# **BIGSdb Documentation**

Release 1.9.0

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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/.

# **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 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

# 1.7 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.

# **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
- Perl
- 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.

- DBI Database Independent interface module used to interact with databases.
- DBD-Pg PostgreSQL database driver for DBI.
- XML::Parser::perlSAX part of libxml-perl Used to parse XML configuration files.
- · Log::Log4perl Configurable status and error logging
- Log::Dispatch::File Object for logging to file
- Error Exception handling

- Config::Tiny Configuration file handling
- Bio::Biblio this used to be part of BioPerl but will need to be installed separately if using BioPerl 1.6.920 or later
- IO::String
- Data::UUID Globally unique identifer handling for preference storage
- List::MoreUtils
- Time::Duration [optional] Used by Job Viewer to display elapsed time in rounded units
- Excel::Writer::XLSX Used to export data in Excel format
- Parallel::ForkManager Required for multi-threading autotagger and autodefiner scripts.

#### 2.1.3 Optional packages

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

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

#### 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 contents of the javascript directory to a javascript directory within the web root tree, i.e. accessible from http://your\_website/javascript/.
- 5. Copy the bigsdb.css stylesheet to the root directory of your website, i.e. accessible from http://your\_website/bigsdb.css.
- 6. Copy the images directory to the root directory of your website, i.e. accessible from http://your\_website/images.
- 7. 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.
- Create a PostgreSQL database user called apache this should not have any special priveleges. 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';
```

9. Create PostgreSQL databases called bigsdb\_auth, bigsdb\_prefs and refs using the scripts in the sql directory. Create the database using the createdb command and set up the tables using the psql command, e.g.

createdb bigsdb\_auth psql -f auth.sql bigsdb\_auth

- 10. Create a writable temporary directory in the root of the web site called tmp, i.e. accessible from http://your\_website/tmp.
- 11. 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/

#### 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
# IPv4 local connections:
host
      all all
                             127.0.0.1/32
                                                  md5
# IPv6 local connections:
host
       all
                 all
                            ::1/128
                                                  md5
```

#### pg\_ident.conf

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

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

```
listen_addresses = '*'
max_connections = 200
shared_buffers = 1024Mb
work_mem = 8Mb
```

effective\_cache\_size = 8192Mb
stats\_temp\_directory = '/dev/shm'

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

See Tuning Your PostgreSQL Server for more details.

Restart PostgreSQL after any changes, e.g.

```
/etc/init.d/postgresql restart
```

# 3.3 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.

#### 3.4 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. Note that CRON does not like '.' in executable filenames, so either rename the script to 'bigsjobs' or create a symlink and call that from CRON, e.g.:

copy bigsjobs.pl to /usr/local/bin
sudo ln -s /usr/local/bin/bigsjobs.pl /usr/local/bin/bigsjobs

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

(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
* * * * * bigsdb sleep 30;xvfb-run -a /usr/local/bin/bigsjobs
```

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
```

#### 3.5 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
```

#### 3.6 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
}
```

# 3.7 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.  $1.8.0 \rightarrow 1.8.1$ , 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. The version number is stored with the bigsdb.pl script, so this should also be updated so that BIGSdb correctly reports its version.

#### **Database setup**

There are two types of BIGSdb database:

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

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

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

# 4.1 Creating databases

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

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

```
sudo su postgres
```

then

```
createdb bigsdb_test_seqdef
psql -f seqdef.sql bigsdb_test_seqdef
```

#### Create an isolate database the same way::

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

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

psql bigsdb\_test\_isolates

and alter the isolate table::

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

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

# 4.2 Database-specific configuration

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

- config.xml the database configuration file. Fields defined here correspond to fields in the isolate table of the database.
- banner.html optional file containing text that will appear as a banner within the database index pages. HTML markup can be used within this text.
- header.html HTML markup that is inserted at the top of all pages. This can be used to set up site-specific menubars and logos.
- footer.html HTML markup that is inserted at the bottom of all pages.
- curate\_header.html HTML markup that is inserted at the top of all curator's interface pages.
- curate\_footer.html HTML markup that is inserted at the bottom of all curator's interface pages.

#### 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 and sample elements must match the physical structure of the database isolate and sample tables respectively.:

<db>

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

<system>

• db

- name of database on system

- required
- dbtype
  - type of database: either 'isolates' or 'sequences'
  - required
- · description
  - Description of database used throughout interface
  - required
- authentication
  - method of authentication: either 'builtin' or 'apache'. See user authentication.
  - required
- webroot
  - URL of web root, which can be relative or absolute. The bigsdb.css stylesheet file should be located in this directory. Default '/'.
  - optional
- view
  - database view containing isolate data, default 'isolates'
  - optional
- script\_path\_includes
  - partial path of the bigsdb.pl script used to access the database. See user authentication.
  - optional
- curate\_path\_includes
  - partial path of the bigscurate.pl script used to curate the database. See user authentication.
  - optional
- noshow
  - comma-separated list of fields not to use in breakdown statistic plugins
  - optional
- 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
  - optional
- 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.
  - optional
- read\_access
  - describes who can view data: either 'public' for everybody, 'authenticated\_users' for anybody who has been able to log in, or 'acl' (access control list) for fine-grained access control to individual isolate records. Default 'public'.

- optional
- write\_access
  - describes who can curate isolate records: either 'acl' (access control list) for fine-grained access control to individual isolate records, or leave empty for anybody with curator permission to alter isolate records.
  - optional
- 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).
  - optional
- 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'.
  - optional
- use\_temp\_scheme\_table
  - sets whether entire schemes are imported in to the isolate database in to an indexed table rather than querying the seqdef scheme view for isolate results tables. Under some circumstances this can be considerably quicker than querying the seqdef scheme view (a few ms compared to >10s if the seqdef database contains multiple schemes with an uneven distribution of a large number of profiles so that the Postgres query planner picks a sequential rather than index scan). This scheme table can also be generated periodically using the update\_scheme\_cache.pl script to create a persistent cache. This is particularly useful for large schemes (>10000 profiles) but data will only be as fresh as the cache so ensure that the update script is run periodically.
  - optional
- labelfield
  - field that is used to describe record in isolate info page, default 'isolate'
  - optional
- tblastx\_tagging
  - sets whether tagging can be performed using TBLASTX: either 'yes' or 'no', default 'no'.
  - optional
- host
  - host name/IP address of machine hosting isolate database, default 'localhost'
  - optional
- port
  - port number that the isolate host is listening on, default '5432'
  - optional
- user
  - username for access to isolates database, default 'apache'
  - optional
- password

- password for access to isolates database, default 'remote'
- optional
- privacy
  - displays E-mail address for sender in isolate information page if set to 'no'. Default 'yes'.
  - optional
- 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
  - optional
- sets
  - use sets: either 'yes' or 'no', default 'no'.
  - optional
- set\_id
  - Force the use of a specific set when accessing database via this XML configuration: Value is the name of the set.
  - optional
- only\_sets
  - when defined, don't allow option to view the 'whole database' only list sets that have been defined: either 'yes' or 'no', default 'no'.
  - optional
- views
  - comma-separated list of views of the isolate table defined in the database. This is used to set a view for a set.
  - optional
- all\_plugins
  - enable all appropriate plugins for database: either 'yes' or 'no', default 'no'.
  - optional
- job\_priority
  - Isolate databases only: Integer with default job priority for offline jobs (default:5) (Version v1.7+)
  - optional
- dbase\_job\_quota
  - isolate databases only:Integer with number of offline jobs that can be queued or currently running for this database (Version 1.7+)
  - optional
- 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. (Version 1.7+)

- optional
- 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. (Version 1.7+)
  - optional
- default\_seqdef\_script
  - isolate databases only: URL of BIGSdb script running the seqdef database (default: '/cgibin/bigsdb/bigsdb.pl'). (Version 1.7+)
  - optional
- 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. (Version 1.7+)
  - optional
- no\_publication\_filter
  - isolate databases only: Switches off display of publication filter in isolate query form by default: either 'yes' or 'no', default 'no'. (Version 1.8+)
  - optional
- seqbin\_size\_threshold
  - Sets the size values in Mbp to enable for the *seqbin filter*.
  - Example: seqbin\_size\_threshold="0.5,1,2,4".
  - optional

#### <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>pandemic</option>

</optlist>

</field>

• type
```

- data type: int, text, float or date
- required
- min
  - minimum value for integer types.(introduced in v1.7)
  - optional

• max

- maximum value for integer types. Special values such as CURRENT\_YEAR can be used. (introduced in v1.7)
- optional
- required
  - is data required for this field? 'yes' or 'no', default 'yes'
  - optional
- maindisplay
  - is field displayed in main table after database search? 'yes' or 'no', default 'yes'. This setting can be overridden by individual user preferences.
  - optional
- length
  - length of field, default 12
  - optional
- optlist
  - does this field have a list of allowed values? default 'no'. Surround each option with an <option> tag
  - optional
- 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.
  - optional
- comments
  - comments about the field
  - optional
- 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.
  - optional
- regex
  - regular expression used to constrain field values, e.g. regex="^[A-Z].\*\$" forces the first letter of the value to be capitalized.
  - optional

#### **Special values**

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

• CURRENT\_YEAR: the 4 digit value of the current year

#### <sample>

Element content: Sample field name + optional list <optlist> of allowed values. Attributes are essentially the same as isolate field attributes, but refer to the samples table rather than the isolates table.

The sample table, if defined, must include isolate\_id and sample\_id fields, which must also be described in the XML file. These must be set as integer fields.

#### 4.3.2 Sequence definition database XML attributes

<db>

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

<system>

- db
  - name of database on system
  - required
- dbtype
  - type of database: either 'isolates' or 'sequences'
  - required
- · description
  - description of database used throughout interface
  - required
- authentication
  - method of authentication: either 'builtin' or 'apache'. See user authentication.
  - required
- webroot
  - URL of web root, which can be relative or absolute. The bigsdb.css stylesheet file should be located in this directory. Default '/'
  - optional
- script\_path\_includes
  - partial path of the bigsdb.pl script used to access the database. See user authentication.
  - optional
- curate\_path\_includes
  - partial path of the bigscurate.pl script used to curate the database. See user authentication.
  - optional
- 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'.
  - optional

- disable\_seq\_downloads
  - prevent users or curators from downloading all alleles for a locus (admins always can). 'yes' or 'no', default 'no'.
  - optional
- materialized\_views
  - enable materialized views: either 'yes' or 'no', default 'no'.
- allele\_flags
  - enable flags to be set for alleles: either 'yes' or 'no', default 'no'.
- 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).
- sets
  - use sets: either 'yes' or 'no', default 'no'.
  - optional
- set\_id
  - force the use of a specific set when accessing database via this XML configuration: Value is the name of the set.
  - optional

# 4.4 User authentication

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

#### 4.4.1 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'.

#### 4.4.2 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.

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

# 4.5 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).:

```
INSERT INTO users (id, user_name, surname, first_name, email, affiliation, status, date_entered,
datestamp, curator) VALUES (1, 'keith', 'Jolley', 'Keith', 'keith.jolley@zoo.ox.ac.uk',
'University of Oxford, UK', 'admin', 'now', 'now', 1);
```

If you are using built-in authentication, set the password for this user using the *add\_user.pl* script. This encrypts the password to a hash 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).

# 4.6 Updating PubMed citations

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 getrefs.pl and can be found in the scripts/maintenance directory. This script needs to know which BIGSdb databases and tables it needs to search for PubMed ids. These are listed in a configuration file (usually called getrefs.conf) which contains two columns - the first is the name of the database, the second is a comma-separated list of tables to search, e.g.

```
pubmlst_bigsdb_neisseria_isolates
pubmlst_bigsdb_neisseria_seqdef
```

refs
profile\_refs,sequence\_refs,locus\_refs

The script can be called as follows:

getrefs.pl getrefs.conf

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

### 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 three 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. Individual isolate records may not be available to every user if access control lists (ACLs) are configured for the database.
- 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 Curator permissions

Individual permissions can be set for each curator:

- disable\_access if set to true, this user is completely barred from access.
- modify\_users allowed to add or modify user records. They can change the status of users, but can not revoke admin priveleges 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\_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\_isolates allowed to add or modify isolate records.
- modify\_isolates\_acl allowed to control who accesses isolate records (provided they themselves have access to a particular isolate).

- 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).

Permissions can be set by clicking the '+' button next to 'user permissions' on the curator's interface:

Users: Add	Query/upda		ies)   Curator's page (database)									
gged in: Keith Jolley (keith). Log out	Change pas	sword										
atabase curator's	interf	ace - Neisser	ia PubMLST									
Datasets												
his database contains multiple o	tatacete Vo	u can choose to display	a single set or the whole database.									
			a single set of the whole database.									
lease select: Whole database	Choose											
Add, update or delet	Bat	tch										
Record type	Add Ad		lelete Comments									
users	+ +											
user groups	+ +		Users can be members of these groups - use for setting access permissions.									
user group members	+ +		Add users to groups for setting access permissions.									
user permissions	+ +	+ ?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.									
isolates	+ +	+ query   brows batch upo	e   list									
isolate field extended attribute values	+ +	+ ?	Add values for additional isolate field attributes.									
projects	+ +	+ ?	Set up projects to which isolates can belong.									
project members	+ +	+ ?	Add isolates to projects.									
isolate aliases	+ +	+ ?	Add alternative names for isolates.									
PubMed links	+ +	+ ?										
allele designations	+	+ ?	Allele designations can be set within the isolate table functions.									
sequences	+ +	+ ?	The sequence bin holds sequence contigs from any source.									
accession number links	+ +	+ ?	Associate sequences with Genbank/EMBL accession number.									
experiments	+ +	+ ?	Set up experiments to which sequences in the bin can belong.									
experiment sequences		?	Add links associating sequences to experiments.									
sequence tags	scan	?	Tag regions of sequences within the sequence bin with locus information.									
Database configurat	ion											
Table	Add Batc	h Add Update or delete	Comments									
loci		+ ?										
	databank											
locus aliases	+ +	+ ?	Add alternative names for loci. These can also be set when you batch add loci.									

Set specific permissions and then click 'Submit'.

	g out   Change password	1	Toggle:
dd new user pe	ermission r	ecord	
Please fill in the fields below	- required fields are	marked with an exclamation mark (!).	
Record			Action
user id:	Jolley, Keith	<b>*</b>	Reset Submit
disable access:	◯ true ◯ false	disable all access to this user.	Treser Oublinit
modify users:	🖲 true 🔘 false	allow user to add or modify users.	
modify usergroups:	◯ true ◯ false	allow user to create or modify user groups and add users to these groups.	
set user passwords:	◯ true  ◯ false	allow user to modify other users' password.	
modify loci:	🔘 true 🔘 false	allow user to add or modify loci.	
modify schemes:	🔘 true 🔘 false	allow user to add or modify schemes.	
modify sequences:	🖲 true 🔘 false	allow user to add sequences to the database.	
modify isolates:	🔍 true 🔘 false	allow user to add or modify isolate records.	
modify isolates acl:	◯ true  ◯ false	allow user to control who accesses isolate records.	
modify projects:	🔍 true 🔘 false	allow user to add isolates to project groups.	
modify composites:	🔘 true 🔘 false	allow user to add or modify composite fields (fields made up of other fields, including scheme fields).	
modify field attributes:	🔘 true 🔘 false	allow user to setup or modify secondary attributes for isolate record fields.	
modify value attributes:	🔘 true 🔘 false	allow user to add or modify secondary attribute values for isolate record fields.	
modify probes:	🔘 true 🔘 false	allow user to define PCR or hybridization reactions to filter tag scanning.	
tag sequences:	🖲 true 🔘 false	allow user to tag sequences with locus information.	
designate alleles:		allow user to designate locus allele numbers.	
	🔘 true 🔘 false	allow user to add or modify sample storage location records.	

If permissions have already been set for a user, click the 'Update or delete' link on the curator's page instead.

gged in: Keith Jolley (keith). Log out								
atabase curator's	; int	terface	- Neisse	ria PubMLST				
Datasets								
- Datasets								
his database contains multiple (	datase	ets. You can c	hoose to displa	y a single set or the whole database.				
lease select: Whole database		Change						
whole database	• •	choose						
1								
Add, update or dele	te re	cords						
		Batch						
Record type	Add	Add	Update or d	lelete Comments				
users	+	++	?					
user groups	+	++	2	Users can be members of these groups - use for setting access permissions.				
user group members	+	++	2	Add users to groups for setting access permissions.				
user permissions	+	++	2	? Set curator permissions for individual users - these are only active for users with a status of 'cur.				
				in the users table.				
isolates	+	++	query   brows batch upo					
isolate field extended attribute values	+	++	?	Add values for additional isolate field attributes.				
projects	+	++	?	Set up projects to which isolates can belong.				
project members	+	++	?	Add isolates to projects.				
isolate aliases	+	++	?	Add alternative names for isolates.				
PubMed links	+	++	?					
allele designations		++	?	Allele designations can be set within the isolate table functions.				
sequences	+	++	?	The sequence bin holds sequence contigs from any source.				
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.				
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.				
experiment sequences			?	Add links associating sequences to experiments.				
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.				
S.								
Database configurat	tion							
Table	Add	Batch	Update or	Comments				
		Add	delete					
loci	+	++	?					
	date	abank scan						
locus aliases	- uaia	++	?	Add alternative names for loci. These can also be set when you batch add loci.				

then search for the user by entering specific criteria, or simply press 'Submit' to display all users. Update a specific user by clicking on the 'Update' link next to their name.

Publ	PublicIST         Database: Species home   Curator's page (species)   Curator's page (database)           Users: Add   Query/update         Isolates: Add   Query/update   Batch insert           Logged in: Keith Jolley (Keith). Log out   Change password         Toggle: if																	
Logged in	: Keith Jo	lley (keith). Lo	g out   Change pas	sword														Toggle: i
Quer	y use	er perm	nissions	for Neis	seria P	PubM	ILST d	latabas	se									
	-		eria below (or le	ave blank and	submit to ret	urn all re												
	arch crite			-			— — Dis				_							
user	r id (id)	-	- •			+ [		rder by: use Display: 25		rds ner n		ending 👻						
	ilter quer		Action					nopiaj. 20	• 1000									
P	iller quer	y by																
			Reset	Submit														
9 records	o roturno	d																
Dele			ase configuration															
Dele	te ALL	Export	configuration/da	ta														
Delete	Update	user id	disable modify		set user	modify	modify	modify	modify	modify isolates	modify	modify	modify field	modify value	modify		designate	
			access users	usergroups	passwords	loci	schemes	sequences	isolates	acl	projects	composites		attributes	probes	sequences	alleles	management
	Update Update	Jolley, Keith Bennett,						true	true							true	true	
Delete	Opuale	Julia	true					true	true							true	true	
Delete	Update	Feavers, Ian	true					false	true		false					false	true	
Delete	Update		true					true	true		true					true	true	
Delete	Undata	Carina Hong, Eva	true						true								true	
	Update		uue						uue							true	true	
		Holly																
Delete	Update	Harrison, Odile	true			true	true	true	true		true					true	true	
Delete	Update	Hill, Dorothea	true					true	true		true					true	true	
Delete	Update	Pannekoek, Yvonne														true	true	
		tvonne																

# 5.3 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':

atabase curator			word		/ 1 8** */*	
	's I	nterfa	ice - Neis	seria locu	is/sequence definitions	
🞽 Add, update or de	elete	records				
Record type	Add	Batch Add	Update	or delete	Comments	
users	+	++		?		
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.	
user group members	+	++		?	Add users to groups for setting access permissions.	
user permissions	+	++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.	
locus descriptions	+	++		?		
scheme curator control list	+	++	query	batch	Define which curators can add or update profiles for particular schemes.	
locus curator control list	+	++	query	batch	Define which curators can add or update sequences for particular loci.	
sequences (all loci)	+	++   FASTA		?		
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.	
ubMed links (to sequences)	+	++		?		
MI OT profiles			query I browse I	list   batch update		
MLST profiles	+	++	query promote j			
rplF species profiles	+	++		list   batch update		
rpIF species profiles	+	**				
rpIF species profiles PubMed links (to profiles)	+	++ ++ on Batch	query   browse   Update or			
rpIF species profiles PubMed links (to profiles) Database configu Table	+ + ratio	++ ++ m Batch Add	query   browse   Update or delete			
rpIF species profiles PubMed links (to profiles) Database configu Table Ioci	+ + ratio	++ ++ Batch Add ++	query   browse   Update or delete ?	list   batch update	Comments	
rpIF species profiles PubMed links (to profiles) Database configu Table Ioci Iocus aliases	+ + ratio	++ ++ Batch Add ++ ++	query   browse   Update or delete ? ?	list   batch update	Comments	
rpIF species profiles PubMed links (to profiles) Database configu Table Ioci Iocus aliases Iocus extended attributes	+ + ratio	+++ +++ Batch Add +++ +++	uery browse   Update or delete ? ? ?	list   batch update Add alternative nam Define additional fie	Comments nes for loci. These can also be set when you batch add loci. elds to associate with sequences of a particular locus.	
rpIF species profiles PubMed links (to profiles) Database configu Table Ioci Iocus aliases	+ + ratio	++ ++ Batch Add ++ ++	Update or delete ? ? ? ?	list   batch update Add alternative nam Define additional fie	Comments tes for loci. These can also be set when you batch add loci. alds to associate with sequences of a particular locus. Is that use locus allele or scheme profile definitions defined in this database - this enables baddlinks and searches of the	se databases when you query
rpIF species profiles PubMed links (to profiles) Database configu Table Ioci Iocus aliases Iocus extended attributes	+ + ratio	+++ +++ Batch Add +++ +++	query   browse   Update or delete ? ? ? ?	list   batch update Add alternative nam Add isolate databas sequences or profile	Comments tes for loci. These can also be set when you batch add loci. alds to associate with sequences of a particular locus. Is that use locus allele or scheme profile definitions defined in this database - this enables baddlinks and searches of the	se databases when you query
rpIF species profiles PubMed links (to profiles) Database configu Table Iocci Ioccus extended attributes client databases	+ + + Add + + + +	+++ +++ Batch Add ++ +++ +++	query   browse   Update or delete ? ? ? ? ?	Add alternative nam Define additional file Add islate database sequences or profile Define loci that are	Comments tes for loci. These can also be set when you batch add loci. taids to associate with sequences of a particular locus. tes that use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of the s in this database.	se databases when you query
rpIF species profiles PubMed links (to profiles) Database configu Table locus extended attributes client database loci client database fields linked	+ + + Add + + + + + +	++ ++ Batch Add ++ ++ ++	update or delete ? ? ? ? ? ? ? ? ? ? ? ?	Add alternative nam Define additional file Add isolate databass sequences or profile Define loci that are Define ioci that are	Comments Nes for loci. These can also be set when you batch add loci. Alds to associate with sequences of a particular locus. es that use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of the s in this database.	se databases when you query
rpIF species profiles PubMed links (to profiles) Database configu Table Iocis Iocus aliases client database loci client database schemes	+ + + Add + + + + + +	++ ++ Batch Add ++ ++ ++ ++ ++	uery browse   Update or delete ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Add alternative nam Define additional fi Add isolate databass sequences or profile Define loci that are Define loci that are Define fields in clier	Comments bies for loci. These can also be set when you batch add loci. bies for loci. These can also be set when you batch add loci. bies to associate with sequences of a particular locus. bies that use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of the sin this database. bies din dient databases. bies used in client databases. You will need to add the appropriate loci to the client database loci table. bit database whose value can be displayed when isolate has matching allele.	se databases when you query
rpIF species profiles PubMed links (to profiles) Database configu Table loci locus adlases client database loci client database loci client database schemes client database fields linked to loci	+ + + + + + + + + + + + + + + +	+++ +++ Batch Add +++ +++ +++ +++	update or delete ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Add alternative nam Define additional file Add isolate databas sequences or profile Define loci that are i Define inclimes that Define fields in dier Desribes schemes co	Comments tes for loci. These can also be set when you batch add loci. alds to associate with sequences of a particular locus. se shat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of the s in this database. used in client databases. Tare used in client databases. You will need to add the appropriate loci to the client database loci table. It database whose value can be displayed when isolate has matching allele. monsisting of collections of loci, e.g. MLST.	se databases when you query
rpIF species profiles PubMed links (to profiles) Database configu Table Iocis aliases Iocus aliases Iocus atiases client database loci client database loci client database schemes client database fields linked to loci schemes	+ + + + + + + + + + + + + +	+++ ++ Batch Add +++ +++ +++ +++ +++ +++ +++	update or delete ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Add alternative nam Define additional factor add isolate databas sequences or profile Define loci that are Define schemes that Define fields in clier Desoribes schemes o Defines which loci b	Comments tes for loci. These can also be set when you batch add loci. alds to associate with sequences of a particular locus. se shat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of the s in this database. used in client databases. Tare used in client databases. You will need to add the appropriate loci to the client database loci table. It database whose value can be displayed when isolate has matching allele. monsisting of collections of loci, e.g. MLST.	se databases when you query
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rpIF species profiles PubMed links (to profiles) Database configu Table Iocis aliases Iocus extended attributes client database schemes client database fields linked to Ioci schemes scheme members scheme groups	+ + + + Add + + + + + + + + + + + +	++ ++ Batch Add ++ ++ ++ ++ ++ ++ ++ ++ ++ ++ ++	uery browse   Update or delete ? ? ? ? ? ? ? ? ? ? ? ? ?	Add alternative nam Define additional file Add isolate databas sequences or profile Define loci that are i Define fields in dier Desribes schemes o Defines which field Defines which field Desribes proups in 1	Comments nes for loci. These can also be set when you batch add loci. alds to associate with sequences of a particular locus. es that use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of the s in this database. used in client databases. You will need to add the appropriate loci to the client database loci table. It database whose value can be displayed when isolate has matching allele. consisting of collections of loci, e.g. MLST. elong to a scheme. belong to a scheme. to which schemes can belong - groups can also belong to other groups.	se databases when you query
rpIF species profiles PubMed links (to profiles) Database configu Table Ioci Iocus atiases Iocus extended attributes client database loci client database schemes client database fields linked to loci scheme members scheme fields scheme groups scheme groups	+ + + + Add + + + + + + + + + + + +	++ ++ Batch Add ++ ++ ++ ++ ++ ++ ++ ++ ++ ++ ++	uery browse   Update or delete ? ? ? ? ? ? ? ? ? ? ? ? ?	Add alternative nam Define additional file Add isolate databas sequences or profile Define loci that are i Define fields in dier Desribes schemes o Defines which field Defines which field Desribes proups in 1	Comments nes for loci. These can also be set when you batch add loci. alds to associate with sequences of a particular locus. es that use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of the s in this database. used in client databases. You will need to add the appropriate loci to the client database loci table. It database whose value can be displayed when isolate has matching allele. consisting of collections of loci, e.g. MLST. elong to a scheme. belong to a scheme. to which schemes can belong - groups can also belong to other groups.	se databases when you query

MLST profiles: Add   Query/update   Batch insert	
Logged in: Keith Jolley (keith). Log out   Change password	
Batch update locus curator access records	
Select user The user status must also be set to curator for permissions to work. Users: Jolley, Keith (keith)  v ([Select])	

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:

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.	Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert
User: Keith Jolley Select values to enable or disable and then click the appropriate arrow button.	Logged in: Keith Jolley (keith). Log out   Change password
Select values to enable or disable and then click the appropriate arrow button.	Batch update locus curator access records
Select loc Available FHbp_segment_E FetA VR NEIS0001 NEIS0001 NEIS0005 NEIS0006 NEIS0006 NEIS0007 NEIS0007 NEIS0008 NEIS008 NEIS08 NEIS008 NEIS008 NEIS08 NEIS08 NEIS08 NEIS08 NEIS	Select values to enable or disable and then click the appropriate arrow button.  Select loc           Select loc         FHbp_segment_D         FHbp_segment_E         FetA VR         NEIS0001         NEIS0005         NEIS0006         NEIS0006         NEIS0007         NEIS0008         NEIS0001         NEIS0001         NEIS0000         NEIS0001         NEIS0000         NEIS0001         NEIS0000         NEIS0000         NEIS0001         NEIS0000         NEIS0001         NEIS0000         NEIS0001         NEIS0000         NEIS0001         NEIS0001         NEIS0001         NEIS0001         NEIS0001         NEIS0001         NEIS0011         All None         All None

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.

## 5.4 Controlling access

#### 5.4.1 Access control lists

If access control lists are in use (set the read\_access attribute to 'acl' in the system tag of the database XML configuration file), viewing and modifying of individual isolates can be restricted to particular users or usergroups.

**Warning:** Please note that access control lists are likely to be deprecated in future releases. This is in favour of creating a new class of user that would be allowed to curate their own data only.

New isolate records are automatically set with the following access control:

- All users: read, not write (all users are members of 'All users' group).
- Curator who added data: read and write.

All access controls can be modified by an admin or curator with appropriate permission. This can be done for individual isolate records or in batch mode following an isolate search in the curation interface.

#### 5.4.2 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.

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.

## 5.5 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 link to 'set user passwords' at the bottom of the curator's index page. Click this.

alla la stan alla a la serie					
allele designations		++	?	Allele designations can be set within the isolate table functions.	
sequences	+	++	?	The sequence bin holds sequence contigs from any source.	
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.	
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.	
experiment sequences			?	Add links associating sequences to experiments.	
sequence tags	\$	scan	?	Tag regions of sequences within the sequence bin with locus information.	
Database configurat	tion				
-		Batch	Update or		
Table	Add	Add	delete	Comments	
loci	+	++	?		
	data	bank scan			
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.	
PCR reactions	+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loc	
nucleotide probes	+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.	
isolate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.	
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.	
sequence attributes	+	++	?	Define attributes that can be set for contigs in the sequence bin.	
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.	
set loci	+	++	?	Add loci to sets.	
set schemes	+	++	?	Add schemes to sets.	
set metadata	+	++	?	Add metadata collection to sets.	
setview	+	++	?	Set database views linked to sets.	
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.	
scheme members	+	++	?	Defines which loci belong to a scheme.	
scheme fields	+	++	?	Defines which fields belong to a scheme.	
	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.	
scheme groups		++	?	Defines which schemes belong to a group.	
scheme groups scheme group scheme members	+				

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

Profitivities: Add   Query/update   Batch insert							
Logged in: Keith Jolley (keith). Log out   Change pas	sword						
Set user password							
User: Jolley, Keith (keith)	*						
New password: •••••							
Retype password:	Set password						

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

### 5.6 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*.

### 5.7 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
              author => 'Keith Jolley',
              affiliation => 'University of Oxford, UK',
              email
                    => 'keith.jolley@zoo.ox.ac.uk',
              description => 'Perform BURST cluster analysis on query results query results',
              category => 'Cluster',
              buttontext => 'BURST',
              menutext => 'BURST',
                       => 'BURST',
              module
              version => '1.0.0',
                        => 'isolates,sequences',
              dbtype
```

```
section => 'postquery',
order => 10,
system_flag => 'BURST',
input => 'query',
requires => 'mogrify',
min => 2,
max => 1000
);
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.

# 5.8 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.

### 5.8.1 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.
```

### 5.8.2 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."
```

# 5.9 Host mapping

During periods of server maintenance, it may be necessary to map a database host to an alternative server. This would allow a backup database server to be used while the primary database server is unavailable. In this scenario, you would probably also want to disable updates. Host mapping can be achieved by editing the /etc/bigsdb/host\_mapping.conf file. Each host mapping is placed on a single line, with the current server followed by any amount of whitespace and then the new mapped host, e.g.

#Existing_host	Mapped_host
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).

## 5.10 Improving performance

#### 5.10.1 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.

#### 5.10.2 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 -d 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.

Note that you will need to run this script periodically as a CRON job to refresh the cache.

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.

#### 5.10.3 Use materialized views for scheme definitions

Because of the way BIGSdb allows any number of profile schemes to be set up, the data are stored in a normalised manner in multiple tables. A database view, e.g. scheme\_1, is created that joins these tables so that they can be queried as you would a single table. A view, however, is only a pre-selected query rather than a physical table and you can not index columns on it to optimise query performance.

A materialized view is a real table that is created from the view and refreshed every time the data in the underlying view changes. Because it is a real table, the database doesn't need to perform these joins every time it is queried and indexes can be set up on it, both of which greatly speeds up querying.

To use materialized views within a sequef database set the following attribute in the system tag of the XML description file:

materialized\_views="yes"

You will then need to run the 'configuration repair' function at the bottom of the administrator's main curation page for each scheme. This rebuilds the view and creates a materialized view called mv\_scheme\_X. This materialized view is updated automatically whenever profile data are added or altered via the web interface.

If you want an isolate database to benefit from this materialized view, make sure you put 'mv\_scheme\_X' (where X is the scheme id) in the dbase\_table field (rather than 'scheme\_X') when setting up the scheme in the isolate database configuration.

Please note that if you make changes to your profile data by means other than the web interface then the materialized view will not be updated. You can update it by running the following SQL command:

```
SELECT refresh_matview('mv_scheme_X');
```

The materialized view is used, for example, for looking up a ST from a profile and vice-versa. Significant speed improvements will only be realised if you have lots of profiles (>5000) and you are doing lots of lookups, e.g. displaying more than the default 25 records per page.

# 5.11 Dataset partitioning

#### 5.11.1 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 and also include additional metadata fields only applicable to that set.

See also:

Sets (concept)

### 5.11.2 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.

sequences				I he sequence bin holds sequence contigs from any source.
accession number links	+	++		Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags	S	can	?	Tag regions of sequences within the sequence bin with locus information.
Database configurat	ion			
Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	datat	oank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
PCR reactions	+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
solate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.
composite fields	+			Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes	+	++		Define attributes that can be set for contigs in the sequence bin.
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.
set loci	+	++	?	Add loci to sets.
set schemes	+	++	?	Add schemes to sets.
setview	+	++	?	Set database views linked to sets.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
cheme group group members	+	++	?	Defines which scheme groups belong to a parent group.
				to log on or change an existing password. and schemes and that required helper applications are properly installed.

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.

Pub	MLST / Breakdown: I	ch   Browse   Profile/ST   List Isolate fields   Scheme/alleles   Publications nts   Home   Options   Profiles/sequences de	finitions	Database sub	missions			
The Nu definiti repres	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.  Datasets This database contains multiple datasets. You can choose to display a single set or the whole database. Please select: Whole database  Choose							
<u>_</u>				Set display     General in     Isolates: 20	I options - including isolati and query options for locu formation 0854 ed: 2014-07-01 tory			
	Breakdown • Single field • Two field • Unique combinations • Scheme and alleles • Publications • Sequence bin	Export • Export dataset • Contigs • Sequences - XMFA / concatenated	I FASTA fo	rmats	Analysis • Codon usage • Presence/absence sta • Genome comparator • BLAST	itus of loci	Miscellaneous <ul> <li>Description of database fields</li> </ul>	

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.

### 5.11.3 Set metadata

Additional metadata fields can be set within the XML configuration file. They are specified as belonging to a metaset by prefixing the field name with 'meta\_NAME:' where NAME is the name of the metaset, e.g.

```
<field type="text" required="no" length="30" maindisplay="no"
optlist="yes">meta_1:clinical_outcome
<optlist>
<option>no sequeleae</option>
```

```
<option>hearing loss</option>
  <option>amputation</option>
  <option>death</option>
  </optlist>
</field>
```

Metaset fields can be defined just like any other *provenance field* and their position in the output is determined by their position in the XML file.

user permissions isolates isolate field extended attribute	+	++	?	)	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the
	+				users table.
isolate field extended attribute		++	query   bro batch u		
values	+	++	?		Add values for additional isolate field attributes.
projects	+	++	?	)	Set up projects to which isolates can belong.
project members	+	++	?	•	Add isolates to projects.
isolate aliases	+	++	?	•	Add alternative names for isolates.
PubMed links	+	++	?		
allele designations		++	?		Allele designations can be set within the isolate table functions.
sequences	+	++	?		The sequence bin holds sequence contigs from any source.
accession number links	+	++	?		Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?		Set up experiments to which sequences in the bin can belong.
experiment sequences			?		Add links associating sequences to experiments.
sequence tags		scan	?	•	Tag regions of sequences within the sequence bin with locus information.
Tabla		atab Add He	adata ar dalata		Commente
			pdate or delete		Comments
loci	+	atch Add Ug ++ ank scan	odate or delete ?		Comments
loci	+	++	?	Add alternative n	Comments ames for loci. These can also be set when you batch add loci.
loci	+ databa	++ ank scan	?		
loci locus aliases	+ databa +	++ ank scan ++	? ?	Set up in silico P	ames for loci. These can also be set when you batch add loci.
loci locus aliases PCR reactions	+ databa + +	++ ank scan ++ ++	? ?	Set up <i>in silico</i> P Define nucleotide	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
loci locus aliases PCR reactions nucleotide probes	+ databa + + +	+++ ank scan ++ ++ ++	? ? ? ? ?	Set up <i>in silico</i> P Define nucleotide Define additional	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.
loci locus aliases PCR reactions nucleotide probes isolate field extended attributes	+ databa + + +	+++ ank scan ++ ++ ++	? ? ? ? ?	Set up <i>in silico</i> P Define nucleotide Define additional Used to construct	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. e probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. I attributes to associate with values of a particular isolate record field.
loci locus aliases PCR reactions nucleotide probes isolate field extended attributes composite fields	+ databa + + + + + +	+++ ank scan +++ ++ ++ ++	? ? ? ? ? ?	Set up <i>in silico</i> P Define nucleotide Define additional Used to construct Define attributes t	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields.
loci locus aliases PCR reactions nucleotide probes isolate field extended attributes composite fields sequence attributes sets set loci	+ databa + 4 + 4 + 4 + 4 + 4 + 4 + 4 + 4 + 4	+++ ank scan 444 444 444 444 444 444 444 444 444 4	? ? ? ? ? ? ? ?	Set up in silico P Define nucleotide Define additional Used to construct Define attributes t Sets describe a co Add loci to sets.	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. e probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. I attributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be set for contigs in the sequence bin. Ollection of loci and schemes that can be treated like a stand-alone database.
loci locus aliases PCR reactions nucleotide probes isolate field extended attributes composite fields sequence attributes sets set loci set schemes	+ databa + + + + + + + + + + + + + +	+++ ank scan +++ 4 +++ 4 ++ 4 \\+++	? ? ? ? ? ? ? ? ?	Set up in silico P Define nucleotide Define additional Used to construct Define attributes to Sets describe a co Add loci to sets. Add schemes to s	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci. I attributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be set for contigs in the sequence bin. ollection of loci and schemes that can be treated like a stand-alone database. ets.
loci locus aliases PCR reactions PCR reactions nucleotide probes isolate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata	+ databa + + + + + + + + + + + + + +	+++ ank scan 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico P Define nucleotide Define additional Used to construct Define attributes to Sets describe a co Add loci to sets. Add schemes to s Add metadata co	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be set for contigs in the sequence bin. ollection of loci and schemes that can be treated like a stand-alone database. ets. liection to sets.
loci locus aliases PCR reactions nucleotide probes isolate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata set view	+ databa + 4 + 4 + 4 + 4 + 4 + 4 + 4 + 4 + 4 + 4	+++ 4 ank scan +++ 4 +++ 4 +++ 4 +++ 4 +++ 4 +++ 4 +++ 4 +++ 4	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in ailico P Define nucleotide Define additional Used to construct Define attributes 1 Sets describe a co Add loci to sets. Add schemes to s Add metadata co Set database view	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. a turbutes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be set for contigs in the sequence bin. collection of loci and schemes that can be treated like a stand-alone database. ets. liection to sets. ws linked to sets.
loci locus aliases PCR reactions nucleotide probes isolate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata set view schemes	+ data ba + 4 + 4 + 4 + 4 + 4 + 4 + 4 + 4	+++ ank scan 444 444 444 444 444 444 444 444 444 4	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico P Define nucleotide Define additional Used to construct Define attributes I Sets describe a co Add loci to sets. Add schemes to s Add ometadata co Set database view Describes scheme	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. a thributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be set for contigs in the sequence bin. collection of loci and schemes that can be treated like a stand-alone database. ets. lilection to sets. we linked to sets. es consisting of collections of loci, e.g. MLST.
loci  locus aliases  PCR reactions nucleotide probes isolate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata set view schemes schemes schemes schemes	+ databa + + + + + + + + + + + + + + + + + +	+++ 7 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico P Define nucleotide Define additional Used to construct Define attributes 1 Sets describe a co Add loci to sets. Add schemes to s Add metadata co Set database view Describes scheme Defines which loc	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci. a ttributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be set for contigs in the sequence bin. ollection of loci and schemes that can be treated like a stand-alone database. ets. liection to sets. ws linked to sets. is consisting of collections of loci, e.g. MLST. is belong to a scheme.
loci locus aliases PCR reactions PCR reactions nucleotide probes isolate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata set view schemes schemes scheme members scheme fields	+ data + + + + + + + + + + + + + + + + + +	+++ ank scan +++ ++ ++ +++ +++ +++ +++ +++ +++ +++	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico P Define nucleotide Define additional Used to construct Define attributes I Sets describe a c Add loci to sets. Add schemes to s Add metadata co Set database view Describes scheme Defines which loc Defines which fiel	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci. a thributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be set for contigs in the sequence bin. ollection of loci and schemes that can be treated like a stand-alone database. ets. lifection to sets. ws linked to sets. is consisting of collections of loci, e.g. MLST. is belong to a scheme. Ids belong to a scheme.
loci locus aliases PCR reactions nucleotide probes isolate field extended attributes composite fields sequence attributes sets set loci set schemes schemes scheme members scheme groups	+ databa + + + + + + + + + + + + + + + + + +	+++ ank scan +++ ++ +++ +++ +++ +++ +++ +++ +++ ++	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico P Define nucleotide Define additional Used to construct Define attributes I Sets describe a co Add loci to sets. Add schemes to s Add metadata co Set database view Describes scheme Defines which fiel Describes groups	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. a turbutes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be set for contigs in the sequence bin. collection of loci and schemes that can be treated like a stand-alone database. ets. liection to sets. ws linked to sets. se consisting of collections of loci, e.g. MLST. is belong to a scheme. lids belong to a scheme. in to which schemes can belong - groups can also belong to other groups.
loci locus aliases PCR reactions nucleotide probes isolate field extended attributes composite fields sequence attributes sets set loci set schemes schemes schemes scheme members scheme fields scheme groups scheme members	+ data + + + + + + + + + + + + + + + + + +	++	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico P Define nucleotide Define additional Used to construct Define attributes I Sets describe a co Add loci to sets. Add schemes to s Add metadata co Set database view Describes scheme Defines which foi Describes groups Defines which sch	ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci. a thributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be set for contigs in the sequence bin. ollection of loci and schemes that can be treated like a stand-alone database. ets. lifection to sets. ws linked to sets. is consisting of collections of loci, e.g. MLST. is belong to a scheme. Ids belong to a scheme.

Metaset fields can then be added to a set using the 'Add set metadata' link on the curator's page.

A new database table needs to be added for each metaset. This should contain all the fields defined for a metaset. The table should also contain an isolate\_id field to act as the foreign key linking to the isolate table, e.g. the SQL would look something like the following:

```
CREATE TABLE meta_1 (
isolate_id integer NOT NULL,
town text,
clinical_outcome text,
PRIMARY KEY (isolate_id),
CONSTRAINT m1_isolate_id FOREIGN KEY (isolate_id) REFERENCES isolates
ON DELETE CASCADE
ON UPDATE CASCADE
);
GRANT SELECT,UPDATE,INSERT,DELETE ON meta_1 TO apache;
```

The above creates the database table for a metaset called '1', defining new text fields for 'town' and 'clinical\_outcome'.

#### 5.11.4 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"
>
</system>
```

