# **BIGSdb Documentation**

Release 1.27.0

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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.

- 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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### 3.2.2 pg\_ident.conf

# MAPNAME	SYSTEM-USERNAME	<i>PG-USERNAME</i>
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.
- 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

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.  $1.7 \rightarrow 1.8$ , 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.

The xml directory of the software archive contains example XML files for sequence definition and isolate databases (rename these to config.xml). The isolates\_config.xml file contains the minimum required isolate table fields and matches the isolate table that will be generated using the isolatedb.sql SQL script.

# 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').
- delete\_retire\_only
  - Set to 'yes' to retire the id of any isolate that is deleted. This prevents re-use of ids. This setting will override the global setting in bigsdb.conf.
- 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: 'secondary metadata'.

- eav\_field\_icon
  - Icon class from FontAwesome to use on isolate info page for sparsely- populated fields. Default 'fas 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. You can add an icon to appear by following the name with a pipe symbol (l) and an icon class from the FontAwesome library, e.g. 'Vaccine reactivitylfas fa-syringe,Risk factors/fas fa-smoking'.
- 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.
- genepresence\_record\_limit
  - Overrides the record number limit (isolates x loci) for the Gene Presence plugin. Default: 500000 (this can also be set globally in bigsdb.conf).
- genepresence\_taxa\_limit
  - Overrides the isolate limit for the Gene Presence plugin. Default: 10000 (this can also be set globally in bigsdb.conf).
- 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 (this can also be set globally in bigsdb.conf).
- 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'.
- itol\_record\_limit
  - Overrides the maximum number of records that can be included in an ITOL job. Default: 2000 (this can also be set globally in bigsdb.conf).
- itol\_seq\_limit
  - Overrides the maximum number of sequences (records x loci) that can be included in an ITOL job. Default: 100,000 (this can also be set globally in bigsdb.conf).
- 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.
- microreact\_record\_limit
  - Overrides the maximum number of records that can be included in a Microreact job. Default: 2000 (this can also be set globally in bigsdb.conf).
- microreact\_seq\_limit
  - Overrides the maximum number of sequences (records x loci) that can be included in an Microreact job.
     Default: 100,000 (this can also be set globally in bigsdb.conf).
- new\_version
  - Set to 'no' to prevent copying field value when creating a new version of the isolate record.
- 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>
<option>carrier</option>
<option>healthy contact</option>
<option>sporadic case</option>
<option>endemic</option>
<option>epidemic</option>
<option>pandemic</option>
</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.
- log\_delete
  - Sets if the field value will be recorded in the log table if the isolate is deleted. Set to 'yes' or 'no', default is 'no'. The id and isolate name are always recorded if deletion is logged.
- 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'. If set to 'yes', then the underlying field in the database must be an ARRAY type, e.g. text[].
- 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'.
- delete\_retire\_only
  - Set to 'yes' to retire the id of any allele or profile that is deleted. This prevents re-use of ids. This setting will override the global setting in bigsdb.conf.
- 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:



Add the following conditions separately:

- $age_year > 0$
- age\_month NOT null

PubMLST D	atabase home Curator home Contents		
Logged in: Keith Jo	iley (keith). 🗭 Log out   Change password		Toggle: (1)
Add new	validation condition		
Please fill in the	e fields below - required fields are marked with an exclamation mark (!).		<b>+</b>
Record		Action	
id	:! 1	Reset Submit	
field	:! age_year  v		
operator	:! >		
value	:! 0 3		
curator	:! Keith Jolley (keith)		
datestamp	2019-06-27		

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

Admin func	tions						OLoci
Permissions	User passwords	Configuration check	Cache refresh	Geocoding setup	Sparse fields	Composite fields	<ul> <li>Schemes</li> <li>Fields</li> <li>Misc</li> <li>Show all</li> </ul>
Extended attribut	tields Validation	t conditions Validation Validation	Seque	nce attributes			

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). HoLog 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 1 * message:! age_mth should only be set when age_yr < 1. curator.! Keith Jolley (keith) datestamp:! 2019-06-27	Action Reset Submit

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



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

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). 🖗 Log out   Change password	Toggle: 🚺 📃
Add new rule condition	
Please fill in the fields below - required fields are marked with an exclamation mark (!).       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 'secondary metadata' 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	ld			
Please fill in the fields below - re Record field:1 value format:1 no curate:1 no submissions:1 curator1 datestamp:1 category: description:	quired fields are marked with an exclamation mark (!).		Action Reset Submit	ľ
length: option list:	\$;];R			
value regex: conditional formatting:		0		
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	Nuth credentials	
Please fill in the fields Record base uni: consumer key: consumer secret: access token: access token: access secret: curator: date entered: datestamp:	s below - required fields are marked with an exclamation mark (!). Action Reset Submit U68_^%HJP9N^1Ax2wemPPkmqrt_J%m_rX6pkgkfdho HTH8jMXsnyhIUvJZFnDF7nj5iZQJsd Keith Jolley (keith) 2017-11-23 21 2017-11-23	E

### 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). (+Log out   Change password Help 🗹						
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 h	nome Curator hon	ne Content	S	
Logged in: Keith	h Jolley (keith). (	Log out   Change passwor	d		Help 🗹
Set cura	ator per	missions			
Select c	urator(s)		Action —		
Clark, Step	ohen (SClark)	<b>^</b>	Select		
Debech, Na	adia (ndebech)	emence) —			
Deghmane	, Ala-Eddin (de	ghmane)			
Diallo, Kan	ny (kdiallo) hol (roxlov)				
Feavers, Ia	an (ifeavers)				
Goodyer-S	ait, Lily (Igoody	er) 🔻			
	All	e			
Check the bo	oxes for the req	uired permissions. Users	s with a status o	f 'submitter	r' have a restricted list of allowed permissions that can be selected. Attributes
with a red ba	ckground add r	estrictions.			
	permissions				— — Action —
		Curator			
Per	mission	Clemence Marianne	Diallo Kanny	All/None	Update
mod	ify users				
modif	fy isolates		<b>V</b>		
modif	y projects	<b>V</b>	<b>V</b>		
modify	sequences	<b>V</b>	<b>V</b>		
tag se	equences		<b>V</b>		
design	ate alleles	<b>V</b>	<b>V</b>		
modify	usergroups				
set user	r passwords				
mo	dify loci	<b>V</b>	<b>V</b>		
modify	y schemes				
modify	composites				
modify fi	eld attributes				
modify va	lue attributes				
modi	fy probes				
modify e	experiments				
de	lete all				
import	t site users				
módify	site users				
only					
disab					
AI	mone				

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								
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 VEIS0004 NEIS0005 NEIS0005 NEIS0007 NEIS0007 NEIS0007 NEIS0010 NEIS0010 NEIS0011 NEIS0012 NEIS014 Meiso12 NEIS014 Meiso12 NEIS014 Neiso12 NEIS014 Neiso14 Neiso12 NEIS014 Neiso14 Nei						

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 funct	ions					O Show all
Permissions	User passwords	Configuration check	Configuration repair	Locus curators	Scheme curators	

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

PubMLST Database	e 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	<i>Mapped_host</i>
serverl	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
Hð 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       .Search or browse database         • Search by combinations of loci (profiles)       .Main public projects         • Your projects       .Set general options - including isolate table field handling.         • Set display and query options for locus, schemes or scheme fields.       .Manage submissions         • Update history       .Update history         • Update history       .About BIGSdb
Breakdown       Export       Analysis       Third party tools         • Single field       • Export dataset       • Coden usage       • Coden usage       • Coden usage         • Unique combinations       • Contigs       • Concatenated FASTA formats       • Coden usage       • Coden usage         • Scheme and alleles       • Sequences - XMFA / concatenated FASTA formats       • Coden usage       • Coden usage       • OrapeTree - Visualization of genomic relationships         • Scheme and alleles       • Sequence bin       • Sequence sector       • BLAST       • PhyloViz - Visualization and phylogenetic inference         • Description of database fields       • Description of database fields       • Description of database fields       • Miscellaneous

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	me Contents	
Logged in: Keith Jolley (keith	n). 🕩 Log out   Change pas	sword	Toggle: 🚺 📃
Add new user	database		
Please fill in the fields be	elow - required fields a	re marked with an exclamation mark (!).	
id1	1		Action
name:!	PubMLST	Site/domain name	Reset Submit
dbase name:!	pubmlst_bigsdb_users	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 database	
dbase host:		<ol> <li>IP address of database host</li> </ol>	
dbase port:		1 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		
<ul> <li>This page allows you to upload locus 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>Download tab-delimited header for your spreadsheet - use 'Paste Special Text' to paste the data.</li> <li>Download submission template (xlsx format)</li> </ul>		ľ
Paste in tab-delimited text (include a field header line).	- Action	
	Reset Sub	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 all
Permissions	User passwords	Configuration chec	k Cache refres	h User database	Extended attribut	te fields
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 - rea	quired fields are marke	ed with an exclamation mark (!).			+
Record				Action	
id:!				Reset Subn	nit
data type:!	DNA 👻				
allele id format!	integer 👻 🚺				
length varies:!	🔘 true 🔘 false 🚺				
coding sequence:	🔍 true 🔘 false				
isolate display:!	allele only 👻 🚺				
main display:!	🔘 true 🔍 false 🚺				
query field:!	🔍 true 🔘 false 🚺				
analysis:	🔍 true 🔘 false 🚺				
curator:	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:	<b>-</b> 0				
genome position:		÷ 0			
match longest:	🔘 true 🔘 false 🕦				
reference sequence:					
				0	
pcr filter:	🔘 true 🔘 false 🜖	Do NOT set to true unless you define	PCR reactions linked to this locus.		
probe filter:	🔘 true 🔘 false 🚺	Do NOT set to true unless you define	probe sequences linked to this locus.		
dbase name:	pubmlst_bigsdb_neiss	eria_seqdef	Name of the database holding allele sequences		
dbase host:			1 IP address of database host		
dbase port:		🔹 🚺 Network port accepting database	connections		
dbase user:			0		
dbase password:			0		
dbase id:	PUT_LOCUS_NAME_H	IERE	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 locus 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
Diseas fill in the fields below some	in d folde one mode d with an evolution mode (1)	
Please ini in the lields below - requ	ired lields are marked with an exclamation mark (!).	
Record		
id:!		
data type:!	DNA 👻	
allele id format:!	integer 👻	
length varies:!	◯ true ● false	
coding sequence:	● true ◯ false	
isolate display:!	allele only 🔻	
main display:!	⊙ true ● false	
query field:!	● true	
analysis:!	● true	
curator:!	Keith Jolley (keith)	
date entered:!	2018-06-18	
datestamp:!	2018-06-18	
formatted name:		
common name:		
formatted common name:		
allele id regex:		
length:	×	
complete cds:	© true	
orf:	▼	
genome position:	A. V	
match longest:	◯ 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	h Jolley (keith). 🗭 Log ou	it   Change password	Toggle: 🚯 📃
Add ne	w locus		Hide tools
Please fill in — Record-	the fields below - requ id:! data type:! allele id format:! length varies:! coding sequence:!	Integer ▼ Otrue @ false @ true ○ 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.
	isolate display:! main display:! query field:! analysis:! curator:! date entered:!	allele only  true  false true  false true  false true  false Keith Jolley (keith) 2018-06-18 2019 4 19	
form	formatted name: common name: atted common name: allele id regex:	2010-00-10	
	length: complete cds: off: genome position:	⊙ true   ☉ false	
	match longest: reference sequence:	© true	

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:

anter or regex.     length:     of     genome position:     match longest:     of true     false 0     por filter:     true     false 0     dbase name:   pubmist_bigsdb_neisseria_seqdef   Name of the database holding allele sequences
ierigui.   orf.   genome position:   match longest:   reference sequence:   reference sequence:   por filter:   probe filter:   true   false 0   dbase name: pubmist_bigsdb_neisseria_seqdef Name of the database holding allele sequences
genome position:       Image: Treference sequence:         reference sequence:       Image: Treference sequence:         por filter:       True Image: Treference sequence:         probe filter:       True Image: Treference sequence:         dbase name:       pubmist_bigsdb_neisseria_seqdef
genome position: match longest reference sequence: profilter: probe filter: dbase name: pubmist_bigsdb_neisseria_seqdef Name of the database holding allele sequences
match longest True Talse reference sequence: por filter: True Talse probe filter: True false dbase name: pubmlst_bigsdb_neisseria_seqdef Name of the database holding allele sequences
reference sequence: pcr filter:  true  false 0 probe filter:  true  false 0 dbase name: pubmlst_bigsdb_neisseria_seqdef Name of the database holding allele sequences
ber filter: probe filter: brue ○ false 0 dbase name: pubmlst_bigsdb_neisseria_seqdef brue ○ false 0 brue ○ false 0 Name of the database holding allele sequences
por filter: O true O false probe filter: O true O false dbase name: pubmist_bigsdb_neisseria_seqdef Name of the database holding allele sequences
por filter: O true O false probe filter: O true O false dbase name: pubmlst_bigsdb_neisseria_seqdef Name of the database holding allele sequences
por filter: O true O false ) probe filter: O true O false ) dbase name: pubmlst_bigsdb_neisseria_seqdef Name of the database holding allele sequences
brote filter: ○ true ○ false 0 probe filter: ○ true ○ false 0 dbase name: pubmlst_bigsdb_neisseria_seqdef Name of the database holding allele sequences
por filter:  true  false  fals
probe filter: O true O false  dbase name: pubmlst_bigsdb_neisseria_seqdef these heat
dbase name: pubmlst_bigsdb_neisseria_seqdef Name of the database holding allele sequences
dhara baab
ODASE NOST. I Paddress of database host
dbase port: 🚔 🚯 Network port accepting database connections
dbase user: 0
dbase password: 0
dbase table: sequences Database table that holds sequence information for this locus
dbase id field: allele_id Primary field in sequence database that defines allele, e.g. 'allele_id'
dbase id2 field: locus I Secondary field that defines allele, e.g. 'locus'
dbase id2 value: PUT_LOCUS_NAME_HERE  I Secondary field value, e.g. locus name
dbase seq field: sequence Field in sequence database containing allele sequence
description un: /cgi-bin/bigsdb/bigsdb.pl?db=pubmlst neisseria segdef&page=locusInfo&
locus=PUT_LOCUS_NAME_HERE
• • • • • • • • • • • • • • • • • • •
UN: /cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_neisseria_seqdef&page=alleleInfo&
locus=PUT_LOCUS_NAME_HERE&allele_id=[?]
0 h.
submission template: 🔿 true 💿 false 🕕 Indude 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					Show all
Permissions	User passwords	Configuration check	Cache refres	h User database	s Extended attribu	ite fields
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). DLog out   Change password			Toggle: 🚺	
Batch insert loci				
This page allows you to upload locus data as tab-delimited text or copied from a spreadsheet.				
<ul> <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 locus as a semi-colon (;) separated list.</li> </ul>				T
Download tab-delimited header for your spreadsheet - use 'Paste Special Stext' to paste the data.     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:	<b>•</b>			Reset Submit
field:				
value format:!	text 🔹			
required:	🔿 true 🔘 false 🚯			
main display:!	🖲 true 🔘 false 🕚			
curator:!	Keith Jolley (keith)			
datestamp:!	2018-06-18			
value regex:		0		
description:				
option list:				
un. Ionath:			•	
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).	Dog 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:!	MLST	
curator:!	Keith Jolley (keith)	
datestamp:!	2018-06-18	
date entered:	2018-06-18	
description:		
display order:		
allow missing loci:	© true ◎ false 3 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 v Use CTRL/SHIFT click to select or deselect values	
PubMed ids:		
links:		
(Format, ORE)description)		
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 functions							
Permissions	User passwords	Configuration check	Configuration repair	User databases	Loci		
Locus aliases	Locus extended att	ributes 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	y (keith). 🗘 Log out   Change password						Toggle: 🜖
Add new s	cheme member						
Please be aware th This does not affec	at any modifications to the structur t allele designations, but any profile	e of this scheme s will have to be r	will result in th reloaded.	e removal o	of all data from it. Th	iis is done to ensure	data integrity.
Please fill in the fie	lds below - required fields are mark	ed with an exclan	nation mark (!). — Action				Et
scheme id:! locus:!	MLST	•	Reset	Submit			
curator:! datestamp:!	Keith Jolley (keith) 2018-06-18						
field order:	1						

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	nfiguration check	Configuration repair	User databases	
Locus aliases	Locus extended attribut	Schemes	Scheme fields	Scheme members	Scheme groups i +++¢

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	<b>y (keith). 🕩</b> Log out	Change password				Toggle: ()
Add new s	cheme fi	eld				
Please be aware th This does not affect	nat any modificati t allele designatio	ons to the structure ons, but any profiles	of this scheme wil will have to be relo	l result in the rer baded.	noval of all data from it. Th	is is done to ensure data integrity.
Please fill in the fie	lds below - requir	ed fields are marked	with an exclamati	ion mark (!).		
					Action	
scheme id:!	MLST		+		Reset Submit	
field:	ST			]		
type:!	integer 👻					
primary key:!	◉ true  ☉ false	8				
dropdown:!	🔘 true 🔘 false	0				
curator:	Keith Jolley (ke	eith)				
datestamp:!	2018-06-18					
description:						
field order:	1	-				
index:	© 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).	Deg out   Change password		Toggle: 🚯 🔳
Add new schen	пе		
Please fill in the fields belo Record	w - required fields are marked with an exclamation mark (!).	Action	Ħ
name: isolate display: main display: query field: query status: analysis: curator! datestamp: date entered: description:	Image: Contract of Cont	reset	
dbase name:	h.		
dbase host			
dbase nort:	×₀		
dbase user:			
dbase password:	0		
dbase id:	A_0		
display order:			
allow missing loci:	True C false 1 This is only relevant to schemes with primary key fields e.g. MI ST		
flags:	citation required experimental in development unpublished Vue CTRL/SHIFT dick to select or deselect values		
PubMed ids:			
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.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). (+Log out   Change password	Help 🗹
Download allele sequences	
Select loci by scheme   Alphabetical list   All loci by scheme Click within the tree to display details of loci belonging to schemes or groups of schemes - clicking a group folder will display the loci for all schemes with Click the nodes to expand/collapse.	hin the group and any subgroups.
Replication and Repair	
i — Jag Genomic islands	
- 🛺 Lineage Schemes	
- 🛺 Metabolism	
- III N. gonorrhoeae AMR	
- Plasmids	
- IVping	
- MIST	
• • • • • • • • • • • • • • • • • • •	
MLST	
Locus Download Type Alleles Length (setting) Min length Max length Full name/product Curator(s) Last updated	
abcZ DNA 879 Fixed: 433 bp 433 434 O. Harrison, K. Jolley 2018-06-11	
adk 2 DIVA 651 FIXed: 405 bp 465 465 O. Harrison, K. Jolley 2018-05-11	
and Sector Secto	
arth  DNA 911 Fixed 405 0p 405 405 0. Harrison K. Jolley 2016-06-11	
adh Anna Anna Anna Anna Anna Anna Anna Ann	
pgm 1 DNA 932 Fixed: 450 bp 447 450 O. Harrison, K. Jolley 2018-06-11	
Download table: tab delimited taut I Evcel format	

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	tions					Show all
Permissions	User passwords	Configuration check	k Cache refresh	User databases	Extended attribut	ite fields
ď		6	Ro	+#⊄	++*	X
Composite fields	Loci	Locus aliases	PCR reactions	PCR locus links	Nucleotide probes	Sequence attributes
+¢	+#🤇 📖	+ <b>#</b> ¢	+#¢	+#	++	
Schemes	Scheme fields	Scheme members	Scheme groups	Group members (s	schemes) Group r	members (groups)
+#¢	+#¢	+#¢	∓#≪	+#0		+#¢

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  name:! 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	3	
Logged in: Keith Jolley (keith). Hog out   Change password		Toggle: 🜖 📃
Add new scheme group scheme me	mber	
Please fill in the fields below - required fields are marked with an exce 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.

Admin functi	ions					Show all
Permissions	User passwords	Configuration che	ck Configurati	User data	Loci Loci ++¢Cille	Locus aliases
Locus extended att	tributes Sche	smes Scheme FC	e fields Schen FC	Schem	e groups	ers (schemes) i t
Group members (g	roups) Classific	ation schemes	Client databases	Client database loci	Client database fields	Locus curators

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

Logged in: Keith Jolley (keith	). Change password	Uniens	Toggle: 🚯 🚍
Add new clien	t database		
Please fill in the fields belo	ow - required fields are marked with	h an exclamation mark (!).	
Record		Action	
id:!	1	Reset Submit	
name:!	PubMLST isolates		
description:!	Contains data for a coll diversity of <u>Neisseria</u> sy database there is at lea isolate may be submitted that it does not represe	ection of isolates that represent the total known pecies. For every allelic profile in the profiles st one corresponding isolate deposited here. Any to this database and consequently it should be noted nt a population sample.	
dbase name:!	pubmlst_bigsdb_neisseria_isolates	s 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:	🖨 🚯 Netwo	ork port accepting database connections	
dbase user:		0	
dbase password:		0	
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 Database	e home Curator hor	me Contents			
Logged in: Keith Jolley (keith	h). ເ⇔Log out   Change passwor	rd			Toggle: 🚺 📃
Add new locu	s to client dat	tabase definit	ion		
Please fill in the fields bel Record client dbase id: locus: curator:! K datestamp:! 20	low - required fields are ma 1) PubMLST isolates abcZ (eith Jolley (keith) 018-06-19	arked with an exclamation r	nark (!).	Action Reset Submit	ľ
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 consequer does not represent a population sample. 5433 isolates	file in the prof tly it should b	files database be noted that it	

## 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	ise home Curator home Contents		
Logged in: Keith Jolley (ke	ith). [+Log out   Change password	Toggle: 🕚	Ξ
Add new loce	us to client database isolate field definition		
Please fill in the fields to Record client dbase id:! locus:! isolate field!! curator:! datestamp! allele query:	below - required fields are marked with an exclamation mark (!).		

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.

PubMLST Databas	e home Contents	
Logged in: Keith Jolley (keit	h). 🕒 Log out   Change password Help 🗹	Ξ
Allele informa	ntion - penA: 9	
Provenance/m	eta data	
locu	s: penA	
allel	e: 9	
sequenc	e: GACGGCGTTT TGCTGCCGGT CAGCTITGAA AAACAGGCGG TGCGCCGCA AGGCAAACGT ATAITITAAAG CAICGACCGC ACGTCAGGTG CGTGAGTTGA TGGTTTCTGT AACCGAAACCT GGCGGTACGG GTACGGCGGG TGCGGTAGAT GGTTTCGACGG TCGGCGCAAA AACCGGTACG GCGCGTAAGGT TGGTTAACGG TCGTTACGTC GATTACAAAC ACGTTGCCAC TTTCATCGGT TTTGCCCCGG CTAAAAATCC GCGGTGGATT GTGGCGGTAA CCATTGACGA GCCGACTGCA AACGGTTACT ACGGCGGCGCT AGTGACAGGT CCGGTCTTCA AACAAGTTAT GGGCGGTAGC CTGGAACATCT TGGGCGTTTC TCCGACCAAA CCTCTGACCA AT	
lengt	h: 402	
statu	s: Sanger trace checked	
date entere	d: 2006-09-04	
datestam	p: 2006-09-04	
sende	r: Muhamed-Kheir Taha, National Reference Center for Meningococci, Institut Pasteur, France	
curato	r: Keith Jolley, University of Oxford, UK	
mutation F504	L: yes	
mutation A510	V: yes	
mutation 1515	V: yes	
mutation H541	N: yes	
mutation 1566	v: yes	
E Publication (1)		
<ul> <li>Taha MK, Vázque Heuberger S, Hoff Stefanelli P, Thulir meningitidis. Antii</li> </ul>	z 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, mann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczynska A, I S, Tzanakaki G, Unemo M, Vogel U, Zarantonelli ML (2007). Target gene sequencing to characterize the penicillin G susceptibility of Neisseria microb Agents Chemother 51:2784-92	
Isolate databa	ses	
PubMLST isolate	s: Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles databas there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted the does not represent a population sample. 494 isolates	se at it
Linked data		
penicillin_rang	e: >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	g 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	
scheme id:	N. meningitidis cgMLST v1.0	
name:!	Nm_cgc_25 0	
inclusion threshold:	25 Aximum number of different alleles allowed between profile and at least one group member profile.	
use relative threshold:!	© true  false Calculate threshold using ratio of shared/present in both profiles in pairwise comparison.	
status:!	experimental 💌	
curator:!	Keith Jolley (keith)	
datestamp:!	2018-06-19	
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:		
Action		
Ponot Submit		
Treser Submit		

### 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.

Admin functions								
Permissions	User passwords	Configuration chee	Cache refres	sh User da	tabases E	xtended attribute	fields Composi	te fields
	Locus aliases	PCR reactions	PCR locus links	Nucleotide p	robes Seq	uence attributes	Schemes	
Scheme fields	Scheme members	Scheme groups	Group members	s (schemes)	Group memi	bers (groups)	Classification sche	mes

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 (!).	Anting	+
Record		Action	
id:!	2	Reset Submit	
scheme id:!	N. meningitidis cgMLST v1.0 -		
name:!	Nm_cgc_25		
inclusion threshold:	25 Aaximum number of different alleles allowed between profile and at least one group member profile.		
use relative threshold:	O true I false Calculate threshold using ratio of shared/present in both profiles in pairwise comparison.		
status:!	experimental 👻		
curator:!	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.		
segdef cscheme id:	2 cscheme_id number defined in segdef 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*.

uisease:	invasive (unspecilied/other)		-	noiogical Stanua	arus anu controis,			
epidemiology:	endemic		F	otters bar, UK				
Publications (2)								
<ul> <li>Feavers IM, Gray SJ, disease outbreak. J C</li> </ul>	Urwin R, Russell JE, Bygrave Clin Microbiol 37:3883-7 14 i	es JA, Kaczmarski E isolates	B, Maiden MC (19	99). Multilocus s	equence typing and	l antigen gen	e sequencing in the investigation o	f a meningococcal
<ul> <li>Jolley KA, Hill DM, B based analysis method</li> </ul>	ratcher HB, Harrison OB, Fea ods. <i>J Clin Microbiol</i> <b>50:</b> 3046-	wers IM, Parkhill J, M 53 14 isolates	laiden MC (2012). I	Resolution of a	meningococcal dise	ase outbreak	from whole-genome sequence dat	a with rapid Web-
X Sequence bin								
contigs:	259	mean length:	8,245 bp	N90 c	ontig number: 63		N95 length (L95):	4,593
total length:	2.135.447 bp N	50 contia number:	18	N9	0 length (L90); 8.(	066	loci tagged:	2.180
max length:	130 716 bp	N50 length (1 50):	38 364	N95 c	ontig number: 79		detailed breakdown:	Display
			,					
	determined by electric	ntion only month						
Similar Isolates (	determined by classific	ation schemes)						
Experimental schemes are s	subject to change and are not	a stable part of the r	omenclature.					
						_		
Classification scheme	Underlying scheme CI	ustering method M	ismatch threshole	d Status	Group			
Nm_cgc_200 N.	meningitidis cgIVILST v1.0	Single-linkage	200	experimental	group: 17 (841 isola	ites)		
Nm_cgc_100 N.	meningitidis cgiviLST v1.0	Single-linkage	50	experimental	group: 36 (566 Isola	nes)		
Nm_cgc_50 N	meningitidis cgMLST v1.0	Single-linkage	25	experimental	group: 45 (4 isolati	es)		
Nill_cgc_25 N.	meningitidia egivicor vito	Olligie-lilikage	23	experimental	group. 45 (4 1301at)	63)		
E Schemes and loci								
🚛 🛄 All loci	Navigate a	and select schemes	within tree to displa	ay allele designa	tions			
Genetic Informa	ation Processing							

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

PubMLST Database home Contents							
Logged in: Keith Jolley (keith). (>Log out   Change password	Help 🛛	Toggle:					
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.			Modif				
Isolate provenance/ohenotype fields Allele designations/scheme fields							
Id							
Diselevicet estima			_				
Orspayson options Action							
Dislay: 15 - records for each of							
Display- 23 V tecutos pel page							
Select project  Add these records Isolate fields  III ST Einstyning	antigens						
isolate aliases country vear disease species servaroup genoaroup capsule aroup ST Icload complex PorA VRI PorA	VR2 FetA	VR					
662 2837 M97/252508 UK 1997 invasive (unspecified/other) Neisseria meningitidis C C 50 ST-11 complex 5-1 10	-4 F3-6	5					
670 2840 M97/252535 UK 1997 invasive (unspecified/other) Neisseria meningitidis C C 50 ST-11 complex 5-1 10	-4 F3-6	5					
671 2844 M97/252781 UK 1997 invasive (unspecified/other) Neisseria meningitidis C C 50 ST-11 complex 5-1 10	-4 F3-6	;					
672 2847 M97/252943 UK 1997 invasive (unspecified/other) Neisseria meningitidis C C 50 ST-11 complex 5-1 10	-4 F3-6	5					
Analysis tools:         Breakdown:       Fields       Two Field       Combinations       Polymorphic sites       Schemes/alleles       Publications       Sequence bin       Tag status         Analysis:       BURST       Codons       Presence/Absence       Genome Comparator       BLAST       rMLST species id							
Export: Dataset Contigs Sequences							
Third party: GrapeTree ITOL PhyloViz Microreact							

# 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.
Accession: AM421808

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

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). @Log out   Change password	Ξ
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	
Download table: tab-delimited text   Excel format (suitable for batch upload of loci).	
Download alleles: tab-delimited text   Excel format (suitable for defining the first allele in the seqdef database).	
Annotation information	
accession: AM421808	
version: 1	
type: dna	
length: 2194961	
description: Neisseria meningitidis serogroup C FAM18 complete genome.	
coding regions: 1975	
Coding sequences	
Locus Aliases Product	Length
NMC0001 IpxC; UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924
emvA	004
NMC002 pist piun (ragment)	291
NMC0003 pn32 united pint NMC0004 fbp	330
NMC0005 pppgrogrammatic province and a province and	219
NMC0006 putative diversite development	954
NMC0007 metG methionvl-tRNA svnhetase	2058
NMC0008 ofmS ofucosamine-fructose-forboshate aminotransferase [isomerizinn]	1839
NMC0009 putative lipoprotein	519
NMC0010 gna33 outer membrane lipoprotein Gna33 1	
NMC0011	1326
putative integral membrane protein	1326 840

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	nome Curator home Contents	
Logged in: Keith	Jolley (keith).	Dog out Change password	Ξ
Scan El	MBL/Ge	nbank record for loci	
This function — Please e Accession:	allows you to nter accessior AM421808	scan an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci. number — Primary identifier — Action —	
Download tabl Download alle	e: tab-delimite les: tab-delimit	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	n informatio	n	
	accession:	AM421808	
	version:	1	
	type:	dna	
	length:	2194961	
	description:	Neisseria meningitidis serogroup C FAM18 complete genome.	
cod	ling regions:	1975	
Coding se	quences		
Locus	Aliases	Product	Length
NMC0001	lpxC;	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924
	envA		
NMC0002	pilS1	pilin (fragment)	291
NMC0003	pilS2	truncated pilin	366
NMC0004	tbp	peptidyi-prolyl cis-frans isomerase	330
NMC0005		putative membrane protein	219
NMC0006		putative glycerate dehydrogenase	954
NIVIC0007	metG	metnionyl-tRVA synthetase	2058
NIVIC0008	gims	giucosamine-itructose-o-priosphate aminotransferase [isomerizing]	1839
NMC0009	ana22	putare inportein	519
NMC0010	gnass	outer memorane lipoprotein Gnass	1320
NMC0012		putative integral memorane protein	040
141410-0012		parative lipoprotein	1107

# 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 - I	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 func	tions			O Show all
Users ++¢¢+	Isolates ++	Sequence bin	Sequence tags	

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

Logged in: Keith Jolley (keith): 60 Log out   Change password       Itel ST       Toggle: •         Isolate query/update         Enter search criteria or leave blank to browse all records. Modify form parameters to filter or enter a list of values.       Modify form parameters to filter or enter a list of values.         Isolate provenance/phenotype fields	PubMLST	Database h	iome Ci	urator home	Contents									
Isolate query/update         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       form         Isolate provenance/phenotype fields       option         Display/sort options       Action         Order by:       id         Display/sort options       Action         Order by:       id         Display:       25 • records per page •         1 record returned. Click the hyperlink for detailed information.         Delete       Tag scanning         Projects       Your projects         Delete ALL       Scan         Select project       Vour projects         Version       id         id       isolate aliases country year disease         serogroup       Gapuer         bin       version         id       isolate aliases country year disease         serogroup       Capsule ST         clonal       PorA         year       Year         Year       Year         Year       Year         Year       Year         Year       Year         Year       Year         Y	Logged in: Kei	Logged in: Keith Jolley (Keith). 🗣 Log out   Change password Toggle: 🚯 📃												
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 isolate  isolate	lsolate	solate query/update												
Display/sort options       Action         Order by: id       ascending         Display: 25       records per page         1 record returned. Click the hyperlink for detailed information.         Delete       Tag scanning         Projects       Your projects         Delete ALL       Scan         Select project       Link         Select project       Add these records         Delete Update       Sequence her version id isolate aliases country year disease species serogroup genogroup group         X       YR1         YR2       YR3         Neisseria       B         B       7         ST32       7         16-2       F1-5	Enter searc	h criteria or leave provenance/phen	e blank to bro otype fields =	owse all record	ds. Modify form p	parameters to fil	ter or enter a	list of values.					M fo op	lodify rm ption
Order by: id <ul> <li>ascending</li> <li>Reset</li> <li>Submit</li> </ul> Display: 25       records per page         1 record returned. Click the hyperlink for detailed information.         Delete       Tag scanning         Projects       Your projects         Delete ALL       Scan         Select project       Link         Select project       Add these records             Delete       Update         Sequence bin       New version         id       isolate aliases country year         disease       species         serogroup       group         ST       complex         VR1       VR2         X       4		/sort options —						ı						
Display: 25  records per page  1 record returned. Click the hyperlink for detailed information.  Delete Tag scanning Projects Vour projects Delete ALL Scan Select project K Select project Add these records	Orde	r by: id			•	ascending	Reset	Submit						
1 record returned. Click the hyperlink for detailed information.         Delete       Tag scanning       Projects         Delete ALL       Scan       Select project       Add these records         Delete ALL       Scan       Select project       Add these records         Delete Update       Sequence bin       New version       Isolate fields Image: Second project       ML ST         Finetyping antigens       id isolate aliases country year disease       serogroup genogroup genogroup       ST       clonal porA porA porA porA porA porA porA porA	Dis	play: 25 🔻 re	cords per pa	age 🚯										
1 record returned. Click the hyperlink for detailed information.         Delete       Tag scanning       Projects         Delete ALL       Scan       Select project       Add these records         Delete ALL       Scan       Select project       Add these records         Delete Update       Sequence bin       New version       Isolate fields ●       MLST       Finetyping antigens         id       isolate aliases       country year       disease       serogroup       group       ST       clonal complex       VR1       VR2       VR         X       Image: Clonal complex in the image: Clon														
Delete       Tag scanning       Projects       Your projects         Delete ALL       Scan       Select project       Link       Select project       Add these records         Delete ALL       Scan       Select project       Link       Select project       Add these records         Delete Update       Sequence bin       New version       id isolate aliases country year disease species serogroup genogroup group       ST       Clonal complex       VR1       VR2       VR         X       Image: Complex Compl	1 record retu	irned. Click the h	yperlink for	detailed inform	ation.									
Delete ALL       Scan       Select project       Link       Select project       Add these records         Delete       Update       Sequence bin       New version       Isolate fields ①       ML ST       Finetyping antigens         X       Image: Sequence bin       New version       Id       isolate aliases country year       disease       species       serogroup       group       ST       clonal complex VR1       VR2       VR         X       Image: Sequence bin       How version       Id       isolate aliases country year       disease species       serogroup genogroup       ST       clonal complex VR1       VR2       VR         X       Image: Sequence bin       How version       Id       Isolate aliases       serogroup genogroup       Group ST       clonal complex VR1       VR2       VR         X       Image: Sequence bin       How Version       Image: Sequence bin       Image: Sequence bin       ST       clonal PorA       PorA <t< td=""><td>Delete</td><td> Tag :</td><td>scanning-</td><td>-Projects-</td><td></td><td></td><td>,</td><td>Your projects</td><td></td><td></td><td></td><td></td><td></td><td></td></t<>	Delete	Tag :	scanning-	-Projects-			,	Your projects						
Delete       Update       Sequence bin       New version       Isolate       Isolate       fields       ML ST       Finetyping antigens         X <td>Delete A</td> <td></td> <td>can</td> <td>Select proje</td> <td>ct</td> <td>- I</td> <td>ink Se</td> <td>elect project</td> <td>. 🔻 Add th</td> <td>ese records</td> <td></td> <td></td> <td></td> <td></td>	Delete A		can	Select proje	ct	- I	ink Se	elect project	. 🔻 Add th	ese records				
Delete       Update       Sequence bin       New version       Id       isolate       aliases       country       year       disease       species       serogroup       genogroup       clonal group       Clonal complex       PorA       PorA       FetA         X       Image: Vera disease       Image: Vera disease       Vera disease       Species       Serogroup       genogroup       Group disease       ST - 200 disease       Vera disease       Vera disease       Serogroup       Serogroup       ST - 200 disease       Vera disease       Vera disease       Vera disease       Serogroup       Serog														
Delete     Update     Sequence bin     New version     Isolate     Isolate     fields     Secuence     MLST     Pinetyping antigense       id     isolate     aliases     country     year     disease     species     serogroup     genogroup     Capsule group     ST     clonal complex     VR1     VR2     VR       *     *     *     *     **     **     **     240     MC58     Z7176     UK     1983     Neisseria meningitidis     B     74     ST-32     7     16-2     F1-5												Eine	4	
Delete       Update       bin       version       id       isolate       aliases       country       year       disease       species       serogroup       genogroup       capsule group       ST       clonal complex       PorA       PorA       VR2       VR         X       //       //       240       MC58       Z7176       UK       1983       Neisseria meningitidis       B       B       74       ST-32 complex       7       16-2       F1-5		Sequence	e New			Isolate	e fields 💷				MLST	ant	igens	
X     Image: Second secon	Delete Up	bin bin	version	id isolate a	liases country	vear disease	species	serogroup	aenoaroup	capsule S	clonal	PorA P	orA Fe	etA
meningitidis complex	×	/ <b>1</b>	+	240 MC58	77176 UK	1983	Neisseria	B		group B 74	ST-32	VR1 1	/RZ V 6-2 F1	IR 1-5
		-		in our			meningitidis	U		0 /-	complex		Ø 6	1

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 Update Upload contigs Create Scan	
Provenance/meta data	
id: 240 seroty	ype: 15
isolate: MC58 sero subt	ype: P1.7,16-2
alias: Z7176 comme	nts: Genome sequenced by TIGR.
strain designation: B: P1.7,16-2: F1-5: ST-74 (cc32) sen country: UK	der: Mumtaz Virji, Dept. Pathology and Microbiology, University of Bristol
continent: Europe cura	tor: Nina Billows, University of Oxford (E-mail: nina.billows@some.ox.ac.uk)
species: Neisseria meningitidis update hist	ory: 313 updates show details
serogroup: B date ente	red: 2001-05-11
capsule group: B datesta	mp: 2018-06-04
Publications (6)	
Z Sequence bin	
contigs: 1	
length: 2272360 bp	
loci tagged: 2,226	
detailed breakdown: Display	

Click the 'Renumber' button:

PubMLST	Database ho	me Curator	home	Contents								
Logged in: Keith	h Jolley (keith). 🗭	.og out   Change pas	sword							Help 🗹	Toggle: 🕚	Ξ
Sequence bin for MC58												
Contig sur	marv statistic	cs										
	Contigs: 1											
	Length: 2,	272,360										
Downlo	ad sequences (H	ASIA format)	MDL form	-+)								
• Downic	au sequences wi	th annotations (E		ac)								
	Sequencing	Original							EMBI	Artomis	Renumber	
Sequence	method	designation	Length	Comments	Locus	Start	End	Direction	format	(i)		
1	Sanger		2272360	whole	NEIS2139	7	498	←	EMBL	Artemis	Renumber	T
				genome	NEIS2140	502	897	←				
					NEIS2141	918	2312	$\leftarrow$				
					NEIS2142	2517	3161	←				
					NEIS2143	3158	3511	$\leftarrow$				
					NEIS2144	3635	4117	$\rightarrow$				
					NEIS2145	4311	4961	$\rightarrow$				
					NEIS2146	4958	5875	$\rightarrow$				
					NEIS2147	5936	6214	$\rightarrow$				
					NEIS2148 (pgk)	6281	7492	←				
					NEIS2149	7573	8826	$\leftarrow$				
					tRNA-lys	9197	9272	←				
					NEIS2150	9346	10317	$\leftarrow$				
					NEIS2151	10350	10811	$\leftarrow$				
					NEICO4CO (L-HA)	40040	40477					

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 Curator home Contents								
Logged in: Keith Jolley (keith). 🗣 Log out   Change passwo								
Renumber locus genome positions based on tagged sequences								
You have selected to renumber the genome positions set in the locus table based on the tagged sequences in sequence id#1.								
Option	Action							
Remove positions for loci not tagged in this set	uence Renumber							
The following designations will be made:								
Locus 🗢 Existing genome po	ion							
NEIS2139	7							
NEIS2140	502							
NEIS2141	918							
NEIS2142	2517							
NEIS2143	3158							
NEIS2144	3635							
NEIS2145	4311							
NEIS2146	4958							
NEIS2147	5936							
NEIS2148	6281							
NEIS2149	7573							
tRNA-lvs	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	ise home Curato	or home	Contents				
Logged in: Keith Jolley (ke	<i>ith).</i> ເ⇔Log out   Change pa	assword					Toggle: 🚺
Add new con	nposite field	d					
Please fill in the fields b	pelow - required fields a	are marked	with an exclamation	mark (!).			<b>F</b> +
id:!	strain_designation			name of the field as it wi	II appear in the web interface	Reset Submit	
position after:!	isolate	✓ field	present in the isolate	table			
main display:!	◯ true 🧕 false	Sets whet	her to display field in i	isolate query results table (c	an be overridden by user preferend	ce).	
curator:	Keith Jolley (keith)						
datestamp:!	2018-06-19						

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				C Show all
Permissions	User passwords	Configuration check	Cache refresh	User databases	Extended attribute fields
Composite fields		Locus aliases	PCR reactions	PCR locus links	Nucleotide probes

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

PubMLST Database home Curator home Contents									
Logged in: Keith Jolley	Logged in: Keith Jolley (keith). [+Log out   Change password								
Update or delete composite field									
1 composite field defi	ined.								
Delete Update	field name	position after	main display	definition	missing data				
× 🥒 st	rain_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 (-)				

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.

PubMLST Database h	nome Cura	ator home Contents							
Logged in: Keith Jolley (keith).	€Log out   Change	e password							=
Update compos	site field	l - strain designati	on						
Position/display									
position after: isolate		-							
main display: 🔘 true 🌒	false								
Update									
field	empty value	regex	curator	datestamp	delete	edit	mo	ve	
capsule_group [isolate field]	ND	rogon	Keith Jolley	2017-08-15	×			•	
: P1.			Keith Jolley	2009-11-12	×		1	4	
PorA_VR1 [locus]	ND		Keith Jolley	2009-11-12	×		$\mathbf{\uparrow}$	•	
			Keith Jolley	2009-11-12	×		1	•	
PorA_VR2 [locus]	ND		Keith Jolley	2009-11-12	×		$\uparrow$	◄	
:			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	×		↑	↓	
clonal_complex [MLST field]	-	s/ST-(\S+) complex.*/cc\$1/	Keith Jolley	2009-11-12	×			◄	
)			Keith Jolley	2009-11-12	×		▲	↓	
Add new field:									
text field:		<del>+</del>							
isolate field:		<b>+</b>							
locus field:		<b>+ +</b>							
scheme field:		<b>.</b>	+						

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
ł.	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					Show all
Permissions	User passwords	Configuration check	Cache refresh	User databases	Extended attribut	te fields
Composite fields		Locus aliases	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 Dat	abase home	Curator home	Contents			
Logged in: Keith Jolle	ey (keith). 🕩 Log out	t   Change password				Toggle: 🕄 📒
Add new s	equence	attribute				 
Please fill in the fie	lds below - requi	red fields are marked	with an exclamat	tion mark (!). — — Action—		- +
key:!	read_length			Reset	Submit	
type:!	integer 👻					
curator:! datestamp:l	Keith Jolley (ke 2018-06-19	eith)				
description:	2010-00-13					

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 o FASTA file. This allows data for multiple isolates to be uploaded.	ther isolate table field that uniquely defines the isolate, can be named in the identifier rows of the
Please note that you can reach this page for a specific isolate by querying isolates and then clicking 'Upload' within t	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: !
	sender: ! Select sender
	method:
	run id:
	assembly id: read length:
	Ontions
	Don't insert sequences shorter than 25 v hos
	Link to experiment:
	Alternatively upload FASTA life
	Browse No file selected
	Action
	Reset Submit

## 5.29 Checking external database configuration settings

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

Admin functions			O Show all
Permissions i C	Sswords 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.

