		Neisseria	meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
20/95	Czech Republic	1995	invasive (unspecified/other)	Neisseria	meningitidis	Х	117			14	
1	Germany	1999	carrier	Neisseria	meningitidis	E	864				
2	Germany	1999	carrier	Neisseria	meningitidis	В	854	ST-18 complex			
3	Germany	1999	carrier	Neisseria	meningitidis	W	174	ST-174 complex			
4	Germany	1999	carrier	Neisseria	meningitidis	В	19	ST-18 complex			
8131 B213; Z1	13 Ghana	1973	invasive (unspecified/other)	Neisseria	meningitidis	Α	4	ST-4 complex/subgroup IV	7	13-1	F1-5
5	Germany	1999	carrier	Neisseria	meningitidis	NG	198	ST-198 complex			
6	Germany	1999	carrier	Neisseria	meningitidis	NG	198	ST-198 complex			
7	Germany	1999	carrier	Neisseria	meningitidis	E	60	ST-60 complex			
8	Germany	1999	carrier	Neisseria	meningitidis	В	32	ST-32 complex/ET-5 complex			
4355 B227; Z1	27 Denmark	1974	invasive (unspecified/other)	Neisseria	meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
9	Germany	1999	carrier	Neisseria	meningitidis	В	930	ST-334 complex			
	99M B99; Z109 0795 2 3 4 4 5 5 6 7 7 8 355 B227; Z12 9	99 B99, 21099 Philippines OP5 Czech Republic Czech Republic Germany Cermany Germany B213, 21213 Ghana Germany Germany Germany Germany Second Cermany Germany Denmark	99M         B99; Z1099         Philippines         1988           0/95         Czech Republic 1995           1         Germany         1999           2         Germany         1999           3         Germany         1999           11         B213; Z1213         Ghana         1973           5         Germany         1999         131         B213; Z1213         Ghana         1973           5         Germany         1999         Germany         1999         1999         1999         36         Germany         1999         1999         37         Germany         1999         38         Germany         1999         38         Germany         1999         36         B227; Z1227         Denmark         1974	99M         B99; Z1099         Philippines         1968           0/95         Czech Republic         1995         invasive (unspecified/other)           1         Germany         1999         carrier           2         Germany         1999         carrier           3         Germany         1999         carrier           11         B213; Z1213         Ghana         1973         invasive (unspecified/other)           5         Germany         1999         carrier           6         Germany         1999         carrier           7         Germany         1999         carrier           8         Germany         1999         carrier           35         B227; Z1227         Denmark         1974         invasive (unspecified/other)	99M         B99; Z1099         Philippines         1968         Neisseria           0/95         Czech Republic         1995         invasive (unspecified/other)         Neisseria           1         Germany         1999         carrier         Neisseria           2         Germany         1999         carrier         Neisseria           3         Germany         1999         carrier         Neisseria           11         B213; Z1213         Ghana         1973         invasive (unspecified/other)         Neisseria           5         Germany         1999         carrier         Neisseria           5         Germany         1999         carrier         Neisseria           6         Germany         1999         carrier         Neisseria           7         Germany         1999         carrier         Neisseria           8         Germany         1999         carrier         Neisseria           355         B227; Z1227         Denmark         1974         invasive (unspecified/other)         Neisseria	99M         B99; Z1099         Philippines         1988         Neisseria meningitidis           0/95         Czech Republic         1995         invasive (unspecified/other)         Neisseria meningitidis           1         Germany         1999         carrier         Neisseria meningitidis           2         Germany         1999         carrier         Neisseria meningitidis           3         Germany         1999         carrier         Neisseria meningitidis           3         Germany         1999         carrier         Neisseria meningitidis           11         B213; Z1213         Ghana         1973         invasive (unspecified/other)         Neisseria meningitidis           12         Germany         1999         carrier         Neisseria meningitidis           131         B213; Z1213         Ghana         1973         invasive (unspecified/other)         Neisseria meningitidis           134         Germany         1999         carrier         Neisseria meningitidis           135         Germany         1999         carrier         Neisseria meningitidis           135         Germany         1999         carrier         Neisseria meningitidis           136         Germany         1999         carrier </td <td>B99; Z1099         Philippines         1968         Neisseria meningittidis         A           0/95         Czech Republic         1995         invasive (unspecified/other)         Neisseria meningittidis         X           1         Germany         1999         carrier         Neisseria meningittidis         E           2         Germany         1999         carrier         Neisseria meningittidis         B           3         Germany         1999         carrier         Neisseria meningittidis         B           3         Germany         1999         carrier         Neisseria meningittidis         B           131         B213; Z1213         Ghana         1973         invasive (unspecified/other)         Neisseria meningittidis         A           6         Germany         1999         carrier         Neisseria meningittidis         NG           6         Germany         1999         carrier         Neisseria meningittidis         NG           7         Germany         1999         carrier         Neisseria meningittidis         B           8         Germany         1999         carrier         Neisseria meningittidis         B           355         B227; Z1227         Denmark         1974<td>B99; Z1099         Philippines         1968         Neisseria meningitidis         A         1           0/95         Czech Republic         1995         invasive (unspecified/other)         Neisseria meningitidis         X         117           1         Germany         1999         carrier         Neisseria meningitidis         B         864           2         Germany         1999         carrier         Neisseria meningitidis         B         864           3         Germany         1999         carrier         Neisseria meningitidis         B         854           3         Germany         1999         carrier         Neisseria meningitidis         B         174           4         Germany         1999         carrier         Neisseria meningitidis         A         4           131         B213; Z1213         Ghana         1973         invasive (unspecified/other)         Neisseria meningitidis         NG         198           6         Germany         1999         carrier         Neisseria meningitidis         NG         198           7         Germany         1999         carrier         Neisseria meningitidis         E         30           8         Germany         1999</td><td>B99; Z1099     Philippines     1968     Neisseria meningitidis     A     1       Cyp5     Czech Republic     1995 invasive (unspecified/other)     Neisseria meningitidis     X     117       1     Germany     1999     carrier     Neisseria meningitidis     E     864       2     Germany     1999     carrier     Neisseria meningitidis     B     854       3     Germany     1999     carrier     Neisseria meningitidis     B     854       3     Germany     1999     carrier     Neisseria meningitidis     B     174       3     Germany     1999     carrier     Neisseria meningitidis     B     19     ST-18 complex       4     Germany     1999     carrier     Neisseria meningitidis     B     19     ST-18 complex       5     Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex       6     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       7     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       8     Germany     1999     carrier     Neisseria meningitidis     B     32     ST-32 co</td><td>99M     B99; Z1099     Philippines     1958     Neisseria meningitidis     A     1     ST-1 complex/subgroup/I/I     5-2       0/95     Czech Republic     1995 invasive (unspecified/other)     Neisseria meningitidis     X     117     117       1     Germany     1999     carrier     Neisseria meningitidis     E     864       2     Germany     1999     carrier     Neisseria meningitidis     B     854       3     Germany     1999     carrier     Neisseria meningitidis     B     117       4     Germany     1999     carrier     Neisseria meningitidis     B     118     117       131     B213; Z1213     Ghana     1973     invasive (unspecified/other)     Neisseria meningitidis     A     4     5T-18 complex       6     Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex       7     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       8     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-18 complex       8     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       <t< td=""><td>B99; Z1099       Philippines       1958       Neisseria meningitidis       A       1       ST-1 complex/subgroup/I/I       5-2       10         0/95       Czech Republic       1995 invasive (unspecified/other)       Neisseria meningitidis       X       117       14       14         1       Germany       1999       carrier       Neisseria meningitidis       E       864       5       117       14         2       Germany       1999       carrier       Neisseria meningitidis       B       854       ST-18 complex       14         3       Germany       1999       carrier       Neisseria meningitidis       B       19       ST-174 complex       14         4       Germany       1999       carrier       Neisseria meningitidis       B       19       ST-18 complex       14         131       B213; Z1213       Ghana       1973       invasive (unspecified/other)       Neisseria meningitidis       NG       198       ST-18 complex       17       13-1         56       Germany       1999       carrier       Neisseria meningitidis       NG       198       ST-198 complex       18       19       18       19       199       13-1       19       13-1       19       <td< td=""></td<></td></t<></td></td>	B99; Z1099         Philippines         1968         Neisseria meningittidis         A           0/95         Czech Republic         1995         invasive (unspecified/other)         Neisseria meningittidis         X           1         Germany         1999         carrier         Neisseria meningittidis         E           2         Germany         1999         carrier         Neisseria meningittidis         B           3         Germany         1999         carrier         Neisseria meningittidis         B           3         Germany         1999         carrier         Neisseria meningittidis         B           131         B213; Z1213         Ghana         1973         invasive (unspecified/other)         Neisseria meningittidis         A           6         Germany         1999         carrier         Neisseria meningittidis         NG           6         Germany         1999         carrier         Neisseria meningittidis         NG           7         Germany         1999         carrier         Neisseria meningittidis         B           8         Germany         1999         carrier         Neisseria meningittidis         B           355         B227; Z1227         Denmark         1974 <td>B99; Z1099         Philippines         1968         Neisseria meningitidis         A         1           0/95         Czech Republic         1995         invasive (unspecified/other)         Neisseria meningitidis         X         117           1         Germany         1999         carrier         Neisseria meningitidis         B         864           2         Germany         1999         carrier         Neisseria meningitidis         B         864           3         Germany         1999         carrier         Neisseria meningitidis         B         854           3         Germany         1999         carrier         Neisseria meningitidis         B         174           4         Germany         1999         carrier         Neisseria meningitidis         A         4           131         B213; Z1213         Ghana         1973         invasive (unspecified/other)         Neisseria meningitidis         NG         198           6         Germany         1999         carrier         Neisseria meningitidis         NG         198           7         Germany         1999         carrier         Neisseria meningitidis         E         30           8         Germany         1999</td> <td>B99; Z1099     Philippines     1968     Neisseria meningitidis     A     1       Cyp5     Czech Republic     1995 invasive (unspecified/other)     Neisseria meningitidis     X     117       1     Germany     1999     carrier     Neisseria meningitidis     E     864       2     Germany     1999     carrier     Neisseria meningitidis     B     854       3     Germany     1999     carrier     Neisseria meningitidis     B     854       3     Germany     1999     carrier     Neisseria meningitidis     B     174       3     Germany     1999     carrier     Neisseria meningitidis     B     19     ST-18 complex       4     Germany     1999     carrier     Neisseria meningitidis     B     19     ST-18 complex       5     Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex       6     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       7     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       8     Germany     1999     carrier     Neisseria meningitidis     B     32     ST-32 co</td> <td>99M     B99; Z1099     Philippines     1958     Neisseria meningitidis     A     1     ST-1 complex/subgroup/I/I     5-2       0/95     Czech Republic     1995 invasive (unspecified/other)     Neisseria meningitidis     X     117     117       1     Germany     1999     carrier     Neisseria meningitidis     E     864       2     Germany     1999     carrier     Neisseria meningitidis     B     854       3     Germany     1999     carrier     Neisseria meningitidis     B     117       4     Germany     1999     carrier     Neisseria meningitidis     B     118     117       131     B213; Z1213     Ghana     1973     invasive (unspecified/other)     Neisseria meningitidis     A     4     5T-18 complex       6     Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex       7     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       8     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-18 complex       8     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       <t< td=""><td>B99; Z1099       Philippines       1958       Neisseria meningitidis       A       1       ST-1 complex/subgroup/I/I       5-2       10         0/95       Czech Republic       1995 invasive (unspecified/other)       Neisseria meningitidis       X       117       14       14         1       Germany       1999       carrier       Neisseria meningitidis       E       864       5       117       14         2       Germany       1999       carrier       Neisseria meningitidis       B       854       ST-18 complex       14         3       Germany       1999       carrier       Neisseria meningitidis       B       19       ST-174 complex       14         4       Germany       1999       carrier       Neisseria meningitidis       B       19       ST-18 complex       14         131       B213; Z1213       Ghana       1973       invasive (unspecified/other)       Neisseria meningitidis       NG       198       ST-18 complex       17       13-1         56       Germany       1999       carrier       Neisseria meningitidis       NG       198       ST-198 complex       18       19       18       19       199       13-1       19       13-1       19       <td< td=""></td<></td></t<></td>	B99; Z1099         Philippines         1968         Neisseria meningitidis         A         1           0/95         Czech Republic         1995         invasive (unspecified/other)         Neisseria meningitidis         X         117           1         Germany         1999         carrier         Neisseria meningitidis         B         864           2         Germany         1999         carrier         Neisseria meningitidis         B         864           3         Germany         1999         carrier         Neisseria meningitidis         B         854           3         Germany         1999         carrier         Neisseria meningitidis         B         174           4         Germany         1999         carrier         Neisseria meningitidis         A         4           131         B213; Z1213         Ghana         1973         invasive (unspecified/other)         Neisseria meningitidis         NG         198           6         Germany         1999         carrier         Neisseria meningitidis         NG         198           7         Germany         1999         carrier         Neisseria meningitidis         E         30           8         Germany         1999	B99; Z1099     Philippines     1968     Neisseria meningitidis     A     1       Cyp5     Czech Republic     1995 invasive (unspecified/other)     Neisseria meningitidis     X     117       1     Germany     1999     carrier     Neisseria meningitidis     E     864       2     Germany     1999     carrier     Neisseria meningitidis     B     854       3     Germany     1999     carrier     Neisseria meningitidis     B     854       3     Germany     1999     carrier     Neisseria meningitidis     B     174       3     Germany     1999     carrier     Neisseria meningitidis     B     19     ST-18 complex       4     Germany     1999     carrier     Neisseria meningitidis     B     19     ST-18 complex       5     Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex       6     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       7     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       8     Germany     1999     carrier     Neisseria meningitidis     B     32     ST-32 co	99M     B99; Z1099     Philippines     1958     Neisseria meningitidis     A     1     ST-1 complex/subgroup/I/I     5-2       0/95     Czech Republic     1995 invasive (unspecified/other)     Neisseria meningitidis     X     117     117       1     Germany     1999     carrier     Neisseria meningitidis     E     864       2     Germany     1999     carrier     Neisseria meningitidis     B     854       3     Germany     1999     carrier     Neisseria meningitidis     B     117       4     Germany     1999     carrier     Neisseria meningitidis     B     118     117       131     B213; Z1213     Ghana     1973     invasive (unspecified/other)     Neisseria meningitidis     A     4     5T-18 complex       6     Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex       7     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       8     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-18 complex       8     Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex <t< td=""><td>B99; Z1099       Philippines       1958       Neisseria meningitidis       A       1       ST-1 complex/subgroup/I/I       5-2       10         0/95       Czech Republic       1995 invasive (unspecified/other)       Neisseria meningitidis       X       117       14       14         1       Germany       1999       carrier       Neisseria meningitidis       E       864       5       117       14         2       Germany       1999       carrier       Neisseria meningitidis       B       854       ST-18 complex       14         3       Germany       1999       carrier       Neisseria meningitidis       B       19       ST-174 complex       14         4       Germany       1999       carrier       Neisseria meningitidis       B       19       ST-18 complex       14         131       B213; Z1213       Ghana       1973       invasive (unspecified/other)       Neisseria meningitidis       NG       198       ST-18 complex       17       13-1         56       Germany       1999       carrier       Neisseria meningitidis       NG       198       ST-198 complex       18       19       18       19       199       13-1       19       13-1       19       <td< td=""></td<></td></t<>	B99; Z1099       Philippines       1958       Neisseria meningitidis       A       1       ST-1 complex/subgroup/I/I       5-2       10         0/95       Czech Republic       1995 invasive (unspecified/other)       Neisseria meningitidis       X       117       14       14         1       Germany       1999       carrier       Neisseria meningitidis       E       864       5       117       14         2       Germany       1999       carrier       Neisseria meningitidis       B       854       ST-18 complex       14         3       Germany       1999       carrier       Neisseria meningitidis       B       19       ST-174 complex       14         4       Germany       1999       carrier       Neisseria meningitidis       B       19       ST-18 complex       14         131       B213; Z1213       Ghana       1973       invasive (unspecified/other)       Neisseria meningitidis       NG       198       ST-18 complex       17       13-1         56       Germany       1999       carrier       Neisseria meningitidis       NG       198       ST-198 complex       18       19       18       19       199       13-1       19       13-1       19 <td< td=""></td<>

Select the isolates for which you wish to export contig data for. If the export function was accessed following a query, isolates returned in the query will be pre-selected.