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

#### 5.11.5 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>
```

# 5.12 Adding new loci

See also:

Loci (concept)

#### 5.12.1 Sequence definition databases

#### Single locus

Click the add (+) loci link on the curator's interface contents page.

Users: Ad	id l C	Query/update			n's page (database)
ogged in: Keith Jolley (keith). Log	out	Change passv	vord		
atabase curato	's	interfa	ce . Nei	sseria loci	is/sequence definitions
	•	meenu		0001111 1000	
🖊 Add, update or de	elete	e records			
Record type	Add	Batch Add	Upda	te or delete	Comments
users	+	++		?	
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.
user group members	+	++		?	Add users to groups for setting access permissions.
user permissions	+	++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++		?	
scheme curator control list	+	++	qu	ery   batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	qu	ery   batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++   FASTA		?	
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	+	++		?	
MLST profiles	+	++	query   brows	e   list   batch update	
rpIF species profiles	+	++	query   brows	e   list   batch update	
PubMed links (to profiles)	+	++			
Database configu Table	rati Add	on Batch Add	Update or delete		Comments
loci	+	++	?		
locus aliases	+	++	?	Add alternative names	for loci. These can also be set when you batch add loci.
locus extended attributes	+	++	?	Define additional fields	to associate with sequences of a particular locus.
client databases	+	++	?		hat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these databases whe r profiles in this database.
client database loci	+	++	?	Define loci that are use	d in client databases.
client database schemes	+	++	?	Define schemes that an	e used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?	Define fields in client d	atabase whose value can be displayed when isolate has matching allele.
schemes	+	++	?	Describes schemes con	sisting of collections of loci, e.g. MLST.
scheme members	+	++	2	Defines which loci held	ing to a scheme

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 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.

Loci: Add		iuery/update Add   Querj	) //update   Batch	insert		
ogged in: Keith Jolley (keith). Log	out	Change passv	vord			
atabase curato	/c	intorfa	co - Nois	seria locu	s/sequence definitions	
	3	IIICIIa	ce - Meia	Sena 1000		
/ Add, update or de	elete	e records				
Record type	Add	Batch Add	Update	or delete	Comments	
users	+	++		?		
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.	
user group members	+	++		?	Add users to groups for setting access permissions.	
user permissions	+	++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.	
locus descriptions	+	++		?		
scheme curator control list	+	++	quer	/   batch	Define which curators can add or update profiles for particular schemes.	
locus curator control list	+	++	quer	/ batch	Define which curators can add or update sequences for particular loci.	
sequences (all loci)	+	++   FASTA		?		
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.	
PubMed links (to sequences)	+	++		?		
MLST profiles	+	++	query   browse	list   batch update		
rpIF species profiles	+	++	query   browse	list   batch update		
PubMed links (to profiles)	+	++				
Database configu Table	rati Add	on Batch Add	Update or delete		Comments	
loci	+	++	?			
locus aliases	+	++	? A	dd alternative names	for loci. These can also be set when you batch add loci.	
locus extended attributes	+	++	? D	efine additional fields	to associate with sequences of a particular locus.	
client databases	+	++			hat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these data profiles in this database.	abases whe
client database loci	+	++	? D	efine loci that are use	d in dient databases.	
client database schemes	+	++	? D	efine schemes that are	e used in client databases. You will need to add the appropriate loci to the client database loci table.	
client database fields linked to loci	+	++	? D	efine fields in client d	atabase whose value can be displayed when isolate has matching allele.	
		++	2 D	seribes schemes con	sisting of collections of loci, e.g. MLST.	
schemes	+			esurbes scrientes cons	and of concentro of foot, e.g. meon.	

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

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			Toggle: i
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 (xisx format)</li> </ul>			
Paste in tab-delimited text (include a field header line).	Action		
	Reset	Submit	
h.			
Back			

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'.

#### 5.12.2 Isolate databases

#### Single locus

Click the add (+) loci link on the curator's interface contents page.

Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update Isolates: Add   Query/update   Batch insert							
gged in: Keith Jolley (keith). Log out   C	hange	password					
atabase curator's i	ntei	rface -	Neisseria F	PubMLST			
		Tuve	neloochu i				
🗡 Add, update or delete	reco	rds					
Record type	Add	Batch Add	Update or d	elete Comments			
users	+	++	?				
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.			
user group members	+	++	?	Add users to groups for setting access permissions.			
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.			
isolates	+	++	query   browse   list				
solate field extended attribute value	s +	++	?	Add values for additional isolate field attributes.			
projects	+	++	?	Set up projects to which isolates can belong.			
project members	+	++	?	Add isolates to projects.			
isolate aliases	+	++	?	Add alternative names for isolates.			
PubMed links	+	++	?				
allele designations		++	?	Allele designations can be set within the isolate table functions.			
sequences	+	++	?	The sequence bin holds sequence contigs from any source.			
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.			
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.			
experiment sequences			?	Add links associating sequences to experiments.			
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.			
Database configuratio		tch Add U	odate or delete	Comments			
loci	+	++	?				
	databa	nk scan					
locus aliases	+	++	? Add a	Iternative names for loci. These can also be set when you batch add loci.			
PCR reactions	+	++	Set up	o in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.			
nucleotide probes	+	++	Define	e nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.			
isolate field extended attributes	+	++	? Define	e additional attributes to associate with values of a particular isolate record field.			
composite fields	+		? Used t	to construct composite fields consisting of fields from isolate, loci or scheme fields.			
sequence attributes	+	++	Define	e attributes that can be set for contigs in the sequence bin.			
schemes	+	++	? Descri	bes schemes consisting of collections of loci, e.g. MLST.			
scheme members	+	++	2 Define	as which lori halono to a schama			

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

PuliMLST / Users: Add	pecies home   Curator's Query/update d   Query/update   Batch	s page (species)   Curator's page (database) insert	
Logged in: Keith Jolley (keith). Log out	t   Change password		Toggle: i
Add new locus			Show tools
Please fill in the fields below - red Record	quired fields are marked	I with an exclamation mark (!).	Action
data type: allele id format! length varies: coding sequence! flag table: isolate display:! main display:! query field; analysis:!	integer ▼ [ true ● false [ ● true ● false [ e true ● false [ allele only ▼ [ true ● false [ ● true ● false [ ● true ● false [ False [ Keith Jolley (keith)	Seqdef database supports allele flags	Reset Submit
datestamp: formatted name: common name: allele id regex: allele id regex: orf: genome position: match longest	▼ Ē	i i i i * i * i	
reference sequence: pcr filter:	◯ true ◯ false []	ي. اب	

- 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.
- flag\_table Set to true to specify that the sequence definition database contains an allele flag table (which is the case for BIGSdb version 1.4 onwards).
  - 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.
- 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\_table - Table in the sequence definition database that contains allele sequences for this locus. If the definition database uses BIGSdb this will be 'sequences'.

- Allowed: any text (no spaces).

• dbase\_id\_field - Primary field in sequence database that defines allele. If the definition database uses BIGSdb this will be 'allele\_id'.

- Allowed: any text (no spaces).

• dbase\_id2\_field - Secondary field in sequence database that defines alleles. If dbase\_id\_field uniquely defines alleles for this locus then this should be left blank. If the definition database uses BIGSdb this will be 'locus'.

- Allowed: any text (no spaces).

• dbase\_id2\_value - Secondary field value in sequence database that defines alleles. If dbase\_id\_field uniquely defines alleles for this locus then this should be left blank. If the definition database uses BIGSdb this will be the name of the locus used in the id field

- Allowed: any text (no spaces).

- dbase\_seq\_field Field in sequence database containing allele sequence. If the definition database uses BIGSdb this will be 'sequence'.
  - 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=[?].

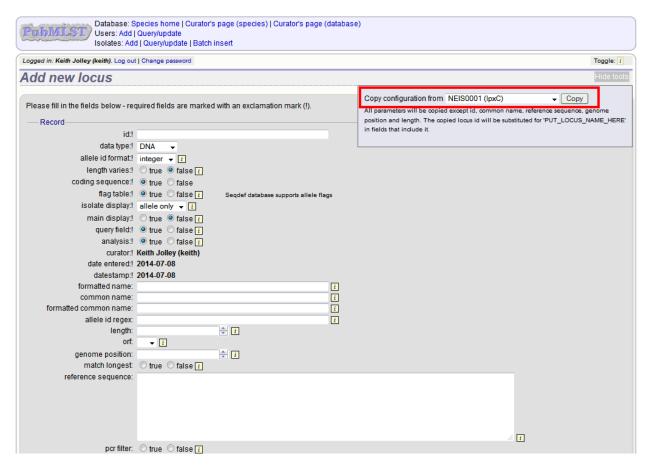
- Allowed: any valid URL.

#### 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:

PTIDMLST / Users: Add	Species home   Curator's   Query/update d   Query/update   Batch	s page (species)   Curator's page ( insert	database)	
Logged in: Keith Jolley (keith). Log ou	t   Change password			Toggle: i
Add new locus				Show tools
Please fill in the fields below - re	quired fields are marked	d with an exclamation mark (!).		
Record				Action
id:!				Reset Submit
data type:!	DNA 👻			Reset
allele id format:!	integer 👻 👔			
	◯ true			
coding sequence:				
	Irue of false i	Segdef database supports allele flag	<b>3</b> 5	
	allele only v i			
main display:	◯ true			
query field:	● true ○ false i			
analysis:	🖲 true 🔘 false i			
curator:	Keith Jolley (keith)			
date entered:!	2014-07-08			
datestamp:!	2014-07-08			
formatted name:			ī	
common name:			i	
formatted common name:			i	
allele id regex:			ī	
length: orf:				
	<b>▼</b> [			
genome position: match longest:	◯ true ◯ false 👔	÷ i		
reference sequence:	O true O faise 1			
Telefence sequence.				
pcr filter:	◯ true ◯ false 👔			

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



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:

	Keitii Jolley (Keitii)	
date entered:		
	2014-07-08	
formatted name:		
common name:		
formatted common name:		
allele id regex:		1
length:	<b>I</b>	
orf:	. 🖻	
genome position:		
-	🔿 true 🔿 false 👔	
reference sequence:		
pcr filter:	◯ true ◯ false 👔	
	○ true ○ false i	
	pubmlst_bigsdb_neisseria_seqdef	Name of the database holding allele sequences
dbase host		i IP address of database host
dbase port		
dbase user:		ī
dbase password:		ī
dbase table:		Database table that holds sequence information for this locus
dbase id field:		Primary field in sequence database that defines allele, e.g. 'allele_id'
dbase id2 field:	-	i Secondary field that defines allele, e.g. 'locus'
	PUT LOCUS NAME HERE	i Secondary field value, e.g. locus name
dbase seq field:		Field in sequence database containing allele sequence
	/cgl-bin/bigsdb/bigsdb.pl?db=pubmlst_ne locus=PUT_LOCUS_NAME_HERE	isseria_seqdef&page=locusInfo&
		<b>i</b> h.
un.	/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_ne locus=PUT_LOCUS_NAME_HERE&allele_id=[?]	-
		ı. ا

Complete the form and click 'Submit'.

### **Batch adding**

Click the batch add (++) loci link on the curator's interface contents page.

Add, update or delete rec		- Neisseria PubMLS	
Record type	oras		
	d Batch Ad	d Update or delete	Comments
users +		?	
user groups +	+ ++	?	Users can be members of these groups - use for setting access permissions.
user group members +	+ ++	?	Add users to groups for setting access permissions.
user permissions +	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates +	+ ++	query   browse   list   batch update	
late field extended attribute values +	+ ++	?	Add values for additional isolate field attributes.
projects +	+ ++	?	Set up projects to which isolates can belong.
project members +	+ ++	?	Add isolates to projects.
isolate aliases +	+ ++	?	Add alternative names for isolates.
PubMed links +	+++	?	
allele designations	++	?	Allele designations can be set within the isolate table functions.
sequences +	+ ++	?	The sequence bin holds sequence contigs from any source.
accession number links +	+ ++	?	Associate sequences with Genbank/EMBL accession number.
experiments +	+++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences		?	Add links associating sequences to experiments.
sequence tags	scan	?	Tag regions of sequences within the sequence bin with locus information.
loci +	++	Jpdate or delete ?	Comments
locus aliases +	bank scan	? Add alternative name	s for loci. These can also be set when you batch add loci.
PCR reactions +	++		eactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes +	++		bes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
olate field extended attributes +	++		butes to associate with values of a particular isolate record field.
composite fields +			posite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes +	++		can be set for contigs in the sequence bin.
schemes +	++		nsisting of collections of loci, e.g. MLST.
scheme members +	++	Pafines which loci hall	
k the link to downlo	home   Curat	tor's page (species)   Curator's page	(database)
Database: Species I Users: Add   Querylu Isolates: Add   Querylu			
IDMLST Users: Add   Query/u	//update   Bat		Te
ISOlates: Add   Query/u Isolates: Add   Query	//update   Bat		T

ste 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'.

# 5.13 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.

user groups user group members user permissions	+				
		++		?	Users can be members of these groups - use for setting access permissions.
upor pormissions	+	++		?	Add users to groups for setting access permissions.
user permissions	+	++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++		?	
scheme curator control list	+	++	q	uery   batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	q	uery   batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++   FASTA		?	
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences	) +	++		?	
MLST profiles	+	++	query   brow	se   list   batch update	
test profiles	+	++	query   brow	se   list   batch update	
test2 profiles	+	++		se   list   batch update	
test2 profiles	+	++		se   list   batch update	
test3 profiles	+	++		se   list   batch update	
PubMed links (to profiles)	+	++		?	
Table	Add	Batch Add	Update or delete		Comments
loci	+	Add ++	delete ?		
		++		Add alternative names f	or loci. These can also be set when you batch add loci
locus aliases	+	++	?		or loci. These can also be set when you batch add loci.
locus aliases locus extended attributes	+ +	++	? ?	Define additional fields	to associate with sequences of a particular locus.
locus aliases	+		?	Define additional fields Add isolate databases th	to associate with sequences of a particular locus. nat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these databas
locus aliases locus extended attributes	+ +	++	? ?	Define additional fields Add isolate databases th	to associate with sequences of a particular locus. Nat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these databas ces or profiles in this database.
locus aliases locus extended attributes client databases	+ + +	++	? ? ?	Define additional fields Add isolate databases th when you query sequent Define loci that are used	to associate with sequences of a particular locus. Nat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these databas ces or profiles in this database.
locus aliases locus extended attributes client databases client database loci	+ + +	++ ++ ++	? ? ? ?	Define additional fields Add isolate databases th when you query sequent Define loci that are used Define schemes that are	to associate with sequences of a particular locus. tat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these databas cas or profiles in this database. i in client databases.
locus aliases locus extended attributes client databases client database loci client database schemes client database fields	+ + + + +	++ ++ ++ ++	? ? ? ? ?	Define additional fields Add isolate databases th when you query sequent Define loci that are used Define schemes that are Define fields in client da	to associate with sequences of a particular locus. nat use locus allele or softeme profile definitions defined in this database - this enables backlinks and searches of these databas ces or profiles in this database. in orient databases. used in client databases. You will need to add the appropriate loci to the client database loci table.
locus aliases locus extended attributes client databases client database loci client database schemes client database fields linked to loci	+ + + + + +	+++   +++   +++   +++	? ? ? ? ?	Define additional fields Add isolate databases th when you query sequent Define loci that are used Define schemes that are Define fields in client da	to associate with sequences of a particular locus. tat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these database as or profiles in this database. I in client databases. Used in client databases. You will need to add the appropriate loci to the client database loci table. Itabase whose value can be displayed when isolate has matching allele.
locus aliases locus extended attributes client databases client database loci client database schemes client database fields linked to loci sets	+ + + + + + + +	+++   +++   +++   +++	? ? ? ?	Define additional fields Add isolate databases th when you query sequent Define loci that are used Define schemes that are Define fields in client da Sets describe a collection	to associate with sequences of a particular locus. tat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these database as or profiles in this database. I in client databases. Used in client databases. You will need to add the appropriate loci to the client database loci table. I tabase whose value can be displayed when isolate has matching allele.
locus aliases locus extended attributes client databases client database loci client database schemes client database fields linked to loci sets set loci	+ + + + + + + + + +	+++ +++ +++ +++ +++	? ? ? ? ? ? ? ? ?	Define additional fields Add isolate databases th when you query sequem Define loci that are used Define schemes that are Define fields in client da Sets describe a collectio Add loci to sets. Add schemes to sets.	to associate with sequences of a particular locus. tat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these database as or profiles in this database. I in client databases. Used in client databases. You will need to add the appropriate loci to the client database loci table. I tabase whose value can be displayed when isolate has matching allele.
locus aliases locus extended attributes client databases client database loci client database schemes client database fields linked to loci sets set loci set schemes	+ + + + + + + + + + + + + + +	+++ +++ +++ +++ +++	? ? ? ? ? ? ? ? ? ? ?	Define additional fields Add isolate databases th when you query sequem Define loci that are used Define schemes that are Define fields in client da Sets describe a collectio Add loci to sets. Add schemes to sets.	to associate with sequences of a particular locus. tat use locus allele or scheme profile definitions defined in this database - this enables baddinks and searches of these database ces or profiles in this database. used in client databases. used in client databases. You will need to add the appropriate loci to the client database loci table. Itabase whose value can be displayed when isolate has matching allele. In of loci and schemes that can be treated like a stand-alone database. isting of collections of loci, e.g. MLST.
locus aliases locus extended attributes client databases client database loci client database schemes client database fields linked to loci sets set loci set schemes schemes	+ + + + + + + + + + + + + + + +	+++   +++   +++   +++   +++   +++	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Define additional fields Add isolate databases it when you query sequen Define loid that are used Define schemes that are Define fields in dilent da Sets describe a collectio Add loci to sets. Add schemes to sets.	to associate with sequences of a particular locus. tat use locus allele or softeme profile definitions defined in this database - this enables backlinks and searches of these database ces or profiles in this database. used in client databases. used in client databases. You will need to add the appropriate loci to the client database loci table. tabase whose value can be displayed when isolate has matching allele. on of loci and schemes that can be treated like a stand-alone database. sting of collections of loci, e.g. MLST. ing to a scheme.
locus aliases locus extended attributes client databases client database loci client database schemes client database fields linked to loci sets set loci set schemes schemes scheme members	+ + + + + + + + + + + + + + + + + +	+++ +++ +++ +++ +++ +++ +++ +++	? ? ? ? ? ? ? ? ? ? ? ? ? ?	Define additional fields Add isolate databases th when you query sequen Define loci that are used Define software shat are Define fields in client da Sets describe a collectio Add loci to sets. Add schemes to sets. Describes schemes com Defines which loci belor Defines which fields beli	to associate with sequences of a particular locus. tat use locus allele or softeme profile definitions defined in this database - this enables backlinks and searches of these database ces or profiles in this database. used in client databases. used in client databases. You will need to add the appropriate loci to the client database loci table. tabase whose value can be displayed when isolate has matching allele. on of loci and schemes that can be treated like a stand-alone database. sting of collections of loci, e.g. MLST. ing to a scheme.
locus aliases locus extended attributes client databases client database loci client database schemes client database fields linked to loci sets set loci set schemes schemes scheme members scheme fields	+ + + + + + + + + + + + + + + + + + +	+++ +++ +++ +++ +++ +++ +++ +++ +++	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Define additional fields Add isolate databases th when you query sequen Define loci that are used Define software shat are Define fields in client da Sets describe a collectio Add loci to sets. Add schemes to sets. Describes schemes com Defines which loci belor Defines which fields beli	to associate with sequences of a particular locus. tat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these database to one or profiles in this database. used in client databases. used in client databases. You will need to add the appropriate loci to the client database loci table. tabase whose value can be displayed when isolate has matching allele. in of loci and schemes that can be treated like a stand-alone database. isting of collections of loci, e.g. MLST. Ig to a scheme. ong to a scheme. hich schemes can belong - groups can also belong to other groups.

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

PubMLST	Database: Species home   Curator's page (species)   Cur Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert	ator's page (database)			
Logged in: Keith Jolley	(keith). Log out   Change password				Toggle: i
Add new loo	cus extended attribute				
Please fill in the field	ds below - required fields are marked with an exclamation	mark (!).			
Record			Action -		
locus:			Reset	Submit	
field:! value format!					
	text ↓ ○ true ● false i				
	Keith Jolley (keith)				
	2014-07-09				
value regex:		1			
description:					
		.ii	-		
option list:					
			i		
length:					
field order:	A V				

- 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.

## 5.14 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)

### 5.14.1 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.

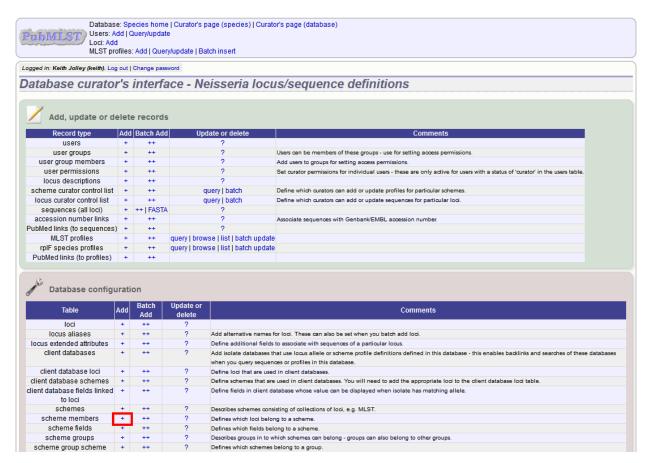
CITERATION USERS: A Loci: Add MLST pr	dd   d ofiles	Query/update s: Add   Quer	e y/update   Bat	age (species)   Curato tch insert	or's page (database)
ogged in: Keith Jolley (keith). Log	g out	Change pass	word		
atabase curato	r's	interfa	ice - Ne	eisseria locu	is/sequence definitions
🗾 Add, update or d	elet	e records	;		
Record type	Ado	Batch Add	Upd	late or delete	Comments
users	+	++		?	
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.
user group members	+	++		?	Add users to groups for setting access permissions.
user permissions	+	++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++		?	
scheme curator control list	+	++	qu	uery   batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	q	uery   batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++   FASTA		?	
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	) +	++		?	
MLST profiles	+	++	query   brow	se   list   batch update	
rpIF species profiles	+	++	query   brow	se   list   batch update	
PubMed links (to profiles)	+	++			
Database configu Table	urat Add	ion Batch Add	Update or delete		Comments
loci	+	++	?		
locus aliases	+	++	?	Add alternative names f	or loci. These can also be set when you batch add loci.
locus extended attributes	+	++	?	Define additional fields	to associate with sequences of a particular locus.
client databases	+	++	?		nat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these databases oes or profiles in this database.
client database loci	+	++	?	Define loci that are used	
client database schemes	+	++	?		used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?		stabase whose value can be displayed when isolate has matching allele.
schemes	+	++	?	Describes schemes cons	isting of collections of loci, e.g. MLST.
schemes					
scheme members	+	++	?	Defines which loci belor	ng to a scheme.
	+++	++ ++	? ?	Defines which loci below Defines which fields below	-
scheme members	+ + +			Defines which fields bel	-

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.

PuliMLST Users	: Add   Query/update	page (species)   Curator's page (o atch insert	latabase)	 
Logged in: Keith Jolley (keith).	Log out   Change password			Toggle: 1
Add new schen	пе			
	MLST Keith Jolley (keith) 2014-07-04	with an exclamation mark (!).	Action Reset Submit	
display order:				

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



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.

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	Toggle: i
Add new scheme member	
Please be aware that any modifications to the structure of this scheme will result in the removal of all data from it. This is done to ensure data integrity. This does profiles will have to be reloaded. Please fill in the fields below - required fields are marked with an exclamation mark (!).	not affect allele designations, but any
Record     Action       scheme id!     MLST       locus!     abcZ       curator!     Keith Jolley (keith)       datestamp!     2014-07-04       field order:     1	

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

bgged in: Keith Jolley (keith). Log out   Change password	
atabase curator's interface - Neisseria locus/sequence definitions	
Add, update or delete records	
Record type Add Batch Add Update or delete Comments	
users + ++ ?	
USEF groups + ++ ? Users can be members of these groups - use for setting access permissions.	
USEr group members + ++ ? Add users to groups for setting access permissions.	
USET PERMISSIONS + + + ? Set ourator permissions for individual users - these are only active for users with a status of 'ourator'	' in the users table.
locus descriptions + ++ ?	
scheme curator control list + +++ query   batch Define which curators can add or update profiles for particular schemes.	
locus curator control list + ++ query   batch Define which curators can add or update sequences for particular loci.	
sequences (all loci) + ++   FASTA ?	
accession number links + ++ ? Associate sequences with Genbank/EMBL accession number.	
MLST profiles + ++ query   browse   list   batch update	
rpIF species profiles + ++ query   browse   list   batch update PubMed links (to profiles) + ++	
PubMed links (to profiles) + ++	
Database configuration           Table         Add         Batch Add         Update or delete         Comments	
Table     Add     Batch     Update or delete     Comments       loci     +     ++     ?	
Table         Add         Batch         Update or delete         Comments           loci         +         ++         ?           locus aliases         +         ++         ?	
Table         Add         Batch Add         Update or delete         Comments           Ioci         +         ++         ?           Iocus aliases         +         ++         ?           Iocus extended attributes         +         ++         ?           Define additional fields to associate with sequences of a particular locus.	
Table         Add         Batch Add         Update or delete         Comments           loci         +         ++         ?         Add alternative names for loci. These can also be set when you batch add loci.         Iocus aliases         +         ++         ?         Add alternative names for loci. These can also be set when you batch add loci.         Iocus extended attributes         +         ++         ?         Define additional fields to associate with sequences of a particular locus.         Iocus aliases         +++         ?         Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks ar when you query sequences or profiles in this database.	nd searches of these databases
Table         Add         Batch Add         Update or delete         Comments           loci         +         ++         ?         Add alternative names for loci. These can also be set when you batch add loci.           locus extended attributes         +         +         ?         Add alternative names for loci. These can also be set when you batch add loci.           locus extended attributes         +         +         ?         Define additional fields to associate with sequences of a particular locus.           client databases         +         ++         ?         Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables baddlinks are when you query sequences or profiles in this database.           client database loci         +         +         ?         Define loci that are used in client databases.	
Table         Add         Batch Add         Update or delete         Comments           loci         +         +         ?         Add alternative names for loci. These can also be set when you batch add loci.           locus extended attributes         +         ?         Add isolate additional fields to associate with sequences of a particular locus.           client databases         +         ?         Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables baddlinks ar when you query sequences or profiles in this database.           client database loci         +         ?         Pefine is of that are used in client databases.           client database schemes         +         +         ?         Define schemes that are used in client databases.	
Table         Add         Batch Add         Update or delete         Comments           loci         +         +++         ?         Add alternative names for loci. These can also be set when you batch add loci.         Incus aliases         +         +++         ?         Add alternative names for loci. These can also be set when you batch add loci.         Incus extended attributes         +         ++         ?         Define additional fields to associate with sequences of a particular locus.         Incus extended attributes         +         +         ?         Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks are when you query sequences or profiles in this database.         Incus extended attributes         +         +         ?         Define loci that are used in client databases.         Incus extended attributes         +         +         ?         Define loci that are used in client databases.         Incus extended attributes         +         +         ?         Define schemes that are used in client databases.         You will need to add the appropriate loci to the dient database loci table         Incus extended attributes         +         +         ?         Define fields in dient database.         You will need to add the appropriate loci to the dient database loci table         Incus extended attribute has matching allele.         Incus extended attribute has matching allele.         Incus extended attribute has matching allele. <t< td=""><td></td></t<>	
Table         Add         Batch Add         Update or delete         Comments           loci         +         ++         ?         Add alternative names for loci. These can also be set when you batch add loci.           locus extended attributes         +++         ?         Add alternative names for loci. These can also be set when you batch add loci.           locus extended attributes         +++         ?         Define additional fields to associate with sequences of a particular locus.           client databases         +++         ?         Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks are when you query sequences or profiles in this database.           client database loci         +++         ?         Define coit that are used in client databases.           client database schemes         +++         ?         Define schemes that are used in client databases. You will need to add the appropriate loci to the dient database loci tabl to loci           tool         -         -         Define fields in client database whose value can be displayed when isolate has matching allele.           tool         -         -         Define schemes consisting of collections of loci, e.g. MLST.	
Table         Add         Batch Add         Update or delete         Comments           loci         +         ++         ?         Add alternative names for loci. These can also be set when you batch add loci.           locus atlases         +         ++         ?         Add alternative names for loci. These can also be set when you batch add loci.           locus extended attributes         +++         ?         Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks ar when you query sequences or profile is in this database.           client database loci         +++         ?         Define schemes that are used in client databases.           client database loci         +++         ?         Define schemes that are used in client databases.           client database fields linked to loci         +++         ?         Define fields in client database whose value can be displayed when isolate has matching allele.           to loci         -         -         Describes schemes consisting of collections of loci, e.g. MLST.           scheme members         +++         ?         Defines which loci belong to a scheme.	
Table         Add         Batch Add         Update or delete         Comments           loci         +         +++         ?         Add alternative names for loci. These can also be set when you batch add loci.         Incurs allases           locus allases         +         ++         ?         Add alternative names for loci. These can also be set when you batch add loci.         Incurs allases           locus extended attributes         +         ++         ?         Define additional fields to associate with sequences of a particular locus.           client databases         +         +         ?         Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks ar when you query sequences or profiles in this databases.           client database loci         +         ++         ?         Define loci that are used in client databases.         Incur of the appropriate loci to the dient database.           client database fields linked         +         +         ?         Define schemes that are used in client databases. You will need to add the appropriate loci to the dient database loci table           dient database fields linked         +++         ?         Define fields in client database whose value can be displayed when isolate has matching allele.           to loci         +++         ?         Defines othermes consisting of collections of loci, e.g. MLST.	
Table         Add         Batch Add         Update or delete         Comments           loci         +         ++         ?         Add alternative names for loci. These can also be set when you batch add loci.           locus aliases         +         ++         ?         Add alternative names for loci. These can also be set when you batch add loci.           locus extended attributes         +++         ?         Define additional fields to associate with sequences of a particular locus.           client databases         +         ++         ?         Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks ar when you query sequences or profiles in this database.           client database loci         +++         ?         Define schemes that are used in client databases.           client database schemes         ++++         ?         Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table client database fields linked           to loci         +++         ?         Define schemes that are used in client databases. You will need to add the appropriate loci to the dient database loci table client database fields linked           to loci         +++         ?         Define schemes consisting of collections of loci, e.g. MLST.           scheme schemes         ++++         ?         Defines which loci belong to a scheme. </td <td></td>	

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

PubMLST	Database: Species home   Curator's page (species)   Curator' Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert	s page (database)
Logged in: Keith Jolle	y (keith). Log out   Change password	Toggle: i
Add new se	cheme field	
Please be aware the profiles will have to		the removal of all data from it. This is done to ensure data integrity. This does not affect allele designations, but any
Please fill in the fie	elds below - required fields are marked with an exclamation mark	t (I).
		Action
scheme id:!	MLST -	Reset Submit
field:	ST	
	integer 👻	
	💿 true 🔘 false 👔	
dropdown:!	🔿 true 🔘 false 👔	
curator:!	Keith Jolley (keith)	
datestamp:!		
description:		
field order:		
	◯ true  ◯ false 👔	
value regex:	1	

- 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

### 5.14.2 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.

Record type	Add	Batch Add	Update	telete	Comments
users	+	++			
user groups	+	++		Users can be members of	of these groups - use for setting access permissions.
user group members	+	++		Add users to groups for :	setting access permissions.
user permissions	+	++			for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query   browse	batch update	
late field extended attribute value	es +	++		Add values for addition	al isolate field attributes.
projects	+	++		Set up projects to which	h isolates can belong.
project members	+	++		Add isolates to projects.	L
isolate aliases	+	++		Add alternative names	for isolates.
PubMed links	+	++			
allele designations		++		Allele designations can	be set within the isolate table functions.
sequences	+	++		The sequence bin hold:	is sequence contigs from any source.
accession number links	+	++		Associate sequences wit	th Genbank/EMBL accession number.
experiments	+	++		Set up experiments to v	which sequences in the bin can belong.
					equences to experiments.
experiment sequences				Add links associating se	equences to experiments.
Database configuration	'n	scan		-	equence to experiments.
Database configuration	'n		pdate or delete	-	
Database configuration	'n		pdate or delete ?	-	es within the sequence bin with locus information.
Database configuratio	n Add Bat	ch Add U ++ k scan	?	-	es within the sequence bin with locus information.
Database configuration	n Add Bat +	ch Add U ++ k scan ++	?	-	es within the sequence bin with locus information.
Database configuratio	n Add Bat + databan	ch Add U ++ k scan	?	Tag regions of sequeno	es within the sequence bin with locus information.
Database configuration	n Add Bat + databan +	ch Add U ++ k scan ++	?	Tag regions of sequeno alternative names for loci. These can also p <i>in silloo</i> PCR reactions. These can be a	Es within the sequence bin with locus information. Comments b be set when you batch add loci.
Sequence tags Database configuratio Table Ioci Iocus aliases PCR reactions	n Add Bat + databan + +	ch Add U ++ k scan ++ ++	?	Tag regions of sequeno alternative names for loci. These can also p <i>in silloo</i> PCR reactions. These can be a	Comments Comments be set when you batch add loci. Used to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci.
Database configuration Table Ioci Iocus aliases PCR reactions nucleotide probes	n Add Bat + databan + +	ch Add U ++ k scan ++ ++ ++	?	Tag regions of sequence alternative names for loci. These can also p in ailico PCR reactions. These can be e nucleotide probes for <i>in ailico</i> hybridizz a dolftional attributes to associate with v	Comments Comments be set when you batch add loci. Used to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci.
Sequence tags	Add Bat + databan + + + + +	ch Add U ++ k scan ++ ++ ++	? ? ? ? ?	Tag regions of sequence alternative names for loci. These can also p in ailico PCR reactions. These can be e nucleotide probes for <i>in ailico</i> hybridizz a dolftional attributes to associate with v	Comments  be set when you batch add loci. used to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ations of a particular isolate record Field.  of fields from isolate, loci or scheme fields.
Sequence tags	Add Bat + databan + + + + + + + + + + + + + + + + + + +	ch Add U ++ k scan ++ ++ ++ ++	? ? ? ? ? ! ?	Tag regions of sequeno alternative names for loci. These can also p <i>in silico</i> PCR reactions. These can be a e nucleotide probes for <i>in silico</i> hybridize e additional attributes to associate with v to construct composite fields consisting o	Comments  b be set when you batch add loci. used to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci.
Sequence tags	Add Bat + databan + + + + +	ch Add U +++ k scan +++ +++ +++ +++	? ? ? ? 1 ?	Tag regions of sequeno alternative names for loci. These can also p in ailico PCR reactions. These can be t e nucleotide probes for <i>in ailico</i> hybridizz e additional attributes to associate with to construct composite fields consisting o e attributes that can be set for contigs in 1	Comments  b be set when you batch add loci. used to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci.
Sequence tags	Add Bat + databan + + + + + + + + + + +	ch Add U ++ k scan ++ ++ ++ ++ ++ ++	? ? ? ? ! ? ! ?	Tag regions of sequence alternative names for loci. These can also p in silico PCR reactions. These can be e nucleotide probes for <i>in silico</i> hybridizz a dottional attributes to associate with v to construct composite fields consisting or e attributes that can be set for contigs in t bies schemes consisting of collections of	Comments  b be set when you batch add loci. used to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci.
Sequence tags	Add Bat + databan + + + + + + + + + + + + +	ch Add U ++ k scan ++ ++ ++ ++ ++ ++ ++	? ? ? ? ! ? ! ? ! ? ! ? ! ? !	Tag regions of sequeno alternative names for loci. These can also p in ailico PCR reactions. These can be t e nucleotide probes for in ailico hybridizz e additional attributes to associate with to to construct composite fields consisting o e attributes that can be set for contigs in tibes schemes consisting of collections of es which loci belong to a scheme.	Comments  b be set when you batch add loci. used to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci.
Sequence tags	Add Bat + databan + + + + + + + + + + + + + + + + + + +	ch Add U ++ k scan ++ ++ ++ ++ ++ ++ ++ ++ ++	?	Tag regions of sequeno alternative names for loci. These can also p in ailico PCR reactions. These can be t e nucleotide probes for in ailico hybridizz e additional attributes to associate with to to construct composite fields consisting o e attributes that can be set for contigs in tibes schemes consisting of collections of es which loci belong to a scheme.	Comments  b be set when you batch add loci. used to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ation reaction to filter genomes for tagging to specific repetitive loci. ations reaction to filter genomes for tagging to specific repetitive loci. ations reaction to filter genomes for tagging to specific repetitive loci. ations reaction to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for tagging to specific repetitive loci. ations reactions to filter genomes for taggi

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

PribMLST / Users	ase: Species home   Ci : Add   Query/update es: Add   Query/update	urator's page (species)   Curator's Batch insert	s page (database)			
Logged in: Keith Jolley (keith).	Log out   Change password					Toggle: i
Add new schen	те					
Please fill in the fields belo	w - required fields are r	marked with an exclamation mark	: (!).			
				— Action —		
id:!	53	* *		Reset	Submit	
description:!			i	10000	Gubinit	
isolate display:!	🔍 true 🔘 false 👔					
main display:!	🔍 true 🔘 false 👔					
query field:	🔍 true 🔘 false 👔					
query status:!	🔘 true 🔍 false 👔					
analysis:	🔍 true 🔘 false 👔					
curator:!	Keith Jolley (keith)					
datestamp:!						
date entered:!	2014-07-08					
dbase name:			i			
dbase host:			i			
dbase port:		÷ 1				
dbase user:			i			
dbase password:			1			
dbase table:			i			
display order:		÷ 1				
allow missing loci:	🔿 true 🔘 false 👔					

- 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\_table Table in the sequence definition database that contains profiles for this scheme. If the definition database uses BIGSdb this will be 'scheme\_X' where X is the scheme id number in the seqdef database.
  - Allowed: any text (no spaces).
- 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).

### 5.15 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.

PTTEMILST 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						
Download allele sequences						
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 within the group and any subgroups. Click the nodes to expand/collapse.						
All loci Capsule Capsu						
MLST						
Locus Download Type Alleles Length Curator(s) abcZ DNA 687 Fixed: 433 bp O. Harrison, K. Jolley						
adk I DNA 463 Fixed: 465 bp O. Harrison, K. Jolley						
aroE DNA 738 Fixed: 490 bp O. Harrison, K. Jolley						
func DNA 700 Fixed: 465 bp 0. Harrison, K. Jolley						
gdh J DNA 708 Fixed: 501 bp O. Harrison, K. Jolley pdhC DNA 713 Fixed: 480 bp O. Harrison, K. Jolley						
punc Diver 715 rised 400 bp 0. Harrison, K. Jolley						
Download in tab-delimited text 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.

	Add	Batch Add	Update or delete	Comments	
users	+	++	?		
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.	
user group members	+	++	?	Add users to groups for setting access permissions.	
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.	
isolates	+	++	query   browse   list   batch up	date	
olate field extended attribute valu	es +	++	?	Add values for additional isolate field attributes.	
projects	+	++	?	Set up projects to which isolates can belong.	
project members	+	++	?	Add isolates to projects.	
isolate aliases	+	++	?	Add alternative names for isolates.	
PubMed links	+	++	?		
allele designations		++	?	Allele designations can be set within the isolate table functions.	
sequences	+	++	?	The sequence bin holds sequence contigs from any source.	
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.	
	+	++	?	Set up experiments to which sequences in the bin can belong.	
experiments					
experiments experiment sequences			?	Add links associating sequences to experiments.	
	on	scan	? ?	Add links associating sequences to experiments. Tag regions of sequences within the sequence bin with locus information.	
experiment sequences sequence tags			?	Tag regions of sequences within the sequence bin with locus information.	
experiment sequences sequence tags					
experiment sequences sequence tags Database configuration Table	Add Ba	tch Add U	? pdate or delete	Tag regions of sequences within the sequence bin with locus information.	
experiment sequences sequence tags Database configuration Table	Add Ba	tch Add U	? pdate or delete ?	Tag regions of sequences within the sequence bin with locus information.	
experiment sequences sequence tags Database configuration Table loci	Add Ba + databar	tch Add U ++ nk scan	? pdate or delete ? Add alternative n	Tag regions of sequences within the sequence bin with locus information. Comments	
experiment sequences sequence tags Database configuration Table Ioci Iocus aliases	Add Ba + databar +	tch Add U ++ nk scan ++	? odate or delete ? Add alternative n Set up in silico P	Tag regions of sequences within the sequence bin with locus information. Comments ames for loci. These can also be set when you batch add loci.	
experiment sequences sequence tags     Database configuration     Table     loci     locus aliases     PCR reactions	Add Ba + databar + +	tch Add U ++ hk scan ++ ++	? pdate or delete ? Add alternative n Set up in allico P Define nucleotid	Tag regions of sequences within the sequence bin with locus information.  Comments  ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci.	
experiment sequences sequence tags Database configuratio Table Ioci Iocus aliases PCR reactions nucleotide probes	Add Ba + databar + + +	tch Add U ++ hk scan ++ ++ ++	Pdate or delete	Tag regions of sequences within the sequence bin with locus information.  Comments  ames for loci. These can also be set when you batch add loci.  CR reactions. These can be used to filter genomes for tagging to specific repetitive loci.  probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.	
experiment sequences sequence tags  Database configuratio  Table Ioci Iocus aliases PCR reactions nucleotide probes isolate field extended attributes	Add Ba + databar + + + + +	tch Add U ++ hk scan ++ ++ ++	? pdate or delete ? Add elternative n Set up in silico P Define nucleotidi ? Define additiona ? Used to construct	Tag regions of sequences within the sequence bin with locus information.  Comments  ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field.	
experiment sequences sequence tags  Database configuration  Table Ioci Iocus aliases PCR reactions mucleotide probes isolate field extended attributes composite fields	Add Ba + databar + + + + +	tch Add U ++ hk scan ++ ++ ++	? pdate or delete ? Add alternative n Set up in allico P Define nucleotid ? Define additiona ? Used to construct Define attributes	Tag regions of sequences within the sequence bin with locus information.  Comments  ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. e probes for <i>in allico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. e attributes to associate with values of a particular lociate record field. composite fields consisting of fields from isolate, loci or scheme fields.	
experiment sequences sequence tags	Add Ba + databar + + + + + + + + + + +	tch Add U ++ hk scan ++ ++ ++ ++	Pdate or delete  P Add alternative n Set up in silico P Define nuclectid Define etributes P Define stributes P Define stribute	Tag regions of sequences within the sequence bin with locus information.  Comments  ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. Probes for <i>inglice</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. Lattributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be as to roung in the sequence bin.	
experiment sequences sequence tags	Add Ba + databar + + + + + + + + + + + + +	tch Add U ++- hk scan ++- ++- ++- ++- ++- ++- ++-	Polate or delete P Polate or delete P Polate or delete Polation Set up in silico P Define nucleotidi Polate additiona Polate additiona Polate atributes Polations softem Polations Pola	Tag regions of sequences within the sequence bin with locus information.  Comments  ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. a probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. athibutes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. that can be set for contigs in the sequence bin. ss consisting of collections of loci, e.g. MLST.	
experiment sequences sequence tags	Add Ba + databar + + + + + + + + + + + + +	tch Add U ++ hk scan ++ ++ ++ ++ ++ ++ ++ ++ ++ ++ ++	Pdate or delete  Add alternative n Set up in allico P Define nucleotid Define additions Used to construct Define attributes P Define attributes P Define shich loc Defines which lice P D D D D D D D D D D D D D D D D D D	Tag regions of sequences within the sequence bin with locus information.    Comments  ames for loci. These can also be set when you batch add loci.  CR reactions. These can be used to filter genomes for tagging to specific repetitive loci.  at the set for <i>in allico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.  at this can be used to filter genomes for tagging to specific repetitive loci.  at the set for <i>in allico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.  at the set for contigs in the sequence bin.  as consisting of fields from isolate, loci or scheme fields.  that can be set for contigs in the sequence bin.  as consisting of solicetions of loci, e.g. MLST.  a belong to a scheme.	
experiment sequences sequence tags	Add Ba + databar + + + + + + + + + + + + +	tch Add U ++ k scan ++ ++ ++ ++ ++ ++ ++ ++ ++ ++ ++ ++ ++	Pdate or delete P Pdate or delete P Pdate or delete P Pdate or delete P Define nuclectif P Define additiona P Used to construct Define stributes P Defines which to P D D D D D D D D D D D D D D D D D D	Tag regions of sequences within the sequence bin with locus information.	

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.

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	Toggle: i
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:! 2014-07-10 description:	Reset Submit
display order:	

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 (+) scheme group scheme members link.

Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	databank scan			
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
ocus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these databases when you query sequences or profiles in this database.
client database loci	+	++	?	Define loci that are used in client databases.
lient database schemes	+	++	?	Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.
set loci	+	++	?	Add loci to sets.
set schemes	+	++	?	Add schemes to sets.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.
	- Che	cks datab	ase connectivit	ole them to log on or change an existing password. y for loci and schemes and that required helper applications are properly installed.

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

Database: Species home   Curator's page (speci Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert	es)   Curator's page (database)
Logged in: Keith Jolley (keith). Log out   Change password	Toggle: i
Add new scheme group scheme meml	ber
Please fill in the fields below - required fields are marked with an excla Record group id:! Typing scheme id:! MLST curator.: Ketur Joney (Ketur) datestamp:! 2014-07-10	amation mark (!). — Action — Reset Submit

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

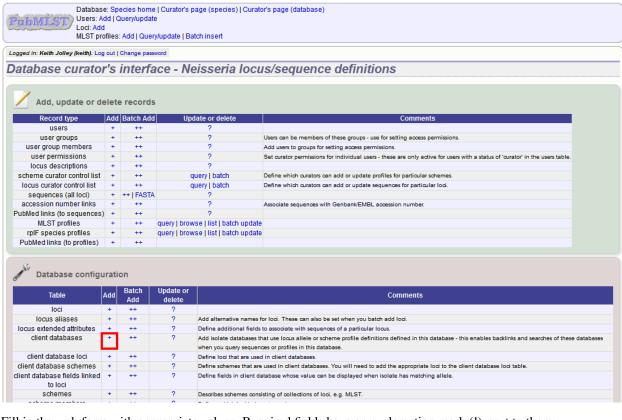
# 5.16 Setting up client databases

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.



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

PubMLST Use	abase: Species home   Curator's page (species ers: Add   Query/update i: Add 3T profiles: Add   Query/update   Batch insert	s)   Curator's page (database)		
Logged in: Keith Jolley (keith	h). Log out   Change password			Toggle: i
Add new clien	t database			
Please fill in the fields b	elow - required fields are marked with an exclan	nation mark (!).		
Record			Action	
id:!	1		Reset Submit	
name:!	PubMLST isolates		Reset	
uescipuon.	diversity of <u>Neisseria</u> species. database there is at least one of	of isolates that represent the total known For every allelic profile in the profile sorresponding isolate deposited here. Any s database and consequently it should be t a population sample.		
dbase name:!	pubmlst_bigsdb_neisseria_isolates	Name of the database holding isolate data		
-	pubmlst_neisseria_isolates	Name of the database configuration		
	Keith Jolley (keith)			
datestamp:!				
dbase host: dbase port:		i IP address of database host		
dbase user		i i		
dbase password:		[]		
dbase view:		View of isolates table to use		
url:	/cgi-bin/bigsdb/bigsdb.pl	Web URL to database sorio	ıt	

- 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.

### 5.16.1 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.

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	Toggle: i
Add new locus to client database definition	
Please fill in the fields below - required fields are marked with an exclamation mark (!).	
Record - Action -	
client dbase id:1 1) PubMLST isolates 👻 Reset Submit	
locus:1 abcZ	
curator! Keith Jolley (keith)	
datestamp:1 2014-07-04 IOCUS 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.

PubMLST / D	tuery: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query Jownload: Alleles   MLST profiles inks: Contents   Home   PorA   FetA   Options   Isolate Database
Allele inform	ation - abcZ: 5
Provenance/meta	a data
locus:	abcZ
allele:	5
sequences:	TTIGATACCE TIGCCGAAGE TITGEGCGAA ATTCGCGATI TATTGCGCCE TTATCAICAI GICAGCCAIG AGTIGGAAAA IGGTICGAGI GAGGCTIIGI IGAAAGAGI TAACGAAIG CAACIIGAA ICGAAGCGAA GGACGGCTGG AAGCIGGATG CGGCAGICAA GCAGACITIG GGIGGACITG GITGGCCAGA AAACGAAAAA AICGGCAACC ICICCGGCGG ACAGAAAAA CGIGIGCCC IAGGGCAGGC IIGGGIGCAG AAGCIIGAIG IAITGCIGCI GGACGAACCG ACCAACCAII IGGACAIIGA CGCGAITAII IGGCIGGAAA AICIGCITAA AGCGIIIGAA GGCAGCCIGG IIGIGAIIAC CCAGGACCGC CGIIIIIIGG ACAAIAICGC CAGCGCAIC GICGAACCG AIC
length:	433
status:	Sanger trace checked
date entered:	2001-02-07
datestamp:	2009-11-11
sender:	Keith Jolley, University of Oxford, UK
curator:	Man-Suen Chan, University of Oxford (E-mail: man-suen.chan@paediatrics.ox.ac.uk)
Profiles containin	ig this allele
MLST:	183 profiles
Isolate databases	3
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. [399 isolates]

### 5.16.2 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.



## 5.16.3 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.

Users: A Loci: Add	dd   ( t	Query/update		age (species)   Curato tch insert	or's page (database)
ogged in: Keith Jolley (keith). Log	out	Change passy	vord		
atabase curato	r's	interfa	ce - Ne	eisseria locu	is/sequence definitions
	-				
🗡 Add, update or de	elet	e records			
Record type	Add	Batch Add	Upd	late or delete	Comments
users	+	++		?	
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.
user group members	+	++		?	Add users to groups for setting access permissions.
user permissions	+	++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++		?	
scheme curator control list	+	++	a	uery   batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++		uery   batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++   FASTA	-	?	
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	+ (	++		?	
MLST profiles	+	++	query I brow	se   list   batch update	
rplF species profiles	+	++		se   list   batch update	
PubMed links (to profiles)	+	++	4		
Database configu	ırati Add	on Batch	Update or		Comments
	Auu	Add	delete		Comments
loci	+	++	?		
locus aliases	+	++	?		or loci. These can also be set when you batch add loci.
locus extended attributes	+	++	?		to associate with sequences of a particular locus.
client databases	+	++	?		nat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these database ces or profiles in this database.
client database loci	+	++	?	Define loci that are used	d in client databases.
client database schemes	+	++	?	Define schemes that are	used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?	Define fields in client da	atabase whose value can be displayed when isolate has matching allele.
schemes	+	++	?	Describes schemes cons	isting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belor	ng to a scheme.
scheme fields	+	++	?	Defines which fields bel	ong to a scheme.
scheme groups	+	++	?	Describes groups in to w	hich schemes can belong - groups can also belong to other groups.
			2	Defines which schemes	

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.

PribMLST La	atabase: Species home   Curator's page (species)   Curator's page (database) sers: Add   Query/update pci: Add LST profiles: Add   Query/update   Batch insert		
Logged in: Keith Jolley (ke	sith). Log out   Change password		Toggle: i
Add new locu	us to client database isolate field definition		
Please fill in the fields	below - required fields are marked with an exclamation mark (!).		
		Action	
	1) PubMLST isolates 👻	Reset Submit	
locus:		inteset Submit	
isolate field:!	penicillin_range		
curator:!	Keith Jolley (keith)		
datestamp:			
allele query:	Itrue C false set to true to display field values when an allele query is done.		

Now, in the allele record or following a sequence query that identifies an allele, all values for the chosen field from

	inks: Contents   Home   PorA   FetA   Options   Isolate Database
lele inform	ation - penA: 9
rovenance/meta	data
locus:	penA
allele:	9
sequences:	GACGGCGTIT IGCTGCCGGI CAGCTITGAA AAACAGGCGG ITGCGCCGCA AGGCAAACGI ATATITAAAG CAICGACCGC ACGICAGGIG CGIGAGIIGA IGGIIICGAI GGCGGTACGG GIACGGCGGG IGCCGGIAGAI GGIIICGACGC ICGGCGCAAA AACCGGIAGG GCGCGIAAGI IGGIIACGG ICGIIACGIC GAIIACAAAC ACGIIGCCAC IIICAICGGI IIIGCCCCGG CIAAAAAICC GCGIGIGAII GIGGCGGIAA CCAIIGACGA GCCGACIGCA AACGGIIACI IGGCGGCGI AGIGACAGGI CCGGICIICA AACAAGIIAI GGGCGGGAC CIGAACAICI IGGCCGIIIC ICCGACCAAA CCICIGACCA AI
length:	402
status:	Sanger trace checked
date entered:	2006-09-04
datestamp:	2006-09-04
sender:	Muhamed-Kheir Taha, National Reference Center for Meningococci, Institut Pasteur, France
curator:	Keith Jolley, University of Oxford, UK (E-mail: keith.jolley@zoo.ox.ac.uk)
mutation F504L:	yes
mutation A510V:	yes
mutation I515V:	yes
mutation H541N:	yes
mutation I566V:	yes
Publication (1)	
Jolley KA, Kadl	uez 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 ubowski 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 . (2007). Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis. <i>Antimicrob Agents Chemother</i> 51:2784-92
solate databases	i
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. 141 isolates
inked data	
penicillin_range:	>0.06 - 1 (intermediate) [n=86] FubMLST isolates

isolates with the corresponding allele are shown.

## 5.17 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.

### 5.17.1 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 ($st eq 'ND') {
 append_html("ST not defined. If individual MLST loci have been found "
  . "they will be displayed below:");
 #The get_scheme_html function automatically formats output for a scheme.
 #Select whether to display in a table rather than a list, list all loci, and/or list fields.
 append_html(get_scheme_html(1, {table=>1, loci=>1, fields=>0}));
}
#Antibiotic resistance
update_status({percent_complete=>80, stage=>'Scanning penA and rpoB'});
scan_locus($_) 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.
   #The min_percentage attribute states that only values that are represented by at least that
   #proportion of all isolates that had a value set are returned (null values are ignored).
   my $range = get_client_field(1,'penA','penicillin_range', {min_percentage => 75});
   append_html(" (penicillin MIC: $range->[0]->{'penicillin_range'})") if @$range;
   append_html("");
  }
 append_html("<i>rpoB</i> allele: $results->{'locus'}->{'rpoB'}");
   my $range = get_client_field(1,'rpoB','rifampicin_range',{min_percentage => 75});
   append_html(" (rifampicin MIC: $range->[0]->{'rifampicin_range'})") if @$range;
```

```
append_html("");
}
append_html("");
}
```

### **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.

## 5.18 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\_table: sequences
- dbase\_id\_field: allele\_id

- dbase\_id2\_field: locus
- dbase\_id\_value: atpD
- dbase\_seq\_field: sequence
- 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\_table: scheme\_1 (or whatever the id of your seqdef scheme is)
- 3. Add scheme\_field ST as before
- 4. Add loci as scheme\_members

## 5.19 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.

PubMed links	-			2
allele designations		++		Allele designations can be set within the isolate table functions.
sequences	-			? The sequence bin holds sequence contigs from any source.
accession number links	-	++		Associate sequences with Genbank/EMBL accession number.
experiments	-	++		? Set up experiments to which sequences in the bin can belong.
experiment sequences				Add links associating sequences to experiments.
sequence tags		scan		? Tag regions of sequences within the sequence bin with locus information.
	Add		Update or delete	Comments
loci		++	?	
locus aliases	data +	bank scan	?	Add allowed in a second for last These and also be estudied and had been
PCR reactions	+	++	f	Add alternative names for loci. These can also be set when you batch add loci.
nucleotide probes	+	++		Set up <i>in silico</i> PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci. Define nucleotide probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.
isolate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.
composite fields	+	**	2	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
	+	++	2	Define attributes that can be set for contias in the sequence bin.
sequence attributes sets	+	++	2	
set loci	+	++	2	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.
set schemes	+		2	Add loci to sets.
		++		Add schemes to sets.
set metadata	+	++	?	Add metadata collection to sets.
setview	+	++	?	Set database views linked to sets.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme groups		++	?	Defines which schemes belong to a group.
	+		?	Defines which scheme groups belong to a parent group.

Click 'Database scan' on the curator's contents pag.

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

Database: Species ho Users: Add   Query/up Isolates: Add   Query/up	
Logged in: Keith Jolley (keith). Log out   Change	password
Scan EMBL/Genbank re	cord for loci
— Please enter accession number — —	or Genbank (whole genome) file in order to create a batch upload file for setting up new loci. — Primary identifier – — Action —

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

PubML	ST/ U	atabase: Species home   Curator's page (species)   Curator's page (database) sers: Add   Query/update plates: Add   Query/update   Batch insert	
Logged in: Keith	ı Jolley (ke	ith). Log out   Change password	
Scan El	/IBL/G	Genbank record for loci	
This function	allowe ve	u ta asan an FURL ar Canhank (whole gangers) file in order to grants a batch upload file for antiing up neu logi	
		u to scan an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci.	
		ssion number — Primary identifier – Action —	
Accession:	AM42180	18 O locus tag Submit	
Download tab	le: tab-del	imited text   Excel format (suitable for batch upload of loci).	
Download alle	eles: tab-d	elimited text   Excel format (suitable for defining the first allele in the seqdef database).	
Annotation	n inform	ation	
aco	ession:	AM421808	
	version:		
	type:	dna	
		2194961	
des	cription:	Neisseria meningitidis serogroup C FAM18 complete genome.	
coding	regions:	1975	
Codina			
Coding se	quence	5	
Locus	Aliases	Product	Length
NMC0001	IpxC;	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924
NMC0002	envA piIS1	pilin (fragment)	291
NMC0003	pilS2	truncated pilin	366
NMC0004	fbp	peptidyl-prolyl cis-trans isomerase	330
NMC0005		putative membrane protein	219
NMC0006		putative glycerate dehydrogenase	954
NMC0007	metG	methionyl-tRNA synthetase	2058
NMC0008	glmS	glucosaminefructose-6-phosphate aminotransferase [isomerizing]	1839
NMC0009		putative lipoprotein	519
NMC0010	gna33	outer membrane lipoprotein Gna33 👔	1326
NMC0011		putative integral membrane protein	840
NMC0012		putative lipoprotein	1167
NMC0013	nhnA	possible membrane protein putative phosphonoacetate hydrolase	1266 330
NMC0014 NMC0015	phnA glmU	bifunctional GImU protein [includes: UDP-N-acetylglucosamine pyrophosphorylase (EC 2.7.7.23) (N-acetylglucosamine-1-phosphate uridyltransferase);	
NWC0015	ginto	onuncional on to protein (includes, ODF-N-acetyigiucosamine pyrophospholylase (EC 2.1.1.23) (N-acetyigiucosamine - phosphate undyitiansierase),	137.1

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.