PubMLST Data	base home Curator home C								
Logged in: Keith Jolley	(keith). 🗭 Log out   Change password								Ξ
Configuration	on check - Neisseria	PubML	ST						
Drogram	Dath	Installed Eve	sutablo						
EMBOSS infealign	/usr/bin/infoalign								
EMBOSS sixpack	/usr/bin/sixpack	<u> </u>	<u> </u>						
EMBOSS stretcher	/usr/bin/stretcher	2	2						
blastn	/usr/local/ncbi-blast+/bin/blastn	~	2						
blastp	/usr/local/ncbi-blast+/bin/blastp	~	~						
blastx	/usr/local/ncbi-blast+/bin/blastx	<b>~</b>	~						
clustalw	/usr/bin/clustalw	×	~						
ipcress	/usr/bin/ipcress	<ul> <li>✓</li> </ul>	<b>~</b>						
mafft	/usr/bin/mafft	×	<b>~</b>						
makeblastdb	/usr/local/ncbi-blast+/bin/makeblastdb	×	~						
mogrify	/usr/bin/mogrify	<ul> <li>✓</li> </ul>	~						
muscle	/usr/bin/muscle	<ul> <li>✓</li> </ul>	~						
tblastx	/usr/local/ncbi-blast+/bin/tblastx	~	~						
Locus databases NEIS0895 (parA) p NEIS0903 (opaD) p NEIS1454 p NEIS1551 (opaC) p NEIS1551 (opaC) p	s (only showing loci with poten Database Hi ubmlst_bigsdb_neissenia_seqdef zoo-a ubmlst_bigsdb_neissenia_seqdef zoo-a ubmlst_bigsdb_neissenia_seqdef zoo-a ubmlst_bigsdb_neissenia_seqdef zoo-a	tial problems ost Port Id berlour 5432 berlour 5432 berlour 5432 berlour 5432	<b>field value D</b> NEIS0895 NEIS0903 NEIS1454 NEIS1551	loci) atabase accessib	e Sequence que	ry Sequences as × × × ×	signed		
NEIS2013 p	ubmist_bigsdb_neisseria_sequer zoo-a	beriour 5432	NEIS2013	~	×.				
Scheme databas	upmist_pigsop_neissena_sequer zoo-a	abaso	Host	Port Id Databa	so accossible Pr	ofile quept			
Scheme	I ST pubmist bigsdt	neisseria seo	def zoo-aberlou	ir 5432 1					
Riboso	mal MLST bigsdb multi	species seadef	zoo-aberlou	ır 5432 1	~	~			
rplF	species pubmlst_bigsdb	_neisseria_seq	def zoo-aberlou	ır 5432 42	× .	×			

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 fun	Admin functions							
Permissions	User passwords	Configuration check	Cache refres	User databases	Extended attribute field	ds Composite fields		
Loci + + - +	Locus aliases	PCR reactions	CR locus links	Nucleotide probes	Sequence attributes	Schemes Schemes	eme fields • <b>+</b> C	

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

PubMLST Data	base home	Curator home	Contents				
Logged in: Keith Jolley	(keith). 🕩 Log ou	t   Change password				Toggle: 🚯	Ξ
Query sche	mes for	<sup>r</sup> Neisseria	PubMLST d	atabase			
Please enter your se	earch criteria be	low (or leave blank a	nd submit to return all re	cords).			
Search criteria-		_		- Display	- according		
lu	• =	•	+	Display: 25		•	
	display:			Action			
mai	n display:			Reset	t		
q	iery field:	▼ 3					
que	y status:	• •					
	analysis:	▼ 3					
allow mis	sing loci:	▼ 3					
	curator:						
	scheme: MLS	Т	▼ 3				

Click the button 'Export configuration/data'.

Logged in: Keith Jolley (keith). 🗘 Log out   Change password	Ξ
Query schemes for Neisseria PubMLST database	
Please enter your search criteria below (or leave blank and submit to return all records).	
Search criteria	
id • = • Order by: id • ascending •	
Display: 25 🔻 records per page 🕚	
Isolate display:	
query field:	
query status:	
analysis: 🔽 🔹	
curator:	
scheme: MLST 3	
1 record returned.	
— Delete — Database configuration —	
Delete ALL Export configuration/data	
dbase dbase dbase isolate main query query , , display allow	da
Delete Update id name dbase name host port id display* display* field* status* analysis* order loci datestamp	ente
X / 1 MLST pubmlst_bigsdb_neisseria_seqdef 1 2 2 2 1 1 Keith 2012-03-22	2009-
۲ الله الله الله الله الله الله الله الل	Þ

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 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
scheme_fields
scheme_id field type primary_key description field_order url isolate_display
→main_display query_field dropdown curator datestamp
1 ST integer 1 1 /cgi-bin/bigsdb/bigsdb.pl?page=profileInfo&db=pubmlst_
→neisseria_seqdef&scheme_id=1&profile_id=[?] 1 1 1 0 2 2010-01-20
1 clonal_complex text 0 2 1 1 1 1 2 2009-11-16

# 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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```
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	Database home	Curator home	Contents	
Logged in: Keith	Jolley (keith). 🗭 Log out	t   Change password		Toggle: 🚺 📃
Databas	se curator's	interface -	Neisseria profile/sequence definition	າຣ
Cura	tor functions			O Show all
Use	rs Sequence of the sequence of	MI	ST 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 (!).		4
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:	true @ false S Receive new submission E-mails (curators only)		
account request emails:	○ true ● false 3 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 +++CC+ Curator functions MLST profiles +++CC+	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*.

Logged in: Keith Jolley (keith	Delog out I Change password	Help 7	Toggle: 🚯	=
Add now allow				-
AUU IIEW alleig	esequence			
Please fill in the fields belo	ow - required fields are marked with an exclamation mark (!).	1		
Record				
locus:!	abcZ 🔹			
allele id:!	878			
sequence:!	ITTGATACCGTTGCCGAAGGTTTGGGTAAAATTCGCGATTTATTGCGCCGTTACCACCGGTCGGT	IGAGTTGGA ICTGGAAGC ICCGGCGGT IACCAACCA ITACCCACG		
status:!	Sanger trace checked			
sender:!	Jolley, Keith (keith)			
curator:!	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 comparison	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:	æ			
Override sequence :	similarity check length check			
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 Million	T profiles				

Download a template Excel file from the following page.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). DLog out   Change password	Help 🗹 🛛 Toggle: 🚯 📃
Batch insert sequences	
<ul> <li>This page allows you to upload allele sequence 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>If the locus uses integer allele ids you can leave the allele_id field blank and the next available number will be u</li> <li>The status defines how the sequence was curated. Allowed values are: 'Sanger trace checked', 'WGS: manual WGS: visually checked', 'WGS: automatically checked', 'unchecked'.</li> <li>Sequence flags can be added as a semi-colon (:) separated list.</li> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special S Text' to paste the data.</li> <li>Download submission template (xlax; format)</li> <li>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: </li> </ul>	ised. extract (BIGSdb)', 'WGS: automated extract (BIGSdb)',
Value will be overridden if you include a sender field in your past     Value will be overridden if you include a sender field in your past     Value will be overridden if you include a sender field in your past     Value will be overridden if you include a sender field in your past     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	ted data. top codon at the ends and no internal stop codons. Existing
— Paste in tab-delimited text ( <b>include a field header line</b> ).	Action 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.

Loged in: Keith Jolley (keith), (% Log out [ Change password] Entern Section Sectio	PubMLST Database home Curator home Contents			
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.  Fit the locus uses integer allele ids you can leave the allele id field blank and the next available number will be used.  Sequence flags can be added as a semi-color () separated list.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Special Text to paste the data.  Download tab-delimited header for your spreadsheet - use Pasts Text Special Text to paste the data.  Download tab-delimited text (Include a field header fine)  Download tab-delimited text (Include a field header fine)  Download tab-delimited text (Include a field header f	Logged in: Keith Jolley (keith). 🗘 Log out   Change password	Help 🗹	Toggle: 🜖	Ξ
This page allows you to upload allele sequence data as tab-delimited text or copied from a spreadsheet.	Batch insert sequences			
Index solution non-net not before         Jolley, Keth (keth) <ul> <li>Value will be overridden if you include a sender field in your pasted data.</li> <li></li></ul>	<ul> <li>This page allows you to upload allele sequence 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>If the locus uses integer allele ids you can leave the allele_id field blank and the next available number will be used.</li> <li>The status defines how the sequence was curated. Allowed values are: 'Sanger trace checked', 'WGS: manual extract (BIGSdb)', 'WGS: an WGS: visually checked', 'WGS: automatically checked', 'unchecked'.</li> <li>Sequence flags can be added as a semi-colon (;) separated list.</li> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special O Text' to paste the data.</li> <li>Download submission template (xlsx format)</li> <li>Please note, some loci have extended attributes which may be required. For affected loci please use the batch insert page specific to that Reload page specific for locus: Select  <ul> <li>Reload</li> </ul> </li> </ul>	utomated extrac	t (BIGSdb)',	
Jolley, Keth (keth)       • Value will be overridden if you include a sender field in your pasted data.	Please select the sender from the list below:			
Paste in tab-delimited text (include a field header line).       Action         locus       allele_id       status       sequence         abcZ       NGS: automated extract (BIGSdb)       Reset       Submit         ITIGATACIGTISECCAAAGACTCAACGAAGTICGCAATTGCAACGAAGGACGCGAAGGACGCGGAAGGACGCGGAAGGACGCGACGA	✓ 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 sequences are also ignored. ☐ Override sequence similarity check	o internal stop c	odons. Exist	ting
locus     allele_id     status     sequence       abc2     WGS: automated extract (BIGSdb)       ITTGATACTGTTGCCGAAGGTTTGGAGGCGAAATTCCGCGTTATCATCATGTCAGCCATGAGTTGGAAAAATG       GTTCGACTGAGGCTTTGGTGGAAGACCCGAACTTCCCAACTGCCAACTGCCGAACGAGCGGCGGAGGAGCGGCGGACGAGCGGCGGACGAGCGGCG	Paste in tab-delimited text (include a field header line).     Action			
	Ibody allele_id       Status Sequence         abg2       MS3: automated extract (BIGSdb)         ITIGATACTECTCGAAGGTTIGEGGGAAATICGCGATTIATICGCGCCGTTATCATCATGICAGCCATGAGTIGGAAAATGGCAAGGCGCTGGGAAAATGGGAAAAGGCGGCGGGGGGGAAAAAGGCGGCGGGGGAAAAAGGCGGC			

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'.

PubML	ST D	atabase home)	Curator home	Contents							
Logged in	Keith Jo	olley (keith). 🕩 Log out	Change password							Help 🗹	Toggle: 🜖
Batc	h ins	sert seque	nces								
Import	status										
Sender:	Keith Jol	lley									
No obvio	us proble	ems identified so far.									
-Acti	on —										
Impo	rt data	1									
_		-									
Data to	o be im	ported									
The follo	wing tab	ble shows your data	Any field with red t	text has a problem and ne	eds to be checked. Note: valid a	sequence flags ar	re display	ed with a	a red backgrour	nd not red text.	
locus	allele_i	d	sequence		status	type_allele	sender	curator	date_entered	datestamp con	ments flags
abcZ	878	TTTGATACTGTTG	CCGAAGG GO	CGAATTGTCGAACTTGACC	WGS: automated extract (BIGS	Sdb)	2	2	2018-06-07	2018-06-07	
abcZ	879	TTTGATACCGTTG	CCGAAGG GO	GGATTGTCGAACTTGACC	WGS: automated extract (BIGS	Sdb)	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.:

PubMLST Database home Curator home Contents						
Logged in: Keith Jolley (keith). (>Log out   Change password					Help 🛛	Toggle: 🚺 📃
Batch insert sequences						
Import status						
Primary key Problem(s)						
locus: abcZ; allele_id: 878 Sequence contains non nucleotide (A C G T) character	ers.					
Data to be imported						
The following table shows your data. Any field with red text has a problem and ne	eds to be checked. Note: valid sequ	ence flags are displa	yed with a	a red backgrour	nd not red text.	
locus allele id sequence	etatus	type allele sende	r curato	date enterer	datestamn comn	nents flags
abcZ 878 TTTGATACTGTTGCCGAAGG GCGAATTGTCGAACTTGACC	WGS: automated extract (BIGSdb)	2	2	2018-06-07	2018-06-07	nento nugo
abcZ 879 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTTGACC	WGS: automated 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). C+Log out   Change password	Toggle: 🚺 📃
Database curator's interface - Neisseria profile/sequence definitions	
Curator functions	O Show all
Users Sequences MLST profiles ++++++++++++++++++++++++++++++++++++	

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	
This page allow next available i	ws you to upload allele sequence data in FASTA format. The identifiers in the FASTA file will be used un id (loci with integer ids only). Do not include the locus name in the identifier in the FASTA file.	less you select the option to use the
Please note th	at you can not use this page to upload sequences for loci with extended attributes.	
Enter para	imeters	
locus:!	abcZ 🗸	
status:!	Sanger trace checked 🔹	
sender:!	Jolley, Keith (keith)	
sequence (FASTA):!	<pre>&gt;isolate1</pre>	
Codons. Exi codons. Exi Coverride Use nex	II sequences that are not complete reading frames - these must have a start and in-frame stop codon a isting sequences are also ignored. sequence similarity check t available id (only for loci with integer ids)	t the ends and no internal 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 Database home Curate	r home Contents		
Logged in: Keith Jolley (keith). 🕩 Log out   Change p	assword	Help 🗗	Toggle: 🚯 📕
Batch insert sequences			
Sequence check			
Locus: abcZ			
Original designation Allele id Status	Action		
isolate1 878 OK	Upload valid sequences		
Isolatez 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	e home	Curator home	Contents							
Logged in: Keit	Logged in: Keith Jolley (keith). 🗘 Log out   Change password Help 🗹 Toggle: 🕚										
Batch i	Batch insert sequences										
Sequence	check										
Locus: abcZ	!										
Original de	esignation	Allele id		Status	-	Action					
isola	ate1	878		OK		Linload valid sequences	)				
isola	ate2	879	Sequence contains no	n nucleotide (A C G T) charact	ers.	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 (kei	ith). C+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 🕚
Filter query by Action
locus: abcZ
status:
type allele:
sender:
curator:
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	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 record	Display							
allele id $\checkmark = \checkmark 4$	+ 3	Order by:	ocus	<b>▼</b> a	scendina 👻				
		Display:	25 <b>•</b> rec	ords per pa	ge 🕚				
──── Filter query by		Action							
locus: abcZ	•	Reset Subr	nit						
status:									
type allele:									
sender:									
curator:	▼ 3								
1 record returned.									
Delete — Database configuration — Flags —									
Delete ALL Export configuration/data Batch set	J								
Delete liedete lesus allele	sequence		type			date	data ata ma		
id sequence	length	status	allele	sender	curator	entered	uatestamp co	niments 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). (>Log out   Change password									
Delete allele se	quence								
You have chosen to delete t	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								
	AAATGAAAAA ATCGGCAACC TITCCGGCGG TCAGAAAAAG CGCGTCGCCT TGGCTCAGGC TIGGGTGCAA AAGCCCGACG TATTGCTGCT GGACGAGCCCG								
	ACLARCAIL IGGALAIGA CGGALAIL IGGEIGAAA AIGIGEIGAA AGCEILIGA GGLAGIIGG IGIGALAC CLACACCGC CGIIIIIGG								
status:	Sanner Geochecked								
type allele:	false								
sender:	Keith Jolley								
curator:	Man-Suen Chan								
date entered:	2001-02-07								
datestamp:	2009-11-11								
comments:									
Action									
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.

um. Reith Joney (Keith	h). C+Log out   Change password	Toggle:
date allele	sequence	
se fill in the fields bel	low - required fields are marked with an exclamation mark (!).	
Record		Action C
locus:	abcZ	Reset Submit
allele id:	4	Inteset Submit
sequence:!	TTTGATACCG TTGCCGAAGG TTTGGGCGAA ATTCGTGATT TATTGCGCCG TTATCATCAT GCTCAGCCATE AGTTGGAAAA TGGTTCGAGT GAGGCTTTGT TGAAAGAACT CAACGAATTG CAACTTGAAA TCGAAGGCGAA GGACGGCTGG AAACTGGATE CGGCAGTCAA GGACGGCTGG GGGGAACTCG GTTTGCCGGA AAATGAAAAA	
status:!	Sanger trace checked -	
sender:!	Jolley, Keith (keith)	
curatoral		
curator.!	Keith Jolley (keith)	
date entered:	Keith Jolley (keith) 2001-02-07	
date entered: datestamp:	Keith Jolley (keith) 2001-02-07 2018-06-07	
date entered: datestamp: type allele:	Keith Jolley (keith)         2001-02-07         2018-06-07         True       false         New allele searches can be constrained to use just type alleles in comparisons	
date entered: datestamp: type allele: comments:	Keith Jolley (keith)         2001-02-07         2018-06-07         True       false         New allele searches can be constrained to use just type alleles in comparisons	
date entered: datestamp: type allele: comments: Flags:	Keith Jolley (keith)         2001-02-07         2018-06-07         True       false         New allele searches can be constrained to use just type alleles in comparisons         atypical contains IS element element frameshift internal stop codon         v       Use Ctrl click to select/deselect multiple choices	н
date entered: datestamp: type allele: comments: Flags: PubMed ids:	Keith Jolley (keith)         2001-02-07         2018-06-07         True       false         New allele searches can be constrained to use just type alleles in comparisons         atypical contains IS element         internal stop codon         use Ctrl click to select/deselect multiple choices	,
Cultor: date entered: datestamp: type allele: comments: Flags: PubMed ids: ENA ids:	Keith Jolley (keith)         2010-02-07         2018-06-07         True       false         New allele searches can be constrained to use just type alleles in comparisons         atypical contains IS element downstream fusion frameshift internal stop codon	
date entered: datestamp: type allele: comments: Flags: PubMed ids: ENA ids: Genbank ids:	Keith Jolley (keith)         2001-02-07         2018-06-07         True       false         Atypical         contains IS element         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 Databas	e home Curator ho	me Contents				
Logged in: Keith Jolley (keit	<b>th). ເ</b> ⇔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 [	atabase home	Curator home	Contents			
Logged in: Keith J	olley (keith). 🗭 Log out   (	Change password				Toggle: 🚯
Add new	retired alle	le id				 
Please fill in the Record locus: allele id: curator: datestamp:	fields below - required NEIS0844 67 Keith Jolley (keith) 2018-06-07	d fields are marked ▼	with an exclama	tion mark (!). Action Reset S	ubmit	ľ

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: Keit	h Jolley (keith). 🕩 Log ou	t   Change password				Toggle: 🜖 📃
Databa	se curator's	; interface -	Neisseria pr	ofile/sequence d	definitions	
Cur.	ator functions					Show all
Use + +	User	groups Use	er group members	Locus descriptions	Locus links +++¢	

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

PubMLST	Database home	Curator home	Contents									
Logged in: Keith	h Jolley (keith). ⊕Log out	Change password									Toggle: 🚯	Ξ
Query l	ocus descri	ptions for	Neisseria	profil	e/sequ	ence	e def	inition	s c	latab	ase	
Please enter	your search criteria be	low (or leave blank a	nd submit to return	n all records	).							
Search c	riteria				Display —							
locus	▼ =	VEIS0620		+ 🚯	Order by:	locus	•	ascending	•			
					Display:	25 🔻	records	per page 🚯				
—⊳ Filter q	uery by	Action										
		Reset Sub	mit									

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

PubMLST Database home Curator home Conten	ents	
Logged in: Keith Jolley (keith). [+Log out   Change password		Toggle: 🜖 📃
<b>Query locus descriptions for Neiss</b>	seria profile/sequence definitions data	abase
Please enter your search criteria below (or leave blank and submit t	it to return all records).	
Search criteria	Display	
locus 🔻 = 👻	+ 1 Order by: locus - ascending -	
	Display: 25 👻 records per page 🕚	
- Filter query by-	Action	
locus: NEIS0620 (maeA)	Reset Submit	
curator:		
common name:	6	

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	
Display: 25 v records per page 3	
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: Comparison of the state of the s	

Fill in the form as needed:

PubMLST Database h	nome Curator home Contents	
Logged in: Keith Jolley (keith).	◆Log out   Change password	Toggle: 🚯 📕
Update locus d	escription	
Please fill in the fields below	- required fields are marked with an exclamation mark (!).	
locus:! curator:!	NEIS0620 Keith Jolley (keith)	
datestamp: full name:	2018-06-07	
product:	malate oxidoreductase (EC 1.1.1.38)	
description:	Final step in TCA cycle producing oxaloacetate.	a
aliases:	NG00240 • NMA0870 • 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 D	)atabas	e home Cui	ator home	Contents			
Logged in: Keith Jo	olley (keith	h). 🕩 Log out   Chan	ge password			Help 🗹	Toggle: 🚺 📃
Add new	MLS	T profile					
Please fill in the	fields bel	low - required fiel	ds are marked	d with an exclamation	in mark (!).		
	ST: 1 3	015					
	abcZ: 1 2	2					
	adk: ! 3	}	×				
4	aroE: 1 4	ł	* *				
f	fumC: 1	.22	*				
	gdh: ! 8	}					
F	pdhC: 1 4	ł	×				
	pgm: ! 6	;	×				
se	ender: !	Jolley, Keith (keit	n)		•		
clonal_co	mplex:						
cu	irator: ! K	eith Jolley (kei	th)				
date_ent	tered: ! 2	018-06-07					
datest	tamp: ! 2	018-06-07	_				
PubMe	led ids:						
-Action-							
Deat	Cubarit	7					
Reset	Submit						

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). C+Log out   Change password	Help 🖪	Toggle: 🚯	Ξ
Batch insert MLST profiles			
<ul> <li>This page allows you to upload profiles 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>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, you is then you must also provide it for each profile record.</li> </ul>	include it in th	ne header li	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	e Curat	or home	Conte	nts					
Logged in: Keit	th Jolley (keith). 🗭 Log	out   Change p	password				Не	elp 🗹	Toggle: 🕚	
Batch insert MLST profiles										
This page allows you to upload profiles as tab-delimited text or copied from a spreadsheet.										
<ul> <li>Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish.</li> <li>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, you include it in the header line, then you must also provide it for each profile record.</li> </ul>										
<ul><li>Down</li><li>Down</li></ul>	nload tab-delimited he nload submission tem	ader for you plate (xlsx f	ur spreadsh format)	eet - use l	Paste Spe	ecial 🛇 Text to paste the data.				
Please	paste in tab-delimited	text ( <mark>inclu</mark>	ıde a field	header li	ne)					
abcZ 2	adk aroE 3 4	fumC 122	gdh 8	pdhC 4	pgm 6	clonal_complex				
Parame	ters					-Action				
Sender: Jolley, Keith (keith)					•	Reset Submit				
Value will b	e overridden if you incl	ude a sende	er field in yo	ur pasted o	iata.					
<ul> <li>Ignore previously defined profiles</li> <li>Ignore duplicate profiles</li> </ul>										

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	Database home	Curator home	Contents		
Logged in: Keith	Jolley (keith). 🗭 Log ou	ut   Change password			Toggle: ()
Databas	e curator's	s interface -	· Neisseria	profile/sequence def	initions
Cura	tor functions				O Show all
Use + +	rs Seq	iuences Mi	LST profiles		

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

PubMLST	Database h	nome	Curator home	e Contents								
Logged in: Kei	th Jolley (keith). 🖲	⇒Log out   C	hange password								Help 🛛	Toggle: 🜖
Query/	update p	orofile	es - Neis	seria prof	file/seq	uence d	defi	nitions				
Schemes												Modit
Please sele	ct the scheme y	ou would l	ike to query:									option
MLST			✓ Select	t								_
Enter search — Locus/s ST	h criteria or leave scheme fields v	e blank to =	browse all recor • 4563	rds. Modify form pa	rameters to fi	lter or enter a li — Display/sort Order by: Display:	option ST 25	ralues. ns ▼ ▼ records pe	ascending er page ()	• [	Action Reset	Submit
1 record retu — Delete — Delete A	rned.											
Delete Up	date ST abcz 4563 2	Z <mark>adk</mark> ard 76	DE <mark>fumC gdh</mark> i i 13 9	pdhC pgm clonal 18 8 ST-16	l complex 7 complex							

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.

PubMLST Database	home Curator home Contents						
Logged in: Keith Jolley (keith).	Log out   Change password						
Delete profile							
You have chosen to delete t	the following record. Select 'Delete and Retire' to prevent the identifier being reused.						
scheme id:	1) MLST						
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	Delete and Retire						
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 (ke	ith). ເ∳Log out   Change password		Help 🗹	Toggle: 🜖 📃
Update profi	le			
		Action		
Update your record as	s required - required fields are marked with an exclamation mark (!):	Reset Submit		
ST: !	4563			
abcZ: !	2			
adk: !	7			
aroE: !	6			
fumC: !	13			
gdh: !	9			
pdhC: !	18			
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:				

## 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). 🗭 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:! MLST (id 1) profile id:! 57232 curator:! Keith Jolley (keith) datestamp:! 2018-06-07	n mark (!). 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	e home Curator hor	ne Contents		
Logged in: Keith Jolley (keit	th). ເ⇔Log out   Change passwor	d		Toggle: 🜖 📃
Database cur	at <mark>or's inter</mark> fac	e - Neisseria	a PubMLST	
Curator funct	ions			O Show all
Users +++C+	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 home Curator home Contents										
Logged in: Keith Jolley (keith). 🕞	Log out   Change password							Help	Toggle:	
Add new isolate	1									
Please fill in the fields below -	required fields are marked	d with an	exclama	tion mark (	!).					
						Allele desigr	nations			
id:!	60465	8								
isolate:	J323_2		0					MLST		
country:	UK	- 8				abcZ	adk	arot	fumC	
species:!	Neisseria meningitidis			- 8		adh	ndhC	nam		
sender:!	Jolley, Keith (keith)				- 3	gun	punc	pym		
curator:!	Keith Jolley (keith) 🕚									
date entered:	2018-06-07 🕚						Finetyp	ing antigens		
datestamp:!	2018-06-07 (3)		-			PorA VR1	PorA VR2	PorA VR3	FetA VR	
region:			0							
year:	2014	0				-Action				
epidemiological year:		~				Reset S	Submit			
age yr.										
age min.	- 0	•								
disease:	meningitis		- 0							
SOURCE:										
epidemiology:										
serogroup:	<b>-</b>									
denogroup:										
MI EE designation:										
serotype:										
sero subtype.										
ET no:										
penicillin:		8								
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 Curato	r home Contents						
Logged in: Keith Jolley (keith). 🍽 Log out   Change pa	ssword		Toggle: 🜖 📃				
Batch insert isolates	Batch insert isolates						
This page allows you to upload isolate data as • Field header names must be included a • Enter aliases (alternative names) for you • Enter references for your isolates as a • You can also upload allele fields along y template for locus names). These will b • You can choose whether or not to inclu • Download tab-delimited header for your • Download submission template (xlsx for Please select the sender from the list below:	tab-delimited text or copied from a spreads ind fields can be in any order. Optional field ur isolates as a semi-colon (;) separated lis semi-colon (;) separated list of PubMed ids with the other isolate data - simply create a e added with a confirmed status and metho de an id number field - if it is omitted, the nu- spreadsheet - use 'Paste Special <b>O</b> Text' t rmat)	sheet. s can be omitted if you wish. t. (non-integer ids will be ignored). new column with the locus name (see the 'allowed_loc d set as 'manual'. ext available id will be used automatically. o paste the data.	i' tab in the Excel				
Select sender	<ul> <li>Value will be overridden if you include</li> </ul>	ude a sender field in your pasted data.					
Paste in tab-delimited text (include a field	ld header 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).

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	Toggle: 🕚	Ξ
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 s	eroarour	ae
60465 J323_2 UK 2014 meningitis CSF Neisseria	B	
< III		Þ

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 ho	ome Contents		
Logged in: Keith Jolley (keith). [+Log out   Change passw	ord		Toggle: ()
Batch insert isolates			
Import status			
Primary key Pr	oblem(s)		
id: 60465 species "Neisseria mengitidis" is n	ot on the list of allowed values for this fiel	d.	
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 reg	ion year epidemiological_year age	yr age_mth sex disease source	epidemiology species serogroup gene
60465 J323_2 UK	2014	meningitis CSF	neisseria B mengitidis
•			Þ

# 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 Databa	ase home Curator ho	ome Contents		
Logged in: Keith Jolley (ke	eith). ເ€Log out   Change passw	ord		Toggle: ()
Database cu	rator's interfa	ce - Neisseri	a PubMLST	
Curator fund	Isolates	Sequence bin	Sequence tags	O Show all
++¢	++	+¢	GIN	

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.

PubML	ST Da	atabase h	ome (	Curato	r home	Contents									
Logged in:	Keith Jol	ley (keith). 😭	Log out   C	hange pa	ssword								Help 🗹	Toggle: 🕻	
Isola	te qu	ery/up	odate												
Enter se	earch crite	eria or leave	blank to l	browse a	all records. N	Aodify form pa	arameters	to filte	er or enter a list of v	alues.				(	Modify
Isol	ate prove	nance/pheno	otype field	ls											
Combi	ne with:	AND 👻													
cour	itry	•	=	-	USA		+	8							
year		•	=	-	2009										
— Dis	play/sort	options							- Action						
C	order by:	id				•	ascendin	g 🔻	Reset S	ubmit					
	Display:	25 <del>•</del> rec	ords per	page 🚯											
30 record	le roturno	d (1 - 25 die	nlaved) (	Click the	a hyperlinke	for detailed in	formation								
JUTECOIL	is returne	u (1 - 25 uis	piayeu).	SICK III	e nypeninks	ior detailed in	Iomation								
Dele	te	– — Tag s	canning-	Pr	ojects —										
Dele	te ALL	Sc	an	Sele	ect project		•	Lir	nk						
Page:															
i age.															
		Sequence	New						lsolate fields 🚯					Seqbin	0.0
Delete	Update	bin	version	id	isolate	aliases	country	year	disease	species	serogroup	genogroup	capsule group	sıze (bp)	Conti
×	ø	<u>1</u>	+	12674	M18700		USA	2009		Neisseria	В		В	0	0
		•	-	12675	M18701		LISA	2009		meningitidis	в		в	0	0
Ŷ	-	-		12075	10110701		USA	2005		meningitidis	D		D	U	U
×		<b>±</b>	+	12676	M18725		USA	2009		Neisseria meningitidis	В		В	0	0
×	1	<b>±</b>	+	13090	M19024	PA09015	USA	2009	meningitis	Neisseria meningitidis	В		В	0	0
×	ø	<b>±</b>	+	14627	M20918		USA	2009		Neisseria meningitidis	A		А	1717803	204(
×	/	*	+	14998	M21319		USA	2009	invasive (unspecified/other)	Neisseria	В		В	0	0
×		+	+	15000	M21323		LISA	2009	invasive	Neisseria	в		В	0	0

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

PubMLST Database	home Curator home	Contents									
Logged in: Keith Jolley (keith). 🕒 Log out   Change password											
 Delete isolate											
You have chosen to delete t	the following record. Select 'E	elete and Retire' to prevent t	he isolate id being reused.								
Provenance/met	a data										
id:	14627	region:	IA	sender:	Xin Zhao, Novartis (formerly						
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:	North America	capsule group:	А	datestamp:	2018-01-31						
Publication (1)     Kislyuk AO, Katz LS     BH, Mayer LW, Jorda     Sequence bin	5, Agrawal S, Hagen MS, Cor an IK (2010). A computationa	nley AB, Jayaraman P, Nelak I genomics pipeline for proka	uditi V, Humphrey JC, Sam ryotic sequencing projects.	mons SA, Govil D, Mair RD, T <i>Bioinformatics</i> <b>26:</b> 1819-26 1	atti KM, Tondella ML, Harcourt 8 isolates						
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						
Action Delete and	Retire										

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 hon	ne Curator home Conte										
Logged in: Keith Jolley (keith). C+Log out   Change password											
Update isolate											
Isolate fields id: 1 isolate: Fields country: species: 1 sender. date entered: 2 datestamp: 1 year: 2 epidemiological year: age yr: age wr: age wr: age wr: age wr: sex: bisease: source: epidemiology: serogroup: genogroup: MLEE designation: serotype: corr outhure:	4627 € M20918 USA • € Neisseria meningitidis Zhao, Xin (xinzhao) Keith Jolley (keith) € 2010-01-26 € 0018-06-07 € KA 2009 • € CSF • € CSF • € A • € • • • •	0 v 0 v 0 v 0 v 0	Loci	splay allele designations • Add/update							

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 h	ome Curator home	Contents
Logged in: Keith Jolley (keith).	◆Log out   Change password	
Update abcZ al	lele for isolate	14627
Provenance/meta	a data	Locus: abcZ
id:	14627	Add new allele designation
isolate: strain designation: country: region: year: source: species: serogroup: capsule group: capsule group: capsule group: sender: curator: update history: date entered: datestamp: Update other loci: Locus: abcZ Add/update	M20918 A: P1.20,9: F3-1: ST-4789,7 USA IA 2009 CSF Neisseria meningitidis A A Xin Zhao Auto Tagger IB updates show details 2010-01-26 2018-01-31	Please fill in the fields below - required fields are marked with an exclamation mark (!).  Record isolate id: 14627 locus:1 abcZ allele id: 5 sender:1 Jolley, Keith (keith) status:1 confirmed v method:1 manual curator:1 Keith Jolley (keith) datestamp:1 2018-06-07 date entered:1 2018-06-07 comments:  Action Reset Submit  Existing designations  Update[Delete lallele id sender status method comments]

## 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: Keit	th Jolley (keith). 🗭 Log ou	t   Change password						Toggle: 🚯 📃
Databa	se curator's	interface -	Neisseria	a PubMLST				
Cur	ator functions							O Show all
-+ -#	CAC + 4	e C 2	+¢	Sequence tags				

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								
This page allows you to batch update provenance fields or alle	ele designations for multiple isolates.							
<ul> <li>The first column should be the isolate id (or unique field that you are selecting isolates on). If a secondary selection field is used (so that together the combination of primary and secondary fields are unique), this should be entered in the second column.</li> <li>The next column should contain the field/locus name and then the final column should contain the value to be entered, e.g.</li> </ul>								
id field value 2 country USA 2 abcZ 5								
<ul> <li>The columns should be separated by tabs. Any other c</li> <li>If you wish to blank a field, enter '<blank>' as the value.</blank></li> </ul>	olumns will be ignored.							
Please enter the field(s) that you are selecting isolates on. Va value(s) used. Usually the database id will be used.	lues used must be unique within this field or combination of fi	elds, i.e. only one isolate has the						
Please paste in your data below:	Options	Allele designations						
id field value	Primary selection field: id 🗸	Add additional new designation						
101 serogroup B	Optional selection field: <none></none>							
	Opdate existing values	- Action						
		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	Databa	ase hon	ne Cura	ator home	Contents					
Logged in: Keith	h Jolley (k	e <i>ith).</i> 🔂 Lo	g out   Chang	e password					Help 🗹	
Batch is	solat	e upo	date							
The following changes, pre	changes ss your b	will be m rowser's	ade to the back buttor	database. Plea 1.	ase check that this	is what you intend a	and then	press 'Upload'. If you do no	ot wish to make these	;
Transaction	ı id F	ield N	lew value	Value(s) curr	ently in database	Action				
1	100 ser	ogroup	В		С	update field with ne	ew value			
2	101 ser	ogroup	В		С	update field with ne	ew value			
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'.

PubMLST Database home Curator	home Contents		
Logged in: Keith Jolley (keith). 🗘 Log out   Change pass	sword		Help 🗹 🛛 Toggle: 🚯
Isolate query/update			
Enter search criteria or leave blank to browse all	I records. Modify form parameters to filte	r or enter a list of values.	Modify
		Display/sort options	form
Combine with: AND -		Order by: id	→ ascending →         →         →         →
date entered • = •	2014-03-18 + 3	Display: 25 👻 records per page 🕚	
curator (surname) 🔹 = 🔹	Jolley	-Action-	
		Reset Submit	
3 records returned. Click the hyperlinks for details	led information		
Delate Tag econoring Brai	ianta		
Tag scanning Proj	ects		
Delete ALL Scan Select	t project • Lin	ĸ	
Delete Undate Sequence bin New version		Isolate fields 🚯	Finetyping antigens
Delete Opdate Sequence bin New version	id isolate aliases country year	disease species serogroup genogroup capsul	e group PorA VR1 PorA VR2 FetA VR
	28788 M22553 USA	Neisseria meningitidis	5-1 2-81 + 5-2 10-96 +
× / ± +	28789 M22568 USA	Neisseria meningitidis	7-2 / 4-39 / +

PubMLST I	Database home Curator home Contents										
Logged in: Keith J	.ogged in: Keith 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). (+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:     46262       curator:!     Keith Jolley (keith)       datestamp:!     2016-12-21	

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 Database home	e Curator home Contents									
Logged in: Keith Jolley (keith). [+Log out   Change password Toggle: ()										
Database curator's interface - Neisseria PubMLST										
Curator functions										
Users Use	User group members	Isolates Isolate aliases	Publications							

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). [0]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. 9. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. 9. Deveload ab-delimited header for your spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 9. Deveload submission template (disk format) 9. Deste nab-delimited text (include a field header line). 1. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 1. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 2. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 2. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 2. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 2. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 2. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use 'Paste Special <b>Q</b> Text to paste the data. 3. Spreadsheet - use '	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 UHS12 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 h	ome Contents				
Logged in: Keith Jolley (keit	<b>h). ⊡</b> Log out   Change passw	rord				Toggle: 🚯 📃
Database cur	ator's interfa	ce - Neisseria Pu	bMLST			
Curator funct	User groups	User group members	Isolates	Isolate aliases	Publications	Show all

Open the Excel template by clicking the link.

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). E+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. <ul> <li>Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish.</li> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special S 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 Reset Submit	E

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									
This page allows yo • Field header • Download tal • Download su Paste in tab-de isolate_id 6160 17517 6162 17517 18968 26515	u to upload PubMe names must be in b-delimited header ibmission template limited text (inclue pubmed_id 841 3523	ed link data as tab cluded and fields o for your spreadsho (xlsx format) de a field header	delimited text or co an be in any order. eet - use 'Paste Spe line).	opied from a spreads Optional fields can l ecial	heet. be omitted if you wish. e the data.	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).	her isolate table field that uniquely defines the isolate, can be named in the identifier rows of the me isolate table.
Paste in sequences in FASTA format: ACCGTCARAATCGGTCGGCATCGATGAATCGATACCGCGCGAAAACAAATTTCTTGGATT TCGCCGTGGTCGTTGTCGTGATGAAGCGGTGAAGGCGGACGAGTGGTTTTAAACAGG CCGGAAGGGCGTGGAAGAATGAAATCCTTCTGTCGATTACTCAAATCGAATGACGG GGAATGCGCCACAAAATCGCGGCCGTTTCTGTCGATTACACGG GGAATGCCGCCACAAAATCGGCGCGTTTTTACCCCCAAATGAAGGAGG GAAATCCGCACCAAAATCGGCGCGTTTCTCCCGCAATGACGGCGCCGTGTGGGCGC CGCCGGCGCGACGACGCATGCGCCGCTTTTGTCGCGCTGTGTGCGCCTTT CGTTAAGGCAAAAATCGCGCCCGCGTTCCCCCGCCGTGTCGCCCGGCTGTCGCGCCTT CGCATCGCGGCGGAGAGCGGCCGTTCCCCCGCCGTTCGCCGCGCCCTTATCGCGGCCCCTT CGCATCGGGCGCGGAGAGCGGCCGTTCCCCGCCGATCGCGCCCGATCGCCCGGCCC CCCGGAGGCGCGCGAAACAGCGCCGCCGATCCGCCGCGCCGGACCGCCTT CGACTGCGGCGCTGTGCCTCCGGCATCCCTCGGGAGCGCCCGGACCGCCTT CGACTGCGGCCGTGTGCCGCCCATCCCCGGACGCGCGGGTCGGCGGGCG	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'.

PubMI	_ST Database home Curator home	e Contents			
Logged i	n: Keith Jolley (keith). 🗣 Log out   Change password				Toggle: 🚯 🗮
Uplo	ad sequences				
——Th	e following sequences will be entered.		Summary —	-Action-	
	Original designation	Sequence length Comments	Number of contigs: 364	Upload	
18	0062 NODE_116_length_5370_cov_18.338547	5408	Minimum length: 100		
1	80063 NODE_267_length_64_cov_54.562500	102	Maximum length: 50093		
18	0064 NODE_1024_length_456_cov_16.434210	494	Total length: 2069108		
18	0065 NODE_367_length_3545_cov_22.858955	3583	Mean length: 5684		
1	80066 NODE_361_length_87_cov_17.862068	125	N50 contig number: 44		
18	0067 NODE_1617_length_297_cov_11.111111	335	N50 contig length (L50): 15404		
1	80068 NODE_909_length_95_cov_9.073684	133	N90 contig number: 146		
18	80069 NODE_699_length_98_cov_110.918365	136	N90 contig length (L50): 3907		
1	80070 NODE_553_length_84_cov_47.964287	122	N95 contig number: 180		
18	0071 NODE_182_length_6772_cov_19.882162	6810	NOS contig langth (LEO): 2205		
18	0072 NODE_928_length_347_cov_35.201729	385	195 contig length (LSU): 2305		
18	0073 NODE_19_length_12542_cov_19.259449	12580			
18	0074 NODE_60_length_5125_cov_18.960781	5163			
18	0075 NODE_168_length_7439_cov_17.615808	7477			
18	0076 NODE_1041_length_109_cov_27.752293	147			
18	0077 NODE_71_length_2120_cov_19.594339	2158			
18	0078 NODE_318_length_1827_cov_15.821566	1865			
18	0079 NODE_207_length_6398_cov_19.577681	6436			
180	080 NODE_162_length_13775_cov_18.618221	13813			
18	0081 NODE_664_length_160_cov_35.068748	198			
18	0082 NODE_56_length_9475_cov_20.244328	9513			
18	0083 NODE_356_length_297_cov_41.383839	335			
18	0084 NODE_778_length_582_cov_42.140892	620			
180	085 NODE_137_length_10168_cov_16.055567	10206			
18	80086 NODE_1102_length_82_cov_43.329269	120			
40	0007ILIODE 007 I II 0007 40 544000	0205			

## 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 hom	Contents		
Logged in: Keith Jolley (keith). 🗘 Log out   Change password			Help 🗹 🛛 Toggle: 🚺
Isolate query/update			
Enter search criteria or leave blank to browse all record	Is. Modify form parameters to filter or enter a list of values.		Modify
Isolate provenance/phenotype fields	Display/sort options	Actio	n form
isolate • = • fam1	+ Order by: id	✓ ascending ✓ Reset	Submit Submit
	Display: 25 👻 records per page 🕚		
1 record returned. Click the hyperlink for detailed inform	ation.		
Delete ALL Scan Select proj	t 👻 Link		
Sequence New	Isolate fields 🕄	MLST	Finetyping antigens
belete update bin version id isola	e aliases country year disease species se	rogroup genogroup capsule ST clonal complex	VR1 VR2 VR
🗙 🥒 🔽 🕂 698 FAM	8 NIBSC_3076; USA 1983 invasive Neisseria	C C 11 ST-11	5 🖋 2 🖋 F1-30
	Z4259 (unspecified/other) meningitidis	complex	1

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). 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 FASTA file. This allows data for multiple isolates to be uploaded.	other isolate table field that uniquely defines the isolate, can be named in the identifier rows of the
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 (I).	
Paste in sequences in FASTA format:	Attributes isolate id: 698) FAM18 sender: ! Select sender  method:  method:  munid: assembly id:  Options 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. 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 o	other isolate table field that uniquely defines the isolate, can be named in the identifier rows of the
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 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: Alternatively upload FASTA file Browse No file selected. Action 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 passv	word		Toggle: 🚯
Database cura	tor's interfa	ice - Neisseri	a PubMLST	
Curator function	Isolates	Sequence bin	Sequence tags	O show al

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 a may be hidden by your operating system.	ecified above), fasta, which
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.

PubMLST	Database ho	ome C	urator home	Contents		
Logged in: Keit	h Jolley (keith). 🗭	Log out   Ch	ange password			Toggle: 🜖 📃
Batch u	ipload se	equer	nce asser	nblies to r	nultiple	isolate records
Please uploa	ad the assembly (	contig files	s for each isolate	record.		
remove row	id isolate	current contigs	sequence bin sta	ate filename	upload status	
	61222 JB_21292	-	-	JB_21292.fasta	×	
	61223 JB_21293	-	-	JB_21293.fasta	×	
Remove	01224 JD_21294	-	-	JD_21294.185ta	<u>^</u>	
3 FASTA file	s left to upload.					
Contig a	ssembly files —					
Please upl	oad contig assen	nblies with	the filenames as	you specified (india	ated in the table	e). Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go.
although y	ou can upload mu	ultiple time	s so that the tota	I size of the upload	can be larger.	,
						· · · · · · · · · · · · · · · · · · ·
- í						i l
			r	Drop filos	horo or a	lick to upload
			L	Jop mes		flick to upload.
L.						
· · · · · ·						
GA						

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.

PubML	ST	Data	abase ho	me Cu	irator home C	ontents		
Logged in:	Keith .	lolley	(keith). 🕩 L	.og out   Char	nge password			Toggle: 🜖
Batc	h up	olo	ad se	quen	ce assemt	olies to n	nultiple	solate records
Please	upload	the a	issembly c	ontig files f	for each isolate reco	ord.		et et
remo row	ve /	id	isolate	current se contigs	equence bin state total size (bp)	filename	upload status	
	61	222	JB_21292	-	-	JB_21292.fasta	<ul> <li>✓</li> </ul>	
	61	223	JB_21293	-	-	JB_21293.fasta	✓	
	61	224	JB_21294	-	-	JB_21294.fasta	✓	
Remo All files — Act Vali	ve upload ion date	ed. T	he sequen	ces have n	ot yet been validate	d. This needs to	be done before	hey 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 ho	ome	Contents						
Logged in: Keith Jolley (keith). 🕩 Log out   Change passw	ord			Toggle: 🚯	Ξ			
Batch upload sequence assemblies to multiple isolate records								
Validation								
id isolate filename valid FASTA	contigs 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 👻		Action
		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). IbLog 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/solates/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 contain and 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 Jolley (keith). (4Log 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 loci, the appropriate scheme description. By default, loci are only scanned for an isolate when no allele designation has been made or sequence tagged. You uselecting the appropriate options.         Isolates       Loc       Schemes         19/9 S3131       10       165_TDNA       ISO_TDNA         13/1 10       10       165_TDNA       ISO_TDNA         13/2 A9 S335       10       235, rNA       10         30/1 4       10.0       235, rNA       10         13/2 30       14       235, rNA       10       10         20/2 33       160       24, S4355       10       10         13/2 30       14       235, rNA       10       10       10         13/2 30       14       10	you can choose to include all loci defined in schemes by selecting can choose to rescan loci with existing designations or tags by Parameters
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.

Publics1 Database finite Culator finite 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       Loc         19 \$3131       1165_DNA         24) \$4355       1165_FNA (SSU_FRNA)         30) 14       125_FNA         31) 10       225_FIAA         322 20       3262         335 26       165_FNA (SSU_FRNA)         3462 (NEISI015)       acef (NEISI2727)         acef (NEISI2727)       acha (NEISI2727)         acha (Neisi acha acha acha acha acha acha acha ach	ou can choose to include all loci defined in schemes by selecting n choose to rescan loci with existing designations or tags by Parameters

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.

Publ	Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Cuery/update Isolates: Add   Cuery/update   Batch insert																
Logged in:	Keith J	olley (kei	th). 🍽	og out   Chan	nge password											Help 🖉	Toggle: 🚯
Segu	ence	e tao	sc	an													
		-															
Isolate	Match	Locus	Allele	% identity	Alianment lenat	h Allele lenath	E-value	Sequence bin io	d Start	End	Predicted start	Predicted end	Orientation	Designate allele	Tag sequence	Flag 🙃	
34) 20	exact	abcZ	1	100.00	433	433	0.0	182791	7064	7496	7064	7496 extract -	←				-
34) 20	exact	adk	3	100.00	465	465	0.0	182750	1392	1856	1392	1856 extract -	$\rightarrow$	<b>V</b>			•
34) 20	exact	aroE	1	100.00	490	490	0.0	182731	32577	33066	32577	33066 extract -	←	<b>V</b>			-
34) 20	exact	fumC	1	100.00	465	465	0.0	182815	19783	20247	19783	20247 extract -	$\rightarrow$	$\checkmark$			-
34) 20	exact	gdh	1	100.00	501	501	0.0	182852	7516	8016	7516	8016 extract -	$\rightarrow$	<b>V</b>			•
34) 20	exact	pdhC	1	100.00	480	480	0.0	182819	13868	14347	13868	14347 extract ->	$\rightarrow$	<b>V</b>			-
34) 20	exact	pgm	3	100.00	450	450	0.0	182831	24559	25008	24559	25008 extract ->	$\rightarrow$				-
														All None	All None		
Actio	on —																
Tag	alleles/	/sequen	ces														
Started:	Thu Jul	2 10:47	:30 20 7:45 0	15													
Elapsed 1	rminie: mu Jui 2 (104/.45.2015)																
Please n	ote that	t scan re	sults	will remain	on the server for	7 days.											