	Profile/ST   List   Scheme/alleles   Publications Options   Profiles/sequences definitions			
			Help 🗗	Toggle: 🚯
Contig analysis and expo	rt			
	ich contigs are associated - use Ctrl or Shift to make multiple gged within the contig - if these loci overlap then the total tagg			
Isolates	Options	Filter by		
1) A4/M1027 2) 120M	Identify contigs with >= 0 • % of sequence untagged FASTA header line: original designation • 0	Sequence method: Project:	<b>•</b> 0	<b>-</b> 0
7) 7891 10) 6748		Experiment:	<b>•</b> 0	
11) 129E 13) 139M		Minimum length:	• 0	
19) S3131 24) S4355	- Action			
All None	Reset Submit			

At its simplest, press submit.

A table will be produced with download links. Clicking these will produce the contigs in FASTA format.

	d the length	of the co	ntig.						
-Is	olates —				Options		— — Filter by —		
	4/M1027			*	Identify contigs with >	>= 0 👻 % of sequence untagged	Sequence method:	<b>•</b> 0	
	20M /891				FASTA header line:	original designation 👻 🜖	Project:		- (
	6748						Experiment:	<b>v</b> 0	
	129E						Minimum length:	<b>•</b> 0	
	139M S3131				Action				
	S4355			-					
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			<u> </u>						
nt	igs with :	>=0% se	quence le	ength	untagged				
			matching	contig	non-matching cor	ntigs			
	isolate 🗢	contigs <del>=</del>	count 🗢 🛛	downloa	d count 🔶 downi	load			
	A4/M1027	364	364	*	0				
2	120M	359	359	*	0				
	7891	199	199	*	0				
)	6748	652	652	*	0				

You can also download all the data in a tar file by clicking the 'Batch download' link.

-Isolates				Or	ptions		-Filter by-	- Filter by				
) A4	4/M1027			Ider	ntify contigs with >= 0	<ul> <li>% of sequence untagged</li> </ul>	Sequence method:	- O				
) 12	20M				STA header line: original		Project:		<b>.</b>			
	891 6748					,	Experiment:	<b>•</b> 0				
1) 1	129E						Minimum length:	- 0				
	139M S3131											
	83131 84355			- Ac	ction							
	_			RE	eset Submit							
	A	I None	)	RE	Submit							
	A	I None	)	Re	Submit							
	A	None None	)	Re	submit							
nti			) uence len									
nti			uence len	ngth unta	agged							
		=0% seq	uence len matching c	ngth unta	agged non-matching contigs							
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i	igs with > solate \$ c A4/M1027	=0% seq ontigs \$ 364	uence len matching c count + do 364	ngth unta contigs n ownload c *	agged non-matching contigs count ¢ download 0							
) i	igs with > solate <del>\$</del> c	=0% seq	uence len matching c count ¢  do	ngth unta contigs n ownload c	agged non-matching contigs count ¢   download							

### 15.1.1 Filtering by tagged status of contigs

You can also export contigs based on the percentage of the sequence that has been tagged. This is useful to find sequences to target for gene discovery.

In order to export contigs where at least half the sequence has been tagged (and also the remaining contigs in a separate file), select '50' in the dropdown box for %untagged.

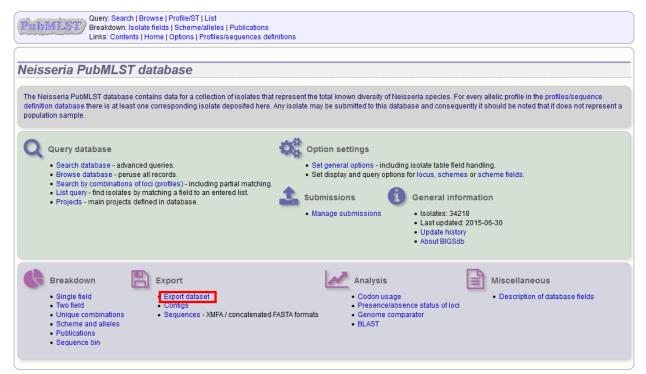
Options					
Identify contigs with	>=	50	•	% of sequ	ence untagged
FASTA header line:	orig	ginal (	les	ignation 🚽	· i

The resulting table has two download links for each isolate, one for contigs matching the condition, and one for contigs that don't match.

Con	Contigs with >=50% sequence length untagged								
id 🔺	isolate 🗢	contigo 🔺	matchin	g contigs	non-match	ning contigs			
iu 👻		conuys 👻	count 🔶	download	count 🔶	download			
1	A4/M1027	364	163	*	201	<u>له</u>			
2	120M	359	81	*	278	*			
7	7891	199	48	*	151	<u>له</u>			
10	6748	652	393	*	259	*			

## **15.2 Isolate record export**

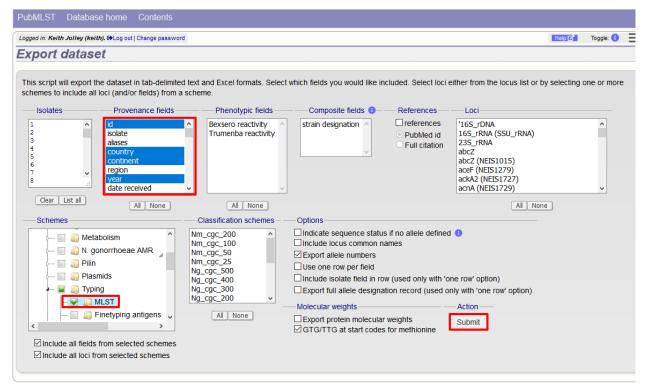
You can export the entire isolate recordset by clicking the 'Export dataset' link in the Export section of the main contents page.



Alternatively, you can export the recordsets of isolates returned from a database query by clicking the 'Dataset' button in the Export list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

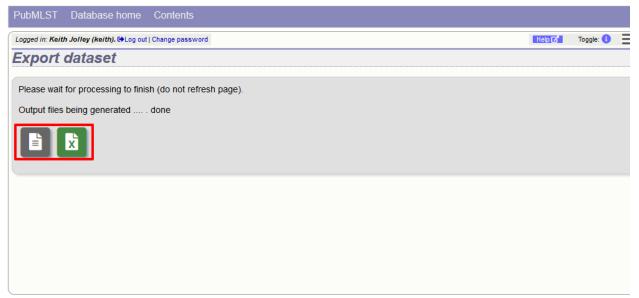
				ls	olate fields 🔢				MLST	Finet	ping antig	ens
id	isolate	aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1		
1	A4/M1027	B1; Z1001	USA	1937	invasive (unspecified/other)		A	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
3	M00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1099		19	15	
4	M1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex/subgroup IV			
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	в	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			

Select the isolate ids (if they have not been pre-selected from your query), isolate fields and schemes to include.



Click Submit.

You can then download the data in tab-delimited text or Excel formats.



#### 15.2.1 Advanced options

Options
Include locus common names
Export allele numbers
Use one row per field
Include isolate field in row (used only with 'one row' option)
Export full allele designation record (used only with 'one row' option)

The options fieldset has the following options.

- Include locus common names any common name for the locus is displayed in parentheses following the primary name.
- Export allele numbers the allele designation is included for any locus included.
- Use one row per field this is an alternative output format where instead of each locus and field having a separate column, each field is export on a separate row.
- Include isolate field in row the name of the isolate is included as a separate column when exporting in 'one row per field' fomrmat.
- Export full allele designation record export sender, curator and datestamp information as separate rows when exporting allele designation data.

#### 15.2.2 Molecular weight calculation

The plugin can also calculate the predicted molecular weight of the gene product of any allele designated in the dataset.

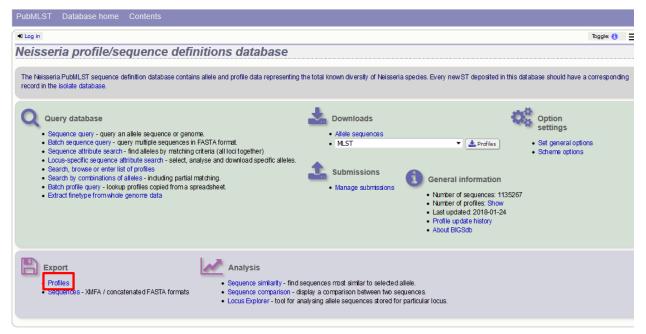
Export protein molecular weights
GTG/TTG at start codes for methionine

Click the 'Export protein molecular weight' checkbox. Additional columns (or rows depending on the output format) will be created to include the molecular weight data.

## **15.3 Profile export**

You can export the allelic profiles for any indexed scheme (those containing a primary key field) defined in the sequence definition database.

The profile export function can be accessed by clicking the 'Profiles' link in the Export section of the contents page.



Alternatively, you can access this function by clicking the 'Profiles' button in the Export list at the bottom of a results table. Please note that the list of functions here may vary depending on the setup of the database.

						pdhC		
1	1	3	1	1	1	1	3	ST-1 complex/subgroup I/II
2	1	3	4	7	1	1	3	ST-1 complex/subgroup I/II
3	1	3	1	1	1	23	13	ST-1 complex/subgroup I/II
4	1	3	3	1	4	2	3	ST-4 complex/subgroup IV
5	1	1	2	1	3	2	3	ST-5 complex/subgroup III
6	1	1	2	1	3	2	11	ST-5 complex/subgroup III
7	1	1	2	1	3	2	19	ST-5 complex/subgroup III
8	2	3	7	2	8	5	2	ST-8 complex/Cluster A4
9	2	3	8	10	8	5	2	ST-8 complex/Cluster A4
10	2	3	4	2	8	15	2	ST-8 complex/Cluster A4
11	2	3	4	3	8	4	6	ST-11 complex/ET-37 complex
12	4	3	2	16	8	11	20	
13	4	10	15	7	8	11	1	ST-269 complex
14	4	1	15	7	8	11	1	ST-269 complex
15	13	3	16	1	3	11	9	ST-364 complex
16	15	9	9	13	8	19	15	ST-4240/6688 complex
17	8	3	13	1	11	12	4	
18	7	8	10	19	10	1	2	ST-18 complex
19	7	8	10	19	8	1	2	ST-18 complex
20	6	8	10	17	10	1	2	ST-18 complex
21	1	5	1	1	2	16	17	on-ro complex
	11	5	18	8	11	24	21	ST-22 complex
22	10	5	18	9	11	9	17	ST-22 complex/Cluster A3
23	2	5	2	7	15	20	5	ST-750 complex
24	6	5	2	12	6	13	14	SI-750 complex
25	0	5	2	12	0	13	14	
۵na	lvsi	is too	ols:					
			_					
		Exp	ort:	rofiles	S	equenc	-	

This will take you to a form with a list box in which the identifiers of the profile definitions you wish to include can be entered. Following a query, these values will be pre-entered. If the box is left empty then all profiles will be included.

PubMLST Database home Conten	ts
•0 Log in	Ξ
Export allelic profiles - N	leisseria profile/sequence definitions
Schemes	
Please select the scheme you would like to que	у:
MLST 💌 (	Select)
This script will export allelic profiles in tab-delim	
Select STs Paste in list of ids to include, start a new	Adion
line for each. Leave blankto include all ids.	Submit
1	
2 = 3	
4 5 *	
6	

Click submit.

The export job will be submitted to the job queue.

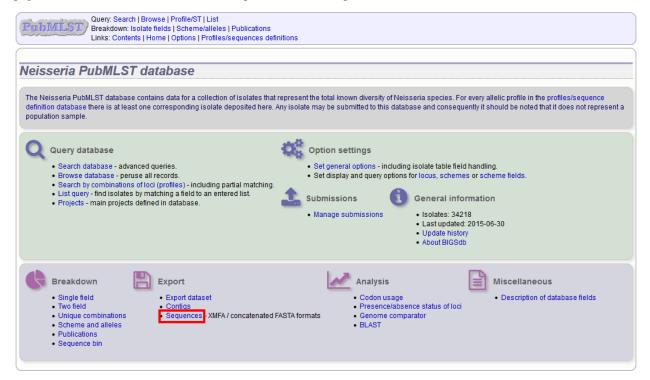
b status viewer					
Status					
Job id: BIG	Sdb_012009_1516786630_99221				
Submit time: 201	8-01-24 09:37:10				
Status: finis	shed				
Start time: 201	18-01-24 09:37:24				
Progress: 100	<b>%</b>				
Stop time: 201	18-01-24 09:37:36				
Total time: 12:	seconds				
tput					
<ul> <li>Profiles - Tab-delimit</li> </ul>	ed text 🖹				
<ul> <li>Profiles - Excel formation</li> </ul>					
<ul> <li>Tar file containing out</li> </ul>					
<ul> <li>rai nie containing ou</li> </ul>					

The profiles will be exported in tab-delimited text and Excel formats.

## 15.4 Sequence export

You can export the sequences for any set of loci designated in isolate records, or belonging to scheme profiles in the sequence definition database.

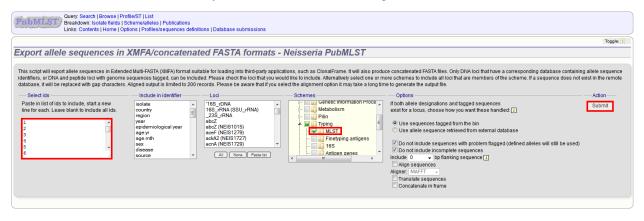
The sequence export function can be accessed by clicking the 'Sequences' link in the Export section of the contents page of isolate databases, or the 'Profile sequences' link of sequence definition databases.



Alternatively, you can access this function by clicking the 'Sequences' button in the Export list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

	M1027	B43; 21043	USA		invasive (unspecified/otner)		A	4	S1-4 complex/subgroup IV				
	M00240227		UK		invasive (unspecified/other)		в		ST-32 complex/ET-5 complex	7	16		
	M00282207		UK		invasive (unspecified/other)		W	1101	ST-22 complex				
7	7891	B54; Z1054	Finland		invasive (unspecified/other)		A	5	ST-5 complex/subgroup III	20	9	F3-1	
	M00242007		UK		invasive (unspecified/other)		В	1102	ST-18 complex		14		
9	0021/84				invasive (unspecified/other)		W	114	ST-22 complex				
10	6748	B73; Z1073	Canada		invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1	
11	129	B92; Z1092	Germany		invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6	
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	в	1015	ST-32 complex/ET-5 complex	7	16		
13	139M	B99; Z1099		1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1	
14	0120/95				invasive (unspecified/other)	Neisseria meningitidis	Х	117			14		
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864					
16	2		Germany	1999	carrier	Neisseria meningitidis	в	854	ST-18 complex				
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex				
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex				
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5	
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex				
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex				
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex				
23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex				
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	5-1	9	F3-1	
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex				

Select the isolate or profile records to analyse - these will be pre-selected if you accessed the plugin following a query. Select the loci to include either directly within the loci list and/or using the schemes tree.



Click submit.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: i
Export allele sequences in XMFA/concatenated FASTA formats - Neisseria PubMLST	
This analysis has been submitted to the job queue.	
Please be aware that this job may take a long time depending on the number of sequences to align and how busy the server is. Alignment of hundreds of sequences can take many hours!	
Follow the progress of this job and view the output.	
Please note that the % complete value will only update after the alignment of each locus.	

The job will be submitted to the job queue. Click the link to follow the progress and download the resulting files.

Sequences will be export in XMFA and FASTA file formats.

Courte Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions				
ob status viewer				
Status				
Job Id: BIGSdb_29565_1405601815_9307 Submit time: 2014-07-17 13:56:55 Status: finished Start time: 2014-07-17 13:57:10 Progress: 100% Stop time: 2014-07-17 13:57:23 Total time: 12 seconds				
Output  XMFA output file (not aligned) Concatenated FASTA (not aligned) Tar file containing output files				
lease note that job results will remain on the server for 7 days.				