	Is		
ogged in: Keitl	h Jolley (ke	(h). Log out   Change password	
can El	MBL/C	Genbank record for loci	
This function	n allows yo	u to scan an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci.	
Plassa	anter acce	ssion number — — Primary identifier – — Action —	
Accession:			
ownload tab	ole: tab-de	imited text   Excel format (suitable for batch upload of loci).	
ownload all	eles: tab-o	elimited text   Excel format (suitable for defining the first allele in the seqdef database).	
nnotatio	n inform	ation	
ac	cession:	AM421808	
	version:		
		1	
	type:	na dna	
	type: length:	1 dna 2194961	
des	type: length: scription:	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome.	
des	type: length:	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome.	
des coding	type: length: cription: regions:	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975	
des coding	type: length: scription: regions: equence	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975	Leng
des coding coding se Locus	type: length: cription: regions:	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S	-
des coding coding se Locus NMC0001	type: length: cription: regions: equence Aliases lpxC; envA	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S Product UDP-3-O-{3-hydroxymyristoy]] N-acetylglucosmine deacetylase	924
des coding se coding se Locus NMC0001 NMC0002	type: length: cription: regions: equence Aliases lpxC; envA pilS1	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 s Product UDP-3-O-[3-hydroxymyristoy]] N-acetylglucosmine deacetylase pillin (fragment)	924 291
des coding se coding se Locus NMC0001 NMC0002 NMC0003	type: length: ccription: regions: equence Aliases lpxC; envA pilS1 pilS2	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 5 Product UDP-3-O-[3-hydroxymyristoy/] N-acety/glucosmine deacety/lase pilin (fragment) truncated pilin	924 291 366
des coding coding se Locus NMC0001 NMC0002 NMC0003 NMC0004	type: length: cription: regions: equence Aliases lpxC; envA pilS1	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 5 Product UDP-3-O-[3-hydroxymyristoy!] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin peptidyl-prolyl cis-trans isomerase	924 291 366 330
des coding se Locus NMC0001 NMC0002 NMC0003 NMC0004 NMC0005	type: length: ccription: regions: equence Aliases lpxC; envA pilS1 pilS2	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 s Product UDP-3-O-[3-hydroxymyristoy!] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin peptidyl-prolyl cis-trans isomerase putative membrane protein	924 291 366 330 219
des coding oding se Locus NMC0001 NMC0002 NMC0003 NMC0003 NMC0005 NMC0006	type: length: cription: regions: equence lpxC; envA pilS1 pilS2 fbp	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 s Product UDP-3-O-[3-hydroxymyristoy!] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin peptidyl-prolyl cis-trans isomerase putative membrane protein putative glycerate dehydrogenase	924 291 366 330 219 954
des coding se coding se Locus NMC0001 NMC0002 NMC0003 NMC0004 NMC0005 NMC0005 NMC0007	type: length: cription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 5  Product UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin peptidyl-prolyl cis-trans isomerase putative membrane protein putative membrane protein putative dehydrogenase methionyl-IRNA synthetase	924 291 366 330 219 954 2058
des coding se coding se Locus NMC0001 NMC0002 NMC0005 NMC0006 NMC0006 NMC0007 NMC0007 NMC0008	type: length: cription: regions: equence lpxC; envA pilS1 pilS2 fbp	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 5  Product UDP-3-0-[3-hydroxymyristoy!] N-acetylglucosmine deacetylase UDP-3-0-[3-hydroxymyristoy!] N-acetylg	924 291 366 330 219 954 2058 1839
des coding se coding se Locus NMC0001 NMC0003 NMC0004 NMC0005 NMC0006 NMC0006 NMC0009	type: length: cription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG glmS	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 s Product UDP-3-O-[3-hydroxymyristoy!] N-acetylglucosmine deacetylase UDP-3-O-[3-hydroxymyristoy!] N-acetylgl	924 291 366 330 219 954 2056 1839 519
des coding se coding se coding se NMC0001 NMC0002 NMC0003 NMC0005 NMC0005 NMC0008 NMC0008 NMC0009 NMC0009 NMC0010	type: length: cription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 s Product UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase pliin (fragment) truncated pilin pliin (fragment) truncated pilin peptidyl-prolyl cis-trans isomerase putative glycerate dehydrogenase methionyl-tRNA synthetase glucosamine=fructose-6-phosphate aminotransferase [isomerizing] putative [ipoprotein outer membrane lipoprotein Gna33 []	924 291 366 330 219 954 2058 1839 519 1326
des coding se coding se coding se NMC0001 NMC0002 NMC0003 NMC0006 NMC0006 NMC0008 NMC0000 NMC0000 NMC0011	type: length: cription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG glmS	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 5 5 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	924 291 366 330 219 954 2058 1839 519 1320 840
des coding se coding se Locus NMC0001 NMC0002 NMC0005 NMC0006 NMC0006 NMC0008 NMC0009 NMC0010 NMC0012	type: length: cription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG glmS	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 5	924 291 366 330 219 954 2058 1839 519 1326 840 116
des coding Coding se	type: length: cription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG glmS	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 5 5 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	924 291 366 330 219 954 205 183 519 132 840

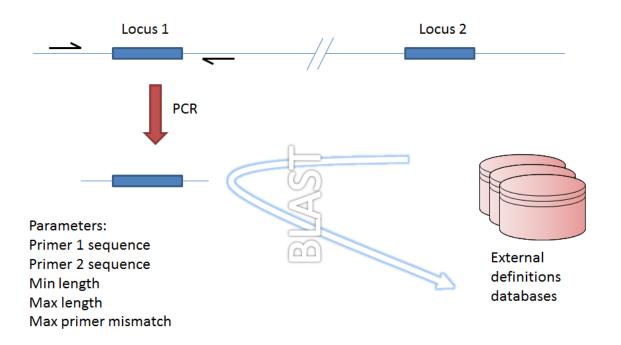
# 5.20 Genome filtering

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.

## 5.20.1 Filtering by in silico PCR

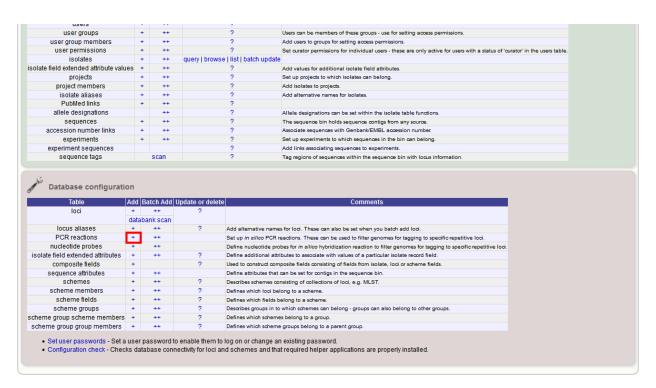
Provided a locus can be predicted to be specifically amplifed by a PCR reaction, the genome can be filtered to only look at regions prediced to fall within amplification products of one or more PCR reactions. Since this is in silico we don't need to worry about problems such as sequence secondary structure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



Locus 1 and locus 2 share allele pool

Figure 5.1: 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.

PTTTMLST Users: Add   Query/update Isolates: Add   Query/update   Batch insert	
Logged in: Keith Jolley (keith). Log out   Change password	Toggle: i
Add new PCR reaction	
Please fill in the fields below - required fields are marked with an exclamation mark (!).	
Record	Action
id! 1	Reset Submit
description:	
primer1:	
primer2:	
curator: Keith Jolley (keith)	
datestamp:/ 2014-07-08	
min length: 🗢 Minimum length of product to return	
max length:	
max primer mismatch: 🚽 🔢 Maximum sequence mismatch per primer	

- 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.

S					
Database configurati	on				
Table	Add	Batch Add	Update or delete	Comments	
loci	+	++	?		
	datal	bank scan			
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.	
PCR reactions	+	++	?	Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.	
PCR locus links	+	++		Link a locus to an <i>in silico</i> PCR reaction.	
nucleotide probes	+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.	
solate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.	
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.	
sequence attributes	+	++	?	Define attributes that can be set for contigs in the sequence bin.	
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.	
set loci	+	++	?	Add loci to sets.	
set schemes	+	++	?	Add schemes to sets.	
set metadata	+	++	?	Add metadata collection to sets.	
setview	+	++	?	Set database views linked to sets.	
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.	
scheme members	+	++	?	Defines which loci belong to a scheme.	
scheme fields	+	++	?	Defines which fields belong to a scheme.	
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.	
cheme group scheme members	+	++	?	Defines which schemes belong to a group.	
cheme group group members	+	++	?	Defines which scheme groups belong to a parent group.	
		•		log on or change an existing password. d schemes and that required helper applications are properly installed.	

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.

### 5.20.2 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.

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.

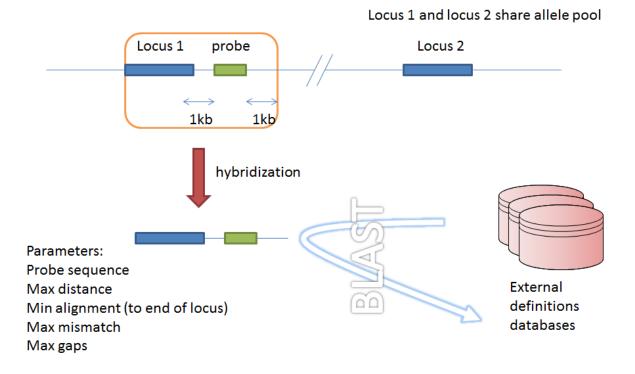


Figure 5.2: Filtering by in silico hybridization

sequence tags		scan		? Tag regions of sequences within the sequence bin with locus information.	
~					
Database configuration	00				
Patabase configuration					
Table	Add	Batch Add	Update or delete	Comments	
loci	+	++	?		
	data	bank scan			
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.	
PCR reactions	+	++	?	Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.	
PCR locus links	+	++		Link a locus to an in silico PCR reaction.	
nucleotide probes	+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.	
solate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.	
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.	
sequence attributes	+	++	?	Define attributes that can be set for contigs in the sequence bin.	
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.	
set loci	+	++	?	Add loci to sets.	
set schemes	+	++	?	Add schemes to sets.	
set metadata	+	++	?	Add metadata collection to sets.	
setview	+	++	?	Set database views linked to sets.	
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.	
scheme members	+	++	?	Defines which loci belong to a scheme.	
scheme fields	+	++	?	Defines which fields belong to a scheme.	
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.	
cheme group scheme members	+	++	?	Defines which schemes belong to a group.	
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.	
				log on or change an existing password. d schemes and that required helper applications are properly installed.	

	_		Update or delete	Comments	
loci	+	++	?		
		bank scan	_		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.	
PCR reactions	+	++	?	Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.	
PCR locus links	+	++		Link a locus to an in silico PCR reaction.	
nucleotide probes	+	++	?	Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.	
probe locus links	+	++		Link a locus to an in silico hybridization reaction.	
solate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.	
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.	
sequence attributes	+	++	?	Define attributes that can be set for contigs in the sequence bin.	
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.	
set loci	+	++	?	Add loci to sets.	
setschemes	+	++	?	Add schemes to sets.	
set metadata	+	++	?	Add metadata collection to sets.	
setview	+	++	?	Set database views linked to sets.	
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.	
scheme members	+	++	?	Defines which loci belong to a scheme.	
scheme fields	+	++	?	Defines which fields belong to a scheme.	
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.	
heme group scheme members	+	++	?	Defines which schemes belong to a group.	
cheme group group members	+	++	?	Defines which scheme groups belong to a parent group.	

- 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.

# 5.21 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.

Isolates: Add				
gged in: Keith Jolley (keith). Log out	Change p	assword		
atabase curator's	inter	face -	Neisseria PubN	ILST
Datasets				
Datasets				
his database contains multiple da	itasets. 1	You can cho	ose to display a single set or	the whole database.
ease select: Whole database 👻	Choos	se		
Add undate or delete	recor	de		
Add, update or delete	Add	ds Batch Add	Update or delete	Comments
		Batch	Update or delete	Comments
Record type	Add	Batch Add	· · · · ·	Comments Users can be members of these groups - use for setting access permissions.
Record type users	Add +	Batch Add ++	?	
Record type users user groups	Add + +	Batch Add ++ ++	? ?	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions.
Record type users user groups user group members	Add + + +	Batch Add +++ ++	? ? ?	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users
Record type users user groups user group members user permissions	Add + + +	Batch Add ++ ++ ++ ++	? ? ? ? query browse   list	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users
Record type users user groups user group members user permissions isolates isolates	Add + + + +	Batch Add +++ + +++ + +++ +++ +++ +++ +++++++++	? ? ? query browse   list   Datch update	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
Record type users user groups user group members user permissions isolates isolates isolate field extended attribute values	Add + + + +	Batch Add +++ = = +++ = = +++ = = +++ = =	? ? ? query browse   list   Datch update ?	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Add values for additional isolate field attributes.
Record type Users User groups User group members User permissions isolates isolate field extended attribute values projects	Add + + + + + + + + + + + + + + + +	Batch Add +++ = = = = = = = = = = = = = = = = = =	? ? ? query browse   list   batch update ?	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Add values for additional isolate field attributes. Set up projects to which isolates can belong.

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

Puli	MLS'	📝 Users: A	dd   Query	/update	urator's pa Batch inse		es) C	urator's p	oage (database)										
Logged in	: Keith Jol	ley (keith). Lo	g out   Chan	ge password								Toggle:	Field	help: id					🗕 😡
Isolat	te qu	ery/up	date																
—Isol	ate prove	nance/phen	otype field	s					— Display/sort of	otions —									Modify
isola	ate	-	=		:58		-	• [	Order by: id	ł			→ asc     →	ending	-				form
									Display: 2	5 👻 recor	ds p	er page 👔							options
Acti	on																		
Res	et S	ubmit																	
1 record	returned	Click the hy	perlink for	detailed in	formation.														
Dele	te	Tag sc	annina -	-Project	s														
	te ALL	Sca		Select p				<b>-</b>	Link										
Dele		000	<u> </u>	ociocrp	0,000			•	LIIK										
0-1-1-		Sequence	New			I	solate	fields i	]	1	<u> </u>	MLST		ping an		test	tes		Loci
Delete	Update	bin	version	id isola	te aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1	PorA VR2	FetA VR	ST	PorA VR1	PorA VR2	'test9
delete	update	upload	create	240 MC	8 Z7176	UK	1983		Neisseria	В	74	ST-32	7	16-2	F1-5		7	16-2	add
									meningitidis			complex/ET-5 complex	update	update	update		update	update	
												comprex							

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

species: Neisseria meningitidis update history: 137 updates show details
Publications (4)
Bennett JS, Bentley SD, Vernikos GS, Quail MA, Cherevach I, White B, Parkhill J, Maiden MC (2010). Independent evolution of the core and accessory gene sets in the genus Neisseria: insights gained from the genome of Neisseria lactamica isolate 020-06. BMC Genomics 11:652 79 isolates
Bennett JS, Jolley KA, Earle SG, Corton C, Bentley SD, Parkhill J, Maiden MC (2012). A genomic approach to bacterial taxonomy: an examination and proposed reclassification of species within the genus Neisseria. Microbiology 158:1570-80 [55 isolates]
Stabler RA, Marsden GL, Witney AA, Li Y, Bentley SD, Tang CM, Hinds J (2005). Identification of pathogen-specific genes through microarray analysis of pathogenic and commensal Neisseria species. Microbiology 151:2907-22 <a href="https://www.secies.org">stable Stable Sta</a>
<ul> <li>Tettelin H, Saunders NJ, Heidelberg J, Jeffries AC, Nelson KE, Eisen JA, Ketchum KA, Hood DW, Peden JF, Dodson RJ, Nelson WC, Gwinn ML, DeBoy R, Peterson JD, Hickey EK, Haft DH, Salzberg SL, White O, Fleischmann RD, Dougherty BA, Mason T, Ciecko A, Parksey DS, Blair E, Cittone H, Clark EB, Cotton MD, Utterback TR, Khouri H, Qin H, Vamathevan J, Gill J, Scarlato V, Masignani V, Pizza M, Grandi G, Sun L, Smith HO, Fraser CM, Moxon ER, Rappuoli R, Venter JC (2000). Complete genome sequence of Neisseria meningitidis serogroup B strain MC58. Science 287:1809-15 (1 isolate)</li> </ul>
Sequence bin
contigs:     1     detailed breakdown:     Display       length:     2272360 bp       loci tagged:     1283
Schemes and loci
All loci Capsule Ca

### Click the 'Renumber' button:

ogged in: Ke	aith Jolley (keith). Log o	ut   Change password										Toggle
equer	nce bin for	MC58										
Contin cu	Immary statistics											
onlig su	ininary statistics	•										
	tber of contigs: 1 ht: 2272360											
-												
	nload sequences (F/											
<ul> <li>Dowr</li> </ul>	nload sequences wi	th annotations (EM	BL format)									
	Sequencing Or	riginal		float SRA	test test te	et				EMBL	Artemis	Renumber
Sequence		ignation Length		test accession			Start	End	Direction	format	i	i
1	Sanger	2272360	whole			NEIS2140	502	897	←	EMBL	Artemis	Renumber
			genome			NEIS2141	918	2312	←			
						NEIS2142	2517	3161	←			
						NEIS2143	3158	3511	←			
						NEIS2144	3635	4117	$\rightarrow$			
						NEIS2145	4311	4961	$\rightarrow$			
						NEIS2145 NEIS2146	4311 4958	4961 5875				
									$\rightarrow$			
						NEIS2146	4958	5875	$\rightarrow$ $\rightarrow$			
						NEIS2146 NEIS2147 NEIS2148 (pgk)	4958 5936 6281	5875 6214 7492	$ \begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \end{array} $			
						NEIS2146 NEIS2147 NEIS2148	4958 5936	5875 6214	$ \begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \end{array} $			
						NEIS2146 NEIS2147 NEIS2148 (pgk)	4958 5936 6281	5875 6214 7492	$\stackrel{\uparrow}{\rightarrow} \stackrel{\uparrow}{\rightarrow} \stackrel{\uparrow}{\leftarrow}$			
						NEIS2146 NEIS2147 NEIS2148 (pgk) NEIS2149	4958 5936 6281 7573	5875 6214 7492 8826	+ + + + + + ↓ ↓			
						NEIS2146 NEIS2147 NEIS2148 (pgk) NEIS2149 NEIS2150 NEIS2151 NEIS2152	4958 5936 6281 7573 9346	5875 6214 7492 8826 10317	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1			
						NEIS2146 NEIS2147 NEIS2148 (pgk) NEIS2149 NEIS2150 NEIS2151	4958 5936 6281 7573 9346 10350	5875 6214 7492 8826 10317 10811	$\uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \downarrow$			

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: Species hor Users: Add   Query/upd Isolates: Add   Query/up	ate	es)   Curator's page (database)
Logged in: Keith Jolle	ey (keith). Log out   Change pa	ssword	
Renumber	locus genom	e positions ba	sed on tagged sequences
i terrarino er	loouo genom		
· · · · ·			
You have selected	to renumber the genome	positions set in the locus	table based on the tagged sequences in sequence id#1.
Option		Actio	n
Remove pos	itions for loci not tagged in	this sequence	umber
		Rent	
The following desi	ignations will be made:		
Lanua de Esta	41	11	
Locus	sting genome position 🗢 2181973	new genome position ≑ 502	
NEIS2140	2182389	918	
NEIS2141	2183899	2517	
NEIS2142	2184552	3158	
NEIS2143	2185029	3635	
NEIS2145	2185705	4311	
NEIS2146	2186352	4958	
NEIS2147	2187330	5936	
NEIS2148	2187675	6281	
NEIS2149	2188934	7573	
NEIS2150	2190551	9346	
NEIS2151	2191558	10350	
NEIS2152	2192048	10840	
NEIS2153	2193382	12174	
NEIS0001	1261	15221	
NEIS0210	209923	17229	
pilS	3271	18127	
NEIS0004	4069	23904	
NEIS0005	4476	24311	
NEIS0007	5843	25679	

# 5.22 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.

acquerices	+	++		The sequence on noise sequence contigs from any source.	
accession number links				- Associate sequences with Genbank/EMBL accession number.	
experiments	+	++		? Set up experiments to which sequences in the bin can belong.	
experiment sequences				? Add links associating sequences to experiments.	
sequence tags		scan		? Tag regions of sequences within the sequence bin with locus information.	
all a second and a second and a second					
Database configuration	on				
Table	Add B	atch Add	Update or delete	Comments	
loci	+	++	?		
	databa	ank scan			
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.	
PCR reactions	+	++	?	Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.	
PCR locus links	+	++		Link a locus to an in silico PCR reaction.	
nucleotide probes	+	++	?	Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.	
probe locus links	+	++		Link a locus to an in silico hybridization reaction.	
isolate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.	
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.	
sequence attributes	+	++	?	Define attributes that can be set for contigs in the sequence bin.	
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.	
set loci	+	++	?	Add loci to sets.	
set schemes	+	++	?	Add schemes to sets.	
set metadata	+	++	?	Add metadata collection to sets.	
setview	+	++	?	Set database views linked to sets.	
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.	
scheme members	+	++	?	Defines which loci belong to a scheme.	
scheme fields	+	++	?	Defines which fields belong to a scheme.	
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.	
cheme group scheme members	+	++	?	Defines which schemes belong to a group.	
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.	

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 U	atabase: Species hon sers: Add   Query/upda olates: Add   Query/up		ior's page (database)		
Logged in: Keith Jolley (ke	e <b>ith)</b> . Log out   Change pa	ssword			Toggle: i
Add new con	nposite field	1			
Recordid:!	strain_designations	s are marked with an exclamation m	ark (!). name of the field as it will appear in the web interface	Action Reset Submit	-
position after:!		<ul> <li>field present in the isolate table</li> </ul>			
	○ true ● false Keith Jolley (keith) 2014-07-08	Sets whether to display field in isolate q	uery results table (can be overridden by user preference).		

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.

loci. epetitive lo
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#### Select the composite field from the list and click 'Update'.

Users: Add   Qu	ery/update			
y (keith). Log out   Ch	nange password	d		
delete con	nposite	e field		
efined. field name	position	main	definition	missing data
	after isolate	display false	[serogroup]: P1.[PorA_VR1],[PorA_VR2]: [FetA_VR]: ST-[scheme 1:ST] ([scheme 1:clonal_complex])	ND: P1.ND,ND: F-ND: ST-ND (-)
	Users: Add   Qu Isolates: Add   Q y (keith). Log out   Ch delete con efined.	Users: Add   Query/update Isolates: Add   Query/update y (keith). Log out   Change passwor delete composite efined. field name position after	Users: Add   Query/update Isolates: Add   Query/update   Batch inser y (keith). Log out   Change password delete composite field efined. field name position main after display	Isolates: Add   Query/update   Batch insert y (keith). Log out   Change password  delete composite field  efined.  field name position after display (serogroup): P1.[PorA_VR2]: [FetA_VR]: ST-[scheme 1:ST]

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 / Users: A	dd   Query/u Add   Query/	update   Batch insert	Curator's page (database)
		- strain_designati	ion
puale composit	e neiu	- Strain_uesiynau	1011
position after: isolate		-	
main display: false 👻 curator: Keith Jolley			
datestamp: 2014-04-09		Update	
	empty value ND	regex	curator datestamp delete edit move
Serogroup [isolate field] ; P1.	ND		Keith Jolley 2009-11-12 delete edit up down
PorA_VR1 [locus]	ND		Keith Jolley 2009-11-12 delete edit up down Keith Jolley 2009-11-12 delete edit up down
	ND		
PorA_VR2 [locus]	ND		Ketth Jolley 2009-11-12 delete edit up down Keith Jolley 2009-11-12 delete edit up down
· · · ·	ND		Keith Jolley 2009-11-12 delete edit up down
FetA VR [locus]	F-ND		Keith Jolley 2009-11-12 delete edit up down
: ST-	1110		Keith Jolley 2009-11-12 delete edit up down
ST [MLST field]	ND		Keith Jolley 2009-11-12 delete edit up down
(			Keith Jolley 2009-11-12 delete edit up down
clonal_complex [MLST field]	-	s/ST-(\S+) complex.*/cc\$1	
)			Keith Jolley 2009-11-12 delete edit up down
Add new field:			
add frem frem.			
		Add new text field	
	-	Add new isolate field	
	•	Add new locus field	
	•	Add new scheme field	
		: Keith Jolley	
	datestamp	: 2014-07-08	

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'.

## 5.23 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.

user groups user group members user permissions isolates olate field extended attribute value projects project members isolate aliases	+ + + + + + + + + + +	+++ ++ ++		2	·· · · · · · · · · · · · · · · · · · ·
user permissions isolates plate field extended attribute value projects project members	+ + es +			- £	Users can be members of these groups - use for setting access permissions.
isolates blate field extended attribute value projects project members	+ es +	++		?	Add users to groups for setting access permissions.
plate field extended attribute value projects project members	es +			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table
projects project members		++	query   browse	list   batch update	
project members	+	++		?	Add values for additional isolate field attributes.
		++		?	Set up projects to which isolates can belong.
icolate aliaces	+	++		?	Add isolates to projects.
Isolate allases	+	++		?	Add alternative names for isolates.
PubMed links	+	++		?	
allele designations		++		?	Allele designations can be set within the isolate table functions.
sequences	+	++		?	The sequence bin holds sequence contigs from any source.
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++		?	Set up experiments to which sequences in the bin can belong.
experiment sequences				?	Add links associating sequences to experiments.
sequence tags		scan		?	Tag regions of sequences within the sequence bin with locus information.
Database configuratio		tch Add II	Indate or delete		Comments
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Table / loci locus aliases PCR reactions	Add Bat + databar + +	++ nk scan	? ?	Set up in silico PCR i	is for loci. These can also be set when you batch add loci. eactions. These can be used to filter genomes for tagging to specific repetitive loci.
Table / loci loci locus aliases PCR reactions nucleotide probes	Add Bat + databar + + +	++ nk scan ++ ++ ++	? ?	Set up <i>in silico</i> PCR i Define nucleotide pro	is for loci. These can also be set when you batch add loci. eactions. These can be used to filter genomes for tagging to specific repetitive loci. ibes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.
Table loci locus aliases PCR reactions nucleotide probes solate field extended attributes	Add Bat + databar + +	++ nk scan ++ ++	? ? ?	Set up <i>in silico</i> PCR i Define nucleotide pro Define additional attr	is for loci. These can also be set when you batch add loci. eactions. These can be used to filter genomes for tagging to specific repetitive loci. bes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. ibutes to associate with values of a particular isolate record field.
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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).



Download the Excel template:

PTRIMIST Users: Add   Query/update Isolates: Add   Query/update   Batch insert	
Logged in: Keith Jolley (keith). Log out   Change password	Toggle: i
Batch insert isolate value extended attributes	
<ul> <li>This page allows you to upload isolate field extended attribute value 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 (xtsx format)</li> </ul>	et.
Paste in tab-delimited text (include a field header line).	
	Reset Submit
Back	

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'.

## 5.24 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.

PubMed links	-	+++		1
allele designations		++		? Allele designations can be set within the isolate table functions.
sequences		+++		? The sequence bin holds sequence contigs from any source.
accession number links	1	+++		? Associate sequences with Genbank/EMBL accession number.
experiments		+ ++		? Set up experiments to which sequences in the bin can belong.
experiment sequences				? Add links associating sequences to experiments.
sequence tags		scan		? Tag regions of sequences within the sequence bin with locus information.
C.				
Database configuration	on			
Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	data	bank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
PCR reactions	+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
solate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes	+	++		Define attributes that can be set for contigs in the sequence bin.
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.
set loci	+	++	?	Add loci to sets.
set schemes	+	++	?	Add schemes to sets.
set metadata	+	++	?	Add metadata collection to sets.
setview	+	++	?	Set database views linked to sets.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
	+	++	?	Defines which schemes belong to a group.
cheme group scheme members		++	2	Defines which scheme groups belong to a parent group.

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'.

Database: Species home   Curator's page (species)   Curator's page (species	ator's page (database)	
Logged in: Keith Jolley (keith). Log out   Change password		Toggle: i
Add new sequence attribute		
Please fill in the fields below - required fields are marked with an exclamation in Record  key:! read_length type:! integer  curator:! Kettn Jolley (Kettn) datestamp:! 2014-07-15 description:	Action Reset Submit	

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

Logged in: Keith Jolley (Reith). 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 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 (!).
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 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.
If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any 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.
If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any 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.
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 (I).
- Paste in sequences in FASTA format - Attributes -
isolate id: 1 Read identifier from FASTA 🗸
identifier fieldt: id
sender: !
memoa. •
assembly id:
read length:
Options
Don't insert sequences shorter than 250 - bps.
Link to experiment
Alternatively upload FASTA file Action Action
Select FASTA file: Reset Submit
Browse No file selected.
Back

# 5.25 Checking external database configuration settings

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

				7	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the table.
isolates	+	++		owse   list   update	
isolate field extended attribute values	+	++		?	Add values for additional isolate field attributes.
projects	+	++		?	Set up projects to which isolates can belong.
project members	+	++		?	Add isolates to projects.
isolate aliases	+	++		?	Add alternative names for isolates.
PubMed links	+	++		?	
allele designations		++		?	Allele designations can be set within the isolate table functions.
sequences	+	++		?	The sequence bin holds sequence contigs from any source.
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++		?	Set up experiments to which sequences in the bin can belong.
experiment sequences				?	Add links associating sequences to experiments.
		scan		?	Tag regions of sequences within the sequence bin with locus information.
b Database configuratio			Indato or doloto		Commonte
Database configuratio	Add	Batch Add	Jpdate or delete		Comments
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Database configuratio	Add f + datat	Batch Add ( ++ pank scan	?		
Database configuration	Add F + datat	Batch Add I ++ pank scan ++		Add alternative	names for loci. These can also be set when you batch add loci.
Database configuration	Add F + datat + +	Batch Add ( ++ pank scan	?	Add alternative Set up in silico	names for loci. These can also be set when you batch add loci. PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
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Database configuration	Add F + datat + + + + + + +	Batch Add   ++ bank scan ++ ++ ++ ++	? ? ?	Add alternative Set up in silico Define nucleoti Define addition Used to constru Define attribute	e names for loci. These can also be set when you batch add loci. PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci. ide probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. al attributes to associate with values of a particular isolate record field. I composite fields consisting of fields from isolate, loci or scheme fields. as that can be set for contigs in the sequence bin.
Database configuration	Add E + datat + + + + + + + + + + +	Batch Add   ++ bank scan ++ ++ ++ ++ ++	? ? ? ?	Add alternative Set up in silico Define nucleoti Define addition Used to constru Define attribute Describes scher	e names for loci. These can also be set when you batch add loci. PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci. de probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. al attributes to associate with values of a particular isolate record field. ct composite fields consisting of fields from isolate, loci or scheme fields.
Database configuration	Add E + datat + + + + + + + + + + + + +	Batch Add   ++ bank scan ++ ++ ++ ++ ++	? ? ? ?	Add alternative Set up in silico Define nucleoti Define addition Used to constru Define attribute Describes scher Defines which I	e names for loci. These can also be set when you batch add loci. PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci. ide probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. al attributes to associate with values of a particular isolate record field. ict composite fields consisting of fields from isolate, loci or scheme fields. Is that can be set for contigs in the sequence bin. mes consisting of collections of loci, e.g. MLST.
Database configuration	Add 4 + datat + + + + + + + + + + + + + +	Batch Add   1 ++ bank scan ++ ++ ++ ++ ++ ++ ++ ++ ++ ++	? ? ? ? ? ?	Add alternative Set up in silico Define nucleoti Define addition Used to constru Define attribute Describes scher Defines which I Defines which I	a names for loci. These can also be set when you batch add loci. PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci. de probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. al attributes to associate with values of a particular isolate record field. ct composite fields consisting of fields from isolate, loci or scheme fields. ss that can be set for contigs in the sequence bin. mes consisting of collections of loci, e.g. MLST. loci belong to a scheme.
Database configuration	Add 4 + 4 datat + 4 + 4 + 4 + 4 + 4 + 4 + 4 + 4 + 4 + 4	Batch Add   ++ bank scan ++ ++ ++ ++ ++ ++ ++ ++ ++	? ? ? ? ? ? ? ?	Add alternative Set up in silico Define nucleoti Define addition Used to constru Define attribute Describes scher Defines which f Describes group	e names for loci. These can also be set when you batch add loci. PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci. al probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. al attributes to associate with values of a particular isolate record field. ct composite fields consisting of fields from isolate, loci or scheme fields. as that can be set for contigs in the sequence bin. mes consisting of collections of loci, e.g. MLST. too belong to a scheme.

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.

	Isolates: Add   Query/update   Batch inse	en								
gged in: Keith Jolley (	keith). Log out   Change password									
onfiguratio	on check - Neisseria F	PubML	ST							
lelper applicati	ons									
Program	Path	netallod E	xecutable							
EMBOSS infoalign	/usr/bin/infoalign	ok	ok							
EMBOSS sixpack	/usr/bin/sixpack	ok	ok							
EMBOSS stretcher	/usr/bin/stretcher	ok	ok							
blastn	/usr/local/ncbi-blast+/bin/blastn	ok	ok							
blastp	/usr/local/ncbi-blast+/bin/blastp	ok	ok							
blastx	/usr/local/ncbi-blast+/bin/blastx	ok	ok							
ipcress	/usr/bin/ipcress	ok	ok							
mafft	/usr/local/bin/mafft	ok	ok							
makeblastdb	/usr/local/ncbi-blast+/bin/makeblastdb	ok	ok							
mogrify	/usr/bin/mogrify	ok	ok							
muscle	/usr/bin/muscle	ok	ok							
tblastx	/usr/local/ncbi-blast+/bin/tblastx	ok	ok							
ocus database	6									
	-									
Locus	Database					Secondary id field value	e Sequence field			
'16S rDNA	pubmlst_bigsdb_neisseria_seqde			allele_id	locus	'16S_rDNA	sequence	ok	ok	197
'porA	pubmlst_bigsdb_neisseria_seqde			allele_id	locus	'porA	sequence	ok	ok	164
'porB	pubmlst_bigsdb_neisseria_seqde			allele_id	locus	'porB	sequence	ok	ok	695
'rpIF	pubmlst_bigsdb_neisseria_seqde			allele_id	locus	'rpIF	sequence	ok	ok	109
BACT000001 (rps			t 5432 sec	allele_id	locus	BACT000001	sequence	ok	ok	8189
BACT000002 (rps			t 5432 sec	allele_id	locus	BACT000002	sequence	ok	ok	6567
BACT000003 (rps			t 5432 sed	allele_id	locus	BACT000003	sequence	ok	ok	5965
BACT000004 (rps			t 5432 sec	allele_id	locus	BACT000004	sequence	ok	ok	6195
BACT000005 (rps			t 5432 sed	allele_id	locus	BACT000005	sequence	ok	ok	5707
BACT000006 (rps			t 5432 sec	allele_id	locus	BACT000006	sequence	ok	ok	4918
BACT000007 (rps BACT000008 (rps			t 5432 sed t 5432 sed	allele_id allele id	locus locus	BACT000007 BACT000008	sequence	ok ok	ok ok	5667 5260

Any problems will be highlighted with a red X.

# Curator's guide

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

## 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.

ed in: Keith Jolley (keith). Log out	Change	password			
tabase curator's	into	rfago	Noiscor	io Dubl	NI CT
Idvase curator s	me	nace	· Neissen	a ruun	
Add, update or delet	e reco	ords			
Record type	Add	Batch Add	Update o	r delete	Comments
users	+	++	?	)	
user groups	+	++	?		Users can be members of these groups - use for setting access permissions.
user group members	+	++	?		Add users to groups for setting access permissions.
user permissions	+	++	?		Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query   bro batch u		
solate field extended attribute values	+	++	?		Add values for additional isolate field attributes.
projects	+	++	?		Set up projects to which isolates can belong.
project members	+	++	?		Add isolates to projects.
isolate aliases	+	++	?		Add alternative names for isolates.
PubMed links	+	++	?		
allele designations		++	?		Allele designations can be set within the isolate table functions.
sequences	+	++	?		The sequence bin holds sequence contigs from any source.
accession number links	+	++	?		Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?		Set up experiments to which sequences in the bin can belong.
experiment sequences			?		Add links associating sequences to experiments.
sequence tags		scan	?		Tag regions of sequences within the sequence bin with locus information.
sequence tags		scan	?		Tag regions of sequences within the sequence bin with locus information.
G					
Database configurati	on				
Table	Add	atab Add L	pdate or delete		Comments
loci		atch Add U	puale of delete		Comments
1001	+		6		
		ank scan			
locus aliases	+	++			names for loci. These can also be set when you batch add loci.
PCR reactions	+	++			PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	++	++		Define nucleoti	ide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
solate field extended attributes		++	2		nal attributes to associate with values of a particular isolate record field.

Enter the user's details in to the form.

PubMLST)	Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update Isolates: Add   Query/update   Batch insert	
Logged in: Keith Jolley	(keith). Log out   Change password	Toggle: i
Add new us	er	
Please fill in the field	is below - required fields are marked with an exclamation mark (!).	Action
id:!	286	Reset Submit
user name:!	jbloggs	
surname:!	Bloggs	
first name:!	Joe	
email:	joe.bloggs@ox.ac.uk	
affiliation:!	University of Oxford, UK	
status:!	user 👻	
date entered:!	2014-07-09	
datestamp:!	2014-07-09	
curator:!	Keith Jolley (keith)	

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.

# 6.2 Adding new allele sequence definitions

## 6.2.1 Single allele

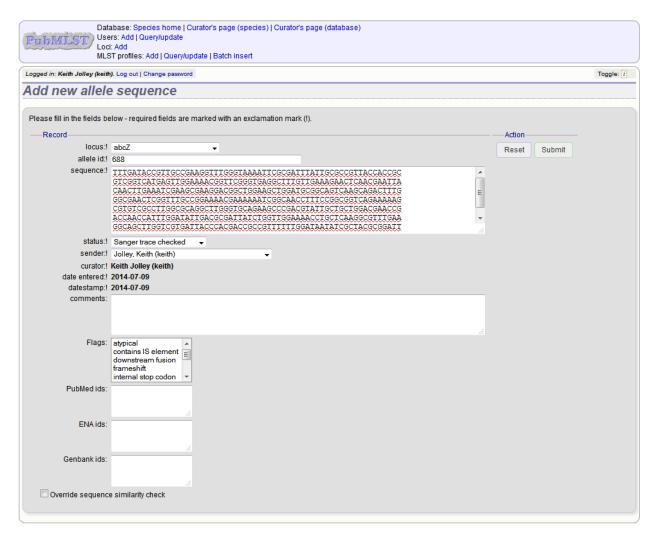
To add a single new allele, click the sequences (all loci) add (+) link on the curator's main page - if only a few loci are defined with permission for the current user to curate then they will be listed individually and the specific locus allele addition links can also be used.

		-		
ged in: Keith Jolley (keith). Log				
tabase curato	r's i	interfa	ce - Neisseria loc	us/sequence definitions
Add, update or de	elete	e records		
Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++	?	
cheme curator control list	+	++	query   batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	query   batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++   FASTA	?	
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	+	++	?	
MLST profiles	+	++	query   browse   list   batch update	
rplF species profiles	+	++	query   browse   list   batch update	
PubMed links (to profiles)	+	++		
Database configu			odate or	
	dd	Add	delete	Comments
loci	+ datat sci		?	
	50			
locus aliases	+	++	2 Add alternative names for	r loci. These can also be set when you batch add loci.

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 can either be:

- Sanger trace checked
- WGS: manual extract
- WGS: automated extract
- unchecked



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.

#### 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 (all loci) link on the curator's main page.

ed in: Keith Jolley (keith). Log	nout I C	banga paraw	ord	
tabase curato	r's I	nterfa	ce - Neisseria loc	sus/sequence definitions
Add, update or de	elete	records		
Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++	?	
cheme curator control list	+	++	query   batch	Define which curators can add or update profiles for particular schemes.
ocus curator control list	+	++	query   batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++ FASTA	?	
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	+	++	?	
MLST profiles	+	++	query   browse   list   batch update	
rpIF species profiles	+	++	query   browse   list   batch update	
ubMed links (to profiles)	+	++		
	Iratio	n		

Download a template Excel file from the following 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	Toggle: i
Batch insert sequences	
This page allows you to upload allele sequence data as tab-delimited text or copied from a spreadsheet. • Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. • If the locus uses integer allele ids you can leave the allele_id field blank and the next available number will be used. • The status defines how the sequence was curated. Allowed values are: 'Sanger trace checked', 'WGS: manual extract, 'W • Sequence flags can be added as a semi-colon (;) separated list • Download tab-delimited header for your spreadsheet - use Paste special → text to paste the data. • Download submission template (vax format) • Please note, some locn have extended attributes which may be required. For affected loci please use the batch insert part Reload page specific for locus: Select ▼ Reload Please select the sender from the list below: Select sender ▼ Value will be overridden if you include a sender field in your pasted data. ③ Ignore existing or duplicate sequences ③ Ignore sequences that are not complete reading frames - these must have a start and in-frame stop codor sequences are also ignored. Paste in tab-delimited text (include a field header line).	ge specific to that locus:

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. 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.

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	Toggle: i
Batch insert sequences	
This page allows you to upload allele sequence data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. If the locus uses integer allele ids you can leave the allele_id field blank and the next available number will be used. The status defines how the sequence was curated. Allowed values are: "Sanger trace checked", "WGS: manual extract Sequence flags can be added as a semi-colon (;) separated list Download tab-delimited header for your spreadsheet - use Paste special → text to paste the data. Download submission template (xisk format) Please note, some loci have extended attributes which may be required. For affected loci please use the batch insert Reload page specific for locus: Select Reload Please select the sender from the list below: Jolley, Keith (keith)  Value will be overridden if you include a sender field in your pasted data. Gingnore existing or duplicate sequences Silently reject all sequences that are not complete reading frames - these must have a start and in-frame stop cod sequences are also ignored. Override sequence similarity check Paste in tab-delimited text (include a field header line).	page specific to that locus:
locus       allele_id       sequence       status       comments       flags         abc2       IITGAIACIGITISCCGAAGGTIIGGEGGAAATICGCGAATIGAACGTIAICATCAIGACAGCCAGGCGGGAGGACGTIGGAAGGC       gattigaAGGCGAAGGCCGAAGGCCGACGTAIGGCGAAGGACGGACGACGCAGGCGAGGACGGACGGACG	Reset Submit

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

PubMLS	Database: Species home   Curator's page (species)   Curator's p Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert	page (database)				
Logged in: Keith J	lley (keith). Log out   Change password					Toggle: i
Batch ins	ert sequences					
Import status						
Sender: Keith Jo	ley					
No obvious prot	iems identified so far.					
Data to be in						
The following ta	ble shows your data. Any field with red text has a problem and needs t	to be checked. Note: V	/alla sequ	ence flags are	displayed with a red bad	ckground not red text.
locus allele_i					datestamp comments	flags
abcZ 688 abcZ 689	TTTGATACTGTTGCCGAAGG GCGGATTGTCGAACTCGATC Sanger tr		2	2014-07-09 2014-07-09		
abcz 089	TTTGATACTGTTGCCGAAGC GCGGATTGTCGAACTCGATC Sanger tr	ace checked 2	2	2014-07-09	2014-07-09	

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

Pub	PTTTTTTTTTST Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert									
Logged in	n: Keith Jo	lley (keith). Log out   Change pass	word							Toggle: i
Batc	h ins	ert sequences								
P	t statu: rimary k abcZ; all		Problem(s) n nucleotide (G A T C) charad	cters.						
The fol		nported ble shows your data. Any field v sequ					-	displayed with a re		ot red text.
abcZ	688	TTTGATACTGTTGCCGAAGG			2	2	2014-07-09			
abcZ	689	TTTGATACTGTTGCCGAAGC	. GCGGATTGTCGAACTCGATC	Sanger trace checked	2	2	2014-07-09	2014-07-09		

### 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.

Users	: Add Add	Query/upda			Curator's page (database)			
ogged in: Keith Jolley (keith).	Log ou	ut   Change pa	ssword					
atabase curat	or's	s interf	ace - N	eisseria lo	ocus/sequence definitions			
dtubuot ourut								
🞽 Add, update or	dele	ete record	s					
Record type	Ad	d Batch Add	Updat	e or delete	Comments			
users	+	++		?				
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.			
user group members	+	++		?	Add users to groups for setting access permissions.			
user permissions	+	++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.			
locus descriptions	+	++		?				
scheme curator control lis	t +	++	que	ry   batch	Define which curators can add or update profiles for particular schemes.			
locus curator control list	+	++	que	ry   batch	Define which curators can add or update sequences for particular loci.			
sequences (all loci)	+	++ FASTA		?				
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.			
PubMed links (to sequences)	+	++		?				
MLST profiles	+	++		wse   list   batch pdate				
rpIF species profiles	+	++		wse   list   batch pdate				
PubMed links (to profiles)	+	++						
Database confi	gura							
Table	Add	Add	pdate or delete		Comments			
loci	+	++	?					
	databank scan							
locus aliases	+	++	? Add	Add alternative names for loci. These can also be set when you batch add loci.				
ocus extended attributes	+	++	? Def	Define additional fields to associate with sequences of a particular locus.				
client databases	+	++	? Add	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks and				

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

PubML	Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert
Logged in: Keith	Jolley (keith). Log out   Change password Toggle: 1
Batch in	sert sequences
	•
(loci with integ	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 fer ids only). Do not include 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.
Enter para	ameters
locus:	abcZ •
status:!	Sanger trace checked 🗸
sender:!	Jolley, Keith (keith)
(FASTA):!	<pre>&gt;isolate1 TITGATACTGTTGCGAAGGTTTGGGCGAAATTCGCGATTTATTGCAACGTTATCATCAT GTCAGCCGGACTTGGCGAAGGTCGAGGCCGTATTGGAGGCCGTAGGAAGGTGGAAGGAGGAGGGCGGAGGTGGAAGGAGGAGGGGGGGG</pre>
sequences	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 are also ignored. e sequence similarity check xt available id (only for loci with integer ids)  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'.

PTTTILLIST Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert							
Logged in: Keith Jolley (keith). Log out   Change password	Toggle: i						
Batch insert sequences							
Sequence check       Original designation Allele id Status isolate1     Action       Upload valid sequences							

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

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									
Batch insert	sequ	iences							
Sequence check Original designation isolate1 isolate2		I Status OK Sequence contains non nucleotide (G[A[T]C) characters.	Action Upload valid sequences						

# 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.

In order to update or delete an allele, first you must select it. Click the query (?) sequences (all loci) link - if only a

few loci are defined with permission for the current user to curate then they will be listed individually and the specific locus query links can also be used.

Users: A Loci: Ad	dd   0 d	Query/upda		age (species)   Curato tch insert	or's page (database)
ogged in: Keith Jolley (keith). Lo	g out	Change pas	sword		
atabase curato	r's	interf	ace - Ne	eisseria locu	is/sequence definitions
🗡 Add, update or d					
Record type	Add	Batch Ad	d Up	late or delete	Comments
users	+	++		?	
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.
user group members	+	++		?	Add users to groups for setting access permissions.
user permissions	+	++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++		?	
scheme curator control list	+	++	q	uery   batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	C	uery   batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++   FAST	A	?	
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
ubMed links (to sequences	) +	++		?	
MLST profiles	+	++	query   brow	/se   list   batch update	
rpIF species profiles	+	++	query   brow	/se   list   batch update	
PubMed links (to profiles)	+	++			
Database configu	urati				
	Add	Batch Add	Update or delete		Comments
loci	+	++	?		
		tabank scan			
locus aliases	+	++	?	Add alternative names fo	r loci. These can also be set when you batch add loci.
locus extended attributes	+	++	?	Define additional fields to	o associate with sequences of a particular locus.
client databases	+	++	2		at use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these

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 and enter the allele number in the allele\_id field.

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.

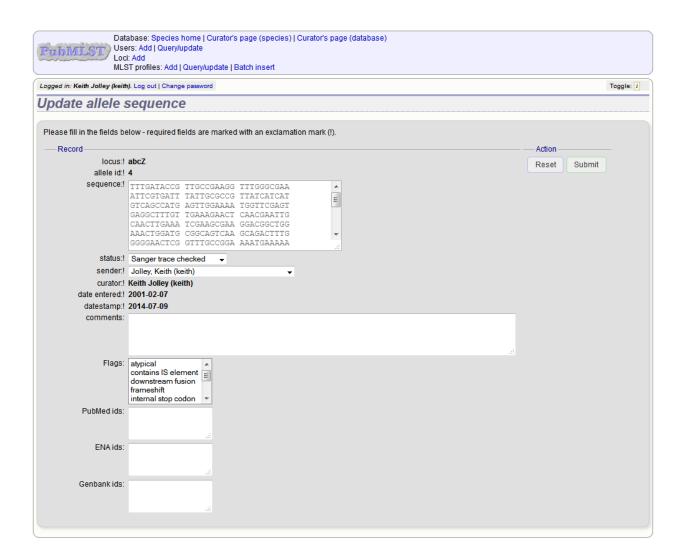
Database: Species home   Curator's page (species)   Curator's page (database) Prifinitizer Loc: Add MLST profiles: Add   Querylupdate   Batch insert
ogged in: Keith Jolley (keith). Log out   Change password
Query sequences for Neisseria locus/sequence definitions database
Some loci have additional fields 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).
- Search criteria Display
allele id v = v 4 + ( Order by: locus v ascending v
Display: 25    records per page []
- Filter query by Action
locus: abcZ  status:
sender:
curator.
allele flag:
I record returned.
Delete — Database configuration — Flags — Flag
Delete ALL Export configuration/data Batch set
Delete Update locus allele id sequence sequence length status sender curator date entered datestamp comments flags
Therefore for the state of the

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.

Database: Species home   Curator's page (database) Users: Add   Query/update Loc: Add MLST profiles: Add   Query/update   Batch insert									
Logged in: Keith Jolley (keith). Log out   Change password									
Delete allele	sequence								
You have chosen to de	elete the following record:								
locus:	abcZ								
allele id:	4								
sequence:	TTIGATACCE TIGCCGAAGE TIGGGCGAA ATICGTGATI TATIGCGCCE TTATCATCAT GTCAGCCATE AGTIGGAAAA IGGTTCGAGT GAGGCTTIGI IGAAAGAACI CAACGAATIG CAACTIGAAA TCGAAGCGAA GGACGGCTGE AAACTGGAIG CGGCGAGCGA GCGAGCTTIG GGGGGAACTCE GTTIGCCGGA AAATGAAAAA ATCGGCAACC TITCCGGCGG TCAGAAAAAG CGCGTCGCCT TGGCTCAGGC TIGGGTGCGA AAGCCCGACG TATIGCTGCI GGACGAGCCGA ACCAACCATI IGGATATCGA CGCGATTATI IGGCTGGAAA ATCGGCTAGA AGCGTTIGAA GGCAGCTTGG TTGIGATTAC CCACGACCGC CGTITITGG ACAATATGGC CACCGGATI GTCGAACTGC ATC								
status:	Sanger trace checked								
sender:	Keith Jolley								
curator:	Man-Suen Chan								
date entered:	2001-02-07								
datestamp:	2009-11-11								
comments:									
Delete!									

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.