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"><img ^="" alt="MRF" src="/images/mrf_20.gif" style="border: 1px solid #a0a0a0; background:white"/></div> <div>&gt;the <a href="http://www.meningitis.org/research/genome">MRF Meningococcus Genome Library</a> 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	r (keith). ➡Log out   Change password		Toggle: 🚺 📃
Add new p	roject member		
Please fill in the fiel — Record project id:! isolate id:! curator:! datestamp:!	ds below - required fields are marked 3) MRF Meningococcus Genome Libra 18968 Keith Jolley (keith) 2018-06-08	with an exclamation mark (!). Action ary Reset Submit	

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. <ul> <li>Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish.</li> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special <sup>O</sup> Text' to paste the data.</li> </ul>		H
Download submission template (xlsx format)		
Paste in tab-delimited text (include a field header line).	Action	
	Reset	

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). C+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_id isolate_id 3 18968 3 18969 3 19023 3 19024 3 19025 3 19026	Action Reset Submit
3 19027 3 19029 3 19030 3 19031 3 19032 3 19032 3 19033 3 19034 	

## 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:

PubMLST Database	home Contents					
Logged in: Keith Jolley (keith).	€ Log out   Change password			Help 🗹	Toggle: 🜖	
Full information	n on isolate I	/17661 (id.	:19377)			
Provenance/met	a data					
id:	19377		species:	Neisseria meningitidi	5	
isolate:	M17661 serogroup:			W		
strain designation:	W: P1.5-1,10-8: F-ND: ST-11 (cc11) capsule grou			W		
country:	USA sender:			Keith Jolley, University of Oxford, UK		
continent:	North America		curator:	Auto Tagger		
region:	MI		update history:	51 updates Show deta	ils	
year:	2008		date entered:	2012-06-27		
disease:	invasive (unspecified/oth	er)	datestamp:	2018-01-31		
Versions More than one version of thi Newer versions:	s isolate record exist. 40500					
Publication (1)						
<ul> <li>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, Harcourt BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. <i>Bioinformatics</i> 26:1819-26 18 isolates</li> </ul>						
X Sequence bin						
contigs:	2,511 N	0 contig number:	591	N95 contig number:	2,006	
total length:	1,805,445 bp	N50 length (L50):	1,011	N95 length (L95):	267	
max length:	4,833 bp NS	0 contig number:	1,720	loci tagged:	1,305	
mean length:	720 bp	N90 length (L90):	366 d	etailed breakdown:	Display	

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:

PubMLS																	
Logged in:	Keith Jolley	(keith). 🗭 Log o	ut   Change pas	ssword											Н	elp 🛃	Toggle: 🚯 📃
Isola	te que	ry/upda	te														
Enter se	earch criteria	or leave blank	to browse a	all reco	rds. Modify	form parameters to filter or	enter a list of valu	es.									Modify
Isola	ate provenar	ice/phenotype	fields			C	lisplay/sort optior	IS				Action					form
id		<b>*</b> =	•	Enter	value	+ 3	Order by: id			<ul> <li>ascend</li> </ul>	ling 👻	Reset Submit					options
						_	Display: 25	▼ rec	cords per page 🕚								
58,801 re	ecords return	ied (1 - 25 disp	olayed). Clicl	k the h	yperlinks fo	r detailed information.											
Dele	te	Tag scann	ing Pro	ojects -			- Private rec	ords -									
Delet	te ALL	Scan	Sele	ct prote	ect	✓ Link	Publish										
Page:	23	4 5 6	7 8 9		Last												
Delete	Update Se	equence bin	New versio	n	lealata	oliosos	a a un tau		Isolate fields 1	anastas			ст	MLST	Finety	ping anti	gens
×		1	+		A4/M1027	B1: NIBSC 2803: 71001	USA	1937	invasive (unspecified/other)	Species Neisseria meningitidis	serogroup A	genogroup capsule gro	4	ST-4 complex	5-2 Z	10 2	FetA VR
×	1	1	÷	2	120M	B35: NIBSC 2822: Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	A	1	ST-1 complex	5-2	10 🖉	F5-1 /
×	1	1	÷	3 N	/00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	В	1099		19 🥒	15 🥒	+
×	1	1	+	4	M1027	B43; NIBSC_3076; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	A	4	ST-4 complex	+	+	+
×	1	1	+	5 N	/00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	В	1100	ST-32 complex	7 🥒	16 🖋	+
×	1	1	+	6 N	/00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	W	1101	ST-22 complex	+	+	+
×		1	+	7	7891	B54; NIBSC_2760; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	A	5	ST-5 complex	20 🥒	9 🥒	F3-1 🥒
×	1	<u>1</u>	+	8 N	/00242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	В	1102	ST-18 complex	+	14 🖋	+
×		±	+	9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	W	114	ST-22 complex	+	+	+
×	1	<b>±</b>	+	10	6748	B73; NIBSC_2784; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	A	1	ST-1 complex	18-1 🥒	3 🥒	F5-1 🥖
×	1	<b>±</b>	+	11	129E	B92; NIBSC_2828; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	A	1	ST-1 complex	5-2 🥒	10 🥒	F3-6 🖋
×	1	<b>1</b>	+	12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	В	1015	ST-32 complex	7 🥒	16 🥒	+
×	1	1	+	13	139M	B99; NIBSC_2795; Z1099	Philippines	1968		Neisseria meningitidis	A	A	1	ST-1 complex	5-2 🥒	10 🥒	F5-1 🥒
×	1	1	+	14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	X	Х	117		+	14 🖋	+
×	1	2	+	15	1		Germany	1999	carrier	Neisseria meningitidis	E	E	864		+	+	+

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.

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). [9Log out   Change password
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_20150623074942_31862_84622_2015-06-23_2015-06-23_Joe Bloggs_NEIS00013
Return to index page

## 7.1 Alleles

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

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 🗗
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_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.

ogged in: Keith Jolley (keith).	Log out   Change password						Hel
urate submiss	sion						
ubmission: BIGSdb_ —Summary	20150709132553_20864_8972	29 — Sequences	s ———				
type: all submitter: Jo datestamp: 20 status: pe locus: NI sequences: 3 technology: Illu read length: 10 coverage: 20	leles le Bloggs, University of Oxford, UK 115-07-09 ending EIS0001 (IpxC) Imina 10-199 1-49x	Identifier Len UK322 92 UK323 92 UK347 92 Batch curate Messages	ength 924 1 924 2 924 1 924 1 te	Sequence AIGCTECAAAGAACTICEGEC ACAICAGAAATTETEGATAA AIGCTECAAAGAACTITIGEC ACAICAGAAATTETEGATAA AIGCTECAAAGAACTITIGEC ACAICAGAAATTETEGATAA Archive Archive of submission and any supp Download	Complete CDS	Status pending • pending •	Assigned allele Curate Curate Curate Update
assembly: de assembly software: Ve	e novo livet	Message: Ap	Append	1 Send now			

There will also be a table summarizing the sequences in the submission and their current submission status.

ied in: Keith Jolley (Kei	th). I+Log out   Change password					He
ırate submi	ssion					
ubmission: BIGSc	lb_20150709132553_20864_897	29 Sequences				
type: submitter: datestamp: status: locus:	alieles Joe Bloggs, University of Oxford, UK 2015-07-09 pending NEIS00001 (IpxC)	Identifier Length UK322 924 UK323 924 UK347 924 Batch curate	Sequence АГССТБСАЛАБААСТІСЕСС АСАГСАБАЛАТІБІББАТАЛ АГССТБСАЛАБААСТІТЕБС АСАГСАБААСТІБІББАТАЛ АГССТБСАЛАБААСТІТЕБС АСАГСАБАЛАТІБІББАТАЛ	Complete CDS	Status pending v pending v	Assigned allele Curate Curate Curate Update
sequences: technology: read length: coverage: assembly:	3 millumina 100-199 20-49x de novo Volunt	Messages Message: Appen	Archive Archive of submission and any supp at Download R	porting files:		

### 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.

ges in real oney freinige position						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	<b>~</b>	pending 👻	Curate 3
submitter: Joe Bloggs, University of Oxford, UK	UK323 924	ATGCTGCAAAGAACT?	TTGGC ACATCAGAACTTGTGGATAA	<b>~</b>	pending 👻	Curate
datestamp: 2015-07-09	UK347 924	ATGCTGCAAAGAACT:	TTGGC ACATCAGAAATTGTGGATAA	<b>~</b>	pending 👻	Curate
status: pending	Batch curate					Undate
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				
doubly. do novo						

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 Bullen	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	n). @Log out   Change password	Help 🖉	Toggle: 🚯
Add new allele	e sequence		
Please fill in the fields be	elow - required fields are marked with an exclamation mark (!).		
Record			
locueit	NEI80001		
allele id:1	210		
sequence:		TOCOLOT	<b>C</b> .
ooquonee	ATGCTGCAAAGAACTTCGGCGAAATCCATCAGCGTTACCGGACTGGCCTGCATTCGGCCGAACGGG ACCAGGCCGCCCGGCGCGGAAACAGGGGATTCCCTCCTCCGCCGTACCGATTGGGCGGGGGAGATGG ATCAAGCTGACCCCTTATTGATCAACGATACCGGCCTTTCCTCCACCATCGTTACCGACAAAGGCG GGCACGATCGAACACATTATGTCCGCGCTGTCCGCCTACGGTATCGACAACGCGCGCG	GCGAACA TGCGCGT ACGCACC ATCAAAA TTACGCC CTTTTGA	
status:	unchecked 🗸		
sender:!	Bloggs, Joe (jbloggs)		
curator:!	Keith Jolley (keith)		
date entered:!	2015-07-09		
datestamp:!	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). @Log out   Change password	Help 🖉	Toggle: 🜖
Add new allele sequence		
Sequence NEIS0001 (lpxC): 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.

gged in: Keith Jolley (keith	). @Log out   Change password						He
urate submis	sion						
Submission: BIGSdl	b_20150709132553_20864_897	29 — Sequences —					
type: submitter: datestamp: status: locus: sequences: technology: read length: coverage: sesmbhy:	alleles Joe Bloggs, University of Oxford, UK 2015-07-09 pending NEIS0001 (IpxC) 3 201 Illumina 100-199 20-49x de novo	Identifier Leng UK322 924 UK323 924 UK347 924 Batch curate Messages	th AIGCIGCAAAGAACTI AIGCIGCAAAGAACTI AIGCIGCAAAGAACTI 	Sequence CGGC ACATCAGAAATTGTGGATA TGGC ACATCAGAAATTGTGGATA IGGC ACATCAGAAATTGTGGATA Archive Archive Download	Complete CDS	Status assigned pending - pending -	Assigned allele 210 Curate Curate Update

### 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.

	ery: Sequences   Batch sequences   Co wnload: Alleles   MLST profiles ks: Contents   Home   PorA   FetA   Opti	ompare alleles   Pro ons   Isolate Databa	file/ST   Batch profiles   List   Browse   Query ase							
ogged in: Keith Jolley (keit	h). HLog out   Change password					Help (2				
Curate submission										
Submission: BIGSd	b_20150709132553_20864_897	29								
summary submitter: datestamp: status: locus: sequences: technology: read length: coverage:	alleles Joe Bloggs, University of Oxford, UK 2015-07-09 pending NEIS0001 (IpxC) 3 the Illumina 100-199 20-49x de novo	Identifier Length UK322 924 UK323 924 UK323 924 UK347 924 Batch curate Messages	Sequence ATECTECAAAGAACTICGEC ACATCAGAAATTGTGGATAA ATECTECAAAGAACTTGEC ACATCAGAAATTGTGGATAA ATECTECAAAGAACTTTGEC ACATCAGAAATTGTGGATAA ATECTECAAAGAACTTTGEC ACATCAGAAATTGTGGATAA Archive Archive f submission and any supp Download	complete CDS	Status assigned pending • pending •	Assigned allele 210 Curate Curate Update				

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). (9Log out   Change password Help 2 Toggle: ()
Batch in	sert sequences
This page allo only). Do not in Please note th	ws 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 integer ids 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.
locus:	NEIS0001 (lpxC)
status:!	unchecked -
sender:!	Bloggs, Joe (ibloggs)
sequence (FASTA):! Reject a ignored. Overrid Verrid	>UK323 ATGCTGCAAAGAACTTTGGCGAAATCGATCAGCGTTACCGGAGTCGGGCTGCATTCGGCG GAACGCGTCGCACCCTGCACCCCGCGCCGCGCACAACGAACG
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 Help	🖸 Toggle: 🚯
Batch insert sequences	
Sequence check       Original designation     Allele id       UK323     211       UK347     212       OK     Upload valid sequences	

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). @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). @Log out   Change password Help											
Curate submission											
Submission: BIGSd	b_20150709132553_20864_897	29 Sequences Identifier Length Sequence CDS Status Assigned allele									
type:	alleles	UK322 924 ATGCTGCAAAGAACTTCGGC ACATCAGAAATTGTGGATAA 🗸 assigned 210									
submitter:	Joe Bloggs, University of Oxford, UK	UK323 924 ATGCTGCAAAGAACTTTGGC ACATCAGAACTTGTGGATAA 🗸 assigned 211									
datestamp:	2015-07-09	UK347 924 ATGCTGCAAAGAACTTTGGC ACATCAGAAATTGTGGATAA 🗸 assigned 212									
status:	pending	Messages Archive Action Action									
IOCUS:	(IpxC)	Archive of submission and any supporting files: Close submission									
technology: read length: coverage: assembly software:	3 Juli Illumina 100-199 20-49x de novo Velvet	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). (HLog out   Change password Help 12											
Curate submission											
Submission: BIGSC — Summary type: submitter: datestamp: status: outcome: locus: sequences: technology: read length: coverage: accombine:	ib_20150709132553_20864_897 alleles Joe Bloggs, University of Oxford, UK 2015-07-09 pending accepted - data uploaded NEIS0001 (lpxC) 3 mi Illumina 100-199 20-49x do pare	29 Sequences Identifier Lengt UK322 924 UK323 924 UK347 924 Batch curate Messages Message: App	h ATGCTGCAAAGAACT ATGCTGCAAAGAACT ATGCTGCAAAGAACT 	Sequence TGGGC ACATCAGAAATIGTGGATAA TTGGC ACATCAGAACTIGTGGATAA TTGGC ACATCAGAAATTGTGGATAA Achive Archive Archive of submission and any supp Download TAR	Complete CDS	Status rejected v rejected v rejected v	Assigned allele Curate Curate Curate Update				
assembly software:	Velvet										

### 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.

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 (kei	th). @Log out   Change password												Help 🗗
Curate submi	ssion												
Submission: BIGS	ib_20150709132553_20864_897	29											
Summary		Sequences											
type:	alleles	Identifier Leng	gth		Sequ	ence		Соп	nplete CDS	Status	6	Assigned allele	
submitter:	Joe Bloggs, University of Oxford, UK	UK322 924	4 ATG	CTGCAAAGAA	CTTCGGC	. ACATCAC	AAATTGTGGAT	TAA	×	rejected	•		
datestamp:	2015-07-09	UK323 924	4 ATG	CTGCAAAGAA	CTTTGGC	. ACATCA	AACTTGTGGAT	TAA	×	rejected	•		
status:	pending	UK347 924	4 A16	LIGCAAAGAA	CITIGGC	. ACAICA	AAAIIGIGGAI	IAA	×	rejected	•		
locus:	NEIS0001 (lpxC)											Update	
sequences:	3 745	— Messages —								nive			
technology:	Illumina	Timesta	amp	User		Me	ssage		Archive	e of subm	issio	n and any suppo	rting files:
read length:	100-199	2015-07-09 12	2:39:35+	00 Keith Joll	ey These se	quences a	e not NEIS000	01 allele	5				-
coverage:	20-49x								Downl	oad TAR			
assembly:	de novo												
assembly software:	Velvet								Acti	on —		-	
					Me	essage: /	oppend Se	end now	Clos	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). [HLog out   Change password	3
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.

PUTIMIST Ownload: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database									
Logged in: Keith Jolley (keith). DLog out   Change password									
Curate submission									
Submission: BIG Sdb_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         Status         As           UK32         43         2         12         32         32         3         2         pending         C           UK32         43         2         12         32         32         3         2         pending         C           UK33         7         56         4         3         2         12         12         pending         C           UK34         76         3         5         3         87         43         34         pending         C           Batch curate	Messages Curate 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.

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													
ogged in: Keith Jolley (keith). @Log out   Change password									Help 🗗				
Curate submission													
Submission: BIGSdb_20150709134405_4219_3553 — Summary	5 Profiles Identifier UK32 UK33 UK34	adk 1 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 pending pending pending	Assigned S Curate			
Messages Archive Archive of submissi  Message: Append Send now	on and any	suppo	orting	files:						Opdate			

Clicking this link takes you to the curation interface *single profile upload page*. 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 Loci: Add MLST profiles: Add   Query/update   Batch insert												
Logged in: Keith Jolley (ke	ith). ⊕Log out   Change passw	ord		Help 🗹	Toggle: 🚺							
Add new MLS	ST profile											
~												
Please fill in the fields	Please fill in the fields below - required fields are marked with an exclamation mark (!).											
ST:1	10056											
adk: !	43											
abcZ: !	2											
aroE: !	12 🚔											
fumC: !	32											
gdh: !	32 🗘											
pdhC: !	3											
pgm: !	2											
sender: !	Bloggs, Joe (jbloggs)	<b>~</b>										
clonal_complex:												
curator: !	Keith Jolley (keith)											
date_entered: !	2015-07-09											
datestamp: !	2015-07-09											
PubMed ids:												
Action												
Reset Subn	nit											

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.

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											Help 🖉
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 urate	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.

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 🖉	
Curate submi	ssion											
Submission: BIGSo — Summary type: submitter: datestamp: status: — Messages	b_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 urate	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 pending	Assigned ST 10056 Curate Update	
Message: Appond	Archive of submissi	on and any	suppo	orting	ïles:							
messaye. Append	Send IUW											

This takes you to the *batch profile upload page* in the curators' interface.

The upload form will be filled with details from the submission.

Database: S Users: Add   Loci: Add MLST profile	Database: Species home   Curator's page (species)   Curator's page (database) PrrhMILST Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert										
Logged in: Keith Jolley (keith). 🗟 Log o	ut   Change password			Help 🗹 🛛 Toggle: 🚯							
Batch insert MLST	profiles										
This page allows you to upload pr Field header names must You can choose whether or it for each profile record. Download tab-delimited h Download submission ter	rofiles as tab-delimited be included and fields r not to include a ST fie eader for your spreadst nplate (xlsx format)	text or copied can be in any Id - if it is omi neet - use Pa	I from a spreadsheet. v order. Optional fields can be d tted, the next available ST will i ste Special <b>O</b> Text to paste the	nitted if you wish. • used automatically. If however, you include it in the header line, then you must also provide lata.							
Prese pase in tao-definitied adk abc2 aroE 7 56 4 76 3 5	fext (include a field new func gdh 3 2 3 87	ader inne) pdhC 12 43	pgm 12 34	Action Reset Submit							

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). I 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.

Profit/TLST Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database												
Logged in: Keith Jolley (keit	th). @Log out   Change password											Help 🖉
Curate submi	ssion											
Submission: BIG Sdb_20150709134405_4219_35535         Summary       Profiles         type:       profiles         submitter:       Joe Bloggs, University of Oxford, UK         datestamp:       2015-07-09         status:       pending         Messages       Archive         Archive of submission and any supporting files:         Download       Image: Status of S												
		Message:	Ap	pend	Se	end no	W	-A	ction lose	submission		

### 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.

PuisMILST Qu Lin	ery: Sequences   Batch sequences   Co wnload: Alleles   MLST profiles ks: Contents   Home   PorA   FetA   Opti	ompare alle ons   Isolati	les   F e Data	Profile/ abase	IST   B	atch p	rofiles	s   List	Bro	wse   Quei	ŋ			
Logged in: Keith Jolley (keit	h). I Log out   Change password													Help 🗹
Curate submi	ssion													
Submission: BIG So — Summary type: submitter: datestamp: status: outcome:	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 uurate ges Ap	abcZ 2 56 3	aroE 12 4 5	fumC 32 3 3 3	gdh 32 2 87	pdhC 3 12 43 — A Arct Dov	pgm 2 12 34 rchive of	Status rejected rejected rejected	• • •	Assigned ST 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.

PubMLST Qu Do Lin	ery: Sequences   Batch sequences   Co wnload: Alleles   MLST profiles ks: Contents   Home   PorA   FetA   Optic	mpare allei ins   Isolate	ies   F e Data	rofile/ base	ST B	atch p	rofile	s   Lis	t   Brov	wse   Query					
Logged in: Keith Jolley (keit	h). Hog out   Change password														Help 🖉
Curate submi	ssion														
Submission: BIGSo — Summary— type: submitter: datestamp: status:	Ib_20150709134405_4219_35535 profiles Joe Bloggs, University of Oxford, UK 2015-07-09 pending	Profiles Identifier UK32 UK33 UK34	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 rejected rejected rejected	A • •	ssigned ST Update			
Timestamp 2015-07-09 12:55:23	User +00 Keith Jolley You need to submit so	M me represe	essag entativ	je ve isol	ates d	lata fo	r thes	e prof	iles.	Archive of	fsub	mission and	any supporting	files:	
			Mes	sage:	Ар	pend	S	end n	i	Download — Action - Close s	d mi	nission			

## 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.

PubMLST)	Query: Search   Browse   P Breakdown: Isolate fields   Links: Contents   Home   C	rofile/ST   List Scheme/alle ptions   Profil	t les   Publications es/sequences defini	tions   Data	ibase su	bmissior	ıs					
Logged in: Keith Jolley	<b>'keith). 🕩</b> Log out   Change pass	word										Help 🖉
Curate subn	nission											
Submission: BIG	Sdb 20150709121747	1342 996	24									
Summarv												
Summary												
typ	e: isolates	- 6 Out										
Submitte	er: Joe Bloggs, University	of Oxford, UK										
stati	is: pendina											
Isolates												
isolate country	disease	source	species	serogroup	abcZ ad	k aroE	fumC gdh	pdhC pg	m FetA_VR	PorA_VR1	PorA_VR2	
UK322 UK n	neningitis and septicaemia	blood Nei	sseria meningitidis	B	2 3	4	3 8	4 6	F1-5	5	2	
Rotob ouroto	Sepucaernia	COP INER	ssena meningidus	D	2 3		5 10	Pacar	d etatue: e	onding.	Lindata	
Baich curate								Recon	u status, pr	ending 👻	Opuale	
Messages	Ar	chive										
	Arch	ive of submis	sion and any suppor	ting files:								
	Dow	nload 📊										
Message: Appor	d Sond now											
Message. Apper	Seliu llow											

#### Click the 'Batch curate' button.

PuinMLST Quer Brea Links	ry: Search   Browse   P akdown: Isolate fields   s: Contents   Home   O	rofile/ST   List Scheme/alleles   Publications )ptions   Profiles/sequences defi	nitions   Databas	e submission:	5			
Logged in: Keith Jolley (keith)	). 🕩Log out   Change pass	word						Help 🕑
Curate submis	sion							
Submission: BIGSdb — Summary type: i submitter: . datestamp: 2 status: j	o_20150709121747 isolates Joe Bloggs, University 2015-07-09 pending	7_1342_99624  of Oxford, UK						
Isolates								-
isolate country	disease	source species	serogroup abc	Z adk aroE fi	ImC gdh pdh	C pgm FetA_VR	PorA_VR1 PorA_VR2	2
UK325 UK	septicaemia	CSF Neisseria meningitidis	B 2	3 4	3 18 4	6 F1-5	5-1 2	
Batch curate						Record status: pe	ending 👻 Update	
Message: Append	Archi Archi Bow Send now	chive ive of submission and any supp mload TAR	orting files:					

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.

Publ	VLST	Data Usei Isola	abase: Spec rs: Add   Qu ates: Add   C	cies home   ery/update Query/update	Curator's p   Batch ins	age (species sert	i)   Curator's	s page (data	base)			
Logged in	: Keith Jolle	ey (keith)	). 🕩Log out	Change passw	vord							Toggle: 🚯
Batcl	h inse	ert is	olates	;								
This pa	ge allows Field head Enter alias Enter refer You can al locus nam You can ch Download Download select the s, Joe (jblo	you to u ler nam ses (alte ences f so uplo les). The tab-del submis sender ggs)	upload isola es must be ernative nar for your isol ad allele fie ese will be vhether or n imited hear ssion templ from the lis	te data as ta included an nes) for your ates as a se ids along w added with a ot to include der for your s tate (xlsx forr st below: v v	ab-delimite isolates a: isolates a: mi-colon (; th the othe a confirmed an id numi preadshee nat)	d text or copi- n be in any o s a semi-col ) separated 1 r isolate data d status and i ber field - if it et - use 'Past	ed from a si rder. Option on () separ ist of PubMi I - simply cr method set is omitted, e Special O	preadsheet. Ial fields can ated list. ed ids (non- eate a new as 'manual' the next ava ) Text' to pasi	be omitted integer ids v column with ilable id will te the data. your pested de	if you wish. vill be ignored). the locus name (s be used automati ata.	see the 'allowed_loci' tab in th tically.	e Excel template for
isol	late cou	ntrv	vear	disease	source	species	serogrou	an	abcZ	adk	Reset Submit	
aroB	fun	ιC	gdh	pdhC	pgm	FetA_VR	PorA_VR	1	PorA_VR2	2	Gubinit	
UK23 meni	33 UK .ngitidi	3	2015 B	meningit 2	is and 3	septicaen 4	nia 3	CSF 8	Neisseri 4	6		
F1-5	5	-	2	-	-	-	-	-	-	-		
UK32	2 UK		2014	meningit	is 9	blood 4	Neisseri	ia mening F1-5	gitidis	B 2_1		
Back	3			5		•	•					

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). DeLog 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). (*Log out   Change password	Help 🖉
Curate submission	
Submission: BICSdb 20150709121747 1342 99624	
Summary	
type: isolates	
submitter: Joe Bloggs, University of Oxford, UK	
catestamp: 2015-07-09 status: pending	
status, penuing	
- 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 blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2	
UN322 UK Septicaetina CSF Veissena mennigiliutis B 2 3 4 3 to 4 0 FT-2 5-1 2	
Baich curate	
Messages Archive Archive	
Archive of submission and any supporting files:	
Download 🔤	
Message Annend Send now	
moodge Append Constrom	