#### 15.4.1 Aligning sequences

By default, sequences will be exported unaligned - this is very quick since no processing is required. You can choose to align the sequences by checking the 'Align sequences' checkbox.

Options
If both allele designations and tagged sequences
exist for a locus, choose how you want these handled: i
Our of the sequences tagged from the bin
O Use allele sequence retrieved from external database
<ul> <li>Do not include sequences with problem flagged (defined alleles will still be used)</li> <li>Do not include incomplete sequences</li> <li>Include 0 = bp flanking sequence i</li> <li>Align sequences</li> <li>Aligner: MAFFT </li> <li>Translate sequences</li> <li>Concatenate in frame</li> </ul>

You can also choose to use MUSCLE or MAFFT as the aligner. MAFFT is the default choice and is usually much quicker than MUSCLE. Both produce comparable results.

# CHAPTER 16

# Submitting data using the submission system

The automated submission system allows users to submit data (new alleles, profiles, or isolates) to the database curators for assignment and upload to the database. The submission system is enabled on a per-database basis so will not always be available.

If the system is enabled, new submissions can be made by clicking the 'Manage submissions' link on the database front page.

PubMLST Database home Contents	
+D Log in	Toggie: (1)
Neisseria profile/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representir a corresponding record in the isolate database.	ng the total known diversity of Neisseria species. Every new ST deposited in this database should have
Query database           Sequence query - query an allele sequence or genome.           Batch sequence query - query multiple sequences in FASTA format.           Sequence attribute search - find alleles by matching criteria (all loci together)           Locus-specific sequence attribute search - select, analyse and download specific alleles.           Search browse or enter list of profiles           Search by combinations of alleles - including partial matching.           Batch profile query - lookup profiles copied from a spreadsheet.           Extract finetype from whole genome data	Downloads     Allele sequences     MLST     Manage submissions     Manage submissions     Muse of sequences: 1,308,331     Number of profiles: Show     Last updated: 2019-06-25     Profile update history     About BIGSab
Sequences - XMFA / concatenated FASTA formats     Sequence comparison - disp	quences most similar to selected allele. play a comparison between two sequences. plysing allele sequences stored for particular locus.

## 16.1 Registering a user account

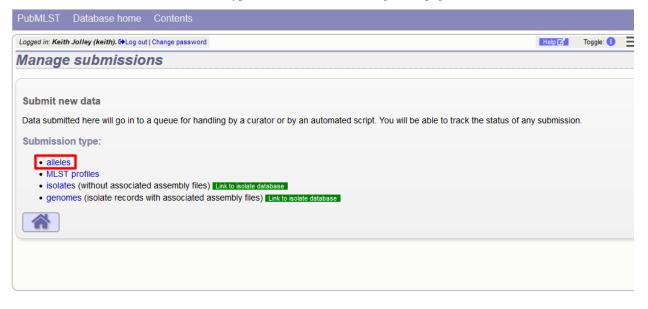
You must have an account for the appropriate database in order to use the submission system. On systems utilizing site-wide databases, such as PubMLST, this can be done automatically via the web. Other sites may require you to contact a curator to set this up.

## 16.2 Allele submission

New allele data can only be submitted from within the appropriate sequence definition database. Submissions consist of one or more new allele sequences for a single locus. You will need to create separate submissions for each locus - this is because different loci may be handled by different curators.

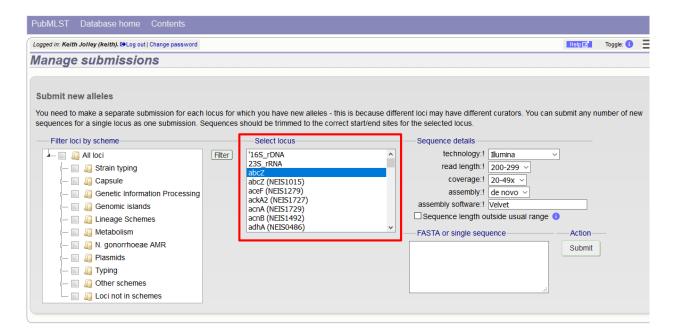
#### 16.2.1 Start

Click the 'alleles' link under submission type on the submission management page.



### 16.2.2 Select the submission locus

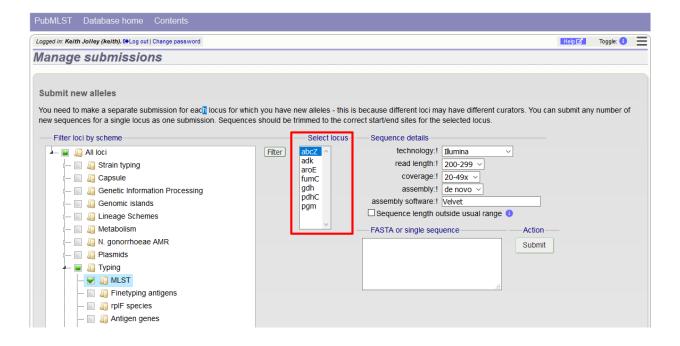
Select the locus from the locus list box:



The locus list may be very long in some databases. It may be possible to filter these to those belonging to specific schemes. If the scheme tree is shown, select the appropriate scheme, e.g. 'MLST' and click 'Filter'.

PubMLST Database home Contents		
Logged in: Keith Jolley (keith). He Log out   Change password		Help 🔀 Toggle: 🚺 🗮
Manage submissions		
Submit new alleles		
	you have new alleles - this is because different loci may have different curators. You car	submit any number of
	should be trimmed to the correct start/end sites for the selected locus.	
Filter loci by scheme	Select locus	
🚛 🔲 🚛 All loci	Filter '16S_rDNA ^	
🔚 🔲 🖉 Strain typing	23S_rRNA abcZ	
- Capsule	abcz (NEIS1015)	
Genetic Information Processing	aceF (NEIS1279)	
— Genomic islands	ackA2 (NEIS1727)	
Lineage Schemes	acnA (NEIS1729) acnB (NEIS1492)	
	adhA (NEIS0486)	
Metabolism	Sequence details FASTA or single	0000000
🔲 🦾 N. gonorrhoeae AMR		sequence
🔲 🚚 Plasmids	technology:! Illumina ~	
🚛 🔲 🛄 Typing	read length: 200-299 V	
- 😪 🔊 MLST	coverage: 20-49x V	
- Sinetyping antigens	assembly: de novo v	
🔲 🔊 rpIF species	assembly software: Velvet	
- 🔲 🛺 Antigen genes	Sequence length outside usual range 1	
	Submit	

The locus list is now constrained making selection easier.



#### 16.2.3 Enter details of sequencing method

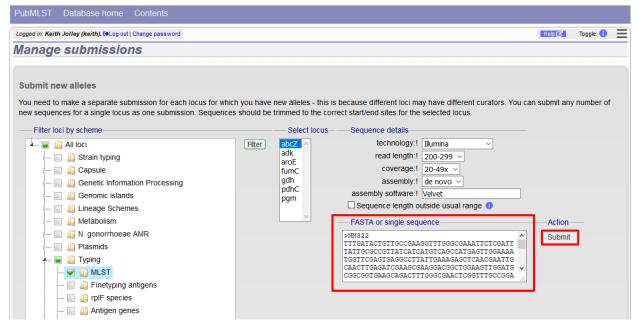
There are a number of fields that must be filled in so that the curator knows how the sequence was obtained:

- technology the sequencing platform used, allowed values are:
  - 454
  - Illumina
  - Ion Torrent
  - PacBio
  - Oxford Nanopore
  - Sanger
  - Solexa
  - SOLiD
  - other
  - unknown
- read length this is the length of sequencing reads. This is a required field for Illumina data, and not relevant to Sanger sequencing. Allowed values are:
  - <100
  - 100-199
  - 200-299
  - 300-499
  - >500
- coverage the mean number of reads covering each nucleotide position of the sequence. This is not relevant to Sanger sequencing, Allowed values are:

- <20x
- 20-49x
- 50-99x
- >100x
- assembly the means of generating the submitted sequence from the sequencing reads. Allowed values are:
  - de novo
  - mapped
- assembly software this is a free text field where you should enter the name of the software used to generate the submitted sequence.

#### 16.2.4 Paste in sequence(s)

Paste in the new variant sequences to the box. This can either be a stand- alone sequence or multiple sequences in FASTA format. The sequences must be trimmed to the start and end points of the loci - check existing allele definitions if in doubt. The submission is likely to be rejected if sequences are not trimmed. Click submit.



The system will perform some basic checks on the submitted sequences. If any of the sequences have been defined previously they must be removed from the submission before you can proceed. Curators do not want to waste their time dealing with previously defined sequences.

ed in: Keith Jolley (keith). 🕩 Log out   Change password			Help 🖍	Toggle: 🚺
nage submissions				
Error: Sequence "NM432" has already been	defined as abcZ-3.			
	th locus for which you have new alleles - this is because differ Sequences should be trimmed to the correct start/end sites f		omit any num	ber of new
Iden loci by scheme      Iden loci by scheme      Iden loci by scheme      Iden loci by scheme      Iden loci biands      Iden	Fiter 1165_rDNA 1235_rRNA 16CZ 16CZ 16CZ 16CZ 16CZ 16CZ 16CZ 16CZ	technology: Illumina  read length: 200-299  coverage: 20-49x  assembly: de novo  assembly software: Velvet Sequence length outside usual range  FASTA or single sequence	-Action	
		>NM322 TTTGATACTGTTGCCGAAGGTTTGGGCGAA ATTCTCGATTTATTGCGCCGTTATCATCAT	Submit	

Assuming the preliminary checks have passed you will then be able to add additional information to your submission.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). [+Log out   Change password	Help 🖓 Toggle: 🚺 🗮
Manage submissions	
Supporting files Please note that if you are submitting alleles determined by Sanger sequencing that you must upload both forward and don't. Please do not pack or compress your files (zip, rar etc).	reverse trace files. Your submission will be rejected if you
Action Abort submission! Submission: BIG Sdb_20190628084417_002033_60338	
Supporting files Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an exp appropriate submission item. Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go (the upload with fewer files at a time if it does), although you can upload multiple times so that the total size of the submission can Drop files here or click to upload	may fail if you try to do more than this - just try again a be larger.
Sequences You are submitting the following abcZ sequences: Download Identifier Length Sequence Status Query Assigned allele NM322 433 TTTGATACTGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending Q NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending Q	Sequence details technology:! Ilumina ~ read length:! 200-299 ~ coverage:! 20-49x ~ assembly:! de novo ~ assembly: oftware:! Velvet Sequence length outside usual range ()
E-mail Action Updates will be sent to keith.jolley@zoo.ox.ac.uk. Finalize submission! ✓ E-mail submission updates Messages Message: Append	

#### 16.2.5 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Append'. This is not normally necessary for routine submissions.

Submission: BIGSdb_20190628084417_002033_60338 Supporting files Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an exp appropriate submission item. Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go (the upload with fewer files at a time if it does), atthough you can upload multiple times so that the total size of the submission ca	d may fail if you try to do more than this - just try again
Drop files here or click to upload	l.
Sequences         You are submitting the following abcZ sequences: Download         Identifier       Length       Sequence       Status       Query Assigned allele         NM322       433       TTTGATACTGTTGCCGAAGG       GCGGATTGTCGAACTCGATC       pending       Q         NM21       433       TTTGATACCGTTGCCGAAGG       GCGGATTGTCGAACTCGATC       pending       Q	Sequence details technology:! Illumina read length:! 200-299 coverage:! 20-49x assembly:! de novo assembly software:! Velvet Sequence length outside usual range
E-mail Action Updates will be sent to keith jolley@zoo.ox.ac.uk. Finalize submission! E-mail submission updates Messages The sequence variant NM322 has been seen in 3 isolates. Message: Append	

The message will be attached. A curator may respond to the message and attach their own, with the full conversation becoming part of the submission record.

Supporting files Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an ex appropriate submission item. Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go (the uploa vith fewer files at a time if it does), although you can upload multiple times so that the total size of the submission ca	ad may fail if you try to do more than this - just try again
Drop files here or click to upload	d.
Sequences	Sequence details
/ou are submitting the following abcZ sequences: Download	technology:! Illumina 🗸
	read length:
Identifier         Length         Sequence         Status         Query         Assigned allele           NM322         433         TTTGATACTGTTGCCGAAGG         GCGGATTGTCGAACTCGAAC         pending         Q	coverage:! 20-49x V
NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending Q	assembly:   de novo ~ assembly software:   Velvet
	Sequence length outside usual range 1
– E-mail – Action – Action –	
Jpdates will be sent to keith.jolley@zoo.ox.ac.uk. Finalize submission!	
E-mail submission updates	
- Messages	
Timestamp User Message	
2019-06-28 07:47:22+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.	
a.	
Message: Append	

# 16.2.6 Add supporting files

Some submissions will require the attachment of supporting files. This will depend on the policies of the individual databases. Sequences determined by Sanger sequencing should normally have forward and reverse trace files attached.

Files can be added to the submission by dragging and dropping in to the large dotted area in the 'Supporting files' section. Alternatively, you can click this area and select files from the local file system.

Supporting files Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an ex- appropriate submission item. Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go (the uploa with fewer files at a time if it does), although you can upload multiple times so that the total size of the submission c	ad may fail if you try to do more than this - just try again
Drop files here or click to upload	d.
Sequences	Sequence details
You are submitting the following abcZ sequences: Download	technology: Ilumina
Identifier Length Sequence Status Query Assigned allele	read length: 200-299 V
NM322 433 TTTGATACTGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending Q	coverage: 20-49x V
NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending Q	assembly:! de novo ~
	Sequence length outside usual range ()
E-mailAction	
Updates will be sent to keith.jolley@zoo.ox.ac.uk. Finalize submission!	
✓ E-mail submission updates	
Messages	
Timestamp User Message	
2019-06-28 07:47:22+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.	
Message: Append	

The files will be uploaded and shown in a table.

Drop files here or click to upload	d.
Uploaded files         Filename Size Delete         NM322_abcZ_Fab1 296.6 KB       NM21_abcZ_Rab1 232.8 KB         NM322_abcZ_R.ab1 232.8 KB       NM322_abcZ_R.ab1 234.9 KB         NM21_abcZ_Fab1 276.4 KB       Delete selected files         Sequences       You are submitting the following abcZ sequences: Download ras         Identifier       Length       Sequence         NM322_433       TTTGATACTGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending Q       Assigned allele         NM21       433       TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending Q	Sequence details technology:! Ilumina read length:! 200-299 coverage:! 20-49x assembly:! de novo assembly: oftware:! Velvet Sequence length outside usual range <b>1</b>
E-mail       Action         Updates will be sent to keith jolley@zoo.ox.ac.uk.       Finalize submission!         ☑ E-mail submission updates       Messages         Messages       1         ☑ 19-06-28 07:47:22+00       Keith Jolley The sequence variant NM322 has been seen in 3 isolates.	
Message: Append	

Files can be removed from the submission by checking the appropriate 'Delete' box and clicking 'Delete selected files'.

# 16.2.7 Finalize submission

Make sure the 'E-mail submission updates' box is checked if you wish to receive E-mail notification of the result of your submission. This setting is remembered between submissions.

Click 'Finalize submission!'.

Drop files here or click to u	pload.
Uploaded files           Filename         Size         Delete           NM322_abcZ_F.ab1         296.6 KB	Sequence details
You are submitting the following abcZ sequences: Download       FAS         Identifier       Length       Sequence       Status       Query       Assigned         NM322       433       TTTGATACTGTTGCCGAAGG       GCGGATTGTCGAACTCGATC       pending       Q         NM21       433       TTTGATACCGTTGCCGAAGG       GCGGATTGTCGAACTCGATC       pending       Q	allele coverage: 20-49x v assembly: de novo v assembly: Velvet
E-mail Action Updates will be sent to keith.jolley@zoo.ox.ac.uk. Finalize submission! ☑ E-mail submission updates Messages <u>Timestamp User Message</u> 2019-06-28 07:47:22+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.	
Message: Append	

Your submission will then be listed under 'Pending submissions' on your submission page.