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



# 6.4 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 next to the scheme name (e.g. MLST):

Users:	Add	Species home   Query/update		page (species)   Curate	or's page (database)		
Loci: A		es: Add   Quer	y/update   B	atch insert			
gged in: Keith Jolley (keith). L	_						
atabaaa auwata	- ul	. interfe		laiaaavia laar	· · · · · · · · · · · · · · · · · · ·		
alabase curalo	or s	s interia	ice - N	eisseria locu	is/sequence definitions		
/ Add, update or o	dele	ete records					
Record type	A	dd Batch Add	Ur	odate or delete	Comments		
users	-	+ ++		?			
user groups	-	+ ++		?	Users can be members of these groups - use for setting access permissions.		
user group members		+ ++		?	Add users to groups for setting access permissions.		
user permissions	-	+ ++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.		
locus descriptions		+ ++		?			
scheme curator control lis	t -	+ ++		query   batch	Define which curators can add or update profiles for particular schemes.		
locus curator control list	-	+ ++		query   batch	Define which curators can add or update sequences for particular loci.		
sequences (all loci)		+ ++   FASTA		?			
accession number links		+ ++		?	Associate sequences with Genbank/EMBL accession number.		
PubMed links (to sequence	s) -	+ ++		?			
MLST profiles	Г	+ ++	query   bro	uery browse   list   batch update			
rpIF species profiles		+ ++	query   bro	uery   browse   list   batch update			
PubMed links (to profiles)		+ ++					
Database config	jura Add	Batch I	Jpdate or delete		Comments		
loci	+	++	?				
	da	atabank					
		scan					
locus aliases	+	++	?	Add alternative names for	loci. These can also be set when you batch add loci.		
locus extended attributes	+	++	?	Define additional fields to	associate with sequences of a particular locus.		
client databases	+	++	?				
client database loci	+	++	?	? Define loci that are used in client databases.			
client database schemes	+	++	?	? Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table.			
client database fields linked to loci	+	++	?	Define fields in client data	abase whose value can be displayed when isolate has matching allele.		

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)	sers: Add   Query/up oci: Add	me   Curator's page (species)   Curato date uery/update   Batch insert	r's page (database)	
Logged in: Keith Jolley (k	e <b>ith)</b> . Log out   Change p	assword		Toggle: i
Add new ML	ST profile			
Please fill in the fields	below - required field	ds are marked with an exclamation ma	'к (1)	
	below required ion		N (.).	
Record				
	10880	×		
abcZ: !		×		
adk: !				
aroE: !				
fumC: !		<b>•</b>		
gdh: !		× ×		
pdhC: !		<u>*</u>		
pgm: !				
sender: !		<b>•</b>		
clonal_complex:				
curator: !	Keith Jolley (keith)			
date_entered: !	2014-07-10			
datestamp: !	2014-07-10			
PubMed ids:				
Action				
Denst Outer	- 14			
Reset Subr	nit			

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:

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								
Database curator's interface - Neisseria locus/sequence definitions								
Add, update or delete records								
Record type	Ad	d Batch Add	U	odate or delete	Comments			
users	+	++		?				
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.			
user group members	+	++		?	Add users to groups for setting access permissions.			
user permissions	+	++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.			
locus descriptions	+	++		?				
scheme curator control list	+	++		query   batch	Define which curators can add or update profiles for particular schemes.			
locus curator control list	+	++		query   batch	Define which curators can add or update sequences for particular loci.			
sequences (all loci)	+	++ FASTA		?				
accession number links	+	++			Associate sequences with Genbank/EMBL accession number.			
PubMed links (to sequences)	) +	++	?					
MLST profiles	+	++	query   bro	wse   list   batch upo	fate			
rpIF species profiles	+	++	query   bro	wse   list   batch upo	fate			
PubMed links (to profiles)	+	++						
Database configuration								
	Table         Add         Batch Add         Update or delete         Comments							
loci	+	++	?					
	databank							
locus aliases	+	scan ++	?	Add alternative names	i for loci. These can also be set when you batch add loci.			

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

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	Toggle: i
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. also provide it for each profile record.</li> </ul>	If however, you include it in the header line, then you must
<ul> <li>Download tab-delimited header for your spreadsheet - use Paste special → text to paste the data.</li> <li>Download submission template (xlsx format)</li> </ul>	
Please paste in tab-delimited text (include a field header line)	—

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'.

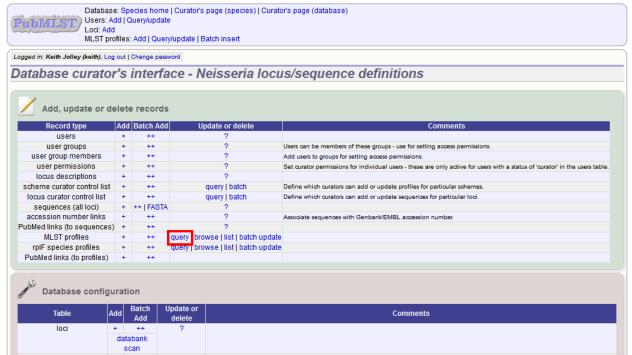
Database: Species home   Curator's page (species Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert	s)   Curator's page (database)
Logged in: Keith Jolley (keith). Log out   Change password	Toggle: i
Batch insert MLST profiles	
This page allows you to upload profiles as tab-delimited text or copied fr	
<ul> <li>Field header names must be included and fields can be in any o</li> <li>You can choose whether or not to include a ST field - if it is omitte you must also provide it for each profile record.</li> </ul>	order. Optional fields can be omitted if you wish. ed, the next available ST will be used automatically. If however, you include it in the header line, then
Download tab-delimited header for your spreadsheet - use Paste     Download automic is a translate (due formal)	e special $\rightarrow$ text to paste the data.
Download submission template (xlsx format)	
Please paste in tab-delimited text (include a field header line) abcz adk aros fumC gdb pdbC	pgm clonal_complex
2 3 4 122 8 4	6
Parameters A	Action
	Reset Submit
Value will be overridden if you include a sender field in your pasted data.	
Ignore duplicate profiles	
Back	

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

Prt11MILST       Database: Species home   Curator's page (species)   Curator's page (database)         Users: Add   Query/update       Loci: Add         Loci: Add       MLST profiles: Add   Query/update   Batch insert	
Logged in: Keith Jolley (keith). Log out   Change password	Toggle: i
Batch insert MLST profiles	
Import status	
Sender: Keith Jolley	
No obvious problems identified so far.	
Import data	
Data to be imported	
The following table shows your data. Any field coloured red has a problem and needs to be checked.	
ST     abcZ     adk     aroE     fumC     gdh     pdhC     pgm     clonal_complex     sender     curator     date_entered     datestamp       10880     2     3     4     122     8     4     6     2     2     2014-07-10     2014-07-10	

# 6.5 Updating and deleting scheme profile definitions

In order to update or delete a scheme profile, first you must select it. Click the query (?) profiles link next to the scheme name (e.g. MLST):



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

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	Toggle: i
Query/update profiles - Neisseria locus/sequence definitions	
Schemes Please select the scheme you would like to query: MLST     Select	
Locus/scheme fields     Display/sort options       ST     •       ST     •       •	
I record returned.       Delete       Delete ALL         Delete Update       ST       abcZ       adk       arce       fumC       gdh       pdh       pdiete       Delete       Delete	

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!'.

PubMLST L	batabase: Species home   Curator's page (species)   Curator's page (database) Isers: Add   Query/update oci: Add ILST profiles: Add   Query/update   Batch insert
	eith). Log out   Change password
Delete profile	3
You have chosen to de	elete the following record:
scheme id:	1) MLST
ST:	4563
abcZ:	2
adk :	
aroE :	
fumC :	
gdh :	
pdhC :	18
pgm :	
clonal_complex :	
	Ana-Belen Ibarz-Pavon
	Keith Jolley
date entered:	
datestamp:	2009-11-11
Delete!	

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'.

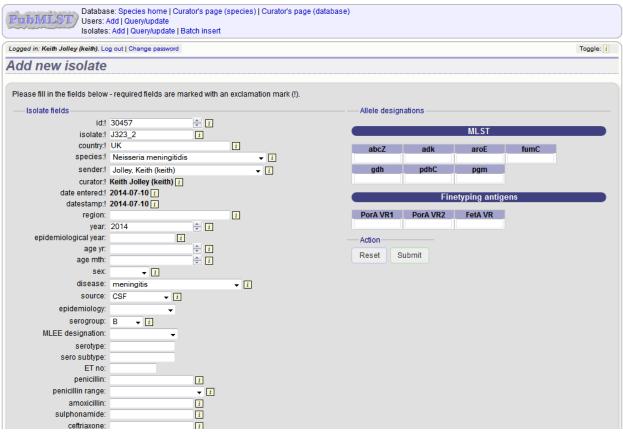
Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update Loci: Add MLST profiles: Add   Query/update   Batch insert									
Logged in: Keith Jolley (k	eith). Log out   Change password		Toggle: i						
Update profi	le								
Record		Action							
Update your record a	as required - required fields are marked with an exclamation mark (!):	Reset Submit							
ST: !	4563								
abcZ: !	2								
adk: !									
aroE: !									
fumC: !									
gdh: !									
pdhC: !	18								
pgm: !									
	ST-167 complex								
	Ibarz-Pavon, Ana-Belen (aibarz)								
date_entered: !	Keith Jolley (keith)								
_	2014-07-10								
PubMed ids:									

# 6.6 Adding isolate records

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

ed in: Keith Jolley (keith). Log out								
	Change	password						
tabase curator's	inte	rface -	Neisser	ia Publ	MLST			
2								
Add, update or delete	e reco	rds						
		Batch						
Record type	Add	Add	Update o	or delete	Comments			
users	+	++	?					
user groups	+	++	?		Users can be members of these groups - use for setting access permissions.			
user group members	+	++	?		Add users to groups for setting access permissions.			
user permissions	+	++	?	>	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.			
isolates	+	++	query   bro batch u					
solate field extended attribute values	+	++	?	, ,	Add values for additional isolate field attributes.			
projects	+	++	?	?	Set up projects to which isolates can belong.			
project members	+	++	?	>	Add isolates to projects.			
isolate aliases	+	++	?	2	Add alternative names for isolates.			
PubMed links	+	++	?	?				
allele designations		++	?	>	Allele designations can be set within the isolate table functions.			
sequences	+	++	?	?	The sequence bin holds sequence contigs from any source.			
accession number links	+	++	?	?	Associate sequences with Genbank/EMBL accession number.			
experiments	+	++	?	>	Set up experiments to which sequences in the bin can belong.			
experiment sequences			?	?	Add links associating sequences to experiments.			
sequence tags		scan	?	>	Tag regions of sequences within the sequence bin with locus information.			
S.								
Database configurati	on							
Table	Add P	atch Add U	pdate or delete		Comments			
loci	Auu B	41CH AUU 0	2		comments			
100		ank scan	f					
locus aliases	+	++	2	Add alternative	a names far lani. These and also be estudion you betch add lani			
	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.				
PCR reactions	+	++			PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.			

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.



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.

Isolates: Add	Query	update   Bato	ch insert		
ed in: Keith Jolley (keith). Log out	Change	password			
tabase curator's	inte	rface -	Neisseri	a Publ	MLST
Add, update or delete	e recc	ords			
Record type	Add	Batch Add	Update or	delete	Comments
users	+	++	?		
user groups	+	++	?		Users can be members of these groups - use for setting access permissions.
user group members	+	++	?		Add users to groups for setting access permissions.
user permissions	+	++	?		Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query   brow batch up		
isolate field extended attribute values	+	++	?		Add values for additional isolate field attributes.
projects	+	++	?		Set up projects to which isolates can belong.
project members	+	++	?		Add isolates to projects.
isolate aliases	+	++	?		Add alternative names for isolates.
PubMed links	+	++	?		
allele designations		++	?		Allele designations can be set within the isolate table functions.
sequences	+	++	?		The sequence bin holds sequence contigs from any source.
accession number links	+	++	?		Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?		Set up experiments to which sequences in the bin can belong.
experiment sequences			?		Add links associating sequences to experiments.
sequence tags		scan	?		Tag regions of sequences within the sequence bin with locus information.
2					
Database configuration	on				
Table	Add B	atch Add Up	date or delete		Comments
	+	++	?		
loci					
loci	databa	ank scan			
loci locus aliases	databa +	ank scan ++	?	Add alternativ	e names for loci. These can also be set when you batch add loci.

Download a submission template in Excel format from the link.

ProforMILSTD Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update   Isolates: Add   Query/update   Batch insert	
Logged in: Keith Jolley (keith). Log out   Change password	Toggle: i
Batch insert isolates	
This page allows you to upload isolate 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 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. 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 automated.</li> <li>Download submission template (xlsx format).</li> </ul>	
Please select the sender from the list below:	
Select sender   Value will be overridden if you include a sender field in your pasted data.	
Paste in tab-delimited text (include a field header line).	Action
	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).

Database: Species home   Curator's page Users: Add   Query/update Isolates: Add   Query/update   Batch insert		
Logged in: Keith Jolley (keith). Log out   Change password		Toggle: i
Batch insert isolates		
You can also upload allele fields along with the other iso method set as 'manual'.     You can choose whether or not to include an id number Download tab-delimited header for your spreadsheet - u Download submission template (xlsx format) Please select the sender from the list below:	e in any order. Optional fields can be omitted if you wish. semi-colon (;) separated list. parated list of PubMed ids (non integer ids will be ignored). plate data - simply create a new column with the locus name. field - if it is omitted, the next available id will be used automat	
— Paste in tab-delimited text (include a field header line).		Action
isolate aliases references country re	egion year epidemiological_year	Reset Submit
penicillin_range anoxicillin si ceftriaxone_range chloramphenicol cl cefotaxime_range rifampicin ri ciprofloxacin_range pending_assembly private_project comments abc2 ac	idemiology species ggrogroup mo subtype ET_no penicillin liphonamide ceftriaxone lioramphenicol_range ceftratime famplein_range ciproflovacin assembly status ENA accession lk arce fumc gdh pdhC 14 12 male Neisseria meningitidia	

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

Logged in: Keith Jolley (i	keith). Log out   Cha	inge pass	word											Toggle: i
Batch insert	isolates													
Import status														
Sender: Keith Jolley														
No obvious problems	identified so far.													
Import data														
Data to be impor	ted													
The following table s	hows your data. A	ny field	with red	text ha	as a problem and needs	to be o	hecked.							
id isolate alia	ses references	country	region	year	epidemiological_year	age_yr	age_mth	sex	disease	source	epidemiology	species	serogroup	MLEE_desig
30457 J392_1		UK		2014		12		male	meningitis and septicaemia	CSF		Neisseria meningitidis	В	
			_											

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

PrinkitsT Users: Add   Query/update Isolates: Add   Query/update   Batch insert										
Logged in: Keith Jolley (keith). Log out   Change password Toggle: 1										
Batch insert isolates										
Import status										
Primary key Problem(s)										
id: 30457 species 'Neisseria meningtidis' is not on the list of allowed values for this field.										
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 serogroup MLEE_desig									
30457 J392_1 UK 2014 12 male meningitis CSF 1	Neisseria B									
and n septicaemia	neningtidis									
	Þ									

# 6.7 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.

Leisseria Publ	Comments         Users can be members of these groups - use for setting access permissions.         Add users to groups for setting access permissions.         Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.         Add values for additional isolate field attributes.         Set up projects to which isolates can belong.
Update or delete ? ? ? ? query   browse   list   batch update ? ? ?	Comments           Users can be members of these groups - use for setting access permissions.           Add users to groups for setting access permissions.           Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.           Add values for additional isolate field attributes.
? ? ? query   browse   list   batch update ? ? ?	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Add values for additional isolate field attributes.
? ? ? query   browse   list   batch update ? ? ?	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Add values for additional isolate field attributes.
? ? ? query   browse   list   batch update ? ? ?	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Add values for additional isolate field attributes.
? ? ? query   browse   list   batch update ? ? ?	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Add values for additional isolate field attributes.
? ? ? query   browse   list   batch update ? ? ?	Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Add values for additional isolate field attributes.
? ? query   browse   list   batch update ? ? ?	Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Add values for additional isolate field attributes.
? ? query   browse   list   batch update ? ? ?	Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Add values for additional isolate field attributes.
? query   browse   list   batch update ? ? ? ?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Add values for additional isolate field attributes.
query   browse   list   batch update ? ? ?	users table. Add values for additional isolate field attributes.
batch update ? ? ?	
? ?	
?	Set up projects to which isolates can belong.
?	Add isolates to projects.
	Add alternative names for isolates.
?	
?	Allele designations can be set within the isolate table functions.
?	The sequence bin holds sequence contigs from any source.
?	Associate sequences with Genbank/EMBL accession number.
?	Set up experiments to which sequences in the bin can belong.
?	Add links associating sequences to experiments.
?	Tag regions of sequences within the sequence bin with locus information.
ite or delete	Comments
?	
? Add alternative	re names for loci. These can also be set when you batch add loci.
	? ? te or delete ?

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.

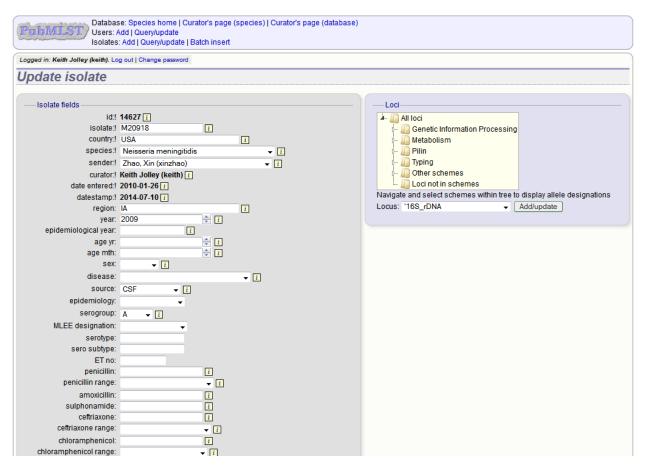
Solate query/update         Isolate provenance/phenotype fields       Display/sort options         Combine with:       AND ~         Country       =       USA       + 1         Display:       25 ~ records per page []         Very arr       =       2009         Action       Reset       Submit         9 records returned. Click the hyperlinks for detailed information.       Delete         Delete       Tag scanning       Projects         Delete ALL       Scan       Select project       Link         MLST       disolate fields I       Sequin       Str clonal comple         delete       update       update       12674       M18700       USA 2009       Neisseria       B       0       7301       ST-32 complexET-5	Md for op
Combine with: AND  Country  e  USA  country  country  country  e  Country  countr	fo
country       =       USA       + i       Display: 25 • records per page i         year       =       • 2009       Action       Reset       Submit         records returned. Click the hyperlinks for detailed information.       Delete       Tag scanning       Projects         Delete       Tag scanning       Projects       • Link         Delete       Scan       Select project       • Link         Delete       Update       Sequence bin       New version       id       isolate       aliases       country year       disease       species       serogroup       ST       clonal comple         telete       upload       create       12674       M18700       USA 2009       Neisseria       B       0       7301       ST-32	fo
year <ul> <li>action</li> <li>Reset</li> <li>Submit</li> </ul> Precords returned. Click the hyperlinks for detailed information.         Delete       Tag scanning - Projects         Delete ALL       Scan         Sequence       New version         id       isolate         aliases       country         year       disease         species       serogroup         Sequence       New version         id       isolate         Jelete       upload         Oreate       12674         MI ST         Strong       Strong         Jelete       upload         Jel	or
Action       Reset       Submit         records returned. Click the hyperlinks for detailed information.	
Reset       Submit         records returned. Click the hyperlinks for detailed information.         Delete       Tag scanning       Projects         Delete ALL       Scan       Select project       Link         Delete ALL       Scan       Select project       Link         Delete Update       New version       id       isolate       aliases       country       year       disease       species       serogroup       ST       clonal comple         telete       upload       create       12674       M18700       USA       2009       Neisseria       B       0       7301       ST-32	
Reset Submit         records returned. Click the hyperlinks for detailed information.         DeleteTag scanningProjects	
records returned. Click the hyperlinks for detailed information.  Delete Tag scanning Projects Delete ALL Scan Select project.  Isolate fields Sequence New Version id isolate aliases country year disease Species Serogroup St clonal comple letet update up	
Delete ALL Scan Select project Link elete Update Sequence New version id isolate aliases country year disease species serogroup size (bp) ST clonal comple elete update upload create 12674 M18700 USA 2009 Neisseria B 0 7301 ST-32	
Delete ALL Scan Select project Link elete Update Sequence New version id isolate aliases country year disease species serogroup size (bp) ST clonal comple elete update upload create 12674 M18700 USA 2009 Neisseria B 0 7301 ST-32	
Delete ALL Scan Select project Link Projects Delete ALL Scan Select project Link Hetete Update Sequence New version id isolate aliases country year disease species serogroup size (bp) ST clonal comple letete update upload create 12674 M18700 USA 2009 Neisseria B 0 7301 ST-32	
Delete ALL       Scan       Select project       Link         Delete ALL       Scan       Select project       Link         Delete Update       Sequence bin       New version id isolate       Isolate fields is       Sequence server to sequence bin isolate       Sequence to server to sequence bin isolate       Null ST         Idelete       Update       Update       Update       Sequence to server to serve	
helete Update Sequence New version id isolate aliases country year disease species serogroup Size (bp) ST clonal comple lelete update upload create 12674 M18700 USA 2009 Neisseria B 0 7301 ST-32	
helete Update Sequence New version id isolate aliases country year disease species serogroup Size (bp) ST clonal comple lelete update upload create 12674 M18700 USA 2009 Neisseria B 0 7301 ST-32	
belete Update Sequence New version id isolate aliases country year disease species serogroup Stream Section Stream St Stream Stream Str	
belete Update Sequence New version id isolate aliases country year disease species serogroup Stream Section Stream St Stream Stream Str	
belete Update Sequence New version id isolate aliases country year disease species serogroup Stream Section Stream St Stream Stream Str	Fi
Id     Isolate     allases     country year     disease     species     serogroup     SI     Cional comple       delete     upload     create     12674     M18700     USA 2009     Neisseria     B     0     7301     ST-32	<u>a</u>
	PorA VR1
meningitidis complex/ET-5	add
lelete update upload create 12675 M18701 USA 2009 Neisseria B 0 7302	-
lelete update upload create 12675 M18701 USA 2009 Neisseria B 0 7302 meningitidis	add
lefete update upload create 12676 M18725 USA 2009 Neisseria B 0 7303	add
meningitidis	
lelete update upload create 13090 M19024 PA09015 USA 2009 meningitis Neisseria B 0 7575	
meningitidis	add
lelete update upload create 14627 M20918 USA 2009 Neisseria A 1718070 4789. ST-5	
meningitidis 7980 complex/subgro	20
	20

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

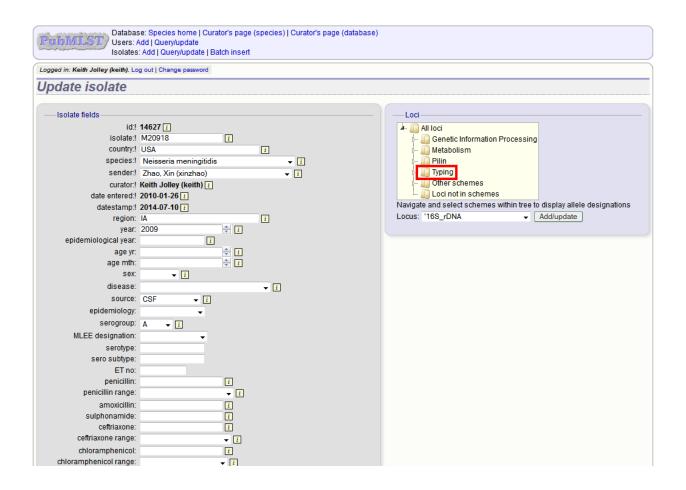
Public LST Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update Isolates: Add   Query/update   Batch insert									
Logged in: Keith Jolley (keith). Log out   Change password									
Delete isolate									
You have selected to d	lelete the following record:								
Provenance/meta	data								
id:	14627	source:	CSF	update history:	28 updates Show details				
isolate:	M20918	species:	Neisseria meningitidis	date entered:	2010-01-26				
strain designation:	A: P1.20,9: F3-1: ST-4789,7980	serogroup:	A	datestamp:	2014-06-17				
	(cc5)	sender:	Xin Zhao, Novartis (formerly at US						
country:	North America	curator	CDC) Carina Brehony, University of Oxford,						
region:		curator.	UK (E-mail:						
-	2009		carina.brehony@zoo.ox.ac.uk)						
Publication (1)									
			Iditi V, Humphrey JC, Sammons SA, Govi ncing projects. <i>Bioinformatics</i> 26:1819-20		l, Tondella ML, Harcourt BH, Mayer LW,				
Sequence bin									
contigs:	2049	N90:	456						
total length:	1718070 bp	N95:	324						
max length:	5436 bp	loci tagged:	979						
mean length:	839 bp	detailed breakdown:	Display						
N50:	1155								
Action									
Delete									
Delete									

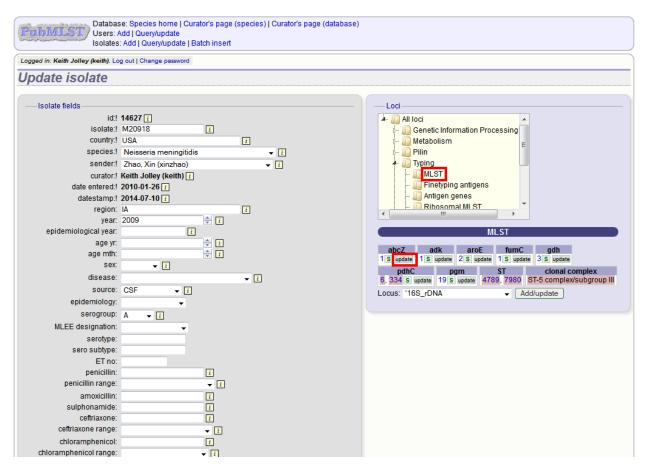
Pressing 'Delete' from this record page confirms the deletion.

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

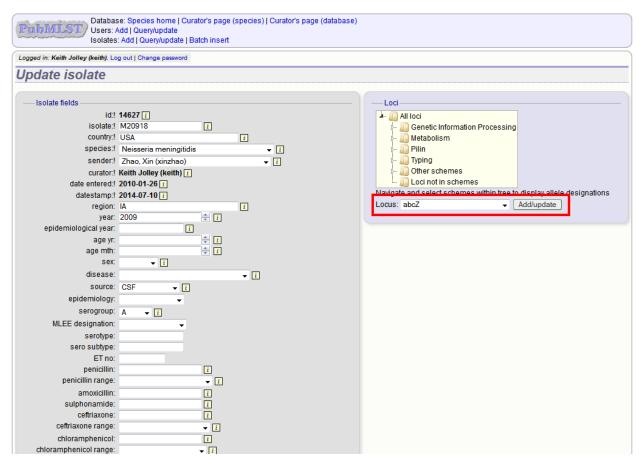


Allele designations can also be updated by clicking within the scheme tree and selecting the 'Add' or 'Update' link next to a displayed locus.





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'.



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 / U	atabase: Species home   Curator's pa sers: Add   Query/update olates: Add   Query/update   Batch inse	ge (species)   Curator's page (database) ert
Logged in: Keith Jolley (ke	aith). Log out   Change password	
Update abcZ	allele for isolate 146	27
Provenance/meta	a data	Locus: abcZ
id:	14627	Add new allele designation
isolate:	M20918	Please fill in the fields below - required fields are marked with an exclamation mark (!).
strain designation:	A: P1.20,9: F3-1: ST-4789,7980	Please fill in the fields below - required fields are marked with an exclamation mark (i).
	(cc5)	Record
country:		isolate id: 14627
region:		locus: abcZ
year:		allele id:1 5
source:		sender.! Jolley, Keith (keith)
-	Neisseria meningitidis	status: confirmed -
serogroup:		method: manual
	Xin Zhao	curator:! Keith Jolley (keith)
	Carina Brehony	datestamp:/ 2014-07-10 date entered:/ 2014-07-10
	26 updates show details	comments:
date entered:		
datestamp:	2014-06-17	Action
Update other loci	:	Reset Submit
Locus: abcZ	✓ Add/update	Existing designations
		Update         Delete         allele id         sender         status         method         comments           Update         Delete         1         Xin Zhao         confirmed         manual

# 6.8 Batch updating multiple isolate records

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

······	Change	password		
atabase curator's	inte	rface -	Neisseria Publ	<i>NLST</i>
2				
Add, update or delet	e reco	rds		
Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the user table.
isolates	+	++	query   browse   list   batch update	
isolate field extended attribute values	+	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences	+	++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
experiment sequences		scan	2	Tag regions of sequences within the sequence bin with locus information.

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 'Overwrite existing data' checkbox. Press 'submit'.

PriDMLST Database: Species home   Curator's page Users: Add   Query/update Isolates: Add   Query/update   Batch insert	(species)   Curator's page (database)	
Logged in: Keith Jolley (keith). Log out   Change password		
Batch isolate update		
This page allows you to batch update provenance fields or allele	e designations for multiple isolates.	
and secondary fields are unique), this should be entered	that you are selecting isolates on). If a secondary selection fiel	
id field value		
2 country USA 2 abcZ 5		
<ul> <li>The columns should be separated by tabs. Any other col         <ul> <li>If you wish to blank a field, enter '<blank>' as the value.</blank></li> <li>The script is compatible with STARS output files.</li> </ul> </li> <li>Please enter the field(s) that you are selecting isolates on. Value the database id will be used.</li> </ul>		s, i.e. only one isolate has the value(s) used. Usually
Please paste in your data below:	Options	Allele designations
id field value	Primary selection field: id 🗸	Add additional new designation
100 serogroup B 101 serogroup B	Optional selection field: <none></none>	Replace existing designations
101 <u>serogroup</u> B	Update existing values	Action
		Reset Submit
	*	

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.

PubML	ST/ Users: Add	Query/u	nome   Curator's page (species) pdate /update   Batch insert	;)   Curator's page (database)
Logged in: Keith	Jolley (keith). Log ou	ut   Change	e password	
Batch is	olate upda	ate		
The following	changes will be m	ade to th	e database. Please check that th	this is what you intend and then press 'Upload'. If you do not wish to make these changes, press your
browser's bac	k button.			
Transaction	id Field N	ew value	Value(s) currently in database	e Action
	100 serogroup	В		update field with new value
	101 serogroup	В	С	update field with new value
Action Upload Back to main	page			

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

# 6.9 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 Query isolates link:

tabase curator's	inte	rface			
Add. update or delet		ace	- Neisser	ia Publ	MLST
Add, update or delet					
Add, update or delet					
rinn, apanto or actor	e rec	ords			
Record type	Add	Batch Add	Update or	delete	Comments
users	+	Auu ++	2		
user groups	+	++	2		Users can be members of these groups - use for setting access permissions.
user group members	+	++	?		Add users to groups for setting access permissions.
user permissions	+	++	?		Set curator permissions for individual users - these are only active for users with a status of 'curator' in th users table.
isolates	+	++	query brow batch up		
isolate field extended attribute values	+	++	?		Add values for additional isolate field attributes.
projects	+	++	?		Set up projects to which isolates can belong.
project members	+	++	?		Add isolates to projects.
isolate aliases	+	++	?		Add alternative names for isolates.
PubMed links	+	++	?		
allele designations		++	?		Allele designations can be set within the isolate table functions.
sequences	+	++	?		The sequence bin holds sequence contigs from any source.
accession number links	+	++	?		Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?		Set up experiments to which sequences in the bin can belong.
experiment sequences			?		Add links associating sequences to experiments.
sequence tags		scan	?		Tag regions of sequences within the sequence bin with locus information.
<i>e</i> .					
Database configurati	on				
j					
Table	Add E	Batch Add	Update or delete		Comments
loci	+	++	?		
	datab	bank scan			
locus aliases	+	++	?	Add alternativ	ve names for loci. These can also be set when you batch add loci.

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

Publ	ALS1	💟 Users:	Add   Qu	ery/upd				)   Cur	ator's page (databas	e)							
Logged in:	Keith Jol	lley (keith). L	og out   Cl	hange pa	assword						Toggle:	i Field	l help: i	d			- Go
Isolat	e qu	ery/up	date														
		enance/phe	notype fie	elds —					Display/so								Modify
	ine with: entered	AND 👻	-		✓ 2014-03-17				Order by:			_		ascending 👻			
	tor (surna	ame) 👻	-		Jolley	3-17		+	i Display:	25 <del>v</del> rec	ords per pag	ge <u>i</u>					options
					,												
Actio																	
Res	et	ubmit															
3 records	returne	d. Click the	hyperlink	s for de	tailed info	ormation											
Dele	te ——	— — Tag s	canning	P	rojects —												
Delet	te ALL	So	an	Se	lect proje	ct			✓ Link								
												o 11			Fi	netypir	Iq
Delete	Update	Sequence	New					Isolate fields 👔			Seqbin size		MLST		ntigen		
		bin	version	id	isolate	aliases	country	year	disease	species	serogroup	(bp)	ST	clonal complex	VR1	PorA VR2	FetA VR
delete	update	upload	create	28783	0012/14		Czech	2014	carrier	Neisseria	W	0	10733		5-2	10-1	
delete	undate	upload	create	28784	0014/14		Republic Czech	2014	carrier	meningitidis Neisseria	В	0	35	ST-35 complex	update 22-1	update 14	update F4-1
defete	upuale	uproad	oreate	20704	0014/14		Republic	2014	Carller	meningitidis	-	5	55	on-oo complex	update	update	update
delete	update	upload	create	28785	0015/14			2014		Neisseria	В	0	10734	ST-41/44	22-1	14	F5-2
							Republic		(unspecified/other)	meningitidis				complex/Lineage 3	update	update	update

You will have a final chance to change your mind:

Public Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update Isolates: Add   Query/update   Batch insert
Logged in: Keith Jolley (keith). Log out   Change password
Delete multiple isolate records
If you proceed, you will delete 3 isolate records. Please confirm that this is your intention. Confirm deletion!

Click 'Confirm deletion!'.

# 6.10 Uploading sequence contigs linked to isolate records

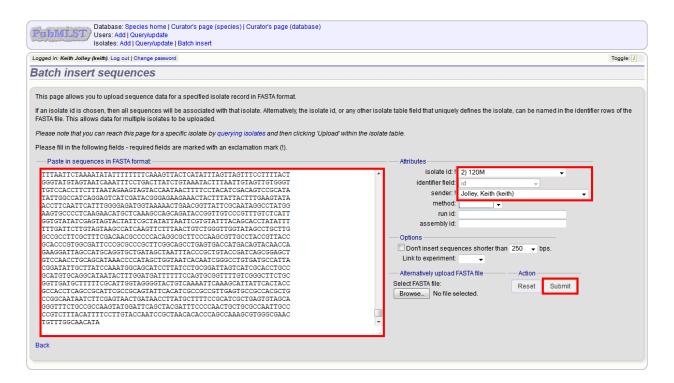
## 6.10.1 Select isolate from drop-down list

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

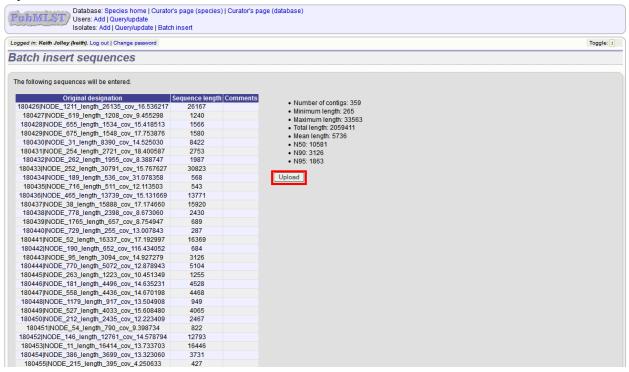
ged in: Keith Jolley (keith). Log out	Chance	a nessword		
tabase curator's	Inte	erface -	- Neisseria Pul	bMLST
/				
Add, update or delete	e rec	ords		
Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query   browse   list   batch update	
isolate field extended attribute values	+	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences	+	++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
S.				
Database configurati	on			
				Commente
Table			Jpdate or delete	Comments
loci	+	++	?	
	datah	ank scan		
locus aliases	+	++	? Add alterna	ative names for loci. These can also be set when you batch add loci.

Select the isolate that you wish to link the sequence to from the dropdown list 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.



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



It is also possible to upload data for multiple isolates at the same time, but these must exist as single contigs for each isolate. To do this, select 'Read identifier from FASTA' in the isolate id field and select the field that you wish to use as the identifier in the 'identifier field', e.g. to use isolate names select 'isolate' here.

PrrhMLST Users: Add   Query/update Isolates: Add   Query/update   Batch insert	
Logged in: Keith Jolley (keith). Log out   Change password	Toggle: 1
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 FASTA file. This allows data for multiple isolates to be uploaded.	any 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	vithin the isolate table.
Please fill in the following fields - required fields are marked with an exclamation mark (!).	
Paste in sequences in FASTA format:	Attributes
>0021/93	▲ isolate id: ! Read identifier from FASTA -
GAAGCGAAAAAAATCATTGACGAAGGCGGCTTGGTGCGCGACGACATCATTATCGGCATG GTCAAAGAACGCATCGCCGAAGACGACTGCAAAAACGGTTTCCTGTTCGACGGTTTCCCG	identifier field: isolate
CGCACATTGGCACAAGCCGAAGCGATGGTTGAAGCAGGCGTGGATTTGGATGCAGTCGTT	sender: ! Jolley, Keith (keith)
GAAATCGACGTGCCTGACAGCGTGATTGTCGACCGTATGAGCGGCCGCCGCGTGCATTTG	method:
GCTTCCGGCCGTACTTACCACGTTACCAACCCGCCCAAAGTTGAAGGCAAAGACGAC GTAACCGGCGAAGATTTCATTCAGCGCGACGACGACAAAGAAGAAGAACCGTGAAAAAAACGC	run id:
CTTGCCGTTTACCACGAGCAAACCGAAGTTTTGGTCGATTTTTACAGCAAACTGGAAGGC	assembly id:
GAACACGCGCCTAAATATATCAAAGTTGACGGCACTCAGCCGGTA	= Options
>0030/93	□ Don't insert sequences shorter than 250 - bps.
GAAGCGAAAAAAAICATIGACGAAGGCGGCTIGGIGCGCGACAACAICATIAICGGCAIG GTCAAAGAACGCAICGCGCAAGACGACIGCAAAAACGGITTCCIGTIIGACGGITICCCG	Link to experiment:
CGCACGCTGGCACAGGCCGAAGCGATGGTTGAAGCAGGCGTGGATTTGGATGCAGTCGTT	
GAAATCGACGTGCCTGACAGCGTGATTGTCGACCGCATGAGCGGCCGCCGCGTGCATTTG	Alternatively upload FASTA file Action
GCTTCCGGCCGTACTTACCACGTTACCTACAACCCGCCCAAAGTTGAAGGCAAAGACGAC GTAACCGGCGAAGATTTGATTCAGCGCGACGACGACAAAGAAGAAGCAGCGTGAAAAAACGC	Select FASTA file: Reset Submit
CTTGCCGTTTACCACGAGCAAACCGAAGTTTTGGTTGATTTTTACAGCAAACTGGAAGGC	Browse No file selected.
GAACACGCGCCTAAATACATCAAAGTTGACGGCACTCAGCCGGTA	
>0033/93 GAAGCGAAAAAAATCATTGACGAAGGCGGCTTGGTGCGCGACGACATCATTATCGGCATG	
GTCAAAGAACGCATCGCGCAAGACGACTGCAAAAACGGTTTCCTGTTCGACGGTTTCCCG	
Back	

Provided the identifier used uniquely identifies the isolate you will get a confirmation screen. If the isolate name does not do this you'll probably have to use the database id number instead. Click 'Upload' to confirm.

ProfatALST Users: Add   Query/update Isolates: Add   Query/update   Batch insert								
Logged in: Keith Jolley (keith). Log ou	t   Change password		Toggle: i					
Batch insert seque	ences							
The following sequences will be BIGSdb id Identifier field (isola			Upload					
938 0021/93	465	Will upload						
944 0030/93	465	Will upload						
946 0033/93	465	Will upload						

### 6.10.2 Select from isolate query

As an alternative to selecting the isolate from a dropdown list (which can become unwieldy for large databases), it is also possible to upload sequence data following an isolate query.

Click the isolate query link from the curator's main page.

tabase curator's in	nter	face -		
/	nei		Noissoria PubMI	с <i>т</i>
		1406 -		<i>J</i>
Add undate or delete				
		rala		
Add, update of delete	recoi	as		
Record type	Add	Batch Ad	d Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query browse   list   batch update	e
te field extended attribute value	s +	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences	+	++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
Database configuration	n			
Table A	dd Ba	tch Add U	Jpdate or delete	Comments
loci	+	++	?	
1001	lataba	nk scan		
	alang			
		++	2 Add alternative name	as for loci. These can also be set when you batch add loci
locus aliases	+ + +	++		es for loci. These can also be set when you batch add loci. reactions. These can be used to filter genomes for tagging to specific repetitive loci.
locus aliases	+		Set up in silico PCR	

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

PTIDI/ILST Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update Isolates: Add   Query/update   Batch insert		
Logged in: Keith Jolley (keith). Log out   Change password	Toggle: 👔 Field help: id	Go
Isolate query/update		
Isolate provenance/phenotype fields     Display/sort options       isolate     ▼     =     ▼ FAM18     +     I       Display.     25     ▼ records per page [	✓ ascending ✓	Modify form options
Action Reset Submit		
1 record returned. Click the hyperlink for detailed information.		
DeleteTag scanningProjects		
Delete ALL Scan Select project		
Setution Index Sequence New Sequence Se	ibin size MLST Finetyping antigen	IS
		A VR
delete update upload create 698 FAM18 Z4259 USA 1983 invasive Neisseria C 219 (unspecified/other) meningitidis	· · · · · · · · · · · · · · · · · · ·	-30 date

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.

Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update Isolates: Add   Query/update   Batch insert			
Logged in: Keith Jolley (keith). Log out   Change password			Toggle: i
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 other iso rows of the FASTA file. This allows data for multiple isolates to be uploaded.	late table field that uniquely defines the isolate	e, can be named in t	he identifier
Please note that you can reach this page for a specific isolate by querying isolates and then clicking 'Upload' within the isola	ite table.		
Please fill in the following fields - required fields are marked with an exclamation mark (!).			
Paste in sequences in FASTA format:	Attributes Isolate Id: 1 698) FAM18 Sender: ! method: run id: assembly id: Options Dont insert sequences shorter than Link to experiment Alternatively upload FASTA file Select FASTA file: Browse_ No file selected.	250 v bps. Action Reset Subm	- It
.: Back			

## 6.10.3 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.

Isolates: Add   Query/update   Batch insert	
Logged in: Keith Jolley (keith). Log out   Change password	gle: i
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 other isolate table field that uniquely defines the isolate, can be named in the ide rows of the FASTA file. This allows data for multiple isolates to be uploaded.	tifier
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 (!).	
isolate id: ! Read identifier from FASTA 👻	
identifier field: id	
sender: !	
method: 🚽	
run id:	
assembly id:	
Options	
□ Don't insert sequences shorter than 250	
Link to experiment	
Alternatively upload FASTA file Action Action	
Select FASTA file: Reset Submit	
Browse No file selected.	
Back	

# 6.11 Automated web-based sequence tagging

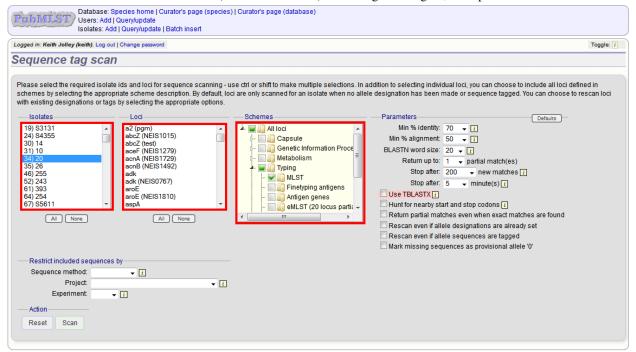
Sequence tagging, or tag-scanning, is the process of identifying alleles by scanning the sequence bin linked to an isolate record. Defined loci can either have a single reference sequence, that is defined in the locus table, or they can be linked to an external database that contains the sequences for 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.

abase curator's in					
abase curator s m	tor	faaa	Noiccori	o DubML S	<i>۲</i>
	ler	lace -	· Neissen		)]
Add, update or delete re	ecor	as			
Record type	Add	Batch Ad	d Update	or delete	Comments
users	+	++		?	
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.
user group members	+	++		?	Add users to groups for setting access permissions.
user permissions	+	++		?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query   browse	list   batch update	
te field extended attribute values	+	++		?	Add values for additional isolate field attributes.
projects	+	++		?	Set up projects to which isolates can belong.
project members	+	++		?	Add isolates to projects.
isolate aliases	+	++		?	Add alternative names for isolates.
PubMed links	+	++		?	
allele designations		++		?	Allele designations can be set within the isolate table functions.
sequences	+	++		?	The sequence bin holds sequence contigs from any source.
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++		?	Set up experiments to which sequences in the bin can belong.
experiment sequences				?	Add links associating sequences to experiments.
sequence tags	_ [	scan		?	Tag regions of sequences within the sequence bin with locus information.
Database configuration					
	d  Ba		Jpdate or delete		Comments
loci +		++	?		
	itabar	nk scan			
		++	? /	Add alternative names	s for loci. These can also be set when you batch add loci.
locus aliases +					

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.

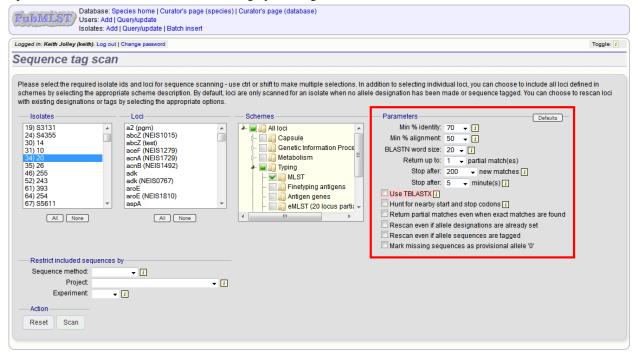


Choose your scan parameters. Lowering the value for BLASTN word size will increase the sensitivity of the search at the expense of time. Using TBLASTX is more sensitive but also much slower. TBLASTX can only be used to identify the sequence region rather than a specific allele (since it will only match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

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



Press 'Scan'. The system takes approximately 1-2 seconds to identify each sequence (depending on machine speed and size of definitions databases). Any identified sequences will be listed in a table, with checkboxes indicating whether allele sequences or sequence regions are to be tagged.

	equence tag scan													
olate Match Locu	ıs Allele	% identity	Alignment length	Allele length	E-value	Sequence bin id	Start	End	Predicted start	Predicted end	Orientation	Designate allele	Tag sequence	Flag 👔
4)20 exact abci	Z 1	100.00	433	433	0.0	182791	7064	7496	7064	7496 extract	←	<b>V</b>		
4) 20 exact adk	3	100.00	465	465	0.0	182750	1392	1856	1392	1856 extract	$\rightarrow$			
4) 20 exact aroE	E 1	100.00	490	490	0.0	182731	32577	33066	32577	33066 extract	←	V		
4) 20 exact fum(	C 1	100.00	465	465	0.0	182815	19783	20247	19783	20247 extract	$\rightarrow$			
4)20 exact gdh	n 1	100.00	501	501	0.0	182852	7516	8016	7516	8016 extract	$\rightarrow$			
4) 20 exact pdh(	C 1	100.00	480	480	0.0	182819	13868	14347	13868	14347 extract	$\rightarrow$			
4) 20 exact pgm ( <sup>a2</sup> )	n 3	100.00	450	450	0.0	182831	24559	25008	24559	25008 extract	$\rightarrow$			
												All None	All	
Action														
Tag alleles/seque	ences													

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

## 6.12 Projects

#### 6.12.1 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.

ged in: Keith Jolley (keith). Log out   C	hange p	password		
tabase curator's i	ntor	rfaco -	Neisseria PubMLS	ST .
	mer	lace -	Neisseria Fubille	21
Add. update or delete				
Add, update or delete	recor	ras		
Record type	Add	Batch Add	I Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query   browse   list   batch update	9
late field extended attribute value	s +	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences	+	++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
e				
Database configuratio	n			
Database configuratio	n			
		tch Add U	pdate or delete	Comments
		atch Add U	pdate or delete ?	Comments
Table A loci	Add Ba			Comments
Table A loci	Add Ba	++	?	Comments es for loci. These can also be set when you batch add loci.
Table /	Add Ba	++ ink scan	? Add alternative name	
Table / loci locus aliases	Add Ba + databai +	++ ink scan ++	? Add alternative name Set up in silico PCR r	ss for loci. These can also be set when you batch add loci.

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 is displayed at the top of an isolate information page. The full description can include HTML formatting, including image links.

Click 'Submit'.

PubMLST Use	abase: Species home   Curator's page (species)   Curator's page (database) rs: Add   Query/update ates: Add   Query/update   Batch insert			
Logged in: Keith Jolley (keith	). Log out   Change password			Toggle: i
Add new proje	ect description			
Please fill in the fields be	elow - required fields are marked with an exclamation mark (!).			
	MRF Meningococcus Genome Library [ Keith Jolley (keith)		Action Reset Submit	
full description:	<pre><div style="float:right; padding: 0 2em">img grg="/images/mif_20.gif" alt="MRF" style="border: lpx solid #a0a0a; background:white' /&gt;</div> <div>The <a href="http://www.meningitis.org/research/genome">MRF Meningccoccus Genome Library</a> is a collaboration between Fublic Health England, The Wellcome Trust Sanger Institute and the University of Oxford, funded by the Meningitis Research Foundation.</div></pre>	• = 		

### 6.12.2 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.

ed in: Keith Jolley (keith). Log out	Change p	bassword		
tabase curator's	inter	face -	Neisseria PubM	LST
2				
Add, update or delete	e recoi	rds		
Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query   browse   list   batch update	
solate field extended attribute values	+	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences	+	++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
Database configuration	on			
Table		tob Add Up	date or delete	Comments

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'.

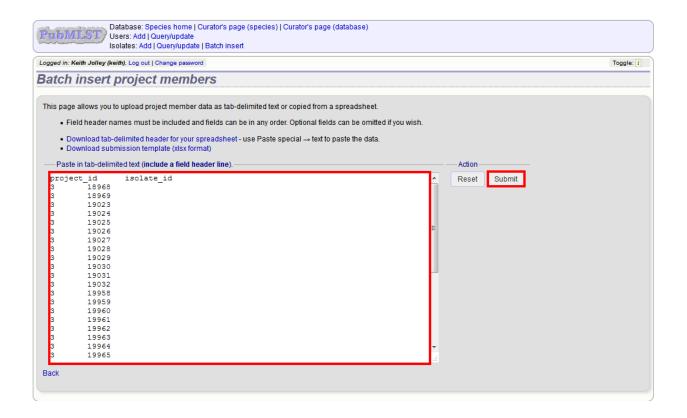
PertinATLST Users: Add   Query/update Isolates: Add   Query/update   Batch insert							
Logged in: Keith Jolley (keith). Log out   Change password	Toggle: i						
Add new project member							
Please fill in the fields below - required fields are marked with an exclamation mark (!).  Record  project id:! MRF Meningococcus Genome Library isolate id:! 18968  curator:! Keith Jolley (keith) datestamp:! 2014-07-10							

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

ed in: Keith Jolley (keith). Log out   Change password										
tabase curator's i	inter	face - I	Veisseria PubM	LST						
2										
Add, update or delete	recor	ds								
		Detab								
Record type	Add	Batch Add	Update or delete	Comments						
users	+	++	?							
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.						
user group members	+	++	?	Add users to groups for setting access permissions.						
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.						
isolates	+	++	query   browse   list   batch update							
isolate field extended attribute values	+	++	?	Add values for additional isolate field attributes.						
projects	+	++	?	Set up projects to which isolates can belong.						
project members	+	++	?	Add isolates to projects.						
isolate aliases	+	++	?	Add alternative names for isolates.						
PubMed links	+	++	?							
allele designations		++	?	Allele designations can be set within the isolate table functions.						
sequences	+	++	?	The sequence bin holds sequence contigs from any source.						
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.						
experiments		++	2	Set up experiments to which sequences in the bin can belong						

Database: Species home   Curator's page (species)   Curator's page (database) Users: Add   Query/update Isolates: Add   Query/update   Batch insert		
Logged in: Keith Jolley (keith). Log out   Change password		Toggle: i
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.		
<ul> <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>		
— Paste in tab-delimited text ( <b>include a field header line</b> ).	Action	
	Reset Submit	
di Back		

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'.