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   Data	tabase submissions	
Logged in: Keith Jolley (keith). GLog out   Change password		Help 🖓
Curate submission		
Submission: DICSdb 20150708191747 1249 88694		
Summary		
type: isolates		
submitter: Joe Bloggs, University of Oxford, UK		
datestamp: 2015-07-09		
status: pending		
Isolates		
isolate country disease source species serogroup	p abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2	
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	
	Record status: accepted 👻 Update	
Messages	Action	
Archive of submission and any supporting files:	Close submission	
	Close submission	
Download TAR		
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
```

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```
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.

PubMLS	Down Links	/: Sequi iload: A : Conte	ences   Batch sec Ileles   MLST pro nts   Home   Por/	quences   Compare alleles   Profile/ST   files A   FetA   Options   Isolate Database	Batch profiles	List   Browse   Q	luery		
									Help 🖉
Download	d allel	e se	quences						
Select loci by so	heme   Alp	habetio	cal list   All loci by	scheme					
Click within the	tree to disp	olay det	ails of loci belong	ging to schemes or groups of schemes -	clicking a grou	ıp folder will disp	play the loci for all	schemes w	vithin the group and any
subgroups. Clic	k the node	es to exp	pand/collapse.						
🛓 🛄 All loci									
🖡 📗 Caps	ule								
🕞 🕞 🚺 Gene	tic Informa	ation Pr	ocessing						
🕞 🖉 🖓 Geno	mic island	ls							
🥼 🛄 Metal	oolism								
🤌 🎧 Typin	q								
	LST								
	netyping a	ntigens	•						
	ir species								
	ALST (201	ocus pa	artial genes)						
🛄 el	ALST (20 1	ocus wi	hole genes)						
🗌 🗌 🛄 N	meningiti	dis cgN	ILST v1.0						
🖓 🖉 🖓 Other	schemes								
🦾 🛴 Loci ı	not in sche	mes							
MLST									
Locus Down	oad Type	Alleles	Length F	ull name/product Curator(s)	Last undated				
abcZ 🕕 🎿	DNA	728	Fixed: 433 bp	O. Harrison, K. Jolley	2015-06-22				
adk 🕦 🔳	DNA	501	Fixed: 465 bp	O. Harrison, K. Jolley	2015-06-08				
aroE 🕕 🎿	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				
	DNA	747	Fixed: 480 bp	O. Harrison, K. Jolley	2015-06-25				
pgm 😈 🚨	DINA	749	Fixed, 450 0p	O. Hamson, K. Jolley	2010-00-22				
Download table	tab-delim	ited tex	t   Excel format						

Click the download link for the required locus

Locus	Download	Type	Alleles	Length	Full name/product	Curator(s)	Last update
abcZ 🕕	*	DNA	728	Fixed: 433 bp		O. Harrison, K. Jolley	2015-06-22
adk 🗊	*	DNA	501	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-08
aroE 🕕	*	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

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ACCATCGGTATGGCGGGCGCGCCGGGGCAATTTCGAGCTGAACGTCTATATGCCCGTCATC	
GCCTACAACCTCTTGCAATCCATCCGCCTGTTGGGCGACGCGTGCAACAGCTTCAACGAA	
CACTGCGCCGTCGGCATTGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC	
CTGATGCTCGTTACCGCGTTAAACCGCAAAATCGGTTACGAAAAC	
>fumC_2	
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG	
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGG	
TTGGGCGAAATCAAAATCCCCGGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC	
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT	
ACCATCGGCATGGCGGGGGGGCGCGGGGGCAATTTCGAGCTGAACGTCTATATGCCCGTTATC	
GCCTACAACCTCTTGCAATCCATCCGCCTCTTGGGCGACGCGTGCAACAGCTTCAACGAA	
CACTGCGCCATCGGCATCGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC	
CTGATGCTCGTTACCGCGTTAAACCGCAAAATCGGTTACGAAAAC	
>fumC_3	
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG	
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGG	
TTGGGCGAAATCAAAATCCCCCGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC	
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT	
ACCATCGGCATGGCGGGCGCGCGGGGCAATTTCGAGCTGAACGTCTATATGCCCGTTATC	
GCCTACAACCTCTTGCAATCCATCCGCCTGTTGGGCGACGCGTGCAACAGCTTCAACGAA	
CACTGCGCCGTCGGCATCGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC	
CTGATGCTGGTTACTGCGTTAAACCGTAAAATCGGCTACGAAAAC	

### 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.

	uery: Sequ ownload: nks: Cont	uences Alleles tents   F	Batch   MLST lome   I	sequences   Compare alleles   profiles PorA   FetA   Options   Isolate Dat	Profile/ST   Batch profiles   List   Browse   Query labase		
							Hel
ownload all	olo si	onu	anco	26			
ownioau an		cyu					
Select loci by scheme	Alphabet	tical list	All loc	ci by scheme			
7							
•							
Locus	Download	i Type	Alleles	Length	Full name/product	Curator(s)	Last updated
ArsR [NEIS1769] 0	*	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] 🕦	<u>*</u>	DNA	493	Variable: No limits set	ABC transporter ATP-binding protein		2015-05-19
aceF [NEIS1279] 🕕	*	DNA	477	Variable: (1563 min; 1641 max)	dihydrolipoamide acetyltransferase (EC 2.3.1.12)		2015-05-19
ackA2 [NEIS1727] 🕕	- ±	DNA	408	Variable: No limits set	acetate kinase		2015-05-20
acnA [NEIS1729] 🕕	. <u>*</u>	DNA	527	Variable: No limits set	aconitate hydratase 1 (EC 4.2.1.3)		2015-05-20
acnB [NEIS1492] 🕕	*	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] 🕕	*	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
atlA [NEIS2274] ()	*	DNA	18	Variable: No limits set	atIA / peptidoglycan transglycosylase	O. Harrison	2014-12-10
autA [NEIS1859] ()	۰.	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.

Query: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query			
Download: Alleles (MLS1) profiles			
			Help 🗗
Download allele sequences			
Select loci by scheme   Alphabetical list   All loci by scheme			
MLST			
Locus Download lype Alleles Length Full name/product Curator(s) Last updated			
acc 0 2 DNA 728 Fixed: 433 bp O. Harrison, K. Jolley, 2015-06-22			
ack 0 2 DNA 501 Fixed 465 0p 0. Harrison, K. Jolley 2015-06-08			
aroe 0 Z DNA //5 Fixed 490 bp O. Harrison, K. Jolley 2015-05-22			
adh C DNA 732 Fixed 400 bp O. Harrison, K. Jolley 2015-06-02			
gdru Z DNA 732 Fixed 301 bp O. Harrison, K. Jolley 2015-05-11			
parte 2 DNA 747 Fixed 480 bp O. Harrison, K. Jolley 2015-06-25			
pgin V Z Diva 749 Pixeu 450 bp V. Hanison, K. Joney 2015-00-22			
Finetyping antigens			
Locus Download Type Alleles Length Full name/product Curator(s) Last updated			
PorA VR1 0 📩 peptide 264 Variable: No limits set PorA variable region 1 K. Jolley 2015-06-16			
PorA VR2 🚺 📩 peptide 735 Variable: No limits set PorA variable region 2 K. Jolley 2015-06-16			
FetA VR 🕦 📩 peptide 581 Variable: No limits set I. Feavers 2015-06-26			
rpir species			
Locus Download Type Alleles Length Full name/product Curator(s) Last undated			
TrolE 0 + DNA 123 Fixed 413 bb 508 ribosmal protein 6 (partial) E Walkins 2015-01-30			
ADP-heptose biosynthesis			
Locus  Download  Type  Alleles  Length Full name/product	Aliases	Curator(s)	Last updated
NEIS0769 (hldA) • ± DNA 244 Variable: No limits set D-beta-D-heptose-7-phosphate kinase	NMB0825; NMC0769; rfaE	C. Kahler	2015-05-18
NEIS0773 (hldD) 0 2 DNA 311 Variable: No limits set ADP-D-beta-D heptose epimerase	NMB0828; NMC0773	C. Kahler	2015-05-17
NEIS2014 (gmhB) 0 216 Variable: No limits set D-alpha,beta,D-Heptose 1,7 bisphosphate phosphatas	e NMB2033; NMC2014	C. Kahler	2015-05-20
NEIS2055 (hldC) 0 206 Variable: No limits set D-beta-D-heptose-1-phosphate adenylyltransferase	NMB2076; NMC2055	C. Kahler	2015-05-21
NEIS2070 (gmhA) () 📩 DNA 230 Variable: No limits set sedoheptulose-7-phosphate isomerase	NMB2090; NMC2070	C. Kahler	2015-05-21

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.

K → MLST	Genetic I Genomic Metaboli Typing MLST M MLST Finet Griffs M Antig M Antig M MLST M M MLST M	Informat c islands ism r yping an species en gene 3T (20 lo 5T (20 lo chemes in scher	tigens s cus pa cus wh lis cgM mes	ntial genes) nole genes) LST v1.0							
Locus	Download	d Type /	Alleles	Length	Full name/product	Curator(s)	Last updated				
abcZ 🕕	<u>*</u>	DNA	728	Fixed: 433 bp		O. Harrison, K. Jolley	2015-06-22				
adk 🕕	*	DNA	501	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-08				
aroE 🕕	<u>*</u>	DNA	775	Fixed: 490 bp		O. Harrison, K. Jolley	2015-06-22				
fumC 🚺	<u>*</u>	DNA	732	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-02				
gdh 🕕	<u>*</u>	DNA	732	Fixed: 501 bp		O. Harrison, K. Jolley	2015-06-11				
pdhC 🚺	<u>*</u>	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	I table tai	b-delimi	ted text	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   Query         Download: Alleles   MLST profiles         Links: Contents   Home   Options   PubMLST.org   Isolate Database										
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									
<ul> <li>Query database</li> <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 attributes.</li> <li>Browse MLST profiles</li> <li>Search MLST profiles matched to entered list.</li> <li>Batch profile query - lookup MLST profiles copied from a spreadsheet.</li> </ul>	Option settings • Set general options • Manage submissions • Manage submissions • Manage submissions • Mumber of sequences: 412175 • Number of profiles (MLST): 7841 • Last updated: 2015-06-17 • Profile update history • About BIGSdb									
Export     Sequences - XMFA / concatenated FASTA formats     Sequence similarity - find sequences most sir     Sequence comparison - display a comparison     Locus Explorer - tool for analysing allele sequence	milar to selected allele. I between two sequences. ences stored for particular locus.									

If multiple schemes are available, you will need to select the scheme in the dropdown box and click 'Download profiles'

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 have a corresponding record in the isolate database.	7 deposited in this database should						
<ul> <li>Query database</li> <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 attributes.</li> <li>Browse profiles</li> <li>List- find profiles matched to entered list.</li> <li>Search by combinations of alleles - including partial matching.</li> <li>Batch sequence from whole genome data</li> <li>Mumber of sequences: 519864</li> <li>Number of sequences: 519864</li> <li>Number of profiles: Show</li> <li>Last updated: 2015-06-26</li> <li>Profile update history</li> <li>About BIGSdb</li> </ul>	Option settings  • Set general options  Submissions • Manage submissions						
<ul> <li>Export         <ul> <li>Sequences - XMFA / concatenated FASTA formats</li> <li>Sequence similarity - find sequences most similar to selected allele.</li> <li>Sequence comparison - display a comparison between two sequences.</li> <li>Locus Explorer - tool for analysing allele sequences stored for particular locus.</li> </ul> </li> </ul>							

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	plex							
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 on Isolate M10 240474         Projects         The Main projects:         MEM Main projects:         Memory is a caliboration between Public Health England, The Waltome Trust Barger Institute and the University of Oxford, Uxr de monte Endering its Research Foundation.         Memory is a caliboration between Public Health England, The Waltome Trust Barger Institute and the University of Oxford, Uxr de monte Endering is Research Foundation.         Memory is a caliboration between Public Health England, The Waltome Trust Barger Institute and the University of Oxford, Uxr de monte Endering is an off-the institute of the Main Park Ma	PubMLST B	uery: Search   Brow reakdown: Isolate fie inks: Contents   Hon	vse   Profile/ST   List elds   Scheme/alleles   Publications ne   Options   Profiles/sequences definition:	s   Database submissions					
Priorets This is a data is a an ender of the bilowing projects:          INFO Manifegeocccus Genome Library         INFO Manifegeocccus Genome Library is a collaboration between Public Health England, The Wailcome Trutt Barger Institute and the University of Control, Kurder (Joneen Library data must be cited in any publication or presentation making use of 4.         INFO Manifegeocccus Genome Library data must be cited in any publication or presentation making use of 4.         INFO         INFO         INFO         MARP Manifegeocccus Genome Library genogroup B leadets from England Wells in 201011 and 201112         INFO         AMPF Manifegeocccus Genome Library genogroup B leadets from England Wells in 201011 and 201112         INFO         AMPF Manifegeocccus Genome Library genogroup B leadets from England Wells in 201011 and 201112         INFO         AMPF Manifegeocccus Genome Library genogroup B leadets from England Wells in 201011 and 201112         INFO	Full informat	ion on iso	late M10 240474						
This locked is a member of the following projects:          MEP Mentageoccus Genome Library ta collaboration below Public Health England. The Wellcome Trust Samper Institute and the University of Colord, funded by the Meningsis Research Foundation.         Library data must be cited in any publication or presentation making use of it.         Second Foundation.         MPE         MPE         MPE         MPE         MPE         MEMMentageoccus Genome Library data must be cited in any publication or presentation making use of it.         MPE         MPE         MEMMentageoccus Genome Library data must be cited in any publication or presentation making use of it.         MERE         AIM MEP Meningpoccus Genome Library data must be cited in any publication or presentation making use of it.         MERE         AIM MEP Meningpoccus Genome Library data must be cited in any publication or presentation making use of it.         MERE         AIM MEP Meningpoccus Genome Library data must be cited in any publication or presentation making use of it.         MERE         Mere Makein 2010/11 ad 2011/12         EMARE         Colspan="2">Colspan="2"         Colspan= Fit<	Projects								
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The MRF Meriopococca Genome Library is a collaboration between Public Health England, The Welcome Trust Sarger Institute and the University of Colord, Junied VI he Manipits Research Foundation.  See of the MRF Genome Library data must be cited in any publication or presentation making use of it.  See of the MRF Genome Library data must be cited in any publication or presentation making use of it.  See of the MRF Genome Library data must be cited in any publication or presentation making use of it.  See of the MRF Genome Library data must be cited in any publication or presentation making use of it.  See of the MRF Genome Library data must be cited in any publication or presentation making use of it.  MRF-MGL Isolates epi years 20102011 to 2011/2012 excluding Northern Ireland  MRF genomes exclu			MRF Menir	ngococcus Genome Library					
BUILD IN THE INSTITUTE OF THE I	The MRF Meningococo Oxford, funded by the M	us Genome Library Ieningitis Research	is a collaboration between Public Health E Foundation.	ngland, The Wellcome Trust Sar	ger Institute and the University of	A			
	Use of the MRF Genon	ne Library data must	be cited in any publication or presentation	making use of it.		Meningitis			
UNRF       MRF-MGL isolates epi years 2010/2011 to 2011/2012 excluding Northem Ireland       EAW_genogroup_ BMRF       All MRF Meningscoccus Genome Library genogroup B isolates from England and Wates in 2010/11 and 2011/12       MRF						Research Foundation			
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EAW_genogroup_B_MRF         All MRF Meningcocccus Genome Library genogroup B isolates from England and Wales in 2010/11 and 2011/12         MRE_no_MI         All MRF genomes excluding Northern Ireland         Provenance/meta data         MRE_no_MI         MRE_no_MI         All MRF genomes excluding Northern Ireland         Provenance/meta data         MRE_no_MI         Genetics M10 240474         serogroup: B         ENA accession: ERR080224 erworete accel         county: UK         county: UK         county: UK         county: UK         county: UK counted on the Multiversity of Oxford, UK (E-mail:         dom counts:: UK         counts:: UK         counts:: UK         counts:: UK         counts:: UK <t< td=""><td>MRF-MGL isolates epi</td><td>years 2010/2011 to</td><td>2011/2012 excluding Northern Ireland</td><td></td><td></td><td></td></t<>	MRF-MGL isolates epi	years 2010/2011 to	2011/2012 excluding Northern Ireland						
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MRE_no_Mi         All MRF genomes excluding Northern Ireland         MRE_no_Mi         Provenance/meta data         Misseria meninglidis         isolation is Br.P.119.1,1511: F3-9: ST-289 (cc269)         ENA accession: ERFN00524 = www.ellevel         contine: UK         contine: UX         contine: UX         contine: UX         contine: UX         contine: Ux         contine: Ux         contine: Uxope         contige: 275       N90: 6405	All MRF Meningococci	us Genome Library (	genogroup B isolates from England and Wa	les in 2010/11 and 2011/12					
All MRF_no_NI All MRF genomes excluding Northern Ireland Provenance/meta data Id: 18968 species: Neisseria meningitidis isolate: M10.240474 serogroup: B strain designation: B: P1.19.1.15.11: F3.9: ST-269 (cc269) ENA accession: ERV0.86224 www.strat.ext country: UK sender: Dorothea Hill continent: Europe curator: Dorothea Hill continent: Europe curator: Dorothea Hill genome and Hill (2000 xa.cu.k) update history: [00 genies frow details epidemiological year: 07/2010-06/2011 date entered: 2012.02-15 disease: invasive (unspecified/other) datestamp: 2014-06-23 Sequence bin contigs: 275 N90: 6405 total length: 2195045 bp loci tagged: 1611 mean length: 1982 bp detailed breakdown: Display N0: 34308 Schemes and loci Wight action and select schemes within tree to display allele designations	_								
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isolate M10 240474 serogroup: B strain designation: B: P1.19-1.15-11: F3-0: ST-269 (cc 269) ENA accession: ERR060224 arWWEblack contry: UK control UK (E-mail: contine: Europe curator Dorothea Hill contine ti Europe curator Dorothea Hill University of Oxford, UK (E-mail: region: South East curator UP 2002-00-08-2011 epidemiological yea: 07/2010-06/2011 date entered: 2012-02-15 disease: Invasive (unspecified/other) date stamp: contigs: 275 N90: 6405 total length: 2195045 bp N95: 3513 max length: 109859 bp locit agged: 1611 mean length: 2195045 bp detailed breakdow: Display N50: 34308 Schemes and loci Schemes and loci Matgate and select schemes within tree to display allele designations National content information Processing Matgate and select schemes within tree to display allele designations Schemes schemes information Processing Matgate and select schemes within tree to display allele designations National content information Processing Matgate and select schemes within tree to display allele designations	id:	18968		species:	Neisseria meningitidis				
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i continet:       Europe       curato:       Dorothea Hill, University of Oxford, UK (E-mall:         region:       South East       dorothea. Hill@200.0X.ac.uk)         year:       2010       update history:       103 updates; show details         epidemiological year:       07/2010-06/2011       date entered:       2012-02-15         disease:       invasive (unspecified/other)       date starup:       2014-06-23         Sequence bin       contigs:       275       N90:       6405         total length:       2195045 bp       N95:       3513         max inght:       109859 bp       locitagged:       1611         mean length:       7982 bp       detailed breakdown:       Display         N50:       34308       34308       Schemes and loci         Mavigate and select schemes within the to display allele designations         i appling       Watabolism       Navigate and select schemes within the to display allele designations         i appling       Other schemes       Other schemes       University of Other schemes	strain designation:	B: P1.19-1,15-11: F	-3-9: ST-269 (cc269)	ENA accession:	ERR086224 → www.ebi.ac.uk				
regin       South East       dorothea.hill@zoo.ox.ac.uk)         year:       2010       update history:       100 updates; show details         epidemiological year:       072010-06/2011       date entered:       2012-02-15         disease:       invasive (unspecified/other)       date entered:       2014-06-23         Sequence bin       275       N90:       6405         total length:       198059 bp       loci tagged:       1611         mean length:       19825 bp       detailed breakdown:       Display         N0:       34308       Sequence bin       Display         Schemes and loci       statistic schemes within the losiplay allele designations       Sequence schemes within the losiplay allele designations         Image: Processing Process	continent:	Europe		curator:	Dorothea Hill, University of Oxford, UK	(E-mail:			
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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     Schemes and locl       All loci     Image: Schemes site of the schemes site o	epidemiological year:	07/2010-06/2011		date entered:	2012-02-15				
Sequence bin         contigs:       275       N90:       6405         total length:       2195045 bp       N91:       3513         max length:       109859 bp       loci tagged:       1611         mean length:       7962 bp       detailed breakdown:       Display         N50:       34308       34308	disease:	invasive (unspecifi	ied/other)	uatestamp.	2014-00-23				
contigs: 275 N90: 6405   total length: 2195045 bp N95: 3513   mean length: 109859 bp loci tagged: 1611   mean length: 7982 bp detailed breakdown: Display   N50: 34308 Display   Schemes and loci   All loci Capsule Genetic Information Processing   Genetic Information Processing Metabolism   Hetabolism Uisplay   Pillin Hetabolism   Wetabolism Other schemes	Sequence bin								
total length:     2195045 bp     N95:     3513       max length:     109859 bp     loci tagged:     1611       mean length:     7982 bp     detailed breakdown:     Display       N50:     34308     34308   Schemes and loci         All loci             Capsule         Genetic Information Processing           Metabolism           Typing            Other schemes	contine	275	N90-	6405					
max length:       109859 bp       locitagged:       1611         mean length:       7962 bp       detailed breakdown:       Display         N50:       34308       Display         Schemes and loc!       All loci       Image: Capsule information Processing informatinformation Processing informatinformation Processing information	total length:	2195045 bp	N95:	3513					
mean length:     7982 bp     detailed breakdown:     Display       N50:     34308       Schemes and locl       All loci       Image: Section of the schemes       Image: Section of the schemes   Navigate and select schemes within tree to display allele designations	max length:	109859 bp	loci tagged:	1611					
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Schemes and locI  All loci Capsule Genetic Information Processing How Metabolism How Dilin How D	N50:	34308							
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All loci     Navigate and select schemes within tree to display allele designations     Gapsule     Gapsule     Metabolism     Metabolism     Pilin     Other schemes			Noviente enderste de la companya de						
Genetic Information Processing     Genetic Inf	All loci		Navigate and select schemes within tree	to display allele designations					
Image: Second	Genetic Info	mation Processing							
Pilin Pilin Typing Pilin Other schemes	⊳- 💭 Metabolism	- 📓 Metabolism							
Company of the schemes	Pilin								
	Other schen	ies							
- 💭 Loci not in schemes	📗 Loci not in s	chemes							

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 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	
🛓 🌆 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     Metabolism	MLST								
Pilin Typing MLST Finetyping antigens	abcZ 4 S	adk 10 S	aroE 15 S	fumC 9S	gdh 8 S	pdhC 11 S	pgm 9 S	<b>ST</b> 269	clonal complex ST-269 complex
Antigen genes     Ribosomal MLST									

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

Profit         Guery: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions											
NEIS0346 all	ele seque	nce: id-18968									
Contig position											
sequence bin id:	4956		length:	744							
contig length:	22993		orientation: f	forward							
end:	14607		method:	yes Illumina							
Sequence											
CACTGTACGC GGCGCA	CGGC TICAGCATI	G CGGGCAGGCG GAAAAACTAT TA	ACCGTACAG CCGACGGT	AA AACCGAAGAT	GCCGTCTTAA	TGGAGAAAAT	ATGTTAAGCG	CGCGCTACCT	CCACCTGCAC	GAAGCCTTGG (	GTTTGGGCCC
AGIGITGGAA ACAACC	GCCG TACATACGC	G CAAACCCGCG CCIGAAACCG AF	ACGCCICI GICCGGCG	TT TCAGACGGCA	TCGCCCCCGT	TCCCGCCGCT	TCGGGCATAA	CCAAACTIGC	CGTTGTCAGC	CIGIGICCGC (	CGACCGAGGA
TATGGTTTAC GGGCAA	CTGT TCCACGGAA	A AGCGGGTGTC CTGCTCGACA AT	ATACTCAA AGCCGTAG	GG CTCGATGCCG	CCTATGTCCA	CAAAACCTGT	TGGGTGAAAA	CCGCCGCCGT	CGGCAACCCG	ATGCCGTCTG	AAGCGGCAAT
CGCCCGGCTG TTGCGC	CAAC CCGLCCGCGA CAAC CCGAACTCA	A ACICGACGCC IGCCGCGCAC CO A AGCCCGCGCC IGGCAGACGC IO	CAAGCAGCT CAAACGTG	TC TTGGCGCAAG	GCGGCGGCAG	TTGAAGCGCG	CCGCACGGGG	CGGTAGAATC	GCAACTGCGT	CCCAATATCT (	GACAGAAAGC
ACAAAATGAC CGATTT	CCGC CAAGATTIC	C TTAAATTCTC CCTC									
Translation											
нст	' R R T A S R G A R T	SALRAGGKT OHCGODFKI	I T V Q P T	VKPK R*NRR	M P S *	WRKY	Y F1 F2				
L Y	AAHGF	SIAGRRKN	YYRTAD	GKTEI	DAVL	мекі	F3				
1 CACTGTA	CGCGGCGCACGGCT	CAGCATTGCGGGCAGGCGGAAAAAC	TATTACCGTACAGCCGA	CGGTAAAACCGAA	GATGCCGTCTT#	ATGGAGAAAA:	T 100				
VK	V K R A L P P P A R S L G F G P D V V E A G S R R P A V R N I A G FI										
T J S R T J T J T L A J G J G F M W J K K G A V V J F S A I L F E 12 C * A R A T S T C T K F W V W A R C G * S G E F S S C R P Q H C R F3											
101 ATGTTAA	GCGCGCGCTACCTC	CACCTGCACGAAGCCTTGGGTTTGGG	CCCGATGTGGTTGAAGC	GGGGAGCCGTCGT	CCTGCCGTCCGC	AACATTGCCG	G 200				
:		::::		:::			I				
K P	DTNPP	AKANRPQHS	SAASVR:	TAYRS	G T A Ç	N H E	F1				
S P K A R	TOTKD	Q K Q T V L S I R K S K P S S A F	RSVRPN	SIPV	RHGS	K P * I	F2 K F3				
201 AAAGCCC	GACACAAATCCGCC	CGCAAAAGCAAACCGTCCTCAGCATI	CCGCAGCGTCCGTCCGA	ACAGCATACCGGT	CAGGCACGGCTC	AAAACCATGA	A 300				
:		::::		:::			1				

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 nks: Contents   Home   PorA   FetA   Options   Isolate Database
Profile inform	nation for ST-11 (MLST)
ST abcZ adk a	aroEfumCgdhpdhCpgmclonal complex43846ST-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. 2899 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

ProfileTATION Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions										
										Toggle
Sequen	ce bin for N	110 240474								
Contig sun	nmary statistics	Contig size	distribution	Cumulative cor	ntig lengt	h				
<ul> <li>Number of contigs: 275</li> <li>Total length: 2195045</li> <li>Miamme length: 10959</li> <li>Mean length: 7082</li> <li>o length: 16244</li> <li>N50: 34308</li> <li>N90: 6405</li> <li>Download sequences (FASTA format)</li> <li>Download sequences with annotations (EMBL format)</li> </ul>										
Sequence	Sequencing 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	<u> </u>			
				NEIS1145	6141	6869	- i			
				NEIS1144	6892	7923	<u> </u>			
				NEIS1143	8005	8313	4			
				NEIS1142	9288	10541	È			
				NEIS1140	10613	12241	4			
				NEIS1139	12391	12744	$\rightarrow$			
				NEIS1138	12824	14362	$\rightarrow$			
				NEIS1137	14426	15046	$\rightarrow$			
				NEIS1136	15102	15392	É			
				NEIS1135	15585	16832				
				NEIS1134	16825	17520	Ś			

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   Lis           Download:         Alleles   MLST profiles           Links:         Contents   Home   PorA   FetA   Options   Isolate Database	( 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 er partial matches will be identified if an exact match is not found. You can query using either DNA or peptide ser — Please select locus/scheme — — — — — — — — Order results by – All loci	xact match against the chosen (or all) loci - they do not need to be trimmed. The nearest quences. [7] ———Alternatively upload FASTA file ————————————————————————————————————
GACGCGGTGCGCGATGAAAAGICAAAGICATGAAGCCATGAAGCCGCTGACCGTCGAA TCIGICAATGAAAAIGICGGCGGGACAAIATACCGCGGCGCAAAGGCATGAACGGCTAT CIIGAAGAAAICGACTAICGGTIIGGCCGACGACAICACGGCGGAGTCAAAAACCAITGCCAT TGAGGGCAAAACCAITIIGCITIIGGCCGGGCGCGGCGCG	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.

Query: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   E Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database	rowse   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 partial matches will be identified if an exact match is not found. You can query using either DNA or peptide seque — Please select locus/scheme — — — — — — — — — — — — — — — — — —	t match against the chosen (or all) loci - they do not need to be trimmed. The nearest nces. [] Alternatively upload FASTA file Action Select FASTA file: Reset Submit Browse No file selected.
1 exact match found.	
Allele Length Start position End 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.

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							
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						
GACGCGGTGCGCGATGAAAAAGTCAAAGTCATCAAGTCATTGAAGCCGCTGACCGTCGAA Select FASTA file:	Reset Submit						
TIGLEARIGEARIGETEGSCEGSALGATIALECESCEGALGALGELARAGECALGALGELARIGETEG CIIGAAGGAATCAALTIGEGITEGSCEAGGCGEGGEGGCAGGACALTIGECAL IGAGGGCAAAACCALTIIGCTITIGGGCGGGGGGGCGGGGGGGGGGGGGGGGGG							
Cineast match aref- 8							
Show alignment							
Differences							
2 differences found.							
258 <sub>T →</sub> 333 <sub>A</sub> 333 <sub>A</sub> → 488 <sub>G</sub>							
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.

Query: Sequences   Download: Alleles   1 Links: Contents   Ho	Batch sequences   Compare alleles   Profile/ST   Batch MLST profiles me   PorA   FetA   Options   Isolate Database	profiles   List   Browse   Query	
Sequence query - Neis	seria locus/sequence definitio	ons	
Please paste in your sequence to query a partial matches will be identified if an exa — Please select locus/scheme All loci — Enter query sequence (single or mult	gainst the database. Query sequences will be checked ct match is not found. You can query using either DNA d Order results by – locus → iple contigs up to whole genome in size)	a first for an exact match against the chosen (or all) loci or peptide sequences. [] Alternatively upload FASTA file Select FASTA file: Browse_ No file selected.	Action Reset Submit

#### 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.

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		
Sequence guery - Neisseria locus/sequence definitions		
Please paste in your sequence to query against the database. Query sequences will be checked first for an exact partial matches will be identified if an exact match is not found. You can query using either DNA or peptide sequen	match against the chosen (or all) loci - they do not need to be trimmed. The nearest ces. $\underline{r}$	
MLST v locus v		
Enter query sequence (single or multiple contigs up to whole genome in size)	Alternatively upload FASTA file — Action — Action	
>4758 NODE 192 length 1326 cov 47.828808	elect FASTA file: Reset Submit	
TAGAACAACAGCAATATICAAAGAITATCIGAAAGICCGAGAIICIAGAIICCCGCIIIC	Browse No file selected.	
CCGGGGAATGACGAAAAGCAAGCCGAGAATCCGACCTAGCTGCCAAACGCCGGCGGCGGCGGCCGGC		
GECAGTTAGTACGCAAAATCGAACAGCACCACAAAAAAAGCCCCGATTCGGATTTTCCAAT		
CGGGCTTTTTTTGCGCCCCGTTTTGTCATCCCGTGAAATATCCGCATGACAAAAATATAGTG ~		
7 exact matches found.		
Allele Length Start position End position Flags Comments		
abcZ: 4 433 203051 203483		
adk: 10 465 938327 938791		
aroE: 15 490 1775325 1775814		
fumC: 9 465 1134240 1134704		
gdh: 8 501 961439 961939		
pdhC: 11 480 1341678 1342157		
pgm. 9 450 1410240 1410095		
MLST		
ST 269		
clonal complex ST-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). @Log out   Change password	3
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 et 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 MLST Incurs Inc	exact match against the chosen (or all) loci - they do not need to be er DNA or peptide sequences. • Alternatively upload FASTA file Select FASTA file:
CAACCGAAAAAAATCATTGACGAAGGCGGCGTGGGCGCGACGACGACATCATTATCGGCATGGTCAAAGAAC GCATCGCGCAAGACGACTGCAAAAACGGTTTCCTGTGGGTTTCCGGCGCACGGGCGA AGCGATGGTTGAAGCAGGCGTGGATTIGGATGCAGTCGTTGAAGGCGACGACGGCGCGACGGGCGACGGGCGACGAGGGTGATGTC GACCGCGATGAAGGGCCGCGCGCGCGATTIGGTTGGATGCGGCCGACGGCGACGACGAGGAGGACGCCGC AAGTTGAAGGCAAAGACGACGTAACCGGCGAAGATTTGGTTGATTCAGCGACGACGACGAAAGAAA	Browse No file selected. Action Reset Submit

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       UIF 1     Partial match found: adk: 2: 2 differences found 100 T = 100 A: 107 T = 107 A
DSH_1 Partial match found: adk: 10: 1 difference found. $^{286}G \rightarrow ^{289}T$
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	<ul> <li>Downloads         <ul> <li>Allele sequences</li> <li>MLST</li> <li>Download profiles</li> </ul> </li> <li>Option settings             <ul> <li>Submissions</li> <li>Set general options</li> <li>Manage submissions</li> </ul> </li> </ul> <li>General information         <ul> <li>Number of profiles: 537919</li> <li>Number of profiles: Show</li> <li>Last updated: 2015-08-27</li> <li>Profile update history</li> </ul> </li>
Export     Sequences - XMFA / concatenated FASTA formats     Sequence similarity - find se     Sequence comparison - disp     Locus Explorer - tool for anal	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.

Query: Seque Download: A Links: Conte	ences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query Jleles   MLST profiles nts   Home   PorA   FetA   Options   Isolate Database		
	Toggle: 1		
Query sequences f	or Neisseria locus/sequence definitions database		
Some loci have additional fields w plugins.	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		
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 l	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		
locus 👻 =	abcZ + i Order by: locus		
	Display. 25 V fecolus per page [		
	- Action		
	Reset Submit		

Click submit.

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
Toolei I
Querv 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
Combine searches with: AND - Order by: locus - ascending -
locus v = vabcZ + i Display: 25 v records per page i
allele id $\checkmark$ = $\checkmark$ 5
> Filter query by
1 record returned. Click the hyperlink for detailed information.
locus         allele id         sequence         sequence length         comments         flags           abc2         5         TTTGATACCETTGCC         TTGGTCGAACTCGATC         433

Click the hyperlinked results to display allele records.

PTIDIALST 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.
Combine searches with: AND  Order by: locus  ascending
locus • = • abcZ + I Display: 25 • records per page I
allele id v = v 5
C Filter query by Action Reset Submit
1 record returned. Click the hyperlink for detailed information.
Iocus     allele id     sequence     sequence length       abcZ     5     TITIGATACCGTIGCC     TITIGATACCGTIGCC

PubMLST	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
Allele inform	ation - abcZ: 5
Provenance/meta	data
locus:	abcZ i
allele:	5
sequences:	ITTGATACCG TIGCCGAAGG TITGGGCGAA ATTCGCGATI TATTGCGCCG ITATCATCAT GICAGCCATG AGTTGGAAAA TGGTTCGAGT GAGGCTITGT TGAAAGAGCT TAACGAATIG CAACTGAAA TCGAAGCGAA GGACGGCTGG AAGCTGGATG CGGCGACTAA GCAGACTTIG GTGGAACTIG GITTGCCAGA AAACGAAAAA ATCGGCAACC TCTCCGGCGG ACGGAAAAAG CGTGTTGCCC TIGGGCGCGG AAGCCTGGATG ITATCGCTG GACGAACCG ACCAACCATI GGACATTGA CGCGATTATI TGGCTGGAAA ATCGGCTAGA GGCAGCCTGG TIGGGACTGC CGCTTTTTGG ACAATAACGC CACGGCATC GICGAACTGG ATC
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	ig this allele
MLST:	183 profiles
Isolate 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: 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
allele id • < • 10 (+) 7 Order by: locus • ascending •
Display: 25 → records per page []
Action Action
locus: abcZ I Reset Submit
status:
sender:
curator:
allele flag:
9 records returned. Click the hyperlinks for detailed information.
abc7 d TTGATACGETTGATCCACC TACCACCACCACCACCACCACCACCACCACCACCACCACC
abez 1 THORRELOGIECC THEFORECOME 433
abc2 3 TITGATACCETIECC TIGTIGAACTIGACC 433
abcz 4 ITIGATACCGTIGCC IIGICGAACICGATC 433
abcZ 5 ITIGATACCETTECC ICEICEAACTCEAIC 433
abcz 6 TITGATACCGTIGCC TIGTCGAACTCGATC 433
abcz 7 TITGATACTGTTGCC TITGTCGAACTCGATC 433
abcZ 8 TITGATACCGTIGCC TIGTCGAACTIGACC 433
abcz 9 TITGATACCGTTGCC TIGTCGAACTCGATC 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 the total known diversity of Neisseria species. Every new ST deposited in this database should have a corresponding record in the isolate database.			
<ul> <li>Query database</li> <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.</li> <li>search, prove or enter rist or promes</li> <li>Search by combinations of alleles - including partial matching.</li> <li>Batch profile query - locup profiles copied from a spreadsheet.</li> <li>Extract finetype from whole genome data</li> </ul>	<ul> <li>Downloads         <ul> <li>Allele sequences</li> <li>MLST</li> <li>Download profiles</li> </ul> </li> <li>Option settings             <ul> <li>Set general options</li> <li>Set general options</li> <li>Set general options</li> <li>Mumber of sequences: 537919</li> <li>Number of profiles: Show                 <ul> <li>Last updated: 2015-08-27</li> <li>Profile update history</li> <li>About BIGSdb</li> </ul> </li> </ul> </li> </ul>		
Export     Sequences - XMFA / concatenated FASTA formats     Sequence similarity - find se     Sequence comparison - disp     Locus Explorer - tool for anal	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.	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.

Profit/ULST Ownload: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database														
											He	lp 🗗	Toggle: 🚯	
Querv	uery PorA VR2 sequences - Neisseria locus/sequence definitions database													
Locus: Po	rA_VR2		→ Page will reload v	when changed									Madifu	
- Eud	hor inform	notion is quailable for this los											form	
• Fuit		nation is available for this for	.us.										options	
Please ente	er your se	arch criteria below (or leave	blank and submit to re	eturn all records).									_	
— Allele fi	ields —			Disi	olav —				Action	ı				
family		2			rder by:	allele i		ascending	-					
idiritiy		• • 2			raor bj.	ancie i		ascending	<ul> <li>Reset</li> </ul>	t Sub	mit			
					Dienlov:	25	recorde pe	r nago 🙃						
					Display:	25 🗸	records pe	r page 🜖						
					Display:	25 🗸	records pe	r page 🕦						
84 records r	eturned (*	1 - 25 displayed) Click the h	vperlinks for detailed i	nformation	Display:	25 👻	records pe	r page 🟮						
84 records r	eturned (*	1 - 25 displayed). Click the hy	yperlinks for detailed i	nformation.	Display:	25 🗸	records pe	r page 🕦						
84 records r Page: 1	eturned (*	1 - 25 displayed). Click the hy	/perlinks for detailed i	nformation.	Display:	25 🗸	records pe	r page 0						
84 records r Page: 1	eturned (* 2 <u>3</u>	1 - 25 displayed). Click the hy	/perlinks for detailed i	nformation.	Display:	25 🗸	records pe	r page 0						
84 records r Page: 1	returned (* 2 3 allele id	1 - 25 displayed). Click the hy 4 > Last sequence	/perlinks for detailed i sequence length	nformation.	Display:	25 ↓ varian	records pe	r page 1) mAb1 r	nAb1 reactivity	/ mAb2 r	nAb2 react	ivity   fla	15	
84 records r Page: 1 Iocus PorA VR2	returned (* 2 3 allele id 2	1 - 25 displayed). Click the hy 4 > Lest Sequence HFVQQTPKSQPTLVP	/perlinks for detailed i sequence length 15	nformation.	Display:	25 ↓ varian	records pe	r page () mAb1 r MN16C13F4	nAb1 reactivity +	/ <b>mAb2</b> r AF202	nAb2 react	ivity fla	gs	
84 records r Page: 1 Iocus PorA VR2 PorA VR2	returned (* 23 allele id 2 2-1	1 - 25 displayed). Click the hy 4 > Last sequence HFVQQTPKSQPTLVP HFVQQPPKSQPTLVP	perlinks for detailed i sequence length 15 15	nformation.	Display: family 2 2	25 ↓ varian	records pe t old name 2b	mAb1 r MN16C13F4 MN16C13F4	nAb1 reactivity + -	/ <b>mAb2</b> r AF202 AF202	nAb2 react - +	ivity fla	gs	
84 records r Page: 1 Iocus PorA VR2 PorA VR2 PorA VR2	returned (* 2 3 allele id 2 2-1 2-10	1 - 25 displayed). Click the hy 4 > Last Sequence HFVQQTPKSQPTLVP HFVQQPPKSQPTLVP HFVQQPPSQSTLVP	perlinks for detailed i sequence length 15 15 15	nformation.	Display: family 2 2 2	25 ↓ varian 1 10	records pe t old name 2b	mAb1 r MN16C13F4 MN16C13F4	nAb1 reactivity + -	/ <b>mAb2</b> r AF202 AF202	nAb2 react - +	ivity flag	gs	
84 records r Page: 1 Iocus PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2	eturned (* 2 3 allele id 2 2-1 2-10 2-11	1 - 25 displayed). Click the hy 4 > Last Sequence HFVQQPPKSQPTLVP HFVQQPPKSQPTLVP HFVQQPQSQSTLVP HFVQQPQSQSTLVP	perlinks for detailed i sequence length 15 15 15 15	nformation.	family 2 2 2 2 2	25 ↓ variant 1 10 11	records pe t old name 2b	mAb1 r MN16C13F4 MN16C13F4	nAb1 reactivity + -	/ mAb2 r AF202 AF202	mAb2 react - +	ivity fla	95	
84 records r Page: 1 Dora VR2 Pora VR2 Pora VR2 Pora VR2 Pora VR2	returned (* 2 3 allele id 2 2-1 2-10 2-11 2-12	1 - 25 displayed). Click the hy 4 > Last Sequence HFVQQTPKSQPTLVP HFVQQPPKSQPTLVP HFVQQPPSQSQPTLVP HFVQQTPKSQPTLVP HFVQQTPKSQPTLVP	perlinks for detailed i sequence length 15 15 15 15 15	nformation.	family 2 2 2 2 2 2	25 ↓ varian 1 10 11 12	records pe t old name 2b	mAb1 r MN16C13F4 MN16C13F4	nAb1 reactivity + -	/ <b>mAb2</b> r AF202 AF202	nAb2 react - +	ivity   fla	95	
84 records r Page: 1 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2	allele id 2 3 2-1 2-10 2-11 2-12 2-13	1 - 25 displayed). Click the hy 4 > Last Sequence HFVQQTPKSQPTLVP HFVQQPPKSQPTLVP HFVQQPPSQSTLVP HFVQQTPQSQPTLVP YFVQQTPQSQPTLVP	perlinks for detailed i sequence length 15 15 15 15 15 15 15	nformation.	family 2 2 2 2 2 2 2 2 2 2 2 2	25 ▼ varian 1 10 11 12 13	records pe	mAb1 r MN16C13F4 MN16C13F4 MN16C13F4	nAb1 reactivity + -	/ mAb2 r AF202 AF202	nAb2 react - +	ivity  fla	95	
84 records r Page: 1 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2	allele id 2 3 2-1 2-10 2-11 2-12 2-13 2-14	1 - 25 displayed). Click the hy 4 > Lest Sequence HFVQQTPKSQPTLVP HFVQQAPQSQSTLVP HFVQQAPQSQSTLVP HFVQQTPKSQPTLVP HFVQQTPKSQPTLVP HFVQQTPSQPTLVP HFVQQTLASKPTLVP	yperlinks for detailed i sequence length 15 15 15 15 15 15 15 15 15 15	nformation.	family 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	25 ▼ Varian 1 10 11 12 13 14	t old name 2b	mAb1 r MN16C13F4 MN16C13F4 MN16C13F4	nAb1 reactivity + - +	/ <b>mAb2 r</b> AF202 AF202	nAb2 react	ivity fla	95	
84 records r Page: 1 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2	eturned (* 2 3 2-1 2-10 2-11 2-12 2-13 2-14 2-15	1 - 25 displayed). Click the hy 4 > Last Sequence HFVQQTPKSQPTLVP HFVQQPPKSQPTLVP HFVQQPQSQSTLVP HFVQQTPQSQPTLVP HFVQQTPQSQPTLVP HFVQQLPKSQPTLVP HFVQQKSTSKPTLVP	perlinks for detailed i sequence length 15 15 15 15 15 15 15 15 15	nformation.	family 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	25 ▼ varian 1 10 11 12 13 14 15	records pe <b>old name</b> 2b 33 33a (33-1)	mAb1 r MN16C13F4 MN16C13F4 MN16C13F4	nAb1 reactivity + - +	/ <b>mAb2</b> r AF202 AF202	nAb2 react	ivity   fla	<b>JS</b>	
84 records r Page: 1 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2 PorA VR2	eturned (* 2 3) allele id 2 2-1 2-10 2-11 2-12 2-13 2-14 2-15 2-16	1 - 25 displayed). Click the hy 4 > Last Sequence HFVQQTPKSQPTLVP HFVQQPPKSQPTLVP HFVQQPPSSQTLVP HFVQQTPSSQPTLVP HFVQQTPSSQPTLVP HFVQQTPSSQPTLVP HFVQQKLSKFTLVP HFVQQKFISKFTLVP	yperlinks for detailed i sequence length 15 15 15 15 15 15 15 15 15 15	nformation.	family 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	25 • varian 1 10 11 12 13 14 15 16	c old name 2b 33a (33-1) 33b (33-2)	mAb1 r MN16C13F4 MN16C13F4 MN16C13F4	nAb1 reactivity + - +	/ mAb2 r AF202 AF202	mAb2 react	ivity   fla	20	

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         Port   FetA   Options         Isolate         Database												
	Help 🗹	Toggle: 🚺										
Query abcZ sequences	s - Neisseria locus/sequence definitions database											
Locus: abcZ  • Further information is available for Please enter your search criteria below (	Page will reload when changed     this focus.     releave blank and submit to return all records)	Modify form options										
Allele fields allele id v =												

A list box can be added by clicking the 'Show' button for 'Allele id list box'.

PubMLST	Query: Sequences   B Download: Alleles   M Links: Contents   Hon	latch sequences   Compare alleles   Profil LST profiles ne   PorA   FetA   Options   Isolate Databas - Neisseria profile/seq	e/ST   Batch profiles   Query e uence definitions databas	Help 67	Toggle: ()
Locus: abcZ • Further inform Please enter your se — Allele fields allele id	nation is available for t arch criteria below (or	Page will reload when changed this locus. I leave blank and submit to return all record	ds). — Display — Order by: allele id → ascending — Display: 25 → records per page ()	X Modify form parameters Click to add or remove additional query • • • 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.

Query: Sequence Download: Allele Links: Contents	es   Batch sequences   Compare alleles   Pro s   MLST profiles Home   PorA   FetA   Options   Isolate Datab	ofile/ST   Batch profiles   ase	List   Browse   Query	
			Help 🗹	Toggle: 🜖
Query abcZ sequence	es - Neisseria locus/seq	uence defini	tions database	
Locus: abcZ	✓ Page will reload when change	:d		Modify
<ul> <li>Further information is available</li> </ul>	e for this locus.			options
Please enter your search criteria belo	w (or leave blank and submit to return all rec + 0	Allele id list	Order by: allele id  ← ascending  ← Display: 25  ← records 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 e	Please enter your search criteria below (or leave blank and submit to return all records).												
	field	S		Allele id list	— — Display — — — — — — — — — — — — — — — — — — —								
allele	id	• = •	+ 1	1	Order by: allele id vascending v								
				2	Display: 25 v records per page 0								
				3									
				4	Action								
				5	Reset Submit								
5 records	return	ed. Click the hyperlinks for detailed information											
loouolo	lolo id	0000000	and an	commonto flogo									
abcZ	1	TTTGATACTGTTGCC TTGTCGAACTCGATC	433	comments hags									
abcZ	2	TTTGATACCGTTGCC TTGTCGAACTCGATC	433										
abcZ	3	TTTGATACCGTTGCC TTGTTGAACTTGACC	433										
abcZ	4	TTTGATACCGTTGCC TTGTCGAACTCGATC	433										
abcZ	5	TITGATACCGTTGCC TCGTCGAACTCGATC	433										
Analysi Export Analysis	FA	DIS: STA Table 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	<ul> <li>Downloads         <ul> <li>Allele sequences</li> <li>MLST</li> <li>Download profiles</li> </ul> </li> <li>Option settings         <ul> <li>Submissions</li> <li>Set general options</li> <li>Manage submissions</li> </ul> </li> <li>General information         <ul> <li>Number of sequences: 537919</li> <li>Number of sequences: 537919</li> <li>Number of profiles: Show</li> <li>Last updated: 2015-08-27</li> <li>Profile update history</li> <li>About BIGSdb</li> </ul> </li> </ul>
Export     Sequences - XMFA / concatenated FASTA formats     Sequence similarity - find se     Sequence comparison - disp     Locus Explorer - tool for anal	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: (	9		
Sea	earch or browse profiles - Neisseria locus/sequence definitions											
Ente	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.	dify		
	Locu	s/sch	eme fi	elds -					Display/sort options Action form			
9	ST ST			-	-				+ O Order by: ST = ascending = Durat Output			
									Display: 25 - records per page 0			
Brows	sing	all red	cords.									
10056	6 rec	ords	returne	ed (1 -	25 di	splaye	d). Cl	ick the hyperlinks for detailed inf	nformation.			
_	_											
Page	: L1	2	3	4	5	8 7		9 > Last				
SI	adk	abc2	aroE	fumC	gdh	pdhC	pgm	clonal complex				
2	3	1	4	7	1	1	3	ST-1 complex/subgroup I/II				
2	2	1	4	1	1	23	12	ST-1 complex/subgroup I/I				
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 07
Profile information for ST-11 (MLST)
ST adk abcZ aroE fumC gdh pdhC pgm clonal complex
sender: Paula Kriz, Paula Kriz and Keith Jolley
currator: 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	<ul> <li>Downloads         <ul> <li>Allele sequences</li> <li>MLST</li> <li>Download profiles</li> </ul> </li> <li>Option settings         <ul> <li>Set general options</li> <li>Set general options</li> <li>Manage submissions</li> </ul> </li> <li>General information         <ul> <li>Number of sequences: 537919</li> <li>Number of profiles: Show</li> <li>Satu update Cu95-08-27</li> <li>Profile update history</li> <li>About BIGSdb</li> </ul> </li> </ul>
Export     Sequences - XMFA / concatenated FASTA formats     Sequence similarity - find se     Sequence comparison - disp     Locus Explorer - tool for anal	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	earch or browse profiles - Neisseria locus/sequence definitions													
Scal														
Entres														
Enters	earc	ch crite	ena or	leave	Diank	to bro	wsea	all records. Modify form paramet	ters to filter of enter a list of values.	Modify				
Lo	cus/	schen	ne fiel	ds —					— Display/sort options — Action — Action	- form				
Com	bine	searc	hes w	ith: Al	ND .	-			Order by: ST 🗸 ascending 🗸 Reset Submit	opuons				
dat	e en	itered		<b>•</b> >	>		•	2013-02-01 +	O Display: 25					
ser	nder	(surna	ime)	<b>v</b> =	•		•	Jolley						
5051 re	cord	ls retu	rned (	1 - 25 (	displa	aved). (	Click	the hyperlinks for detailed inforn	nation.					
	_													
Page:	1	2	3 4	5	6	][7]	8	9 > Last						
ST	adk	abcZ	aroE	fumC	gdh	pdhC	pgm	clonal complex						
5001	6	12	12	352	9	18	9	07.4444						
5002	5	2	9	1/2	9	110	8 10	S1-41/44 complex/Lineage 3						
5003	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							
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.

PTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT														
														Toggle: 🚯
Search	n or	bro	ws	e n	rofi	iles	- Neisseria Io	cus/s	equence	e definitio	ns			
- cui oi														
Enter sear	rch crit	eria or	leave	blank	to bro	wse a	Il records. Modify form par	ameters to	filter or enter a	listofvalues				
Enter ocu				Jun			in records, modify form par							Modify
Locus	/scher	ne fielo	ds —						— Display/sor	t options			Action	torm
Combine	e sear	ches w	ith: A	ND -	•			_	Order by:	ST	<ul> <li>ascending</li> </ul>	-	Reset Submit	opuons
date er	ntered		<b>•</b>	>		-	2013-02-01	+ 0	Display:	25 - records	per page 🜖			
sender	r (surn	ame)	•	-		-	Jolley							
5051 record	ds retu	irned (*	1 - 25	displ:	ayed). (	Click 1	he hyperlinks for detailed i	information	Ι.					
				_										
ST adk	abcī		fumC	adb	ndhC	nam	cional 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.

Public International Alleles   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	Search or browse profiles - Neisseria locus/sequence definitions											
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.												
ST +	= •	+	] 🛛	Order by:	ST	→ ascending     →	Reset	Submit	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'.

Profit MILST 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	ry terms: Iues			

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.

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 browse profiles - Neisseria locus/sequence definitions											
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	ields - +	=		,	+ 0 Fi	Attribute values list	Display/sort options Order by: ST ← ascending ←	form options
								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	adk	abcZ	aroE	fumO	gdh	pdhC	pgm	clonal complex			
1	3	1	1	1	1	1	3	ST-1 complex/subgroup I/II			
2	3	1	4	1	1	1	3	SI-1 complex/subgroup I/II			
3	3	1	1	1	1	23	13	ST-1 complex/subgroup I/I			
Ana Ana E	4       3       1       3       1       4       2       3       ST-4 complex/subgroup IV         Analysis tools:										

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'.

Pro15/VILST Query: Sequences   Batch sequences   Compare alleles   Profile/ST []] Batch profiles   Query Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database									
Cogges In: Relationey (Relat): By Cog Stirl Change passions			neipter Toggie.						
Search or browse profiles - Neisseria p	profile/sequence definitions								
Enter search onteria or leave blank to browse all records. Modify form pa Locus/scheme fields ST • = •	Arameters to filter or enter a list of values. Attribute values list Field: ST 1 2 3 4 	Display/sort options Order by: ST Display: 25 V recorr Click to add or remove Locus/s O Attribute Filters	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   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query           Download: Alleles   MLST profiles           Links: Contents   Home   PorA   FetA   Options   Isolate Database								
		Toggle: 🕄						
Search or browse profiles - Neisse	eria locus/sequence definitions	\$						
Enter search criteria or leave blank to browse all records. Modil	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	olex ogroup IV							

# 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	
el Log in	Toggle: ()
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 diffue a corch, find fullelos he gratebile a criteria (all led to the corch).	Allele sequences     MLST     Scheme options     Scheme options
Sequence autobase sector - into aneles of inacting direct a (an oct togetter)     Locus-specific sequence attribute search - select, analyse and download specific alleles.     Search, browse or enter list of profiles	submissions
<ul> <li>Search by combinations of alleles - including partial matching.</li> <li>Batch profile query - lookup profiles copied from a spreadsheet.</li> </ul>	Manage submissions
Extract finetype from whole genome data	General information
	Number of sequences: 943149     Number of profiles: Show
	Last updated: 2016-12-20     Profile undate history
	About BIGSdb
Export     Sequences - XMFA / concatenated FASTA formats     Sequence similarity - find sequence     Sequence comparison - display a     Locus Explorer - tool for analysing	ces most similar to selected allele. comparison between two sequences. 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			
49 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 aok aroc rumo gun pano pgm Sr. Autofill			
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		
49 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		
abcz     adk     aroi:     rumi:     gdn     pani:     pgm     ST:     Autofill       2     3     4     3     8     4     6		
Options Display/sort options Action		
Search: Exact or nearest match 🖌 Order by: ST 🔹 ascending 👻 Reset Submit		
Display: 25 v records per page 0		

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			