PubMLST Database home Contents			
Logged in: Keith Jolley (keith). C+Log out   Change password	Help 🗹	Toggle: 🚺	Ξ
Manage submissions			
Submit new data			
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission	on.		
Submission type:			
<ul> <li>alleles</li> <li>MLST profiles</li> <li>isolates (without associated assembly files) Linkto isolate database</li> <li>genomes (isolate records with associated assembly files) Linkto isolate database</li> </ul>			
Pending submissions You have submitted the following submissions that are pending curation:			
Submission idSubmittedUpdatedTypeDetailsBIGSdb_20190628084417_002033_603382019-06-282019-06-28alleles2 abcZ sequences			

# 16.3 Profile submission

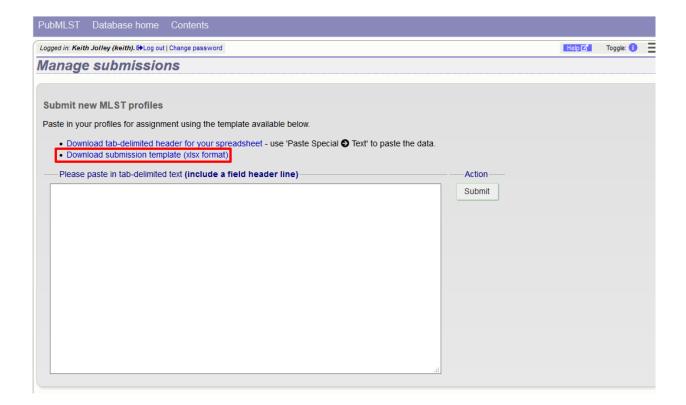
# 16.3.1 Start

**Note:** Most MLST databases on PubMLST.org require you to submit an isolate record for each new ST that you wish to be defined. In these cases, you should add the isolate name to the id field of your profile submission and make a corresponding *isolate submission* containing the allelic profile.

Click the appropriate profiles link under submission type on the submission management page.

PubMLST Database home Contents			
Logged in: Keith Jolley (keith). GLog out   Change password	Help 🗹	Toggle: 🚺	Ξ
Manage submissions			
Submit new data			
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any	/ submission	n.	
Submission type:			
alleles     MLST profiles     isolates (without associated assembly files) Link to isolate database     genomes (isolate records with associated assembly files) Link to isolate database			

Download the Excel submission template.



# 16.3.2 Paste in profile(s)

Fill in the template. The first column 'id' can be used to enter an identifier that is meaningful to you - it is used to report back the results but is not uploaded to the database. It can be left blank, or the entire column can be removed - in which case individual profiles will be identified by row number.

Copy and paste the entire contents of the submission worksheet. Click submit.

Pub	MLST	Databa	ise hom	e Cont										
Logg	ged in: Keit	h Jolley (ke	e <i>ith).</i> 🔂 Log	out   Change	password							Help 🔀	Toggle: 🚺	Ξ
Ма	anage	e subi	missi	ions										
Su	ıbmit n	ew MLS	T profile	es										
Pa	ste in yo	ur profiles	for assig	nment usi	ng the tem	plate ava	ilable belov	V.						
						eadsheet -	- use 'Paste	e Special	Text' to paste the	data.				
				emplate (xl	1									
		-		ited text (ir							-Action-			
1	id	abcZ 8	adk 5	aroE 32	fumC 2	gdh 6	pdhC 43	pgm 32			Submit			
		5 3	7 2	3 4	6 3	33 8	12 4	2 6						
		9	6	9	9	9	6	9						

Some basic checks will be performed. These include whether the profile has already been assigned and whether each allele identifier exists. The submission cannot proceed if the checks fail.

Publ	MLST	Datab	ase hom	ie Cont	ents										
Logge	d in: Ke	ith Jolley (k	ke <i>ith).</i> 🔂 Log	out   Change	password								Help 🖍	Toggle: 🕕	Ξ
Ма	nag	e sub	missi	ions											
>	٢	Error: Row 4: Pi	rofile has a	already be	en defined	l as ST-44									
		new MLS			ng the terr	iplate ava	ilable belov	N.							
	• Dow	vnload sub	omission te	emplate (xl	sx format)			e Special	Text' to p	paste the d	ata.	Action			
i		abcZ 8 5	adk 5 7	aroE 32 3	fumC 2 6	field head gdh 6 33 8 9	pdhC 43 12 4 6	pgm 32 2				Submit			
		3 9	2 6	4 9	8 3 9			6 9							

Provided the checks pass, you will then be able to add additional information to your submission. New profile submissions usually don't require supporting files directly in the submission. You generally will need to make a corresponding *submission to the isolate database* though.

# 16.3.3 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Append'.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). 🔂 Log out   Change password Toggle: 1 Toggle:
Manage submissions
Isolate submission required Please note that you must make a corresponding submission to the isolate database - this is not the same as attaching an isolate template file to this submission. Please see the submission guide for details. Every newly defined ST should have a representative isolate record in the isolate database. Your submission will be rejected if you do not do this.
Action Abort submission! Submission: BIG Sdb_20190628091104_018718_08755
Supporting files
Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an explanatory note so that they can be linked to the appropriate submission item. Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go (the upload may fail if you try to do more than this just try again with fewer files at a time if it does), although you can upload multiple times so that the total size of the submission can be larger. Drop files here or click to upload. ProfilesE-mail
You are submitting the following MLST profiles: Download csv Updates will be sent to keith.jolley@zoo.ox.ac.uk.
Identifier       abcZ       adk       aroE       fumC       gdh       pdhC       pgm       Status       Query       Assigned ST         Row 1       8       5       32       2       6       43       32       pending       Q       Action       Action       Finalize submission!         Row 3       3       2       4       3       8       4       6       pending       Q       Finalize submission!       Finalize submission!         Messages       Corresponding isolate submission has been made -       -       -       -       -
BIGSdb_20190530060244_022168_38354

The message will be attached. A curator may respond to the message and attach their own, with the full conversation becoming part of the submission record.

,*				time if i 				
					D	rop file	s h	re or click to upload.
Profiles								E-mail
You are sub	mittin	a the follo	vina ML	ST pro	ofiles: Do	vnload 🔜		Updates will be sent to keith.jolley@zoo.ox.ac.uk.
						m Status (	Query	
luenuner		5 32	2	6	43 3	1 0	Q	Action
Row 1	8					2 pending	Q	Finalize submission!
Row 1 Row 2	5	7 3	6	33 8			Q	
Row 1 Row 2 Row 3	5 3		6 3	8	4 6		Q	
Row 1 Row 2 Row 3 Messages	5 3 s	7 3 2 4	3	8			Q	
Row 1 Row 2 Row 3 Messages	5 3 s	7 3 2 4	3 User	8	4 6	5 pending		Message has been made - BIGSdb 20190530060244 022168 38354.
Row 1 Row 2 Row 3 Messages	5 3 s	7 3 2 4	3 User	8	4 6	5 pending		Message

### 16.3.4 Finalize submission

Make sure the 'E-mail submission updates' box is checked if you wish to receive E-mail notification of the result of your submission. This setting is remembered between sessions.

Click 'Finalize submission!'.

								I up to 64 MB in one go (the upload may fail if you try to do more th nes so that the total size of the submission can be larger.	,
						Drop file	s here or c	lick to upload.	
Profiles								E-mail	
						Download csv	Query Accidned ST	Updates will be sent to keith.jolley@zoo.ox.ac.uk.	
dentifier	abcZ	adk a	roE fum	C gdh	pdhC	pgm Status	Query Assigned ST		
		adk a				_	Query Assigned ST Q Q	E-mail submission updates	
dentifier Row 1	abcZ 8	adka 5	roE fum 32 2	C gdh 6	pdhC 43	pgm Status 32 pending	Q	E-mail submission updates	
dentifier Row 1 Row 2 Row 3	abcZ 8 5 3	adka 5 7	roE fum 32 2 3 6	C gdh 6 33	<b>pdhC</b> 43 12	pgmStatus32pending2pending	Q Q	E-mail submission updates	
dentifier Row 1 Row 2 Row 3 Message	abcZ 8 5 3	adk a 5 7 2	roE fum 32 2 3 6 4 3	C gdh 6 33 8	<b>pdhC</b> 43 12	pgmStatus32pending2pending	Q Q Q	E-mail submission updates  Action  Finalize submission!	
dentifier Row 1 Row 2 Row 3 Message Tim	abcZ 8 5 3 es	adk a 5 7 2	roE fum 32 2 3 6 4 3	C gdh 6 33 8	<b>pdhC</b> 43 12 4	pgmStatus32pending2pending6pending	Q Q Q M(	E-mail submission updates	
dentifier Row 1 Row 2 Row 3 Message Tim	abcZ 8 5 3 es	adk a 5 7 2	roE fum 32 2 3 6 4 3	C gdh 6 33 8	<b>pdhC</b> 43 12 4	pgmStatus32pending2pending6pending	Q Q Q M(	E-mail submission updates Action Finalize submission! essage	

Your submission will then be listed under 'Pending submissions' on your submission page.

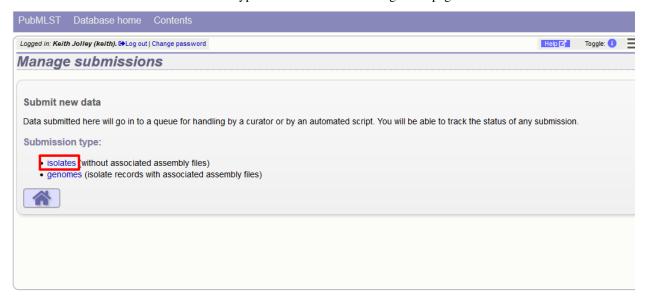


# 16.4 Isolate submission

New isolate data can only be submitted from within the appropriate isolate database. You may be required to submit isolate data if you would like to get a new MLST sequence type defined, but this depends on individual database policy.

### 16.4.1 Start

Click the 'isolates' link under submission type on the submission management page.



Download the Excel submission template.

PubMLST Database home Contents												
Logged in: Keith Jolley (keith). [+Log out   Change password	Help 🗹	Toggle: 🚺										
Manage submissions												
Submit new isolates												
Paste in your isolates for addition to the database using the template available below.												
• Enter aliases (alternative names) for your isolates as a semi-colon (;) separated list.												
<ul> <li>Enter references for your isolates as a semi-colon (;) separated list of PubMed ids.</li> <li>You can also upload additional allele fields along with the other isolate data - simply create a new column with the locus name.</li> </ul>												
Download tab-delimited header for your spreadsheet - use 'Paste Special SText' to paste the data.												
Download submission template (xlsx format)												
Please paste in tab-delimited text (include a field header line)     Action												
Submit												

### 16.4.2 Paste in isolate data

Fill in the template. Some fields are required and cannot be left blank. Check the 'Description of database fields' link on the database contents page to see a description of the fields and allowed values where these have been defined. Where allowed values have been set, the template will have dropdown boxes (although these require newer versions of Excel to work).

Some databases may have hundreds of loci defined, and most will not have a column in the template. You can add new columns for any loci that have been defined and for which you would like to include allelic information for. These locus names must be the primary locus identifier. A list of loci can be found in the 'allowed_loci' tab of the Excel submission template.

Copy and paste the entire contents of the submission worksheet. Click submit.

agged in: Keth Johry (Weith). (PLog out] Change password       Togget.         Anage submissions         Submit new isolates         Paste in your isolates for addition to the database using the template available below.         • Enter references for your isolates as a semi-colon (:) separated list.         • Enter references for your isolates as a semi-colon (:) separated list.         • Download additional allee fields along with the other isolate data - simply create a new column with the locus name.         • Download additional allee fields along with the other isolate data - simply create a new column with the locus name.         • Download submission template (xist format)         Please paste in tab-delimited text (include a field header line)         ceforaxine_range       chloramphenicol_range         cefora	PubMLST	Datab	ase home	e Cont	ents											
Submit new isolates Paste in your isolates for addition to the database using the template available below.	ogged in: Keit	h Jolley (k	re <i>ith).</i> 🔂 Log	out   Change	password									Help 🖌	Toggle: 🜖	
Paste in your isolates for addition to the database using the template available below. • Enter aliases (alternative names) for your isolates as a semi-colon (;) separated list. • Enter references for your isolates as a semi-colon (;) separated list. • You can also upload additional allele fields along with the other isolate data - simply create a new column with the locus name. • Download tab-delimited header for your spreadsheet - use 'Paste Special Text' to paste the data. • Download submission template (xisx format) Please paste in tab-delimited text (include a field header line) Ceftriaxon_range chloramphenicol chloramphenicol_range ceftotaxime otiporofloxacin range tetracycline ceftixime azithromyclin spectionwyclin ENR_accession private_project comments abc2 adk arcof fumC gdh phC pgm PorA_VRI PorA_VR2 FetA_VR gyra penA rpoB UK322 UK 2 3 4 3 8 4 6 5 2 FI-5 W 2 3 4 3 8 4 6 5 2 FI-5 W 2 3 4	lanage	e sub	missi	ons												
Paste in your isolates for addition to the database using the template available below. • Enter aliases (alternative names) for your isolates as a semi-colon (;) separated list. • Enter references for your isolates as a semi-colon (;) separated list. • You can also upload additional allele fields along with the other isolate data - simply create a new column with the locus name. • Download tab-delimited header for your spreadsheet - use 'Paste Special Text' to paste the data. • Download submission template (xisx format) Please paste in tab-delimited text (include a field header line) Ceftriaxon_range chloramphenicol chloramphenicol_range ceftotaxime otiporofloxacin range tetracycline ceftixime azithromyclin spectionwyclin ENR_accession private_project comments abc2 adk arcof fumC gdh phC pgm PorA_VRI PorA_VR2 FetA_VR gyra penA rpoB UK322 UK 2 3 4 3 8 4 6 5 2 FI-5 W 2 3 4 3 8 4 6 5 2 FI-5 W 2 3 4																
<ul> <li>Enter allases (alternative names) for your isolates as a semi-colon (;) separated list.</li> <li>Enter references for your isolates as a semi-colon (;) separated list of PubMed ids.</li> <li>You can also upload additional allele fields along with the other isolate data - simply create a new column with the locus name.</li> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special Text' to paste the data.</li> <li>Download submission template (xlsx format)</li> </ul> Please paste in tab-delimited text (include a field header line) Action   ceftriaxon=_range chloramphenicol chloramphenicol_range cefotaxime   ciprofloxacin_range chloramphenicol chloramphenicol_range cefotaxime   ciprofloxacin_range chloramphenicol comments abcZ   gyrA penA rpoB   W W ymain problem   Septicaemia Blood Neisseria meningitidis Neisseria meningitis Neisseria meningitis Neisseria meningitis Neisseria meningitis	Submit n	ew isola	ates													
<ul> <li>Enter references for your isolates as a semi-colon (;) separated list of PubMed ids.</li> <li>You can also upload additional allele fields along with the other isolate data - simply create a new column with the locus name.</li> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special Text' to paste the data.</li> <li>Download submission template (xisx format)</li> </ul> Please paste in tab-delimited text (include a field header line) Action   ceftriaxone_range chloramphenicol chloramphenicol_range cefotaxime   ciprofloxacin_range rifampicin_range ciprofloxacin   ciprofloxacin_range tetracycline ceftxime   spectinomycin ENA accession private-project comments   acce gmx penA   2 3 4   3 8 4 6   5 2 FI-5   UX3225 UK   2 3 4	Paste in yo	ur isolate	s for addit	ion to the	database	using the	e template a	vailable b	elow.							
<ul> <li>You can also upload additional allele fields along with the other isolate data - simply create a new column with the locus name.</li> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special Text' to paste the data.</li> <li>Download submission template (xisx format)</li> </ul> Please paste in tab-delimited text (include a field header line) Action   ceftriaxone_range chloramphenicol chloramphenicol_range ceftotaxime   ceftriaxone_range chloramphenicol chloramphenicol_range ceftotaxime   ceftriaxone_range chloramphenicol_range ceftotaxime   ceftriaxone_range chloramphenicol_range ceftotaxime   ceftriaxone_range chloramphenicol_range ceftotaxime   ceftriaxone_range chloramphenicol_range ceftotaxime   ceftriaxone_range chloramphenicol_range ceftotaxime   ceftriaxone_range chloramphenicol_range ceftotaxime   ceftriaxone_range ceftraine athromycin   spectinorycin path ppm   gyrah penA rpoB   UX322 UK meningitis and   c 2 3   3 8 4 6   5 2 Fil-5   UX325 UK   2019 septicaemia   W 2 3   2 3 4			•	· · · · · ·												
<ul> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special C Text' to paste the data.</li> <li>Download submission template (xisx format)</li> <li>Please paste in tab-delimited text (include a field header line)</li> <li>Ceftriaxone_range chloramphenicol chloramphenicol_range cefotaxime ciprofloxacin range tritracycline cefixime azithromycin spectinomycin ENA accession private project comments abc2 adk arob fumC gdm pdhC pdm PorA_VR1 PorA_VR2 FetA_VR gyrA penA rpoB</li> <li>UK322 UK 2019 meningitis and septicaemia blood Neisseria meningitidis C</li> <li>3 8 4 6 5 2 FI-5 UK septicaemia</li> <li>3 8 4 6 5 2 FI-5 UK septicaemia</li> <li>3 8 4 6 5 2 FI-5 UK septicaemia</li> <li>3 8 4 6 5 2 FI-5 UK septicaemia</li> <li>3 8 4 6 5 2 FI-5 UK septicaemia</li> <li>3 8 4 6 5 2 FI-5 UK septicaemia</li> <li>3 8 4 6 5 2 FI-5 UK septicaemia</li> </ul>										create a new	colur	nn with the locus na	me			
• Download submission template (xisx format) Please paste in tab-delimited text (include a field header line) Ceftriaxone_range chloramphenicol chloramphenicol_range cefotaxime cefotaxime_range rifampicin rifampicin_range ciprofloxacin ciprofloxacin_range tetracycline cefixime azithromycin spectinomycin ENA_accession private_project comments abc2 adk arcc funC gdh pdhC pgm PorA_VR1 PorA_VR2 FetA_VR gvrA penA rpoB UK322 UK 2019 meningitis and septicaemia blood Neisseria meningitidis C 3 8 4 6 5 2 F1-5 UK325 UK 2019 septicaemia CSF Neisseria meningitis W 2 3 4			· · · ·			Ŭ										
Ceftriaxone_range       chloramphenicol chloramphenicol_range       cefotaxime       for the second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second secon							I-USC FASI	e opeciai		paste trie da	11.01.					
cefotaxime_range rifampicin_rifampicin_range ciprofloxacin ciprofloxacin_range tetracycline cefixime azithromycin spectinomycin FNA_accession_private_project comments abc2_adk aroE_fumC_gdh_pdhC_pgm_PorA_VR1_PorA_VR2_FetA_VR gyrA_penA_rpoB_ UK3225_UK_2019	Please	paste in	tab-delimi	ted text (ii	nclude a f	field hea	ader line) –					Action —				
ciprofloxačin range tetračycline cefixime azithromycin spectinomycin ENA accession private project comments abcZ adk arcE fumC gdh pdhC pgm PorA_VR1 PorA_VR2 FetA_VR gyrA penA rpoB UK322 UK 2019 meningitis and septicaemia blood Neisseria meningitidis C 3 8 4 6 5 2 F1-5 UK325 UK 2019 septicaemia CSF Neisseria meningitis W											^	Submit				
aroE fumC gdh pdhC pgm PorA_VR1 PorA_VR2 FetA_VR gyrA penA rpoB UK 2019 meningitis and septicaemia blood Neisseria meningitidis C 3 8 4 6 5 2 F1-5 UK 2019 CSF Neisseria meningitis W 2019 septicaemia CSF Neisseria meningitis	ciprofl	oxacin_	range	tetrac	ycline					0110xacin						
gyrA penA rpoB																
2019 meningitis and septicaemia blood Neisseria meningitidis C 3 8 4 6 5 2 F1-5 UK325 UK 2019 septicaemia CSF Neisseria meningitis W	gyrA			-	1.2											
C 2 3 4 3 8 4 6 5 2 F1-5 UK325 UK 2019 septicaemia CSF Neisseria meningitis W 2 3 4	2019			OR					menin	ngitis and						
3 8 4 6 5 2 F1-5 UK325 UK 2019 septicaemia CSF Neisseria meningitis W		emia	D1000		Neisse	ria mer	iingitidis									
UK325 UK 2019 septicaemia CSF Neisseria meningitis W 2 3 4		_			_	_		2	3	4						
CSF Neisseria meningitis W 2 3 4	UK325	8	4		5	2	F1-5									
W 2 3 4			Neisse	ria meni	ngitis				septi	caemia						
3 18 4 6 5-1 2 F1-5 ✓								2	3	4						
	3	18	4	6	5-1	2	F1-5				×.					