## 6.13 Isolate record versioning

New in version 1.9.0.

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:



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:

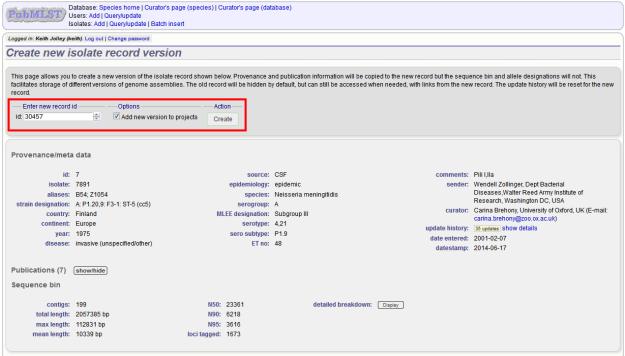
Profit/ILST Users: Add   Query/update Isolates: Add   Query/update   Batch insert											
Logged in: Keith Jolley (Keith). Log out   Change password											
Database curator's interface - Neisseria PubMLST											
Datasets											
This database contains multiple datasets. You can choose to display a single set or the whole database.											
Please select: Whole database 👻	Choos	ie									
Add, update or delete i	Add, update or delete records										
Record type	Add	Batch Add	Update or delete	Comments							
users	+	++	?								
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.							
user group members	+	++	?	Add users to groups for setting access permissions.							
user permissions	+	++	?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.							
isolates	+	++	query   browse   list   batch update								
isolate field extended attribute values	s +	++	?	Add values for additional isolate field attributes.							
projects	+	++	?	Set up projects to which isolates can belong.							
project members	+	++	?	Add isolates to projects.							
isolate aliases	+	++	?	Add alternative names for isolates.							
PubMed links	+	++	?								
allele designations		++	?	Allele designations can be set within the isolate table functions.							
sequences	+	++	?	The sequence bin holds sequence contigs from any source.							
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.							
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.							
experiment sequences			?	Add links associating sequences to experiments.							
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.							
Database configuration	Database configuration										
Table A	dd Ba	tch Add U	pdate or delete	Comments							
	+	++	?								
d	latabar	nk scan									
locus aliases	+	++	? Add alternative name	is for loci. These can also be set when you batch add loci.							
PCR reactions	+	++	Set up in silico PCR n	reactions. These can be used to filter genomes for tagging to specific repetitive loci.							
nucleotide probes	+	++	Define nucleotide pro	bes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.							

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

																	_
		ey (keith). Log										Tog	gle: i	Field help: id			-
rowse	e Ne	eisseria	a Pub	ML	.ST dat	abase											
Browse	e criteri:	a				— — Actic	n										
Orde	er by: 📊	d			•	Brow	se all record	s									
Direct	tion: a	ascending	•														
Disp	play: 2	25 👻 reco	ords per pa	age [	i												
🗌 Inclu	ide old i	record versi	ons														
56 recon	rds retu	rned (1 - 25	displayed	n Cl	ck the hyperli	nks for deta	iled informat	ion									
Delete -		— Tag sca	anning	_P	rojects												
Delete A	ALL	Scar	n	Se	ect project			▼ Li	nk								
pe: 🚺	2 3	4 5															
			1 6 1 7	1 8	1 9 1 > 1	Loct											
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elete Up	odate	Sequence	New				country		e fields <u>i</u> disease	species	serogroup	Seqbin size		MLST	PorA	/ping ant PorA	Fet
	date	Sequence bin	New version	id	isolate	aliases	country	year	disease	species	serogroup	(bp)	ST	cional complex	PorA VR1	PorA VR2	Fet/ VR
	date	Sequence	New	id		aliases B1;	country USA		disease invasive	Neisseria	serogroup A			cional complex ST-4	PorA VR1 5-2	PorA VR2 10	Fet/ VR F1-
elete up	odate	Sequence bin	New version	id	isolate	aliases		year	disease			(bp)	ST	cional complex	PorA VR1	PorA VR2	Fet/ VR F1-
elete up	odate odate odate	Sequence bin upload upload	New version create create	id 1 2	isolate A4/M1027 120M	aliases B1; Z1001	USA Pakistan	year 1937 1967	disease invasive (unspecified/other) meningitis and septicaemia	Neisseria meningitidis Neisseria meningitidis	A	(bp) 2069108 2059411	ST 4 1	cional complex ST-4 complex/subgroup IV	PorA VR1 5-2 update 5-2 update	PorA VR2 10 update 10 update	Fet VR F1- updat F5- updat
elete up	odate odate odate	Sequence bin upload	New version create	id 1 2	isolate A4/M1027	aliases B1; Z1001 B35;	USA	year 1937	disease invasive (unspecified/other) meningitis and septicaemia invasive	Neisseria meningitidis Neisseria meningitidis Neisseria	A	(bp) 2069108	ST 4	Clonal Complex ST-4 Complex/Subgroup IV ST-1	PorA VR1 5-2 update 5-2 update 19	PorA VR2 10 update 10 update 15	Fet/ VR F1- updat F5- updat
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elete up elete up elete up	odate odate odate odate	Sequence bin upload upload upload	New version create create create	id 1 2 3 4	isolate A4/M1027 120M M00242905	aliases B1; Z1001 B35; Z1035 B43;	USA Pakistan UK	year 1937 1967 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria	A A B	(bp) 2069108 2059411 0	ST 4 1 1099	Clonal Complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-32 complex/ET-5	PorA VR1 5-2 update 5-2 update 19 update	PorA VR2 10 update 10 update 15 update add	Fet/ VR F1- upda F5- upda add
elete up elete up elete up elete up	odate odate odate odate odate	Sequence bin upload upload upload upload upload	New version create create create create create	id 1 2 3 4 5	isolate A4/M1027 120M M00242905 M1027 M00240227	aliases B1; Z1001 B35; Z1035 B43;	USA Pakistan UK USA UK	year 1937 1967 2000 1937 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B	(bp) 2069108 2059411 0 0 0	ST 4 1099 4 1100	cional complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-32 complex/ET-5 complex	PorA VR1 5-2 update 5-2 update 19 update add 7 update	PorA VR2 10 update 10 update 15 update add 16 update	Fetz VR F1- updat F5- updat add add
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elete up elete up elete up elete up elete up elete up	odate odate odate odate odate odate	Sequence bin upload upload upload upload upload	New version create create create create create	id 1 2 3 4 5	isolate A4/M1027 120M M00242905 M1027 M00240227	aliases B1; Z1001 B35; Z1035 B43;	USA Pakistan UK USA UK	year 1937 1967 2000 1937 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B	(bp) 2069108 2059411 0 0 0	ST 4 1099 4 1100	cional complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-32 complex/ET-5 complex	PorA VR1 5-2 update 5-2 update 19 update add 7 update	PorA VR2 10 update 10 update 15 update add 16 update	Fet/ VR F1-3 updat F5- updat add add add
elete up elete up elete up elete up elete up elete up	odate odate odate odate odate odate	Sequence bin upload upload upload upload upload upload upload	New version create create create create create create	id 1 2 3 4 5 6 7	isolate A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891	aliases B1; Z1001 B35; Z1035 B43; Z1043	USA Pakistan UK USA UK UK Finland	year 1937 2000 1937 2000 2000 1975	disease invasive (unspecified/dother) meningitis and septicaemia invasive (unspecified/dother) invasive (unspecified/dother) invasive (unspecified/dother) invasive (unspecified/dother)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B W A	(bp) 2069108 2059411 0 0 0 0 2057385	ST 4 1099 4 1100 1101 5	Clonal complex ST-4 complex/subgroup IV ST-4 complex/subgroup I/I ST-32 complex/ET-5 complex/subgroup IV ST-22 complex ST-22 complex ST-5 complex/subgroup III	PorA VR1 5-2 update 5-2 update 19 update add 7 update add	PorA VR2 10 update 10 update 15 update add 16 update add	Fet/ VR F1-5 updat F5- <sup>-1</sup> updat add add
elete up elete up elete up elete up elete up elete up	odate odate odate odate odate odate odate	Sequence bin upload upload upload upload upload upload	New version create create create create create create	id 1 2 3 4 5 6 7	isolate A4/M1027 120M M00242905 M1027 M00240227 M00282207	aliases B1; Z1001 B35; Z1035 B43; Z1043 B54;	USA Pakistan UK USA UK UK	year 1937 1967 2000 1937 2000 2000	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive	Neisseria meningittdis Neisseria meningittdis Neisseria meningittdis Neisseria meningittdis Neisseria meningittdis Neisseria meningittdis Neisseria	A A B A B W	(bp) 2069108 2059411 0 0 0 0	ST 4 1099 4 1100 1101	Cional complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-32 complex/ET-5 complex ST-22 complex ST-5	PorA VR1 5-2 update 5-2 update 19 update add 7 update add 20	PorA VR2 10 update 10 update 15 update add 16 update add 9 update 14	Fet/ VR F1-5 updat add add add F3-1
belete Up delete up delete up delete up delete up delete up delete up delete up delete up	odate odate odate odate odate odate odate odate	Sequence bin upload upload upload upload upload upload upload	New version create create create create create create create	id 1 2 3 4 5 6 7	isolate A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891	aliases B1; Z1001 B35; Z1035 B43; Z1043 B54;	USA Pakistan UK USA UK UK Finland	year 1937 2000 1937 2000 2000 1975	disease invasive (unspecified/dother) meningitis and septicaemia invasive (unspecified/dother) invasive (unspecified/dother) invasive (unspecified/dother) invasive (unspecified/dother)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B W A	(bp) 2069108 2059411 0 0 0 0 2057385	ST 4 1099 4 1100 1101 5	Clonal complex ST-4 complex/subgroup IV ST-4 complex/subgroup I/I ST-32 complex/ET-5 complex/subgroup IV ST-22 complex ST-22 complex ST-5 complex/subgroup III	PorA VR1 5-2 update 5-2 update 19 update add 7 update add 20 update	PorA VR2 10 update 10 update 15 update add 16 update add 9 update	Fett VR F1- upda add add add add F3- upda

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.



### **Offline curation tools**

### 7.1 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
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. -h, --help This help page. -i, --isolates LIST Comma-separated list of isolate ids to scan (ignored if -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. -q, --quiet Only error messages displayed. -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. -T, --already\_tagged Scan even when sequence tagged (no designation). -w, --word\_size SIZE BLASTN word size.

```
-x, --min ID
Minimum isolate id.
-y, --max ID
```

```
Maximum isolate id.
```

## 7.2 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.
-A, --alignment INT
    Percentage alignment (default: 100).
-B, --identity INT
    Percentage identity (default: 99).
-c, --coding_sequences
    Only return complete coding sequences.
-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). -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. -T, --already\_tagged Scan even when sequence tagged (no designation). -w, --word\_size SIZE BLASTN word size. -x, --min ID Minimum isolate id. -y, --max ID Maximum isolate id.

# 7.3 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 terminte 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

## **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.

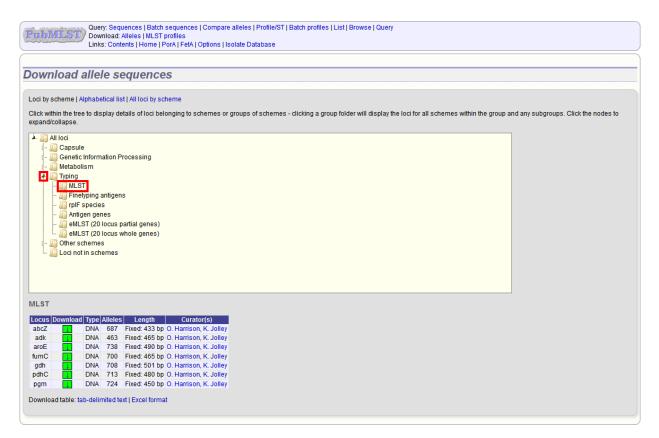
## 8.1 Allele sequence definitions

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.

### 8.1.1 Scheme tree

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
Download allele sequences
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 within the group and any subgroups. Click the nodes to expand/collapse.
All loci Capsule Genetic Information Processing Metabolism Joint schemes Loci not in schemes

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.



#### Click the green download link for the required locus



#### Alleles will be downloaded in FASTA format, e.g.

>fumC\_1

### 8.1.2 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.

ownload all						
ownioad all	ala aggina					
	ele seque	ICE	!5			
oci by scheme   Alpha	abetical list   All lo	ci by so	heme			
Locus	Download Type	Allolos	Length	Full name/product	Curator(s)	
ArsR [NEIS1769]	Dowilload Type	54	Variable: No limits set	ArsR family transcriptional regulator	Curator(S)	
AsnC [NEIS1566]	DNA DNA	121	Variable: No limits set	transcription regulator AsnC		
abcZ	DNA	687	Fixed: 433 bp	a ano anguara ta garata na na na	O. Harrison, K. Jollev	
abcZ [NEIS1015]	DNA	330	Variable: No limits set	ABC transporter ATP-binding protein		
aceF [NEIS1279] i	DNA	333		x) dihydrolipoamide acetyltransferase (EC 2.3.1.12)		
ackA2 [NEIS1727]	DNA	260	Variable: No limits set	acetate kinase		
acnA [NEIS1729]	DNA	396	Variable: No limits set	aconitate hydratase 1 (EC 4.2.1.3)		
acnB [NEIS1492] i	L DNA	349	Variable: No limits set	aconitate hydratase 2 (EC 4.2.1.3)		
adhA [NEIS0486] i	DNA	415	Variable: No limits set	alcohol dehydrogenase		
adhC [NEIS1241] i	1 DNA	169	Variable: No limits set	alcohol dehydrogenase		
adk	1 DNA	463	Fixed: 465 bp		O. Harrison, K. Jolley	
adk [NEIS0767] i	L DNA	169	Variable: No limits set	adenylate kinase		
aldA [NEIS1942] i	1 DNA	306	Variable: No limits set	aldehyde dehydrogenase		
apaH [NEIS0610] i	1 DNA	92	Variable: No limits set	diadenosine tetraphosphatase		
argH [NEIS0580] i	1 DNA	288	Variable: No limits set	argininosuccinate lyase		
aroE	1 DNA	738	Fixed: 490 bp		O. Harrison, K. Jolley	
aroE [NEIS1810] i	L DNA	223	Variable: No limits set	shikimate dehydrogenase		
aspA	1 DNA	97	Fixed: 432 bp		K. Jolley	
aspA [NEIS1185] i	1 DNA	326	Variable: No limits set	aspartate ammonia-lyase		
atIA [NEIS2274] i	1 DNA	4	Variable: No limits set	atIA / peptidoglycan transglycosylase		
autA [NEIS1859] i	DNA	178	Variable: No limits set	autotransporter A		

Click the green download links for the required locus.

#### 8.1.3 All loci by scheme

Loci can also be displayed by scheme with all schemes displayed.

PubMLST	📝 Downloa	d: Alleles	MLST		lleles   Profile/ST   Batch profiles   List   Browse   ate Database	Query		
Download	allele	seque	nce	S				
Loci by scheme	Alphabetical	list   All Io	ci by sci	heme				
MLST								
Locus Downloa				Curator(s)				
abcZ 👔				O. Harrison, K. Jolley				
adk 🔒				O. Harrison, K. Jolley				
aroE 1				O. Harrison, K. Jolley O. Harrison, K. Jolley				
qdh				O. Harrison, K. Jolley				
pdhC				O. Harrison, K. Jolley				
pgm 1				O. Harrison, K. Jolley				
Finetyping an	tigens							
Locus Do	wnload Ty	e Allele	s	Length Full r	name/product Curator(s)			
PorA VR1 i					ariable region 1 K. Jolley			
PorA VR2 i		ide 713			ariable region 2 K. Jolley			
FetA VR		ide 426	Varia	ble: No limits set	I. Feavers			
rpIF species								
Locus Downloa	ad Type Alle	les Le	ngth	Full name/prod	uct Curator(s)			
'rplF i				50S ribosomal protein				
ADP-heptose	biosynthe	SIS						
Locus	Downl	oad Type	Alleles	Lenath	Full name/product	Aliases	Curator(s)	
NEIS0769 (hld/		DNA	187	Variable: No limits set	D-beta-D-heptose-7-phosphate kinase	NMB0825; NMC0769; rfaE		
NEIS0773 (hldE			241	Variable: No limits set	ADP-D-beta-D heptose epimerase	NMB0828; NMC0773	C. Kahler	
NEIS2014 (gmh		DNA		Variable: No limits set	D-alpha,beta,D-Heptose 1,7 bisphosphate phosp		C. Kahler	
NEIS2055 (hldC		DNA	156	Variable: No limits set	D-beta-D-heptose-1-phosphate adenylyltransfe		C. Kahler	
NEIS2070 (gmh		DNA	158	Variable: No limits set	sedoheptulose-7-phosphate isomerase	NMB2090; NMC2070	C. Kahler	

Click the green download links for the required locus.

### 8.1.4 Download locus table

The locus table can be downloaded in tab-delimited text or Excel formats by clicking the links following table display.

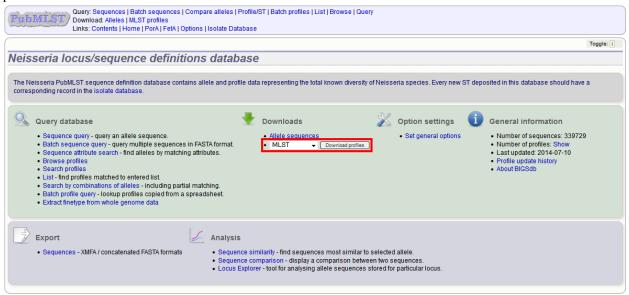
	Capsule		
	Genetic Information Processing		
	Metabolism		
н 🚛 т	Typing		
	MLST		
	Finetyping antigens		
	rpIF species		
	Antigen genes		
	eMLST (20 locus partial genes)		
	MLST (20 locus whole genes)		
	Other schemes		
	Loci not in schemes		
···· @ •			
MLST			
	undered Torse Allesters Landth Constants		
abcZ	wnload Type Alleles Length Curator(s) DNA 687 Fixed: 433 bp O. Harrison, K. Jolley		
adk	DNA         687         Fixed: 433 bp O. Harrison, K. Jolley           DNA         463         Fixed: 465 bp O. Harrison, K. Jolley		
aroE			
fumC gdh			
pdhC			
pgm	DNA 724 Fixed: 450 bp O. Harrison, K. Jolley		
Download t	table tab-delimited text   Excel format		

# 8.2 Scheme profile definitions

Scheme profiles, e.g. those for MLST, can be downloaded by clicking the appropriate link on the contents page.

PUTITATION 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 known diversity of C. jejuni and C. coli. corresponding record in the isolate database.	Every new ST deposited in this database should have a
🔍 Query database 🕹 Downloads 🕺 Option settings 🧃 d	General information
Batch sequence query - query multiple sequences in FASTA format.     Sequence attribute search - find alleles by matching attributes.     Browse MLST profiles	Number of profiles (MLST), 7281     Vamber of profiles (MLST), 7281     Last updated: 2014-07-10     Profile update history     About BIGSdb
Export     Sequences - XMFA / concatenated FASTA formats     Sequence similarity - find sequences most similar to selected allele.     Sequence comparison - display a comparison between two sequences.     Locus Explorer - tool for analysing allele sequences stored for particular locus.	

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



#### 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 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

# **Data records**

Record pages for different types of data can be accessed following a query by clicking appropriate hyperlinks.

# 9.1 Isolate records

An Isolate record page displays everything known about an isolate.

PUDMLST B	reakdown: Isolate fie	se   Profile/ST   List alds   Scheme/alleles   Publications ne   Options   Profiles/sequences definition:	s   Database submissions		
Full informat	ion on iso	late M10 240474			
Projects					
This isolate is a membe	r of the following pro	jects:			
			ngococcus Genome Library		
The MRF Meningococo Oxford, funded by the N		is a collaboration between Public Health E Foundation.	ngland, The Wellcome Trust Sar	ger Institute and the University of	À
		be cited in any publication or presentation	making use of it.		Meningitis A Research Foundation
			899_MRF		
MRF-MGL isolates epi	vears 2010/2011 to	2011/2012 excluding Northern Ireland	005_mm		
	,	-			
			/_genogroup_B_MRF		
All MRF Meningococci	us Genome Library (	genogroup B isolates from England and Wa	ales in 2010/11 and 2011/12		
			MRF_no_NI		
All MRF genomes excl	uding Northern Irela	nd			
Provenance/meta	data				
	18968			Neisseria meningitidis	
	M10 240474	22 0: ST 260 (co260)	serogroup:		
strain designation: country:		-3-9. 51-209 (CC209)		ERR086224 → www.ebi.ac.uk Dorothea Hill	
continent:				Dorothea Hill, University of Oxford, UK	(E-mail:
region:	South East			dorothea.hill@zoo.ox.ac.uk)	
year:	2010			103 updates show details	
epidemiological year:			date entered:		
disease:	invasive (unspecifi	ied/other)	datestamp:	2014-06-23	
Sequence bin					
contigs:	275	N90:	6405		
total length:	2195045 bp	N95:	3513		
max length:		loci tagged:			
mean length:		detailed breakdown:	Display		
N50:	34308				
Schemes and loci					
		Noviente and select actions of the	to display all de destructions		
All loci		Navigate and select schemes within tree	to display allele designations		
	mation Processing				
- 🚺 Metabolism					
🗁 🛄 Pilin					
b. In Typing					
Other schem Loci not in se					

Each record will have some or all of the following sections:

### 9.1.1 Projects



This displays a list of projects that the isolate is a member of. Only projects that have a full description will be displayed.

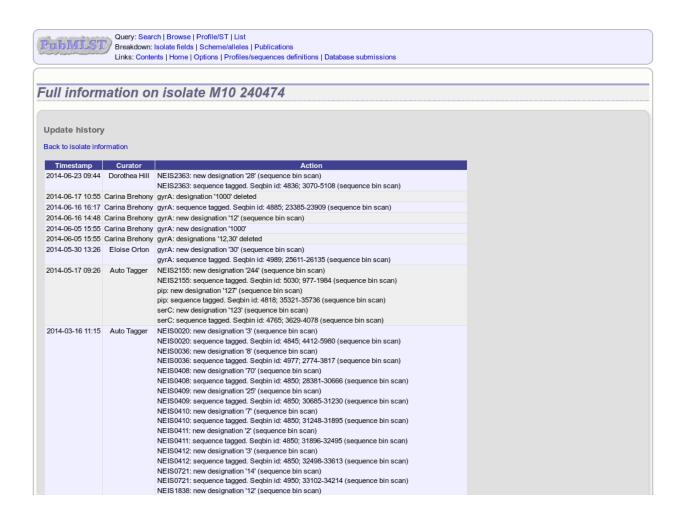
### 9.1.2 Provenance metadata

Provenance/meta	data		
id:	18968	species:	Neisseria meningitidis
isolate:	M10 240474	serogroup:	В
strain designation:	B: P1.19-1,15-11: F3-9: ST-269 (cc269)	ENA accession:	ERR086224 → www.ebi.ac.uk
country:	UK	sender:	Dorothea Hill
continent:	Europe	curator:	Dorothea Hill, University of Oxford, UK (E-mail:
region:	South East		dorothea.hill@zoo.ox.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)	datestamp:	2014-06-23

This section includes:

- 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.



#### 9.1.3 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 [578 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 [24 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, Unvin 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
   Torisolates
- 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.

#### 9.1.4 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*.

#### 9.1.5 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					М	LST			
Pilin Typing MLST Finetyping antigens	abcZ 4 S	adk 10 S	aroE 15 S	fumC 9 S	gdh 8 S	pdhC 11 S	pgm 9 S	<b>ST</b> 269	clonal complex ST-269 complex
They ping antigens     They ping antigens									

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*.

## 9.2 Allele definition records

An allele definition record displays information about a defined allele in a sequence definition database.

(	uery: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query
	unit or defances of advances for the and of the advances for the advances for the advances of
Li	nks: Contents   Home   PorA   FetA   Options   Isolate Database
Allala informa	ation - abcZ: 2
Allele Informa	auon - adc2: Z
Provenance/meta	data
locus:	abcZ i
allele:	2
	TITGATACCG TIGCCGAAGG TITGGGTGAA ATTCGCGATT TATTGCGCCG TTACCACCGC GTCGGCCATG AGTGGAAAA CGGTTCGGTG GAGGCTTTGT IGAAAGAACT CAACGAATA CAACTIGAAA ICGAAGCGAA GGACGGCTGG AAGCTGGATG CGGCAGTCAA GCAGACTTTG GGGGAACTCG GTTTGCCGGA AAACGAAAAA ATCGGCAACC TITCCGGCG TCAGAAAAG GTGTCGCCT IGGCGAGCA TIGGGTGCAG AAGCCGAACCGATTGTGAAGCGAACCG ACCAACCAATT IGGATATCGAC GCCGATTATT IGGCTGGAAA ATCTGCTCAA AGCGTTGAA GGCAGCTTGG TIGTGATTAC CCACGACCG CGTTTTIGG ACAATATCGA CACGGATTATT IGGCTGGAAA ATCTGCTCAA AGCGTTGAA GGCAGCTTGG TIGTGATTAC CCACGACCG CGTTTTIGG ACAATATCGA CACGGACTGG ACCG GTCGAACTCG ATC
length:	433
status:	Sanger trace checked
date entered:	
datestamp:	
	Keith Jolley, University of Oxford, UK
curator:	Man-Suen Chan, University of Oxford (E-mail: man-suen.chan@paediatrics.ox.ac.uk)
Profiles containin	g this allele
MLST:	993 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. 5041 isolates

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.

### 9.3 Sequence tag records

Query: Search   Browse   Profile Breakdown: Isolate fields   Sch	me/alleles   Publications
Links: Contents   Home   Optio	s   Profiles/sequences definitions   Database submissions
NEIS0346 allele sequence: id	18968
Contig position	
sequence bin id: 4956	length: 744
contig length: 22993	orientation: forward
start: 13864 end: 14607	complete: yes method: Illumina
	nicarda, maninia
Sequence	
	CG GAAAAACTAT TACCGTACAG CCGACGGTAA AACCGAAGAT GCCGTCTTAA TGGAGAAAAT <b>ATGTTAAGCG CGCGCTACCT CCACCTGCAC GAAGCCTTGG GTTTGGGCCC</b> CA ACATIGCCGG AAAGCCCGAC ACAAATCCGC CCGCAAAAGC AAACCGTCCT CAGCATTCCG CAGCGTCCGT CCGAACAGCA TACCGGTCAG GCACGGCTCA AAACCATGAA
AGTGTTGGAA ACAACCGCCG TACATACGCG CAAACCC	CS CCTGAAACCG AAACGCCTCT GICCGGCGTI ICAGACGGCA ICGCCCCCGI ICCCGCCGCI ICGGGCAIAA CCAAACTIGC CGIIGICAGC CIGIGICCGC CGACCGAGGA
	IC CIGCICGACA ATATACICAA AGCCGIAGGG CICGAIGCCG CCIAIGICCA CAAAACCIGI IGGGIGAAAA CCGCCGCCGI CGGCAACCCG AIGCCGICIG AAGCGGCAAI SC IGCCGCGCAC CCGCCGICCI GIICCICGGA CAGGCGIIIG ICAAACCGGA ACGGCAGGCG AIGAIIGAAA CIIIGIGCGC CGGCCGCCCC IICIICAICA ICGACCAICC
CGCCCGGCTG TTGCGCCAAC CCGAACTCAA AGCCCGC	CC IGGCAGACGC ICAAGCAGCT CAAACGIGIC IIGGCGCAAG GCGCGCGCAG IIGAAGCGCG CCGCACGGGG CGGIAGAAIC GCAACIGCGI CCCAAIAICI GACAGAAAGC
ACAAAATGAC CGATTICCGC CAAGATITCC TIAAATI	
Translation	
HCTRRTASAL	AGGKTITVQPTVKPKMPS 🖁 WRKYF1
	G Q A E K L L P Y S R R S N R R C R L N G E N F2
	G R R K N Y Y R T A D G K T E D A V L M E K I F3 GGGCAGGCGGAAAAACTATTACCGTACAGCCGACGGTAAAACCGAAGATGCCGTCTTAATGGAGAAAAT 100
: : :	; ; ; ; ;
VKRALPPPAR	SLGFGPDVVEAGSRRPAVRNIAG F1
	ALGLGPMWLKRGAVVLPSATLPE F2
	K P W V W A R C G X S G E P S S C R P Q H C R F3 AAGCCTTGGGTTGGGCCCGATGTGGTTGAAGCGGGGAGCGGCGCGCCGCAACATTGCCGG 200
:: :	: : : : :
KPDTNPPAKA	NRPQHSAASVRTAYRSGTAQNHE F1
S P T Q I R P Q K Q K A R H K S A R K S	TVLSIPQRPSEQHTGQARLKTMK F2 PSSAFRSVRPNSIPVRHGSKP 🕏 KF3
	ACCGTCCTCRGCATTCCGCAGCGTCCGGACAGCATACCGGTCRGGCACGGCTCAAAACCATGAA 300
:: :	: : : : :

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.

# 9.4 Profile records

PubMLST Dow	ry: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query rrload: Alleles   MLST profiles s: Contents   Home   PorA   FetA   Options   Isolate Database
Profile informa	ation for ST-11 (MLST)
ST abcZ adk aro 11 2 3 4	E         fumc         gdh         pdfc         pgm         clonal complex           3         8         4         6         ST-11 complex/ET-37 complex
Client database	
	ontains 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 eposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample. 2699 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.

# 9.5 Sequence bin records

	Links. Conte	nts   Home   Options   Pr		•							
											Togg
equen	ce bin for N	110 240474									
ontig sum	nmary statistics		Contig size	distribution	Cumulative conti	g lengt	h				
<ul> <li>Total le</li> <li>Minimu</li> <li>Maxim</li> <li>Mean l</li> <li>σ lengi</li> <li>N50: 3</li> <li>N90: 6</li> <li>N95: 3</li> </ul>	6405		Click to enlarg	re pad lengths							
		STA format) annotations (EMBL form	nat)								
• Downl	load sequences with	annotations (EMBL form		Length Comments	Locus	Start	End [	Direction	EMBL format	Artemis 🖬	
• Downi		annotations (EMBL form Original de:	signation	Length Comments	Locus NEIS1151	Start 488			EMBL format		
• Downl	load sequences with Sequencing method	annotations (EMBL form	signation				End [ 1144 2913	←	EMBL format	Artemis i Artemis	
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151	488	1144				
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150	488 1141	1144 2913	↓ ↓			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149	488 1141 3155	1144 2913 3733	$\begin{array}{c} \leftarrow \\ \leftarrow \\ + \end{array}$			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1148	488 1141 3155 3896	1144 2913 3733 4513	$\downarrow$ $\uparrow$ $\uparrow$ $\uparrow$			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147	488 1141 3155 3896 4521	1144 2913 3733 4513 5384 5831 6869	1 1 1 1			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146	488 1141 3155 3896 4521 5397	1144 2913 3733 4513 5384 5831 6869 7923	1 + + + 1 1 + + + 1			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146 NEIS1145	488 1141 3155 3896 4521 5397 6141 6892 8005	1144 2913 3733 4513 5384 5831 6869 7923 8313	$\downarrow \downarrow \uparrow \uparrow \uparrow \downarrow \downarrow \uparrow$			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146 NEIS1145 NEIS1144 NEIS1143 NEIS1142	488 1141 3155 3896 4521 5397 6141 6892 8005 9288	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541	1 + + + + + + + + + + + + + + + + + + +			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146 NEIS1145 NEIS1144 NEIS1143 NEIS1142 NEIS1142 NEIS1142	488 1141 3155 3896 4521 5397 6141 6892 8005 9288 10613	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241	1 1 1 1 1 1 1 1 1 1			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146 NEIS1145 NEIS1143 NEIS1143 NEIS1142 NEIS1140 NEIS1139	488 1141 3155 3896 4521 5397 6141 6892 8005 9288 10613 12391	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241 12744	1111111			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1145 NEIS1145 NEIS1144 NEIS1143 NEIS1142 NEIS1139 NEIS1138	488 1141 3155 3896 4521 5397 6141 6892 8005 9288 10613 12391 12824	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241 12241 12744 14362	1111111111			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1146 NEIS1145 NEIS1144 NEIS1143 NEIS1143 NEIS1142 NEIS1142 NEIS1142 NEIS1139 NEIS1138 NEIS1137	488 1141 3155 3896 4521 5397 6141 6892 8005 9288 10613 12391 12824 14426	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241 12241 122744 14362 15046	L T T T L T L L L T T T			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1147 NEIS1146 NEIS1146 NEIS1145 NEIS1143 NEIS1142 NEIS1142 NEIS1140 NEIS1139 NEIS1138 NEIS1137 NEIS1136	488 1141 3155 3896 4521 5397 6141 6892 8005 9288 10613 12391 12824 14426 15102	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241 12241 122744 14362 15046 15392	<u> </u>			
• Downl	load sequences with Sequencing method	annotations (EMBL form Original de:	signation		NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1146 NEIS1145 NEIS1144 NEIS1143 NEIS1143 NEIS1142 NEIS1142 NEIS1142 NEIS1139 NEIS1138 NEIS1137	488 1141 3155 3896 4521 5397 6141 6892 8005 9288 10613 12391 12824 14426 15102	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241 12744 14362 15046 15392 16832	L L L T T T T L T L L L T T T			

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.

# **Querying data**

# 10.1 Querying sequences to determine allele identity

Sequence queries are performed in the sequence definition database. Click 'Sequence query' from the contents page.

Query: Sequences   Batch sequences   Compare alleles   Profile Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database		rowse   Query
		Toggle: 1
Neisseria locus/sequence definitions database	2	
The Neisseria PubMLST sequence definition database contains allele and profile dat have a corresponding record in the isolate database.	a representing the total kno	wn diversity of Neisseria species. Every new ST deposited in this database should
🔍 Query database 🗸 🦊	Downloads	💥 Option settings
Sequence query Batch sequence query - query multiple sequences in FASTA format.	Allele sequences     MLST	Set general options vnload profiles
Sequence attribute search - find alleles by matching attributes.     Browse profiles		General information
Search profiles     List - find profiles matched to entered list.		Number of sequences: 341811     Number of profiles: Show
<ul> <li>Search by combinations of alleles - including partial matching.</li> <li>Batch profile guery - lookup profiles copied from a spreadsheet.</li> </ul>		<ul> <li>Last updated: 2014-07-11</li> </ul>
Extract finetype from whole genome data		Profile update history     About BIGSdb
Export Analysis		
Sequence co	mparison - display a comp	ost similar to selected allele. arison between two sequences. sequences stored for particular locus.

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'.

PubMLST Download: Alleles   M	Batch sequences   Compare alleles   Profile/ST   Batch pro /LST profiles me   PorA   FetA   Options   Isolate Database	files   List   Browse   Query	
Sequence query - Neiss	seria locus/sequence definition	S	
partial matches will be identified if an example and the select locus/scheme All loci Enter query sequence (single or mult GACGCGETCGCGCGATAAAASTCAAA TCTGTCCATCGCGCGGGATCGCGCGGGATCGAAAASTCAACTATCGGCGCGGGGGGGGAGAAACCATTICGCTTIGGCTGGGGGGGGAAACCATTICGCTTIGGGTGGAAAGAAACCATTICGCTTIGGGTGGAAAGAAACCATTICGCCGGAATTIGAAAGAAACCATTICGCCGGGATTICGAAAGAAACCATTICGCCGGCGGAATTICAAAAGAAACCATTICGCCGGAATTICAAAAGAAACCATTICGCCGGAATTICAAAAGAAACCATTICGCCGGAATTICGAAAGAAACCATTICGCCGGAATTICGAAAGAAACCATTICGCCGGAATTICGAAAGAAACCATTICGCCCGCAAATTICGAAAGAAACCATTICGCCGGAATTICGAAAGAAACCATTICGCCGGAATTICGAAAGAAACCATTICGCCGGAATTICGCCGGAATTICGAAAGAAACCATTICGCCGGAATTICGCCGGAATTICGCCGGAATTICGCCGGAATTICGCCGGAATTICGCCGGAATTICGAAAGAAACCATTICGCCGCGAATTICGCCGGAATTICGCCGGAATTICGAAAGAAACCATTICGCCCGCGCAATTICGCCGGAATTICGAAAGAAACCAATTICGCCGCGAATTICGCCGGAATTICGCCGGAATTICGCCGGAATTICGAAAGAAACCATTICGCCGGAATTICGCCGGAATTICGCCGGAATTICGAAAGAAACCATTICGCCGGAATTICGCCGGAATTICGCCGGAATTICGCCGGAATTICGCCGGAATTICGCCGGCGCGCCGCCCGCCGCAATTICGCCGGAATTICGCGGAACGACCGCGCCCGCCGCCGCCGCGAATTICGCGGAATTICGCGGAACGACCGCGCCCGCCGCGCGCGCGCGCGCGCGC	gainst the database. Query sequences will be checked firs ct match is not found. You can query using either DNA or pe Order results by- locus · liple contigs up to whole genome in size) VSTCATCAAGTCATTGAAGCCGTCGACCGTCGAA CCAATTACCGCCGCCAAAGCCATTGCCAT CCAACGACTCACGCAGCCAAAAACATTGCCAT CCACGGACTACGCAGCCGACGCGACACCGTCGAA CCACGACTCACGCAGCCGACGCGACACCGCGACACGCGACGCACGC		i - they do not need to be trimmed. The nearest Action Reset Submit

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   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 exa partial matches will be identified if an exact match is not found. You can query using either DNA or peptide seque Please select locus/schemeOrder results by	
1 exact match found. Translate query	
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 pro Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database	files   List   Browse   Query	
Sequence query - Neisseria locus/sequence definition	5	
Please paste in your sequence to query against the database. Query sequences will be checked first partial matches will be identified if an exact match is not found. You can query using either DNA or perpendicular and the set of the second seco		- they do not need to be trimmed. The nearest Action Reset Submit
Translate query         Closest match: aroE: 8         Show alignment         Differences         2 differences found. []         28°F		

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         Batch         sequences         Compare alleles         Profile/ST         Batch         profiles         L           Download:         Alleles         MLST         profiles         L         Links:         Contents         Home         PorA         FetA         Options         Isolate         Database	List   Browse   Query	
Sequence query - Neisseria locus/sequence definitions Please paste in your sequence to query against the database. Query sequences will be checked first for ar partial matches will be identified if an exact match is not found. You can query using either DNA or peptide s Please select locus/scheme - Order results by - All loci  Enter query sequence (single or multiple contigs up to whole genome in size)		est

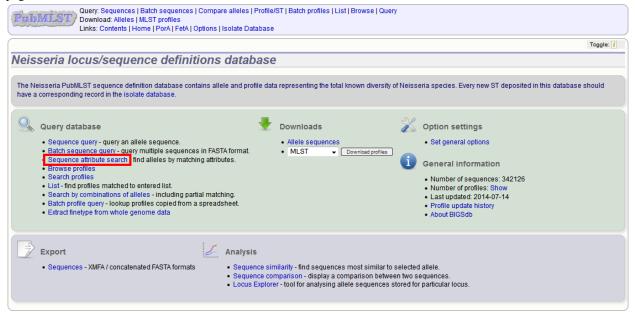
#### 10.1.1 Querying whole genome data

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.

PubML	Profit/ILST Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database														
Sequend	ce o	werv - I	Veisser	ia loc	us/se	quence defini	tions								
ocquein	ve y	uciy i	Telooen	u 100	40/00	quenee uenin									
	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															
MLST				-	locus										
Enter que	erv sea	wence (sinale	e or multiple co	ontias up	to whole a	enome in size)									
			1326_cov			·····,		Select FASTA file:	Reset Submit						
TAGAACAA	ACAGC	AATATTCAA	AGATTATCTO	AAAGTC	CGAGATTO	TAGATICCCGCTITC		Browse No file selected.	Treser Submit						
						GACAAAAGCCTGCCAT									
						ATTCGGATTTTCCAAT									
						IGACAAAAATATAGTG	-								
AATTAACA	AAAAA	TCAGGACAA	GGCGACGAAG	CCGCAG	ACAGTACI	AGATAGTACGGTAAGG									
7 exact matche	es four	nd.													
			<b>F</b> 1 10	51 0											
	angtn s 433	203051	End position 203483	Flags Co	omments										
	465	938327	938791												
	490	1775325	1775814												
fumC: 9 4	465	1134240	1134704												
	501	961439	961939												
	480	1341678	1342157												
pgm: 9 4	450	1416246	1416695												
MLST															
ST clonal comp	26 Iov ST														
cional comp		200 complex													

# 10.2 Searching for specific allele definitions

To retrieve specific allele designations, click 'Sequence attribute search' on a sequence definition database contents page.



Enter your query using the dropdown search box - additional terms can be added by clicking the '+' button.

#### Designations can be queried using standard operators.

PubMLST / Download: A	ences   Batch sequences   Compare al dieles   MLST profiles ents   Home   PorA   FetA   Options   Isol		rofiles   List   Browse	Query		
					1	Toggle: i
Query sequences t	for Neisseria locus/se	equence defin	itions datab	ase		
Some loci have additional fields v plugins.	which are not searchable from this gen	eral page. Search for thes	e at the locus-specific	query page. Us	e this page also for access to the sequence analysis or	export
Also note that some loci in this da locus that uses integer allele ids		strings. Queries using the	'<' or '>' modifiers will	work alphabeti	cally rather than numerically unless you filter your search	n to a
Please enter your search criteria	below (or leave blank and submit to ret	turn all records). Matching	sequences will be retu	urned and you v	vill then be able to update their display and query setting	JS.
locus 👻 =	✓ abcZ	+ i Order by:	locus 👻	ascending .	-	
		Display:	25 👻 records per p	oage 👔		
> Filter query by	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
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 - Display
Combine searches with: AND • Order by: locus • ascending •
locus • = • abcZ + i Display: 25 • records per page i
allele id 🔹 = 🔹 5
> Filter query by
1 record returned. Click the hyperlink for detailed information.
locus     allele id     sequence     sequence length     comments     flags       abc2     5     TITGATACCGTTGCC     TOGTCGAACTCGATC     433

Click the hyperlinked results to display allele records.

PubMLST/c	uery: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query Jownload: Alleles   MLST profiles inks: Contents   Home   PorA   FetA   Options   Isolate Database
	Toggle: i
Query seque	nces for Neisseria locus/sequence definitions database
query ocque	
plugins.	onal 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
-	r allele ids using the drop-down list. rch 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	→ Display with: AND ▼ Order by: locus ▼ ascending ▼
locus	mini. Altor ♥ abcZ + I Display: 25 ♥ records per page []
allele id	
── > Filter query by -	Action Reset Submit
1 record returned. Click	the hyperlink for detailed information.
locus allele id abcZ 5 TTTG	sequence sequence length comments flags ATACCGTIGCC TCGTCGAACTCGATC 433
PubMLST/c	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	a data
locus:	abcZ i
allele:	5
sequences:	TITGATACCE TIGCCGAAGE TITGGGCGAA ATTCGCGATI TATTGCGCCE ITATCATCAT GICAGCAIG AGTIGGAAAA TGGTICGAGI GAGGCITIGI IGAAAGAGCI TAACGAAITG CAACITGAA TCGAAGCGAA GGACGGCIGE AAGCIGGAIG CGGCAGICAA GCAGACITIG GICGAACITG GITGCCCAGA AAACGAAAAA AICCGCAACC TCICCCGCCG ACAGAAAAAG CGTGTIGCCC TAGGCGACGE TIGGGIGCGA GAACCIGGIGI TATICGIG GGACGAACCG ACCAACCAI TGGACAIGA CGCGAITAIT IGGCTGGAAA AICTGCITAA AGCGITIGAA GGCAGCCIGG TIGGIGAITAC CCACGACCGC CGITITIIGG ACAATAICGC CACGCGCAIC GICGAACICG AIC
length:	
	Sanger trace checked
date entered:	
datestamp:	
	Keith Jolley, University of Oxford, UK Man-Suen Chan, University of Oxford (E-mail: man-suen.chan@paediatrics.ox.ac.uk)
Profiles containir	ig this allele
	183 profiles
Isolate databases	3
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 analys plugins.	sis 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 so locus that uses integer allele ids using the drop-down list.	earch to a
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 search criteria below (or leave blank and submit to return all records).	ettings.
- Search criteria - Display -	
allele id 🔹 < 💌 10 (+) 👔 Order by: locus 💌 ascending 💌	
Display: 25 🗸 records per page 👔	
Filter query by     Action       locus: abcZ     I       status:     Image: Constraint of the status       sender:     Image: Constraint of the status       curator:     Image: Constraint of the status       allele flag:     Image: Constraint of the status	
9 records returned. Click the hyperlinks for detailed information.	
locus allele id sequence sequence length comments flags	
abcZ 1 TITGATACTGTIGCC TIGTCGAACTCGATC 433	
abcz 2 TITIGATACCETIGCC TIGTICGAACTCGATC 433	
abcZ     3     TTTGATACCGTTGCC      TTGATACCGTTGCC     433       abcZ     4     TTTGATACCGTTGCC      TTGCGAACTCGATC     433	
abcz 4 Indefacemente 135 abcz 5 ITIGARCCATECC TEGECGARCEGARC 433	
abcZ 6 TITGATACCGTTGCC TIGTCGAACCCGATC 433	
abcz 7 TITGATACIGTIGCC TIGICGAACTCGAIC 433	
abcz 8 ITTGATACCGTIGCC TIGTCGAACTTGACC 433	
abcz 9 TITGATACCGITGCC ITGICGAACTCGAIC 433	

### 10.2.1 Locus-specific attributes

Some loci have *extended attribute fields*. To query these, you need to navigate to a locus-specific query page, by clicking the 'locus-specific query' link on the sequence attribute search page.

(PubMLST) D	ownload: Al	eles   MLST pi	ofiles	ipare alleles   Profi is   Isolate Databa		rofiles   List	Browse	Query								
																Toggle: i
Query seque	nces f	o <mark>r Neis</mark> s	seria locu	is/sequen	ce defin	itions d	lataba	ase								
Some loci have additio plugins.	nal fields w	hich are not se	earchable from th	nis general page. S	Search for thes	e at the locus	-specific (	query page. U	Useth	nis pag	e also f	or acces	s to the	sequence	e analysis	or export
Also note that some loo locus that uses integer				as text strings. Que	eries using the	'<' or '>' modi	fiers will v	vork alphabe	etically	y rather	than n	umerica	lly unles:	s you filter	r your sear	rch to a
Please enter your sear	ch criteria b	elow (or leave	blank and subm	iit to return all reco	rds). Matching	sequences w	/ill be retu	rned and you	u will t	then be	able to	update	their dis	play and	query setti	ngs.
Search criteria					Display											
locus	▼ =	*		+ i	Order by:			ascending	•							
					Display:	25 <del>v</del> reco	ords per pa	age <u>i</u>								
Filter query by		Action —														
		Reset	Submit													

Pick the required locus from the dropdown box.

(PubMLST)	Downlo	ad: Allele	es   MLS	r profiles		are alleles   Pr   Isolate Datal		Batch p	orofiles   List	Browse	Query						
																	Toggle: i
Query PorA	VR2	seq?	uenc	es - I	leisse	ria locu	s/seq	juer	nce def	initio	ns dat	abas	se				
Locus: PorA_VR2  • Further information Please enter your sea			le for this	locus.	when change		cords)										
Locus fields	ron on			ine blankt			— Displa	av					— Filter qu	ierv by			
allele id	<b>•</b> =		•			(+) <u>i</u>			allele id	•	ascending	-		tus:		-	
							Dis	splay:	25 👻 rec	ords per p	age i		allele f	lag:	•		
Action																	
Reset Submi	it																

The fields specific for that locus will be added to the dropdown query boxes.

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													
												Toggl	jle: i
Query I	PorA	VR2 sequences	s - Neisseri	a locus/seq	uen	ce d	efinitio	ons data	base				
Locus: Por	A_VR2		reload when changed										
• Furti	her inforr	mation is available for this loc	us.										
Please ente	eryourse	earch criteria below (or leave l	blank and submit to r	eturn all records).									
	Subr	1 - 25 displayed). Click the hy	perlinks for detailed	Dis	erby: a	allele id 25 👻	▼ records per	ascending page [		uery by — atus: flag:		•	
	allele id	sequence	sequence length 15	comments		variant	old name	mAb1 MN16C13F4			mAb2 reactivity	flags	
PorA VR2 PorA VR2	2 2-1	HFVQQTPKSQPTLVP HFVQQPPKSQPTLVP	15		2	1	2b	MN16C13F4 MN16C13F4	+	AF202 AF202	-+		
PorA VR2	2-10	HFVQQAPQSQSTLVP	15		2	10	20	WINTOG ISP4	-	AF202			
PorA VR2		HFVLQTPQSQPTLVP	15		2	11							
PorA VR2		HFVQQIPKSQPTLVP	15		2	12							
PorA VR2		YFVQQTPQSQPTLVP	15		2	13		MN16C13F4	+				
PorA VR2	2-14	HFVQQKLASKPTLVP	15		2	14	33						
PorA VR2	2-15	HFVQQKSTSKPTLVP	15		2	15	33a (33-1)						
PorA VR2	2-16	HFVQQKPTSKPTLVP	15		2	16	33b (33-2)						
PorA VR2	2-17	HFVQQQPTSEPTLVP	15		2	17	33c (33-3)						
PorA VR2	2-18	HFVQQIPKSQPILVP	15		2	18							
PorA VR2	2-19	HFVQQTSQSQPTLVP	15		2	19							

# **10.3 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, click the link to 'Browse profiles'.

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 d should have a corresponding record in the isolate database.	ata representing the total known diversity of <i>C. jejuni</i> and <i>C. co</i>	vii. Every new ST deposited in this database					
🔍 Query database 🚽	Downloads 🕺 Option settings i	General information					
Sequence query - query an allele sequence.     Batch sequence query - query multiple sequences in FASTA format.     Sequence attribute search - find alleles by matching attributes.     Browse MLST profiles     Search MLST profiles     List - find MLST profiles matched to entered list.     Search by combinations of MLST alleles - including partial matching.     Batch profile query - lookup MLST profiles copied from a spreadsheet.	Allele sequences     Set general options     MLST profiles	Number of sequences: 364232     Number of profiles (MLST): 7281     Last updated: 2014-07-11     Profile update history     About BIGSdb					
Sequence comp	trity - find sequences most similar to selected allele. arison - display a comparison between two sequences. tool for analysing allele sequences stored for particular locus						

Choose the field to order the results by, the number of results per page to display, and click 'Browse all records'.