Please enter your allelic profile below. Blank loci will be ignored.       Autofill profile         abcZ       adk       aroE       fumC       gdh       pdhC       pgm       ST: 11       Autofill         Options       Options       Action       Action       Action       Search:       Exact or nearest match       Order by: ST       v ascending       Reset       Submit			
Display: 25 👻 records per page 🕄			

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		
Please enter your allelic profile below. Blank loci will be ignored.       Autofill profile         abcZ       adk       aroc       fumC       gdh       pdhC       pgm         ST:       11       Autofill       Autofill         Options       Display/sort options       Action         Search:       Exact or nearest match ▼       Order by:       ST       ▼ ascending ▼       Reset       Submit         Display:       25       ▼ records per page ●       Itecord returned. Click the hyperlink for detailed information.		
ST       abcZ       adk       aroE       fumC       pdhC       pgm       clonal complex         11       2       3       4       3       8       4       6       ST-11 complex/ET-37 complex         Analysis tools:       Export       Sequences       Sequences       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 in	in: Kei	ith Joi	iley (ke	eith). 🕩	Log ou	ut   Cha	inge p	assword	Help 🖾	Toggle: 🚯
ear	ch	Ne	eiss	seri	a p	rofi	ile/s	sequence definitions database by combinations of loci		
scher	mes									
lease	esele	ectitn	e sche	eme yo	bu wo		e to q	uery.		
MLST								▼ Select		
-Ple	ease	ente	r your	allelic	profil	e belo	w. Bla	ank loci will be ignored Autofill profile		
at	bcZ		adk		aroE	1	fumC	gdh pdhC pgm ST: 11 Autofil		
	2		3		4		3	8 4 6		
0	otions							- Display/sort options - Action -		
	Sear	ch:	4 or p	ooro n	aatichu	20	_			
	ocui		4 01 11	nore n	accin	35	_	Diselar ascending V Reset Submit		
								Display. 25 V records per page ()		
9 reci	ords	retur	ned (1	1 - 25 (	displa	ved), (	Click	he hyperlinks for detailed information.		
ige:	1	2	3	4 5		7	8	9 > Last		
ST a	ibcZ	adk	aroE	fumC	gdh	pdhC	pgm	cional complex		
0	2	3	4	2	8	15	2	ST-8 complex/Cluster A4		
1	2	3	4	3	8	4	6	S1-11 complex/E1-37 complex		
1	2	2	19	22	0	6	6	ST-11 complex/ET-37 complex		
2	7	3	4	3	8	4	6	ST-11 complex/ET-37 complex		
7	2	3	4	24	8	4	6	ST-11 complex/ET-37 complex		
55	2	3	4	48	8	4	6	ST-11 complex/ET-37 complex		
6	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		
47	2	3	4	5	8	4	6	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). @Log out   Change password	Toggle: 🜖 🚍
Neisseria profile/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing should have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in this database
Q Query database	Lownloads
<ul> <li>Sequence query - query an allele sequence.</li> <li>Batch sequence query - query multiple sequences in FASTA format.</li> </ul>	Allele sequences     MLST     V
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	Option settings 1 Submissions
Search by combinations of alleles - including partial matching.     Batch profile query - lookup profiles copied from a spreadsheet.     Editad finatione from whole genome data	Set general options     Manage submissions     Scheme options
	General information
	Number of sequences: 943149     Number of profiles: Show
	Last updated: 2016-12-20     Profile update history
	About BIGSdb
Export  Sequences - XMFA / concatenated FASTA formats  Analysis  Sequence similarity - find se  Sequence comparison - dis	equences most similar to selected allele. play a comparison between two sequences.
Locus Explorer - tool for ana	iysnig anere sequences stored for particular fOCUS.

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). HoLog out   Change password	3
Batch profile query - Neisseria profile/sequence definition	ons
Schemes	
Please select the scheme you would like to query:	
MLST   Select	
whitespace. The first column should be an isolate identifier and the remaining columns should compris data. Non-numerical characters will be stripped out of the query. — Paste in profiles	e the allele numbers (show column order). Click here for example

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.

eo m. Rein Jolley	neidij. e <del>v</del> edg o	or I change p	-							
tch profil	e query	/ - Neis	sseria	profile	/seque	ence de	efinitions			
homos										
liemes										
ase select the sc	heme you wo	ould like to q	uery:							
CT.			Calast	-						
.51			<ul> <li>Select</li> </ul>							
er allelic profiles	helow in tab-	delimited te	vt format usi		d naste (for e	avample dire	ctly from a sprea	dsheet) Colum	nns can be senarated by any am	ount of whites no
ter allelic profiles	below in tab-	delimited te	xt format usi	ing copy and	d paste (for e	example dire	ectly from a sprea	adsheet). Colum	nns can be separated by any am	ount of whitespa
ter allelic profiles e first column sho aracters will be st	below in tab- uld be an iso ipped out of i	delimited te late identifie the query	xt format usi er and the re	ing copy and maining co	d paste (for e lumns shou	example dire Id comprise	ectly from a sprea the allele numbe	adsheet). Colum ers (show colun	nns can be separated by any am nn order). Click here for example	ount of whitespa data. Non-num
ter allelic profiles e first column sho aracters will be str	below in tab- uld be an iso ipped out of t	delimited te plate identifie the query.	xt format usi er and the re	ing copy and maining co	d paste (for e lumns shou	example dire Id comprise	ectly from a sprea the allele numbe	adsheet). Colum ers (show colun	nns can be separated by any am nn order). Click here for example	ount of whitespa data. Non-num
er allelic profiles e first column sho aracters will be str - Paste in profiles	below in tab- uld be an iso ipped out of l	delimited te date identifie the query.	xt format usi er and the re	ing copy and maining co	d paste (for e lumns shou	example dire Id comprise	ectly from a sprea the allele numbe	adsheet). Colum ers (show colun	nns can be separated by any am nn order). Click here for example Action	ount of whitespa data. Non-num
ter allelic profiles e first column sho aracters will be str -Paste in profiles .solate 6	below in tab- uld be an iso ipped out off 3	delimited te plate identifie the query. 6	xt format usi er and the re 9	ing copy and maining co 5	d paste (for e lumns shou 8	example dire Id comprise 6	ectly from a sprea the allele numbe	adsheet). Colum ers (show colum	nns can be separated by any am nn order). Click here for example — Action — Reset Submit	ount of whitespa data. Non-num
er allelic profiles e first column sho aracters will be str - Paste in profiles .solate_6 .solate_7	below in tab- uld be an iso ipped out of t 3 6	delimited te plate identifie the query. 6 6	xt format usi er and the re 9 365	ing copy and maining co 5 55	d paste (for e lumns shou 8 72	example dire Id comprise 6 6	ectly from a sprea the allele numbe 9 20	adsheet). Colum ers (show colun	nns can be separated by any am nn order). Click here for example — Action Reset Submit	ount of whitespa e data. Non-num
ter allelic profiles e first column sho aracters will be str - Paste in profiles .solate_6 .solate_7 .solate_8	below in tab- uld be an iso ipped out of f 3 6 4	delimited te late identifie the query. 6 6 3	xt format usi er and the re 9 365 5	ing copy and maining co 5 55 4	d paste (for e lumns shou 8 72 315	example dire Id comprise 6 6 21	ectly from a sprea the allele numbe 9 20 8	adsheet). Colum ers (show colun	nns can be separated by any am nn order). Click here for example Action Reset Submit	ount of whitespa e data. Non-num
er allelic profiles e first column sho racters will be str Paste in profiles solate_6 solate_7 solate_8 solate_9	below in tab- uld be an iso ipped out of 1 3 6 4 2	delimited te plate identifie the query. 6 6 3 273	xt format usi er and the re 9 365 5 19	ing copy and maining co 5 55 4 3	d paste (for e lumns shou 8 72 315 8	example dire Id comprise 6 6 21 4	ectly from a sprea the allele numbe 9 20 8 6	adsheet). Colum ers (show colun	nns can be separated by any am nn order). Click here for example — Action Reset Submit	ount of whitespa ⊧ data. Non-num
er allelic profiles first column sho aracters will be stu- Paste in profiles solate 6 solate 7 solate 8 solate 9 solate 10	below in tab- uld be an iso ipped out of i 3 6 4 2 2	delimited te plate identifie the query. 6 6 3 273 7	y st format usi and the re 365 5 19 159	ing copy and maining co 5 55 4 3 92	d paste (for e lumns shou 8 72 315 8 93	example dire Id comprise 6 6 21 4 6	ectly from a sprea the allele numbe 9 20 8 6 2	adsheet). Colum ers (show colum	nns can be separated by any am nn order). Click here for example — Action Reset Submit	ount of whitespa data. Non-num
er allelic profiles e first column sho rracters will be str Paste in profiles solate_6 solate_7 solate_8 solate_9 solate_10 solate_11	below in tab- uld be an iso ipped out of t 3 6 4 2 2 2 2	delimited te plate identifie the query. 6 6 3 2 73 7 5	9 365 5 19 12	5 55 4 3 92 143	d paste (for e lumns shou 8 72 315 8 93 29	example dire Id comprise 6 6 21 4 6 285	9 20 8 6 2 7	adsheet). Colum	nns can be separated by any am nn order). Click here for example Action Reset Submit	ount of whitespa data. Non-num
er allelic profiles first column sho racters will be sti Paste in profiles solate 6 solate 7 solate 8 solate 9 solate 10 solate 11 solate 12	below in tab- uld be an iso ipped out of 1 3 6 4 2 2 2 6	delimited te plate identifie the query. 6 6 3 273 7 5 7 5 7	xt format usi er and the re 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	ectly from a sprea the allele numbe 9 20 8 6 2 7 8	adsheet). Colum ers (show colun	nns can be separated by any am nn order). Click here for example — Action Reset Submit	ount of whitesp: data. Non-num
er allelic profiles first column sho racters will be sh Paste in profiles solate 6 solate 7 solate 8 solate 9 solate 10 solate 11 solate 12 solate 13	below in tab- uld be an iso ipped out of i 3 6 4 2 2 2 2 6 11	delimited te vlate identifie the query. 6 6 3 273 7 5 7 5 5 7 5	9 365 5 19 159 12 9 18	5 55 4 3 92 143 56 5	8 8 72 315 8 93 29 26 9	6 6 21 4 6 285 18 24	ectly from a sprea the allele number 9 20 8 6 2 7 8 3	adsheet). Colum ers (show colun	nns can be separated by any am nn order). Click here for example Action Reset Submit	ount of whitespa data. Non-num
ter allelic profiles e first column sho aracters will be str - Paste in profiles .solate_6 .solate_7 .solate_8 .solate_9 .solate_10 .solate_11 .solate_12 .solate_13 .solate_14	below in tab- uld be an iso ipped out of 1 6 4 2 2 2 6 11 222	delimited te late identifie the query. 6 6 3 2 7 3 7 5 7 5 7 5 2 3 1	xt format usi er and the re 365 5 19 12 9 12 9 18 406	5 55 4 3 92 143 56 5 12	8 72 315 8 93 29 26 9 161	6 6 21 4 6 285 18 24 2	9 20 8 6 2 7 8 3 16	adsheet). Colum	nns can be separated by any am nn order). Click here for example — Action Reset Submit	ount of whitespa : data. Non-num

#### A results table will be displayed.

PubMLST	Dat	abas	e hor		Cont				
Logged in: Keit	th Joll	ey (kei	ith). 🕩 L	.og out	Cha	nge pa	ssword		
Batch p	rot	ïle	au	erv	- N	leis	ser	ia p	rofile/sequence a
aton prome query - Neloocha prometocquenoc deminiono									
Isolate	abc7	adk	aroE	fumC	adh	pdhC	pam	ST	cional complex
isolate 1	8	3	5	4	1	3	8	290	ST-32 complex/ET-5 complex
isolate 2	2	3	4	86	8	110	118	5639	ST-11 complex/ET-37 complex
isolate 3	4	26	15	9	8	11	18	8381	ST-269 complex
isolate 4	20	5	144	35	8	130	123	942	
isolate 5	214	6	13	5	9	6	9	3312	ST-41/44 complex/Lineage 3
isolate 6	3	6	9	5	8	6	9	485	ST-41/44 complex/Lineage 3
isolate 7	6	6	365	55	72	6	20	4053	
isolate 8	4	3	5	4	315	21	8	3770	ST-32 complex/ET-5 complex
isolate 9	2	273	19	3	8	4	6	6070	ST-11 complex/ET-37 complex
isolate_10	2	7	159	92	93	6	2	10908	
isolate_11	2	5	12	143	29	285	7	4658	
isolate_12	6	7	9	56	26	18	8	10620	ST-175 complex
isolate_13	11	5	18	5	9	24	3	10202	ST-22 complex
isolate_14	222	231	406	12	161	2	16	8927	
isolate_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 roffles           • 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>
Export     Sequences - XMFA / concatenated FASTA formats     Sequence similarity     Ind sec     Sequence comparison - disp     Locus Explorer - tool for analy	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.

Prohi/LIST         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
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     Number of results: 10 -

A list of nearest alleles will be displayed, along with the percentage identity and number of gaps between the se-

quences.

		uery: Seque ownload: Al inks: Conter	nces   leles   I nts   Ho	Batch seque /ILST profiles me   PorA   F	nces   Compare alleles   Profile/ST []] Batch profiles   Query s ietA   Options   Isolate Database
Logged in: Ke	eith Jolley (ke	eith). 🗭Log ou	t   Chan	ge password	Help 🗹
Find m	ost sii	nilar a	llele	es - Nei	sseria profile/sequence definitions
					· · · · · · · · · · · · · · · · · · ·
This page	allows you t	o find the m	ost sim	ilar sequend	ces to a selected allele using BLAST.
	parameters				Action
	Locu	s: abcZ		•	Pasat Submit
	Allel	e: 5			
Numb	per of result	s: 10 👻			
abcZ-5					
abcZ-5	% Identity	Nismatches	Gaps	Alignment	Compare
abcZ-5 Allele abcZ: 453	% Identity   99.77	Mismatches 1	Gaps	Alignment 433/433	Compare
abcZ-5 Allele abcZ: 453 abcZ: 405	% Identity   99.77 99.77	Mismatches 1 1	Gaps 0 0	Alignment 433/433 433/433	Compare ④ 실실
abcZ-5 Allele abcZ: 453 abcZ: 405 abcZ: 404	% Identity   99.77 99.77 99.77	Mismatches 1 1 1	Gaps 0 0 0	Alignment ( 433/433 433/433 433/433	Compare ④ ④ ④
abcZ-5 Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213	% Identity   99.77 99.77 99.77 99.77	Mismatches 1 1 1 1	Gaps 0 0 0 0	Alignment ( 433/433 433/433 433/433 433/433	Compare ④ ④ ④ ④
<b>Allele</b> abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166	% Identity         I           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9	Aismatches 1 1 1 1 1 1	Gaps 0 0 0 0 0 0	Alignment   433/433 433/433 433/433 433/433 433/433	Compare ④같 ④같 ④같 ④같
abcZ-5 Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166 abcZ: 114	% Identity         I           99.77         99.77           99.77         99.77           99.77         99.77           99.77         99.77           99.77         99.77           99.77         99.77	Mismatches 1 1 1 1 1 1 1	Gaps 0 0 0 0 0 0 0	Alignment 433/433 433/433 433/433 433/433 433/433 433/433	전값
abcZ-5 Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166 abcZ: 114 abcZ: 103	% Identity         I           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9           99.77         9	Mismatches 1 1 1 1 1 1 1 1 1	Gaps 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Alignment 433/433 433/433 433/433 433/433 433/433 433/433 433/433	Compare ④ 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
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Click the appropriate 'Compare' button to display a list of nucleotide differences and/or a sequence alignment.

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
Allele sequence comparison - Neisseria locus/sequence definitions
This tool allows you to select two alleles and highlight the nucleotide differences between them.         Select parameters       Action         Locus:       abcZ       Submit         Allele #1:       5         Allele #2:       453
Nucleotide differences between abcZ: 5 and abcZ: 453 Identity: 99.77 % Show alignment Differences: 1 $300: G \rightarrow A$

#### 11.8.2 Sequence comparison

To directly compare two sequences click 'Sequence comparison' from the contents page of a sequence definition database.



Enter the locus and two allele identifiers to compare. Press submit.

Query: Sequences   Download: Alleles   Links: Contents   Ho	atch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query LST profiles ne   PorA   FetA   Options   Isolate Database
Allele sequence compa	rison - Neisseria locus/sequence definitions
This tool allows you to select two alleles	nd highlight the nucleotide differences between them.
Select parameters Locus: abcZ Allete #1: 5 Allete #2: 8	✓ Submit

A list of nucleotide differences and/or an alignment will be displayed.
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										
Allele sequence comparison - Neisseria locus/sequence definitions										
This tool allows you to select two alleles and highlight the nucleotide differences between them.										
Locus: abcZ										
Allele #1: 5										
Allele #2: 8										
Nucleotide differences between abcZ: 5 and abcZ: 8										
Identity: 90.53 %										
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$72: G \rightarrow 1$ $72: A \rightarrow G$										
79: A - C										
81: T → C										
82: G → A										
$83: 6 \rightarrow A$										
$\sigma : \sigma \to A$ 8: $A \to G$										
89: G → A										
90: $T \rightarrow C$										
$93:G \rightarrow C$										
$30, G \rightarrow 1$ $90, G \rightarrow \Lambda$										
$102: G \rightarrow A$										

#### See also:

Locus explorer plugin.

# 11.9 Browsing isolate data

Isolate records can be browsed by clicking the link to 'Search or browse database'.



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'.

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Clicking the hyperlink for any record will display full information about the profile.

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3	M00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1099	·	19	15			
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5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1100	ST-32 complex	7	16			
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# 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.

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Publications     Sequence bin	-		BLAST     Species identification	<ul> <li>Microreact - Open data</li> </ul>	visualization and sharing for genomic epidemiology
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	_	Description of database fields			

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'.

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After the search has been submitted, the results will be displayed in a table.

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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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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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2316	M7086		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	v	V	22	ST-22	complex	6	3			
2317	M7084		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	v	V	22	ST-22	complex	6	3			
2322	M7092		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	V	V	1065	ST-22	complex	6	3			

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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	Allele designation status
	Tagged sequence counts
	Tagged sequence status
	Attribute values list
	Filters

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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						Allele designation counts
						Allele designation status
						Tagged sequence counts
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						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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1	A4/M1027	B1; NIBSC_2803; Z10	01 USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex	5-2	10	F1-5	
2	120M	B35; NIBSC_2822; Z10	35 Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	1	ST-1 complex	5-2	10	F5-1	
7	7891	B54; NIBSC_2760; Z10	54 Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex	20	9	F3-1	
10	6748	B73; NIBSC_2784; Z10	73 Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex	18-1	3	F5-1	
11	129E	B92; NIBSC_2828; Z10	92 Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex	5-2	10	F3-6	

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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id	isolate	aliases	country	year	disease	species	capsule group	ST	cional complex	PorA_VR1	PorA_VR2	FetA_VR	
451	14/1455	NIBSC_2732; Z4717	Russia	1970	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex	20	9	F3-1	
887	OX9930357		UK [England]	1999	carrier	Neisseria meningitidis	В	43	ST-41/44 complex	19	15-1	F1-98	
3412	OX9931676		UK [England]	1999	carrier	Neisseria meningitidis	В	1228	ST-41/44 complex	7-1	1		
3415	OX9931776		UK [England]	1999	carrier	Neisseria meningitidis	В	1644	ST-213 complex	22	14	F5-5	
4193	OX9931563		UK [England]	1999	carrier	Neisseria meningitidis	С	136	ST-41/44 complex	5	2	F1-20	
34733	LNP15075		Burkina Faso	1997		Neisseria meningitidis				20	10-1	F3-1	
57890	15134		Spain	2002	invasive (unspecified/other)	Neisseria meningitidis	W			5-1	10-4	F1-18.F1-7	

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.

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		Allele designation counts
		Allele designation status
		Tagged sequence counts
		Tagged sequence status
		Attribute values list
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Select a locus from the dropdown box and either 'provisional' or 'confirmed'. Additional query fields can be displayed by clicking the '+' button. Click 'Submit'.

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Isolate fields ()         MLST         Finetyping anti- id isolate aliases country year disease species capsule group         ST         clonal complex         PorA_VR1         PorA_VR1           14733         NJ9703         BennettTree32         Unknown         Neisseria subflava         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304         10304<	<b>FetA_VR</b> F5-8
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Isolate fields ①       MLST       Finetyping anti-         id       isolate       aliases       country       year       disease       species       capsule group       ST       clonal complex       PorA_VR1       PorA_VR1         14733       NJ9703       BennettTree32       Unknown       Neisseria subflava       10304       10304       10304         19363       961-5945       Unknown       Neisseria meningitidis       B       153       ST-8 complex       21       16         Analysis tools:         Image: Stress Two Field       Combinations       Polymorphic sites       Publications       Sequence bin	<b>F5-8</b>
Isolate fields ①       MLST       Finetyping anti id isolate aliases country year disease species capsule group       ST       clonal complex PorA_VR1 PorA_VR1         14733       NJ9703       BennettTree32       Unknown       Neisseria subflava       10304       10304         19363       961-5945       Unknown       Neisseria meningitidis       B       153       ST-8 complex       21       16         Analysis tools:         Image: Species Component Comparator       BLAST       rMLST species id       PCR	FetA_VR F5-8
Isolate fields ()       MLST       Finetyping anti-         id       isolate       aliases       country       year       disease       species       capsule group       ST       clonal complex       PorA_VR1       PorA_VR1         14733       NJ9703       BennettTree32       Unknown       Neisseria subflava       10304       10304         19363       961-5945       Unknown       Neisseria meningitidis       B       153       ST-8 complex       21       16         Analysis tools:         Image: Struct Str	gens FetA_VR F5-8

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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	Allele designation status     Tagged sequence counts
	Tagged sequence status     Attribute values list
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For example, to find all isolates that have sequence tags at >1000 loci, select 'total tags > 1000', then click 'Submit'.

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id	isolate	aliases	country	year	disease	species	group	ST	complex	PorA_VR1	PorA_VR2	FetA_VR
1	A4/M1027	B1; NIBSC_2803; Z1001	USA	1937	invasive	Neisseria	А	4	ST-4 complex	5-2	10	F1-5
					(unspecified/other)	meningitidis						
2	120M	B35; NIBSC_2822; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	1	ST-1 complex	5-2	10	F5-1
7	7891	B54; NIBSC_2760; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex	20	9	F3-1
10	6748	B73; NIBSC_2784; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	А	1	ST-1 complex	18-1	3	F5-1

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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1	A4/M1027	B1; NIBSC_2803; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex	5-2	10	F1-5
2	120M	B35; NIBSC_2822; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	1	ST-1 complex	5-2	10	F5-1
7	7891	B54; NIBSC_2760; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex	20	9	F3-1
11	129E	B92; NIBSC_2828; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	А	1	ST-1 complex	5-2	10	F3-6

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.

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	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.

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1 record returned. Click the hyperlink for detailed information.           Isolate fields ()         MLST         Finetyping antigens           id         isolate         aliases         country         year         disease         species         capsule group         ST         clonal complex         PorA_VR1         PorA_VR2         FetA_VR			
2017       153       aipha153       Germany 1999       carrier       Neissena meningitidis       E       60       S1-60       complex       5       2       F1-7         Analysis tools:       Image: Stand			

#### 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.

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	Allele designations/scheme field values
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	Contraction status     Tagged sequence counts
	Tagged sequence status
	Attribute values list
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Select the attribute to query and enter a list of values.

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isolate leads de le
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(unspecified/other) meningitidis
120M         B35; NIBSC_2822;         Pakistan         1967         meningitis and septicaemia         Neisseria         A         1         ST-1 complex         5-2         10
120M     B35; NIBSC_2822; Z1035     Pakistan     1967     meningitidis septicaemia     Neisseria meningitidis     A     1     ST-1 complex     5-2     10       M00242905     UK     200     invasive (unspecified/other)     Neisseria meningitidis     B     109     19     15
120M     B35; NIBSC_2822; Z1035     Pakistan     1967     meningitis and septicaemia     Neisseria meningitidis     A     1     ST-1 complex     5-2     10       M00242905     UK     200     invasive (unspecified/other)     Neisseria meningitidis     B     109     19     15       M1027     B43; NIBSC_3076; 77043     USA     1937     invasive (unspecified/other)     Neisseria meningitidis     A     4     ST-4 complex
Isolate fields 🚯 MI ST Einstyning antigen
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A4/M1027 B1; NIBSC_2803; Z1001 USA 1937 invasive Neisseria A 4 ST-4 complex 5-2 10
(unspecified/other) meningitidis
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120M         B35; NIBSC_2822;         Pakistan         1967         meningitis and septicaemia         Neisseria         A         1         ST-1 complex         5-2         10
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120M     B35, NIBSC_2822; Z1035     Pakistan     1967     meningitis and septicaemia     Neisseria meningitidis     A     1     ST-1 complex     5-2     10       M00242905     UK     200     invasive (unspecified/other)     Neisseria meningitidis     B     109     19     15       M1027     B43; NIBSC 3076;     USA     1937     invasive invasive     Neisseria     A     4     ST-4 complex
120M     B35; NIBSC_2822; Z1035     Pakistan     1967     meningitis and septicaemia     Neisseria meningitidis     A     1     ST-1 complex     5-2     10       M00242905     UK     200     invasive (unspecified/other)     Neisseria meningitidis     B     109     19     15       M1027     B43; NIBSC_3076; Z1043     UK     103     103     invasive (unspecified/other)     Neisseria meningitidis     A     4     ST-4 complex     7     16
A4/M1027 B1; NIBSC_2803; Z1001 USA 1937 invasive (unspecified/other) meningitidis A 4 ST-4 complex 5-2 10

### 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.

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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 fields Id  T = T Enter value  Display/sort options  Action  Order by: Id  Display: 25 T records per page  Reset Submit	<ul> <li>Modify form parameters</li> <li>Click to add or remove additional query terms:</li> <li>Provenance fields</li> <li>Vaccine coverage</li> <li>Allele designations/scheme field values</li> <li>Allele designation counts</li> <li>Allele designation status</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>
	• 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.

### 11.10.8 Bookmarking an isolate query

Once you have made an isolate database query, you can bookmark it so that it can be repeated in the future. You need to have an account and be logged in to the database to be able to bookmark.

Following a query, there will be a 'Bookmark query' section in the results header section. Enter a name for the bookmark (a default name based on the date will be shown) and click 'Add bookmark'.

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20155	240001		LIK [England]	Midlands	2014	(unspecified/other)	meningitidis	M	2 122 950	142	11	COMPLEX	5	2	E1 1	
30133	240002		on [England]	Midlands	2014	(unspecified/other)	meningitidis	vv	2,102,009	142		complex	5	2	1 1-1	
30156	M14 240007		UK [England]	South and West	2014	invasive (unspecified/other)	Neisseria	W	2,136,323	118	11	ST-11 complex	5	2	F1-1	
30157	M14 240013		UK [England]	West	2014	invasive (unspecified/other)	Neisseria	W	2,133,927	134	11	ST-11	5	2	F1-1	
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30154	M14		UK [England]	West	2014	invasive	Neisseria	W	2,134,099	155	11	ST-11	5	2	F1-1
30155	240001 M14		UK [England]	West	2014	(unspecified/other)	Neisseria	w	2.132.859	142	11	ST-11	5	2	E1-1
	240002			Midlands		(unspecified/other)	meningitidis					complex			
30156	M14 240007		UK [England]	South and West	2014	invasive (unspecified/other)	Neisseria meningitidis	W	2,136,323	118	11	ST-11 complex	5	2	F1-1
30157	M14 240013		UK [England]	West Midlands	2014	invasive (unspecified/other)	Neisseria meningitidis	W	2,133,927	134	11	ST-11 complex	5	2	F1-1

You can also access your bookmarks from the main contents page. A link will appear in the query section once you have saved a bookmark.



This will take you to a page where you can manage your bookmarks.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). (+Log out   Change password
Bookmarks
Please note that only you will be able to access a query defined by a bookmark if it is shown as locked. Click the padlock icon to make it publicly shareable - you can then copy the URL from the 'Run query' field and share this with colleagues. Delete Name + Database configuration + Created + Share Run query × 2020-03-06:1 pubmist neisseria isolates 2020-03-06 • Q

You can go to a bookmarked search by clicking on the 'Run query' icon. By default, a bookmark can only be used by the logged-in user who created it. This is for privacy reasons to prevent other users from finding out what terms are being used for a search. If, however, you wish to share the URL to the query, you can make it shareable by clicking the padlock icon.



The icon will change to a green open padlock. You can right-click on the 'Run query' link to copy the URL if you wish to share it with others.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). [+Log out   Change password
Bookmarks
Please note that only you will be able to access a query defined by a bookmark if it is shown as locked. Click the padlock icon to make it publicly shareable - you can then copy the URL from the 'Run query' field and share this with colleagues. Delete Name + Database configuration + Created + Share Run query × 2020-03-06:1 pubmist_neisseria_isolates 2020-03-06  Q

Bookmarks can be deleted by clicking on the delete icon.

# 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.

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 a sample.	For every allelic profile in the profiles/sequence definition should be noted that it does not represent a population
Query database Search or browse database Search by combinations of loci (profiles) 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  • 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         • Presence/absence status of Io       • Genome comparator       • BLAST	Miscellaneous     • Description of database fields ci

If multiple schemes are defined, you may have to select the scheme you wish to query in the 'Schemes' dropdown box and click 'Select'.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definition	ns   Database submissions		
			Toggle: i
Search Neisseria PubMLST database by comb	inations 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.	<ul> <li>Autofill profile by searching remote data</li> </ul>	base ——	
abcZ adk aroE fumC gdh pdhC pgm	ST:	Autofill	
- Filters - Ontions -	Display/soft of	ntions	
Project: Vitility Search: Ex	xact or nearest match - Order by:	id 👻	ascending 👻
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.

Output         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	
abcZ     adk     aroE     fumC     gdh     pdhC     pgm     ST:     Autofill       2     3     4     3     8     4     Autofill     Autofill	
Project:	
□ Include old record versions Display: 25	
Reset	

Alternatively, for scheme profiles, you can enter a primary key value (e.g. ST) and select 'Autofill' to automatically fill in the associated profile.

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.	
MI ST _ 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 Options Display/soft options	
Include old record versions Display: 25  records per page [7]	
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 - 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(soft ontions	
Project:	
□ Include old record versions Display: 25  v records per page []	
Reset Submit	

#### Click 'Submit'.

Publ	MLST	Query: Search Breakdown: Is Links: Content	Browse   Profile/ olate fields   Sche ts   Home   Option:	ST   Li me/all s   Pro	st eles   Publications files/sequences definitions	Database submissions	i					
												Toggle: i
Sear	ch Neis	seria Pu	ubMLST d	ata	base bv combir	nations of loc	i					
Schen	nes											
Please	select the so	cheme you wou	Id like to query:									
MUST			-	Seler	+							
			• (	00.00								
Dia			halaw Diasisiani									
-Pie	ase enter yo	ur allelic profile	below. Blank loch	will be	Ignored.	Automi prome by searc	ning remote	data	ibase			
ab		K aroe		an 9	panc pgm	51. 44			Autofill			
			, , , , , , , , , , , , , , , , , , ,		0.1		Dist					
Filt	Project				Options	and a second	Display/ Order	SOR	options		Langer	
	Project.				• [] Search. Exact	or nearest match 👻	Dian	Dy.			<ul> <li>ascend</li> </ul>	ng 👻
	nciude old re	cord versions					Disp	Idy.	25 Tecords per page 1			
Acti Res	set Subi	mit										
		_										
Eventury		(71)										
Exactima	atches tound	(7 1001).										
119 reco	ords returned	(1 - 25 display	ed). Click the hype	rlinks	for detailed information.							
Page:	1 2 3	4 5 >	Last									
-												
				Isola	te fields 👔				MLST	Finet	vping antig	ens
id	isolate	aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1	PorA VR2	FetA VR
41	19		Germany	1999	carrier	Neisseria meningitidis	В	44	ST-41/44 complex/Lineage 3			
70	38		Germany	1999	carrier	Neisseria meningitidis	NG	44	ST-41/44 complex/Lineage 3			
427	NG E30	Z4692	Norway	1988	carrier	Neisseria meningitidis	B	44	SI-41/44 complex/Lineage 3	21	16	F1-7
792	99 182		Canada	1999	invasive (unspecified/other)	Neisseria meningitidis	B	44	ST-41/44 complex/Lineage 3			
975	0069/93		Czech Republic	1993	carrier	Neisseria meningitidis	NG	44	ST-41/44 complex/Lineage 3	22	14-4	F1-7
1097	3532	Z7184	The Netherlands	1975	Califor	Neisseria meningitidis	B	44	ST-41/44 complex/Lineage 3		4	
1603	0213/93		Czech Republic	1993	carrier	Neisseria meningitidis	В	44	ST-41/44 complex/Lineage 3	22	14-4	F1-19
1604	0214/93		Czech Republic	1993	carrier	Neisseria meningitidis	NG	44	ST-41/44 complex/Lineage 3	22	14-4	F1-7
1633	0244/03		Czech Republic	1003	carrier	Neisseria meningitidis	R	11	ST-11/11 complex/Lineage 3	22	14-4	F1_7

# 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. I database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it a sample.	For every allelic profile in the profiles/sequence definition should be noted that it does not represent a population
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       Export       Analysis         • Single field       • Export dataset       • Contigs         • Unique combinations       • Scheme and alleles       • Sequences - XMFA / concatenated FASTA formats       • Codon usage         • Publications       • Sequence bin       • Sequence bin       • BLAST	Miscellaneous     Description of database fields

A list of publications linked by isolates within the database will be displayed.

PubMLS	Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions						
Publicatio	on breakdown of dataset						
	by Display	Action					
Author:	All authors    Order by: number of isolates   descending	Submit					
Year:	All years 👻 Display: 25 👻 records per page						
73 records return Page: 1 2	ned (1 - 25 displayed). Click the hyperlinks for detailed information.						
PubMed id Yea	Ir Citation	Title	Isolates in database				
17517841 200	17 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, Voqel 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 200	5 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	14 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	55 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 200	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.

PubML	ST	Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions		
Publica	tio	n breakdown of dataset		
Filter qu Auth Ye	iery by hor: ear:	Jolley KA		
13 records re PubMed	eturne Year	d. Click the hyperlinks for detailed information. Citation	Title	Isolates in
17517841 :	2007	Taha MK, Vázquez JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enriquez 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 Neisserla 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 191: 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,	378 isolates

To display the isolate records for any of the displayed publications, click the button to the right of the citation.

PuisMLST	Ouery: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions		
Dublicatio	hundedawa of dataaat		
uplicatio	i preakdown of dataset		
	Display Action		
Author:	olley KA    Order by: number of isolates   descending   Submit		
Year:	Il years   Display: 25   records per page		
13 records returne	. Click the hyperlinks for detailed information.		
PubMed id Year	Citation	Title	lsolates in database
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 J, Feil F J, 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.

	MLS'	Direction Control Cont	earch   Browse vn: Isolate field ntents   Home	Profi ds   Scl   Optic	le/ST   List heme/alleles   Publications ons   Profiles/sequences defi	initions   Database subm	nissions					
Puk	licatio	ons cite	d in the	Nei	isseria PubMLS	T database						
lita	ion que	ry (Publi	ed Id: 178	2505	91)							
Spec The popu three 576 m	ies status seven loci N lation gene species. A cords retur	of Neisseria g leisseria MLS tic inferences nalysis of varia	splayed). Click	evoluti s readi acludin le locu	onary and epidemiological in ly adapted to N. gonorrhoeae g direct comparisons with N. s, gdh, provided a rapid meal perlinks for detailed informat	ion.	us sequenc hly discrimir amica. Exan sified isolate	e typi natory ninatic es anc	ng. typing method. In addition, th on of these data demonstrate I determining whether mixed	ese data p d that allele cultures we	ermitted phy es were rare ere present.	logenetic ly shared
					solate fields				MI ST	Finat	vning antige	ane
id	isolate	aliases	country	l vear	solate fields 1	species	serogroup	ST	MLST clonal complex	Finet	yping antige PorA VR2	ens FetA VR
id 1	isolate A4/M1027	aliases B1; Z1001	country USA	l year 1937	solate fields [] disease invasive (unspecified/other)	species Neisseria meningitidis	serogroup A	ST 4	MLST clonal complex ST-4 complex/subgroup IV	Finet PorA VR1 5-2	yping antige PorA VR2 10	ens FetA VR F1-5
id 1 2	isolate A4/M1027 120M	aliases B1; Z1001 B35; Z1035	country USA Pakistan	year 1937 1967	solate fields [] disease invasive (unspecified/other) meningitis and septicaemia	species Neisseria meningitidis Neisseria meningitidis	serogroup A A	ST 4 1	MLST clonal complex ST-4 complex/subgroup I/I ST-1 complex/subgroup I/I	Finet PorA VR1 5-2 5-2	yping antige PorA VR2 10 10	ens FetA VR F1-5 F5-1
id 1 2 7	isolate A4/M1027 120M 7891	aliases B1; Z1001 B35; Z1035 B54; Z1054	country USA Pakistan Finland	l year 1937 1967 1975	solate fields [] disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup A A A	ST 4 1 5	MLST clonal complex ST-4 complex/subgroup I/I ST-5 complex/subgroup I/I ST-5 complex/subgroup III	Finet PorA VR1 5-2 5-2 20	yping antige PorA VR2 10 10 9	ens FetA VR F1-5 F5-1 F3-1
id 1 2 7 10	isolate A4/M1027 120M 7891 6748	aliases B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073	country USA Pakistan Finland Canada	year 1937 1967 1975 1971	solate fields [] disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup A A A A	ST 4 1 5 1	MLST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	Finet PorA VR1 5-2 5-2 20 18-1	yping antige PorA VR2 10 10 9 3	ens FetA VR F1-5 F5-1 F3-1 F5-1
id 1 2 7 10 11	isolate A4/M1027 120M 7891 6748 129	aliases B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092	country USA Pakistan Finland Canada Germany	year 1937 1967 1975 1971 1964	solate fields [] disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup A A A A A A	ST 4 1 5 1 1	MLST clonal complex 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	Finet PorA VR1 5-2 5-2 20 18-1 5-2	yping antige PorA VR2 10 10 9 3 10	ens FetA VR F1-5 F5-1 F3-1 F5-1 F3-6
id 1 2 7 10 11 13	isolate A4/M1027 120M 7891 6748 129 139M	aliases B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099	country USA Pakistan Finland Canada Germany Philippines	year 1937 1967 1975 1975 1971 1964 1968	solate fields [] disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup A A A A A A A	ST 4 1 5 1 1 1	ML ST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup III ST-5 complex/subgroup III ST-1 complex/subgroup I/II ST-1 complex/subgroup I/I	Finet PorA VR1 5-2 5-2 20 18-1 5-2 5-2 5-2	yping antige PorA VR2 10 10 9 3 10 10	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1
id 1 2 7 10 11 13 19	isolate A4/M1027 120M 7891 6748 129 139M S3131	aliases B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1072 B99; Z1099 B213; Z1213	country USA Pakistan Finland Canada Germany Philippines Ghana	year 1937 1967 1975 1971 1964 1968 1973	solate fields [] disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	Serogroup A A A A A A A A A	ST 4 1 5 1 1 1 1 4	MLST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup III ST-5 complex/subgroup III ST-1 complex/subgroup I/II ST-1 complex/subgroup I/I ST-4 complex/subgroup IV	Finet PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7	yping antige 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 F5-1 F1-5
id 1 2 7 10 11 13 19 24	isolate A4/M1027 120M 7891 6748 129 139M S3131 S4355	aliases B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227	country USA Pakistan Finland Canada Germany Philippines Ghana Denmark	year 1937 1967 1975 1971 1964 1968 1973 1974	solate fields [] disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	Serogroup A A A A A A A A A A	ST 4 1 5 1 1 1 4 5	MLST clonal complex ST-4 complex/subgroup I/I ST-1 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 I/I ST-5 complex/subgroup II	Finet PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1	yping antige PorA VR2 10 10 9 3 10 10 13-1 9	ens FetA VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1 F1-5 F3-1
id 1 2 7 10 11 13 19 24 31	isolate A4/M1027 120M 7891 6748 129 139M S3131 S4355 10	aliases B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B268; Z1269	country USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso	year 1937 1967 1975 1971 1964 1968 1973 1974 1963	solate fields [] disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup A A A A A A A A A A A A	ST 4 1 5 1 1 1 4 5 4	ML ST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup III ST-5 complex/subgroup III ST-1 complex/subgroup IVI ST-4 complex/subgroup IV ST-5 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup IV	Finet PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-1 7 5-1 7	yping antige PorA VR2 10 9 3 10 10 13-1 9 13-1	Ens FetA VR F1-5 F5-1 F3-1 F3-1 F3-6 F5-1 F1-5 F3-1 F1-5
id 1 2 7 10 11 13 19 24 31 34	isolate A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 20	aliases B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B275; Z1275	Country USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger	year 1937 1967 1975 1971 1964 1968 1973 1974 1963 1963	solate fields [] disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	Serogroup A A A A A A A A A A A A A	ST 4 1 5 1 1 1 4 5 4 1	MLST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup III ST-5 complex/subgroup III ST-1 complex/subgroup III ST-1 complex/subgroup IV ST-5 complex/subgroup III ST-4 complex/subgroup III ST-4 complex/subgroup III ST-4 complex/subgroup III ST-4 complex/subgroup III ST-4 complex/subgroup III	Finet PorA VR1 5-2 20 18-1 5-2 5-2 7 5-1 7 5-1 7 5-2	yping antige PorA VR2 10 9 3 10 10 13-1 9 13-1 10	ns FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F1-5 F3-1 F1-5 F1-7
id 1 2 7 10 11 13 19 24 31 34 35	isolate A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 20 20 26	aliases B1; 21001 B35; 21035 B54; 21054 B73; 21073 B92; 21092 B99; 21099 B213; 21213 B227; 21227 B269; 21269 B275; 21275 B276; 21278	country USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Niger	year 1937 1967 1975 1971 1964 1968 1973 1974 1963 1963 1963	solate fields [] disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	Serogroup A A A A A A A A A A A A A A	ST 4 1 5 1 1 1 4 5 4 1 4 4	MLST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup III ST-5 complex/subgroup III ST-1 complex/subgroup IVI ST-1 complex/subgroup IVI ST-4 complex/subgroup IV ST-5 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup IVI ST-4	Finet PorA VR1 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1 7 5-2 7	yping antige PorA VR2 10 9 3 10 10 13-1 9 13-1 10 13	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F3-6 F5-1 F3-1 F1-5 F3-1 F1-5 F1-7 F1-5
id 1 2 7 10 11 13 19 24 31 34 35 46	isolate A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 20 26 255	aliases B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1227 B276; Z1275 B278; Z1278 B318; Z1318	country USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso	year 1937 1967 1975 1971 1964 1968 1973 1974 1963 1963 1963	solate fields [] disease 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)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup A A A A A A A A A A A A A A A	ST 4 1 5 1 1 1 4 5 4 1 4 4 4	MLST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-5 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I	Finet PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1 7 5-1 7 5-1 7 7 5-2 7 7 7-2	yping antige PorA VR2 10 9 3 10 10 13-1 9 13-1 10 13 13-1	ms FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F1-5 F3-1 F1-5 F1-7 F1-5 F1-5
id 1 2 7 10 11 13 19 24 31 34 35 46 52	isolate A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 20 26 255 243	aliases B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B276; Z1275 B276; Z1278 B318; Z1318 B362; Z1362	country USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Cameroon	year 1937 1967 1975 1971 1964 1968 1973 1974 1963 1963 1966 1966	solate fields [] 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)	species Neisseria meningitidis Neisseria meningitidis	serogroup A A A A A A A A A A A A A A A A A A	ST 4 1 5 1 1 1 4 5 4 1 4 4 4 4 4	MLST Clonal complex ST-4 complex/subgroup I// ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I	Finet 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 7	yping antige [PorA VR2] 10 9 3 10 10 13-1 10 13-1 10 13 13-1 13 13 13 13 13 13 13 13 13 1	ms FetA VR F1-5 F5-1 F3-1 F3-1 F3-1 F3-6 F5-1 F1-5 F1-7 F1-5 F1-5 F1-5 F1-5
id 1 2 7 10 11 13 19 24 31 34 35 46 52 61	isolate A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 20 26 255 243 393	aliases B1; Z1001 B35; Z1035 B54; Z1054 B92; Z1092 B92; Z1092 B9213; Z1213 B227; Z1227 B269; Z1269 B275; Z1275 B278; Z1278 B318; Z1318 B362; Z1362 B392; Z1392	Country USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso Cameroon Greece	year 1937 1967 1975 1971 1964 1968 1973 1963 1963 1966 1966 1966	solate fields [] disease invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis	Serogroup A A A A A A A A A A A A A A A A A A A	ST 4 1 5 1 1 1 4 5 4 4 1 4 4 4 4 4 4 1	MLST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup III ST-5 complex/subgroup III ST-1 complex/subgroup IVI ST-1 complex/subgroup IVI ST-4 complex/subgroup IV ST-5 complex/subgroup IVI ST-4 complex/subgroup IVI S	Finet PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-2 7 5-2 7 5-2 7 7-2 7 5-2 7	yping antige PorA VR2 10 9 3 10 10 13-1 9 13-1 10 13 13-1 13 13-1 13 10	ens FetA VR F1-5 F5-1 F3-1 F3-1 F3-6 F5-1 F1-5 F3-1 F1-5 F1-5 F1-5 F1-5 F5-1
id 1 2 7 10 11 13 19 24 31 34 35 46 52 61 64	isolate A4/M1027 120M 7891 6748 129 139M 83131 833131 84355 10 20 26 255 243 393 254	aliases B1; 21001 B35; 21035 B54; 21054 B73; 21073 B92; 21092 B99; 21099 B213; 21213 B227; 21227 B269; 21269 B276; 21275 B278; 21278 B318; 21318 B362; 21362 B392; 21392 B392; 21392	country USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso Cameroon Greece Dibbouti	year 1937 1967 1975 1971 1964 1968 1973 1974 1963 1963 1966 1966 1968 1966	solate fields [] disease invasive (unspecified/other) invasive (unspecified/other) carrier	species Neisseria meningitidis Neisseria meningitidis	serogroup A A A A A A A A A A A A A A A A A A A	ST 4 1 5 1 1 1 1 4 5 4 1 4 4 4 4 4 1 1	MLST Clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup IV ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I 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-4 complex/subgroup IV ST-4 complex/subgroup IV	Finet PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-1 7 5-1 7 5-1 7 7 5-2 7 7 2 5-2 5-2 5-2	yping antige PorA VR2 10 9 3 10 10 13-1 13-1 13 13-1 13 13-1 13 10 10	PINS FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F1-5 F1-7 F1-5 F1-5 F1-5 F1-5 F1-7
id 1 2 7 10 11 13 19 24 31 34 35 46 52 61 64 67	isolate A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 20 26 255 243 393 254 243 393 255	aliases B1; 21001 B35; 21035 B54; 21054 B73; 21073 B92; 21092 B99; 21099 B213; 21213 B227; 21227 B269; 21269 B275; 21275 B278; 21278 B318; 21382 B362; 21362 B392; 21392 B439; 21436	country USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Cameroon Greece Djibouti Australia	I year 1937 1967 1975 1971 1964 1964 1963 1963 1963 1966 1966 1966 1966 1968 1967	solate fields [] 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) invasive (unspecified/other) carrier invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis	Serogroup A A A A A A A A A A A A A A A A A A A	ST 4 1 5 1 1 1 1 4 5 4 1 4 4 4 4 4 1 1 1	MLST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup III ST-5 complex/subgroup III ST-1 complex/subgroup III ST-4 complex/subgroup IV ST-5 complex/subgroup IV ST-4 complex/subgroup IVI ST-4 complex/subgroup IVI ST-1 complex/	Finet PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-1 7 5-1 7 5-2 7 7 -2 7 5-2 5-2 5-2 5-2	yping antige PorA VR2 10 9 3 10 13-1 9 13-1 10 13 13-1 10 13 13-1 13 13 10 10 10	Pns FetA VR F1-5 F5-1 F3-1 F3-1 F3-6 F5-1 F1-5 F1-5 F1-7 F1-5 F1-7 F5-1 F1-7 F5-1

## 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.	For every allelic profile in the profiles/sequence definition should be noted that it does not represent a population Submissions • Manage submissions • General information • Isolates: 35423 • Last updated: 2015-08-27 • Update history • About BIGSdb
Breakdown       Export       Analysis         • Single field       • Export dataset       • Codon usage         • Unique combinations       • Scheme and alleles       • Sequences - XMFA / concatenated FASTA formats       • Codon usage         • Publications       • Sequence bin       • Sequences - 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.

Putin/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
➤ 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.

Ouery:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/sequences definitions   Database submissions
Help 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.  Joifferentiate 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). I bisplay locus aliases if set.
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
Differentiate provisional allele designations.     Display sender, curator and last updated details for allele designations (tooltip).     Display information about sequence bin records tagged with locus information (tooltip).     Display information about whether alleles have flags defined in sequence definition database (shown in sequence detail tooltip).     Display information about sample records (tooltip).     Display information about sample records (tooltip).
Set options
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.

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 tootlips (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.

Profinition Streakdown: Isolate fi Links: Contents   Hor	se   Profile/ST   List elds   Scheme/alleles   Publications ne   Options   Profiles/sequences definitions   I	Database submissions	
Set database options			
Here you can set options for your use of the when you next go to a query page, try refres	website. Options are remembered between s hing the page (Shift + Refresh) as some page:	essions and affect the current database (Neisseria s are cached by your browser.	a PubMLST) only. If some of the options don't appear to set
<ul> <li>General options</li> </ul>			
▶ Main results table			
Isolate record display			
<ul> <li>Provenance field display</li> </ul>			