Some basic checks will be performed. These include checking all field values conform to allowed lists or data types. The submission cannot proceed if any checks fail.

PubMLST Database home Contents			
Logged in: Keith Jolley (keith). Co Log out   Change password	Help 🗹	Toggle: 🚺	Ξ
Manage submissions			
Error: UK325 has problems - species: value is not on the list of allowed values for this field.			
Submit new isolates Paste in your isolates for addition to the database using the template available below.			
<ul> <li>Enter aliases (alternative names) for your isolates as a semi-colon (;) separated list.</li> <li>Enter references for your isolates as a semi-colon (;) separated list of PubMed ids.</li> </ul>			
• You can also upload additional allele fields along with the other isolate data - simply create a new column with the locus name.			
<ul> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special Statt' to paste the data.</li> <li>Download submission template (xisx format)</li> </ul>			
Please paste in tab-delimited text (include a field header line)     Action			
isolate aliases references country region year date_received date_sampled non_culture epidemiological_year age_yr age_mth sex disease source epidemiology species serogroup genogroup MLEE_designation serotype sero_subtype ET_no penicillin penicillin_range amoxicillin sulphonamide ceftriaxone ceftriaxone_range chloramphenicol chloramphenicol_range cefotaxime cefotaxime_range rifampicin rifampicin_range ciprofloxacin ciprofloxacin parge tetracycline cefixime ciprofloxacin parge			

Provided the checks pass, you will then be able to add additional information to your submission.

# 16.4.3 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Append'.

PubMLST	Datal	base hoi	me Contents															
Logged in: Keit	h Jolley (	(keith). 🔂	og out   Change password													Help 🗹	Toggle: 🚺	Ξ
Manage	e sul	bmiss	sions															
	te recor	d contain	is a new combination of assigned and that you				e subr	nissic	on to ti	he sequ	ience	e datab	ase. F	Please see ti	ne submissio	on guide fo	or details. T	ĥis
Isolates	Ab on: Bl		ission! 20191204090508_01 owing isolates: Downloa		933													
isolate	country	y year	disease	source	species	serogroup	abcZ	adk	aroE	fumC	gdh	pdhC	pgm	PorA_VR1	PorA_VR2	FetA_VR	ST (MLST)	
UK322	UK	2019	meningitis and septicaemia	blood	Neisseria meningitidis	С	2	3	4	3	8	4	6	5	2	F1-5	11	
UK325	UK	2019	meningitis	CSF	Neisseria meningitidis	W	2	3	4	3	18	4	6	5-1	2	F1-5	-	
Messag	ges —				E-mail					Actio	۱ <u> </u>							
will al	so sub ion fo	mit a n r this	new MLST profile. I ew profile to the sequence Message: Append	✓ ✓	odates will be sent to		200.0X.	ac.uk	c.	Finali	ze su	bmissic	n!					

The message will be attached. A curator may respond to the message and attach their own, with the full conversation becoming part of the submission record.

-Isolate ou are			20191204090		7012_99933												
solate	country	year	disease	source	species	serogroup	abcZ	adk	aroE	fumC	gdh	pdhC	pgm	PorA_VR1	PorA_VR2	FetA_VR	ST (MLST
UK322	UK	2019	meningitis and septicaemia	blood	Neisseria meningitidis	С	2	3	4	3	8	4	6	5	2	F1-5	11
UK325	UK	2019	meningitis	CSF	Neisseria meningitidis	W	2	3	4	3	18	4	6	5-1	2	F1-5	-
	limestam		User 0 Keith Jolley I	think UK3	25 has a new l	MLST profile.	l will a	IISO SI		Messa a new p		e definit	ion fo	r this to the	sequence d	efinition da	tabase

# 16.4.4 Finalize submission

Make sure the 'E-mail submission updates' box is checked if you wish to receive E-mail notification of the result of your submission. This setting is remembered between sessions.

Click 'Finalize submission!'.

isolate country yea UK322 UK 201		source													
UK322 UK 201			species	serogroup	abcZ	adk	aroE	fumC	gdh	pdhC	pgm	PorA_VR1	PorA_VR2	FetA_VR	ST (MLST
	9 meningitis and septicaemia	blood	Neisseria meningitidis	С	2	3	4	3	8	4	6	5	2	F1-5	11
UK325 UK 201	9 meningitis	CSF	Neisseria meningitidis	W	2	3	4	3	18	4	6	5-1	2	F1-5	-
Messages Timestamp 2019-12-04 09:08:41-	User +00 Keith Jolley	I think UK3	25 has a new l	MLST profile.	l will a	also si		Messa a new p		definit	on foi	r this to the	sequence d	efinition da	tabase

Your submission will then be listed under 'Pending submissions' on your submission page.

PubMLST Database home Contents			
Logged in: Keith Jolley (keith). (+Log out   Change password	Help 🖪	Toggle: 🚺	Ξ
Manage submissions			
Submit new data			
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any sub-	mission.		
Submission type:			
<ul> <li>isolates (without associated assembly files)</li> <li>genomes (isolate records with associated assembly files)</li> </ul>			
Pending submissions			
You have submitted the following submissions that are pending curation:			
Submission id Submitted Updated Type Details			
BIGSdb_20190628093907_003732_26733 2019-06-28 2019-06-28 isolates 2 isolates			

# 16.5 Genome submission

Submitting genomes uses the same process as standard *isolate submission*. The only difference is that there are a couple of extra required fields in the submission table:

- assembly_filename this is the name of the FASTA file containing the assembly contigs. This must be uploaded as a supporting file you will not be able to finalize the submission until every isolate record has a matching contig file.
- sequence_method the sequencing technology used to generate the sequences. The allowed values are listed on the submission page.

To start the submission, click the 'genomes' link under submission type on the submission management page.

PubMLST Database home Contents			
Logged in: Keith Jolley (keith). (+Log out   Change password	Help 🛃	Toggle: 🚺	Ξ
Manage submissions			
Submit new data			
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of an	y submission	n.	
Submission type:			
<ul> <li>isolates (without associated assembly files)</li> <li>genomes isolate records with associated assembly files)</li> </ul>			

Then follow the steps for *isolate submission*, uploading the contigs files as supporting files.

# 16.6 Removing submissions from your notification list

Once a submission has been closed by a curator, the results will be displayed in your 'Manage submissions' area. You can remove submissions once you have noted the result by clicking the 'Remove' link.



Alternatively, submissions will be removed automatically a specified period of time after closure. By default, this time is 90 days, but this can vary depending on the site configuration.

# CHAPTER 17

# **RESTful Application Programming Interface (API)**

The REST API allows third-party applications to retrive data stored within BIGSdb databases or to send new submissions to database curators. To use the REST API, your application will make a HTTP request and parse the response. The response format is JSON (except for routes that request a FASTA or CSV file).

Access to protected resources, i.e. those requiring an account, can be accessed via the API using OAuth authentication.

# 17.1 Passing additional/optional parameters

If you are using a method called with GET, optional parameters can be passed as arguments to the query URL by adding a '?' followed by the first argument and its value (separated by a '='). Additional parameters are separated by a '&', e.g.

http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates?page=2&page_size=100

Methods called with POST require their arguments to be sent as JSON within the post body.

# 17.2 Paging using request headers

Paging of results can be selected using query parameters as described above. In this case, methods that support paging will include a paging object in the JSON response. This will contain links to the next page, last page etc.

The API also supports paging using request headers. The following request headers are supported:

- X-OFFSET
- X-PER-PAGE

e.g.

If either of these headers are used, the paging object is no longer returned as part of the JSON response. The response will include the following headers:

- X-OFFSET
- X-PER-PAGE
- X-TOTAL-PAGES

# **17.3 Resources**

- GET / or /db List site resources
- *GET /db/{database}* List database resources
- *GET /db/{database}/classification_schemes* List classification schemes
- *GET /db/{database}/classification_schemes/{classification_scheme_id}* Retrieve classification scheme information and groups
- *GET /db/{database}/classification_schemes/{classification_scheme_id}/groups/{group_id}* List isolates belonging to a classification scheme group
- GET /db/{database}/loci List loci
- GET /db/{database}/loci/{locus} Retrieve locus record
- GET /db/{database}/loci/{locus}/alleles Retrieve list of alleles defined for a locus
- GET /db/{database}/loci/{locus}/alleles_fasta Download alleles in FASTA format
- GET /db/{database}/loci/{locus}/alleles/{allele_id} Retrieve full allele information
- POST /db/{database}/loci/{locus}/sequence Query sequence to identify allele
- POST /db/{database}/sequence Query sequence to identify allele without specifying locus
- GET /db/{database}/sequences Get summary of defined sequences
- GET /db/{database}/schemes List schemes
- GET /db/{database}/schemes/{scheme_id} Retrieve scheme information
- GET /db/{database}/schemes/{scheme_id}/loci Retrieve scheme loci
- GET /db/{database}/schemes/{scheme_id}/fields/{field} Retrieve information about scheme field
- GET /db/{database}/schemes/{scheme_id}/profiles List allelic profiles defined for scheme
- GET /db/{database}/scheme_id}/profiles_csv Download allelic profiles in CSV (tab-delimited) format
- GET /db/{database}/schemes/{scheme_id}/profiles/{profile_id} Retrieve allelic profile record
- *POST /db/{database}/scheme_id}/sequence* Query sequence to extract allele designations/fields for a scheme
- GET /db/{database}/isolates Retrieve list of isolate records
- GET /db/{database}/genomes Retrieve list of isolate records that have genome assemblies
- POST /db/{database}/isolates/search Search isolate database
- GET /db/{database}/isolates/{isolate_id} Retrieve isolate record
- GET /db/{database}/isolates/{isolate_id}/allele_designations Retrieve list of allele designations

- GET /db/{database}/isolates/{isolate_id}/allele_designations/{locus} Retrieve full allele designation record
- GET /db/{database}/isolates/{isolate_id}/allele_ids Retrieve allele identifiers
- *GET /db/{database}/isolate_id}/schemes/{scheme_id}/allele_designations* Retrieve scheme allele designation records
- *GET /db/{database}/isolate_id}/schemes/{scheme_id}/allele_ids* Retrieve list of scheme allele identifiers
- GET /db/{database}/isolates/{isolate_id}/contigs Retrieve list of contigs
- GET /db/{database}/isolates/{isolate_id}/contigs_fasta Download contigs in FASTA format
- GET /db/{database}/isolates/{isolate_id}/history Retrieve isolate update history
- GET /db/{database}/contigs/{contig_id} Retrieve contig record
- *GET /db/{database}/fields* Retrieve list of isolate provenance field descriptions
- GET /db/{database}/fields/{field} Retrieve values set for a provenance field
- GET /db/{database}/users/{user_id} Retrieve user information
- GET /db/{database}/projects Retrieve list of projects
- *GET /db/{database}/projects/{project_id}* Retrieve project information
- GET /db/{database}/projects/{project_id}/isolates Retrieve list of isolates belonging to a project
- GET /db/{database}/submissions Retrieve list of submissions
- POST /db/{database}/submissions Create new submission
- GET /db/{database}/submissions/{submission_id} Retrieve submission record
- DELETE /db/{database}/submissions/{submission_id} Delete submission record
- GET /db/{database}/submissions/{submission_id}/messages Retrieve submission correspondence
- POST /db/{database}/submissions/{submission_id}/messages Add submission correspondence
- GET/db/{database}/submissions/{submission_id}/files retrieve list of supporting files uploaded for submission
- POST /db/{database}/submissions/{submission_id}/files Upload submission supporting file
- GET /db/{database}/submissions/{submission_id}/files/{filename} Download submission supporting file
- DELETE /db/{database}/submissions/{submission_id}/files/{filename} Delete submission supporting file

#### 17.3.1 GET / or /db - List site resources

#### Required route parameters: None

**Optional query parameters:** None

#### Example request URI: http://rest.pubmlst.org/

**Response:** List of resource groupings (ordered by name). Groups may consist of paired databases for sequence definitions and isolate data, or any set of related resources. Each group contains:

- name [string] short name (usually a single word)
- description [string] fuller description
- databases [array] list of database objects, each consists of three key/value pairs:
  - name [string] name of database config

- description [string] short description of resource
- href [string] URI to access resource

### 17.3.2 GET /db/{database} - List database resources

These will vary depending on whether the resource is an isolate or a sequence definition database.