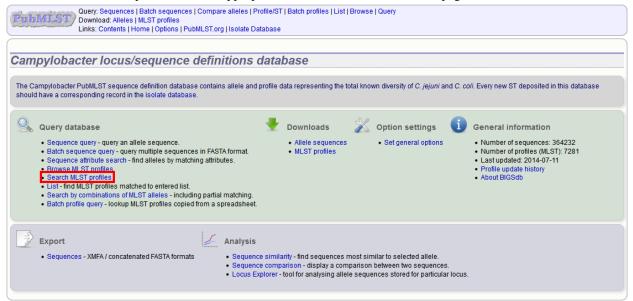
	Query: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query								
Pu	Publid LST Download: Alleles   MLST profiles Links: Contents   Home   Options   PubMLST.org   Isolate Database								
	Links, contents   nonte   options   nonte   options   nonte balande								
									Toggle: i
Bro	ws	e p	rof	ïles	s -	Ca	mr	vlobacter	locus/sequence definitions
	Brows	e crite	ria –					Action -	
	Ord	er by:	ST			-		Desures	all records
		ction:		andin				Browse	antecords
		splay:			-				
	Dis	spiay.	25		econ	is pe	i pag		
7281	7281 records returned (1 - 25 displayed). Click the hyperlinks for detailed information.								
Page	: 1	2	3	4	5	6	7	8 9 > L	asi
ST	aspA	gInA		glyA	pgm	tkt	uncA	clonal complex	
1	2	1	54	3	4	1	5	ST-21 complex	
2	4	7	51	4	1	7	1	ST-45 complex	
3	3	2	5	10	11	11	6	ST-49 complex	
4	10	11	16	7	10	5	7	ST-403 complex	
5	7	2	5	2	10	3	6	ST-353 complex	
6	63	34	27	33	45	5	7		
7	8	10	2	2	14	12	6	ST-354 complex	
8	2	1	1	3	2	1	6	ST-21 complex	
9	1	6	22	24		7	1	ST-508 complex	
10	2	59	4	38	17	12	5	ST-433 complex	
11	48	7	10	4	1	7	1	ST-45 complex	
12	7	1	5	2	11	3	6	ST-353 complex	
13	2	1	1	9	2	1	5	ST-21 complex	

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

(PubMLST)	tuery: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query ownload: Alleles   MLST profiles inks: Contents   Home   Options   PubMLST.org   Isolate Database
Profile inform	nation for ST-8 (MLST)
STaspAglnA821	gltA     glyA     pgm     tkt     uncA     clonal complex       1     3     2     1     6     ST-21 complex
sender:	Frances Colles
	Frances Colles, University of Oxford, UK (E-mail: frances.colles@medawar.ox.ac.uk)
date entered:	
datestamp:	2001-05-02
Client database	
PubMLST isolates:	Contains data for a collection of isolates that represent the total known diversity of C, jejuni and C, coli. 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.

# 10.4 Querying scheme profile definitions

click the link to 'Search profiles' for the appropriate scheme on the main contents page.



Enter the search criteria you wish to search on. You may also see some drop-down list boxes that allow further filtering of results. You can add search criteria by clicking the '+' button in the 'Locus/scheme fields' section. These can be combined using 'AND' or 'OR'.

														Togg
earc	h j	oro	file	<mark>s -</mark>	Cá	amp	oylo	obacter loo	us/sequ	ence defi	nitions			
-Locu	ıs/sc	heme	field	;—						Display/so	t options			
Combir				_	ND -					Order by		→ ascendin	a <b>-</b>	
date				<b>-</b>		•	-	2014-02-01	(+) [i		25 v recor		<b>y</b> •	
sende			(a)	Ţ				Cody		Display	25 + 10001	is her hade [1]		
senu	ci (S	uman	ic)	× .	_		•	Couy						
- Filter	r que	ry by-						Acti	n —					
	c	lonal	com	lex:				▼ i Res	et Submit					
record	s ret	urned	Clic	the	hyper	links	for de	tailed information.						
ecord	s ret	urned	Clic	the	hyper	links	for de	tailed information.						
record	s ret	urned	Clic	the	hyper									
ST as	spA	ginA	gitA	jiyA	pgm	tkt	uncA	tailed information.						
ST as 117 3	spA 33	ginA 66	gitA 65	<b>jiyA</b> 192	pgm 189	tkt 44	uncA 17	cional complex						
ST as 117 3 162	spA 33 1	ginA	gitA 65 3	9 <mark>1yA</mark> 192 539	pgm 189 5	tkt 44 9	uncA 17 3	clonal complex ST-42 complex						
ST as 117 3 162 172	spA 33 1 8	ginA 66 2 1	gitA 65 3 6	192 539 3	pgm 189 5 2	tkt 44 9 1	uncA 17 3 384	Clonal complex ST-42 complex ST-21 complex						
Tas 117 162 172 176	spA 33 1 8 7	ginA 66 2 1 448	gitA 65 3 6 5	2 <mark>192</mark> 192 539 3 2	pgm 189 5 2 10	tkt 44 9 1 3	uncA 17 3 384 6	clonal complex ST-42 complex						
ST as 117 3 162 172 176 177 8	spA 33 1 8	gInA 66 2 1 448 21	gitA 65 3 6 5 2	192 539 3 2 566	pgm 189 5 2 10 11	tkt 44 9 1 3 37	uncA 17 3 384 6 3	Clonal complex ST-42 complex ST-21 complex ST-353 complex						
ST as 117 3 162 172 176 177 9 178	spA 33 1 8 7 55 7	ginA 66 2 1 448 21 17	0ltA 65 3 6 5 2 5	2 192 539 3 2 566 2	pgm 189 5 2 10 11 705	tkt 44 9 1 3 37 37	uncA 17 3 384 6 3 6	cional complex ST-42 complex ST-21 complex ST-353 complex ST-353 complex						
ST as 117 3 162 172 176 177 9 178	spA 33 1 8 7 55 7 3	gInA 66 2 1 448 21 21 17 495	gltA 65 3 6 5 2 5 5 5	2 192 539 3 2 566 2 10	pgm 189 5 2 10 11	tkt 44 9 1 3 37	uncA 17 3 384 6 3 6 6 6	Clonal complex ST-42 complex ST-21 complex ST-353 complex						
ST as 117 3 162 172 176 177 5 178 179 180 3	spA 33 1 8 7 55 7 3 79	ginA 66 2 1 448 21 17 495 496	gitA 65 3 6 5 2 5 5 5 420	2 539 3 2 566 2 10 372	pgm 189 5 2 10 11 705 11 20	tkt 44 9 1 3 37 3 68 1	uncA 17 3 384 6 3 6 6 6 6 17	cional complex ST-42 complex ST-21 complex ST-353 complex ST-353 complex						
ST as 117 3 162 172 176 177 5 178 178 179 180 3	spA 33 1 8 7 55 7 3 79	gInA 66 2 1 448 21 21 17 495	gitA 65 3 6 5 2 5 5 5 420	2 539 3 2 566 2 10 372	pgm 189 5 2 10 11 705 11 20	tkt 44 9 1 3 37 3 68 1 560	uncA 17 3 384 6 3 6 6 6	cional complex ST-42 complex ST-21 complex ST-353 complex ST-353 complex						

Each field can be queried using standard operators.

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

Pub	Mİ	ST	/ Do	wnloa	ad: All	eles	MLS	T profiles	npare alleles   Profile/ F.org   Isolate Databa		List Brows	e   Query			
															Toggle: i
Sear	ch	pro	file	es -	Ca	m	ovl	obacter loo	cus/sequen	ce definit	ions				
							_		4						
Lo	cus/s	chem	e field	ls —						-Display/sort opti	ons				
Com	bine s	earch	es wi	ith: A	ND -	-				Order by: ST		<ul> <li>ascending</li> </ul>	•		
dat	e ente	ered		•	>		•	2014-02-01	+ i	Display: 25	+ records	per page 👔			
ser	nder (s	surnar	ne)	•	=		•	Cody							
— Filt	ter qu	ery by						Acti	on						
		clonal	com	plex:				▼ i Res	et Submit						
17 recor	rds re	turnec	I. Clic	k the	hyper	links	for de	etailed information.							
ST	asn∆	alnA	altA	αlvA	nam	tkt	uncA	clonal complex							
7117		66	-	192			17	cional complex							
7162	1	2		539	5	9	3	ST-42 complex							
7172		1	6	3	2	1	384								
7176		448	5	2	10	3	6	ST-353 complex							
7177	55	21		566	11	37	3	07.050							
7178	3	17 495	5 5	2 10	705	3 68	6	ST-353 complex ST-49 complex							
7179	79	495				1	17	S1-45 Complex							
7180	121	490				560	94								
7182	7	2			22										

# 10.5 Investigating allele differences

#### 10.5.1 Sequence similarity

To find sequences most similar to a selected allele within a sequence definition database, click 'Sequence similarity' on the contents page.

		Toggle: i
Neisseria locus/sequence definition	s database	
The Neisseria PubMLST sequence definition database contains a have a corresponding record in the isolate database.	allele and profile data representing the total known diver	sity of Neisseria species. Every new ST deposited in this database should
Query database	🛃 Downloads	🔀 Option settings
Sequence query - query an allele sequence.     Batch sequence query - query multiple sequences in FA	Allele sequences     ASTA format.     MLST	Set general options
Back sequence duely - quely multiple sequences in F     Sequence attribute search - find alleles by matching att     Browse profiles		General information
Search profiles     List - find profiles matched to entered list.		Number of sequences: 341811     Number of profiles: Show
<ul> <li>Search by combinations of alleles - including partial ma</li> <li>Batch profile guery - lookup profiles copied from a spre</li> </ul>		<ul> <li>Last updated: 2014-07-11</li> </ul>
Extract finetype from whole genome data	BUSITEEL	Profile update history     About BIGSdb
Export	Analysis	
Sequences - XMFA / concatenated FASTA formats	Sequence similarity find sequences most similar	ar to selected allele.
	<ul> <li>Sequence comparison - display a comparison be</li> <li>Locus Explorer - tool for analysing allele sequence</li> </ul>	

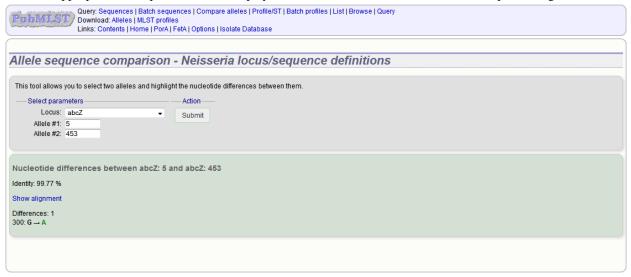
Enter the locus and allele identifier of the sequence to investigate and the number of nearest matches you'd like to see, then press submit.

Query:         Sequences         Batch sequences         Compare alleles         Profile/ST         Batch profiles         List         Browse         Query           Download:         Alleles         MLST profiles         Links:         Contents         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     Image: AbcZ       Allele: 5     Submit       Number of results: 10     Image: AbcZ

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

ind m	nost si	milor o	مامال	s - Noi	ssoria loc	ue/eonua	ence defii	nitions		
mu m	1031 31	iiiiai a	IICIC	3 - MCI	556114 100	uərəcyud	ence dem	1100113		
This page	allows you	to find the m	ost simil	lar sequenc	es to a selected a	lele using BLAS	ST			
	t parameters		1001 01111	iai sequene		Icie dolling DENO	51.			
Seleci	1	s IS: abcZ								
		le: 5			<ul> <li>Reset</li> </ul>	Submit				
Num	Allel ber of result									
Num	berorresult	is. 10 👻								
abcZ-5										
	% Identity	Mismatches	s Gaps A	Alignment	Compare					
		Mismatches 1		Alignment 433/433 (	Compare Compare abcZ: (	57				
Allele	99.77		0		· · ·					
Allele abcZ: 657	99.77 99.77	1	0	433/433 (	Compare abcZ: (	53				
Allele abcZ: 657 abcZ: 453	99.77 99.77 99.77	1 1	0 0 0	433/433 ( 433/433 (	Compare abcZ: 6 Compare abcZ: 4	53 05				
Allele abcZ: 657 abcZ: 453 abcZ: 405	99.77 99.77 99.77 99.77	1 1 1	0 0 0 0 0	433/433 ( 433/433 ( 433/433 (	Compare abcZ: ( Compare abcZ: 4 Compare abcZ: 4 Compare abcZ: 4	53 05 04				
Allele abcZ: 657 abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213	99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1	0 0 0 0 0 0	433/433 ( 433/433 ( 433/433 ( 433/433 (	Compare abcZ: ( Compare abcZ: 4 Compare abcZ: 4 Compare abcZ: 4 Compare abcZ: 2	53 05 04 13				
Allele abcZ: 657 abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166	99.77 99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1 1	0 0 0 0 0 0 0	433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 (	Compare abc2: ( Compare abc2: 4 Compare abc2: 4 Compare abc2: 4 Compare abc2: 2 Compare abc2: 2	53 05 04 13 66				
Allele abcZ: 657 abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166 abcZ: 114	99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1 1 1 1 1	0 0 0 0 0 0 0 0 0 0	433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 (	Compare abc2: 4 Compare abc2: 4 Compare abc2: 4 Compare abc2: 4 Compare abc2: 2 Compare abc2: 2 Compare abc2: 2	53 05 04 13 66 14				
Allele abcZ: 657 abcZ: 405 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 116 abcZ: 114 abcZ: 103	99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1 1 1 1 1 1 1	0 0 0 0 0 0 0 0 0 0 0 0 0	433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 (	Compare abc2: ( Compare abc2: 4 Compare abc2: 4 Compare abc2: 2 Compare abc2: 2 Compare abc2: 2 Compare abc2: 2 Compare abc2: 2	53 05 04 13 66 14 03				
Allele abcZ: 657 abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166 abcZ: 114	99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1 1 1 1 1	0 0 0 0 0 0 0 0 0 0 0 0 0 0	433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 ( 433/433 (	Compare abc2: 4 Compare abc2: 4 Compare abc2: 4 Compare abc2: 4 Compare abc2: 2 Compare abc2: 2 Compare abc2: 2	53 155 24 13 66 14 23 46				

Click the appropriate 'Compare' button to display a list of nucleotide differences and/or a sequence alignment.



#### 10.5.2 Sequence comparison

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

Query: Sequences   Batch sequences   Compare alleles   Profiles Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database		ery
		Toggle: i
Neisseria locus/sequence definitions database	ð	
The Neisseria PubMLST sequence definition database contains allele and profile dat have a corresponding record in the isolate database.	a representing the total known diversit	y of Neisseria species. Every new ST deposited in this database should
🔍 Query database 😽	Downloads	🔀 Option settings
<ul> <li>Sequence query - query an allele sequence.</li> <li>Batch sequence query - query multiple sequences in FASTA format.</li> <li>Sequence attribute search - find alleles by matching attributes.</li> <li>Browse profiles</li> <li>Search profiles</li> <li>List - find profiles matched to entered list.</li> <li>Search by combinations of alleles - including partial matching.</li> <li>Batch profile query - lockup profiles copied from a spreadsheet.</li> <li>Extract finetype from whole genome data</li> </ul>	Allele sequences     MLST      Download profiles	Set general options     General information     Number of sequences: 341811     Number of profiles: Show     Last updated: 2014-07-11     Profile update history     About BIGSdb
Sequence co	milarity - find sequences most similar t Imparison - display a comparison betw er - tool for analysing allele sequences	/een two sequences.

Enter the locus and two allele identifiers to compare. Press 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
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:     8

A list of nucleotide differences and/or an alignment will be displayed.

PubMLST / Download: Allele	es   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query es   MLST profiles   Home   PorA   FetA   Options   Isolate Database
Allele sequence com	parison - Neisseria locus/sequence definitions
This tool allows you to select two allel	eles and highlight the nucleotide differences between them.
	Action
Locus: abcZ Allele #1: 5 Allele #2: 8	▼ Submit
Nucleotide differences betwe Identity: 90.53 % Show alignment Differences: 41	en abcZ: 5 and abcZ: 8
72: G → T	
78: $A \rightarrow G$ 79: $A \rightarrow C$	
81: T → C 82: G → A	
83: <b>G</b> → A	
87: G → A 88: A → G	
$89: \mathbf{G} \rightarrow \mathbf{A}$	
90: $T \rightarrow C$	
93: G → C 95: C → T	
99: G → A	
102: $G \rightarrow A$	

#### See also:

Locus explorer plugin.

## 10.6 Querying isolate data

The 'Search database' page of an isolate database allows you to search by combinations of provenance criteria, scheme and locus data, and more.

Pub	MLST) Breakdown: Is	Browse  Profile/ST  List solate fields  Scheme/alleles  Publications ts  Home  Options  Profiles/sequences de		missions		
Neis	seria PubMLST	database				
		contains data for a collection of isolates the esponding isolate deposited here. Any isola				
Q	Query database		🔏 Option set	tings	i	General information
			<ul> <li>Set display</li> </ul>	I options - including isolate table field and query options for locus, schemes		Isolates: 29172     Last updated: 2014-07-11     Update history     About BIGSdb
	Breakdown	Fxport	5	Analysis	Miscellaneous	
	<ul> <li>Single field</li> <li>Two field</li> <li>Unique combinations</li> <li>Scheme and alleles</li> <li>Publications</li> <li>Sequence bin</li> </ul>	Export dataset     Contigs     Sequences - XMFA / concatenated	I FASTA formats	Codon usage     Presence/absence status of loci     Genome comparator     BLAST	Description of da	atabase 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'.

Query:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/sequences definition	s   Database submissions		
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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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- 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.
- Filters
  - Various filters may be available, including
    - \* Publications
    - \* Projects
    - \* MLST profile completion status
    - \* Clonal complex
    - \* Sequence bin size
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If the interface is modified, a button to 'Save options' becomes available within the tab. If this is clicked, the modified form will be displayed the next time you go to the query page.

### 10.6.1 Query by allele\_designation/scheme field

Queries can be combined with allele designation/scheme field values.

Make sure that the allele designation/scheme field values fieldset is displayed by selecting it in the 'Modify form options' tab.

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Designations can be queried using standard operators.

Additional search terms can be combined using the '+' button.

Add your search terms and click 'Submit'. Allele designation/scheme field queries will be combined with terms entered in other sections.

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id isolate alias 341 M7085 2281 M7089 2299 M7257 9369 M13519 9371 M15141 9374 M16917 9377 M17661	ES COUNTRY USA USA USA USA USA USA USA	Iso year 2000 invasiv 2000 invasiv 2000 invasiv 2005 invasiv 2006 invasiv 2007 invasiv 2008 invasiv	late fields [] disease e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other)	Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me	ningitidis ningitidis ningitidis ningitidis ningitidis ningitidis ningitidis	W W W C NG	11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c	clonal complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex	PorA VR1 5 5-1 5-1 5-1 5-1 5-1	PorA VR2 2 10-8 10-8 10-8	FetA VR F3-6	
id isolate aliaso 341 M7085 2281 M7089 2299 M7257 9369 M13519 9371 M15141 9374 M16917	ES COUNTRY USA USA USA USA USA USA USA	Iso year 2000 invasiv 2000 invasiv 2000 invasiv 2005 invasiv 2006 invasiv 2007 invasiv 2008 invasiv	late fields [] disease e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other)	Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me	ningitidis ningitidis ningitidis ningitidis ningitidis ningitidis ningitidis	W W W C NG W	11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c	clonal complex complex/ET-37 complex complex/ET-37 complex complex/ET-37 complex complex/ET-37 complex complex/ET-37 complex complex/ET-37 complex complex/ET-37 complex	PorA VR1 5 5-1 5-1 5-1 5-1 5-1	PorA VR2 2 10-8 10-8 10-8 10-8 10-8	FetA VR F3-6	
id isolate aliase 341 M7085 2281 M7089 2299 M7257 9371 M1519 9371 M15141 9377 M16917 9377 M17661 9379 M18774 nalysis tools:	es country USA USA USA USA USA USA USA	year 2000 invasiv 2000 invasiv 2005 invasiv 2006 invasiv 2007 invasiv 2008 invasiv 2009 invasiv	late fields [] disease e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other)	Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me	ningitidis ningitidis ningitidis ningitidis ningitidis ningitidis ningitidis	W W W C NG W W	11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c	clonal complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex	PorA VR1 5 5-1 5-1 5-1 5-1 5-1 5	PorA VR2 2 10-8 10-8 10-8 10-8 10-8	FetA VR F3-6	
id isolate aliase 341 M7085 2281 M7089 2299 M7257 9369 M13519 9371 M15141 9374 M16917 9374 M16917 9377 M17661 9379 M18774	ES COUNTRY USA USA USA USA USA USA USA	Iso year 2000 invasiv 2000 invasiv 2000 invasiv 2005 invasiv 2006 invasiv 2008 invasiv 2008 invasiv 2009 invasiv	late fields [] disease e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other)	Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me Neisseria me	ningitidis ningitidis ningitidis ningitidis ningitidis ningitidis ningitidis	W W W C NG W W	11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c 11 ST-11 c	clonal complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex omplex/ET-37 complex	PorA VR1 5 5-1 5-1 5-1 5-1 5-1	PorA VR2 2 10-8 10-8 10-8 10-8 10-8	FetA VR F3-6	

#### 10.6.2 Query by allele designation status

Allele designations can be queried based on their status, i.e. whether they are confirmed or provisional. Queries will be combined from the values entered in all form sections.

Make sure that the allele designation staus fieldset is displayed by selecting it in the 'Modify form options' tab.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles Links: Contents   Home   Options   Profiles/	Publications sequences definitions   Database submissions	
	Toggle: i Field	help: id 🗸 Go
Search Neisseria PubMLST databas	se	
id • Enter value	Display/sort options     (X)     (X)     Display: 25	ers Modify
Action Reset Submit	Click to add or remove add Show Allele de Show Allele de	

Select a locus from the dropdown box and either 'provisional' or 'confirmed'. Additional query fields can be displayed by clicking the '+' button. Click 'Submit'.

11 31	WLS7	📝 Break	down: Is	olate fi	se   Profile/ST   List elds   Scheme/alleles   F me   Options   Profiles/se		ns   Database	e submissions				
									Toggle: <i>i</i> Field help: id			- G
eard	ch Ne	eisser	ia P	ubM	LST databas	е						
-Iso	late prove	enance/ph	enotype	fields -			— Display/s	ort options				Modi
id			- =		<ul> <li>Enter value</li> </ul>	+ 1	Order b	y: id				form
							Displa	ay: 25 👻 records per page 👔				optic
ecord	s returne	d. Click th	e hyperli		detailed information.				ст	Finot	vning an	tiaone
ecord: id				1	detailed information. solate fields 👔 disease	species	serogroup	ML ST	ST clonal complex	PorA	yping ant PorA VR2	FetA
id		aliases		l: year	solate fields 👔	species Neisseria meningitidis	serogroup B					
id 10735	isolate N 56/99	aliases	country	l: year 1999	solate fields <mark>i</mark> disease invasive	Neisseria		ST	clonal complex	PorA VR1	PorA VR2	FetA VR
id	isolate N 56/99 8/00	aliases	country Norway	year 1999 2000	solate fields I disease invasive (unspecified/other) invasive	Neisseria meningitidis Neisseria	В	ST 45, <mark>2183, 4363, 9838</mark>	clonal complex ST-41/44 complex/Lineage 3, ST-41/44 complex/Lineage 3,	PorA VR1 5-1	PorA VR2 10-1	FetA VR F5-5
id 10735 10756	isolate N 56/99 8/00 10/00	aliases	country Norway Norway	year 1999 2000 2000	solate fields disease invasive (unspecified/other) invasive (unspecified/other) invasive	Neisseria meningitidis Neisseria meningitidis Neisseria	B	ST 45, 2183, 4363, 9838 43, 1644, 2433, 4163	cional complex ST-41/44 complex/Lineage 3, ST-41/44 complex/Lineage 3, ST-213 complex ST-41/44 complex/Lineage 3,	PorA VR1 5-1 22	PorA VR2 10-1 14	FetA VR F5-5 F5-5
id 10735 10756 10758	isolate N 56/99 8/00 10/00	aliases	country Norway Norway Norway	year 1999 2000 2000 2000 2000	solate fields [2] disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) Invasive	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria	B B	ST 45, 2183, 4363, 9838 43, 1644, 2433, 4163 110, 1419, 1844, 6617	cional complex ST-41/44 complex/Lineage 3, ST-41/44 complex/Lineage 3, ST-213 complex ST-41/44 complex/Lineage 3, ST-1157 complex	PorA VR1 5-1 22 21-7	PorA VR2 10-1 14 16	FetA VR F5-5 F5-5 F5-36 F1-5
id 10735 10756 10758 10812	isolate N 56/99 8/00 10/00 64/00 Mk	aliases	country Norway Norway Norway	year 1999 2000 2000 2000 1996	solate fields disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria	B B B	ST 45, 2183, 4363, 9838 43, 1644, 2433, 4163 110, 1419, 1844, 6617 146, 41, 303, 1788, 1823, 3142	cional complex ST-41/44 complex/Lineage 3, ST-41/44 complex/Lineage 3, ST-213 complex ST-41/44 complex/Lineage 3, ST-41/44 complex/Lineage 3	PorA VR1 5-1 22 21-7 7-2	PorA VR2 10-1 14 16 4	FetA VR F5-5 F5-5 F5-36

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.

### 10.6.3 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.

PubMLST	📝 Breakdown: Isola	rowse   Profile/ST   List te fields   Scheme/alleles   Pi Home   Options   Profiles/sec		s   Database submissions						
					Toggle: i Field help: id	🗕 🕒				
Search Ne	earch Neisseria PubMLST database									
	nance/phenotype fiel			Display/sort options	rva.	Modify				
id		<ul> <li>Enter value</li> </ul>	+ 1	Order by: id	[X]	form				
				Display: 25 👻 records per page	Modify form parameters	options				
Action					Click to add or remove additional query terms:					
Reset S	ubmit				Show Allele designations/scheme field values					
					Show Allele designation status					
					Show ] Tagged sequence status					
					Show 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.

Query: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
Toggle: 1 Field help: id	▼ Go
Search Neisseria PubMLST database	
- Isolate provenance/phenotype fields Display/sort options	Modify
id	form options
	opuono
Tagged sequence status     Action     NEIS0001 (lpxC)  ▼ is flaqqed: internal stop codon  ▼ + ii Recet     Submit	
NEIS0001 (lpxC) → is flagged: internal stop codon → + i Reset Submit	
1 record returned. Click the hyperlink for detailed information.	
Isolate fields 🖬 MLST Finetyping antigens	
id isolate aliases country year disease species serogroup ST clonal complex PorA VR1 PorA VR2 FetA VR 2077 153 alpha153 Germany 1999 carrier Neisseria meningitidis E 60 ST-60 complex 5 2 F1-7	
Analysis tools:	
Breakdown: Fields Two Field Codons Polymorphic sites Combinations Schemes/alleles Publications Sequence bin Tag status	
Analysis: Presence/Absence Genome Comparator BLAST	
Export: Dataset Contigs Sequences	

#### See also:

Sequence tag flags

#### 10.6.4 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.

(PubMLST) Br	reakdown: Isolate	wse   Profile/ST   List fields   Scheme/alleles   Pu ome   Options   Profiles/seq		is   Database submissions							
					Toggle: i Field help: id	▼ Go					
Search Neiss	earch Neisseria PubMLST database										
Isolate provenance		✓ Entervalue		Display/sort options Order by: id	X	Modify					
Id	▼ =	Enter value	+ 1	Display: 25 - records per page		form options					
Action Reset Submit					Click to add or remove additional query terms: Show Allele designations/scheme field values Show Allele designation status Show Tagged sequence status Show Fitters						

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*.

### 10.7 Querying by allelic profile

If a scheme, such as MLST, has been defined for either 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. This can also be done in sequence definition databases if the scheme has a primary key field defined.

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.

Pub	MILST / Breakdown: I	ch   Browse   Profile/ST   List Isolate fields   Scheme/alleles   Publications ints   Home   Options   Profiles/sequences defi	nitions   Database su	bmissions		
Neis	seria PubMLS	T database				
		e contains data for a collection of isolates that rresponding isolate deposited here. Any isolate				
Q				nttings ral options - including isolate table field ay and query options for locus, scheme		General information • Isolates: 29174 • Last updated: 2014-07-14 • Update history • About BIGSdb
	Breakdown • Single field • Two field • Unique combinations • Scheme and alleles • Publications • Sequence bin	Export • Export dataset • Contigs • Sequences - XMFA / concatenated F	FASTA formats	Analysis Codon usage Presence/absence status of loci Genome comparator BLAST	Miscellaneous  • Description of da	atabase fields

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   Put Links: Contents   Home   Options   Profiles/sequ				
			Тод	ggle: i
Search Neisseria PubMLST database	by combinations of loc	i		
Schemes				
Please select the scheme you would like to query:				
MLST				
Please enter your allelic profile below. Blank loci will be ignored.		ning remote database		
abcZ adk aroE fumC gdh pdhC	pgm ST:	Autofill		
Filters	Options	Display/sort options		
Project:	Search: Exact or nearest match 👻	Order by: id	→ ascending         →	
Include old record versions		Display: 25 🗸 records per page i		
Action				
Reset Submit				

Enter the combination of alleles that you want to query for. Fields can be left blank.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: [i]
Search Neisseria PubMLST database by combinations of loc	i
Schemes	
Please select the scheme you would like to query:	
MLST Velect	
Please enter your allelic profile below. Blank loci will be ignored. — Autofill profile by search	hing remote database ——
abcZ         adk         aroE         fumC         gdh         pdhC         pgm         ST:           2         3         4         3         8         4         3         3         3         4         3         3         4         3         3         4         3         3         4         3         3         3         4         3         3         4         3         3         4         3         3         4         3         3         4         3         3         4         3         3         4         3         3         4         3         3         4         3         3         4         3         3         4         3         3         4         3         3         3         4         3         3         3         4         3         3         3         4         3         3         3         4         3         3         3         4         3         3         4         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3         3	Autofill
- Filters - Options	Display/sort options
Project: Version Search: Exact or nearest match Version	Order by: id     ascending
Include old record versions	Display: 25 👻 records per page 👔
Action	
Reset Submit	

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

Ouery:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: i
Search Neisseria PubMLST database by combinations of loci	
Schemes	
Please select the scheme you would like to query:	
MLST	
abcZ     adk     aroE     fumC     gdh     pdhC     pgm     ST:     44     Autofill       9     6     9     9     6     9	
- Filters - Display/sort options	
Project: • Search: Exact or nearest match • Order by: id • ascending •	
□ Include old record versions Display: 25  v records per page i	
Action	
Reset Submit	

Select the number of loci that you'd like to match in the options dropdown box. Available options are:

- Exact or nearest match
- · Exact match only
- x or more matches
- y or more matches
- z or more matches

Where x,y, and z will range from n-1 to 1 where n is the number of loci in the scheme.

Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/Sequences definitions   Database submissions	
Tog	gle: i
Search Neisseria PubMLST database by combinations of loci	
Schemes	
Please select the scheme you would like to query:	
MLST - Select	
abcZ adk aroE fumC gdh pdhC pgm ST: 44 Autofill	
- Filters - Options - Display/sort options	
Project:	
□ Include old record versions Display: 25	
Action	
Reset Submit	

Click 'Submit'.

		Links: Conten										
												Toggle
ar	ch Neis	sseria Pi	ubMI ST d	ata	base by combin	nations of loc	i					
ar		Jocha i v		ata								
hei	mes											
ease	select the se	cheme vou wou	Id like to query:									
					_							
ILST			-	Selec	*							
Ple	ease enter yo	ur allelic profile	below. Blank loci	will be	ignored. — — —	-Autofill profile by search	ning remote	data	base ——			
al	ocZ ad	lk aroE	fumC g	jdh	pdhC pgm	ST: 44			Autofill			
	96	9	9	9	6 9							
-Filf	ters				Options		-Display/s	sort o	options			
	Project:				I Search: Exact	t or nearest match 👻	Order	by:	id	_	ascendi	ng 👻
	nciude old re	cord versions							25 v records per page 7			
	nciude old re	cord versions			_		Displ		25 👻 records per page 👔			
	nciude old re tion	cord versions			_				25 👻 records per page 👔			
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Act Re Ict m	tion set Sub atches found ords returned	mit I (7 loci). I (1 - 25 display		rlinks	for detailed information.				25 → records per page [			
Act Re ct m reco	tion set Sub atches found ords returned	mit I (7 loci). I (1 - 25 display									Ding antic	ens
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- Act Re ct m recc ge: ( 1 41 70 27	tion set Sub atches found ords returned 1 2 3 isolate 19 38 NG E30	mit 4 (7 loci). 4 (1 - 25 display ) (4 (5 ≥	Country Germany Germany Norway	Isolat year 1999 1999 1988	te fields 1 disease carrier carrier carrier	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	Displ serogroup B NG B	ay: ST 44 \$ 44 \$	ML ST clonal complex ST-41/44 complex/Lineage 3 ST-41/44 complex/Lineage 3 ST-41/44 complex/Lineage 3	Finety		
- Acl Re ct m recc ge: ( 11 70 27 74	ion set Sub atches found ords returned 1 2 3 isolate 19 38 NG E30 99 182	mit 4 (7 loci). 4 (1 - 25 display ) 4 5 > aliases	Country Germany Germany Norway Canada	Isolat year 1999 1999 1988 1999	te fields 👔 disease carrier carrier carrier invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	Serogroup B NG B B B	ay: 51 44 44 44 44 44	ML ST clonal complex ST-41/44 complex/Lineage 3 ST-41/44 complex/Lineage 3 ST-41/44 complex/Lineage 3 ST-41/44 complex/Lineage 3	Finety PorA VR1	PorA VR2	FetA VR
- Acl Re ct m recc ge: ( 11 70 27 74 92	tion set Sub atches found ords returned 1 2 3 isolate 19 38 NG E30 99 182 99-132	mit 4 (7 loci). 4 (1 - 25 display ) 4 5 > aliases	Country Germany Germany Norway Canada Canada	Isolat 9999 1999 1988 1999 1999	te fields [] disease carrier carrier carrier invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	Displ serogroup B NG B B B B B B B B	ay: 5T 44 44 44 44 44 44 44 44 5 5 5 5 5 5 5 5 5 5 5 5 5	MLST clonal complex ST-41/44 complex/Lineage 3 ST-41/44 complex/Lineage 3 ST-41/44 complex/Lineage 3 ST-41/44 complex/Lineage 3	Finety PorA VR1 21	PorA VR2	FetA VR F1-7
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# 10.8 Retrieving list of isolates or profiles

Both isolate and sequence definition databases can be queried against a list of values matching any criteria (isolate provenace fields, alleles, or scheme fields).

Click 'List query' on the main contents page.

Publ	MLST / Breakdown: Is	Browse   Profile/ST   List solate fields   Scheme/alleles   Publ ts   Home   Options   Profiles/seque		missions		
Neise	seria PubMLST	database				
				wn diversity of Neisseria species. Fo this database and consequently it sh		
0			<ul> <li>Set display natching.</li> </ul>	tings al options - including isolate table fiel v and query options for locus, schem		General information • Isolates: 29174 • Last updated: 2014-07-14 • Update history • About BIGSdb
	Breakdown Single field Two field Unique combinations Scheme and alleles Publications Sequence bin	Export • Export dataset • Contigs • Sequences - XMFA / conc	atenated FASTA formats	Analysis • Codon usage • Presence/absence status of loci • Genome comparator • BLAST	Miscellaneous  • Description of d	

Select the attribute you wish to search against in the drop-down list box and enter the list of attributes in the box (one per line). Click 'Submit'.

Ouery:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/sequences definitions   Database submissions								
		Toggle: <i>i</i> Field help: id	← Go					
Query Neisseria PubMLST database	e matching a field against a	list						
Please select attribute isolate Enter your list of attribute values below (one per line) H44/76 MC58 alpha14	Filters Display/sort	t options						
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237 H44/76 44/76-3; Z3842 Norway 1976 invasive (unspe 240 MC58 Z7176 UK 1983		ST-32 complex/ET-5 complex         7         16         F3-3           ST-32 complex/ET-5 complex         7         16-2         F1-5						
20477 H44/76 44/76-3; Z3842 Norway 1976 invasive (unspe		ST-32 complex/ET-5 complex 7 16 F3-3						
Analysis tools: Breakdown: Fields Two Field Codons Polymorphic sites Analysis: BURST Presence/Absence Genome Comparator Export: Dataset Contigs Sequences	Combinations Schemes/alleles Publications	Sequence bin Tag status						

## 10.9 Retrieving isolates by linked publication

Click 'Publications' in the Breakdown section of the contents page.

Pub	MLST / Breakdown: Isola	rowse   Profile/ST   List te fields   Scheme/alleles   Publications Home   Options   Profiles/sequences d		bmissions		
Neis	seria PubMLST d	latabase				
		ntains data for a collection of isolates th conding isolate deposited here. Any isol				
Q	Query database		💥 Option se	ttings	()	General information
			<ul> <li>Set displa</li> </ul>	al options - including isolate table field y and query options for locus, scheme		Isolates: 29174     Last updated: 2014-07-14     Update history     About BIGSdb
	Breakdown	Export	1	Analysis	Miscellaneous	5
	Single field     Two field     Unique combinations     Scheme and alleles     Publications     Sequence bin	Export dataset     Contigs     Sequences - XMFA / concatenate	d FASTA formats	Codon usage     Presence/absence status of loci     Genome comparator     BLAST	Description of d	latabase fields

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

ublica	atio	n breakdown of dataset			
- Filter q	uery by	——————————————————————————————————————		Action	
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Y	'ear:	All years   Display: 2	5 👻 records per page		
		d (1 - 25 displayed). Click the hyperlinks for detail	ed mornation.		
PubMed id	Year	Citation	1	Title	lsolates in database
id	Year 2007		and S, Bukovski S, Cafferkey MT, Carion 12 R, Fazio C, Frosch M, Heuberger S, 3, Kesanopoulos K, Kriz P, Lambertsen L nska A, Stefanelli P, Thulin S, Tzanakaki	Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis.	
id 7517841	Year 2007 2008	Citation Taha MK, Vázquez JA, Hong E, Bennett DE, Bertr F, Christensen JJ, Diggle M, Edwards G, Enríque Hoffmann S, Jolley KA, Kadlubowski M, Kechrid J Levenet I, Musilek M, Paragi M, Saguer A, Skoczy	and S, Bukovski S, Cafferkey MT, Carion z R, Fazio C, Frosch M, Heuberger S, A, Kesanopoulos K, Kriz P, Lambertsen L nska A, Stefanelli P, Thulin S, Tzanakaki imicrob Agents Chemother <b>51</b> : 2784-92	Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis.	database
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These can be filtered by author and/or year, and the sort order changed.

TM din	ST	Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions		
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18815379 2		uckee CO, Jolley KA, Recker M, Penman B, Kriz P, Gupta S, Maiden MC (2008) Proc Natl Acad Sci U S A 05: 15082-7	Role of selection in the emergence of lineages and the evolution of virulence in Neisseria meningitidis.	1054 isolates
15776372 2		Haus H, Maiden MC, Wilson DJ, McCarthy ND, Jolley KA, Urwin R, Hessler F, Frosch M, Vogel U (2005) J Ifect Dis <b>191:</b> 1263-71	Genetic analysis of meningococci carried by children and young adults.	822 isolates
15528708 2		azdankhah SP, Kriz P, Tzanakaki G, Kremastinou J, Kalmusova J, Musilek M, Alvestad T, Jolley KA, Wilson J, 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 2	2007	ennett 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 2	005	olley 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.

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blica           ation           nnett JS           secies st           seven           pulation           records           records           ation           1           1           1           2           1           2           3           3           3           3           3           3           3           3           3           3           3           4           2           5	atio quer 3, Jolley 1 loci Ne geneti 1 loci Ne loci	Breakdow Links: Co <b>ns cited</b> <b>y (PubMe</b> <b>y (PubMe</b> <b>y (PubMe</b> <b>y (A Sparling</b> <b>f Veisseria g</b> <b>alisseria MLS'</b> <b>i cinferences</b> <b>alisseria g</b> <b>alisses</b> <b>b (1 - 25 dis</b> <b>aliases</b> <b>B (1 - 25 dis</b> <b>b (1 - 25 dis</b> ) <b>b (1 - 25 dis</b> ) <b>b (1 - 10 dis)</b> <b>b (1 - 10 d</b>	m: Isolate field ntents   Home d in the ed id: 178 approximation of the approximation of the approximati	ts   Sctore Nei 2509 N, H 2509 N, H 2509 100 100 100 100 100 100 100 1	neme/alleles   Publication nns   Profiles/sequences (	Idefinitions   Database subn     ST database     Statement     Stat	us sequence hly discrimin amica. Exam sified isolates serogroup A A A A A A A A A A A A A A A A A A A	atory t inatior s and s and 1 1 1 1 4 5 1 1 1 1 4 5 4 1 1 4	MLST clonal complex MLST clonal complex ST-4 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-2 complex/subgroup I/II ST-4 complex/subgroup I/II ST-4 complex/subgroup I/II ST-4 complex/subgroup I/II	Finetyping antigens           PorA VR1         PorA VR2         Fer           5-2         10         F           20         9         F           18-1         3         F           5-2         10         F           5-1         9         F           5-1         9         F           5-2         10         F           5-2         10         F           7         13-1         F           5-2         10         F           7         13-1         F           5-2         10         F           7         13         F	A VR 1-5 5-1 3-1 5-1 3-6 5-1 1-5 3-1 1-5 1-5
d         isol           d         isol           i         isol	atio           quer           quer           s, Jolley           loci Nc           genetic           loci Nc           genetic           atus o           loci Nc           genetic           loci Nc           genetic           loci Nc           genetic           loci Nc	Breakdow Links: Co <b>ns cited</b> <b>y (PubM</b> <b>y (PubM</b> <b></b>	In: Isolate field Intents   Home and in the ed id: 178 ed id: 178	ts   Sctore Neir 2509 NJ, H evolution readilities readilities 1937 1975 1971 1963 1963 1963 1963 1966 1966	neme/alleles   Publication pons   Profiles/Sequences ( sseria Publication part CA, Feavers IM, Maider onary and epidemiologica y adapted to N. gonorrhoe g direct comparisons with s, gdh, provided a rapid m perlinks for detailed inform > Last solate fields [] disease invasive (unspecified/oth invasive (unspecified/oth	Initions   Database subn     ST database     Statement     Statem	us sequence hly discrimin amica Exam sified isolates A A A A A A A A A A A A A A A A A A A	atory t inatior s and 4 1 5 1 1 1 4 5 4 1 1 4 4 4 4 4 4	MLST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-1 complex/subgroup IV ST-1 complex/subgroup III ST-1 complex/subgroup III ST-1 complex/subgroup III ST-4 complex/subgroup IV ST-4 complex/subgroup IV	Finetyping antigens           PorA VR2   ForA VR	A VR 1-5 5-1 3-1 5-1 3-6 5-1 1-5 3-1 1-5 1-5 1-5 1-5 1-5 1-5 1-5 1-5
ation           Innet JS           secies st           e Seven           pulation           ge:           1           A4MM           2           2           2           3	atio           quer           quer           s, Jolley           loci Ne           genetic           loci Ne           loci N	Breakdow Links: Co <b>ns cited</b> <b>y (PubM</b> <b>y (PubM</b> <b>y (PubM</b> <b>y (PubM</b> <b>y (A Sparling</b> <b>f Veisseria g</b> <b>aisseria MLS'</b> <b>isseria MLS'</b> <b>isseria MLS'</b> <b>isseria MLS'</b> <b>isseria MLS'</b> <b>isseria MLS'</b> <b>isseria MLS'</b> <b>isseria g</b> <b>aisseria MLS'</b> <b>isseria MLS'</b> <b></b>	m: Isolate field Intents   Home d in the ed id: 178 ed id: 178 PF, Saunders jonorrhoeae: a T scheme wass to be made, ir ation at a singl splayed). Click c 7 & Country USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso Cameroon Greece	Is   Sci   Optic	neme/alleles   Publication nns   Profiles/Sequences ( Sseeria Publication art CA, Feavers IM, Maider nary and epidemiologic y dapted to N. gonorrhoe g direct comparisons with s, gdh, provided a rapid m perlinks for detailed inform berlinks for detailed inform berlinks for detailed inform berlinks for detailed inform berlinks and septicaen invasive (unspecified/oth invasive(unspecified/oth invasive	definitions   Database subn     ST database     ST databa	us sequence hly discrimin amica. Exam sified isolates A A A A A A A A A A A A A A A A A A A	atory t inatior s and s and 4 1 5 1 1 1 4 5 4 1 1 4 4 4 4 1	MLST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-1 complex/subgroup IV ST-1 complex/subgroup III ST-1 complex/subgroup III ST-1 complex/subgroup IV ST-2 complex/subgroup IV ST-4 complex/subgroup IV	Finetyping antigens           PorA VR1         PorA VR2         Fef           5-2         10         F           7         13-1         F           5-1         9         F           7         13-1         F           5-2         10         F           7         13-1         F           7-2         13-1         F           7-2         13-1         F           7-2         13-1         F           5-2         10         F           5-2         10         F	A VR 1-5 5-1 3-6 5-1 1-5 3-1 1-5 3-1 1-5 1-5 1-7 1-5 1-5 1-5 5-1
Iblication           ation           nnetJS           secies st           e seven           pulation           is records	atio           quer           s, Jolley           tatus o           loci N: No           genetitics. An           s return           2           1027           1004           999           131           1325           100           1335           131           1335           131           1325           131           1325           131           1355           1355           136           137           138           1399           131           132           133           143           143           143           143           143           143           143           143           143           143           143           143           144           145           145	Breakdow Links: Co <b>ns cited</b> <b>y (PubM</b> <b>y (PubM</b> <b></b>	In: Isolate field Intents   Home and in the ed id: 178 ed id: 178	Is   Science   S	neme/alleles   Publication nns   Profiles/sequences ( Sseeria Publication ant   Profiles/sequences ( Sseeria Publication ant CA, Feavers IM, Maider onary and epidemiologica y adapted to N. gonorrhoe g direct comparisons with s, gdh, provided a rapid m perlinks for detailed inform i>> Lest solate fields [] disease invasive (unspecified/oth  invasive(unspecified/oth) invasive(unspecified	Initions   Database subn     ST database     Statement     Statem	us sequence hly discrimin amica Exam sified isolates A A A A A A A A A A A A A A A A A A A	atory t inatior s and 4 1 5 1 1 1 4 5 4 1 1 4 4 4 4 4 1 1	MLST clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-1 complex/subgroup IV ST-1 complex/subgroup III ST-1 complex/subgroup III ST-1 complex/subgroup III ST-4 complex/subgroup IV ST-4 complex/subgroup IV	Finetyping antigens           PorA VR1 PorA VR2 Fei           5-2         10         F           5-2         10         F           20         9         F           5-2         10         F           7         13-1         F           7         13-1         F           7         13-1         F           7-2         13-1         F           7-2         13-1         F           7-2         13-1         F           5-2         10         F           5-2         10         F           5-2         10         F           5-2         10         F	A VR 1-5 5-1 3-1 5-1 3-6 5-1 1-5 3-1 1-5 1-5 1-5 1-5 1-5 1-5 1-5 1-5

## 10.10 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.

	ofile/ST   List cheme/alleles   Publications titions   Profiles/sequences definitions   Database submis	ssions	
	SC for a collection of isolates that represent the total known late deposited here. Any isolate may be submitted to this		
Query database • Search database - advanced queries. • Browse database - peruse all records. • Search by combinations of loci (profiles • List query - find isolates by matching a	<ul> <li>Set display and s) - including partial matching.</li> </ul>	gs <mark>otions l</mark> including isolate table field handling d query options for locus, schemes or scheme field	General information • Isolates: 29173 • Last updated: 2014-07-14 • Update history • About BIGSdb
Two field     Cont	ort dataset • tigs • uences - XMFA / concatenated FASTA formats •		llaneous ription of database fields

### 10.10.1 General options

The general options tab is displayed by default. If another tab is being shown, click the 'General options' header.

Query: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions
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 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.

#### 10.10.2 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   Indeeddes per line in seddene alginiens. Display 100   nucleotides of flanking sequence (where available).
✓ Display locus aliases if set. ✓ Enable tooltips (beginner's mode).
Set options
→ Main results table
► Isolate record display
Provenance field display
Query filters
Reset
Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences.
Reset all to defaults

The '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
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
<ul> <li>Hyperlink allele designations where possible.</li> <li>Differentiate provisional allele designations.</li> <li>Display information about sequence bin records tagged with locus information (tooltip).</li> <li>Display sequence bin size.</li> <li>Set options</li> </ul>
▹ 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.

- 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.

#### 10.10.3 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.
<ul> <li>✓ General options</li> </ul>
Display 25 v records per page. Page bar position: top and bottom v Display 100 v nucleotides per line in sequence alignments. Display 100 v nucleotides of flanking sequence (where available). Ø Display locus aliases if set. Ø Enable tooltips (beginner's mode). Set options
► Main results table
► Isolate record display
Provenance field display
➤ Query filters
Reset
Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences.
Reset all to defaults

The 'Isolate record display' tab will scroll up.

Ouery:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/sequences definitions   Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
General options
► Main results table
✓ Isolate record display
<ul> <li>Differentiate provisional allele designations.</li> <li>Display sender, curator and last updated details for allele designations (tooltip).</li> <li>Display information about sequence bin records tagged with locus information (tooltip).</li> <li>Display information about whether alleles have flags defined in sequence definition database (shown in sequence detail tooltip).</li> <li>Display full information about sample records (tooltip).</li> <li>Set options</li> </ul>
Provenance field display
Query filters
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences. Reset all to defaults

This tab allows the following options to be modified:

- Differentiate provisional allele designations Allele designations can be set as confirmed or provisional, usually depending on the method of assignment. Selecting this option will display provisional designations in a different colour to confirmed designations.
- Display sender, curator and last updated records Displays a tooltip containing sender information next to each allele designation.
- Sequence bin information Displays a tooltip with information about the position of the sequence if tagged within the sequence bin.
- Allele flags Displays information about whether alleles have flags defined in sequence definition databases.
- Display full information about sample records Used when the database is used as part of a basic laboratory information management system (LIMS). This option will display records of samples available for the displayed isolate.

#### 10.10.4 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).
I objegio rocca anazza a sec. III cable toollips (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.

Links: Contents   Hor Set database options Here you can set options for your use of the	elds   Scheme/alleles   Publications ne   Options   Profiles/sequences definitions   C	essions and affect the current database (Neisseria	a PubMLST) only. If some of the options don't appear to set
General options     Main results table     Isolate record display			
	and then selecting the 'Customize' option.	table following a query. Settings for displaying loc amoxicillin sulphonamide cettriaxone cettriaxone_range chloramphenicol chloramphenicol cefotaxime cefotaxime cefotaxime_range fifampicin fifampicin_range 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	ettings for this database - this includes locus ar	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'.

#### 10.10.5 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
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).
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.

Isolate record display		
Provenance field display		
Query filters		
	n lists containing known values on which to filter query results. These w PNA_accession private_project comments sender curator date_entered datestamp MLST profile completion Finetyping antiges profile completion 165 profile completion ADP-heptose biosynthesis profile completion Antipodynamic Profile completion Antipodynamic Profile completion Antipodynamic Profile completion Antipodynamic Profile completion Capsule Region A - Serogroup A profile completion Capsule Region A - Serogroup B profile completion Capsule Region A - Serogroup B profile completion Capsule Region A - Serogroup L profile completion Capsule Region A - Serogroup Y profile completion Capsule Region A - Serogroup X profile completion Capsule Region C profile completion Capsule Region C profile completion Capsule Region D and D' profile completion Capsule Region C profile completion DNA replication profile completion DNA replication 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 inner core transferases profile completion         LOS transport/export profile completion         Lipid A biosynthesis: acyltransferases profile completion         Lipid A biosynthesis: acyltransferases profile completion         Nucleotide excision repair profile completion         Nucleotide excision repair profile completion         Prius genes profile completion         Protein glycosylation profile completion         Pyruwate dehydrogenase complex profile completion         Pyruwate dehydrogenase complex profile completion         RNA polymerase profile completion         Pyruwate dehydrogenase complex profile completion         RNA polymerase profile completion         Small regulatory RNAs profile completion         UDP-GlcNAc synthesis profile completion         UDP-glcoxes and UDP-galactose biosynthesis profile completion         UDP-GlcVAc synthesis profile completion         WIB T4SS profile completion         MLST (20 locus whole genes) profile completion         PMLST (20 locus whole genes) profile completion         PUBications

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'.