Select the isolate provenance fields ti locus, scheme or scheme field query isolate aliases strain_designation country continent region year epidemiological_year age_mth sex All None Default Set op	at you wish to be displayed in the main results and then selecting the 'Customize' option.	stable following a query. Settings for displaying loc amoxicillin sulphonamide cettriaxone chiraramphenicol chiraramphenicol chiraramphenicol- chiraramphenicol- cefotaxime cefotaxime cefotaxime frifampicin_ange ciprofloxacin	us and scheme data can be made by performing a ciprofloxacin_range pending_assembly assembly_status ENA_accession private_project comments sender curator date_entered datestamp
Query filters  Reset  Click the reset button to remove all user so  Reset all to defaults	attings 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	
et database options	
ere 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 then you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.	to set
✓ General options	
Display 25 ▼ records per page. Page bar position: top and bottom ▼ Display 100 ▼ nucleotides of flanking 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 'Query filters' tab will scroll up.

<ul> <li>Isolate record display</li> </ul>		
Provenance field display		
Query filters		
Select the fields for which you would like dropdow isolate country continent region year epidemiological_year age_mth sex disease source epidemiology species serogroup MLEE_designation serotype sero_subtype ET_no penicillin_range amoxicillin sulphonamide ceftriaxone_range chloramphenicol_range cefotaxime_range rffampicin_range iffampicin_range pendingical_range ciprofloxacin_range pendingical_range pendingical_range pendingical_range pending_assembly assembly_status AI None Default Set options	vn lists containing known values on which to filter query results. These w PNL accession Private_project comments ender curator date_entered datestamp MLST profile completion Finetyping antigens profile completion ADP-heptose biosynthesis profile completion ADP-heptose biosynthesis 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 A - Serogroup Y profile completion Capsule Region C profile completion Capsule Region D - Serogroup Y profile completion Capsule Region D - Serogroup Y profile completion Capsule Region D profile completion Capsule Region D mofile completion Conjugative Plasmid profile completion Gonococcal Genetic Island profile completion Kdo addition profile completion	ill be available in the filters section of the query interface. LOS alpha chain transferases profile completion LOS transport/export profile completion LIPId A biosynthesis: acyltransferases profile completion Lipid A biosynthesis: acyltransferases profile completion Neisseria genus core genes profile completion Nucleotide excision repair profile completion Protein glycosylation profile completion Pruina metabolism profile completion Pruna metabolism profile completion Prunate dehydrogenase complex profile completion RNA polymerase profile completion TCA cycle profile completion UDP-GlycAcs and UDP-galactose biosynthesis profile completion UDP-glucose and UDP-galactose biosynthesis profile completion MT T4SS profile completion WTR T4SS profile completion MT T4SS profile completion Prific profile completion WDP-glucose strail genes) profile completion WDP-glucose strail genes) profile completion WDP-glucose strail profile completion WDP-glucose strail genes) profile completion WDP-glucose strail genes) profile completion WTR T4SS profile completion WDP-glucose strail genes) profile completion WDP-glucose strail genes) profile completion WDP-glucose strail genes) profile completion WDP-glucose strail genes) profile completion MUST (20 locus strail genes) profile

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.

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. 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 <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>Option settings</li> <li>Set display and query options for locus, schemes or scheme fields.</li> <li>Set display and query options for locus, schemes or scheme fields.</li> <li>General information <ul> <li>Isolates: 35423</li> <li>Last update history</li> <li>About BIGSdb</li> </ul> </li> </ul>
<ul> <li>Breakdown</li> <li>Single field</li> <li>Two field</li> <li>Unique combinations</li> <li>Scheme and alleles</li> <li>Sequences - XMFA / concatenated FASTA formats</li> <li>Sequence bin</li> </ul>

Either select the locus id by querying for it directly.

Query:         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 settings.	
— Search criteria — Display — Display	
id • = • abcZ + [ Order by: id • • ascending •	
Display. 25 V fecords per page []	
-> Filter query by	
Reset	
1 record returned. Click the hyperlink for detailed information.	
Customize	
locus options	
id data type lailete id format length varies coding sequence orf genome position isolate display* [query field* analysis*	
autz Drvk integer 4-55 raise uue i intro-4-0 allele only faise true true -	

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	<b>/ILST</b>	Query: Sea Breakdown Links: Cont	rch   Brows I: Isolate fie tents   Hon	se   Profile/S elds   Schen ne   Options	T   List ne/alleles   Publi   Profiles/seque	cations nces de	finitions   [	Database	submissions					
														Toggle: i
Quer	/ loci	for Neis	sseria	PubM	LST data	abas	е							
Please	enter your	search criteria	a below (or	r leave blank	and submit to r	eturn all	records). I	Matching I	ci will be ret	urned and you wil	l then be ab	le to update	their display and query settings.	
Sea	rch criteria	a					— — D	isplay —						
id		<b>→</b> =		•		+	i	Order by:	id	-	ascendin	g 👻		
								Display:	25 👻 rec	ords per page 👔				
⊽ Fi	Iter query	by-					Action -							
		data type:	-				Reset	Submit	1					
	allele	id format:	•						-					
	len	gth varies:	<b>v</b> i											
	coding	sequence:	-											
		orf:	<u> </u>											
	mate	n longest:	<u> </u>											
		robo filtor:												
	P	flag table:												
	isola	te display:		-										
	ma	in display:		<u>.</u>										
	c	query field:	- i											
		analysis:	▼ i											
		curator:			i									
		scheme: M	ILST			i								
7 records	returned	Click the hype	erlinks for	detailed info	rmation									
Cust	omize													
locus	options													
id c	lata type	allele id forma	at length I	length varie:	s coding seque	nce orf	genome	position is	olate display	/* main display*	query field	* analysis*		
abcZ	DNA	integer	433	false	true	1	1176	340	allele only	false	true	true		
adk	DNA	integer	465	false	true	1	9919	151	allele only	false	true	true		
fumC	DNA	integer	465	false	true	1	1592	943	allele only	false	true	true		
gdh	DNA	integer	501	false	true	1	1514	394	allele only	false	true	true		
pdhC	DNA	integer	480	false	true	1	1453	970	allele only	false	true	true		
* Default	UNA values are	Integer displayed for thi	450 is field The	talse se may be ove	true prridden hy user n	1 reference	9654	181	allele only	false	true	true		
Default	values alle	ulapiayeu for th	ia neid. The	se may be ove	moden by user p	reference								

7 records returned. Click the hyperlinks for detailed information. Customize locus options id data type ele id forı 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 integer fumC DNA 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). (+Log out   Change password
User projects
New private projects Projects allow you to group isolates so that you can analyse them easily together. Rease enter the details for a new project. The project name ended to be unique on the system. A description is entired 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'.

ged in	: Keith Jolley (ke	eith). 🕩 Log ou	t   Chan	ge password														Help 🗹	Togg	le: 🚯
arc	ch or bro	owse N	leis	seria PubM	LST a	latabas	9													
toro	aarab aritaria ar	leave bleek	te brev	waa all raaarda. Madii	h form no	remeters to filt	or or optor o	list of volue	_											
-Isol	late provenance	e/phenotype	fields	wse all records. Modi	iy ionn pa	rameters to mit	Allele desig	nations/sch	s. eme field	s										M fo
omb	oine with: AND	•					ST (MLST)	•	=		<b>v</b> 11					+ 0				0
cour	ntry	<b>~</b> =		▼ UK		+ 0		ontione								_		tion		
sero	group			▼ W			Order by:	id							<b>-</b> 3	cendi		aon	Qubmi	
year	r			✓ 2016			Display:	25 <b>•</b> re	cords ner	nage	6					canta	S R	eset	Submi	
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K gra	oup W ST-11 2	016 V A	Add the	se records										MI	ST			Fir	nefvping ;	antio
C gra e: [ d	pup W ST-11 2 1 2 3 4 isolate alias	016 ▼ A	Add the	se records	source	species	serogroup	Seqbin size (bp)	Contigs	abcZ a	adk a	IroE fu	ımC g	ML dh pd	.ST hC pgi	n ST	clonal comple	Fir x Po X VF	netyping a rA PorA	antig
( gra e: <b>(</b> d 451	isolate alias M16 240077	016 V A	Add the 7	se records	source sputum	species Neisseria meningitidis	serogroup W	Seqbin size (bp) 2111799	Contigs 257	abcZ a	adk a 3	troE fu	ımC g 3	ML dh pd 8 4	.ST hC pgi 4 6	n ST 11	cional comple ST-11 complex/ET-3 complex	Fir x Po VF 7	netyping a rA PorA R1 VR2 5 2	antig F
( grc a: (* 1 175	isolate alias M16 240077 M16 240003	016 - A	Add the 7 9 9 2016 2016	se records > Last Isolate fields • disease invasive (unspecified/other)	source sputum	species Neisseria meningitidis Neisseria meningitidis	serogroup W W	Seqbin size (bp) 2111799 2098168	Contigs 257 222	abcZ a 2 2	adk a 3 3	troE fu 4	ImC g 3 3	ML dh pd 8 4	.ST hC pgr 4 6	n ST 11 11	clonal comple ST-11 complex/ET-3 complex/ET-3 complex/ET-3 complex/ET-3	Fir × Po × VF 7 7	retyping a rA PorA R1 VR2 5 2 5 2	antig F F
( grd e: 451 475 478	M16         M16           240003         M16	016 ▼ A S COUNTRY UK UK UK	Add the 7 2016 2016 2016	se records > Last Isolate fields • disease (unspecified/other) invasive (unspecified/other)	source	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup W W	Seqbin size (bp) 2111799 2098168 2108815	Contigs 257 222 265	abcZ a 2 2 2	adk a 3 3 3	troE ft 4 4	1 <b>mC</b> g 3 3 3	ML dh pd 8 4 8 4	.ST hC pg1 4 6 4 6	n ST 11 11	clonal complex ST-11 complex/ET-3 complex/ET-3 complex/ET-3 complex/ET-3 complex/ET-3 complex/ET-3	Fir x Po 7 5 7 7	netyping a rA PorA 1 VR2 5 2 5 2 5 2	ntig F F F
( grd e: 2 4 451 475 478 480	M16         M16           240007         M16           M16         M16           240003         M16           M16         M16           240008         M16	es country UK UK UK	Add the 7 2016 2016 2016 2016	se records > Lest isolate fields ① disease invasive (unspecified/other) invasive (unspecified/other)	source	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup W W W	Seqbin size (bp) 2111799 2098168 2108815 2117414	Contigs 257 222 265 338	abcZ 4 2 2 2 2 2	adk a 3 3 3 3	ITOE fl 4 4 4 4	1mC g 3 3 3 3	ML dh pd 8 · 8 · 8 ·	ST hC pgi 4 6 4 6 4 6	n ST 11 11 11	clonal complex ST-11 complex/ET-3 complex/ET-3 complex/ET-3 complex/ET-3 complex/ET-3 complex/ET-3 complex/ET-3 complex/ET-3	Fir           x         Po           7         E           7         E           7         E           7         E           7         E           7         E           7         E           7         E	rA PorA TA PorA 2 2 5 2 5 2 5 2 5 2	F F
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).
New project
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	I Data	ibase h	ome	Conte	nts																
Logged in	: Keith Jolle	y (keith).	€+Log out	Chang	e password														Help 🖉	Toggle	: <b>()</b> =
Searc	ch or l	brow	se N	eiss	seria PubN	ILST d	atabase														
Enter se	earch criter	ia 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 proven	ance/ph	enotype	fields -			F	Filters													form
id		•	- =		<ul> <li>Enter value</li> </ul>		+	P	ublication:									÷ (	•		options
									Project:	1 selecte	ed				÷	0					
								MLS	T profiles:	✓ Checl	k all	× Unch	eck al	l i	0						
							(	cional comple	ex (MLST):	Irish N	/lening	ococcus	s Geno	me Lib	ra 🔨						
								becomol MI 6	T profiles:	MRF	Mening	gococcu	s Gen	ome Lil	br						
							RI.	Seni Seni	ionco hin:	NI_EX	(CL_M	RF									
							F	uplo ebular	record versi	penA	seque	nce ana	lysis								
									record vers	C rpoB	sequer	ICE anai	ysis malih	rany	=						
Dis	play/sort of	ptions —					and the second second	- Action		UK ar	oup W	ST-11 2	2016	iaiy	11						
U U	Display: 7		o o o r do u			•	ascending	Rese	t Subi	UK &	Ireland	MGL 2	010/11	-2013/	14 👻						
	Dispidy. 2	.J 🔻 I	ecorus p	er pag	eu					•		III			Þ.						
163 reco	rds returne	ed (1 - 25	display	ed). Cli	ck the hyperlinks fo	r detailed in	formation.														
-Your	projects -																				
Select	project		▼ A	dd thes	e records																
Page:	1 2 3	4	5 6	7)>	Last																
					Isolate fields 🛈				Soubin						MLST				Finety	/ping an	tigens
id	isolate	aliases	country	year	disease	source	species	serogroup	size (bp)	Contigs	abcZ	adk arol	E fumC	gdh p	odhC	pgm	ST	clonal complex	PorA VR1	PorA VR2	FetA 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). [HLog 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: Description:
Your projects
Delete     Add/remove records     Modify users     Project     Description     Administrator     Isolates     Browse       Image: Control of the second
Note that deleting a project will not delete its member isolates.
*

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.
$\odot$
Add user  Enter username hbratcher You need to know the username or any user you wish to add.

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). (Honge 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)     Users       Jolley, Keith (keith)     Image: Comparison of the second secon
Add user Action Enter username: hbratcher Add user You need to know the username of any user you wish to add.
Θ

# 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 Adion Name: Description:
Your projects
Petete     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.     Isolates     Isolates     Isolates       You can also add isolates to projects from the results of a query.     Isolates     Isolates     Isolates     Isolates
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).
X 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
Description:
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.     G     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
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). House out   Change password	Toggle: 🜖 🚍
Batch insert isolates	
Private data upload These isolates will count against your quota of private data. Quota available: 100	ŧ
<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 a 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 automatically</li> <li>Download tab-delimited header for your spreadsheet - use 'Paste Special O Text' to paste the data.</li> <li>Download submission template (xlsx format)</li> </ul>	the 'allowed_loci' tab in the Excel template y.
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). @Log out   Change password
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       • Main public projects       • Set general options - including isolate table field handling.       • Manage submissions         • Search by combinations of loci (profiles)       • Main public projects       • Set general options - including isolate table field handling.       • Manage submissions         • Search by combinations of loci (profiles)       • Main public projects       • Set display and query options for locus, schemes or scheme fields.       • Manage submissions         • Isolates: 43172       • Isolates: 43172       • Last updated: 2017-06-23       • Defined field values       • Update history         • Update history       • About BIGSdb       • About BIGSdb       • Main general options       • Main general options
Breakdown       Export       Analysis       Miscellaneous         • Single field       • Export dataset       • Contigs       • Codon usage       • Description of database fields         • Two field       • Contigs       • Sequences - XMFA / concatenated FASTA formats       • Codon usage       • Description of database fields         • Publications       • Sequence bin       • Sequence bin       • BLAST       • 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.

M0024027 M00282207         UK         2000         invasive (unspecified/other)         Neisseria meningitidis W1101         B         1100         ST-32 complex/ET-5 complex visubgroup III         7         16           7891         B54, 21054         Finland         1975         invasive (unspecified/other)         Neisseria meningitidis W1102         A         5         55- complex/subgroup III         20         9         F3-1           M00242007         UK         2000         invasive (unspecified/other)         Neisseria meningitidis W114         ST-18 complex/subgroup III         20         9         F3-1           0021/84         Czech Republic         1984         invasive (unspecified/other)         Neisseria meningitidis W114         ST-12 complex/subgroup III         5-2         10         F3-6           0090/89         Czech Republic         1988         invasive (unspecified/other)         Neisseria meningitidis W117         T1 complex/subgroup III         5-2         10         F5-1           0120095         Czech Republic         1986         invasive (unspecified/other)         Neisseria meningitidis W117         T1         F1-0         F1-0         F2-2         10         F5-1           0120095         Czech Republic         1996         carrier         Neisseria meningitidis W117         T1	-					,		· · · · · · · · · · · · · · · · · · ·						
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781       B54, Z1054       Finland       1975       invasive (unspecified/other)       Neisseria meningitidis       A       5       ST-5 complex/subgroup III       20       9       F3-1         M00242007       UK       2000       invasive (unspecified/other)       Neisseria meningitidis       B       1102       ST-18 complex       14         6748       B73, Z1073       Canad       1971       invasive (unspecified/other)       Neisseria meningitidis       A       1       ST-1 complex/subgroup III       18-1       3       F5-1         129       B92, Z1092       Canad       1971       invasive (unspecified/other)       Neisseria meningitidis       A       1       ST-1 complex/subgroup III       18-1       3       F5-1         0390/89       Czech Republic       1985       invasive (unspecified/other)       Neisseria meningitidis       A       1       ST-1 complex/subgroup III       5-2       10       F5-1         102095       Czech Republic       1985       invasive (unspecified/other)       Neisseria meningitidis       X       117       14       14       14       14       14       14       14       14       14       14       14       14       14       14       14       14       14       14	6	100282207		UK	2000	invasive (unspecified/other)	Neisseria m	neningitidis	W	1101	ST-22 complex			
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002184         Czech Republic 1984 invasive (unspecified/other) Neisseria meningitidis         W         114         ST-22 complex         Image: Complex invasive (unspecified/other) Neisseria meningitidis         A         1         ST-1 complex/subgroup III         18-1         3         F5-1           129         B92, 21092         Germany 1984         invasive (unspecified/other) Neisseria meningitidis         A         1         ST-1 complex/subgroup III         5-2         100         F5-3           0090/089         Czech Republic 1989         invasive (unspecified/other) Neisseria meningitidis         A         1         ST-1 complex/subgroup III         5-2         10         F5-1           0120/95         Czech Republic 1995         invasive (unspecified/other) Neisseria meningitidis         X         117         T1	8	100242007		UK	2000	invasive (unspecified/other)	Neisseria m	neningitidis	В	1102	ST-18 complex		14	
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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.

AST	Τ															
ase se	elect the requ	uired isolate	ids to BLAST ag	ainst (use cti	rl or shif	ft to make r	nultiple sel	ections) and paste	in your que	ery seque	nce. Nucleot	ide or pept	de sequences can be	queried.		
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H ankii Use 1 2 7 0 1 1 3 9 9	lits per isolat ng length (br e TBLASTX [ A4/M1027 120M 7891 6748 129 139M S3131 S4355	Ke         I           p):         100           Image:	<ul> <li>Ignment length</li> <li>465</li> </ul>	Mismatche 7 7 7 7 7 7 7 7 7 7	s Gaps 0 0 0 0 0 0 0 0 0	Seqbin id 180177 180583 180965 181186 181867 182004 182318 215673	Start 19444 4782 19869 19181 35889 36775 19090 4534	End (0 19908 extract - 20333 extract - 19645 extract - 36355 extract - 19554 extract - 19554 extract - 4998 extract -	$\begin{array}{c} \text{Drientation} \\ \rightarrow \\ \leftarrow \\ \rightarrow \\ \leftarrow \end{array}$	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	Bit score 807 807 807 807 807 807 807 807 807					
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H ankii Use 1 2 7 0 0 1 1 3 9 9 2 4 50 51	lits per isolat ng length (br e TBLASTX[ A4/M1027 120M 7891 6748 129 139M \$3131 \$4365 14 10	<ul> <li>identity A</li> <li>98.49</li> </ul>	<ul> <li>Ignment length</li> <li>465</li> </ul>	Mismatche 7 7 7 7 7 7 7 7 7 7 12 7	s Gaps 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Seqbin id 180177 180583 180965 181186 181866 181867 182004 182318 215673 8 182380	Start           19444           4782           19869           19181           35889           36775           19090           4534           1363524           5559	End   0 5246 extract - 2033 extract - 19645 extract - 19645 extract - 37239 extract - 19554 extract - 19558 extract - 136398 extract - 136398 extract -	$\begin{array}{c} \text{Drientation} \\ \rightarrow \\ \downarrow \\ \rightarrow \\ \rightarrow \\ \uparrow \\ \rightarrow \\ \downarrow \\ \uparrow \\ \downarrow \\ \downarrow$	1 E-value 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.	Bit score 807 807 807 807 807 807 807 807 807 807					
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H ankii Usi ate id 1 2 7 7 10 11 13 39 9 24 30 31 13 4 35 52 31 34 52 31 34 57	Its per isolat           ng length (br)           e TBLASTX[           A4/M1027           120M           7891           7891           139M           5748           129           6748           129           6748           129           6748           129           6748           129           33311           S4355           14           10           20           26           255           243           393           254           25611	Image: Provide and	<ul> <li>Ignment length</li> <li>465</li> </ul>	Mismatche 7 7 7 7 7 7 7 12 7 7 7 7 7 7 7 7 7 7 7	s Gaps 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Seqbin Id 180177 180583 180965 181186 181867 182004 182318 215673 8 182380 182815 182880 182380 183381 1833818 1833818 1834143	Start           19444           4782           19869           19181           35889           36775           19090           4534           1363524           5559           19783           18879           4982           4532           7217           4716           4804	End         CI           19900         extract           5246         extract           20333         extract           19645         extract           38353         extract           19554         extract           20247         extract           20247         extract           7681         extract           7681         extract           7681         extract           5268         extract	$\begin{array}{c} \text{Drientation} \\ \uparrow \\ \downarrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \downarrow \\ \uparrow \\ \uparrow$	E-value 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.	Bit Score 807 807 807 807 807 807 807 807 807 807					
H ankii Usi ate id 1 2 7 7 10 11 13 3 9 9 24 30 31 13 4 35 5 6 52 31 34 57 32	Its per isolation           ng length (br)           e TBLASTX[           A4/M1027           120M           7891           6748           129           139M           S31311           S4355           14           10           26           255           243           393           254           S5611           11-004	<ul> <li>identity A</li> <li>identity A</li> <li>98.49</li> </ul>	<ul> <li>Ignment length</li> <li>465</li> </ul>	Mismatche 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	s Gaps 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Seqbin id 180177 180583 180965 181186 181867 182004 182318 216673 8 182380 182815 182880 183179 1833818 183648 183413 183443 184297	Start           19444           17829           19869           19181           35889           36775           19090           4534           1363524           5559           19783           18879           4982           4532           7217           4716           4804           19518	End         C           19008         settest         -           5246         settest         -           19045         settest         -           36353         settest         -           37239         settest         -           37238         settest         -           37238         settest         -           36353         settest         -           37238         settest         -           19654         settest         -           37239         settest         -           37238         settest         -           37239         settest         -           37239         settest         -           36308         settest         -           5446         settest         -           5180         settest         -           5268         settest         -           5268         settest         -           19962         settest         -	$\begin{array}{c} \text{Drientation} \\ \uparrow \\ \downarrow \\ \uparrow \\ \downarrow \\ \uparrow \\ \downarrow \\ \uparrow \\ \downarrow \\ \downarrow$	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           0.0           0.0           0.0           0.0           0.0	Eit score 807 807 807 807 807 807 807 807 807 807					
H lankii Usi ate id 1 2 7 10 11 13 19 24 30 31 34 35 5 46 52 31 34 55 46 52 31 34 35 54 34	Its per isolat           ng length (b;           e TBLASTX[           A4M1027           120M           7891           6748           129           139M           S3131           S4355           14           10           20           255           243           393           254           S5611           11-004           IAL2229	Image: second system         Image: second system           Image: second system	<ul> <li>Ignment length</li> <li>465</li> </ul>	Mismatche 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	S Gaps 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Seqbin id 180177 180583 180965 181186 181867 182044 182318 215673 8 182380 182815 182800 183179 183381 1834297 183688 184455	Start 19444 4782 19869 19181 35879 36775 19090 4534 1363524 5559 19783 138379 4982 4532 7217 4716 4804 19518 4530	End         C           19908 settract         1           5246 settract         2           19645 settract         1           19645 settract         3           19645 settract         1           19645 settract         1           19645 settract         1           19645 settract         1           19534 settract         1           20247 settract         1           20248 settract         1           20247 settract         1           20448 settract         1           5268 settract         1           19982 settract         1           19982 settract         1           19982 settract         1           19982 settract         1	$\begin{array}{c} \text{Drientation} \\ \uparrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \downarrow \uparrow \uparrow \downarrow \downarrow	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           0.0           0.0           0.0           0.0           0.0	Eit score 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 🛶	←	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

Query: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/Sequences definitions   Database submissions				
Extracted sequence: Seqbin id#:182318 (19090-19554)				
sequence bin id#182318				
sequence Solexa Coechcosoff TIGAACAGOC ATCCCCGAAAA GCCGCCGCCA AACTCGCCGGA ATTGCCGGG TIGCCGTITG TCAGCGCGCC GAACAAATTT GAAGCCTIGG GCGGACGCGA IGCCGCTGI GCCGCCGI GCCGCCGCGA				
method GCCCATIGAA AACCTGGCG GCAAGCCTGA ATAAAATCCC CAACGACATC CGCTGGCTGGGC GCCGCGCGGCT TIGGGCGAA TCAAAATCCC CGAAAACGAC CGCGGCTGGT CCATCATGCC GGGCAAAGCC start 19900 AACCCGACC AATCCGAAGC GGTGCCCG CAACGACGGC CACGACGGTA GCGCGGGCGC GCCGGGCAAT TICGACGCAAT GCCGGCTAAGC CGGCGAAAGCC				
end 19554 CAICCOCCCG IIGGGCGACG CETGCAACAG CTICAACGAA CACTGCGCCG ICGGCATIGA ACCOETACCG GAAAAAACG ACTATIICCT GCACCATICC CIGAIGCICG IIACCGCGTI AAACGGCAAA AICGGTIACG				
ength 465 AAAADSCOEC CAAASTCECC AAAACCSCCT ACAAAACCAA CAAATCSTIE CECEAAACCS CCETTEAET BEETTECTE ACBABACCAA ACTBE				
translation				
R H G F E Q P S R I R R K S R R Q T R R I V R L A V C Q R A E Q I 🕴 F1				
ARV * TAIPNTPKKPPPNSPNCPACRISARTNL F3				
1 CGGCACGGGTTTGAACAGCCATCCCGAATACGCCGAAAAAGCCGCCGAAATCGCCGGAATTGCCGGGCTTGCCGTTTGCCAGCGCGCCGAACAATTT 100				
SLGRTRCRRCRFGRIENAGGKPE 🚪 NRQRHPLAG F1				
E A L G G R D A A V A A S G A L K T L A A S L N K I A N D I R W L A F2 V D W D D M D T D T D A H V D W D D D T T V C D T T C A G W F3				
101 GAASCETTSGECGKACGCATGCCCCCETTSCCCCTTCGGGCCCATTGAAAACGCTGGCGCGCAACCTGAATAAAATCGCCAACGACATCCGCTGGCTG				
KRPALRF GRN QNPRKRAGF VHHAG QS QPDPMRS F1				
S G P R C G L G E I K I P E N E P G S S I M P G K V N P T Q C E A F2				
Q A A R A A V W A K S K S P K T S R V R P S C R A K S T R P N A K R F3 20 Chargescorecentergentingencentationalancealecorectrotecorecentercharges and				
D D H G V L P S V R O R R Y H R Y G G R V G O F R A F R L Y A R H R FI				
M T M V C C Q V F G N D V T I G M A G A S G N F E L N V Y M P V I F2				
* P W C A A K C S A T T L P S V W R A R R A I S S * T S I C P S S F3				
AYN LOSIR LLGDACNSFNEH CAVGLE PVPEKID F2				
PTTSCNPSACWATRATASTNTAPSALNPYRKKS F3				
401 GCCTACAACCTCTGCAATCCATCCGCCGTGTGGGGGACGCCGGGAACACCTCCAACGACACTGCGGCCGTCGGCCATGGACCCGGAAAAATCG 500				

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	30.45	400	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
Download FASTA   FASTA with flanking i   Table (tab-delimited text)   Excel format											

#### 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 sequences by					
restrict monded bequenees by					
Sequence method:	▼ i				
Project:		▼ 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 N	100282207		UK	2000	invasive (unspecified/other)	Neisseria meningitio	lis W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitio	lis A	5	ST-5 complex/subgroup III	20	9	F3-1
8 N	100242007		UK	2000	invasive (unspecified/other)	Neisseria meningitio	tis B	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitio	tis W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitio	lis A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitio	lis A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitio	tis B	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitio	lis A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitio	tis X	117			14	
15	1		Germany	1999	carrier	Neisseria meningitio	tis E	864				
16	2		Germany	1999	carrier	Neisseria meningitio	tis B	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitio	tis W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitio	tis B	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitio	lis A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitio	dis NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitio	lis NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitio	tis E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitio	tis B	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitio	lis A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitio	tis B	930	ST-334 complex			
Analysis tools: Breakdown: Fields Two Field Codons Polymorphio sites Combinations Schemes/alleles Publications Sequence bin Tag status												
An	nalysis: B	JRST Prese	noe/Absence	Senome	Comparator BLAST							
	Export D	atarat Conti	an Converse	٦								
	Export D	ataset Conti	as									
Page: 1 2 3 4 5 6 7 8 > Last												

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.
<ul> <li>Divide strains into groups according to their allelic profiles.</li> <li>Count the number of Single Locus Variants (SLV), Double Locus Variants (DLV) and Satellites (SAT) for ea</li> <li>Identify the potential Ancestral Type (AT). These are shown with an asterisk next to their names in the resu</li> </ul>	ch sequence type (ST). Its table.
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 - 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
Neisseria PubMLST database	epresent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition
Query database Search 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.     General information     Isolates: 34221     Last updated: 2015-07-02     Update history     About BIGSdb
Breakdown Single field Two field Unique combinations Scheme and alleles Publications Sequence bin	Analysis Codon usage Presence/absence status of loci STA formats BLAST Miscellaneous - Description of database fields

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.

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.

Query: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publicati           Links: Contents   Home   Options   Profiles/sequence	ions is definitions   Database submissions	
		Toggle: [i]
Codon usage analysis		
This plugin will analyse the codon usage for individual loci and overall for correct identification of codons can only be achieved for loci for which the c would like to include. Output is limited to 500 records.	an isolate. Only loci that have a corresponding c correct ORF has been set (if they are not in read	database containing sequences, or with sequences tagged, can be included. It is important to note that ling frame 1). Partial sequences from the sequence bin will not be analysed. Please check the loci that you
	Loci	Schemes
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 • • • • • • • • • • • • •	165_CNA     155_CRNA (SSU_rRNA)     155_CRNA (SSU_rRNA)     235_CRNA     abc2     abc2 (NEIS1279)     ac46 (NEIS1729)     ac46 (NEIS1727)     ac46 (NEIS1727)     ac48 (NEIS1727)     ac48 (NEIS1727)	Cenetic Information Proce
Sequence retrieval	Codons	— — Action —
If both allele designations and tagged sequences	Select codon order:	Submit
exist for a focus, choose now you want these handled. [1]	eliphabetical	
Ose sequences tagged from the bin Use allele sequence retrieved from external database	C or G ending codons first	
$\ensuremath{\overline{\mathbb{V}}}$ Do not include sequences with problem flagged (defined alleles will	still 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.

Durp:         Search   Browse   Profile/STI List           Breakdown:         Isolate fields   Schemeralieles   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

Ouery:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Schemefalleles   Publications           Links:         Contents   Home   Options   Profile/Sequences definitions   Database submissions
Job status viewer
Status
Job id:         BIGSdb_13269_1405586315_76138           Submit time:         2014-07-17 09:38:35           Status:         finished           Statu:         grade           Progress:         10%           Stop time:         2014-07-17 09:39:05           Total time:         20 seconds
Output  Absolute frequency of codon usage by isolate Absolute frequency of codon usage by isolate 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. 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 does	e profiles/sequence definition s not represent a population sample.		
<ul> <li>Query database</li> <li>Search database - advanced queries.</li> <li>Showse 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       Miscellance         Single field       - two field       - Export dataset       - Contigs       - Contigs       - Contigs       - Description of         • Unique combinations       - Sequences - XMFA / concatenated FASTA formats       - Codon usage       - Presence/absence status of loci       - Description of         • Publications       - Sequence bin       - Sequence for the security of the secure security of the secure security of the sec	us 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.

			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			
Ana	lysis tools	3:				meningitidis					complex			
G	Breakdown	Fields Two Fie	d Combin	ations	Polymorphic sites	Publications S	equence bin	Tag status						
	Analysis	BURST Codo	ns Presenc	e/Abse	nce Genome Compa	arator BLAST	rMLST spe	cies id						
	Export	Dataset Cont	igs Sequer	nces										
ß	Third party	: GrapeTree IT	OL PhyloVi	z Mic	croreact									
Page:	123	4 5 6 7	89>	Las	t									

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.

PubMLST Database	e home Cont	ents
Logged in: Keith Jolley (keith	). 🕩 Log out   Change	password
Breakdown by	/ country	
121 values.		
country A	Frequency A	Percentade A
	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	550	0.76
Cuba	497	0.71
Slovenia	432	0.62
Australia	321	0.46
Quiterdand	021	0.40

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	
+9 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 definition database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be note population sample.	n the profiles/sequence ed that it does not represent a
Q Query database 📰 Projects 👯 Option settings	1 Submissions
Search or browse database     Search by combinations of loci (profiles)     Search by combinations     Search by comb	Manage submissions
	General information Isolates: 48,296 Last updated: 2019-01-28 Defined field values Update history About BIGSdb
Breakdown       Export       Analysis       Third party tools         • Single field       • Export dataset       • Contigs       • Contigs       • Contigs         • Unique combinations       • Sequences - XMFA / concatenated FASTA formats       • Codon usage       • GrapeTree - Visualization on         • Publications       • Sequences - XMFA / concatenated FASTA formats       • Genome comparator       • BLAST         • Description of database fields       • Description of database fields       • Description of database fields       • Output	of genomic relationships with data overlays d phylogenetic inference ualization and sharing for

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.

	0120/30		02001	1990	IIIVGSIVC	Nelaacha	л				1-4	
			Republic	1000	(unspecified/other)	meningitiais	5	004				
5	1		Germany	1999	carner	meningitidis	E	864				
6	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
7	3		Germany	1999	carrier	Neisseria meningitidis	w	174	ST-174 complex			
8	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
9	S3131	B213; NIBSC_2813; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex	7	13-1	F1-5
0	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
1	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
2	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
3	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex			
4	S4355	B227; NIBSC_2806; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	А	5	ST-5 complex	5-1	9	F3-1
5	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

PubMLST Database home Contents		
+D Log in		Toggle: ()
Gene Presence - Neisseria PubMLST	•	
Please select the required isolate ids and loci for comparison - us loci defined in schemes by selecting the appropriate scheme desc Interactive analysis is limited to 500,000 data points (isolates x loc	e CTRL or SHIFT to make multiple selections in cription.	ist boxes. In addition to selecting individual loci, you can choose to include all e restricted to static tables.
	Loci	Recommended schemes
Isolates       Optionally include data not in the database.         Quitonally include data not in the database.       Upload assembly FASTA file (or zip file containing multiple FASTA files - one per genome): The selected.         Clear Let al       Browse       No file selected.         Schemes       Parameters / Min % alig         W. gonorrhoeae cgMi       Min % alig         BLASTN work       Min % alig         BLASTN work       Ribosomal MLST	'165_rDNA       *         165_rRNA (SSU_rRNA)       235_rRNA         abcZ       abcZ         abcZ (NEIS1015)       ack42 (NEIS1279)         ack42 (NEIS1727)       acn4 (NEIS1727)         acn4 (NEIS1729)       *         All None Pastelist       options         options       •         of size:       20 * •	Recommended schemes below or use the full schemes list. MLST Ribosomal MLST N. meningtidis cgMLST v1.0 N. gonorrhoeae cgMLST v1.0 Clear
🔤 🛄 rpIF species		
Action Reset Submit		

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 home	e Contents
Logged in: Keith Jolley (keith). 🗣 Log o	but   Change password
Job status viewer	
Status	
Job id: BIC	3Sdb 194879 1548675927 08172
Submit time: 20	19-01-28 11:45:27
Status: fini	ished
Start time: 20	19-01-28 11:45:43
Progress: 10	0%
Stop time: 20	19-01-28 11:46:38
Total time: 54	seconds
Output Pivot Table Hea Files Presence/absence	e (Excel) Presence/absence (text)
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 Conte	ents										
Logged in: Keith Jolley (keith). 🗭 Log out   Change	bassword				Toggle: 🜖 📃						
Gene Presence - Neisse	eria PubMLS	; <b>7</b>									
158,895 data points (isolates x loci) used Please note that table updates may be slow if you try to combine id (or isolate) with 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 axes	. Multiple fields can be	e combined.			Change analysis						
Table •	id • isolate •	complete •	know	n allele • designated • tagged •							
Count  ▼ ↓ ↔	presence •	-									
locus *	presence ab	osent present	Totals								
	NEIS0001	80 19	99								
	NEIS0004	80 19	99								
	NEIS0005	80 19	99								
	NEISO007	80 19	99								
	NEIS0008	80 19	99								
	NEIS0009	80 19	99								
	NEIS0010	80 19	99								
	NEIS0011	80 19	99								

The table will be re-drawn including these fields.

Divet table										
Ivot table										
ag and drop fields on to the table axes. Multiple fields can be combined.										
Table 🔹	id 🔹	isolate	• co	mplete 🔹	know	n allele 🔻	)			
Count	pres	ence v	designa	ted 🔹 👔	added	•				
			1						_	
locus 🔻		presence absent				pre	sent			
		designated	not de	esignated	des	ignated	not de	signated	Totals	
		tagged	taggod	untaggod	taggod	untaggod	taggod	untegrad	rotaio	
	locus		lagged	untaggeu	laggeu	untaggeu	layyeu	untayyeu		
	NEIS00	001		80	19				99	
	NEIS00	04		80	19				99	
	NEIS00	05		80	19				99	
	NEIS00	006		80	19				99	
	NEIS00	107		80	19				99	
	NEIS00	008		80	19				99	
	NEIS00	009		80	19				99	
	NEISOO	)10		80	19				99	
	NEIS00	)11		80	18		1		99	
	NELSOO	112		80	19				99	
	NELS00	113		80	19				99	
	NEISOO	14		80	10				00	
	ME1300			00	13				33	
	NEISOO	15		80	19				99	
	NFIS00	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). Go out   Change password		Toggle: 🚯
Gene Presence - Neisseria PubMLST		
Heatmap	— Change analysis – Pivot Table	Controls Attribute Complete sequences
4		F

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 i 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 c	n the profiles/sequence definition does not represent a population sample.
<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       Miscellar         • Single field       • Export dataset       • Contigs       • Contigs       • Description         • Two field       • Contigs       • Sequences - XMFA / concatenated FASTA formats       • Codon usage       • Description         • Scheme and alleles       • Sequence bin       • Sequence bin       • BLAST       • Description	neous on 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.

19022 M10 240481       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1831       22       9       F33         19026 M10 240482       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       3754       ST-41/44 complex/Lineage 3       7-2       4       F5-1         19028 M10 240485       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1097       ST-41/44 complex/Lineage 3       7-2       4       F5-1         19028 M10 240485       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1049       ST-269 complex       12-1       15-1       F5-1         19028 M10 240489       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       461       ST-461 complex       19-2       13-1       F3-9         19031 M10 240489       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       411       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19032 M10 240490       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       911       ST-213 complex       22       9       F5-12         19032 M10 240490       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       9812 <td< th=""><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th></td<>											
19026 M10 240482       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       3754 ST-41/44 complex/Lineage 3       7-2       4       F5-1         19027 M10 240484       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1097       ST-41/44 complex/Lineage 3       17-1       23       F1-5         19028 M10 240487       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1049       ST-268 complex       122       9       F5-12         19030 M10 240487       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1161       ST-461 complex       19-2       13-1       F3-9         19031 M10 240490       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1161       ST-474 complex/Lineage 3       7-2       4       F1-5         19958 M10 240476       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       418       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19958 M10 240499       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       418       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19958 M10 240500       UK       2010 invasive (unspecified/other) Neisseria meningitidis       <	19025 M10 240481	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	1831		22	9	F3-3	
19027       M10 240484       UK       2010       imvasive (unspecified/other) Neisseria meningitidis       B       1097       ST-41/44 complex/Lineage 3       17-1       2.3       F1-5         19028       M10 240485       UK       2010       imvasive (unspecified/other) Neisseria meningitidis       B       275       ST-269 complex       22       9       F5-12         19028       M10 240489       UK       2010       imvasive (unspecified/other) Neisseria meningitidis       B       1049       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19031       M10 240490       UK       2010       imvasive (unspecified/other) Neisseria meningitidis       B       411       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19031       M10 240490       UK       2010       imvasive (unspecified/other) Neisseria meningitidis       B       911       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19950       M10 240490       UK       2010       imvasive (unspecified/other) Neisseria meningitidis       B       314       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19960       M10 240500       UK       2010       imvasive (unspecified/other) Neisseria meningitidis       B       310       ST-4	19026 M10 240482	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	3754	ST-41/44 complex/Lineage 3	7-2	4	F5-1	
19028       M10 240485       UK       2010       invasive (unspecified/other)       Neisseria meningitidis       B       275       ST-269 complex       12       9       F5-12         19029       M10 240487       UK       2010       invasive (unspecified/other)       Neisseria meningitidis       B       1049       ST-269 complex       19-2       13-1       F5-3         19031       M10 240489       UK       2010       invasive (unspecified/other)       Neisseria meningitidis       B       416       ST-249 complex       22       9       F5-12         19032       M10 240498       UK       2010       invasive (unspecified/other)       Neisseria meningitidis       B       411       ST-4144 complex/Lineage 3       7.2       4       F5-5         19959       M10 240498       UK       2010       invasive (unspecified/other)       Neisseria meningitidis       B       415       ST-4144 complex/Lineage 3       7.2       4       F1-5         19961       M10 240500       UK       2010       invasive (unspecified/other)       Neisseria meningitidis       B       340       ST-4144 complex/Lineage 3       7.2       4       F1-5         19962       M10 240500       UK       2010       invasive (unspecified/other)	19027 M10 240484	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	1097	ST-41/44 complex/Lineage 3	17-1	23	F1-5	
19029 M10 240487       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1049       ST-269 complex       19-1       15-11       F5-12         19030 M10 240489       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       461       ST-461 complex       19-2       13-1       F3-9         19031 M10 240498       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       4161       ST-4144 complex/Lineage 3       7-2       4       F1-5         19958 M10 240498       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       275       ST-269 complex       22       9       F5-12         19958 M10 240499       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       275       ST-269 complex       22       9       F5-12         19960 M10 240500       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       41       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19961 M10 240500       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       411       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19962 M10 240505       UK       2010 invasive (unspecified/other) Neisseria meningitidis       Y	19028 M10 240485	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	275	ST-269 complex	22	9	F5-12	
19030 M10 240499       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       411       ST-461 complex       19-2       13-1       F3-9         19031 M10 240490       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1161       ST-269 complex       22       9       F5-12         19032 M10 240498       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       411       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19956 M10 240499       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       9812       ST-213 complex       22       9       F5-12         19956 M10 240499       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       411       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19960 M10 240500       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       340       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19962 M10 240500       UK       2010 invasive (unspecified/other) Neisseria meningitidis       Y       33       ST-23 complex/Luser A3       5-1       10-10       F4-11         19964 M10 240505       UK       2010 invasive (unspecified/other) Neisseria meningitidis <t< td=""><td>19029 M10 240487</td><td>UK</td><td>2010 invasive (unspecified</td><td>Vother) Neisseria meningitid</td><td>is B</td><td>1049</td><td>ST-269 complex</td><td>19-1</td><td>15-11</td><td>F5-1</td></t<>	19029 M10 240487	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	1049	ST-269 complex	19-1	15-11	F5-1	
19031 M10 240490       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1161       ST-269 complex       22       9       F5-12         19032 M10 240498       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       911       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19958 M10 240476       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       9212       ST-213 complex       22       14       F5-5         19950 M10 240499       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       275       ST-269 complex       22       9       F5-12         19960 M10 240500       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       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       F1-95         19963 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 <td< td=""><td>19030 M10 240489</td><td>UK</td><td>2010 invasive (unspecified</td><td>Vother) Neisseria meningitid</td><td>is B</td><td>461</td><td>ST-461 complex</td><td>19-2</td><td>13-1</td><td>F3-9</td></td<>	19030 M10 240489	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	461	ST-461 complex	19-2	13-1	F3-9	
1902/1012/40498       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       41       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19958       M10 2404076       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       9812       ST-213 complex       22       9       F5-12         19956       M10 240499       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       275       ST-289 complex       22       9       F5-12         19961       M10 240500       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       41       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19961       M10 240500       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       41       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       10-10       F4-1         19964       M10 240505       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       175       5       72       11       F5-12         19966       M10 240504       UK	19031 M10 240490	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	1161	ST-269 complex	22	9	F5-12	
19956 M10 240476       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       9812       ST-213 complex       22       14       F5-5         19959 M10 2404049       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       275       ST-269 complex       22       9       F5-12         19950 M10 240500       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       41       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19961 M10 240502       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       340       ST-41/44 complex/Lineage 3       7-2       4       F1-5         19962 M10 240502       UK       2010 invasive (unspecified/other) Neisseria meningitidis       Y       33       ST-23 complex/Cluster A3       5-1       12-2       F1-96         19962 M10 240505       UK       2010 invasive (unspecified/other) Neisseria meningitidis       Y       183       ST-23 complex/Cluster A3       5-1       10-10       F4-1         19964 M10 240507       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1575       7-2       13-1       F1-7         19966 M10 240511       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       41	19032 M10 240498	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	41	ST-41/44 complex/Lineage 3	7-2	4	F1-5	