Required route parameter: database [string] - Database configuration name

**Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates

**Response:** Object containing a subset of the following key/value pairs:

- *fields* [string] URI to isolate provenance field information
- isolates [string] URI to isolate records
- genomes [string] URI to genome records
- · schemes [string] URI to list of schemes
- loci [string] URI to list of loci
- projects [string] URI to list of projects

#### 17.3.3 GET /db/{database}/classification_schemes - List classification schemes

Required route parameter: database [string] - Database configuration name

**Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/classification_schemes

Response: Object containing:

- records [integer] Number of classification schemes.
- classification_schemes [array] List of URIs to classificaton schemes.

# 17.3.4 GET /db/{database}/classification_schemes/{classification_scheme_id} - Retrieve classification scheme information and groups

Sequence definition databases only.

#### **Required route parameters:**

- database [string] Database configuration name
- classification_scheme_id [integer] Classification scheme id number

**Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/classification_schemes/1

Response: Object containing some or all of:

- id [integer] Classification scheme id
- name [text] Name of classification scheme
- description [text] Description of classification scheme

- relative_threshold [boolean] True if a relative thresold is used
- inclusion_threshold [integer] The threshold for number of loci difference used to group
- groups [array] (sequence definition databases only) list of group objects consisting of:
  - id [integer] group id
  - profiles [array] list of URIs to profiles belonging to the group

## 17.3.5 GET /db/{database}/classification_schemes/{classification_scheme_id}/groups/{group_id - List isolates belonging to a classification scheme group

Isolate databases only.

#### **Required route parameters:**

- database [string] Database configuration name
- classification_scheme_id [integer] Classification scheme id number
- group_id [integer] Group id number

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/classification_schemes/4/groups/65

#### Response: Object containing of:

- records [integer] Number of isolates
- isolates [array] List of *URIs to isolate records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

### 17.3.6 GET /db/{database}/loci - List loci

#### Required route parameter: database [string] - Database configuration name

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.
- alleles_added_after [date] Include only loci with alleles added after specified date (ISO 8601 format). Only recognized in sequence definition databases.

• alleles_updated_after [date] - Include only loci with alleles last modified after specified date (ISO 8601 format). Only recognized in sequence definition databases.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci

Response: Object containing:

- records [integer] Number of loci
- loci [array] List of *URIs to defined locus records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

**Note:** See also the *scheme specific version*, allowing filtering by date of last allele update for just the loci that are members of a scheme.

# 17.3.7 GET /db/{database}/loci/{locus} - Retrieve locus record

Provides information about a locus, including links to allele sequences (in seqdef databases).

#### **Required route parameters:**

- database [string] Database configuration name
- locus [string] Locus name
- **Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ

Response: Object containing a subset of the following key/value pairs:

- id [string] locus name
- data_type [string] 'DNA' or 'peptide'
- allele_id_format [string] 'integer' or 'text'
- allele_id_regex [string] regular expression constraining allele ids
- common_name [string]
- aliases [array] list of alternative names of the locus
- length_varies [boolean]
- length [integer] length if alleles are of a fixed length
- coding_sequence [boolean]
- orf [integer] 1-6
- schemes [array] list of scheme objects, each consisting of:
  - scheme [string] URI to scheme information

- description [string]
- min_length [integer] (seqdef databases) minimum length for variable length loci
- max_length [integer] (seqdef databases) maximum length for variable length loci
- alleles [string] (seqdef databases) URI to list of allele records
- alleles_fasta [string] (seqdef databases) URI to FASTA file of all alleles of locus
- curators [array] (seqdef databases) list of URIs to user records of curators of the locus
- publications [array] (seqdef databases) list of PubMed id numbers of papers describing the locus
- full_name [string] (seqdef databases)
- product [string] (seqdef databases)
- description [string] (seqdef databases)
- extended_attributes [array] (seqdef databases) list of extended attribute objects. Each consists of a subset of the following fields:
  - field [string] field name
  - value_format [string] 'integer', 'text', or 'boolean'
  - value_regex [string] regular expression constraining value
  - description [string] description of field
  - length [integer] maximum length of field
  - required [boolean]
  - allowed_values [array] list of allowed values
- genome_position [integer] (isolate databases)

# 17.3.8 GET /db/{database}/loci/{locus}/alleles - Retrieve list of alleles defined for a locus

#### **Required route parameters:**

- database [string] Database configuration name
- locus [string] Locus name

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.
- added_after [date] Include only alleles added after specified date (ISO 8601 format).
- added_on [date] Include only alleles added on specified date (ISO 8601 format).
- updated_after [date] Include only alleles last modified after specified date (ISO 8601 format).
- updated_on [date] Include only alleles last modified on specified date (ISO 8601 format).

#### Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles

#### Response: Object containing:

- records [integer] Number of alleles.
- last_updated [date] Latest allele addition/modification date (ISO 8601 format).
- alleles [array] List of *URIs to defined allele records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

# 17.3.9 GET /db/{database}/loci/{locus}/alleles_fasta - Download alleles in FASTA format

#### **Required route parameters:**

- database [string] Database configuration name
- locus [string] Locus name

#### **Optional parameters:**

- added_after [date] Include only alleles added after specified date (ISO 8601 format).
- added_on date] Include only alleles added on specified date (ISO 8601 format).
- updated_after [date] Include only alleles last modified after specified date (ISO 8601 format).
- updated_on [date] Include only alleles last modified on specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles_fasta

Response: FASTA format file of allele sequences

# 17.3.10 GET /db/{database}/loci/{locus}/alleles/{allele_id} - Retrieve full allele information

#### **Required route parameters:**

- database [string] Database configuration name
- locus [string] Locus name
- allele_id [string] Allele identifier

#### **Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles/5

Response: Object containing the following key/value pairs:

- locus [string] URI to locus description
- allele_id [string] allele identifier
- sequence [string] sequence

- status [string] either 'Sanger trace checked', 'WGS: manual extract', 'WGS: automated extract', or 'unchecked'
- sender [string] URI to user details of sender
- curator [string] URI to user details of curator
- date_entered [string] record creation date (ISO 8601 format)
- datestamp [string] last updated date (ISO 8601 format)

### 17.3.11 POST /db/{database}/loci/{locus}/sequence - Query sequence to identify allele

#### **Required route parameters:**

- database [string] Database configuration name
- locus [string] Locus name

#### **Required additional parameters (JSON-encoded in POST body):**

• sequence [string] - Sequence string or base64-encoded FASTA file

#### **Optional parameters (JSON-encoded in POST body):**

- details [true/false] Return detailed exact match parameters
- base64 [true/false] Sequence is a base64-encoded FASTA file

**Response:** Object containing the following key/value pairs:

- exact_matches [array] list of match objects, each consisting of:
  - allele_id
  - href URI to allele record.

additionally if 'details' parameter passed:

- start start position on query
- end end position on query
- orientation forward/reverse
- length length of matched allele
- contig contig name if FASTA file is uploaded

If the locus is linked to field data in client isolate databases, there may also be an object called 'linked_data' containing values and frequencies of the field for the returned allele.

- best_match [object] consisting of key/value pairs (if no exact matches)
  - allele_id
  - href URI to allele record.
  - start start position on query (predicted taking account of allele length)
  - end end position on query (predicted taking account of allele length)
  - orientation forward/reverse
  - length length of matched allele
  - alignment length of BLAST alignment

- mismatches number of mismatches
- identity %identity of match
- gaps number of gaps in alignment

# 17.3.12 POST /db/{database}/sequence - Query sequence to identify allele without specifying locus

#### **Required route parameters:**

• database [string] - Database configuration name

#### **Required additional parameters (JSON-encoded in POST body):**

• sequence [string] - Sequence string or base64-encoded FASTA file

#### **Optional parameters (JSON-encoded in POST body):**

- details [true/false] Return detailed exact match parameters
- base64 [true/false] Sequence is a base64-encoded FASTA file

#### **Response:**

- exact_matches [object] consisting of locus keys, each consisting of array of match objects consisting of:
  - allele_id
  - href URI to allele record.

additionally if 'details' parameter passed:

- start start position on query
- end end position on query
- orientation forward/reverse
- length length of matched allele
- contig contig name if FASTA file is uploaded

If the locus is linked to field data in client isolate databases, there may also be an object called 'linked_data' containing values and frequencies of the field for the returned allele.

**Note:** This method only supports exact matches. If no match is indicated for a specific locus, use the *locus-specific call* to identify the closest match.

#### 17.3.13 GET /db/{database}/sequences - Get summary of defined sequences

Required route parameter: database [string] - Database configuration name

#### **Optional parameters:**

- added_after [date] Count only alleles added after specified date (ISO 8601 format).
- added_on [date] Count only alleles added on specified date (ISO 8601 format).
- updated_after [date] Count only alleles last modified after specified date (ISO 8601 format).
- updated_on [date] Count only allele updated on specified date (ISO 8601 format).

#### Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/sequences

Response: Object containing a subset of the following key/value pairs:

- *loci* [string] URI to list of loci
- records [integer] Number of alleles defined
- last_updated [date] Latest allele addition/modification date (ISO 8601 format).

### 17.3.14 GET /db/{database}/schemes - List schemes

Required route parameter: database [string] - Database configuration name

**Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes

#### **Response:**

- records [integer] Number of schemes
- schemes [array] list of scheme objects, each containing:
  - scheme [string] URI to scheme information
  - description [string]

## 17.3.15 GET /db/{database}/schemes/{scheme_id} - Retrieve scheme information

Includes links to allelic profiles (in seqdef databases, if appropriate). Required route parameters:

- database [string] Database configuration name
- scheme_id [integer] Scheme id number

#### **Optional parameters:**

- added_after [date] Count only profiles added after specified date (ISO 8601 format).
- added_on [date] Count only profiles added on specified date (ISO 8601 format).
- updated_after [date] Count only profiles last modified after specified date (ISO 8601 format).
- updated_on [date] Count only profiles updated on specified date (ISO 8601 format).

#### Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1

Response: Object containing a subset of the following key/value pairs:

- id [integer]
- description [string]
- · locus_count [integer] number of loci belonging to scheme
- loci [array] list of URIs to locus descriptions
- has_primary_key_field [boolean]
- fields [array] list of URIs to scheme field descriptions
- primary_key_field [string] URI to primary key field description
- profiles [string] URI to list of profile definitions (only seqdef databases)
- profiles_csv [string] URI to tab-delimited file of all scheme profiles

- curators [array] (seqdef databases) list of URIs to user records of curators of the scheme
- records [integer] Number of profiles
- last_added [date] Latest profile addition/modification date (ISO 8601 format).
- last_updated [date] Latest profile addition/modification date (ISO 8601 format).

# 17.3.16 GET /db/{database}/schemes/{scheme_id}/loci - Retrieve scheme loci

#### **Required route parameters:**

- database [string] Database configuration name
- scheme_id [integer] Scheme id number

#### **Optional parameters:**

- alleles_added_after [date] Include only loci with alleles added after specified date (ISO 8601 format). Only recognized in sequence definition databases.
- alleles_updated_after [date] Include only loci with alleles last modified after specified date (ISO 8601 format). Only recognized in sequence definition databases.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/loci

#### Response: Object containing:

- records [integer] Number of loci
- loci [array] List of URIs to defined locus records.

# 17.3.17 GET /db/{database}/schemes/{scheme_id}/fields/{field} - Retrieve information about scheme field

#### **Required route parameters:**

- database [string] Database configuration name
- scheme_id [integer] Scheme id number
- field [string] Field name

#### **Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/fields/ST

Response: Object containing the following key/value pairs:

- field [string] field name
- type [string] data type of field (integer or text)
- primary_key [boolean] true if field is the scheme primary key

# 17.3.18 GET /db/{database}/schemes/{scheme_id}/profiles - List allelic profiles defined for scheme

#### **Required route parameters:**

• database [string] - Database configuration name

• scheme_id [integer] - Scheme id

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.
- added_after [date] Include only profiles added after specified date (ISO 8601 format).
- added_on [date] Include only profiles added on specified date (ISO 8601 format).
- updated_after [date] Include only profiles last modified after specified date (ISO 8601 format).
- updated_on [date] Include only profiles last modified on specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles

#### Response: Object containing:

- records [integer] Number of profiles
- last_updated [date] Latest profile addition/modification date (ISO 8601 format).
- profiles [array] List of *URIs to defined profile records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

**Note:** This method also supports content negotiation. If the request accepts header includes TSV or CSV, then the call is redirected to /*db*/{*database*}/*scheme_id*}/*profiles_csv*.

# 17.3.19 GET /db/{database}/schemes/{scheme_id}/profiles_csv - Download allelic profiles in CSV (tab-delimited) format

#### **Required route parameters:**

- database [string] Database configuration name
- scheme_id [integer] Scheme id

#### **Optional parameters:**

- added_after [date] Include only profiles added after specified date (ISO 8601 format).
- added_on [date] Include only profiles added on specified date (ISO 8601 format).
- updated_after [date] Include only profiles last modified after specified date (ISO 8601 format).
- updated_on [date] Include only profiles last modified on specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles_csv

Response: Tab-delimited text file of allelic profiles

# 17.3.20 GET /db/{database}/schemes/{scheme_id}/profiles/{profile_id} - Retrieve allelic profile record

#### **Required route parameters:**

- database [string] Database configuration name
- scheme_id [integer] Scheme id
- profile_id [string/integer] Profile id

#### **Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles/11

Response: Object containing the following key/value pairs:

- *primary_key_term* [string/integer] The field name is the primary key, e.g. ST. The value is the primary key value (primary_id used as an argument).
- alleles [object] list of URIs to allele descriptions
- *other_scheme_fields* [string/integer] Each scheme field will have its own value if defined. The field name is the name of the field.
- sender [string] URI to user details of sender
- curator [string] URI to user details of curator
- date_entered [string] record creation date (ISO 8601 format)
- datestamp [string] last updated date (ISO 8601 format)

# 17.3.21 POST /db/{database}/schemes/{scheme_id}/sequence - Query sequence to extract allele designations/fields for a scheme

#### **Required route parameters:**

- database [string] Database configuration name
- scheme_id [integer] Scheme id

#### Required additional parameters (JSON-encoded in POST body):

• sequence [string] - Sequence string or base64-encoded FASTA file

#### **Optional parameters (JSON-encoded in POST body):**

- details [true/false] Return detailed exact match parameters
- base64 [true/false] Sequence is a base64-encoded FASTA file

**Response:** Object containing the following key/value pairs:

- exact_matches [array] list of match objects, each consisting of:
  - allele_id
  - href URI to allele record.

additionally if 'details' parameter passed:

- start start position on query
- end end position on query
- orientation forward/reverse
- length length of matched allele
- contig contig name if FASTA file is uploaded

If the locus is linked to field data in client isolate databases, there may also be an object called 'linked_data' containing values and frequencies of the field for the returned allele.

Example curl call to upload a FASTA file 'contigs.fasta' and extract MLST results from Neisseria database:

**Note:** This method only supports exact matches. If no match is indicated for a specific locus, use the *locus-specific call* to identify the closest match.