### 10.10.6 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.

Pub	MLST / Breakdown: Is	h   Browse   Profile/ST   List solate fields   Scheme/alleles   Publications nts   Home   Options   Profiles/sequences defi	initions   Database sub	missions		
The N	ase there is at least one corr	<b>T database</b> e contains data for a collection of isolates that responding isolate deposited here. Any isolat				
				ttings al options - including <u>isolate table field</u> y and query options fo <mark>r locus, scheme</mark>		General information • Isolates: 29174 • Last updated: 2014-07-14 • Update history • About BIGSdb
	Breakdown • Single field • Two field • Unique combinations • Scheme and alleles • Publications • Sequence bin	Export • Export dataset • Contigs • Sequences - XMFA / concatenated I	FASTA formats	Analysis • Codon usage • Presence/absence status of loci • Genome comparator • BLAST	Miscellaneous  Description of da	tabase fields

Either select the locus id by querying for it directly.

Ouery:         Search   Browse   Profile/ST   List           Breakdown:         Isolate fields   Scheme/alleles   Publications           Links:         Contents   Home   Options   Profiles/Sequences definitions   Database submissions	
T	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	
id • = • abcZ + 12 Order by: id • ascending •	
Display: 25    records per page []	
Filter query by Action	
Reset Submit	
1 record returned. Click the hyperlink for detailed information.	
Customize	
locus options	
id data type allele id format length length varies coding sequence orf genome position isolate display* main display* query field* analysis* abcZ DNA integer 433 false true 1 1176340 allele only false true true	
* Default values are displayed for this field. These may be overridden by user preference.	

Designations can be queried using standard operators.

Alternatively, you can search by filtering loci by schemes. Click the 'Filter query by' header and select the scheme in the dropdown box.

	<b>MLST</b>			lds   Scheme/ ie   Options   F			nitions   Databas	e submissions					
													Toggle: i
uer	y loci	for Neis	sseria	PubML	ST data	base	•						
Please	enter your	search criteria	below (or	leave blank a	nd submit to re	turn all r	ecords). Matchin	g loci will be returr	ned and you wi	ill then be ab	le to update	their display and query settings.	
Sea	rch criteria	a					— — Display—						
id				•		+	Order b	y: id	•	ascending			
							Displa	iy: 25 👻 record	ds per page 🚺	]			
—⊽ Fi	Iter query I	by -					Action						
		data type:	-				Reset Subr	nit					
	allele	id format:	•				- Oubr						
	leng	gth varies:	- <u>i</u>										
	coding s	sequence:	-										
		orf:	•										
	matc	h longest:	- -										
		pcr filter:	▼ i										
	р	robe filter:	▼ 1										
		flag table:	<b>-</b> i										
		te display:		•									
	mai	in display:	▼ 1										
	q	query field:	<b>-</b> i										
		analysis:	<b>v</b> <u>i</u>										
		curator:		-		_							
		scheme: M	LST		-	i							
records	s returned.	Click the hype	rlinks for o	letailed inform	ation.								
Curd	omize —												
locus	options												
id o	lata type	allele id forma	t length l	ength varies	coding sequen	ice orf g	genome position	isolate display*	main display*	query field*	analysis*		
abcZ	DNA	integer	433	false	true	1	1176340	allele only	false	true	true		
adk	DNA	integer	465	false	true	1	991951	allele only	false	true	true		
aroE fumC	DNA DNA	integer integer	490 465	false false	true true	2	2079469 1592943	allele only allele only	false false	true true	true		
gdh	DNA	integer	501	false	true	1	1514394	allele only	false	true	true		
pdhC	DNA	integer	480	false	true	1	1453970	allele only	false	true	true		
pgm	DNA	integer	450	false	true	1	965481	allele only	false	true	true		
		displayed for thi	C 11 Th										

Once loci have been selected, click Customize 'locus options'.

	tomize											
locus	options											
_				_		ce on g		i isolate display*				
abcZ	DNA	integer	433	false	true	1	1176340	allele only	false	true	true	
adk	DNA	integer	465	false	true	1	991951	allele only	false	true	true	
aroE	DNA	integer	490	false	true	2	2079469	allele only	false	true	true	
fumC	DNA	integer	465	false	true	1	1592943	allele only	false	true	true	
	DNA	integer	501	false	true	1	1514394	allele only	false	true	true	
gdh	DNA	integer	480	false	true	1	1453970	allele only	false	true	true	
gdh pdhC	DINA		450	false	true	1	965481	allele only	false	true	true	

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).

### Data analysis plugins

## 11.1 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.

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
	Toggie: /
Neis	sseria locus/sequence definitions database
	leisseria 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 d in the isolate database.
Q	Query database       Image: Downloads       Option settings       Image: Option settings         • Sequence query - query multiple sequences in FASTA format.       • Allele sequences       • Set general options       • Number of sequences: 342758         • Back h sequence attribute search infind alleles by matching attributes.       • MLST       • Download profiles       • Number of profiles: Show         • Beguence attribute search profiles       • MLST       • Download profiles       • Number of profiles: Show         • Beguence search profiles       • MLST       • Download profiles       • Number of profiles: Show         • Search profiles       • Search profiles       • MLST       • Download profiles         • List - Ind profiles matched to entered list.       • About BIGSdb       • About BIGSdb
	Search by combinations of alleles - including partial matching.     Batch profile query - lookup profiles copied from a spreadsheet.     Extract finetype from whole genome data
	Export Sequences - XMFA / concatenated FASTA formats Sequences smolt similarity - find sequences most similar to selected allele. Sequence comparison - display a companison between two sequences. Locus Explorer tool for analysing allele sequences stored for particular locus.

### 11.1.1 Polymorphic site analysis

Select the locus you would like to analyse in the Locus dropdown box. The page will reload.

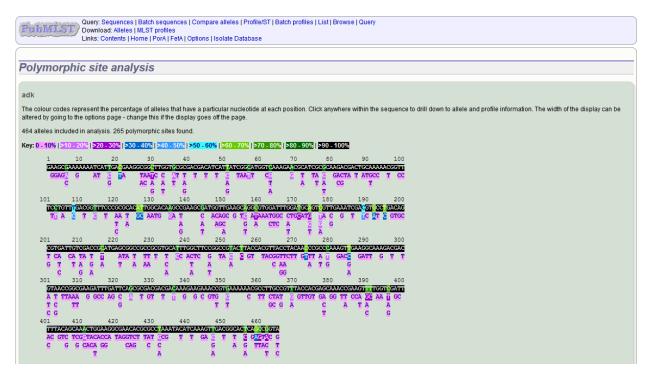
Query: Sequences   Batch sequences   Compare alleles   Profile/ST   Batch profiles   List   Browse   Query Download: Alleles   MLST profiles Links: Contents   Home   PorA   FetA   Options   Isolate Database
Locus Explorer - Neisseria locus/sequence definitions
Please select locus for analysis: Locus: adk • rege will reload when changed Select sequences - Analysis functions Polymorphic sites Display polymorphic site frequencies and sequence schematic Codon Calculate G+C content and codon usage Codon Calculate G+C content and codon usage Translate Translate DNA to peptide sequences All None

Select the alleles that you would like to include in the analysis. Variable length loci are limited to 200 sequences or fewer since these need to be aligned. Click 'Polymorphic sites'.

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     Polymorphic sites       451     Codon       462     Codon       463     Translate       All     None

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 -	- 50%	>50 -	60%	>60	- 70%	>70 - 80%	
	40		50		60		
GGT	r <mark>gcgcg</mark>	ACGA	CATO	CATTA	TCGG <mark>C</mark> A	TGGT <mark>C</mark> AAA	
С	AT T	Т	T 1	r 🖸	TAATT	CG	
A	ΤA			Α		Т	
Т	G			G		A	
Pul	DIALST / Do	wnload: Allel	es   MLST pro	ofiles		e/ST   Batch profiles   List   B	
	LIN	ks: Contents	Home   Por	A   FetA   Option	ns   Isolate Database	3	
Site	Explorer						
adk p	osition 51						
	leles included in a						
Base T	Number of alleles 370	Percentag 79		MLST profiles 10619 / 10883 (97.57%)			
С	92	19	83	262 / 10883 (2.41%)			
A	1 (adk-351)		22	1/10883 (0.01%)			
G	1 (adk-413)	0.:	22	1 / 10883 (0.01%)			

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

• 1		••			4					
C										
401		410		42			30	44		450
									TCAAAG	
C			ACA			GTCT T CAG	C C	• T	T GA	G
<u> </u>	9	90	T	66		CAG	A			A
			- 1							
lucleotid	le fre	que	ncie	es 🛛						
						Nucleoti	do			
osition 🗢		r ≜	c 🔺	T 🔺		%A ≑		KC A	%T \$ 9	
2	463	0	1	0	0	99.78	100	0.22		
3	462	0	2	0	0	99.57		0.43		
4	1	0	463	0	0	0.22		99.78		
5	0	463	1	0	0		99.78			
6	52	7	405	0	0	11.21	1.51	87.28		
9	463	0	1	0	0	99.78		0.22		
14	1	0	0	463	0	0.22			99.78	
15	0	452	0	12	0		97.41		2.59	
18	0	76	7	381	0		16.38	1.51	82.11	
21	0	295	0	169	0		63.58		36.42	
22	8	0	456	0	0	1.72		98.28		
27	3	451	0	10	0		97.20		2.16	
28	2	1	461	0	0		0.22			
29	1	0	463	0	0	0.22		99.78		
30	-	341	1	119	0	0.65	73.49			
31	0	10		454	0		2.16		97.84	
33	2	5	455		0		1.08			
36	51	0	410			10.99		88.36		
37	0	463	0	1	0		99.78		0.22	

See also:

- Investigating allele differences.
- Polymorphism analysis following isolate query.

### 11.1.2 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'.

PTISIALST 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									

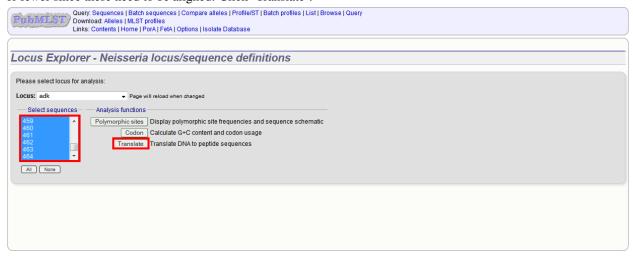
The GC content of the alleles will be determined and a table of the codon frequencies displayed.

Coden Usage           adk           DRF used: 1           444 alleles included in analysis.           GC content           Coding: C0 52 47%           Tistleffer: C0 53 173%           Zord of 25 37%           Zord of 25 30 412 216           GCC         A           OC 0 27 7 353 1248           GCC         A           OC 0 37 6 650           GCC         A           GCC         A           Code 3 0 581 2 484           TC C         0 013 0 083 6           GCC         A           GCA 4         0 246 17 535 1248           GCA 4         0 248 17 595 1450           GCA 4         0 248 17 595 1200     <	1. ISML	ST / Do	ery: Sequence wnload: Allele: ks: Contents	s   MLST profil	es
PR used: 1         464 alleles included in analysis.         5C content         Config: GC 52.47% ist letter: GC 63.17% ist letter: GC 63.17% ist letter: GC 63.17%         Content         Cont       A         Cot	don l	Jsage			
RF used: 1         64 alleles included in analysis.         Solid Colspan="2">Solid Colspa= 2: Colspan="2">Solid Colspan="2: Colspa="	ĸ				
44 alleles included in analysis.         5C content         Soding: GC 52.47%, Ist letter: GC 65.31%         Ist letter: GC 65.31%         Valid tetter: GC 80.37%         Codons         Traction: Proportion of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid). requency: Usage of given codon per 1000 codons.         Codons         Codon 4       0.262       17.353       1248         GCC       A       0.246       16.254       1169         GCG       A       0.245       16.254       1169         GCG       A       0.246       16.254       1169         GCG       A       0.245       16.254       1169         GCG       A       0.245       16.452       464         TGT       C       0.081       6.452       464         TGT       D       0.253       30.812       2216         GAA       E       0.916       82.297       592.6         GGG					
Coding: GC 52 47%         Ist letts: GC 66 31%         2nd letts: GC 60 31%         Stal letts: GC 60 37%         Codons         Fraction: Proportion of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         Frequency: Usage of given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         Frequency: Usage of given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         Frequency: Usage of given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         Frequency: Usage of given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         GCC       A       0.242       17.25         GCC       A       0.242       16.254       1169         GCC       C       0.987       6.452       464         TCT       D       0.253       30.812       2216         GAA       E       0.916 <td></td> <td></td> <td></td> <td></td> <td></td>					
Coding: GC 52.47%         Ist letter: GC 31.73%         Val letter: GC 60.37%         Codons         Fraction: Proportion of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         requency: Usage of given: codon per 1000 codons.         Codon 4       0.262       17.353       1248         GCC       A       0.262       17.353       1248         GCC       A       0.246       16.254       1169         GCG       A       0.246       16.254       1169         GCG       A       0.246       16.254       169         GCG       A       0.039       25.751       1852         GCT       A       0.103       6.813       490         TGC       C       0.937       6.850       6         GAA       E       0.916       82.397       5926         GAA       E       0.916       82.397       5926         GAA       G       0.070       0.542       39         GAA       G       0.070       0.542       39         GAA       G       0.001       0.042       3         GAA       G       0.001	alleles inc	cluded in a	nalysis.		
Coding: GC 52.47%         Ist letter: GC 31.73%         Val letter: GC 60.37%         Codons         Fraction: Proportion of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         requency: Usage of given: codon per 1000 codons.         Codon 4       0.262       17.353       1248         GCC       A       0.262       17.353       1248         GCC       A       0.246       16.254       1169         GCG       A       0.246       16.254       1169         GCG       A       0.246       16.254       169         GCG       A       0.039       25.751       1852         GCT       A       0.103       6.813       490         TGC       C       0.937       6.850       6         GAA       E       0.916       82.397       5926         GAA       E       0.916       82.397       5926         GAA       G       0.070       0.542       39         GAA       G       0.070       0.542       39         GAA       G       0.001       0.042       3         GAA       G       0.001	content				
isiteliar: GC 63:31%         colors         colors         iraction: Proportion of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         requency: Usage of given codon per 1000 codons.         codon 4       0.0262       17.33         codon 4       0.246       162.54       1169         GCC       A       0.246       162.54       1189         GCC       A       0.246       162.54       1189         GCC       A       0.246       162.54       1189         GCC       A       0.246       162.54       1169         GCC       A       0.246       162.54       1189         GCC       A       0.246       162.54       1189         GCC       A       0.389       25.751       1852         GCT       A       0.03       6.616       6         GAC       D       0.747       91.073       6550         GAT       D       0.253       30.812       2216         GAA       E       0.946       7.564       544         TTC       F       0.594       152.95       1100         TTT       F					
2nd letter: CC 3173%         Srd letter: CC 60.37%         Codons         Fraction of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         Fraction of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         Fraction of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         Fraction of its redundant set (i.e. the set of codons which code for this codon's amino acid).         Fraction of its redundant set (i.e. the set of codons which code for this codon's amino acid).         Fraction of its redundant set (i.e. the set of codons which code for this codon's amino acid).         Fraction of its redundant set (i.e. the set of codons which code for this codon's amino acid).         Fraction of its redundant set (i.e. the set of codons which code for this codon's amino acid).         Godon of its redundant set (i.e. the set of codons which code for this codon's amino acid).         Godon of its redundant set (i.e. the set of codons which code for this codon's amino acid).         Godon of its redundant set (i.e. the set of codons which code for this codon's amino acid).         Godon of its redundant set (i.e. the set of codons which code for this codon's amino acid).         Godon of its redundant set (i.e. the set of codons which code for this c					
Bit letter: GC 60.37%         Cocons         Fraction: Proportion of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         Frequency: Usage of given codon per 1000 codons.         Codon 4       Amino acid 7         GCA       A       0.262       17.733         GCA       A       0.262       17.733         GCC       A       0.103       6.813         GCC       C       0.987       6.452         GCA       D       0.747       91.073         GCA       D       0.747       91.073         GCA       E       0.084       7.564         GAA       E       0.016       15.295         GCA       G       0.007       0.542         GCA       G       0.007       0.542         GCA       G       0.001       0.042         GCA       G       0.001       0.042         GCA       G <t< td=""><td></td><td></td><td></td><td></td><td></td></t<>					
Fraction: Proportion of Usage of given: codon among its redundant set (i.e. the set of codons which code for this codon's amino acid).         Codon *       Amino acid *       Fraction *       Frequency *       Number *         GCA       A       0.262       17.353       1248         GCC       A       0.262       17.353       1248         GCC       A       0.262       17.353       1248         GCC       A       0.246       16.254       1189         GCG       A       0.389       25.751       1852         GCT       A       0.013       6.813       490         TGC       C       0.977       6.452       464         TGT       C       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         GGG       G       0.024       7.564       544         TT       F       0.406       10.470       753         GGA       G       0.001       0.042       3         GGG       G       0.025       59.497					
Amino acid       Fraction e       Frequency       Number e         GCA       A       0.262       17.353       1248         GCC       A       0.262       17.353       1248         GCC       A       0.262       17.353       1248         GCC       A       0.262       17.551       1852         GCT       A       0.103       6.813       490         TCC       C       0.907       6.452       464         TGT       C       0.013       0.083       6         GAA       E       0.916       82.397       5926         GAA       E       0.916       82.397       5926         GAA       E       0.944       7.564       544         TTC       F       0.406       10.470       753         GGA       G       0.007       0.542       39         GGC       G       0.075       59.497       4279         GGG       G       0.001       0.042       3         GGT       G       0.227       17.659       1270         GAC       H       0.749       19.258       135					
Frequency: Usage of given codon per 1000 codons.         Codon \$       Amino acid \$       Frequency \$       Number \$         GCA       A       0.262       17.353       1248         GCC       A       0.246       16.254       1119         GCC       A       0.389       25.751       1852         GCT       A       0.103       6.813       490         TGC       C       0.987       6.452       464         TGT       C       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       0.406       10.470       753         GGC       G       0.0765       59.497       4279         GGC       G       0.0765       59.497       1270         GAC       H       0.749       19.258       1385	ions				
Color       Amino acid       Fraction       Frequency       Number +         GCA       A       0.262       17.353       1248         GCC       A       0.246       16.254       1169         GCG       A       0.349       25.751       1852         GCT       A       0.103       6.813       490         TGC       C       0.987       6.452       464         TGT       C       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       0.944       544       544         TTC       F       0.406       10.470       753         GGA       G       0.007       0.542       39         GGC       G       0.755       59.497       4279         GGG       G       0.001       0.042       3         GGT       G       0.227       17.659       1270         GGC       G       0.271       17.659       1270         GGC					g its redunda
GCA       A       0.262       17.353       1248         GCC       A       0.246       16.254       1189         GCG       A       0.039       25.751       1852         GCT       A       0.103       6.813       490         TGC       C       0.907       6.452       464         TGT       C       0.013       0.083       6         GAC       D       0.747       91.073       6550         GAC       D       0.747       91.073       6550         GAC       D       0.747       91.073       6550         GAT       D       0.253       30.812       2216         GAA       E       0.916       82.397       5926         GAG       E       0.944       7.564       544         TTC       F       0.406       10.470       753         GGA       G       0.007       0.542       39         GGC       G       0.755       5.9497       4279         GGG       G       0.042       3       3         GGT       G       0.227       17.659       1270         GAC       H	quency: Us	sage of give	n codon per 1	000 codons.	
GCA       A       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       C       0.967       6.452       464         TGT       C       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       0.944       7.564       544         TTC       F       0.406       10.470       753         GGC       G       0.075       59.497       4279         GGC       G       0.0765       59.497       4279         GGC       G       0.075       59.497       1270         GAC       H       0.749       19.258       135	lon ≜ Am	nino acid ≜	Fraction A	requency 🔺	Number 🔺
GCC         A         0.246         16.254         1169           GCG         A         0.389         25.751         1852           GCT         A         0.013         6.813         490           TGC         C         0.987         6.452         464           TGT         C         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         592.6           GAG         E         0.916         82.397         592.6           GAG         E         0.916         82.397         592.6           GAG         G         0.007         0.542         39           GGC         G         0.075         59.497         42.79           GGC         G         0.001         0.042         3           GGT         G         0.227         17.659         1270           CAC         H         0.749         19.258         1385					
GCT       A       0.103       6.813       490         TGC       C       0.987       6.452       464         TGT       C       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       G       0.004       7.564       544         TTC       F       0.496       10.470       753         GGA       G       0.007       0.542       39         GGC       G       0.075       59.497       4279         GGG       G       0.001       0.042       3         GGT       G       0.227       17.659       1270         CAC       H       0.749       19.258       1385					
TGC         C         0.987         6.452         464           TGT         C         0.013         0.083         6           GAC         D         0.747         91.073         6650           GAT         D         0.253         30.812         2216           GAA         E         0.916         82.397         5926           GAG         E         0.084         7.564         544           TTC         F         0.406         10.470         753           GGA         G         0.007         0.542         39           GGC         G         0.007         0.542         39           GGC         G         0.001         0.042         3           GGT         G         0.227         17.659         1270           CAC         H         0.749         19.258         1385					
TCT       C       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       0.916       82.397       5926         GAG       E       0.944       15.295       1100         TTC       F       0.406       10.470       753         GGA       G       0.007       0.542       39         GGC       G       0.075       59.497       4279         GGG       G       0.001       0.042       3         GGT       G       0.227       17.659       1270         CAC       H       0.749       19.258       1385	3CT	Α	0.103	6.813	490
GAC         D         0.747         91.073         6550           GAT         D         0.253         30.812         2216           GAA         E         0.916         82.397         5926           TTC         F         0.406         10.470         753           GGA         G         0.007         0.542         39           GGC         G         0.075         59.497         4279           GGG         G         0.001         0.042         3           GGT         G         0.227         17.659         1270           CAC         H         0.749         19.288         1385	rGC	С	0.987	6.452	464
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           TTT         F         0.406         10.470         753           GGA         G         0.007         0.542         39           GGC         G         0.001         0.042         3           GGG         G         0.001         0.042         3           GGT         G         0.227         17.659         1270           CAC         H         0.749         13258         1385	IGT	С	0.013	0.083	6
GAA         E         0.916         82.397         5926           GAG         E         0.084         7.564         544           TTC         F         0.594         15.295         1100           TTT         F         0.406         10.470         753           GGA         G         0.007         0.542         39           GGC         G         0.755         59.497         4279           GGG         G         0.001         0.042         3           GGT         G         0.227         17.659         1270           CAC         H         0.749         139258         1385	GAC	D	0.747	91.073	6550
GAG         E         0.084         7.564         544           TTC         F         0.594         15.295         1100           TTT         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         H         0.749         19.258         1385	GAT	D	0.253	30.812	2216
GAG         E         0.084         7.564         544           TTC         F         0.594         15.295         1100           TTT         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         H         0.749         19.258         1385	GAA	E	0.916	82.397	5926
TTC         F         0.594         15.295         1100           TTT         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         H         0.749         19.258         1385					544
TTT         F         0.406         10.470         753           GGA         G         0.007         0.542         39           GGC         G         0.755         59.497         4279           GGG         G         0.001         0.042         3           GGG         G         0.001         0.042         3           GGT         G         0.227         17.659         1270           CAC         H         0.749         19.258         1385					
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         H         0.749         19.258         1385					
GGC         G         0.765         59.497         4279           GGG         G         0.001         0.042         3           GGT         G         0.227         17.659         1270           CAC         H         0.749         19258         1385	GA				39
GGG         G         0.001         0.042         3           GGT         G         0.227         17.659         1270           CAC         H         0.749         19258         1335					
GGT         G         0.227         17.659         1270           CAC         H         0.749         19.258         1385					
CAC H 0.749 19.258 1385					
CAT H 0.251 6.438 463		н	0.251	6.438	463
ATA I 0.001 0.083 6					

#### 11.1.3 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'.



An aligned amino acid sequence will be displayed.

433 I	
34 1	L
135 1	Т
436 1	
437 1	
438 1	
439 1	
440 1	ĸ
441 1	
442 1	
443 1	ь
444 1	
445 1	
446 1	
440_1	
448 1	
449 1	
450 1	
-	
451_1	КТ.
452_1 453 1	
	IA. T.
454_1	
455_1	
456_1	
457_1	
458_1	
459_1	
460_1	S
461_1	
462_1	
463_1	
464_1	I
Consensus	EAKKIIDEGGLVRDDIIIGMVKERIAQDDCKNGFLFDGFPRILAQAEAMVEAGVDLDAVVEIDVPDSVIVDRMSGRRVHLASGRTYHVTYNPPKVEGKDD
	110 120 130 140 150
	:
1_1	
2_1	
3_1	
4_1	
5_1	
6_1	
7_1	
8 1	

If there appear to be a lot of stop codons in the translation, it is possible that the orf value in the *locus definition* is not set correctly.

## 11.2 Field breakdown

The field breakdown plugin for isolate databases displays the frequency of each value for fields stored in the isolates table. *Allele and scheme field breakdowns* are handled by a different plugin.

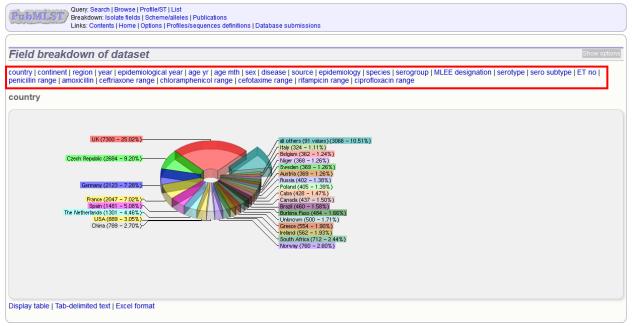
The breakdown function can be selected for the whole database by clicking the 'Single field' link in the Breakdown section of the main contents page.

Query: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/Sequences definitions   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 one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it doe										
Query database       Option settings         • Search database - advanced queries.       Search database - peruse all records.         • Search by combinations of loci (profiles) - including partial matching.       • Set display and query options for locus, schere         • List query - find isolates by matching a field to an entered list.       • Set display and query options for locus, schere										
Breakdown       Export       Analysis         Single field       • Export dataset       • Configs         • Invo field       • Configs       • Sequences - XMFA / concatenated FASTA formats       • Codon usage         • Scheme and alleles       • Sequence bin       • Sequence bin       • BLAST	Miscellaneous     Description of database fields									

Alternatively, a breakdown can be displayed of the dataset returned from a query by clicking the 'Fields' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the

								-							
5 M002	240227		UK	2000	invasive (	unspecified/other)	Neisser	ia meningiti	dis	в	1100	ST-32 complex/ET-5 complex	7	16	
6 M002	282207		UK	2000	invasive (	unspecified/other)	Neisser	ia meningiti	dis	W	1101	ST-22 complex			
7 7	891	B54; Z1054	Finland	1975	invasive (	unspecified/other)	Neisser	ia meningiti	dis	Α	5	ST-5 complex/subgroup III	20	9	F3-1
8 M002	242007		UK	2000	invasive (	unspecified/other)	Neisser	ia meningiti	dis	в	1102	ST-18 complex		14	
9 002	21/84		Czech Republic	1984	invasive (	unspecified/other)	Neisser	ia meningiti	dis	W	114	ST-22 complex			
10 6	748	B73; Z1073	Canada	1971	invasive (	unspecified/other)	Neisser	ia meningiti	dis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11 1	129	B92; Z1092	Germany	1964	invasive (	unspecified/other)	Neisser	ia meningiti	dis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12 009	90/89		Czech Republic	1989	invasive (	unspecified/other)	Neisser	ia meningiti	dis	В	1015	ST-32 complex/ET-5 complex	7	16	
13 1	39M	B99; Z1099	Philippines	1968			Neisser	ia meningiti	dis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14 012	20/95		Czech Republic	1995	invasive (	unspecified/other)	Neisser	ia meningiti	dis	Х	117			14	
15	1		Germany	1999		carrier	Neisser	ia meningiti	dis	E	864				
16	2		Germany	1999		carrier	Neisser	ia meningiti	dis	В	854	ST-18 complex			
17	3		Germany	1999		carrier	Neisser	ia meningiti	dis	W	174	ST-174 complex			
18	4		Germany	1999		carrier	Neisser	ia meningiti	dis	в	19	ST-18 complex			
19 S3	3131	B213; Z1213	Ghana	1973	invasive (	unspecified/other)	Neisser	ia meningiti	dis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999		carrier	Neisser	ia meningiti	dis 1	NG	198	ST-198 complex			
21	6		Germany	1999		carrier	Neisser	ia meningiti	dis 1	NG	198	ST-198 complex			
22	7		Germany	1999		carrier	Neisser	ia meningiti	dis	E	60	ST-60 complex			
23	8		Germany	1999		carrier	Neisser	ia meningiti	dis	в	32	ST-32 complex/ET-5 complex			
24 S4	4355	B227; Z1227	Denmark	1974	invasive (	unspecified/other)	Neisser	ia meningiti	dis	A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999		carrier	Neisser	ia meningiti	dis	в	930	ST-334 complex			
1	s tools wn: Fie sis: Bu	Ids Two Fi		<u> </u>	norphic sites • Comparate		Schem	es/alleles	Publicati	ons	Sequer	noe bin Tag status			

A series of charts will be displayed. Pick the field to display from the list at the top.



The values used to generate the chart can be displayed or extracted by clicking the 'Display table' link at the bottom of the page.

ProDMLST Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions
Field breakdown of dataset Show options
country   continent   region   year   epidemiological year   age yr   age mth   sex   disease   source   epidemiology   species   serogroup   MLEE designation   serotype   sero subtype   ET no   penicillin range   amoxicillin   ceftriaxone range   chloramphenicol range   cefotaxime range   rifampicin range   ciprofloxacin range
country
UK (7300 - 25,02%)       all others (91 values) (3066 - 10.51%)         Italy (324 - 1.11%)       Beglum (362 - 1.24%)         Negr (368 - 1.26%)       Negr (368 - 1.26%)         France (2047 - 7.02%)       France (2047 - 7.02%)         The Netherstand (1301 - 4.44%)       Cranal (430 - 1.56%)         USA (888 - 3.05%)       USA (888 - 3.05%)         China (789 - 2.70%)       France (2047 - 7.02%)         The Netherstand (1301 - 4.44%)       France (2047 - 7.02%)         The Netherstand (1301 - 4.44%)       France (2047 - 1.17%)         Distail (480 - 1.56%)       France (2047 - 7.02%)         The Netherstand (1301 - 4.44%)       France (2047 - 7.02%)         The Netherstand (1301 - 4.44%)       France (2047 - 7.02%)         Norway (760 - 1.37%)       France (2047 - 7.02%)         Norway (760 - 2.00%)       France (2047 - 7.02%)
Display table Tab-delimited text   Excel format

### This displays a table that can be ordered by clicking the appropriate header.

<b>bMLST</b> / Brea	kdown: Isolate	rse   Profile/ST   List ields   Scheme/alleles   Publications me   Options   Profiles/sequences definitions   Database submissions	
eakdown by	countr		Show o
earuowii by	country		
5 values.			
country 🔶	Frequency 🗢	ercentage 🖕	
UK	7300	25.02%	
Czech Republic	2684	9.20%	
Germany	2123	7.2%	
France	2047	7.02%	
Spain	1481	5.08%	
The Netherlands	1301	4.46%	
USA	889	3.05%	
China	789	2.70%	
Norway	760	2.60%	
South Africa	712	2.44%	
Ireland	562	1,93%	
Greece	554	1.90%	
Unknown	500	1.71%	
Burkina Faso	484	1.66%	
Brazil	460	1.58%	
Canada	437	1.50%	
Cuba	428	1.47%	
Poland	405	1.39%	
Russia	402	1.38%	
Austria	369	1.26%	
Sweden	369	1.26%	
Niger	368	1.26%	
Belgium	362	1.24%	
Italy	324	1.11%	
Finland	312	1.07%	
Denmark	307	1.05%	
Japan	238	0.82%	

The data can also be downloaded in tab-delimited text or Excel formats by clicking the appropriate links.

PublicST Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions
Field breakdown of dataset Show options
country   continent   region   year   epidemiological year   age yr   age mth   sex   disease   source   epidemiology   species   serogroup   MLEE designation   serotype   sero subtype   ET no   penicillin range   amoxicillin   ceftriaxone range   chloramphenicol range   cefotaxime range   rifampicin range   ciprofloxacin range
country
UK (7300 - 25.02%)         I czech Republic (2684 - 9.20%)         Germany (2123 - 7.28%)         Prance (2047 - 7.02%)         Spin (1681 - 5.05%)         U kthrima Ravo (488 - 1.38%)         Dispin (1681 - 5.05%)         U kthrima Ravo (484 - 1.95%)         Dispin (1691 - 5.05%)         Dirk (759 - 2.70%)
Display table Tab-delimited text   Excel format

# 11.3 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.

PubMLST Bre	ary: Search   Browse   Profile/ST   List akdown: Isolate fields   Scheme/alleles   Publicat ks: Contents   Home   Options   Profiles/sequence		
		as that rannasant tha total known diversity of Neisseria s	pecies. For every allelic profile in the profiles/sequence definition database there is at least
Query databa Search datab Browse datab Search by cor	te deposited here. Any isolate may be submitted	to this database and consequently it should be noted th Option settings Set general options - including isolate Set display and query options for locu	at it does not represent a population sample.  General information  table field handling  isolates: 29177
Single field - Single field - Two field - Scheme and - Publications - Sequence bir	alleles	Analysis - Codon usage - Presence/absence stat - Genome comparator - BLAST	Miscellaneous  • Description of database fields tus of loci

Alternatively, a two field breakdown can be displayed of the dataset returned from a query by clicking the 'Two field' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitio	dıs W	1101	SI-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         M00242007         UK         2000         invasive (unspecified/other)         Neisseria meningitidis         B         1102         ST-18 complex         14													
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria meningitio	dis B	1102	ST-18 complex		14		
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitio	dis W	114	ST-22 complex				
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitio	dis A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1	
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitio	dis A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6	
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitio	dis B	1015	ST-32 complex/ET-5 complex	7	16		
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitio	dis A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1	
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitio	dis X	117			14		
15	1		Germany	1999	carrier	Neisseria meningitio	dis E	864					
16	2		Germany	1999	carrier	Neisseria meningitio	dis B	854	ST-18 complex				
17	3		Germany	1999	carrier	Neisseria meningitio	dis W	174	ST-174 complex				
18	4		Germany	1999	carrier	Neisseria meningitio	dis B	19	ST-18 complex				
19		B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitio		4	ST-4 complex/subgroup IV	7	13-1	F1-5	
20			Germany	1999	carrier	Neisseria meningitio		198	ST-198 complex				
21	6		Germany	1999	carrier	Neisseria meningitio		198	ST-198 complex				
22	7		Germany	1999	carrier	Neisseria meningitio	dis E	60	ST-60 complex				
23			Germany	1999	carrier	Neisseria meningitio	dis B		ST-32 complex/ET-5 complex				
24		B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitio	dis A	5	ST-5 complex/subgroup III	5-1	9	F3-1	
25	9		Germany	1999	carrier	Neisseria meningitio	dis B	930	ST-334 complex				

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/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profile/Sequences definitions   Database submissions												
Two field breakdown of dataset		Show options										
Here you can create a table breaking down one field by another, e.g. breakdown of a Select fields	Calculate percentages by Action     Other 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 less than 30.

Selected options: Display values only.         Selected options: Display values only.         Ares       Show         Reverse       Values and percentages         Selected options: Display values only.         Selected option: 13         Selected option: 13         Selected colspan="2">Selected option: 13         Selected complex       1 <th colspa<="" th=""><th></th><th></th><th></th><th></th><th>is   Pro</th><th>ofiles/s</th><th>equences</th><th>s definitio</th><th>ns   Database submissions</th></th>	<th></th> <th></th> <th></th> <th></th> <th>is   Pro</th> <th>ofiles/s</th> <th>equences</th> <th>s definitio</th> <th>ns   Database submissions</th>					is   Pro	ofiles/s	equences	s definitio	ns   Database submissions
searcogroup:         searcogroup:         Ares       Show         Reverse       Values and percentages         searcogroup         searcogroup         searcogroup         searcogroup         searcogroup         searcogroup         searcogroup         searcogroup         structure         structure       searcogroup         structure       searcogroup         structure       structure       structure         structure       structure       structure         structure       structure       structure         structure       structure         structure       structure         structure       structure         structure       structure         structure       structure         structure       structure         structure       stru										
Heted options: Display values only. Axes Show Reverse Values and percentages tonal_complex (MLST) $4$ $A = B + C + E + NG + V + X + Y + Z + Total + No value 1 3 1 1 4 1 1 12 ST-1 complex/Subgroup III 1 1 1 1 2 ST-1 complex/Subgroup III 1 1 1 2 3 ST-177 complex 5 0 5 5 7 ST-167 complex 5 0 5 5 ST-167 complex 1 1 1 1 3 ST-174 complex 2 1 1 1 1 3 ST-174 complex 2 2 2 2 ST-226 complex 1 1 1 1 1 1 ST-226 complex 1 1 1 1 1 1 ST-246 complex 2 1 1 1 1 ST-35 complex 2 1 1 1 1 ST-35 complex 1 1 1 1 1 ST-44 complex Subgroup IV 9$	vo field breakdo	vn of	f da	atas	set				Shov	
Aves Show Reverse Values and percentages Stonal_complex (MLST)										
elected options: Display values only. Aves Show Reverse Values and percentages tonal_complex (MLST) $\diamond$ A $\diamond$ B $\diamond$ C $\diamond$ E $\diamond$ NG $\diamond$ W $\diamond$ X $\diamond$ Y $\diamond$ Z $\diamond$ Total $\diamond$ No value 1 3 1 1 4 1 1 12 ST-1 complex/subgroup  N 1 3 6 6 6 5 ST-1 complex/subgroup  N 1 6 6 6 5 ST-167 complex 1 6 16 ST-162 complex 5 5 6 6 5 ST-174 complex 1 1 1 1 1 3 ST-174 complex 3 6 7 ST-260 complex 2 1 1 1 1 1 ST-226 complex 3 6 1 1 1 ST-226 complex 1 1 1 1 ST-260 complex 2 1 1 1 ST-260 complex 1 1 1 ST-260 complex 2 1 1 ST-260 complex 1 1 1 ST-260 complex 1 1 1 ST-260 complex 1 1 1 ST-35 complex Number N 6 7 ST-36 complex 1 1 1 ST-35 complex Number N 6 7 ST-36 complex 1 1 1 ST-35 complex Number N 9 7 ST-36 complex 1 1 1 ST-36 complex 1 1 1 ST-36 complex 1 1 1 ST-36 complex 1										
Aves       Show         Reverse       Values and percentages         clonal_complex (MLST)       A + B + C + E + NG + W + X + Y + Z + Total +         No value       1       1       1         ST-100 pelex/subgroup (MLST)       A + B + C + E + NG + W + X + Y + Z + Total +       13         To nonjex/subgroup (MLST)       A + B + C + E + NG + W + X + Y + Z + Total +         No value       1       3       1       1       1       13         Efformation (MLST)       A + B + C + E + NG + W + X + Y + Z + Total +       13       13       14       1       11       13         ST-100 pelex/subgroup (MLST)       16       15       16       16       16       16         ST-174 complex       1       1       2       3       4       1       1       1       3       3       3       3 <td>reakdown of clonal_cor</td> <td>plex (N</td> <td>MLST</td> <td>í) by :</td> <td>sero</td> <td>group</td> <td>p:</td> <td></td> <td></td>	reakdown of clonal_cor	plex (N	MLST	í) by :	sero	group	p:			
Aves         Show           Reverse         Values and percentages           clonal_complex (MLST)         A + B + C + F + NG + W + X + Y + Z + Total +           No value         1         1         1           ST-1 complex/subgroup (MLST)         A + B + C + F + NG + W + X + Y + Z + Total +         1           ST-1 complex/subgroup (MLST)         A + B + C + F + NG + W + X + Y + Z + Total +         1           ST-1 complex/subgroup (MLST)         A + B + C + F + NG + W + X + Y + Z + Total +         1           ST-1 complex/subgroup (MLST)         A + B + C + F + NG + W + X + Y + Z + Total +         1           ST-1 complex/subgroup (MLST)         B + C + F + NG + W + X + Y + Z + Total +         1           ST-1 complex/subgroup (MLST)         B + C + F + NG + W + X + Y + Z + Total +         1           ST-162 complex         1         1         1         3           ST-174 complex         1         1         3         3           ST-198 complex         2         2         2         2           ST-226 complex         1         1         1         1           ST-240 complex F1-5 complex         1         1         1         3           ST-426 complex         1         1         1         1           ST-280 comp	elected options: Display value	only								
Values and percentages           Serogroup           clonal_complex (MLST) ◆ A ◆ B ◆ C ◆ F ◆ NG ◆ NV ◆ X ◆ Y ◆ Z ◆ Total ◆           No value         1<										
Serogroup           clonal_complex (MLST)         A         B         C         E         NG         Y	Axes — Show —									
Starting         A + B + C + E + NG + W + X + Y + Z + Total + No value         No value         1         3         1         4         1	Reverse Values and	percentag	iges							
clonal_complex (MLST)         A         B         C         E         VM d         X         Y         Z         F Total           No value         1         3         1         4         1         1         12           ST-1 complex/Stubgroup (ML         13         1         4         1         1         12           ST-1 complex/Stubgroup (ML         16         6         5         16         5           ST-167 complex         1         1         2         3           ST-174 complex         1         1         1         1           ST-18 complex         2         2         2           ST-226 complex         2         2         2           ST-226 complex         1         1         1           ST-269 complex         1         1         1           ST-260 complex         1         1         1           ST-32 complex/ST-55 complex         1         1         1           ST-40 complex/Subgroup (M <td> r</td> <td></td> <td></td> <td></td> <td>_</td> <td></td> <td></td> <td></td> <td></td>	r				_					
No value         1         3         1         1         4         1<	cional complex (MLST) 🔺	<b>▲ B ▲  </b>		F 🔺 🛙				Z ≜ Tot		
ST-1 complex/Subgroup I/I     13     16     13       T-11 complex/ET-37 complex     16     16     16       ST-162 complex     5     1     2     3       ST-174 complex     1     1     2     3       ST-174 complex     1     1     2     3       ST-174 complex     2     1     1     1       ST-176 complex     3     4     3       ST-176 complex     3     4     3       ST-176 complex     2     2     3       ST-18 complex     3     4     4     3       ST-18 complex     2     2     2       ST-22 complex     2     2     2       ST-22 complex     1     1     1       ST-226 complex     1     1     1       ST-268 complex     2     1     1       ST-268 complex     2     1     1       ST-34 complex/ET-55 complex     1     1       ST-426 complex     1     1										
T-11 complex/ET-37 complex     16     1     16       ST-162 complex     5     1     2     3       ST-176 complex     1     1     1     3       ST-176 complex     1     1     1     1       ST-176 complex     1     1     1     1       ST-176 complex     3     1     1     1       ST-176 complex     3     1     1     1       ST-18 complex     3     2     2     3       ST-198 complex     2     2     2       ST-226 complex     1     1     1       ST-268 complex     1     1     1       ST-269 complex     2     1     1       ST-269 complex     1     1     1       ST-269 complex     1     1     1       ST-269 complex     1     1       ST-269 complex     2     1       ST-269 complex     1     1       ST-260 complex									13	
ST-167 complex       1       1       2       3         ST-174 complex       1       1       1       3         ST-176 complex       1       1       1       1       3         ST-176 complex       3       1       1       1       1       3         ST-176 complex       3       2       1       1       3         ST-18 complex       3       2       2       2         ST-22 complex       2       2       2       2         ST-22 complex       1       1       1       1         ST-22 complex       1       1       1       1         ST-22 complex       1       1       1       1       1         ST-254 complex       1       1       1       1       1       1         ST-324 complex       1       5       6       5			16						16	
ST-174 complex       1       1       1       1       3         ST-176 complex       1       1       1       1       1         ST-180 complex       3       2       3         ST-190 complex       2       2       2         ST-22 complex       2       2       2         ST-22 complex       1       1       1         ST-22 complex       2       2       2         ST-22 complex       1       1       1         ST-256 complex       1       1       1         ST-256 complex       1       1       3         T-32 complexUFLF-5 complex       6       6         ST-334 complex       1       1       1         ST-45 complex       1       1       1         ST-35 complex       1       1       1         ST-46 complex/subgroup IV       9       9       9	ST-162 complex	5							5	
ST-178 complex       1       1       1         ST-18 complex       3       4       3         ST-196 complex       2       2       2         ST-196 complex       2       2       2         ST-20 complex       1       2       2         ST-226 complex       1       1       1         ST-254 complex       1       1       1         ST-269 complex       1       1       3         ST-260 complex       2       1       3         ST-260 complex       1       1       1         ST-269 complex       2       1       3         ST-324 complex       6       6       6         ST-334 complex       1       1       1         ST-35 complex       1       1       1         ST-44 complex/subgroup IV       9       9       9	ST-167 complex						2			
ST-18 complex     3     3     3     3       ST-198 complex     2     2     2       ST-22 complex     2     2     2       ST-226 complex     1     1     1       ST-226 complex/Cluster A3     1     1     1       ST-246 complex     1     1     1       ST-246 complex     1     1     1       ST-250 complex/F5-complex     2     1     1       ST-324 complex     1     1     1       ST-35 complex/Subgroup IV     9     9     9				1	1	1				
ST-198 complex     2     2       ST-22 complex     2     2       ST-22 complex     1     1       ST-22 complex/Cluster A3     1     1       ST-254 complex     1     1       ST-256 complex     1     1       ST-256 complex     2     1       ST-256 complex     6     6       ST-324 complex     1     1       ST-334 complex     1     1       ST-35 complex/subgroup IV     9     9					1					
ST-22 complex     2     2       ST-226 complex     1     1       ST-226 complex/Cluster A3     1     1       ST-25 complex/Cluster A3     1     1       ST-26 complex/ST-26 complex     1     1       ST-26 complex/ST-56 complex     1     3       ST-32 complex/ST-56 complex     1     1       ST-35 complex     1     1       ST-46 complex/Subgroup IV     9     9		3								
ST-226 complex       1       1         ST-23 complex/Cluster A3       1       1         ST-254 complex       1       1         ST-256 complex       2       1       3         ST-266 complex       2       1       3         ST-260 complex/ET-5 complex       6       6         ST-334 complex/ET-5 complex       6       6         ST-355 complex       1       1         ST-44 complex/subgroup IV       9       9					2					
ST-23 complex/Cluster A3       1       1       1         ST-254 complex       1       1       1         ST-256 complex       2       1       3         ST-360 complex       6       6         ST-34 complex/ST-5 complex       6       6         ST-35 complex       1       1         ST-35 complex/Strapper/						2				
ST-254 complex     1     1       ST-269 complex     2     1     3       T32 complexETF-5 complex     6     6       ST-334 complex     1     1       ST-35 complex subgroup IV     9     9		1								
ST-269 complex     2     1     3       ST-32 complexET-5 complex     6     6       ST-334 complex     1     1       ST-35 complex     1     1       ST-42 complex/subgroup IV     9     9							1			
3T-32 complex/ET-5 complex         6         6           ST-334 complex         1         1           ST-55 complex         1         1           ST-42 complex/bufgroup IV         9         9										
ST-334 complex         1         1           ST-35 complex         1         1           ST-4 complex/subgroup IV         9         9					1					
ST-35 complex         1         1           ST-4 complex/subgroup IV         9         9										
ST-4 complex/subgroup IV 9 9 9					1					
		9								
51-41/44 complex/Lineage 3 5 1 1 6	T-41/44 complex/Lineage 3	- 5			1				6	
ST-461 complex 1 1									1	
ST-5 complex/subgroup III 6 6									6	
ST-53 complex 2 2 2					2					
ST-60 complex 1 1										
Total 29 27 17 3 15 3 1 99		9 27	17	3	15	3	1 3	1	99	
	ownload as tab-delimited text.									

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.

# 11.4 Scheme and allele breakdown

The scheme and allele breakdown plugin displays the frequency of each allele and scheme field (e.g. ST or clonal complex).

The function can be selected for the whole database by clicking the 'Scheme and allele breakdown' link on the main contents page.

Publ		vse   Profile/ST   List fields   Scheme/alleles   Publications me   Options   Profiles/sequences def	initions   Database sub	missions		
The Ne						offies/sequence definition database there is at least
0,	Query database • Search database - advanced q Browse database - peruse all • Search by combinations of loci • List query - find isolates by ma	records. i (profiles) - including partial matching.		tings I options - including isolate table field rand query options for locus, scheme		General information • Isolates: 29177 • Last updated: 2014-07-16 • Update history • About BIGSdb
	Breakdown • Single field • Two field • Unique combinations • Scheme and alleles • Publications • Sequence bin	Export • Export dataset • Contigs • Sequences - XMFA / concatenated	FASTA formats	Analysis • Codon usage • Presence/absence status of loci • Genome comparator • BLAST	Miscellaneous     Oescription of da	tabase fields

Alternatively, a breakdown can be displayed of the dataset returned from a query by clicking the 'Schemes/alleles' 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.

r -	0		I I											
1 A4/	M1027	B1; Z1001	USA	1937	invasive (	unspecified/other)	Neisseria	meningiti	idis A	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2 1	120M	B35; Z1035	Pakistan	1967	meningitis	s and septicaemia	Neisseria	meningiti	idis A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
3 M00	242905		UK	2000	invasive (	unspecified/other)	Neisseria	meningiti	idis B	1099		19	15	
4 M	1027	B43; Z1043	USA	1937	invasive (	unspecified/other)	Neisseria	meningiti	idis A	4	ST-4 complex/subgroup IV			
5 M00	240227		UK	2000	invasive (	unspecified/other)	Neisseria	meningiti	idis B	1100	ST-32 complex/ET-5 complex	7	16	
6 M00	282207		UK	2000	invasive (	unspecified/other)	Neisseria	meningiti	idis W	1101	ST-22 complex			
7 7	7891	B54; Z1054	Finland	1975	invasive (	unspecified/other)	Neisseria	meningiti	idis A	5	ST-5 complex/subgroup III	20	9	F3-1
8 M00	242007		UK	2000	invasive (	unspecified/other)	Neisseria	meningiti	idis B	1102	ST-18 complex		14	
9 00	21/84		Czech Republic	1984	invasive (	unspecified/other)	Neisseria	meningiti	idis W	114	ST-22 complex			
10 6	5748	B73; Z1073	Canada	1971	invasive (	unspecified/other)	Neisseria	meningiti	idis A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (	unspecified/other)	Neisseria	meningiti	idis A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12 00	90/89		Czech Republic	1989	invasive (	unspecified/other)	Neisseria	meningiti	idis B	1015	ST-32 complex/ET-5 complex	7	16	
13 1	139M	B99; Z1099	Philippines	1968			Neisseria	meningiti	idis A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14 01	20/95		Czech Republic	1995	invasive (	unspecified/other)	Neisseria	meningiti	idis X	117			14	
15	1		Germany	1999		carrier	Neisseria	meningiti	idis E	864				
16	2		Germany	1999		carrier	Neisseria	meningiti	idis B	854	ST-18 complex			
17	3		Germany	1999		carrier	Neisseria	meningiti	idis W	174	ST-174 complex			
18	4		Germany	1999		carrier	Neisseria	meningiti	idis B	19	ST-18 complex			
19 S	3131	B213; Z1213	Ghana	1973	invasive (	unspecified/other)	Neisseria	meningiti	idis A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999		carrier	Neisseria	meningiti	idis NG	198	ST-198 complex			
21	6		Germany	1999		carrier	Neisseria	meningiti	idis NG	198	ST-198 complex			
22	7		Germany	1999		carrier	Neisseria	meningiti	idis E	60	ST-60 complex			
23	8		Germany	1999		carrier	Neisseria	meningiti	idis B	32	ST-32 complex/ET-5 complex			
24 S	4355	B227; Z1227	Denmark	1974	invasive (	unspecified/other)	Neisseria	meningiti	idis A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999		carrier	Neisseria	meningiti	idis B	930	ST-334 complex			
Breakdo Analy	sis: BU	elds Two Fie	noe/Absence		morphic sites e Comparato		Schemes	/alleles	Publications	Seque	nce bin Tag status			

A scheme tree is shown. Select any combination of schemes to analyse.