1995 M10 240499       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       275       ST-269 complex       22       9       F5-12         19960 M10 240500       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       41       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       23       ST-23 complex/Cluster A3       5-1       2-2       F1-96         19964 M10 240507       UK       2010 invasive (unspecified/other) Neisseria meningitidis       Y       183       ST-23 complex/Cluster A3       5-1       10-10       F4-1         19964 M10 240507       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       4713       T2-2       9       F5-12         19966 M10 240518       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       4713       T2-2       1-1       F1-5         19966 M10 240512       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       411       ST-41/44 complex/Line	19958 M10 240476	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	9812	ST-213 complex	22	14	F5-5	
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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       B       1575       7-2       13-1       F1-7         19966 M10 240511       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       4713       22       9       F5-12         19967 M10 240512       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       41       ST-41/44 complex/Lineage 3       7-1       1       F1-5         19968 M10 240514       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       18       ST-260 complex       5-1       2.2       F1-1         19968 M10 240514       UK       2010 invasive (unspecified/other) Neisseria meningitidis       W       11       ST-1260 complex       5-1       2.2       F5-1         19970 M10 240515       UK       2010 invasive (unspecified/other) Neisseria meningitidis       Y       1655       ST-280 complex       5-1       10-1       F4-1         Analysis tools:       Breakdown:       Fields       Two Field       Codons       Polymorphic sites       Combinations       Schemes/	19963 M10 240505	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is Y	1655	ST-23 complex/Cluster A3	5-1	10-10	F4-1	
19965 M10 240508       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       1575       7-2       13-1       F1-7         19966 M10 240511       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       4713       22       9       F5-12         19966 M10 240511       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       41       ST-41/44 complex/Lineage 3       7-1       1       F1-5         19968 M10 240514       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       41       ST-41/44 complex/Lineage 3       7-1       1       F1-5         19968 M10 240514       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       269       ST-269 complex       5       2       F1-1         19969 M10 240515       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       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 Field Codons Polymorphic sites Combinations Schemes/alleles Publications Sequence bin </td <td>19964 M10 240507</td> <td>UK</td> <td>2010 invasive (unspecified</td> <td>Vother) Neisseria meningitid</td> <td>is Y</td> <td>183</td> <td>ST-23 complex/Cluster A3</td> <td>21</td> <td>16-5</td> <td>deleted</td>	19964 M10 240507	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is Y	183	ST-23 complex/Cluster A3	21	16-5	deleted	
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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       B       269       ST-260 complex       5-1       2-2       F5-1         19970 M10 240515       UK       2010 invasive (unspecified/other) Neisseria meningitidis       Y       1655       ST-23 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 Field       Codons       Polymorphio sites       Combinations       Schemes/alleles       Publications       Sequence bin         Analysis:       Presence/Abance       Genome Comparator       BLAST       Export       Dataset       Contigs       Sequences         Page:       1       3       4       6       7       9       Last	19967 M10 240512	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	41	ST-41/44 complex/Lineage 3	7-1	1	F1-5	
19969 M10 240515       UK       2010 invasive (unspecified/other) Neisseria meningitidis       B       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:	19968 M10 240514	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is W	11	ST-11 complex/ET-37 complex	5	2	F1-1	
19970 M10 240520       UK       2010 invasive (unspecified/other) Neisseria meningilidis       Y       1655       ST-23 complex/Cluster A3       5-1       10-1       F4-1         Analysis tools:       Breakdown:       Fields       Two Field       Codons       Polymorphic sites       Combinations       Schemes/alleles       Publications       Sequence bin         Analysis:       Presence/Absence       Genome Comparator       BLAST       Export:       Dataset       Contigs       Sequences         Page:       1       2       3       4       6       7       8       >       Last	19969 M10 240515	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is B	269	ST-269 complex	5-1	2-2	F5-1	
Analysis tools: Breakdown: Fields Two Field Codons Polymorphicistes Combinations Schemes/alleles Publications Sequence bin Analysis: Presence/Abence Genome Comparator BLAST Export Dataset Contigs Sequences Page: 1 2 3 4 5 6 7 8 9 > Last	19970 M10 240520	UK	2010 invasive (unspecified	Vother) Neisseria meningitid	is Y	1655	ST-23 complex/Cluster A3	5-1	10-1	F4-1	
Page: 1 2 3 4 5 6 7 8 9 > Last	Analysis tools: Breakdown: Fields Two Field Codons Polymorphic sites Combinations Schemes/alleles Publications Sequence bin Analysis: Presence/Absence Genome Comparator BLAST Export: Dataset Contigs Sequences										
	Page: 123456789 > Last										

# 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.

PubMLST Databas					
Logged in: Keith Jolley (ke	eith). @Log out   Change password			Help 🖸 Toggle: (	
Genome Con	nparator - Neisseria Pub	MLST			
Please select the required the appropriate schem	ired isolate ids and loci for comparison - usi e description. Alternatively, you can enter the User genomes Optionally include data not in the database. Upload FASTA file (or zip file containing multiple FASTA files - one per genome); Browse No file selected.	e CTRL or SHIFT to make multiple selections accession number for an annotated reference Loci 165_rRNA (SSU_rRNA) _235_RNA abc2 4bc2 (HEIS1015) accf (HEIS1027) acA2 (NEIS1272) acAA (NEIS1727) acAA (NEIS1729)	in list boxes. In addition to selecting individu e genome and compare using the loci define Include in identifiers country region year epidemiological year age yth sex desase	al loci, you can choose to include all loci defined in schemes by selected in that.	ing
		All None Paste list	source		
- Reference genom	e Parameters / optic	Distance matrix calculation	.n Alignments	Core genome analysis	
or choose annotated	igenome: Min % identi genome: BLASTN word siz	t. 50 v 0 Complete loc: Completely exclude fro Treat as distinct allele	m analysis // Include ref sequences in Align all loci (not only vari	alignment Calculate mean distances ()	
or upload Genbank/E Browse No file	EMBL/FASTA file: selected.	Exclude paralogous loc	panson Aligner: MAFFT 👻		
Filter by					
Sequence method	d: 🗾 🗸 🚺	Reset Submit			
Experimen	tt 🔹 🕖	U			

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.

ProfileIST Query: Search   Browse   ProfileIST   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.

Profile/ST Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions									
Job Status viewer									
Job id:         BIGSdb_27748_1405410063_94241           Submit time:         2014-07-15 08:41:03           Status:         finished           Status:         finished           Status:         finished           Stop time:         2014-07-15 08:41:05           Stop time:         2014-07-15 08:41:22           Total time:         17 seconds									
Analysis against defined loci									
Allele numbers are used where these have been defined, otherwise sequences will be marked as 'New#1. 'New#2' etc. Missing alleles are marked as 'X'. Truncated alleles (located at end of contig) are marked as 'T									
Locus  644 (L93/4286)  662 (2837)  663 (2839)  664 (2838)  665 (2845)  666 (2843)  667 (2842)  669 (2846)  670 (2840)  671 (2844)  672 (2847)  698 (FAM18)   abcZ 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2									
aroE 4 19 4 4 4 4 4 4 19 19 19 4 two 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2									
Mile         S         S         S         Z4         Z3         Z3         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S         S </td <td></td>									
Loci with sequence differences among isolates:									
Variable loci: 4									
Locus         644 (L93/4286)         662 (2837)         663 (2839)         664 (2838)         665 (2845)         666 (2843)         667 (2842)         670 (2840)         671 (2844)         672 (2847)         698 (FAM18)           abc2         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									
Exactly matching loci									
These loci are identical in all isolates.									
Matches: 3									
Locus         644 (L93/4286)         662 (2837)         663 (2839)         664 (2838)         665 (2845)         666 (2843)         667 (2842)         670 (2840)         671 (2844)         672 (2847)         698 (FAM18)           adk         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									
Unique strains									
Unique strains: 5									
Strain 1         Strain 3         Strain 4         Strain 5           644 (L93)4286)         662 (2837)         666 (2843)         665 (2845)         669 (2846)           653 (2839)         671 (2840)         667 (2842)         669 (5845)         669 (5847)           698 (FAM18)         672 (2847)         672 (2847)         672 (2847)         672 (2847)									
Text output file     Excel format     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_PNG format)									
(click to enlarge)  • Splits graph (Neighbour-net, SVG format) - This can be edited in Inkscape or other vector graphics editors  • Locus presence frequency:									
Locus presence frequency chart (PNG format)									
(dick to enlarge)									
Tar file containing output files									
Please note that job results will remain on 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 Databa	ase home Contents												
Logged in: Keith Jolley (	(keith). @Log out   Change password		Help 🗹	Toggle: 🚯									
Genome Co	mparator - Neisseria Pub	MLST											
Please select the rec the appropriate sche	Please select the required isolate ids and loci for comparison - use CTRL or SHIFT to make multiple selections in list boxes. In addition to selecting individual loci, you can choose to include all loci defined in schemes by selecting the appropriate scheme description. Alternatively, you can enter the accession number for an annotated reference genome and compare using the loci defined in that.												
Isolates		Include in identifiers											
662 663 664 665	Optionally include data not in the database. Upload FASTA file (or zp file containing multiple FASTA files - one per genome): • Browse No file selected.	Isolate <ul> <li>Country</li> <li>region</li> <li>region</li> <li>gear</li> <li>epidemiological year</li> <li>age mth</li> <li>sex</li> <li>disease</li> <li>source</li> <li> </li> </ul>											
Reference geno	me Parameters / option	is — — — Distance matrix calculation — — Alignments — — Core genome analysis — —											
Enter accession nu	umber: Min % identity	70 • 6 With incomplete loci: Produce alignments 6 Core threshold (%): 90 • 6											
or choose annotate FAM18 (Nm) or upload Genbank Browse No fi	ed genome: Min % alignmen BLASTN word size REMBL/FASTA file: ile selected.	50 • 0       O make erg sectore non analysis         20 • 0       Incude ref sequences in alignment         20 • 0       Incude ref sequences in alignment         Align all loci (not only variable)         Aligner:       MAFFT •											
Filter by Sequence meth Proj	10d: • • •	Action Reset Submit											
Experime	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.

Profit ALST Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions																
Job status viewer																
Status	Status															
Job id: Submit time: Status: Start time: Progress: Stop time: Total time: Output Analysis by t accession version type length	Image: Status         BiGSd5_21911_1405410488_8452           Submit time:         2014-07-15 08:48:38           Status:         finished           Stop time:         2014-07-15 08:48:34           Total time:         2014-07-15 08:12:58           Total time:         214-07-15 08:12:58           Output         Analysis by reference genome           accession         AM421808           version         1           type         dna															
description coding region	Neisseria meningitidis serogroup C FAM18 complete genome.															
All Iooi																
All IOCI																
Each unique a	lleie is defined a number starting at 1. Missing alleies are marked as 'X	. Truncated	alleles (loc	ated at end o	f contig) are	marked	as 'l'.									
Locus	Product	Sequence	Genome	Reference	644	662	663 (2930)	664 (2939)	665	666	667	669	670 (2940)	671	672	698 (EAM19)
IpxC   envA   NMC0001	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924	1261	1	1	1	1	1	1	1	1	1	1	1	1	1
piIS1   NMC0002	pilin (fragment)	291	3341	1	1	1	1	1	1	1	1	1	1	1	1	1
pilS2   NMC0003	truncated pilin	366	3675		2	2	2	2	2		2	2		2		1
fbp   NMC0004	peptidyl-prolyl cis-trans isomerase	330	4069		2	2	2	2	2	2	2	Т	2	2	2	1
NMC0005	putative membrane protein	219	4476		2	3	3	3	3		3	4		5		1
NMC0006	putative glycerate dehydrogenase	954	4816		2	2	2	2	2		2	2		2		1
metG   NMC0007	methionyl-tRNA synthetase	2058	5843	1	2	2	3	3	2	2	2	2	2	2	2	1
gImS	glucosaminefructose-6-phosphate aminotransferase [isomerizing]	1839	8016	1	2	2	2	2	2	2	2	2	2	2	2	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	Ŧ

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.

Alianmente									
Aiginnenia									
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 the pr 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 no	ofiles/sequence definition t represent a population sample.									
Query database       Option settings       Image: Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of Comparison of C	Submissions • Manage submissions General information • Isolates: 34221 • Last updated: 2015-07-02 • Update history • About BIGSdb									
Breakdown       Export       Analysis       Miscellaneous         • Single field       • Export dataset       • Codon usage       • Codon usage       • Description of dataset         • Two field       • Unique combinations       • Sequences - XMFA / concatenated FASTA formats       • Codon usage       • Description of dataset         • Publications       • Sequence bin       • Sequences - XMFA / concatenated FASTA formats       • Description of dataset       • Description of dataset	atabase 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 (unsp	ecified/other)	Neisseria m	eningitidis	в	1831		22	9	F3-3
	19026 M10 240482		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	3754	ST-41/44 complex/Lineage 3	7-2	4	F5-1
	19027 M10 240484		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	В	1097	ST-41/44 complex/Lineage 3	17-1	23	F1-5
	19028 M10 240485		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	275	ST-269 complex	22	9	F5-12
	19029 M10 240487		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	1049	ST-269 complex	19-1	15-11	F5-1
	19030 M10 240489		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	461	ST-461 complex	19-2	13-1	F3-9
	19031 M10 240490		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	1161	ST-269 complex	22	9	F5-12
	19032 M10 240498		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	41	ST-41/44 complex/Lineage 3	7-2	4	F1-5
	19958 M10 240476		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	9812	ST-213 complex	22	14	F5-5
	19959 M10 240499		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	275	ST-269 complex	22	9	F5-12
	19960 M10 240500		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	41	ST-41/44 complex/Lineage 3	7-2	4	F1-5
	19961 M10 240502		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	340	ST-41/44 complex/Lineage 3	7-2	4	F1-5
	19962 M10 240503		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	Y	23	ST-23 complex/Cluster A3	5-1	2-2	F1-96
	19963 M10 240505		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	Y	1655	ST-23 complex/Cluster A3	5-1	10-10	F4-1
	19964 M10 240507		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	Y	183	ST-23 complex/Cluster A3	21	16-5	deleted
	19965 M10 240508		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	1575		7-2	13-1	F1-7
	19966 M10 240511		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	4713		22	9	F5-12
	19967 M10 240512		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	41	ST-41/44 complex/Lineage 3	7-1	1	F1-5
	19968 M10 240514		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	W	11	ST-11 complex/ET-37 complex	5	2	F1-1
	19969 M10 240515		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	в	269	ST-269 complex	5-1	2-2	F5-1
	19970 M10 240520		UK	2010 invasive (unsp	ecified/other)	Neisseria m	eningitidis	Y	1655	ST-23 complex/Cluster A3	5-1	10-1	F4-1
Analysis tools: Breakdown: Fields Two Field Codons Polymorphic sites Combinations Schemes/alleles Publications Sequence bin Analysis: Presence/Abence Genome Comparator BLAST Export: Dataset Contigs Sequences													
P	age: 1 2 3	4 5	6	7 8 9 > L	ast								

# 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.

PubMLST Databas					
Logged in: Keith Jolley (ke	eith). @Log out   Change password			Help 🖸 Toggle: (	
Genome Con	nparator - Neisseria Pub	MLST			
Please select the required the appropriate schem	ired isolate ids and loci for comparison - usi e description. Alternatively, you can enter the User genomes Optionally include data not in the database. Upload FASTA file (or zip file containing multiple FASTA files - one per genome); Browse No file selected.	e CTRL or SHIFT to make multiple selections accession number for an annotated reference Loci 165_rRNA (SSU_rRNA) _235_RNA abc2 4bc2 (HEIS1015) accf (HEIS1027) acA2 (NEIS1272) acAA (NEIS1727) acAA (NEIS1729)	in list boxes. In addition to selecting individu e genome and compare using the loci define Include in identifiers country region year epidemiological year age yth sex desease	al loci, you can choose to include all loci defined in schemes by selected in that.	ing
		All None Paste list	source		
- Reference genom	e Parameters / optic	Distance matrix calculation	.n Alignments	Core genome analysis	
or choose annotated	igenome: Min % identi genome: BLASTN word siz	t. 50 v 0 Complete loc: Completely exclude fro Treat as distinct allele	m analysis // Include ref sequences in Align all loci (not only vari	alignment Calculate mean distances ()	
or upload Genbank/E Browse No file	EMBL/FASTA file: selected.	Exclude paralogous loc	panson Aligner: MAFFT 👻		
Filter by					
Sequence method	d: 🗾 🗸 🚺	Reset Submit			
Experimen	tt 🔹 🕖	U			

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.

ProfileIST Query: Search   Browse   ProfileIST   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.

PTIMIST Guery, Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions
Job status viewer
Status           Job id:         BIGSdb_27748_1405410063_94241           Submit time:         2014-07-15 08:41:03           Status:         finished           Statu:         2014-07-15 08:41:05
Progress: 100% Stop time: 2014-07-15 08:41:22 Total time: 17 seconds Output
Analysis against defined loci
Allele numbers are used where these have been defined, otherwise sequences will be marked as 'New#1, 'New#2' etc. Missing alleles are marked as 'X'. Truncated alleles (located at end of contig) are marked as 'T'.
Locus 644 (L93/4286) 662 (2837) 663 (2839) 664 (2838) 665 (2845) 666 (2843) 667 (2842) 669 (2846) 670 (2840) 671 (2844) 672 (2847) 698 (FAM18)
abc2     2     2     2     2     2     2     2     2       adk     3     3     3     3     3     3     3     3     3
aroE 4 19 4 4 4 4 4 19 19 19 4 fumC 3 3 3 3 24 23 23 3 3 3 3 3 3
gdh 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
pgm 6 6 6 6 6 6 6 6 6 6 6 6
Loci with sequence differences among isolates:
Variable loci: 4
Locus  644 (L93/4286) 662 (2837) 663 (2839) 664 (2838) 665 (2845) 666 (2843) 667 (2842) 669 (2846) 670 (2840) 671 (2844) 672 (2847) 698 (FAM18)
abo2 2 2 2 2 2 2 2 2 2 7 2 2 2 2 2 2 2 2 2
func         3         3         3         24         23         23         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 </td
Exactly matching loci
Inese loci are identical in all isolates.
adk 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
gan 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
Unique strains
Unique strains: 5
Strain 1         Strain 3         Strain 4         Strain 5           644 (L934/286) 665 (2843) 665 (2843) 665 (2845) 669 (2846)         663 (2839)         670 (2840) 665 (2842)           664 (2838)         671 (2844)         671 (2844)         671 (2844)
698 (FAM18) 672 (2847)
Text output the     Excel format     Excel format     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, PNG format)
(click to enlarge)
Splits graph (Neighbour-net; SVG format) - This can be edited in Inkscape or other vector graphics editors     Locus presence frequency     Locus presence frequency chart (PNG format)
Tar file containing output files
Places and that is the could will comple as the second for 7 days
Frease note unacjou results with remain on 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 Database	e home Contents				
Logged in: Keith Jolley (keith	h). @Log out   Change password		Help 🗗	Toggle: 🜖	Ξ
Genome Com	parator - Neisseria Pub	MLST			
Please select the require	ed isolate ids and loci for comparison - use	CTRL or SHIFT to make multiple selections in list boxes. In addition to selecting individual loci, you can choose to include all loci defini	ed in scheme	s by selectin	ig
the appropriate scheme	description. Alternatively, you can enter the a	accession number for an annotated reference genome and compare using the loci defined in that.			
Isolates	User genomes	Include in identifiers			
662 663	Optionally include data not in the database.	country			
664 665	Upload FASTA file (or zip file containing multiple	region year epidemiological year			
	FASTA files - one per genome): 1	age yr age mth			
	biomac No me selected.	disease Source •			
	Parameters / optior	is Distance matrix calculation Alignments Core genome analysis			
Enter accession numb	per: Min % identity	: 70 🗸 🜒 With incomplete loci: Produce alignments 🛈 Core threshold (%): 90 💌 6			
or choose apportated o	Min % alignment	50 V O Completely exclude from analysis Include ref sequences in alignment Calculate mean distances (	•		
FAM18 (Nm) -	BLASTN word size	20 - 0 Index as usually and a set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set of the set			
or upload Genbank/EM	BL/FASTA file:	Exclude paralogous loci			
Browse No file se	elected. ()				
Filter by		Action			
Sequence method:	- O	Reset			
Project:	-				
Experiment:	• 0				

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.

Public         Ouer: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profile/Sequences definitions   Database submissions																
Job state	is viewer															
Status																
Job id: Submit time: Status: Start time: Progress: Stop time: Total time: Output Analysis by t accession version type length	BIGSdb_21911_1405410488_8452 2014-07-15 08:48:08 finished 2014-07-15 08:48:34 form 2014-07-15 09:12:58 24 minutes and 24 seconds <b>eference genome</b> AM421808 1 1 1 2194961															
description coding region	Neisseria meningitidis serogroup C FAM18 complete genome.															
All Iooi																
All IOCI																
Each unique a	lleie is defined a number starting at 1. Missing alleies are marked as 'X	. Truncated	alleles (loc	ated at end o	f contig) are	marked	as 'l'.									
Locus	Product	Sequence	Genome	Reference	644	662	663 (2930)	664 (2939)	665	666	667	669	670 (2940)	671	672	698 (EAM19)
IpxC   envA   NMC0001	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924	1261	1	1	1	1	1	1	1	1	1	1	1	1	1
piIS1   NMC0002	pilin (fragment)	291	3341	1	1	1	1	1	1	1	1	1	1	1	1	1
pilS2   NMC0003	truncated pilin	366	3675		2	2	2	2	2		2	2		2		1
fbp   NMC0004	peptidyl-prolyl cis-trans isomerase	330	4069		2	2	2	2	2	2	2	Т	2	2	2	1
NMC0005	putative membrane protein	219	4476		2	3	3	3	3		3	4		5		1
NMC0006	putative glycerate dehydrogenase	954	4816		2	2	2	2	2		2	2		2		1
metG   NMC0007	methionyl-tRNA synthetase	2058	5843	1	2	2	3	3	2	2	2	2	2	2	2	1
gImS	glucosaminefructose-6-phosphate aminotransferase [isomerizing]	1839	8016	1	2	2	2	2	2	2	2	2	2	2	2	1

# 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.

— Include in identifiers –	
isolate	
country	
region	-
year	
epidemiological year	
age yr	
age mth	
sex	
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.

- Alianments
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:	▼ i	
Project:		<b>√</b> [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.

PubMLST Database home Contents	
Neisseria PubMLST database	Ξ
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 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 sate	profiles/sequence definition database there is at least one mple.
Query database       Search or browse database       • Main public projects       • Set general options - including isolate table field handling.         • Search by combinations of loci (profiles)       • Your projects       • Set display and query options for locus, schemes or scheme fields.	Submissions • Manage submissions • Ceneral information • Isolates: 44,865 • Lastupdated: 2018-02-20 • Defined field values • Update history • About BICSdb
Breakdown       Export       Analysis       Third party is         • Single field       • Export dataset       • Contigs       • Contigs       • Contigs         • Unique combinations       • Sequences - XMFA / concatenated FASTA formats       • Contigs       • Contigs       • Third party is         • Publications       • Sequences - XMFA / concatenated FASTA formats       • Contigs       • Contigs       • Contigs       • Third party is         • Description of database fields       • Description of database fields	tools isualization of genomic relationships netic trees with data overlays alization and phylogenetic inference pen data visualization and sharing for genomic

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.

024 M10 240480 025 M10 240481					
025 M10 240481	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2267206	267 1194 ST-41/44 com	nplex 7-2	4 F1-5
	UK 2010 invasive (unspecified/other) Neisseria meningituis	B 2194837	274 1831	22	9 E3-3
026 M10 240482	LIK 2010 invasive (unspecified/other) Neisseria meningituis	B 2184823	263 3754 ST-41/44 com	nlex 7-2	4 F5-1
027 M10 240484	UK 2010 invasive (unspecified/other) Neisseria meningituis	B 2168050	253 1097 ST-41/44 com	nplex 17-1	23 E1-5
028 M10 240485	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2193457	294 275 ST-269 com	nlex 22	9 E5-12
029 M10 240487	LIK 2010 invasive (unspecified/other) Neisseria meningituis	B 2188678	241 1049 ST-269 com	nlex 19-1	15-11 E5-1
030 M10 240489	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2218969	275 461 ST-461 com	plex 19-2	13-1 F3-9
031 M10 240490	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2175692	293 1161 ST-269 com	plex 22	9 F5-12
032 M10 240498	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2154070	235 41 ST-41/44 com	nplex 7-2	4 F1-5
958 M10 240476	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2242902	284 9812 ST-213 com	plex 22	14 F5-5
959 M10 240499	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2189734	198 275 ST-269 com	plex 22	9 F5-12
960 M10 240500	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2197545	223 41 ST-41/44 com	nplex 7-2	4 F1-5
961 M10 240502	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2173298	188 340 ST-41/44 com	nplex 7-2	4 F1-5
962 M10 240503	UK 2010 invasive (unspecified/other) Neisseria meningitidis	Y 2101043	197 23 ST-23 comp	olex 5-1	2-2 F1-96
963 M10 240505	UK 2010 invasive (unspecified/other) Neisseria meningitidis	Y 2090713	189 1655 ST-23 comp	lex 5-1	10-10 F4-1
964 M10 240507	UK 2010 invasive (unspecified/other) Neisseria meningitidis	Y 2108738	170 183 ST-23 comp	olex 21	16-5 deleted
965 M10 240508	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2233910	196 1575	7-2	13-1 F1-7
966 M10 240511	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2174583	219 4713	22	9 F5-12
967 M10 240512	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2203751	205 41 ST-41/44 com	nplex 7-1	1 F1-5
968 M10 240514	UK 2010 invasive (unspecified/other) Neisseria meningitidis	W 2110464	160 11 ST-11 comp	olex 5	2 F1-1
969 M10 240515	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2181841	205 269 ST-269 com	plex 5-1	2-2 F5-1
970 M10 240520	UK 2010 invasive (unspecified/other) Neisseria meningitidis	Y 2095486	190 1655 ST-23 comp	lex 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.

ogged in: Keith Jolley (keit	th). I Log out   Change password			loggle: 😈 🗧
GrapeTree: Vi	isualization of genomi	c relationships - Neisseria PubMLST		
	This pl	lugin generates a minimum-spanning tree and visualizes within GrapeTi	ree:	
	Grap	eTree: Visualization of core genomic relationships		
	Grape	Tree is developed by:		
2		Zhemin Zhou (1) Nabil-Fareed Alikhan (1) Martin J. Sergeant (1) Nina Luhmann (1) Cáta Vaz (2,5) Alexandre P. Francisco (2,4) João André Carrigo (3) Marté Achtmog (1)		
	1 2 3 3 4 5 Publici	Warwick Medical School, University of Warwick, UK Instituto de Engenharia de Sistemas e Computadores: Investigação e I Universidade de Lisboa, Faculdade de Medicina, Instituto de Microbiolo Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal ADEETC, Instituto Superior de Engenharia de Lisboa, Instituto Politécni ation: Zhou at al. (2017) GrapeTree: Visualization of core genomic relatio	Desenvolvimento (INESC-ID), Lisboa, Portugal gia and Instituto de Medicina Molecular, Lisboa, Portugal ico de Lisboa, Lisboa, Portugal Inships among 100,000 bacterial pathogens. bioRxiv 216788	
This tool will generate n Analysis is limited to 50	ninimum spanning trees trees from alleli 0,000 records.	c profiles. Please check the loci that you would like to include. Alternative	ily select one or more schemes to include all loci that are mer	nbers of the scheme.
Isolates	- Loci		<ul> <li>Include fields</li> <li>Select additional fields to include in CraneTree metadata</li> </ul>	-Action
18968  18969 19023 19024 19025 19026 19027	165_TWA (SSU_RNA) _235_RNA abcZ abcZ (NEIS1015) aceF (NEIS1279) ackA2 (NEIS1727)	Antigen genes     Bell ST (20 locus partial genes)     Bell ST (20 locus whole genes)     Bell ST (20 locus whole genes)     Dentified and 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 second s	country  Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrient Contrie	Submit

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). (Honge password
Job status viewer
Status           Job id:         BIGSdb_141866_1519311802_19416           Submit time:         2018-02-22 15:03:22           Status:         fnished           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)     Metadata (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.

	A4/IVI1027	BT, NIBSC_2803, 21001	USA	1937	invasive (unspecilied/other)	Neissena meningluois	А	4	S1-4 complex	0-2	10	F1-0
2	120M	B35; NIBSC_2822; Z1035	Pakistan 1	1967	meningitis and septicaemia	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
7	7891	B54; NIBSC_2760; Z1054	Finland 1	1975	invasive (unspecified/other)	Neisseria meningitidis	А	5	ST-5 complex	20	9	F3-1
10	6748	B73; NIBSC_2784; Z1073	Canada 1	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	18-1	3	F5-1
11	129E	B92; NIBSC_2828; Z1092	Germany 1	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F3-6
13	139M	B99; NIBSC_2795; Z1099	Philippines 1	1968		Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
19	S3131	B213; NIBSC_2813; Z1213	Ghana 1	1973	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13-1	F1-5
24	S4355	B227; NIBSC_2806; Z1227	Denmark 1	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	5-1	9	F3-1
30	14	alpha14; BennettTree10	Germany 1	1999	carrier	Neisseria meningitidis	cnl	53	ST-53 complex	7	30-3	F5-5
31	10	B269; NIBSC_2825; Z1269	Burkina Faso 1	1963	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13-1	F1-5
34	20	B275; NIBSC_2767; Z1275	Niger 1	1963	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F1-7
35	26	B278; NIBSC_2764; Z1278	Niger 1	1963	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13	F1-5
52	243	B362; NIBSC_2779; Z1362	Cameroon 1	1966		Neisseria meningitidis	Α	4	ST-4 complex	7	13	F1-5
61	393	B392; NIBSC_2823; Z1392	Greece 1	1968	carrier	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
64	254	B439; NIBSC_2812; Z1439	Djibouti 1	1966	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F1-7
67	S5611	B466; NIBSC_2765; Z1466	Australia 1	1977	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
82	11-004	B503; NIBSC_2826; Z1503	China 1	1984	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	20	9	F3-8
84	IAL2229	B506; NIBSC_2816; Z1506	Brazil 1	1976		Neisseria meningitidis	Α	5	ST-5 complex	20	9	F2-1
90	CN100	B534; NIBSC_2768; Z1534	UK 1	1941	invasive (unspecified/other)	Neisseria meningitidis	Α	21		5-2	10	F3-9
An	alysis too	ols:										
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-	1 mild pai	ing. Graperice HOL FI	ingiovaz inicio	redet								

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	home Contents			
+D Log in				Toggle: 🚺
In silico PCR				
Use this tool to simulate I ipcress program written b Please select the require	PCR reactions run using genomes by Guy Slater. ed isolate ids to run the PCR react	s stored in the database. This is us ion against. These isolate records	seful for designing and testing primer must include genome sequences.	s. The plugin is a wrapper for the exonerate
Isolates	Primer 1	Primer 2 GAGAACGAGCCGGGATAGGA	Reported products Min length: 0 🔅 Max length: 10000 🔄 Export sequences	ActionSubmit

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.

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.

PubMLST Database home					
+) Log in					Ξ
Neisseria PubMLS	ST database				
The Neisseria PubMLST datab is at least one corresponding i	base contains data for a c solate deposited here. Ar	ollection of isolates that represe ny isolate may be submitted to th	ent the total known diversity of Neisse is database and consequently it sho	ria species. For every allelic profile uld be noted that it does not repres	in the profiles/sequence definition database there ent a population sample.
Q Query database	E	Projects	Option settings		
<ul> <li>Search or browse data</li> <li>Search by combination</li> </ul>	base is of loci (profiles)	<ul><li>Main public projects</li><li>Your projects</li></ul>	<ul> <li>Set general options - including iso</li> <li>Set display and query options for</li> </ul>	plate table field handling. locus, schemes or scheme fields.	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
	5		1.0	-1	
Breakdown	Export		Analysis	Third party tools	
Single field	<ul> <li>Export dataset</li> </ul>		Codon usage	<ul> <li>GrapeTree - Visualization</li> </ul>	of genomic relationships
Two field	<ul> <li>Contigs</li> </ul>		<ul> <li>Gene presence</li> </ul>	iTOL Phylogenetic trees	with data overlays
<ul> <li>Unique combinations</li> </ul>	<ul> <li>Sequences - XM</li> </ul>	IFA / concatenated FASTA forma	ets • Genome comparator	<ul> <li>PhyloViz - Visualization at</li> </ul>	nd phylogenetic inference
<ul> <li>Publications</li> </ul>			BLAST	<ul> <li>Microreact - Open data vi</li> </ul>	isualization and sharing for genomic
<ul> <li>Sequence bin</li> </ul>			<ul> <li>Species identification</li> </ul>	epidemiology	
	Miscellaneou	S	<ul> <li>In silico PCR</li> </ul>		
	Description of d	atabase fields			

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.

2 120M 1 3 M00242905 4 M1027 8 5 M00240227	B35: NIBSC 2822: Z1035		1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex	5-2	10	F1-5
3 M00242905 4 M1027 8 5 M00240227		Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	Α	1	ST-1 complex	5-2	10	F5-1
4 M1027 H		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1099		19	15	
5 M00240227	B43; NIBSC_3076; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex			
		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 I	B73; NIBSC_2784; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	18-1	3	F5-1
11 129E I	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 I	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 E	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 B	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 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 hor							
Logged in: Keith Jolley (keith). 🔂	og out   Change password					Toggle: ()	Ξ
iTOL - Interactive	e Tree of Life - Neisse	eria PubMLST					
PubMLST Database ho Loged in Kaith Jolity (keith). (e TTOL - Interactiv TOL - Interactiv This tool will generate neig Please check the loci that y Analysis is limited to 2,000 Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Iso	This plugin uploads data for analy Interactive tree of life (iTOL) ITOL is developed by: • NKa Letunic (1) • Peer Bork (2,3,4) 1. Biobyte solutions GmbH, Bo 2. European Molecular Biolog 3. Max Delbrück Centre for Mo 4. Department of Bioinformatic Web site: https://tol.embl.de/ Publication. Letunic & Bork (2016) and annotation of phylogenetic an	sis within the interactive Tree of Life onl : an online tool for the display a thestr 142, 69126 Heidelberg, Germany / Laboratory, Meyerhofstrasse 1, 60117 iecular Medicine, 13125 Berlin, German s, Biocenter, University of Würzburg, 97 Interactive tree of life (ITOL) v3: an onl d other trees. <i>Nucleic Acids Res</i> <b>44(W1</b>	ne service: nd annotation of Heidelberg, German y 774 Würzburg, Germ ne tool for the displa ;W242-5.	ohylogenetic and other tre , any	es		
This tool will generate neight Please check the loci that yo Analysis is limited to 2 000 re	bor-joining trees from concatenated no would like to include. Alternatively s	ucleotide sequences. Only DNA loci that elect one or more schemes to include a	have a correspondi I loci that are membe	g database containing allele sec rs of the scheme.	quence identifiers, or DNA and peptide loci with genome s	equences, can be include	:d.
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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	
poged in: Keith Jolley (keith). Gelog out   Change password	Ξ
ob status viewer	
Status	
Job Id: BIGSdb 190460 1562236303 79711	
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lasse adde that lob zonills will zomals as the source for 7 days	
rease note that you results with remain on the server rol / Udys.	

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.

Query: S Downloa Links: C	sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse ad: Alleles   MLST profiles contents   Home   PorA   FetA   Options   Isolate Database	Query
		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'.

Query: Downl Links:	: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query Ioad: Alleles   MLST profiles : Contents   Home   PorA   FetA   Options   Isolate Database	
		Help 🖉
Locus Explorer	<ul> <li>Neisseria locus/sequence definitions</li> </ul>	
Please select locus for ana	alysis:	
Locus: adk	<ul> <li>Page will reload when changed</li> </ul>	
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	>50 - 60	>6	0 - 1	70	>70	- 80  >8	0 - 90	>9
30		40			5	0		50	
GCGG <mark>C</mark> T	TGG	TGCGCG	ACG	ACA	TCA	TTA	TCGGCA	rggt <mark>c</mark> a	AA(
TAATC	С	ATCT	Т	Т	Т	С	TAAT T	CG	G
AC A	А	ΤG				Α	C	Т	
G	Т	A				G		A	

Publ	Query Down Links:	: Sequences   Batch Ioad: Alleles   MLST : Contents   Home	i sequences   Com profiles PorA   FetA   Optior	npare alleles   Profile/ST   Batch profiles   List   Browse   Query Is   Isolate Database
				Help 🖉
Site L	Explorer			
adk po	osition 51			
EQ1 alla	las issluded is see	-lusis		
501 alle	eles included in ana	alysis.		
Base	Number of alleles	Percentage of allel	es MLST profiles	
Т	401	80.04	11130 / 11407 (97.57%)	
С	98	19.56	275 / 11407 (2.41%)	
A	1 (adk-351)	0.20	1 / 11407 (0.01%)	
G	1 (adk-413)	0.20	1 / 11407 (0.01%)	

The second part of the page shows a table listing nucleotide frequencies at each of the variable positions.

A	C TT/	AA TTT	GCCC	C AG	C	A T	GT T	<u> </u>	G	CGGTG T	CCTG	C	TT	CTAT	C	GTTG	TAG/	GG	T	0	CA	GC	A	A	0 7	C	
c	G		00			•								00 0	•				1		•	A			G		
401		410		42	0	4	30	44	10	45	50	4	60									Ξ.					
TT	TACAO	ICAA/	CTGC	AAGG	CGA	ACACGO	GCC <mark>T</mark> A	AATACA	TCAA	AGT <mark>T</mark> GA	ACGGCA	C <mark>T</mark> CA	GCC	GTA													
AC	GTC/	<b>TCG</b>	TACA	CCAA	TAG	GTCTCT	'AT GC	GCGCTC	CT	GAA <mark>C</mark> CO	<b>TAAT</b>	T <mark>C</mark> TG	AGT/	A <mark>A G</mark>													
C	G	GC	CACA	GGC	ATC	CAG	C CG	A	G	ΤG	A	GC	TTA(	сс т													
			GT			G	A			A	G	A	G	гс													
lucieotic	ie me	eque	encie	:5																							
opition A					I	lucleot	ide																				
	A 🗢	C 🗢	G ≑	T 🜩	- 🜲	%A ≑	%C ≑	%G ≑	%T ≑	%- ≑																	
2	499	1	1	0	0	99.60	0.20	0.20																			
3	498	0	2	1	0	99.40		0.40	0.20																		
4	1	0	500	0	0	0.20		99.80																			
5	0	500	1	0	0		99.80	0.20																			
6	53	8	440	0	0	10.58	1.60	87.82																			
9	499	0	2	0	0	99.60		0.40																			
12	500	0	1	0	0	99.80		0.20																			
13	500	0	1	0	0	99.80		0.20																			
14	1	0	0	500	0	0.20			99.80	D																	
15	0	488	1	12	0		97.41	0.20	2.40																		
18	0	86	8	407	0		17.17	1.60	81.24	4																	
21	0	315	1	185	0		62.87	0.20	36.93	3																	
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	0.60	97.41		2.00																		
28	2	2	497	0	0	0.40	0.40	99.20																			
29	2	0	499	0	0	0.40		99.60																			
30	3	367	2	129	0	0.60	73.25	0.40	25.75	5																	
31	0	11	0	490	0		2.20		97.80	D																	
33	2	5	492	2	0	0.40	1.00	98.20	0.40																		
36	53	0	445	3	0	10.58		88.82	0.60																		
37	0	499	0	2	0		99.60		0.40																		
38	0	1	500	0	0		0.20	99.80																			
20		40.4	0	4	0	0.00	00.00	0.40	0.00																		

#### 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.

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											
Codon	Usage	<u>)</u>									
adk											
ORF used: 1	ORF used: 1										
464 alleles included in analysis.											
GC conten	GC content										
Coding: GC 52.47% 1st letter: GC 65.31% 2nd letter: GC 31.73% 3rd letter: GC 60.37%											
Codons											
Fraction: Pro Frequency: U Codon ¢ A	portion of u Usage of giv mino acid (	sage of a giver ven codon per Fraction ¢	n codon amon 1000 codons. Frequency ¢	g its redunda Number ¢	ant set (i.e. the set of codons which code for this codon's amino acid).						
GCA	Α	0.262	17.353	1248							
GCC	A	0.246	16.254	1169							
GCG	A	0.389	25.751	1852							
GCT	A	0.103	6.813	490							
TGC	С	0.987	6.452	464							
TGT	С	0.013	0.083	6							
GAC	D	0.747	91.073	6550							
GAT	D	0.253	30.812	2216							
GAA	E	0.916	82.397	5926							
GAG	E	0.084	7.564	544							
TTC	F	0.594	15.295	1100							
111	F	0.406	10.470	753							
GGA	G	0.007	0.542	39							
GGC	G	0.765	59.497	4279							
GGG	G	0.001	0.042	3							
GGT	G	0.227	17.659	1270							
CAC	н	0.749	19.258	1385							
CAT	н	0.251	6.438	463							
ATA	- I	0.001	0.083	6							
ATO		0.600	40 760	0000							

### 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       Analysis functions         460       Analysis functions         461       Codon Calculate G+C content and codon usage         463       Translate         464       Translate         All None       None

An aligned amino acid sequence will be displayed.

433 <sup>T</sup>	······ð
434_1	L
435_1	Т
436_1	
437_1	
438_1	
439_1	
440_1	. К
441 1	
442 1	
443 1	н.
444 1	
445 1	
445 1	
447 1	
449 1	
440_1	
445_1	
450_1	
451_1	
452_1	К.
453_1	
454_1	IAT
455_1	
456_1	
457_1	GGG
458_1	
459_1	
460_1	
461_1	
462 1	
463 1	
464 1	I
Consensu	EAKKIIDEGGLVRDDIIIGNVKERIAODDCKNGFLFDGFPRILAOAEAMVEAGVDLDAVVEIDVPDSVIVDRMSGRRVHLASGRIYHVIYNPPKVEGKDD
	110 120 130 140 150
1.1	
2 1	
2 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	A	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	A	4	ST-4 complex	7	13-1	F1-5
24	S4355	B227; NIBSC_2806; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	5-1	9	F3-1
31	10	B269; NIBSC_2825; Z1269	Burkina Faso	1963	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex	7	13-1	F1-5
34	20	B275; NIBSC_2767; Z1275	Niger	1963	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex	5-2	10	F1-7
35	26	B278; NIBSC_2764; Z1278	Niger	1963	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex	7	13	F1-5
52	243	B362; NIBSC_2779; Z1362	Cameroon	1966		Neisseria meningitidis	A	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	А	1	ST-1 complex	5-2	10	F1-7
67	S5611	B466; NIBSC_2765; Z1466	Australia	1977	invasive (unspecified/other)	Neisseria meningitidis	А	1	ST-1 complex	5-2	10	F5-1
82	11-004	B503; NIBSC_2826; Z1503	China	1984	invasive (unspecified/other)	Neisseria meningitidis	А	5	ST-5 complex	20	9	F3-8
84	IAL2229	B506; NIBSC_2816; Z1506	Brazil	1976		Neisseria meningitidis	A	5	ST-5 complex	20	9	F2-1
90	CN100	B534; NIBSC_2768; Z1534	UK	1941	invasive (unspecified/other)	Neisseria meningitidis	A	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	А	5	ST-5 complex	20	9	F3-1
160	1014	NIBSC_2821; Z3667	Sudan	1985	invasive (unspecified/other)	Neisseria meningitidis	А	4	ST-4 complex	7	13-1	F1-5
210	H1964	NIBSC_2796; Z3771	UK	1987	invasive (unspecified/other)	Neisseria meningitidis	А	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	А	6	ST-5 complex	20	9	F3-1
Anal	Analysis tools: Breakdown: Fields Two Field Combinations Polymorphic sites Publications Sequence bin Analysis: BURST Codons Gene Presence Genome Comparator BLAST rMLST species id PCR B Export: Dataset Contigs Sequences Third party: GrapeTree TTOL Phylo/Iz Microreact											
Page:	123	3 4 5 > Last										

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	
Jvothish NT	
- Stenhano	
• Stephano	
in the Aanensen Research Group at Imperial College London and The Centre for Genomic F	Pathogen Surveillance.
Web site: https://misrorgast.org	
web site. https://microreact.org	
Publication: Argimon 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.	
Applying in limited to 2,000 records or 100,000 conjugators (records x loci)	
Analysis is infinited to 2,000 records or 100,000 sequences (records x loci).	
Isolates Loci Schemes	
1 ^ '16S_rDNA ^ '	·····
2 16S_rRNA (SSU_rRNA)	Ismids
7 23S rRNA	bing
10 abcZ	
11 abc7 (NEIS1015)	MLST
13 aceE (NEIS1279)	Einetyning antigens
	r metyping antigens
24 acrA (NEIS1720)	16S
	Antigen genes
Clear List all All None Paste list	Devene Arthur Ora M
	Bexsero Antigen Seq *
Descriptions	Include fields Action Action
Modify the values below - these will be displayed within the created Microreact project.	Select additional fields to include in Microreact data table
	(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: Neigeeria RubMLST	continent
Description. Relabella Publica	region
	date received
li.	date samed
	uate sampled
	non culture
	epidemiological year v

The job will be sent to the job queue. When it has finished, click the button marked 'Launch Microreact'.

↔ Log in									
Job status viev	ver								
-									
Status									
Job id	BIGSdb 034939 15632	78919 45263							
Submit time	2019-07-16 13:08:39	-							
Status	Status: finished								
Start time	Start time: 2019-07-16 13:08:42								
Progress	Progress: 100%								
Stop time	2019-07-16 13:09:13								
Total time	: 30 seconds								
Output Launch Microre: Files	act								
Concatenate	d FASTA	NJ tree (Newick format)	Microreact TSV file	Tar file containing all output files					

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.

C_2828; Z1092 Germa Czech Re C_2795; Z1099 Philippi Czech Re Germa Germa Germa SC_2813; Z1213 Ghan	1964         Inva           public         1989         Inva           1968         1968         Inva           ipublic         1995         Inva           any         1999         Inva	isive (unspecified/other) isive (unspecified/other) carrier carrier carrier carrier	<ul> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> <li>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 B A X E B W	1 1015 1 117 864 854 174	ST-1 complex ST-32 complex ST-1 complex ST-18 complex ST-174 complex	5-2 7 5-2	10 16 10 14	F3-6 F5-1
Czech Re C_2795; Z1099 Philippi Czech Re Germa Germa Germa Germa Germa	Public         1989         inva           ines         1968	sive (unspecified/other) carrier carrier carrier carrier carrier	<ul> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> </ul>	B A X E B W	1015 1 117 864 854 174	ST-32 complex ST-1 complex ST-18 complex ST-18 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 complex ST-174 comp	7 5-2	16 10 14	F5-1
C_2795; Z1099 Philippi Czech Re Germa Germa Germa Germa Germa Germa	ines         1968           epublic         1995         inva           any         1999         any	sive (unspecified/other) carrier carrier carrier carrier carrier	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A X E B W	1 117 864 854 174	ST-1 complex ST-18 complex ST-174 complex	5-2	10 14	F5-1
Czech Re Germa Germa Germa Germa SC_2813; Z1213 Ghan	Public         1995         inva           any         1999         -	sive (unspecified/other) carrier carrier carrier carrier carrier	<ul> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> <li>Neisseria meningitidis</li> </ul>	X E B W	117 864 854 174	ST-18 complex ST-174 complex		14	
Germa Germa Germa Germa Germa GC_2813; Z1213 Ghan	any 1999 any 1999 any 1999 any 1999 any 1999	carrier carrier carrier carrier	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	E B W	864 854 174	ST-18 complex ST-174 complex			
Germa Germa Germa SC_2813; Z1213 Ghan	any 1999 any 1999 any 1999 any 1999	carrier carrier carrier	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	B	854 174	ST-18 complex ST-174 complex			
Germa Germa GC_2813; Z1213 Ghan	any 1999 any 1999 aa 1973 inva	carrier carrier	Neisseria meningitidis Neisseria meningitidis	W	174	ST-174 complex			
Germa SC_2813; Z1213 Ghan	any 1999 na 1973 inva	carrier	Neisseria meningitidis	-					
SC_2813; Z1213 Ghan	na 1973 inva			в	19	ST-18 complex			
		sive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex	7	13-1	F1-5
Germa	any 1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
Germa	any 1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
Germa	any 1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
Germa	any 1999	carrier	Neisseria meningitidis	В	32	ST-32 complex			
SC_2806; Z1227 Denma	ark 1974 inva	sive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex	5-1	9	F3-1
Germa	any 1999	carrier	Neisseria meningitidis	В	930	ST-334 complex			
	SC_2806; Z1227 Denm Germa SC_2806; Z1227 Denm	Germany 1999 Germany 1999 Germany 1999 Germany 1999 SC_2806; Z1227 Denmark 1974 inva Germany 1999	Germany 1999 carrier Germany 1999 carrier Germany 1999 carrier SC_2806; Z1227 Denmark 1974 invasive (unspecified/other) Germany 1999 carrier	Germany         1999         carrier         Neisseria meningitidis           Germany         1999         carrier         Neisseria meningitidis           Germany         1999         carrier         Neisseria meningitidis           Germany         1999         carrier         Neisseria meningitidis           SC_2806; Z1227         Denmark         1974 invasive (unspecified/other)         Neisseria meningitidis           Germany         1999         carrier         Neisseria meningitidis	Germany         1999         carrier         Neisseria meningitidis         NG           Germany         1999         carrier         Neisseria meningitidis         E           Germany         1999         carrier         Neisseria meningitidis         E           Germany         1999         carrier         Neisseria meningitidis         B           SC_2806; Z1227         Denmark         1974         invasive (unspecified/other)         Neisseria meningitidis         A           Germany         1999         carrier         Neisseria meningitidis         B	Germany     1999     carrier     Neisseria meningituis     NG     198       Germany     1999     carrier     Neisseria meningituis     NG     198       Germany     1999     carrier     Neisseria meningituis     E     60       Germany     1999     carrier     Neisseria meningituis     B     32       SC_2806, Z1227     Denmark     1974 invasive (unspecified/other)     Neisseria meningituis     A     5       Germany     1999     carrier     Neisseria meningituis     B     32	Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex       Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       Germany     1999     carrier     Neisseria meningitidis     B     32     ST-32 complex       SC_2806, Z1227     Denmark     1974 invasive (unspecified/other)     Neisseria meningitidis     A     5     ST-5 complex       Germany     1999     carrier     Neisseria meningitidis     B     32     ST-32 complex	Germany       1999       carrier       Neisseria meningituis       NG       198       ST-198 complex         Germany       1999       carrier       Neisseria meningituis       NG       198       ST-198 complex         Germany       1999       carrier       Neisseria meningituis       E       60       ST-60 complex         Germany       1999       carrier       Neisseria meningituis       B       32       ST-32 complex         SC_2806, Z1227       Denmark       1974 invasive (unspecified/other)       Neisseria meningituis       A       5       ST-5 complex         Germany       1999       carrier       Neisseria meningituis       B       930       ST-334 complex	Germany     1999     carrier     Neisseria meningitidis     NG     198     ST-198 complex       Germany     1999     carrier     Neisseria meningitidis     E     60     ST-60 complex       Germany     1999     carrier     Neisseria meningitidis     B     32     ST-32 complex       Germany     1999     carrier     Neisseria meningitidis     B     32     ST-32 complex       SC_2806, Z1227     Denmark     1974 invasive (unspecified/other)     Neisseria meningitidis     A     5     ST-5 complex       Germany     1999     carrier     Neisseria meningitidis     B     930     ST-334 complex