#### 17.3.22 GET /db/{database}/isolates - Retrieve list of isolate records

Required route parameter: database [string] - Database configuration name

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.
- added_after [date] Include only isolates added after specified date (ISO 8601 format).
- added_on [date] Include only isolates added on specified date (ISO 8601 format).
- updated_after [date] Include only isolates last modified after specified date (ISO 8601 format).
- updated_on [date] Include only isolates updated on specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates

#### Response: Object containing:

- · records [integer] Number of isolates
- isolates [array] List of *URIs to isolate records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

# 17.3.23 GET /db/{database}/isolates/{isolate_id} - Retrieve isolate record

#### **Required route parameters:**

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

#### **Optional parameter:**

• provenance_only [integer] - Set to non-zero value to only return provenance metadata

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1

Response: Object containing some or all of the following key/value pairs:

- provenance [object] set of key/value pairs. Keys are defined by calling the */fields route* route. The fields will vary by database but will always contain the following:
  - id [integer]
  - sender [string] URI to user details of sender
  - curator [string] URI to user details of curator
  - date_entered [string] record creation date (ISO 8601 format)
  - datestamp [string] last updated date (ISO 8601 format)
- publications [array] (seqdef databases) list of PubMed id numbers of papers that refer to the isolate
- sequence_bin [object] consists of the following key/value pairs:
  - contigs_fasta [string] URI to FASTA file containing all the contigs belonging to this isolate
  - contigs [string] URI to list of contig records
  - contig_count [integer] number of contigs
  - total_length [integer] total length of contigs
- allele_designations [object] consists of the following key/value pairs:
  - allele_ids URI to list of all allele_id values defined for the isolate
  - designation_count number of allele designations defined for the isolate
  - full_designations URI to list of full allele designation records
- schemes [array] list of scheme objects, each containing some of the following:
  - description [string] description of scheme
  - loci_designated_count [integer] number of loci within scheme that have an allele designated for this isolate.
  - allele_ids [string] URI to list of all allele_id values defined for this scheme for this isolate
  - full_designations [string] URI to list of full allele designation records for this isolate
  - fields [object] consisting of key/value pairs where the key is the name of each scheme field
  - classification_schemes [object] consisting of key/value pairs, where each key is the name of the classification scheme and the value is an object consisting of:
    - * href [string] URI to classification scheme description
    - * groups [array] list of group objects consisting of:
      - · group [integer] group id

- · records [integer] number of isolates in group
- · isolates [string] URI to classification group record containing URIs to member isolate records
- projects [array] list of project objects, each containing the following:
  - id [string] URI to project information
  - description [string] description of project
- history [string] URI to isolate history record
- new_version [string] URI to newer version of record
- old_version [string] URI to older version of record

# 17.3.24 GET /db/{database}/isolates/{isolate_id}/allele_designations - Retrieve list of allele designation records

#### **Required route parameters:**

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_designations

#### Response: Object containing:

- records [integer] Number of allele designations
- allele_designations [array] List of *URIs to allele designation records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

### 17.3.25 GET /db/{database}/isolates/{isolate_id}/allele_designations/{locus} - Retrieve full allele designation record

#### **Required route parameters:**

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier
- locus [string] Locus name

#### **Optional parameters:** None

**Example request URI:** http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_designations/ BACT000065

**Response:** List of allele_designation objects (there may be multiple designations for the same locus), each containing:

- locus [string] URI to locus description
- allele_id [string]
- method [string] either 'manual' or 'automatic'
- status [string] either 'confirmed' or 'provisional'
- comments [string]
- sender [string] URI to user details of sender
- curator [string] URI to user details of curator
- datestamp [string] last updated date (ISO 8601 format)

## 17.3.26 GET /db/{database}/isolates/{isolate_id}/allele_ids - Retrieve allele identifiers

#### **Required route parameters:**

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_ids

#### Response: Object containing:

- records [integer] Number of allele id objects
- allele_ids [array] List of allele id objects, each consisting of a key/value pair where the key is the locus name. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

## 17.3.27 GET/db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_designations - Retrieve scheme allele designation records

#### **Required route parameters:**

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier
- scheme_id [integer] Scheme identifier

#### **Optional parameters:** None

**Example request URI:** http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/schemes/1/allele_designations

#### **Response:**

- records [integer] Number of allele designation objects
- allele_designations [array] List of *allele designation objects* for each locus in the specified scheme that has been designated.

## 17.3.28 GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_ids -Retrieve list of scheme allele identifiers

#### **Required route parameters:**

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier
- scheme_id [integer] Scheme identifier

#### **Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/schemes/1/allele_ids

#### **Response:**

- records [integer] Number of allele id objects
- allele_ids [array] List containing allele id objects for each locus in the specified scheme that has been designated. Each allele_id object contains a key which is the name of the locus with a value that may be either a string, integer or array of strings or integers (required where there are multiple designations for a locus). The data type depends on the allele_id_format set for the specific locus.

# 17.3.29 GET /db/{database}/isolates/{isolate_id}/contigs - Retrieve list of contigs

#### **Required route parameters:**

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/contigs

Response: Object containing:

- records [integer] Number of contigs
- contigs [array] List of *URIs to contig records* Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

## 17.3.30 GET /db/{database}/isolates/{isolate_id}/contigs_fasta - Download contigs in FASTA format

#### **Required route parameters:**

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

#### **Optional parameter:**

• header [string] - either 'original_designation' or 'id' (default is 'id'). This selects whether the FASTA header lines contain the originally uploaded FASTA headers or the sequence bin id numbers.

**Example request URI:** http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/contigs_fasta?header= original_designation

Response: FASTA format file of isolate contig sequences

# 17.3.31 GET /db/{database}/isolates/{isolate_id}/history - Retrieve isolate update history

#### **Required route parameters:**

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

**Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/1/history

Response: Object containing:

- records [integer] Number of updayes
- contigs [array] List of update objects each consisting of the following key/value pairs:
  - curator [string] URI to user details of curator
  - timestamp [string] Time of update
  - actions [array] List of update descriptions [strings]

# 17.3.32 GET /db/{database}/genomes - Retrieve list of isolate records that have genome assemblies

**Required route parameter:** database [string] - Database configuration name

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.
- added_after [date] Include only isolates added after specified date (ISO 8601 format).
- added_on [date] Include only isolates added on specified date (ISO 8601 format).
- updated_after [date] Include only isolates last modified after specified date (ISO 8601 format).
- updated_on [date] Include only isolates updated on specified date (ISO 8601 format).
- genome_size [integer] Filter to only include records with a sequence bin of at least the specified size (default is 500,000bp).

#### Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/genomes

#### Response: Object containing:

- records [integer] Number of isolates
- isolates [array] List of *URIs to isolate records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

## 17.3.33 POST /db/{database}/isolates/search - Search isolate database

#### **Required route parameters:**

• database [string] - Database configuration name

#### **Optional parameters (appended to URI):**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

#### Query parameters (JSON-encoded in POST body):

You must include at least one query parameter.

Parameter names in the following forms are supported:

• field.{field} - key/value pairs for provenance fields. Supported field names can be found by calling the */fields route*. The fields will vary by database.

- locus.{locus} key/value pairs of locus and its allele designation. Supported locus names can be found by calling the */loci route*.
- scheme_id}.{scheme_field} key/value pairs of scheme fields and their values. Supported field names can be determined by following routes from the */schemes route*.

**Example method call using curl:** The following searches for *Neisseria* ST-11 isolates from Europe in 2015 (MLST is scheme#1 in this database).

```
curl -s -H "Content-Type: application/json" -X POST \
"http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/search" \
-d '{"field.continent":"europe","field.year":2015,"scheme.1.ST":11}'
```

#### Response: Object containing:

- · records [integer] Number of isolates
- isolates [array] List of *URIs to isolate records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

### 17.3.34 GET /db/{database}/contigs/{contig_id} - Retrieve contig record

#### **Required route parameters:**

- database [string] Database configuration name
- contig_id [integer] Contig identifier

#### **Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/contigs/180062

Response: Contig object consisting of the following key/value pairs:

- id [integer] contig identifier
- isolate_id [integer] isolate identifier
- sequence [string] contig sequence
- length [integer] length of contig sequence
- method [string] sequencing method
- sender [string] URI to user details of sender
- curator [string] URI to user details of curator
- date_entered [string] record creation date (ISO 8601 format)
- datestamp [string] last updated date (ISO 8601 format)
- loci [array] list of sequence tag objects consisting of:

- locus [string] URI to locus description
- locus_name [string]
- start [integer]
- end [integer]
- direction [string] forward/reverse
- complete [boolean] true/false

## 17.3.35 GET /db/{database}/fields - Retrieve list of isolate provenance field descriptions

#### **Required route parameters:**

• database [string] - Database configuration name

#### **Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/fields

Response: Array of field objects, each consisting of some or all of the following key/value pairs:

- name [string] name of field
- type [string] data type (int, text, date, float)
- length [integer] maximum length of field
- required [boolean] true if field value is required
- min [integer] minimum value for integer values
- max [integer] maximum value for integer values
- regex [string] regular expression that constrains the allowed value of the field
- comments [string]
- allowed values [array] list of allowed values for the field
- values [string] URI to list of used field values

### 17.3.36 GET /db/{database}/fields/{field} - Retrieve values set for a provenance field

#### **Required route parameters:**

- database [string] Database configuration name
- field [string] Provenance metadata field name

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

#### Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/fields/country

Response: Object containing:

• records [integer] - Number of values

- values [array] List of values used in isolate records. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

## 17.3.37 GET /db/{database}/users/{user_id} - Retrieve user information

Users may be data submitters or curators.

#### **Required route parameters:**

- database [string] Database configuration name
- user_id [integer] User id number

#### **Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/users/2

**Response:** Object containing the following key/value pairs:

- id [integer] user id number
- first_name [string]
- surname [string]
- affiliation [string] institutional affiliation
- email [string] E-mail address

## 17.3.38 GET /db/{database}/projects - Retrieve list of projects

Required route parameter: database [string] - Database configuration name

**Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/projects

#### **Response:**

- projects [array] List of project objects, each containing:
  - project [string] URI to project information
  - description [string]
  - isolate_count [integer] number of isolates in project

## 17.3.39 GET /db/{database}/projects/{project_id} - Retrieve project information

#### **Required route parameters:**

- database [string] Database configuration name
- project_id [integer] Project id number

#### **Optional parameters:** None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/projects/3

Response: Object containing a subset of the following key/value pairs:

- id [integer]
- description [string]
- isolates [string] URI to list of URIs of member isolate records.

# 17.3.40 GET /db/{database}/projects/{project_id}/isolates - Retrieve list of isolates belonging to a project

#### **Required route parameter:**

- database [string] Database configuration name
- project_id [integer] Project id number

#### **Optional parameters:**

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/projects/3/isolates

#### Response: Object containing:

- records [integer] Number of isolates in the project
- isolates [array] List of URIs to isolate records. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

## 17.3.41 GET /db/{database}/submissions - retrieve list of submissions

Required route parameter: database [string] - Database configuration name

#### **Optional parameters:**

• type [string] - either 'alleles', 'profiles' or 'isolates'

- status [string] either 'closed' or 'pending'
- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/submissions

#### Response: Object containing:

- records [integer] Number of submissions
- submissions [array] List of URIs to submission records
- paging [object] Some or all of the following:
  - previous URI to previous page of results
  - next URI to next page of results
  - first URI to first page of results
  - last URI to last page of results
  - return_all URI to page containing all results (paging disabled)

### 17.3.42 POST /db/{database}/submissions - create new submission

Required route parameter: database [string] - Database configuration name

#### **Required additional parameters (JSON-encoded in POST body):**

- type [string] either:
  - alleles (sequence definition databases only)
  - profiles (sequence definition databases only)
  - isolates (isolate databases only)
  - genomes (isolate databases only)

The following are required with the specified database type:

#### Allele submissions

- locus [string] name of locus
- technology [string] name of sequencing technology: either '454', 'Illumina', 'Ion Torrent', 'PacBio', 'Oxford Nanopore', 'Sanger', 'Solexa', 'SOLiD', or 'other'
- read_length [string] read length of sequencing: either '<100', '100-199', '200-299', '300-499', '>500', or any positive integer (only required for Illumina)
- coverage [string] mean coverage of sequencing: either '<20x', '20-49x', '50-99x', '>100x', or any positive integer (only required for Illumina)
- assembly [string] assembly method: either 'de novo' or 'mapped'
- software [string] name of assembly software
- sequences [string] either single raw sequence or multiple sequences in FASTA format

#### **Profile submissions**

· scheme_id [integer] - scheme id number

• profiles [string] - tab-delimited profile data - this should include a header line containing the name of each locus

#### **Isolate submissions**

• isolates [string] - tab-delimited isolate data - this should include a header line containing each field or locus included

#### Genome submissions

• isolates [string] - tab-delimited isolate data - this should include a header line containing each field or locus included as well as for 'assembly_filename' and 'sequence_method'. The 'sequence_method' should be either '454', 'Illumina', 'Ion Torrent', 'PacBio', 'Oxford Nanopore', 'Sanger', 'Solexa', 'SOLiD', or 'other'. Follow-ing submission, contig files should be uploaded with the same names as set for 'assembly_filename'. This can be done using the *file upload route*.

#### **Optional parameters:**

- message [string] correspondence to the curator
- email [integer] set to 1 to enable E-mail updates (E-mails will be sent to the registered user account address).

#### Response: Object containing:

• submission - URI to submission record

For genome submissions, the response object will also contain:

- missing_files [array] List of filenames that need to be uploaded to complete the submission. These filenames are defined in the 'assembly_filename' field of the isolate record upload. The files should contain the contig assemblies.
- message [string] 'Please upload missing contig files to complete submission.'

# 17.3.43 GET /db/{database}/submissions/{submission_id} - Retrieve submission record

#### **Required route parameters:**

- database [string] Database configuration name
- submission_id [string] Submission id

#### **Optional parameters:** None

ExamplerequestURI:http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740

**Response:** Object containing some of the following:

- id [string] Submission id
- type [string] Either 'alleles', 'profiles', 'isolates'
- date_submitted [string] Submission date (ISO 8601 format)
- datestamp [string] Last updated date (ISO 8601 format)
- submitter [string] URI to user details of submitter
- curator [string] URI to user details of curator
- status [string] either 'started', 'pending', or 'closed'
- outcome [string] either 'good' (data uploaded), 'bad' (data rejected), or 'mixed' (parts of submission accepted)
- correspondence [array] List of correspondence objects in time order. Each contains:

- user [string] URI to user details of user
- timestamp [string]
- message [string]

#### Allele submissions

- · locus [string] name of locus
- technology [string] name of sequencing technology: either '454', 'Illumina', 'Ion Torrent', 'PacBio', 'Oxford Nanopore', 'Sanger', 'Solexa', 'SOLiD', or 'other'
- read_length [string] read length of sequencing: either '<100', '100-199', '200-299', '300-499', '>500', or any positive integer (only required for Illumina)
- coverage [string] mean coverage of sequencing: either '<20x', '20-49x', '50-99x', '>100x', or any positive integer (only required for Illumina)
- assembly [string] assembly method: either 'de novo' or 'mapped'
- software [string] name of assembly software
- seqs [array] List of sequence objects each containing:
  - seq_id [string] Sequence identifier
  - assigned_id [string] Allele identifier if uploaded to the database (otherwise undefined)
  - status [string] Either 'pending', 'assigned', or 'rejected'
  - sequence [string]

#### **Profile submissions**

- scheme [string] URI to scheme information
- profiles [array] List of profile record objects. Each contains:
  - profile_id [string] Record identifier
  - assigned_id [string] Profile identifier if uploaded to the database (otherwise undefined)
  - status [string] Either 'pending', 'assigned', or 'rejected'
  - designations [object] containing key/value pairs for each locus containing the allele identifier

#### Isolate submissions

isolates [array] - List of isolate record objects. Each contains key/value pairs for included fields.

# 17.3.44 DELETE /db/{database}/submissions/{submission_id} - Delete submission record

You must be the owner and the record must be closed.

#### **Required route parameters:**

- database [string] Database configuration name
- submission_id [string] Submission id

#### **Optional parameters:** None

```
Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740
```

Response: message [string] - 'Submission deleted.'

# 17.3.45 GET /db/{database}/submissions/{submission_id}/messages - Retrieve submission correspondence

#### **Required route parameters:**

- database [string] Database configuration name
- submission_id [string] Submission id

#### **Optional parameters:** None

**Example request URI:** http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740/messages

Response: Array of correspondence objects in time order. Each contains:

- user [string] URI to user details of user
- timestamp [string]
- message [string]

### 17.3.46 POST /db/{database}/submissions/{submission_id}/messages - Add submission correspondence

#### **Required route parameters:**

- database [string] Database configuration name
- submission_id [string] Submission id

#### Required additional parameter (JSON-encoded in POST body):

• message [string] - Message text

#### **Optional parameters:** None

Response: message [string] - 'Message added.'

# 17.3.47 GET /db/{database}/submissions/{submission_id}/files - Retrieve list of supporting files uploaded for submission

#### **Required route parameters:**

- database [string] Database configuration name
- submission_id [string] Submission id

#### **Optional parameters:** None

ExamplerequestURI:http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740/files

**Response:** Array of URIs to files

# 17.3.48 POST /db/{database}/submissions/{submission_id}/files - Upload submission supporting file

#### **Required route parameters:**

- database [string] Database configuration name
- submission_id [string] Submission id

#### Required additional parameters (JSON-encoded in POST body):

- filename [string] Name of file to store within submission
- upload [base64 encoded data] Raw file data

#### **Optional parameters:** None

Response: message [string] - 'File uploaded.'

## 17.3.49 GET /db/{database}/submissions/{submission_id}/files/{filename} - Download submission supporting file

#### **Required route parameters:**

- database [string] Database configuration name
- submission_id [string] Submission id
- filename [string] Name of file

#### **Optional parameters:** None

Response: File download

## 17.3.50 DELETE /db/{database}/submissions/{submission_id}/files/{filename} Delete submission supporting file

#### **Required route parameters:**

- database [string] Database configuration name
- submission_id [string] Submission id
- filename [string] Name of file

#### **Optional parameters:** None

Response: message [string] - 'File deleted.'

## **17.4 Authentication**

Protected resources, i.e. those requiring a user to log in, can be accessed via the API using OAuth (1.0A) authentication (see IETF RFC5849 for details). Third-party client software has to be registered with the BIGSdb site before they can access authenticated resources. The overall three-legged flow works as follows:

- 1. Developer signs up and gets a consumer key and consumer secret specific to their application.
- 2. Application gets a request token and directs user to authorization page on BIGSdb.

- 3. BIGSdb *asks user for authorization* for application to access specific resource using their credentials. A verifier code is provided.
- 4. The application exchanges the request token and OAuth verifier code for an *access token and secret* (these do not expire but may be revoked by the user or site admin).
- 5. Application uses access token/secret to request session token (this is valid for 12 hours).
- 6. All calls to access protected resources are signed using the session token/secret and consumer key/secret.

It is recommended that application developers use an OAuth library to generate and sign requests.

**Note:** There are Python and Perl example scripts available at https://github.com/kjolley/BIGSdb/tree/develop/scripts/ rest_examples to demonstrate and test OAuth authentication.

### 17.4.1 Developer sign up to get a consumer key

Application developers should apply to the site administrator of the site running BIGSdb. The administrator can *generate a key and secret* using a script - both of these will need to be used by the application to sign requests.

The client id is usually a 24 character alphanumeric string. The secret is usually a 42 character alphanumeric (including punctuation) string, e.g.

- client_id: efKXmqp2D0EBlMBkZaGC2lPf
- client_secret: F\$M+fQ2AFFB2YBDfF9fpHF^qSWJdmmN%L4Fxf5Gur3

### 17.4.2 Getting a request token

- Relative URL: /db/{database}/oauth/get_request_token
- Supported method: GET

The application uses the consumer key to obtain a request token. The request token is a temporary token used to initiate user authorization for the application and will expire in 60 minutes. The request needs to contain the following parameters and to be signed using the consumer secret:

- oauth_consumer_key
- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_timestamp (UNIX timestamp seconds since Jan 1 1970) this must be within 600 seconds of the current time.
- oauth_callback ('oob' for desktop applications)
- oauth_nonce (random string)
- oauth_version ('1.0')

If the application has been registered and has been granted permission to access the specific resource, a JSON response will be returned containing the following parameters:

oauth_token

- This is the request token. It is usually a 32 character alphanumeric string.
- e.g. fKFm0WNhCfbEX8zQm6qhDA8K23FOWDGE
- oauth_token_secret
  - This is the secret associated with the request token. It is usually a 32 character alphanumeric string.
  - e.g. aZ0fncP7i5w5jlebdK5zyQ4vrRRVcdnv
- oauth_callback_confirmed
  - This parameter is always set to true.

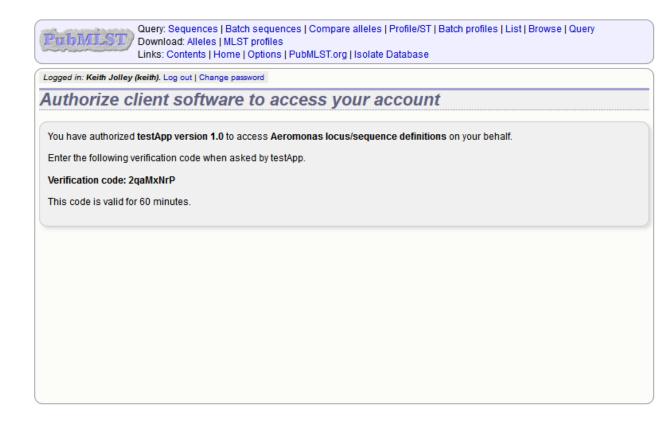
### 17.4.3 Getting user authorization

Once a request token has been obtained, this can be used by the end user to grant permission to access a specific resource to the application. The application should direct the user to the client authorization page (authorizeClient) specific to a database within BIGSdb, e.g. http://pubmlst.org/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_neisseria_seqdef& page=authorizeClient&oauth_token=fKFm0WNhCfbEX8zQm6qhDA8K23FOWDGE

The user will be asked if they wish to grant access to the application on their behalf:

Query: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query           Download: Alleles   MLST profiles           Links: Contents   Home   Options   PubMLST.org   Isolate Database	
Logged in: Keith Jolley (keith). Log out   Change password	
Authorize client software to access your account	
Do you wish for the following application to access data on your behalf?	
Application Resource	Action —
testApp version 1.0 Aeromonas locus/sequence definitions	Cancel Authorize
You will be able to revoke access for this application at any time.	

If they authorize the access, they will be presented with a verifier code. This should be entered in to the client application which will use this together with the request token to request an access token.



The verifier code is valid for 60 minutes.

## 17.4.4 Getting an access token

- Relative URL: /db/{database}/oauth/get_access_token
- Supported method: GET

The application uses the request token, verifier code and its consumer key to obtain an access token. The access token does not expire but can be revoked by either the end user or the site administrator. The request needs to contain the following parameters and to be signed using the consumer secret and request token secret:

- oauth_consumer_key
- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_token (request token)
- oauth_timestamp (UNIX timestamp seconds since Jan 1 1970) this must be within 600 seconds of the current time.
- oauth_nonce (random string)
- oauth_version ('1.0')

If the application has been registered and has been granted permission to access the specific resource, a JSON response will be returned containing the following parameters:

- oauth_token
  - This is the access token. It is usually a 32 character alphanumeric string.
  - e.g. SDrC74ZV15SYSqY8IWZqrRxnyDnNGVFO
- oauth_token_secret
  - This is the secret associated with the access token. It is usually a 32 character alphanumeric string.
  - e.g. tYI2SPzgiO02IRVzW4JR1ez6Vvm4gVyv

### 17.4.5 Getting a session token

- Relative URL: /db/{database}/oauth/get_session_token
- Supported method: GET

The application uses the access token and its consumer key to obtain a session token. The session token is valid for 12 hours before it expires. The request needs to contain the following parameters and to be signed using the consumer secret and access token secret:

- oauth_consumer_key
- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_token (access token)
- oauth_timestamp (UNIX timestamp seconds since Jan 1 1970) this must be within 600 seconds of the current time.
- oauth_nonce (random string)
- oauth_version ('1.0')

If the application has been registered and has been granted permission to access the specific resource, a JSON response will be returned containing the following parameters:

- oauth_token
  - This is the session token. It is usually a 32 character alphanumeric string.
  - e.g. H8CjIS8Ikq6hwCUqUfF1l4pTaCYl8Ljw
- oauth_token_secret
  - This is the secret associated with the session token. It is usually a 32 character alphanumeric string.
  - e.g. RfponbaNPO7tkZ2miHFISk0pMndePNfJ

### 17.4.6 Accessing protected resources

The application uses the session token and its consumer key to access a protected resource. The request needs to contain the following parameters and to be signed using the consumer secret and session token secret:

- oauth_consumer_key
- oauth_request_method ('GET')

- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_token (session token)
- oauth_timestamp (UNIX timestamp seconds since Jan 1 1970) this must be within 600 seconds of the current time.
- oauth_nonce (random string)
- oauth_version ('1.0')

# CHAPTER 18

## Frequently asked questions (FAQs)

## 18.1 General

#### 1. What is the minimum specification of hardware required to run BIGSdb?

The software will run on fairly modest hardware - a number of PubMLST mirrors have been set up on virtual machines with 1 processor core and 4 GB RAM. This should be considered an absolute minimum specification though. For an installation with only local users, the following minimum is recommended:

- 4 processor cores
- 16 GB RAM
- 50 GB partition for temporary files
- 100 GB partition for databases

As usual, the more RAM that is available the better. Ideally you would want enough RAM that the whole database(s) can reside in memory (an approximation is roughly twice the total size of your contigs), although this is not absolutely required.

Offline jobs, such as *Genome Comparator* will use multiple cores (depending on the settings in bigsdb.conf), so if you want to run multiple jobs in parallel then you may want more cores (and memory). Tagging of new genomes using the offline *autotagger* is usually run in multi-threaded mode so the more cores available the faster this will be.

As a comparison, the PubMLST site is run on two machines - separate web and database servers. All offline jobs and tagging of genomes is performed on the database server. These have the following specification:

- web server: 40 cores, 128GB RAM
- database server: 64 cores, 1TB RAM, 3TB RAID 10 local storage

#### 2. Why might icons be missing when using Internet Explorer?

This can occur if you have Compatibility Mode enabled. BIGSdb generates valid HTML5 and Compatibility Mode should not be used. Please ensure this is not enabled in the Internet Explorer tools section.

## **18.2 Installation**

#### 1. BIGSdb is accumulating files in various temp directories - is this normal and how do I clean them out?

See: Periodically delete temporary files.

#### 2. BIGSdb is complaining of an invalid script path - what does this mean?

In your database config.xml file system tag are two attributes - script_path_includes and curate_path_includes. These contain regexes that the web url to your script (bigsdb.pl and bigscurate.pl respectively) must match. This prevents somebody from accessing a private database using an instance of bigsdb.pl that is not in a protected directory if you're using apache authentication.

So, if you access the script from http://localhost/cgi-bin/bigsdb/bigsdb.pl then you can set script_path_includes to something like "/bigsdb/" (which is the default), or "/cgi-bin/" or just "/" if you don't care about this check.

## **18.3 Administration**

#### 1. How can I make some isolates public but not others?

The easiest way to do this is to set up two or more separate configuration directories that refer to the database. The URLs to access these will differ by the value of the 'db' attribute, which refers to the name of the configuration directory (in /etc/bigsdb/dbases/). The database view accessed by each of these configurations can be different as can the access restrictions.

Example:

We have a database 'bigsdb_test' that contains data, only some of which we wish to make publicly available. The isolates to make public are all members of a project. First we can make a view of the isolates table that contains only isolates within this project.

For isolates in project id 3, create a database view by logging in to psql as the postgresql user. We will name this view 'public'.:

```
sudo su postgres
psql bigsdb_test
CREATE VIEW public AS SELECT * FROM isolates WHERE id IN (SELECT isolate_id
FROM project_members WHERE project_id=3);
GRANT SELECT ON public TO apache;
```

Create a private configuration that can access everything in the database in /etc/bigsdb/dbases/test_private. This will be accessible from http://IP_ADDRESS/cgi-bin/bigsdb/bigsdb.pl?db=test_private.

The important attributes to set in the system tag of the config.xml file in this directory are::

```
view="isolates"
read_access="authenticated_users"
```

This means that anyone with an account can log in and view all the isolates (because the view is set to the isolates table).

Now create a public configuration in /etc/bigsdb/dbases/test_public. This will be accessible from http: //IP_ADDRESS/cgi-bin/bigsdb/bigsdb.pl?db=test_public. It is better to create a symlink to the private config.xml and then override the attributes that are different. So create a symlink to the private config file:

```
cd /etc/bigsdb/dbases/test_public
sudo ln -s ../test_private/config.xml .
```

You can now override the view and access settings. Within /etc/bigsdb/dbases/test_public, create a file called system.overrides and add the following:

```
view="public"
read_access="public"
```

See also Restricting particular configurations to specific user accounts.

# CHAPTER 19

# Appendix

## **19.1 Query operators**

Various query forms have operators for use with field values. Available operators are:

- =
- Exact match (case-insensitive).
- contains
  - Match to a partial string (case-insensitive), e.g. searching for clonal complex 'contains' st-11 would return all STs belonging to the ST-11 complex.
- starts with
  - Match to values that start with the search term (case-insensitive).
- ends with
  - Match to values that end with the search term (case-sensitive).
- >
- Greater than the search term.
- >=
  - Greater than or equal the search term.

• <

- Less than the search term.
- <=
  - Less than or equal the search term.

• NOT

- Match to values that do not equal the search term (case-insensitive).

- NOT contain
  - Match to values that do not contain the search term (case-insensitive).

## 19.2 Sequence tag flags

Sequences tagged in the sequence bin can have features indicated by specific flags. The presence of these flags can be queried. These are a superset of *flags available for allele sequences*. Available flags are:

- ambiguous read
  - Genome sequence contains ambiguous nucleotides in coding sequence.
- apparent misassembly
  - Sequence has a region of very high identity to existing allele in one region but looks completely different in another.
- atypical
  - Catch-all term for a sequence that is unusual compared to other alleles of locus.
- · contains IS element
  - Coding sequence is interrupted by insertion sequence.
- downstream fusion
  - No stop codon present resulting in translation continuing.
- frameshift
  - Frameshift in sequence relative to other alleles, not resulting in internal stop codon.
- indel
  - Insertion/deletion in sequence that is uncommon compared to other alleles.
- · internal stop codon
  - Frameshift in sequence relative to other alleles, resulting in internal stop codon.
- · no start codon
  - No apparent start codon in immediate vicinity of usual start.
- · no stop codon
  - No stop codon in immediate vicinity of usual stop.
- · phase variable: off
  - Coding sequence has a homopolymeric run with a frameshift resulting in a stop codon preventing complete translation.
- truncated
  - Coding sequence is unusually short resulting in a truncated protein (not the same as running off the end of a contig).
- · upstream fusion
  - No apparent start codon in immediate vicinity of usual start, likely due to a gene fusion (sequence is transcribed together with upstream coding sequence).

# 19.3 Allele sequence flags

Sequences can be flagged with specific attributes - these are searchable when doing a sequence attribute query. These are a subset of *flags available for tagged sequences*. These are mainly for use with whole genome MLST type data. Multiple flags can be selected by Ctrl-clicking the list. Available flags are:

- atypical
  - Catch-all term for a sequence that is unusual compared to other alleles of locus.
- · contains IS element
  - Coding sequence is interrupted by insertion sequence.
- downstream fusion
  - No stop codon present resulting in translation continuing.
- frameshift
  - Frameshift in sequence relative to other alleles, not resulting in internal stop codon.
- indel
  - Insertion/deletion in sequence that is uncommon compared to other alleles.
- internal stop codon
  - Frameshift in sequence relative to other alleles, resulting in internal stop codon.
- no start codon
  - No apparent start codon in immediate vicinity of usual start.
- no stop codon
  - No stop codon in immediate vicinity of usual stop.
- phase variable: off
  - Coding sequence has a homopolymeric run with a frameshift resulting in a stop codon preventing complete translation.
- truncated
  - Coding sequence is unusually short resulting in a truncated protein (not the same as running off the end of a contig).
- upstream fusion
  - No apparent start codon in immediate vicinity of usual start, likely due to a gene fusion (sequence is transcribed together with upstream coding sequence).

# CHAPTER 20

Database schema

- Sequence definition database
- Isolate database

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