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'.

PubMLST Database h	ome Contents	
+) Log in		Toggle: 🚺
PhyloViz: phylo	genetic tree vizualisation - Neisseria PubMLST	
Non T	This plugin uploads data for analysis within the PhyloViz online service:	
C C 237	PHYLOViZ Online: Web-based tool for visualization, phylogenetic inference, analysis and sharing.	
till	PHYLOVIZ Online is developed by:	
	Bruno Gonçalves (1)     João André Carriço (1)     Alexandre P. Francisco (2,3)     Cátia Vaz (2,4)     Mário Ramirez (1)	
	<ol> <li>Instituto de Microbiologia, Instituto de Medicina Molecular, Faculdade de Medicina, Universidade de Lisboa, Lisboa, Portugal</li> <li>INESC-ID, R. Alves Redol 9, 1000-029 Lisboa, Portugal</li> <li>Instituto Superior Técnico, Universidade de Lisboa, Lisboa, Portugal</li> <li>Instituto Superior de Engenharia de Lisboa, Instituto Politécnico de Lisboa, 007 Lisboa, Portugal</li> </ol>	
	Web site: https://online.phyloviz.net/	
Please wait for processing Data are being processed	to finish (do not refresh page). and sent to PhyloViz Online.	
Generating profile data file	e✔	
Generating auxiliary file	✓	
Sending data to PhyloViz of	online 🗸	
Launch PhyloViz		

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	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	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	Α	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			
20     9     Germany 1999     camer     resissena meningilious     B     930     S1-334 Complex       Analysis tools:       Breakdown:     Fields     Two Field     Polymorphicaites     Combinations     Schemes/alleles     Publications     Sequence bin     Tag status       Analysis:     BURST     Codons     Presence/Absence     Genome Comparator     BLAST       Export     Dataset     Contigs     Sequences												
Page	1 2	3 4 5	678	> (	Last							

Select the locus that you would like to analyse from the list.

Ouery: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profile/Stequences definitions   Database submissions									
Тода	le: 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         '16S, rDNA       If both allel designations and tagged sequences tasts for a locus, choose how you want these handled:       Analyse         23S, rRNA       Image: Comparison of the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the sequence set and the set and the sequence set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the set and the s									

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			
The Neisseria PubMLST data one corresponding isolate de	base contains data for a collection of isolates that represent the posited here. Any isolate may be submitted to this database a	he total known diversity of Neisseria nd consequently it should be noted	a species. For every allelic profile in I that it does not represent a popula	the profiles/sequence definition database there is at least tion sample.
Q Query database	Projects	Option settings		1 Submissions
<ul> <li>Search or browse dat</li> <li>Search by combination</li> </ul>	abase • Main public projects • S ns of loci (profiles) • Your projects • S	Set general options - including isola Set display and query options for lo	te table field handling. cus, schemes or scheme fields.	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>	f genomic relationships
Two field	Contigs	Gene presence	<ul> <li>iTOL - Phylogenetic trees w</li> </ul>	vith data overlays
Unique combinations     Publications	<ul> <li>Sequences - XMFA / concatenated FASTA formats</li> </ul>	Genome comparator     BLAST	<ul> <li>PhyloViz - Visualization and</li> <li>Microreact Open data visu</li> </ul>	phylogenetic inference
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).

Clonal complex (MLST): N. gonorrhoeae cgMLS OMV peptide typing p Cluster (OMV peptide Ribosomal MLST profiles: Sequence bin: Sequence bin											
7 records returned. Click the hyperlinks for detailed information.											
Isolate fields			MIST	Fine	typing antig	one					
Isolate fields ()	species	capsule group	MLST ST clonal complex	Fine	typing antig	ens Fetà VR					
Isolate fields Id isolate aliases country year disease 1 A4/M1027 B1: NIBSC 2803:21001 USA 1937 inysave (unsonerified/other	species Neisseria meningifidis	capsule group A	MLST ST clonal complex 4 ST-4 complex	Fine PorA_VR1 5-2	typing antig PorA_VR2 10	ens FetA_VR F1-5					
Isolate fields O           Id         Isolate         aliases         country         year         disease           1         A4/M1027         B1; NIBSC_2803; Z1001         USA         1937         Invasive (unspecified/other           2         120M         B35         MIBSC_2822; Z1035         Pakistan         1997         meniontis and sectionamic	species Neisseria meningitidis Neisseria meningitidis	capsule group A A	MLST ST clonal complex 4 ST-4 complex 1 ST-1 complex	Fine PorA_VR1 5-2 5-2	typing antig PorA_VR2 10 10	ens FetA_VR F1-5 E5-1					
Isolate fields ①           Id         isolate         allases         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 septicaemila           7         7891         B54; NIBSC_7206; Z1054         Finland         1975         invasive (unspecified/other	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	capsule group A A A	MLST ST clonal complex 4 ST-4 complex 1 ST-1 complex 5 ST-5 complex	Fine PorA_VR1 5-2 5-2 20	typing antig PorA_VR2 10 10 9	ens FetA_VR F1-5 F5-1 F3-1					
Isolate fields ①           Id         isolate         aliases         country         year         disease           1         A4/M1027         B1; NIBSC_2803; Z1001         USA         1997 invasive (unspecified/other           2         120M         B35; NIBSC_2822; Z1035         Pakistan         1967 meningitis and septicaemia           7         7891         B54; NIBSC_2760; Z1054         Finland         1975 invasive (unspecified/other           0         6748         B73; NIBSC 2764; Z1073         Canada         1971 invasive (unspecified/other	species ) Neisseria meningitidis Neisseria meningitidis ) Neisseria meningitidis ) Neisseria meningitidis	capsule group A A A A	MLST ST clonal complex 4 ST-4 complex 1 ST-1 complex 5 ST-5 complex 1 ST-1 complex	Fine PorA_VR1 5-2 5-2 20 18-1	typing antig PorA_VR2 10 10 9 3	ens FetA_VR F1-5 F5-1 F3-1 F5-1					
Isolate fields 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 meningitis and septicaemia           7         7891         B54; NIBSC_2760; Z1054         Finland         1975 invasive (unspecified/other           10         6748         B73; NIBSC_2762; Z1023         Gamany         1964 invasive (unspecified/other           11         120E         B92; NIBSC_2828; Z1002         Germany         1964 invasive (unspecified/other	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	capsule group A A A A A A	MLST           ST clonal complex           4         ST-4 complex           1         ST-1 complex           5         ST-5 complex           1         ST-1 complex           1         ST-1 complex           5         ST-5 complex           1         ST-1 complex           1         ST-1 complex           1         ST-1 complex	Fine PorA_VR1 5-2 5-2 20 18-1 5-2	typing antig PorA_VR2 10 10 9 3 10	ens FetA_VR F1-5 F5-1 F3-1 F5-1 F3-6					
Isolate fields 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         meningitis and septicaemic           7         7891         B54; NIBSC_2760; Z1054         Finland         1975         invasive (unspecified/other           10         6748         B73; NIBSC_2784; Z1073         Canada         1971         invasive (unspecified/other           11         129E         B92; NIBSC_2785; Z1029         Germany         1964         invasive (unspecified/other           13         139M         B99; NIBSC_2755; Z1099         Philippines         1968	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	capsule group A A A A A A A A	MLST ST cional complex 4 ST-4 complex 5 ST-5 complex 1 ST-1 complex 1 ST-1 complex 1 ST-1 complex 1 ST-1 complex	Fine PorA_VR1 5-2 20 18-1 5-2 5-2 5-2	typing antig PorA_VR2 10 10 9 3 10 10	ens FetA_VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1					
Isolate fields 0           Id         Isolate         Isolate         Isolate         Isolate           1         Ad/M1027         B1; NIBSC_2803; 21001         USA         1937         invasive (unspecified/other           2         120M         B35; NIBSC_2802; 21035         Pakistan         1967         meningtis and septicaemia           7         7891         B54; NIBSC_2822; 21035         Pakistan         1975         invasive (unspecified/other           10         6748         B73; NIBSC_2784; 21073         Canada         1971         invasive (unspecified/other           11         129E         B92; NIBSC_2828; 21092         Germany         1964         invasive (unspecified/other           13         139M         B90; NIBSC_2813; 21213         Ghana         1973         invasive (unspecified/other           19         S313         B213; NIBSC_2813; 21213         Ghana         1973         invasive (unspecified/other	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	capsule group A A A A A A A A A	MLST       ST-1 complex       4     ST-4 complex       5     ST-5 complex       1     ST-1 complex       1     ST-1 complex       1     ST-1 complex       1     ST-1 complex       4     ST-4 complex	Fine PorA_VR1 5-2 20 18-1 5-2 5-2 5-2 7	etyping antig PorA_VR2 10 10 9 3 10 10 10 13-1	ens FetA_VR F1-5 F5-1 F3-1 F3-6 F5-1 F5-1 F1-5					

Finally, the analysis is also possible directly from an isolate record, if the isolate has a genome assembly associated with it.

	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											
	• Bratcher HB, Corton C, Jolley KA, Parkhill J, Maiden MC (2014). A gene-by-gene population genomics platform: de novo assembly, annotation and genealogical analysis of 108 representative Neisseria meningitidis genomes. BMC Genomics 15:1138 [108 isolates]											
	Didelot X. Unvin R. Malden MC, Falush D (2009). Genealogical typing of Neisserla meningitidis. Microbiology 155:3176-86 93 isolates											
	$\sim$											
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						
<b>=</b>	Schemes and lo	ci										
à 🧸	All loci		Navigate and select sche	emes within tree	to display allele designatio	ns						
	🏭 Capsule											
- P-	🏭 Genetic Inform	ation Processing										
	- Ji Genomic Islan	ds										
	Motabolism	mes										
1	Dilin											
	🛄 Typing											
ļ.,	- A Other scheme	s										
	🌆 Loci not in sch	iemes										
Lad	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
+D Log in Toggle: ①
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 linked to validated genomes in the rMLST database.
Please select the required isolate ids to run the species identification for. These isolate records must include genome sequences.
Isolates — Action —
1 Submit
13 19
Clear List all
List al

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.

υτρι	ıt						
d is	solate		Identified rSTs				
1 A4	I/M1027	Rank	Taxon Neisseria meningitidis	Taxonomy Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meninglildis	100%	2504	Species Neisseria meningitidis
2	120M	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2532	Neisseria meningitidis
'	7891	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2434	Neisseria meningitidis
D	6748	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis		2530	Neisseria meningitidis
1	129E	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2528	Neisseria meningitidis
3	139M	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2433	Neisseria meningitidis
9 5	53131	SPECIES	Neisseria meningitidis	Proteobacteria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria > Neisseria meningitidis	100%	2285	Neisseria meningitidis
es							

Clicking the '+' icon on any row will display further details about the matches.

id isola	Prediction from identified rMLST alleles linked to genomes									Identified rSTs		
		Rank	Ta	xon		Taxonomy Support Matches						
1 A4/M1	027 SPECIES Neisseria meningitidi				Proteobacte	ria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria >	100%	0	2504	Neisseria meningitid		
					Neisseria me	eningitidis						
2 120	/ S	PECIES	Neisseria	meningitidis	Proteobacte	ria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria >	100%	0	2532	Neisseria meningitid		
					Neisseria me	eningitidis						
7 789	1 S	PECIES	Neisseria	meningitidis	Proteobacte	ria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria >	100%	0	2434	Neisseria meningitio		
					Neisseria me	eningitidis		_				
674	3 S	PECIES	Neisseria	meningitidis	Proteobacte	ria > Betaproteobacteria > Neisseriales > Neisseriaceae > Neisseria >	100%	•	2530	Neisseria meningitid		
					Neisseria me	eningitidis						
3 loci mat	ched (r	MLSTuse	es 53 in to	otal)								
				Start	End							
Locus	Allel	e Length	Contig	position	position	Linked data values						
BACT0000	01 174	1680	181603	32429	34108	species: Neisseria meningitidis [n=1759]						
BACT0000	02 9	729	181098	6971	7699	species: Neisseria meningitidis [n=674]						
BACT0000	03 1	693	181315	13840	14532	species: Neisseria meningitidis [n=1701]						
BACT0000	03 1	693	181474	5814	6506	species: Neisseria meningitidis [n=1701]						
BACT0000	04 2	621	181315	5569	6189	species: Neisseria meningitidis [n=7346]; Neisseria sp. [n=1]						
BACT0000	05 1	519	181315	9345	9863	species: Neisseria meningitidis [n=15997]; Neisseria sp. [n=1]						
BACT0000	05 1	519	181474	10483	11001	species: Neisseria meningitidis [n=15997]; Neisseria sp. [n=1]						
BACT0000	06 5	369	181603	53216	53584	species: Neisseria meningitidis [n=1945]; Neisseria sp. [n=1]						
BACT0000	07 1	471	181145	2253	2723	species: Neisseria meningitidis [n=13786]; Neisseria sp. [n=1]						
BACT0000	07 1	471	181374	2271	2741	species: Neisseria meningitidis [n=13786]; Neisseria sp. [n=1]						
BACT0000	08 2	393	181315	10796	11188	species: Neisseria meningitidis [n=6991]						
BACT0000	09 1	393	181193	16935	17327	species: Neisseria meningitidis [n=2942]						
BACT0000	09 1	393	181591	20941	21333	species: Neisseria meningitidis [n=2942]						
BACT0000	10 1	312	181315	19833	20144	species: Neisseria meningitidis [n=898]						
BACT0000	10 1	312	181474	202	513	species: Neisseria meningitidis [n=898]						
BACT0000	11 2	396	181315	6209	6604	species: Neisseria gonorrhoeae [n=9494]; Neisseria meningitidis [n=6718	3]; Neisseria 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.

2	120M	B35; NIBSC_2822; Z10	35 Pakistan	1967 meningit	s 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; Z10	043 USA	1937 invasive	(unspecified/other)	Neisseria meningitidis	А	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; Z10	54 Finland	1975 invasive	(unspecified/other)	Neisseria meningitidis	А	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; Z10	73 Canada	1971 invasive	(unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex	18-1	3	F5-1
11	129E	B92; NIBSC_2828; Z10	92 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; Z10	99 Philippines	1968		Neisseria meningitidis	A	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; Z1:	213 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; Z1:	227 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			
Ana	lysis tools	:			_							
G	Breakdown:	Fields Two Field	Combinations Pc	olymorphic sites	Publications Se	equence bin						
	Analysis:	BURST Codons	Gene Presence	Genome Compara	tor BLAST rM	ILST species id PCR						
	Export:	Dataset Contigs	Sequences									
Ø	Third party:	GrapeTree ITOL	PhyloViz Microre	act								
	-											
Page	1 2 3	4 > 1ast										

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.

Log in      Breakdown of sequence bin contig properties  Please select the required isolate ids for comparison - use Ctrl or Shift to make multiple selections. Select loci/schemes to use for calculating percentage of alleles designated or tagged.	PubMLST Databas	e home Contents			
Breakdown of sequence bin contig properties Please select the required isolate ids for comparison - use Ctrl or Shift to make multiple selections. Select loci/schemes to use for calculating percentage of alleles designated or tagged.	+) Log in			Help	3
Please select the required isolate ids for comparison - use Ctrl or Shift to make multiple selections. Select loci/schemes to use for calculating percentage of alleles designated or tagged.	Breakdown of	f sequence bin contig	properties		
Isolates       Loci       Schemes       Options         93       165_rRNA (SSU; rRNA)       235_rRNA       Calculate %GC         96       97       3bcZ       abcZ       Genetic Information Proc         99       acef (NESI 127)       acef (NESI 1272)       Genomic Islands         acA2 (NEISI 1272)       acad (NEISI 1272)       Metabolism         Clear List all       All None Paste list       W go control and All Information Proc	Please select the requi	Loci Loci 165_rDNA 165_rRNA (SSL_rRNA) 235_rRNA abcz abcz (NEIS1015) acf42 (NEIS1015) ack22 (NEIS1279) ack24 (NEIS1727) ach42 (NEIS1727) ach42 (NEIS1727) ach42 (NEIS1729)	or Shift to make multiple selections. Select loci/schemen Schemes All loci Genomic Islands Capsule Genomic Islands Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule Capsule	s to use for calculating percentage of alleles designated or tagged.  Options Contig analysis (min, max, N50 etc.) Calculate %GC Fitter by Sequence method: Project: Experiment Contignation 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.

PubMLS1 Database home Contents												
+) Log in										Help 🖌	Ξ	
Please sele	own of	seque ed isolate id Loci	nce bin co	- use Ctrl or Shift to	rties make multiple selections. S Schemes	elect loci/schemes	to use for calculat Options	ing percentage of allel /sis (min, max, N50 etc	es designated or tagged. )			
2       165_RNA (SSU_RNA)         3       235_RNA         3 d       225_RNA         3 d       abcZ         abcZ       abcZ         abcZ       abcZ         abcZ       abcZ         abcZ       abcZ         abcZ       abcZ         abcZ       ack4 (NEIS1015)         ack4 (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)       acna (NEIS1727)         acna (NEIS1727)												
Loci selecte	ed: 3050											
Isolate id a	≑ Isolate ≑	Contigs 🗢	Total length 🗧	Alleles designated	I 🗢 % Alleles designated	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 →				

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	f contigs	То	otal length								
Overall mea	n: 254.3; σ: 12	3.7 O	verall mean: 21889	922.1; σ: 497829.9							
			nideredapetersslagidens	televistender							

Sequence bin records can also be accessed by clicking the 'Display' button for each row of the table.

Clear ( Loci selecte	List all	acnA (NEI	S1729)	v site list	👻 🤑 Caps	ule Region / ule Region / >	Experi Action Reset Sut	ment: v 3
Isolate id a	+ Isolate +	Contigs ¢	Total length 4	Alleles designated +	% Alleles designated \$	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	717	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	e profiles/sequence definition s not represent a population sample.
<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.

Select the two fields you wish to breakdown and how you would like the values displayed (percentage/absolute values and totaling options).

Query: Search   Browse   Profile/S Breakdown: Isolate fields   Schem Links: Contents   Home   Options	T   List ne/alleles   Publications   Profiles/sequences definitions	Database submissions		
Two field breakdown of datase	et			Show options
Here you can create a table breaking down one field by Select fields Field 1: clonal complex (MLST) • Field 2: serogroup •	another, e.g. breakdown of serv Display values only values and percentages percentages only	ogroup by year. — Calculate percentages by- @ dataset	Action 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.

Two field breakdo Breakdown of clonal_con Selected options: Display value	<b>WI</b>	n o	f da	nta					
Two field breakdo Breakdown of clonal_co Selected options: Display value	wi npl	n o	f da	nte					
Breakdown of clonal_con Selected options: Display value	npl			2 C C C	set				
Breakdown of clonal_col Selected options: Display value	npl								
Breakdown of clonal_co. Selected options: Display value	npl								
Selected options: Display value		ex (I	VLST	í) by	sero	grou	p:		
	s on	ily.							
Avoc Chow									
- Silow									
Reverse Values and	l per	centa	ges	J					
					ser	ogroup	)		
clonal_complex (MLST) \$	4 \$	B \$	C \$	E 🕈	NG 🗢	W \$	X 🗢 Y	* Z ≑	Total 🗢
No value	1	3	1	1	4		1	1	12
SI-1 complex/subgroup I/II	13		16						13
ST-11 Complex/E1-37 Complex ST-162 complex		5	10						10
ST-167 complex		3			1			2	3
ST-174 complex				1	1	1			3
ST-178 complex					1				1
ST-18 complex		3							3
ST-198 complex					2	2			2
ST-22 complex		1				2			2
ST-220 complex/Cluster A3								1	1
ST-254 complex					1				1
ST-269 complex		2			1				3
ST-32 complex/ET-5 complex		6							6
ST-334 complex		1							1
ST-35 complex					1				1
ST-4 complex/subgroup IV	8	5			1				8
ST-41/44 complex/Lineage 3		2			1				0
ST-5 complex/subgroup III	6								6
ST-53 complex	-				2				2
ST-60 complex				1					1
Total	28	27	17	3	15	3	1	3 1	98

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 home	Contents				
↔ Log in					
Neisseria PubMLS	T database				
The Neisseria PubMLST databa definition database there is at le population sample.	east one corresponding	collection of isolates that repre- isolate deposited here. Any iso	sent the total known diversity of Neisseria blate may be submitted to this database ar	species. For every allelic profile in nd consequently it should be noted	the profiles/sequence that it does not represent
Q Query database	E	Projects	Option settings		1 Submissions
Search or browse databa	ase	Main public projects	Set general options - including isolate	e table field handling.	Manage
<ul> <li>Search by combinations</li> </ul>	of loci (profiles)	<ul> <li>Your projects</li> </ul>	<ul> <li>Set display and query options for loc</li> </ul>	us, schemes or scheme fields.	submissions
<ul> <li>Isolates: 51,359</li> <li>Last updated: 2019-06-1</li> <li>Defined field values</li> <li>Update history</li> <li>About BIGSdb</li> </ul>	19				
Breakdown	Export		Analysis	Third party tools	
Single field	<ul> <li>Export dataset</li> </ul>		Codon usage	GrapeTree - Visualization of	f genomic relationships
Two field	Contigs		Gene presence	<ul> <li>ITOL - Phylogenetic trees w</li> </ul>	ith data overlays
Unique combinations     Publications	<ul> <li>Sequences - X</li> </ul>	MFA / concatenated FASTA for	mats • Genome comparator	<ul> <li>PhyloViz - Visualization and</li> <li>Microreact Open data view</li> </ul>	phylogenetic inference
Sequence bin			Species identification	<ul> <li>microreact - Open data visu genomic epidemiology</li> </ul>	anzauon and sharing for
	Miscellaneou	IS	In silico PCR	J	
	Description of	latabaco fioldo			
	<ul> <li>Description of elements</li> </ul>	Jalabase lielus			

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.

E 1400040007											
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 B	54; 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 B	73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11 129 B	92; 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 B	99; 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 B2	213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	Α	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 B2	227; 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			
Analysis tools: Breakdown: Field Analysis: BURS Export Datas	ds Two Fi ST Codo set Conti	eld Polymorph ns Presence/Al gs Sequences	ic sites bsence	Combinations Schemes Genome Comparator BL	AST	Sequence b	in	Tag status			

Select the combination of fields to analyse, e.g. serogroup and finetyping antigens.

PubMLST Database home Contents	
+D Log in	Help Cr Toggle: (1)
Frequencies of field combinations	
Here you can determine the frequencies of unique field combinations in the dataset. Please set one or more schemes to include all loci (and/or fields) from a scheme.	ect your combination of fields. Select loci either from the locus list or by selecting
Isolates       Provenance fields       Phenotypic fields       Composition         1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1	e fields • Loci lation • Loci 165_rRNA (SSU_rRNA) 235_rRNA abc2 abc2 (NEIS1015) aceF (NEIS1279) acKA2 (NEIS1727) acrA (NEIS1729) All None
⊡ Include all fields 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	
The Neisseria PubMLST database contains data for a collection of isolates that repres- database there is at least one corresponding isolate deposited here. Any isolate may b sample.	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         • Bolates: 34218       • Last updated: 2015-06-30         • Update history       • About BIGSdb
Breakdown     Single field     Two field     Unique combinations     Scheme and alleles     Publications     Sequence bin	Analysis Codon usage Presence/absence status of loci Genome comparator BLAST Analysis 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.

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.

Query: Search   Browse   Breakdown: Isolate fields Links: Contents   Home	Profile/ST   List ;   Scheme/alleles   Publications Options   Profiles/sequences definitions			
			Help 🖉	Toggle: 🜖
Contig analysis and expo	rt			
Please select the required isolate ids from wh calculated by adding up the length of all loci ta the length of the contig.	ich contigs are associated - use Ctrl or Shift to make multiple gged within the contig - if these loci overlap then the total tagg	selections. Please note t ed length will be reported	that the total length of tagged sequenc I as being longer than it really is but it v	e is von't exceed
Isolates	Options	Filter by		
1) A4/M1027 2) 120M	Identify contigs with >= 0	Sequence method: Project	<b>▼</b> 0	- 0
7) 7891 10) 6748		Experiment:	<b>v</b> 0	•••
11) 129E 13) 139M		Minimum length:	<b>▼</b> 0	
19) \$3131 24) \$4355	- 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.

	u ine tengi	n of the co	ntig.								
-Is	olates —				Options			— Filter by ———			
I) A	4/M1027			*	Identify contigs wi	th >= 0 →	% of sequence untagged	Sequence metho	od:	- 0	
2) 1	20M				FASTA header line	e: original desi	gnation 👻 🕕	Proje	ect:		- 0
10)	6748							Experime	nt: 📃 🗸 🕕		
1)	129E							Minimum leng	th: 🚽	0	
3) 9)	S3131				Action						
24)	S4355			-	Action						
			-		Reset Subr	nit					
nt	igs with 3	>=0% se	quence le	ength	untagged						
			matching	config	non-matching	contins					
<b>+</b>	isolate 🗢 🛛	contigs 🖨	count 🔶 🛛	downloa	d count 🔶 do	wnload					
	A4/M1027	364	364	*	0						
2	120M	359	359	*	0						
'	7891	199	199	*	0						
	0740	650	652		0						

You can also download all the data in a tar file by clicking the 'Batch download' link.

-15				(	Ontiono		Filter by		
-							Cogueres method:		
i) A 2) 1	4/1/11/27				entity contig	s with ≥= 0	Sequence metriod.	<b>v</b> U	
ń7	7891			L FA	IS IA neader	TINE: original designation 👻 🚺	Project.		<b>*</b> (
$\frac{10}{11}$	6748 120E						Experiment	<b>v</b> 0	
13)	139M						Minimum length:	<b>→ ()</b>	
19)	S3131				Action				
24)	S4355					Nucleon 14			
	(A)	None	ר		Reset	Submit			
			_						
		- 00%							
ont	tigs with >	=0% seq	uence le	ength un	itagged				
ont	tigs with >	=0% seq	uence le matching	ength un contigs	itagged non-match	ing contigs			
ont ¢	t <mark>igs with</mark> > isolate ≑ co	=0% seq ontigs +	uence le matching count + d	ength un contigs lownload	ntagged non-match count 🗢	ing contigs download			
ont ¢	tigs with > isolate	=0% seq ontigs ¢ 364	uence le matching count + d 364	ength un contigs lownload	ntagged non-match count ¢ 0	ing contigs download			
ont ¢ 1 2	tigs with > isolate \$ co A4/M1027 120M	= <b>0% seq</b> ontigs ¢ 364 359	uence le matching count \$ d 364 359	ength un contigs lownload ±	ntagged non-match count ¢ 0 0	ing contigs download			
ont € 1 2 7	tigs with >= isolate \$ co A4/M1027 120M 7891	<b>=0% seq</b> ontigs <b>\$</b> 364 359 199	uence le matching count ¢ d 364 359 199	ength un contigs lownload ± ± ±	non-match count ¢ 0 0 0	ing contigs 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 seq	uence untagged
FASTA header line:	orig	ginal o	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.

	Contigs with >=50% sequence length untagged										
id A		icolato 🔺	contigo 🔺	matchin	g contigs	non-matching contig					
	u 🕈		conuys 👻	count 🔶	download	count 🔶	download				
	1	A4/M1027	364	163	<u>*</u>	201	*				
	2	120M	359	81	*	278	*				
	7	7891	199	48	*	151	<u>*</u>				
	10	6748	652	393	<u>خ</u>	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.

id isolate 1 A4/M1027 2 120M	aliases B1; Z1001	country	year			Isolate fields <b>FI</b> MLST Finetyning antigens										
1 A4/M1027 2 120M	B1; Z1001	country		dicoaco	spacias	serogroup	ет	clonal complex		DorA VR2	EotA VR					
2 120M	D1, 21001		1037	invasive (unspecified/other)	Neisseria meningitidis	Δ	1	ST-4 complex/subgroup IV	5-2	10	E1-5					
	B35: 71035	Pakistan	1967	meningitis and senticaemia	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/I	5-2	10	F5-1					
3 M00242905	200,21000	UK	2000	invasive (unspecified/other)	Neisseria meningitidis	B	1099		19	15						
4 M1027	B43: 71043	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						
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								
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					
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					
4 0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14						
5 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 I	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	Α	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 I	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 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

-Op	ptions
	Include locus common names
V	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.

Expert protein melecular weights
CTO/TTO at start as day for mothisming
GIG/IIG 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.

r age.		2		4 0	6	][7]	8	9 > Last
ST	abcZ	adk	aroE	fumC	gdh	pdhC	pgm	cional 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 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	
22	11	5	18	8	11	24	21	ST-22 complex
23	10	5	18	9	11	9	17	ST-23 complex/Cluster A3
24	2	5	2	7	15	20	5	ST-750 complex
25	6	5	2	12	6	13	14	
Analysis tools:								

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 Content	3
● Log in	Ξ
Export allelic profiles - N	eisseria profile/sequence definitions
Schemes	
Please select the scheme you would like to query	
MLST 👻 S	elect)
This seciel will support effective profiles in the definition	ad had and Final formula
oute d otte	o text and excertormats.
Paste in list of ids to include, start a new	Action
line for each. Leave blank to include all ids.	SUMIR
1	
3	
5 *	
6	

Click submit.

The export job will be submitted to the job queue.

PubMLST Database home Co						
+D Log in						
Job status viewer						
Status						
Job id: BIGSdb_012009 Submit time: 2018-01-24.09	9_1516786630_99221 37-10					
Status: finished	a. 10					
Start time: 2018-01-24 09:37:24						
Progress: 100%						
Stop time: 2018-01-24 09:	37:36					
Total time: 12 seconds						
Output						
<ul> <li>Profiles - Tab-delimited text </li> <li>Profiles - Excel format </li> <li>Tar file containing output files</li> </ul>						
Please note that job results will remain on	the server for 7 days.					

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.

4 1	/1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	S1-4 complex/subgroup IV			
5 M0	0240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16	
6 M0	0282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	20	9	F3-1
8 M0	0242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1102	ST-18 complex		14	
9 0	021/84		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	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 0	090/89		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/I	5-2	10	F5-1
14 0	120/95		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 5	33131	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 \$	64355	B227: Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subaroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			
Analysis tools: Breakdown: Fields Two Field Polymorphicaites Combinations Schemesialleles Publications Sequence bin Tag status Analysis: BURST Codons Presence/Abence Genome Comparator BLAST Export: Dataset Contigs Sequences												

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.

PTIDI/JJST 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						
• 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:
Our of the sequences tagged from the bin
O Use allele sequence retrieved from external database
Do not include sequences with problem flagged (defined alleles will still be used)
Do not include incomplete sequences
Include 0 - bp flanking sequence i
Align sequences
Aligner: MAFFT 👻
Iransiate sequences
Concatenate in frame

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: 🕚 🗧
Neisseria profile/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representin a corresponding record in the isolate database.	g 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)           Locue-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     Submissions     Manage submissions     Mumber of sequences: 1,308,331     Number of profiles: Show     Last updated: 2019-06-25     Profile update history     About BIGSdb
Export     Profiles     Sequences - XMFA / concatenated FASTA formats     Sequence comparison - disp     Locus Explorer - tool for anal	quences most similar to selected allele. lay a comparison between two sequences. lysing 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). HeLog out   Change password		Help 🔀 Toggle: 🚺 🗮
Manage submissions		
Submit new alleles		
You need to make a separate submission for each locus for which you have new alleles - this is because different loci may have different curators. You can submit any number of		
new sequences for a single locus as one submission. Sequences	should be trimmed to the correct start/end sites for the selected locus.	
Filter loci by scheme		
🛓 🔲 🛄 All loci	Filter 16S_rDNA ^	
🔲 🛺 Strain typing	23S_rRNA abc7	
— 🔲 🛺 Capsule	abcz (NEIS1015)	
Genetic Information Processing	aceF (NEIS1279)	
Genomic islands	ackA2 (NEIS1727)	
	acnB (NEIS1/29)	
Motobolism	adhA (NEIS0486)	
	Sequence details EASTA or single s	equence
N. gonormoeae AMR	technologuel de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la companya de la compan	cquence
F D Plasmids		
🚛 🔲 🚛 Typing	read length !! 200-299 V	
- 😪 🎧 MLST	coverage:! 20-49x V	
🛄 🚛 Finetyping antigens	assembly:! de novo ~	
🔲 🌆 rpIF species	assembly software: Velvet	
- 🔲 🛄 Antigen genes	Sequence length outside usual range 1 Action	
	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.

Logged in: Keith Jolley (keith). Cog out   Change password				Help 🗹	Toggle: 🚺	=
Manage submissions						
Error:						
Sequence "NM432" has already been defined	d as abcZ-3.					
Submit new alleles						
You need to make a separate submission for each locus	s for which you have new alleles - this is	s because differe	ent loci may have different curators. You can su	bmit any num	ber of new	
sequences for a single locus as one submission. Seque	nces should be trimmed to the correct	start/end sites fo	r the selected locus.			
Filter loci by scheme	Select locus		Sequence details			
🗕 📃 🔊 All loci	ter '16S_rDNA	^	technology: ! Illumina ~			
🔲 🔊 Strain typing	23S_rRNA abcZ	_	read length: 200-299 V			
🔜 🌆 Capsule	abcZ (NEIS1015)		coverage:! 20-49x ~			
🔲 🍶 Genetic Information Processing	aceF (NEIS1279)		assembly:! de novo ~			
🔲 🛄 Genomic islands	acnA (NEIS1727)		assembly software: Velvet			
🔜 🛄 Lineage Schemes	acnB (NEIS1492)		Sequence length outside usual range 0			
- 🛄 🚛 Metabolism	adna (NEIS0486)	· · · · ·	FASTA or single sequence	-Action		
🖙 🔲 🏭 N. gonorrhoeae AMR			>NM322	Submit		
🔲 🥼 Plasmids			ATTCTCGATTTATTGCGCCGAAGGTTTGGGCGAA			
🔲 🍶 Typing			GTCAGCCATGAGTTGGAAAATGGTTCGAGT			
📖 🔲 🥼 Other schemes			CAACTTGAGATCGAAGCGAAGGACGGCTGG			
📖 🔲 🚛 Loci not in schemes						

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 i don't. Please do not pack or compress your files (zip, rar etc).	everse trace files. Your submission will be rejected if you
Action Abort submission! Submission: BIGSdb 20190628084417 002033 60338	
Supporting files	
Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an expla appropriate submission item. Individual filesize is limited to 64 MB. You can upload up to 64 MB in one go (the upload r 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 apprendent of the submission can be apprendent of the submission can be apprendent of the submission can be apprendent.	natory note so that they can be linked to the nay fail if you try to do more than this - just try again be larger.
Drop files here or click to upload.	
Sequences	- Sequence details
You are submitting the following abcZ sequences: Download ras           Identifier         Length         Sequence         Status         Query         Assigned allele           NM322         433         TTGATACCGTTGCCGAAGG         GCGGATTGTCGAACTCGATC         pending         Q           NM21         433         TTTGATACCGTTGCCGAAGG         GCGGATTGTCGAACTCGATC         pending         Q	technology:! Ilumina ~ read length:! 200-299 ~ coverage:! 20-49x ~ assembly:! de novo ~ assembly: Velvet Sequence length outside usual range <b>1</b>
E-mailAction	
Updates will be sent to keith.jolley@zoo.ox.ac.uk. Finalize submission!	
E-mail submission updates	
Message: Append	
indexage. 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 expropriate 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 ca	planatory note so that they can be linked to the d may fail if you try to do more than this - just try again n be larger.
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! Jlumina ~ read length.! 200-299 ~ coverage! 20-49x ~ assembly! de novo ~ assembly: oftware! Velvet
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. 	

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.

h fewer files at a time if it does), although you can upload multiple times so that the total size of the submission c	an be larger.
Drop files here or click to upload	d.
Sequences	Sequence details
u are submitting the following abcZ sequences: Download Tras	technology: Ilumina
lantifiar Longth Converse Status Query Accience allele	read length: 200-299 V
NM322 433 TTTGATACTGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending Q	coverage: 20-49x V
NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending Q	assembly software 1 Velvet
	Sequence length outside usual range 1
E-mail — Action — Action	
dates will be sent to keith.jolley@zoo.ox.ac.uk. Finalize submission!	
E-mail submission updates	
Messages	
Timestamp User Message	
Timestamp         User         Message           019-06-28 07:47:22+00         Keith Jolley         The sequence variant NM322 has been seen in 3 isolates.	

# 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 ca	planatory note so that they can be linked to the ad may fail if you try to do more than this - just try again an be larger.
Drop files here or click to upload	d.
- Sequences You are submitting the following abcZ sequences: Download	Sequence details technology:! Illumina v read length:! 200-299 v
Identifier         Length         Sequence         Status         Query         Assigned allele           NM322         433         TTTGATACTGTTGCCGAAGG         GCGGATTGTCGAACTCGATC pending         Q           NM21         433         TTTGATACCGTTGCCGAAGG         GCGGATTGTCGAACTCGATC pending         Q	coverage:   20-49x v assembly:   de novo v assembly software: ! Velvet
E-mail     Action       Updates will be sent to keith.jolley@zoo.ox.ac.uk.     Finalize submission!       Image: Description of the sent to keith.jolley@zoo.ox.ac.uk.     Finalize submission!	
Messages           Timestamp         User         Message           2019-06-28 07:47:22+00         Keith Jolley         The sequence variant NM322 has been seen in 3 isolates.	

The files will be uploaded and shown in a table.

Uploaded files           Filename         Size         Delete           NM322_abcZ_Fab1         296.6 KB	
Delete selected files         Sequences         You are submitting the following abcZ sequences: Download       Fas         Identifier Length       Sequence       Status       Query       Assigned allele         NM322       433       TTTGATACTGTTGCCGAAGG       GCGGATTGTCGAACTCGATC pending       Q         NM21       433       TTTGATACCGTTGCCGAAGG       GCGGATTGTCGAACTCGATC pending       Q	Sequence details technology:1 Illumina ~ read length:1 200-299 ~ coverage:1 20-49x ~ assembly:1 de novo ~ assembly software:1 Velvet Sequence length outside usual range ()
E-mail       Action         Updates will be sent to keith.jolley@zoo.ox.ac.uk.       Finalize submission!         Image: Provide the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequence of the sequ	

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 uploa	ad.
Filename         Size         Delete           NM322_abcZ_F.ab1         296.6 KB	Sequence details
Sequences       Status       Query       Assigned allele         Identifier       Length       Sequence       Status       Query       Assigned allele         NM322       433       TTTGATACCGTTGCCGAAGG       GCGGATTGTCGAACTCGATC       pending       Q         NM21       433       TTTGATACCGTTGCCGAAGG       GCGGATTGTCGAACTCGATC       pending       Q	technology: I flumina read length: I 200-299 coverage: I 20-49x assembly: I de novo assembly software: I Velvet
E-mail     Action       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.	

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: 🚺 📃
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) Link to isolate database</li> <li>genomes (isolate records with associated assembly files) Link to isolate database</li> </ul>		
Pending submissions You have submitted the following submissions that are pending curation: Submission id Submitted Updated Type Details		
BIGSdb_20190628084417_002033_60338 2019-06-28 2019-06-28 alleles 2 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). [+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	submissior	<b>1</b> .	
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.

PubN	<b>ILST</b>	Databa	ase hom	e Cont											
Logged	d in: Keit	h Jolley (ke	e <i>ith).</i> 🔂 Log	out   Change	password							Не	ip 🗹	Toggle: 🚺	Ξ
Mai	nage	e sub	miss	ions											
Sub	mit n	ew MLS	T profil	es											
Past	e in yo	ur profiles	s for assig	gnment usi	ng the terr	iplate ava	lable below	N.							
	• Down	load tab-	delimited	header fo	r your spre	eadsheet -	use 'Paste	e Special	Text' to paste the	data.					
1	<ul> <li>Down</li> </ul>	lload sub	mission to	emplate (xl	sx format)										
	Please	paste in t	tab-delim	ited text (ir	nclude a f	ield head	ler line)—				Action —				
10	1	abcZ 8	adk 5	aroE 32	fumC 2	gdh 6	pdhC 43	pgm 32		_   L	Submit				
		5	7	3	6	33	12	2							
		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.

PubMLST Da	tabase hom	e Conte	ents								
Logged in: Keith Joli	ley (keith). 🔂 Log	out   Change	password						Help 📝	Toggle: 🚺	Ξ
Manage s	ubmissi	ions									
Error Row 4	r: 4: Profile has a MLST profile	already be	en defined	l as ST-44							
Paste in your pr • Download • Download	ofiles for assig tab-delimited submission te	inment usi header foi emplate (xi	ng the tem r your spre sx format)	iplate avai eadsheet -	lable belov use 'Paste	ø. e Special <b>€</b> Text' to	o paste the data.				
Please past id abc 8 5 3 9	e in tab-delim Z adk 5 7 2 6	ited text (ir aro£ 32 3 4 9	nclude a f fumC 2 6 3 9	field head gdh 6 33 8 9	pdhC 43 12 4 6	pgm 32 2 6 9		- Action Submit			

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). HoLog out   Change password	elp 🖪	Toggle: 🚺	Ξ
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 Please see the submission guide for details. Every newly defined ST should have a representative isolate record in the isolate database. Your so rejected if you do not do this.	to this su submissi	ubmission ion will be	
Action Abort submission! Submission: BIG Sdb_20190628091104_018718_08755			
Supporting files			
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 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.           Profiles         E-mail	do more	than this	
You are submitting the following MLST profiles: Download solution to keith.jolley@zoo.ox.ac.uk.			
Identifier abcZ adk aroE fumC gdh pdhC pgm Status Query Assigned ST       Image: Constraint of the submission updates         Row 1       8       5       32       2       6       43       32       pending Q       Image: Constraint of the submission updates         Row 2       5       7       3       6       33       12       2       pending Q       Image: Constraint of the submission updates         Row 3       3       2       4       3       8       4       6       pending Q       Image: Constraint of the submission has been made - BIGsdt_20190530060244_022168_38354       Finalize Submission       Finalize Submission			

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.

just try agai	in with	h fewer fi	les at a	time if	it does	), althc	ough you	can uj	load multiple times so that the total size of the submission can be larger	
						Dro	op file	s h	ere or click to upload.	
Profiles	nitting	g the follo	wing M	LST pr	ofiles:   pdhC 43	Downlo	oad csv Status	Querj	E-mail     Updates will be sent to keith.jolley@zoo.ox.ac.uk.      ✓E-mail submission updates     ✓Action	
Row 1	8	5 32 7 3	6	33	12	2	pending	Q	Tingling submission!	
Identifier a Row 1 Row 2 Row 3	8 5 3	5 32 7 3 2 4	6	33 8	12 4	2 6	pending pending	Q Q	Finalize submission!	
Identifier Row 1 Row 2 Row 3 -Messages	8 5 3	5 32 7 3 2 4	63	33 8	12 4	2 6	pending pending	Q	Finalize submission!	

## 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!'.

ust try ag	ain wit	th fewer	files at a	time if	it does	s), although you	can upload multipl	le times so that the total size of the submission can be larger.
						Drop file	es here or	click to upload.
Profiles					rofiles			E-mail
ou are su	bmittin	g the fo			ndhC	nom Status		E-mail submission updates
ou are su dentifier Row 1	abcZ	g the fo	roE fum	C gdh	pdhC	pgm Status	Query Assigned	ST E-mail submission updates
ou are su dentifier Row 1 Row 2	bmittin abcZ 8 5	g the fo adk a 5 7	roE fum 32 2 3 6	C gdh 6 33	pdhC 43 12	pgm Status 32 pending 2 pending	Query Assigned Q Q	ST CE-mail submission updates
dentifier Row 1 Row 2 Row 3	abcZ 8 5 3	g the fo adk a 5 7 2	roE fum 32 2 3 6 4 3	C gdh 6 33 8	pdhC 43 12 4	pgm Status 32 pending 2 pending 6 pending	Query Assigned Q Q Q Q	ST       ☑ E-mail submission updates         Action
dentifier Row 1 Row 2 Row 3 Message	bmittin abcZ 8 5 3	g the fo adk a 5 7 2	roE fum 32 2 3 6 4 3	C gdh 6 33 8	pdhC 43 12 4	pgm Status 32 pending 2 pending 6 pending	Query Assigned Q Q Q	ST E-mail submission updates Action Finalize submission!
dentifier Row 1 Row 2 Row 3 Message	abcZ 8 5 3 es	g the fo	roE fum 32 2 3 6 4 3	C gdh 6 33 8	pdhC 43 12 4	pgm Status 32 pending 2 pending 6 pending	Query Assigned Q Q Q	ST E-mail submission updates Action Finalize submission!
entifier Row 1 Row 2 Row 3 Message Tim 019-06-2	bmittin abcZ 8 5 3 es estan 28 08:1	g the fo adk a 5 7 2 1p 6:16+0	Ilowing N           roE         fum           32         2           3         6           4         3           Use         Use           0         Keith J	C gdh 6 33 8 er Iolley C	pdhC 43 12 4	pgm Status 32 pending 2 pending 6 pending	Query Assigned Q Q Q Q	ST       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 State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State State Stat
are su dentifier Row 1 Row 2 Row 3 Message Tim 019-06-2	abcZ 8 5 3 es estan 28 08:1	g the fo adk a 5 7 2 10 6:16+0	Iowing N           roE         fum           32         2           3         6           4         3           Use         0           Keith J	C gdh 6 33 8 er Iolley C	pdhC 43 12 4 Corresp	pgm Status 32 pending 2 pending 6 pending onding isolate s	Query Assigned Q Q Q ubmission has bee	ST       Image: State of the Kellinging (getter out, det data)         Action       Finalize submission!         Message       Message         en made - BIGSdb_20190530060244_022168_38354.

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 lds.</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 S Text' 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.

PubMLST	Datab	ase hom	e Cont												
.ogged in: Kei	ith Jolley (F	ke <i>ith).</i> 🔂 Log	out   Change	password								Не	ip 🗹	Toggle: 🔒	-
lanag	e sub	missi	ions												
Submit r	new isol	ates													
Paste in yo	our isolate	es for addi	tion to the	database	using the	e template a	ivailable t	pelow.							
• Ente	er aliases	(alternativ	e names)	for your is	olates as	a semi-colo	on (;) sep	arated list							
<ul> <li>Ente</li> <li>You</li> </ul>	er referen can also	ces for yo upload ad	ur isolates ditional all	as a semi ele fields a	i-colon (;) along with	) separated i the other i	list of Pul solate da	bMed ids. ta - simply	create a new	r colur	mn with the locus name.				
• Dow	nload tab	-delimited	header fo	r vour spr	eadsheet	t - use 'Past	e Special	S Text' to	paste the da	ita.					
• Dow	Inload sub	omission te	emplate (xl	sx format)				•							
Please	e paste in	tab-delim	ited text (ii	nclude a	field hea	ader line)-					- Action —				
ceftria cefota:	axone_ra xime ran	inge ige	chlora rifamp	mphenico icin	ol chlor rifan	ramphenico mpicin rar	ol_range nge	cefot cipro	axime floxacin	^	Submit				
ciprof	loxacin	range	tetrac	ycline	cefix	kime -	azith	romycin							
aroE	fumC	gdh	pdhC	privat	PorA	VR1	PorA	VR2	adk FetA_VR						
gyrA UK322	penA	rpoB	UK		_	-	_		_						
2019							_	menir	ngitis and						
C	aemia	D1000		Neisse	eria mer	iingitiais	5								
							2	3	4						
3 UK325	8	4	6 UK	5	2	F1-5									
2019 CSF		Neisse	ria meni	ngitis				septi	caemia						
W															
							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). 🕒 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			
Deste in your isolates for addition to the database using the template available below			
Este ni your isolates for addition to the database using the template available below.			
<ul> <li>Enter references 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.			
Download tab-delimited header for your spreadsheet - use 'Paste Special S Text' to paste the data.			
Download submission template (disk format)			
Please paste in tab-delimited text (include a field header line) Action			
date sampled non culture epidemiological_year age_yr age_mth sex			
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_range tetracycline cefixime azithromycin			

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	Data	base ho	me Contents															
Logged in: Keit	h Jolley	(keith). 🔂	og out   Change password													Help 🗗	Toggle: 🚺	Ξ
Manage	e sul	bmiss	sions															
New MLS If your isola ensures that	T prof te recor at your \$	<b>iles?</b> rd contair STs will be	ns a new combination of e assigned and that you	MLST alle get notifie	eles, please also mak ed of these assignme	e a new profil nts.	e subr	nissic	on to t	he sequ	ience	e datab	ase. F	Please see ti	he submissio	on guide fo	r details. Th	nis
Submissi —Isolates	Ac At on: Bl	tion ort subm GSdb_2	ission! 20191204090508_01	7012_99	933													
You are s	ubmittin	g the foll	owing isolates: Downloa	d csv														
isolate	countr	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	jes —				E-mail					Actio	۱—							
I think will al definit definit	UK325 so sub ion fo ion da	has a mit a n r this tabase.	new MLST profile. I ew profile to the sequence Message: Appen	∧ Up v ⊡ d	odates will be sent to	keith.jolley@a	200.0X.	ac.uk	с. (	Finali	ze su	bmissio	on!					

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	submitting	the fo	_20191204090	Downloa	d csv												
isolate	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	-
-Messa 2019-1:	ages fimestam 2-04 09:08	р 8:41+0	User 0 Keith Jolley I	think UK3	25 has a new l	MLST profile.	l will a	ilso si	ubmit a	Messa a new p	age profile	definit	iion fo	r this to the	sequence d	efinition da	itabase

# 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 ′ou are :	es submitting	g the fo	pllowing isolates:	Downloa	d csv												
isolate	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	-
- Messa T 2019-12	ages Timestam 2-04 09:08	р 8:41+0	User 0 Keith Jolley I	think UK3	25 has a new l	MLST profile.	l will a	IISO SI	ubmit a	Messa a new p	age profile	definit	ion fo	r this to the	sequence d	efinition da	itabase

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 s	submission.		
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 idSubmittedUpdatedTypeDetailsBIGSdb_20190628093907_003732_267332019-06-282019-06-28isolates2			

# 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	/ 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:**

• with\_pk [integer] - Set to non-zero value to only show indexed schemes, i.e. those with a primary key field that defines each unique combination of alleles, e.g. MLST.

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:

```
(echo -n '{"base64":true,"sequence": "'; base64 contigs.fasta; echo '"}') |
curl -s -H "Content-Type: application/json" -X POST "http://rest.pubmlst.org/db/
→pubmlst_neisseria_seqdef/schemes/l/sequence" -d @-
```

**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_
20151013081	836_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				
Tou will be able to revoke access for any application at any unite.				

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. H8CjIS8Ikq6hwCUqUfF1l4pTaCY18Ljw
- 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:

- alternative start codon
  - A start codon other than ATG, GTG, or TTG is used. This can be the case with some yeasts.
- · 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:

- alternative start codon
  - A start codon other than ATG, GTG, or TTG is used. This can be the case with some yeasts.
- 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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