Query: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
Scheme field and allele breakdown of dataset	Show options
Select schemes or groups of schemes within the tree. A breakdown of the individual fields and loci belonging to these schemes will then be performed.	

### Click 'Select'.

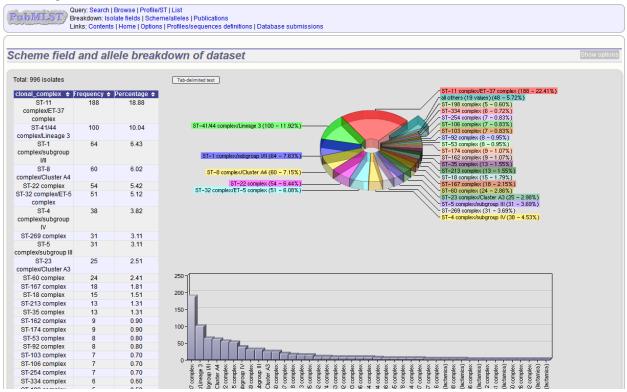
A table showing the number of unique values for each locus and scheme field will be displayed.

PubMLS	Breakdown		s   Sche	me/alleles   Pub		ions   Databa	abase submissions	
Scheme fi	eld and	allele b	reak	down of	datase	t	Show	v options
🛓 🔟 💭 All loci	psule netic Informatio tabolism n			e. A breakdown o	of the individu	al fields and	nd loci belonging to these schemes will then be performed.	
	Fields Unique values			Unique alleles		Download		
ST clonal complex	554 43	Breakdown Breakdown	abcZ adk aroE	64 57 80	Breakdown Breakdown Breakdown	Download Download Download		
			fumC gdh pdhC	85 79 83	Breakdown Breakdown Breakdown	Download Download Download		
			pgm	68	Breakdown	Download		

A detailed display of allele or field frequencies can be displayed by clicking the appropriate 'Breakdown' button.

chomo fi	ield and a	allala br	oakde	own of	datasat		Show option
Jileille II	ieiu aliu a	allele Di	eanuu	JWII OI	ualasel		Choir opa
		to a second second to be at			and the standard strength	distain an eite	
elect schemes	or groups of sci	nemes within t	ie tree. A t	breakdown o	t the individual	fields and lo	ci belonging to these schemes will then be performed.
🛓 🔛 🔝 All loci	i			*			
- 📃 順 Ca				=			
	enetic Information	n Processing					
- 🔚 🌆 Me							
👘 🤚 🌆 Pili	in						
🔺 👿 🛄 Typ	ping			+			
	ping			•			
	ping			•			
	ping			-			
Select	ping			•			
Select	bing The ot			Ŧ			
Select	ping Fields				leles		
Select ILST Field name	ping Lucot Fields Unique values			ique alleles	Analyse [	Download	
Select ALST Field name ST	Fields Unique values 554	Breakdown	abcZ	ique alleles 64 (	Analyse [ Breakdown	Download	
Select ILST Field name ST	Fields Unique values 554	Breakdown Breakdown	abcZ adk	ique alleles 64 ( 57 (	Analyse E Breakdown Breakdown	Download Download	
Select ALST Field name ST	Fields Unique values 554	Breakdown Breakdown	abcZ adk aroE	ique alleles 64 ( 57 ( 80 (	Analyse [ Breakdown ] Breakdown ] Breakdown ]	Download Download Download	
Select ALST Field name ST	Fields Unique values 554	Breakdown Breakdown	abcZ adk aroE umC	ique alleles 64 ( 57 ( 80 ( 85 (	Analyse [ Breakdown ] Breakdown ] Breakdown ] Breakdown ]	Download Download Download Download	
Select ALST Field name	Fields Unique values 554	Breakdown Breakdown	abcZ adk aroE	ique alleles 64 ( 57 ( 80 (	Analyse [ Breakdown ] Breakdown ] Breakdown ] Breakdown ] Breakdown ]	Download Download Download	

The sorting of the table can be changed by clicking the appropriate header - this toggles between ascending and descending order.



The table values can be exported in a format suitable for copying in to a spreadsheet by clicking the 'Tab-delimited text' button.

Fotal: 996 isolates			Tab-delimited text	
clonal_complex + Fi	requency 🗢	Percentage 🔶		ST-11 complex/ET-37 complex (188 - 22.4)
ST-11 complex/ET-37 complex	188	18.88		rail others (19 values) (48 - 5.72%)           ST-198 complex (5 - 0.60%)           ST-34 complex (6 - 0.72%)           ST-254 complex (7 - 0.83%)
ST-41/44 complex/Lineage 3	100	10.04	ST-41/44 complex/Lineage 3 (100 - 11.92%)	ST-106 complex (7 - 0.83%) ST-103 complex (7 - 0.83%) ST-92 complex (8 - 0.95%)
ST-1 complex/subgroup I/II	64	6.43	ST-1 complex/subgroup I/II (64 - 7.63%)	ST-53 complex (8 - 0.95%) ST-174 complex (9 - 1.07%) ST-162 complex (13 - 1.55%)
ST-8 complex/Cluster A4	60	6.02	ST-8 complex/Cluster A4 (60 - 7.15%)	ST-213 complex (13 - 1.55%) ST-18 complex (15 - 1.79%)
ST-22 complex	54	5.42	ST-22 complex (54 - 6.44%)	ST-167 complex (18 - 2.15%)
ST-32 complex/ET-5 complex	51	5.12	ST-32 complex/ET-5 complex (51 - 6.08%)	ST-60 complex (24 - 2,86%) ST-23 complex/Cluster A3 (25 - 2,98%) ST-5 complex/cluster A3 (25 - 2,98%)
ST-4 complex/subgroup	38	3.82		ST-269 complex (31 - 3.69%) ST-4 complex/subgroup IV (38 - 4.53%)

You can also download the sequences for alleles designated in the dataset for the loci belonging to the scheme by clicking the appropriate 'Download' button in the first results table.

		n: Isolate field ntents   Home				ions   Datab	ase submissions
cheme fie	eld and	allele b	reak	down o	f datase	t	Show option
oneme m		untere is	- curr	uomno	, addoo	•	
Select schemes o	r groups of s	chemes withir	n the tree	. A breakdow	n of the individu	al fields and	l loci belonging to these schemes will then be performed.
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clonal complex			aroE	80	Breakdown	Download	
cional complex			fumC	85	Breakdown	Download	
clonal complex			gdh	79	Breakdown	Download	
cional complex			pdhC	83	Breakdown	Download	
cional complex			pgm	68	Breakdown	Download	

#### Sequences will be served in FASTA format in order of frequency.

>2

>1

>4

## 11.5 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.

Pub		vse   Profile/ST   List fields   Scheme/alleles   Publications me   Options   Profiles/sequences defir	nitions   Databas	e submissions			
Neis	seria PubMLST da	tabase					
		ins data for a collection of isolates that re. Any isolate may be submitted to this					ofiles/sequence definition database there is at least ample.
Q	Query database Search database - advanced q Browse database - peruse all Search by combinations of loci List query - find isolates by ma	records. i (profiles) - including partial matching.	Set g	n settings eneral options - including iso isplay and query options for i		fields.	General information Isolates: 29177 Last updated: 2014-07-16 Update history About BIGSdb
	Breakdown • Single field • Two field • Unique combinations • Scheme and alleles • Publications • Sequence bin	Export • Export dataset • Contigs • Sequences - XMFA / concatenated F	ASTA formats	Analysis • Codon usage • Presence/absence • Genome comparate • BLAST	• D status of loci	cellaneous escription of da	tabase fields

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.

4 5 M	100242905	B35; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	S A	1	SI-1 complex/subgroup I/II	5-2	10	F5-1
			UK	2000	invasive (unspecified/other)	Neisseria meningitidis	s B	1099		19	15	
	M1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	s A	4	ST-4 complex/subgroup IV			
6 M	100240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	s B	1100	ST-32 complex/ET-5 complex	7	16	
	100282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	s W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	s A	5	ST-5 complex/subgroup III	20	9	F3-1
8 M	100242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	s B	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	s W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	s A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	в А	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	s B	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	s A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	s X	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	s E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	s B	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	s W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	s B	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	s A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	s NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	s NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	s E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	s B	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	в А	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	s B	930	ST-334 complex			

Select the isolate records to analyse - these will be pre-selected if you accessed the plugin following a query. Click submit.

	Profile/ST   List ds   Scheme/alleles   Publications   Options   Profiles/sequences definitions   Database submissions	
Breakdown of sequence	bin contig properties	
Please select the required isolate ids for con Isolates 67) 55611 82) 11-004 82) 11-229 90) CN100 120) F4598 128) F6124 160) 1014 All None Pestellat	nparison - use Ctri or Shift to make multiple selections. — Filter by Sequence method: Project: Experiment: ¥ []	Action Reset Submit

If there are fewer than 100 isolates selected, the table will be generated immediately. Otherwise it will be submitted to the job queue.

A table of sequence bin stats will be generated.

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Breakd	own of	seque	ence bin	n cont	ig pro	perti	es									
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Please sele	ect the require	d isolate id	is for comparis	son - use C	trl or Shift	to make	multiple	e selectio	ns.							
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1) A4/M10				Bequence r	nethod:		<b>-</b> [	-								
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10) 6748 11) 129				Expe	sinnent.	<b>▼</b> [	1									
13) 139M																
19) S313 24) S4355	1															
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Isolate id 🗢			Total length 🖨			Mean 🗢		N50 🗢	N90 \$			ated 🗢 🎋 Loc		Sequence bin 🗢	l i i i i i i i i i i i i i i i i i i i	
1	A4/M1027	364	2069108	100	50093	5685	8182	15404	3907	2305	82.9		87.4	Display ->		
2	120M	359	2059411	265	33563	5737	6303	10581	3126	1863	83.4		87.5	Display		
7	7891	199	2057385	267	112831	10339			6218	3616	86.4		88.4	Display 🛶		
10	6748	652	4241338	100	175414		13847		6190	3227	86.0		88.0	Display 🛶		
11	129	272	2072690	250	79861	7621	9439	14589	4150	2758	84.8		88.0	Display		
13	139M	293	2141711	113	149689			26154	6394	4214	85.4		87.8	Display		
19	S3131	173	2061338	250	96136			24737	8348	3961	85.5		87.8	Display		
24	S4355	198	2071992	250	89288			22947	6226	3728	85.5		87.4	Display ->		
30	14	1	2145295		2145295				2145295		84.6		84.6	Display ->		
31	10	275	2059146	262	53317	7488		14091	3975	2480	84.7		87.6	Display ->		
34	20	213	2067373	252	54815			19311	5317	3235	85.6		87.8	Display		
35	26	194	2056454	251	74067	10601	13102	24734	5428	3319	85.6		87.7	Display		
46	255	194	2052090	265	74202	10578	12873	20445	7237	3801	85.0		87.5	Display -		
52	243	229	2057666	252	77632	8986	10969	17283	5032	2902	85.3		87.7	Display →		
61	393	282	2064767	255	47836	7322	7919	14444	4057	2487	84.0		87.5	Display		
64	254	251	2054183	257	69510	8184	9379	15763	4488	2543	83.7		87.7	Display		
67	95611	104	2004212	255	102457	10744	14516	22222	6156	2521	95.2		077	Disalary		

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.

	A4/M1027	364	2069108	100	50093	5685	8182	15404	3907	2305	82.9	87.4	Display ->
2	120M	359	2059411	265	33563	5737	6303	10581	3126	1863	83.4	87.5	Display -
7	7891	199	2057385	267	112831	10339	13596	23361	6218	3616	86.4	88.4	Display -
10	6748	652	4241338	100	175414	6506	13847	26424	6190	3227	86.0	88.0	Display -
11	129	272	2072690	250	79861	7621	9439	14589	4150	2758	84.8	88.0	Display -
13	139M	293	2141711	113	149689	7310	15303	26154	6394	4214	85.4	87.8	Display ->
19	S3131	173	2061338	250	96136	11916	15196	24737	8348	3961	85.5	87.8	Display -
24	S4355	198	2071992	250	89288	10465	13482	22947	6226	3728	85.5	87.4	Display -
30	14	1	2145295	2145295	5 2145295	2145295	i :	2145295	2145295	2145295	84.6	84.6	Display -
31	10	275	2059146	262	53317	7488	8917	14091	3975	2480	84.7	87.6	Display -
34	20	213	2067373	252	54815	9706	10784	19311	5317	3235	85.6	87.8	Display ->
35	26	194	2056454	251	74067	10601	13102	24734	5428	3319	85.6	87.7	Display -
46	255	194	2052090	265	74202	10578	12873	20445	7237	3801	85.0	87.5	Display →
52	243	229	2057666	252	77632	8986	10969	17283	5032	2902	85.3	87.7	Display -
61	393	282	2064767	255	47836	7322	7919	14444	4057	2487	84.0	87.5	Display ->
64	254	251	2054183	257	69510	8184	9379	15763	4488	2543	83.7	87.7	Display ->
67	S5611	194	2084213	255	103457	10744	14516	22332	6156	3531	85.3	87.7	Display ->
82	11-004	258	2055227	251	47478	7966	8518	13854	4751	2921	84.9	87.8	Display
84	IAL2229	188	2051679	256	96122	10914	13975	21515	6282	3629	85.8	88.3	Display -
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Sequence bin records can also be accessed by clicking the 'Display' button for each row of the table.

7       7891       199       2057385       267       112831       10339       13596       23361       6218       3616       86.4       88.4       Desity-         10       6748       652       4241338       100       175414       6506       1347       24424       6190       3227       86.0       88.0       Desity-         13       139M       293       2141711       113       149689       7310       15303       26154       6394       4214       85.5       87.8       Desity-         19       S3131       173       2061338       250       96136       11916       1416       2145295       2145295       2145295       2145295       2145295       85.5       87.4       Desity-         30       14       1       2145295       2145295       2145295       2145295       84.6       84.6       84.6       Desity-         31       10       275       2059146       262       5317       7488       8917       1015       537       2450       84.7       87.6       Desity-         34       20       213       206737.3       252       54815       97.6       10781       1937       233 <t< th=""><th>1</th><th>A4/M1027</th><th>364</th><th>2069108</th><th>100</th><th>50093</th><th>5685</th><th>8182</th><th>15404</th><th>3907</th><th>2305</th><th>82.9</th><th>87.4</th><th>Display</th></t<>	1	A4/M1027	364	2069108	100	50093	5685	8182	15404	3907	2305	82.9	87.4	Display
10       6748       652       4241338       100       175414       6506       13847       28424       6190       3227       86.0       88.0       Display         11       129       272       2072890       250       79861       7621       9439       14509       4150       2778       84.4       87.8       Display         19       33131       173       2061338       250       96136       11016       15196       24737       8348       3961       85.5       87.8       Display         24       S4355       198       2071992       250       89288       10465       13482       22947       6226       3728       85.5       87.4       Display       931       10       275       2059146       262       53317       7488       8917       14091       3975       2480       84.7       87.6       Display       935       246       944       2056454       251       74067       10601       13102       24734       5428       3319       85.6       87.7       Display       935       266       194       2056454       251       74067       10601       13102       24734       5428       3319       85.6       87.	2	120M	359	2059411	265	33563	5737	6303	10581	3126	1863	83.4	87.5	Display 🛶
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13       139M       293       2141711       113       149689       7310       15303       26154       6394       4214       85.4       87.8       Digay	10	6748	652	4241338	100	175414	6506	13847	26424	6190	3227	86.0	88.0	Display
19       S3131       173       2061338       250       96136       11916       15196       2477       8348       3961       85.5       87.8       Display         24       \$84355       198       2071992       250       89288       10455       13482       22947       6226       3728       85.5       87.4       Display       208139         24       24       2145295       2145295       2145295       2145295       2145295       84.6       84.6       84.6       Display       208139       2061373       255       54815       9706       10744       1931       3217       2480       84.7       87.6       Display       208139       2064767       2145295       2145295       2145295       84.6       87.8       Display       20817       206706       205770       214707       100113102       21474       5428       319       85.6       87.7       Display       20819       2064767       255       77632       8986       10969       7223       73801       85.0       87.7       Display       208109       265       255       10347       184.4       4057       248.0       83.7       87.7       Display       208104       205427       251 <td>11</td> <td>129</td> <td>272</td> <td>2072690</td> <td>250</td> <td>79861</td> <td>7621</td> <td>9439</td> <td>14589</td> <td>4150</td> <td>2758</td> <td>84.8</td> <td>88.0</td> <td>Display 🛶</td>	11	129	272	2072690	250	79861	7621	9439	14589	4150	2758	84.8	88.0	Display 🛶
24       \$4355       198       2071992       250       89288       10455       13482       2297       6226       3728       85.5       87.4       Depty         30       14       1       2145295       214529       21657       216733       216733<	13	139M	293	2141711	113	149689	7310	15303	26154	6394	4214	85.4	87.8	Display 🛶
30       14       1       2145295       214529       214529       2165       6351       6350       637.5       Display       Display       2056767       255       47305       102323       21515       2531<	19	S3131	173	2061338	250	96136	11916	15196	24737	8348	3961	85.5	87.8	Display -
31       10       275       2059146       262       53317       7488       8917       14091       3975       2480       84.7       87.6       Display         34       20       213       2067373       252       54815       9706       10784       19311       5317       3235       86.6       87.8       Display       -         35       26       194       2056454       251       74067       10601       13102       2474       5428       3319       85.6       87.7       Display       -         46       255       194       2057666       252       77632       8986       10969       17283       5032       2902       85.3       87.7       Display       -         61       393       282       2064767       255       193457       10744       444       4057       248.0       83.7       87.7       Display       -         64       254       251       2054183       257       69510       8184       9379       15763       4488       2543       83.7       87.7       Display       -       Display       2       84.0       87.7       Display       2       84.0       87.7	24	S4355	198	2071992	250	89288	10465	13482	22947	6226	3728	85.5	87.4	Display -
34       20       213       2067373       252       54815       9706       10784       19311       5317       3235       85.6       87.8       Dagay         35       26       194       2066454       251       74067       10601       13102       247.34       5428       3319       85.6       87.7       Dagay       Daga	30	14	1	2145295	2145295	2145295	2145298	5	2145295	2145295	2145295	84.6	84.6	Display ->
35       26       194       2056454       251       74067       10601       13102       24734       5428       3319       85.6       87.7       10507         46       255       194       2052090       265       74202       10578       12873       20445       723       3801       85.0       87.7       Display         61       393       282       2067666       252       7762       8986       10969       1723       5032       2902       85.3       87.7       Display       -         64       254       251       204767       255       47836       7322       7919       14444       4057       2467       84.0       87.5       Display       -         64       254       251       204767       255       103457       10744       14516       2232       616       5531       85.3       87.7       Display       -         82       11-004       258       2055227       251       47478       7966       8518       13854       4751       2921       84.9       87.8       Display       -         90       CN100       236       2118544       261       73069       8977	31	10	275	2059146	262	53317	7488	8917	14091	3975	2480	84.7	87.6	Display -
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52       243       229       2057666       252       77632       8986       10969       17283       5032       2902       85.3       87.7       Display_         61       393       282       2064767       255       47836       7322       7919       14444       4057       2487       84.0       87.5       Display_         64       254       251       205418       257       6950       814       9379       1573       4488       2543       83.7       87.7       Display_         67       S5611       194       2064/13       255       103457       10744       14516       2232       6156       3531       85.3       87.7       Display_         82       11-004       258       2055227       251       47478       7966       8518       13854       4751       2921       84.9       87.8       Display_       0       0       CN100       236       2118544       261       73069       8977       11101       19065       4570       2839       84.5       87.2       Display_       0       0       0       0       0       0       0       0       0       0       0       0       0	35	26	194	2056454	251	74067	10601	13102	24734	5428	3319	85.6	87.7	Display
61       393       282       2064767       255       47836       7322       7919       1444       4057       2487       84.0       87.5       Dagtay         64       254       251       2054183       257       69510       8184       9379       15763       4488       2543       83.7       87.7       Digety       Digety       657       56611       194       2064213       255       103457       10744       14516       2232       6156       5531       85.3       87.7       Digety       -         82       11-004       258       2055227       251       47478       7966       8518       13854       4751       2921       84.9       87.8       Digety       -         84       IAL2229       188       2051679       256       96122       10914       13975       21515       6282       3629       88.8       88.3       Digety       -       -       Digety       -       Digety       -       -       Digety       -       -       Digety       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -       -	46	255	194	2052090	265	74202	10578	12873	20445	7237	3801	85.0	87.5	Display ->
64       254       251       2054183       257       69510       8184       9379       15763       4488       2543       83.7       87.7       Display         67       S5611       194       2004213       255       103457       10744       14516       22332       6156       3531       86.3       87.7       Display       Display       205227       251       47478       7966       8561       1354       4751       2221       84.9       87.8       Display       2       84.9       87.2       Display       2       0       0.0       0.0       0.0       100.0       23.6       21185.44       261       73069       8977       11101       19065       4570       2839       84.5       87.2       Display       0       Display       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0 <td>52</td> <td>243</td> <td>229</td> <td>2057666</td> <td>252</td> <td>77632</td> <td>8986</td> <td>10969</td> <td>17283</td> <td>5032</td> <td>2902</td> <td>85.3</td> <td>87.7</td> <td>Display 🛶</td>	52	243	229	2057666	252	77632	8986	10969	17283	5032	2902	85.3	87.7	Display 🛶
67       S5611       194       2084213       255       103457       10744       14516       2232       6156       5531       85.3       87.7       Display_         82       11-004       258       2055227       251       47478       7966       8518       13854       4751       2921       84.9       87.8       Display_         90       CN100       236       2118544       261       73069       8977       11101       19055       4570       2839       84.5       87.2       Display_         90       CN100       236       2118544       261       73069       8977       11101       19065       4570       2839       84.5       87.2       Display_         • Download in tab-delimited text format       • Download in Excel format       • Download in Excel format       • Display_       •	61	393	282	2064767	255	47836	7322	7919	14444	4057	2487	84.0	87.5	Display 🛶
82       11-004       258       2055227       251       47478       7966       8518       13854       4751       2921       84.9       87.8       Depay         84       JLL2229       188       2051679       256       96122       10914       13975       21515       6282       3629       85.8       88.3       Depay	64	254	251	2054183	257	69510	8184	9379	15763	4488	2543	83.7	87.7	Display 🛶
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<ul> <li>Download in tab-delimited text format</li> <li>Download in Excel format</li> <li>Download in Excel format</li> <li>Total length</li> <li>Mean contig length</li> <li>Contig lengths</li> <li>Overall mean: 2182080.5; or 485517.0</li> <li>Overall mean: 115617.0; or 477740.1</li> <li>Overall mean: 2182080.5; or 485517.0</li> <li>Overall mean: 115617.0; or 477740.1</li> <li>Overall mean: 2684.9; or 32339.5</li> <li>Impact of the following control of the following co</li></ul>	84	IAL2229	188	2051679	256	96122	10914	13975	21515	6282	3629	85.8	88.3	Display 🛶
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	on the	following char			jth		1	Vlean d	contig le	ength		Contig lengths		
	all mea	n: 251.3; σ: 12	1.2	Overall mea	n: 218208	0.5; σ: 485	517.0	Overall m	nean: 115	617.0; σ:	477740.1	Overall mean: 8684.9; o	r: 32339.5	
					the the sector	ati ati sticati	-		222.000.000					

## 11.6 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   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 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 of the second seco	
Query database       Query database         • Search database - advanced queries.       Search database - peruse all records.         • Browse database - peruse all records.       • Set general options - including isolate table field handling         • List query - find isolates by matching a field to an entered list.       • Set display and query options for locus, schemes or scheme fields.	i General Information • Isolates: 29177 • Last updated: 2014-07-15 • Update history • About BIGSdb
Single field       Export       Miscellanee         • Single field       • Export dataset       • Configs         • Unique combinations       • Sequences - XMFA / concatenated FASTA formats       • Codon usage       • Description         • Presence/absence status of loci       • Genome comparator       • BLAST	Dus 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.

I								
19025 M10 240481	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	1831		22	9	F3-3
19026 M10 240482	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	3754	ST-41/44 complex/Lineage 3	7-2	4	F5-1
19027 M10 240484	UK	2010 invasive (unspecified/other) Neisseria meningitidis	В	1097	ST-41/44 complex/Lineage 3	17-1	23	F1-5
19028 M10 240485	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	275	ST-269 complex	22	9	F5-12
19029 M10 240487	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	1049	ST-269 complex	19-1	15-11	F5-1
19030 M10 240489	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	461	ST-461 complex	19-2	13-1	F3-9
19031 M10 240490	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	1161	ST-269 complex	22	9	F5-12
19032 M10 240498	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	41	ST-41/44 complex/Lineage 3	7-2	4	F1-5
19958 M10 240476	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	9812	ST-213 complex	22	14	F5-5
19959 M10 240499	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	275	ST-269 complex	22	9	F5-12
19960 M10 240500	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	41	ST-41/44 complex/Lineage 3	7-2	4	F1-5
19961 M10 240502	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	340	ST-41/44 complex/Lineage 3	7-2	4	F1-5
19962 M10 240503	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	23	ST-23 complex/Cluster A3	5-1	2-2	F1-96
19963 M10 240505	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	1655	ST-23 complex/Cluster A3	5-1	10-10	F4-1
19964 M10 240507	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	183	ST-23 complex/Cluster A3	21	16-5	deleted
19965 M10 240508	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	1575		7-2	13-1	F1-7
19966 M10 240511	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	4713		22	9	F5-12
19967 M10 240512	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	41	ST-41/44 complex/Lineage 3	7-1	1	F1-5
19968 M10 240514	UK	2010 invasive (unspecified/other) Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex	5	2	F1-1
19969 M10 240515	UK	2010 invasive (unspecified/other) Neisseria meningitidis	в	269	ST-269 complex	5-1	2-2	F5-1
19970 M10 240520	UK	2010 invasive (unspecified/other) Neisseria meningitidis	Y	1655	ST-23 complex/Cluster A3	5-1	10-1	F4-1
nalysis tools: Breakdown: Fields Two Analysis: Presence/Absen Export: Dataset Cor	œ Ge	Codons Polymorphic sites Combinations Schemes'alleles nome Comparator BLAST Bequences	) Publi	ications	Sequence bin			

## 11.6.1 Analysis using defined loci

Select the isolate genomes that you wish to analyse and then either the loci from the list or a set of schemes. Press submit.

	Profile/ST   List   Scheme/alleles   Publications Options   Profiles/sequences definition	ons   Database submissions		
				Toggle: i
Genome Comparator - Ne	isseria PubMLST			Show options
appropriate scheme description. Alternatively,	you can enter the accession number	nake multiple selections. In addition to selecting indivi- for an annotated reference genome and compare us		defined in schemes by selecting the
Isolates 658) 890326 659) A22 660) 71/94 661) 860800 6672 2837 663) 2839 664) 2838 065) 2845 All None Pastelist	Lod 165_rCNA 165_rCNA 235_rCNA abcZ abcZ (NEIS1015) ackA2 (NEIS1279) ackA2 (NEIS1727) acrA (NEIS1727) acrA (NEIS1729) All None Paste list	country region year epidemiological year age yr age mth sex dicease	E ST etyping antigens	
Reference genome Enter accession number: I or choose annotated genome: or upload Genbank/EMBL/FASTA file: Browse_ No file selected.	Parameters / options Min % identity: 70 • [ Min % alignment: 50 • [ BLASTN word size: 15 • [ Use TBLASTX[] V Use tagged designations if avai Disable HTML output []	Distance matrix calculation With truncated loci: © Completely exclude from analysis Treat as distinct allele © Ignore in pairwise comparison Exclude paralogous alleles	Alignments Produce alignments Produce alignments Align all loci (not only variable) Aligner: MAFFT	Core genome analysis Core threshold (%): 90 • [ Calculate mean distances [
Filter by Sequence method: • ? Project: Experiment: • ?	→ Adti Res			

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.

Public Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
	Toggle: i
Genome Comparator - Neisseria PubMLST	Show options
This analysis has been submitted to the job queue. Please be aware that this job may take a long time depending on the number of comparisons and how busy the server is.	
Follow the progress of this job and view the output	

There will be a series of tables displaying variable loci, colour-coded to indicate allelic differences. Finally, there will be links to a distance matrix which can be loaded in to SplitsTree for further analysis and to a NeighborNet chart showing relatedness of isolates. Due to processing constraints on the web server, this NeighborNet is only calculated if 200 or fewer genomes are selected for analysis, but this can be generated in the stand-alone version of SplitsTree using the distance matrix if required.

PubMLST) Breakdown: Isola	Browse   Profile/ST   List ate fields   Scheme/alleles   P Home   Options   Profiles/se	ublications quences definitions   Database s	submissions			
ob status viewer						
Status						
Job id: BIGSdb_27748_14054	10063 94241					
Submit time: 2014-07-15 08:41:03 Status: finished						
Start time: 2014-07-15 08:41:05						
Progress: 100% Stop time: 2014-07-15 08:41:22 Total time: 47						
Total time: 17 seconds Dutput						
nalysis against defined loci						
llele numbers are used where these	have been defined, otherwis	e sequences will be marked as	'New#1, 'New#2' etc. Mi	ssing alleles are marked	as 'X'. Truncated alleles (located	at end of contig) are marked as "
.ocus 644 (L93/4286) 662 (2837) 6	63 (2839) 664 (2838) 665 (	845) 666 (2843) 667 (2842) 66	69 (2846) 670 (2840) 6	71 (2844) 672 (2847) 6	98 (FAM18)	
abcZ 2 2 2 adk 3 3	2 2 2 3 3 3	2 2 2 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	7         2           3         3	2 2 3 3	2 3	
aroE 4 19 fumC 3 3					4 3	
gdh 8 8 pdhC 4 4	8 8 8 4 4 4		8 8 4 4	8 8 4 4	8 4	
pgm 6 6	6 6 6		6 6	6 6	6	
oci with sequence differences a	imong isolates:					
ariable loci: 4				74 (00 4 0) 000 000 000		
.ocus 644 (L93/4286) 662 (2837) 6 abcZ 2 2	2 2 2	2 2	7 2	2 2	2	
aroE 4 19 iumC 3 3	4 4 4 3 3 2	4 23 23	4 19 3 3	19 19 3 3	4 3	
odhC 4 4	4 4 4	6 6	4 4	4 4	4	
xactly matching loci						
hese loci are identical in all isolates. latches: 3						
Locus  644 (L93/4286)   662 (2837)  6	63 (2839) 664 (2838) 665 (	2845) 666 (2843) 667 (2842) 66	69 (2846) 670 (2840) 6	71 (2844) 672 (2847) 6	98 (FAM18)	
adk 3 3 gdh 8 8	3 3 3 8 8 8	3 3	3 3 8 8	3 3 8 8	3	
pgm 6 6	6 6 6		6 6	6 6	6	
nique strains						
nique strains: 5						
Strain 1         Strain 2         Strain 3           44 (L93/4286)         662 (2837)         666 (2843)           63 (2839)         670 (2840)         667 (2842)           64 (2838)         671 (2844)           98 (FAM18)         672 (2847)	3) 665 (2845) 669 (2846)					
Text output file						
<ul> <li>Excel format</li> <li>Distance matrix (Nexus format)</li> </ul>		plitsTree. Distances between tax	a are calculated as the	number of loci with differ	ent allele sequences	
<ul> <li>Splits graph (Neighbour-net, P</li> </ul>	NG format)					
	-					
<ul> <li>Splits graph (Neighbour-net; S)</li> </ul>		ed in Inkscape or other vector gra	aphics editors			
<ul> <li>Locus presence frequency</li> <li>Locus presence frequency cha</li> </ul>	art (PNG format)					
Tar file containing output files	(click to enlarge)					
ease note that job results will remain	on the server for 7 days.					

## 11.6.2 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.

	a for comparison - use ctrl or shift to make multi you can enter the accession number for an and Include in identifiers			defined in schemes by selecting the
Reference genome         Enter accession number.         I         or choose annotated genome:         FAM18 (Nm)         or upload Genbank/EMBL/FASTA file:         BrowseNo file selected.	Parameters / options Min % identity: 70 • 1 Min % alignment 50 • 1 BLASTN word size: 15 • 1 Use TBLASTX [] Use tagged designations if available [] Disable HTML output []	Distance matrix calculation With truncated loci: © Completely exclude from analysis Treat as distinct allele C Ignore in pairwise comparison Exclude paralogous alleles	Alignments Produce alignments Cludde ref sequences in alignment Align all loci (not only variable) Aligner: MAFFT	Core genome analysis Core threshold (%): 90
Filter by Sequence method: Project Experiment	Action Reset Su	ibmit		

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.

PrINTIST Query Search   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/Sequences definitions   Database submissions																
Job statı	us viewer															
Status																
Submit time: Status: Start time: Progress: Stop time: Total time: Output Analysis by r accession	Job id:         BIGSdb_21911_1405410488_8452           Submit time:         2014-07-15 08.48:08           Status:         finished           Start time:         2014-07-15 08.48:34           Progress:         100%           Stop time:         2014-07-15 09.12:58           Total time:         24 minutes and 24 seconds           Output         Analysis by reference genome															
version type length description coding region																
All loci	llele is defined a number starting at 1. Missing alleles are marked as ">	" Truncotod		ated at end o	f contig) oro	marked	00 T									
Each unique a	inere is defined a number starting at 1. Missing alletes are marked as A	Sequence			644	662	663	664	665	666	667	669	670	671	672	698
Locus	Product	length	position	genome	(L93/4286)			(2838)				(2846)				(FAM18)
IpxC   envA   NMC0001	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924	1261	1												1
pilS1   NMC0002	pilin (fragment)	291	3341	1	1	1	1	1	1	1	1	1	1	1	1	1
pilS2   NMC0003	truncated pilin	366	3675	1	2	2	2	2	2	2	2	2	2	2	2	1
fbp   NMC0004	peptidyl-prolyl cis-trans isomerase	330	4069	1	2		2		2		2	Т	2			1
NMC0005	putative membrane protein	219	4476	1	2	3	3	3	3		3	4	3	5		1
NMC0006	putative glycerate dehydrogenase	954	4816	1	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

## 11.6.3 Include in identifiers fieldset

This selection box allows you to choose which isolate provenance fields will be included in the results table and sequence exports.

— 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.

## 11.6.4 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.

## 11.6.5 Parameters/options fieldset

This section allows you to modify BLAST parameters. This affects sensitivity and speed.

-Parameters / options							
Min % identity:	70 🔻 👔						
Min % alignment:	50 👻 🚺						
BLASTN word size:	15 👻 👔						
Use TBLASTX i							
🗹 Use tagged desigr	nations if available 👔						
Disable HTML output 👔							

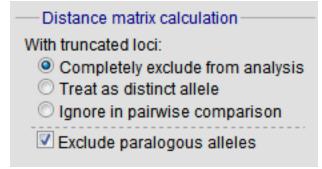
- Min % identity This sets the threshold identity that a matching sequence has to be in order to be considered (default: 70%). Only the best match is used.
- Min % alignment This sets the percentage of the length of reference allele sequence that the alignment has to cover in order to be considered (default: 50%).
- BLASTN word size This is the length of the initial identical match that BLAST requires before extending a match (default: 15). Increasing this value improves speed at the expense of sensitivity. The default value gives good results in most cases, but increasing this to 20 is almost as good (there was 1 difference among 2000 loci in a test run) and will speed up the analysis approximately two-fold.
- Use TBLASTX This compares the six-frame translation of your nucleotide query sequence against the sixframe translation of the contig sequences. Sequences will be classed as identical if they result in the same translated sequence even if the nucleotide sequence is different. This is significantly slower than using BLASTN.

Additionally, two other options are available in this fieldset:

- Use tagged designations When analysing using defined loci, Genome Comparator can use the designations stored within the database (this is the default). This is much quicker since it doesn't need to run BLAST against these sequences. If a designation is missing, BLAST will be run for that locus anyway.
- Disable HTML output If running Genome Comparator against a large number of genomes, the resulting table may get so large that your web browser struggles to render it properly and may use up too much memory on your computer. Clicking this button prevents this output this output is not required for further analysis since everything present in it is also generated in Excel format at the end. HTML output is automatically disabled when more than 150 genomes are analysed.

## 11.6.6 Distance matrix calculation fieldset

This section provides options for the treatment of truncated and paralogous loci when generating the distance matrix.



For truncated 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 truncated in at least one isolate will be removed from the analysis completely (default). Using this option means that if there is one bad genome with a lot of truncated 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 truncated sequences as a specific allele 'T'. This varies from any other allele, but all truncated sequences will be treated as though they were identical.
- Ignore in pairwise comparison This is probably the best option (and will likely become the default). In this case, truncated 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 affect 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.

## 11.6.7 Alignments fieldset

This section enables you to choose to produce alignments of the sequences identified.

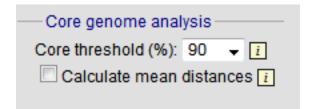
- Alignments
Aigintenta
Produce alignments i
🗹 Include ref sequences in alignment
Align all loci (not only variable)
Aligner: MAFFT 🚽

Available options are:

- Produce alignments Selecting this will produce the alignment files, as well as XMFA and FASTA outputs of aligned sequences. This will result in the analysis taking approximately twice as long 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 issued otherwise.

### 11.6.8 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).



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.

## 11.6.9 Filter fieldset

This section allows you to further filter your collection of isolates and the contigs to include.

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.

## 11.6.10 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.

# 11.7 **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.

Pub	MLST / Breakdown: Is	Browse   Profile/ST   List olate fields   Scheme/alleles   Publications ts   Home   Options   Profiles/sequences defi	nitions   Database sub	omissions		
The Ne						offles/sequence definition database there is at least
Q				ttings al options - including isolate table field y and query options for locus, scheme		General information • Isolates: 29178 • Last update: 2014-07-17 • Update history • About BIGSdb
	Breakdown • Single field • Two field • Unique combinations • Scheme and alleles • Publications • Sequence bin	Export • Export dataset • Contigs • Sequences - XMFA / concatenated F	-ASTA formats	Analysis • Codon usage • Presence/absence status of loci • Genome comparator • BLAST	Miscellaneous  • Description of da	tabase fields

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.

5         M00240227         UK         2000 invasive (unspecified/other) Neisseria meningitidis         B         1100         ST-32 complex/ET-5 complex         7           5         M00282207         UK         2000 invasive (unspecified/other) Neisseria meningitidis         W         1100         ST-32 complex/ET-5 complex         7           7         7891         B54; 21054         Finland         1975         invasive (unspecified/other) Neisseria meningitidis         A         5         ST-52 complex/ET-5 complex         7	16								
7 7001 DE4: 71054 Finland 1075 invasive (unapagified/other) Najagaria manipajitidia A E OT 5 complex/substraus III 00									
7 7891 B54, 21054 Finianu 1975 invasive (unspecified/outer) iveissena meningliudis A 5 51-5 complexisubgroup in 20	9 F3-1								
8 M00242007 UK 2000 invasive (unspecified/other) Neisseria meningitidis B 1102 ST-18 complex	14								
9 0021/84 Czech Republic 1984 invasive (unspecified/other) Neisseria meningitidis W 114 ST-22 complex									
10 6748 B73; Z1073 Canada 1971 invasive (unspecified/other) Neisseria meningitidis A 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 B 1015 ST-32 complex/ET-5 complex 7	16								
13 139M B99; Z1099 Philippines 1968 Neisseria meningitidis A 1 ST-1 complex/subgroup I/II 5-2	10 F5-1								
14 0120/95 Czech Republic 1995 invasive (unspecified/other) Neisseria meningitidis X 117	14								
15 1 Germany 1999 carrier Neisseria meningitidis E 864									
16 2 Germany 1999 carrier Neisseria meningitidis B 854 ST-18 complex									
17 3 Germany 1999 carrier Neisseria meningitidis W 174 ST-174 complex									
18 4 Germany 1999 carrier Neisseria meningitidis B 19 ST-18 complex									
19 S3131 B213; Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningitidis A 4 ST-4 complex/subgroup IV 7	13-1 F1-5								
20 5 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex									
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 B 32 ST-32 complex/ET-5 complex									
24 S4355 B227; Z1227 Denmark 1974 invasive (unspecified/other) Neisseria meningitidis A 5 ST-5 complex/subgroup III 5-1	9 F3-1								
25 9 Germany 1999 carrier Neisseria meningitidis B 930 ST-334 complex									
Analysis tools: Breakdown: Fields Two Field Codons Polymorphic sites Combinations Schemes/alleles Publications Sequence bin Tag status Analysis: BURST Presence/Absence Genome Comparator BLAST Export: Detaset Contigs Sequences									

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.

	Profile/ST   List ;   Scheme/alleles   Publications Options   Profiles/sequences definitions   Database submissions			
				Toggle: i
BLAST				
Please select the required isolate ids to BLAS	T against (use ctrl or shift to make multiple selections) and paste in you Paste sequence	r query sequence. Nucleotide or pepti	de sequences can be queried. — Include in results table —	
64) 254 67) 55611 82) 11-004 84) 1/4L2229 90) CK1100 120) F4698 128) F6124 160) 1014	GAASCCTTISSECGEACSCEATESCCGCCTTISCCGCTTCGESCCGATES SCAASCCTEAATAAAATCSCCAACGEACTCCGCTBGCTBSCAAGCGEC TTSSECGEAATAAATCCCCCEAAAACGACCGSGETCGTCCTCCATEATE AACCCGACCCAATGCGAAGCGATGACCATSGTGTSCTSCCAAGTGTTC ACCATGSCCAATGCGAGCGATGACCATSGTGTSCTSCCAAGTGTTC ACCATGSCCTGTGSGCACCGGSGCAATTTCGGCTGACGCCGTGCAC CACTGCGCCGTCGSGCACCGGGCACCGTGTGSGCGACGCGTGCAC CACTGCGCCGTCGSGCACCGGTACCGGGAAAAAASCGACTATTTC CTGATGCTGGCTACCGCTAACGCGTAACGGCTACCGAAAA	CCGCGCIGCGGI CCGGGCAAAGIC GGCAACGACGII AGCCCGIIAIC AGCTICAACGAA	country region year epidemiological year age yr age mth sex disease source epidemiology •	
Parameters	Options	Restrict included sequences by		- Action
BLASTN word size: 11 👻 👔	Show 0% matches in table	Sequence method:	<b>▼</b> [	Reset Submit
BLASTN scoring: reward:2; penalty:-3	; gap open:5; gap extend:2 👻 i	Project:	<b>▼</b> [i	
Hits per isolate: 1 👻		Experiment: 🚽 👔		
Flanking length (bp): 100 🚽 🧵				
USE IBLASIA I				

#### Click submit.

A table of BLAST results will be displayed.

														Тор
IST	Γ													
se se	lect the requ	uired isolate	ids to BLAST ag	gainst (use ctr	l or shif	it to make m	nultiple se	lections) and paste	in your que	ery sequei	nce. Nucleoti	de or peptide sequences can be que	eried.	
solat	es		F	aste sequend	.e ——								e —	
A4/M 120N 7891 ) 674 ) 129 ) 139 ) 331 ) \$43	8 M 31 55	None	GC TT AA AC GC	AAGCCTGAA GGGCGAAAT CCCGACCCA CATCGGCAT CTACAACCT CTGCGCCGT	TAAAA CAAAA ATGCG GGCGG CTTGC CGGCA	ICGCCAAC ICCCCGAA AAGCGATG GCGCGTCG AATCCATC ICGAACCC	GACATCO AACGAGO ACCATGO GGCAATI CGCCTGI	CCGCTTCGGGCGC GCTGGCTGGCAAG CGGGTTCGTCCAT TGTGCTGCCAAGT TCGAGCTGAACGT TCGGGCGACGCGTG AAAAAATCGACTA TCGGCTACGAAAA	CGGCCCG CATGCCG GTTCGGC CTATATG CAACAGC ATTTCCTG	CGCTGCG GGCAAAG AACGACG CCCGTTA TTCAACG	GT STC STT ATC SAA	country region year age wr age mth sex disease source source	A E	
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	neters TN word size	ze: 11 🖵 🛛	7				- Optio	ns ow 0% matches in t		Sequence	cluded seque			Action
			<ol> <li>penalty:-3; gaj</li> </ol>		outond	·2 🗖	5H	ow 0% matches in t	lable	Sequence	Project:	<b>▼</b> []		Reset Submit
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ankir	ng length (bj e TBLASTX [	p): 100	• [											
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ankir Use te id 1 2 7 0	Isolate A4/M1027 120M 7891 6748 129	<ul> <li>p): 100</li> <li>f</li> <li>identity A</li> <li>98.49</li> <li>98.49</li> <li>98.49</li> <li>98.49</li> <li>98.49</li> <li>98.49</li> <li>98.49</li> <li>98.49</li> </ul>	Alignment lengti 465 465 465 465 465	7 7 7 7 7 7	0 0 0 0 0 0 0 0	180177 180583 180965 181186 181867	19444 4782 19869 19181 35889	19908 extract	1 <b>↓</b> 1 <b>↑</b> 1	0.0 0.0 0.0 0.0 0.0	807 807 807 807 807 807			
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ankir Use te id 1 2 7 0 1 3 9	Isolate A4/M1027 120M 7891 6748 129 139M	<ul> <li>b): 100</li> <li>b): 100</li> <li>b): 100</li> <li>c): 100</li> <lic): 100<="" li=""> <lic): 100<="" li=""> <lic): 100<="" li=""> <li< td=""><td>Alignment lengti 465 465 465 465 465</td><td>7 7 7 7 7 7 7</td><td>0 0 0 0 0</td><td>180177 180583 180965 181186 181867</td><td>19444 4782 19869 19181 35889 36775</td><td>19908 extract</td><td>1 <b>↓</b> 1 <b>↑</b> 1</td><td>0.0 0.0 0.0 0.0 0.0</td><td>807 807 807 807 807 807</td><td></td><td></td><td></td></li<></lic):></lic):></lic):></ul>	Alignment lengti 465 465 465 465 465	7 7 7 7 7 7 7	0 0 0 0 0	180177 180583 180965 181186 181867	19444 4782 19869 19181 35889 36775	19908 extract	1 <b>↓</b> 1 <b>↑</b> 1	0.0 0.0 0.0 0.0 0.0	807 807 807 807 807 807			
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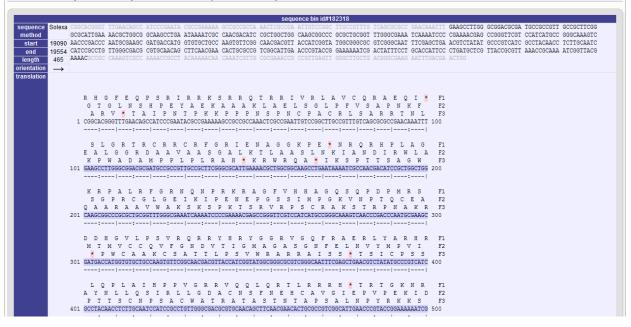
Clicking any of the 'extract' buttons will display the matched sequence along with a translated sequence and flanking sequences.

181867	35889	36353 extract>	$\rightarrow$	0.0	807
182004	36775	37239 extract →	$\rightarrow$	0.0	807
182318	19090	19554 <mark>extract →</mark>	$\rightarrow$	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)



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	53011	30.43	400	1	v	104143	4004	JZ00 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

## 11.7.1 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	$\overline{\mathbf{v}}$

Multiple values can be selected by clicking while holding down Ctrl.

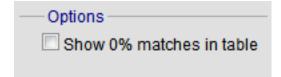
### **11.7.2 Parameters fieldset**

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 🚽	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.

## 11.7.3 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.

## 11.7.4 Filter fieldset

This section allows you to further filter your collection of isolates and the contig sequences to include.

-Restrict included sec	nuences by	
Sequence method:	<b>▼</b> [i]	
Droject		
Project:		<b>▼</b> [i]
Experiment:	▼ i	

Available options are:

- Sequence method Choose to only analyse contigs that have been generated using a particular method. This depends on the method being set when the contigs were uploaded.
- Project Only include isolates belonging to the chosen project. This enables you to select all isolates and filter to a project.
- Experiment Contig files can belong to an experiment. How this is used can vary between databases, but this enables you to only include contigs from a particular experiment.

## **11.8 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.

	00282207		UK		invasive (unspecified/other)	-	W	1101	ST-22 complex			
	7891	B54; Z1054	Finland		invasive (unspecified/other)		A	5	ST-5 complex/subgroup III	20	9	F3-1
	00242007		UK		invasive (unspecified/other)		В	1102	ST-18 complex		14	
9	0021/84				invasive (unspecified/other)		W	114	ST-22 complex			
10	6748	B73; Z1073	Canada		invasive (unspecified/other)	-	A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany		invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89				invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099		1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic		invasive (unspecified/other)		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			

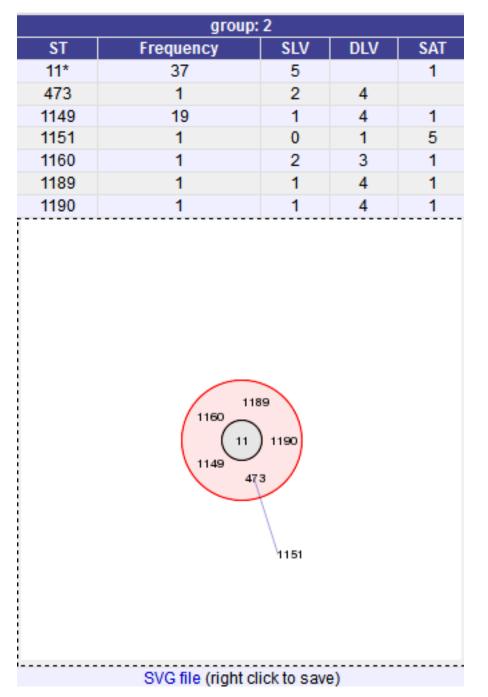
If there multiple schemes that can be analysed, these can then be selected along with the group definition.

Ouery: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profile/Sequences definitions   Database submissions
BURST analysis
This is the original BURST algorithm, developed by Ed Feil, first implemented by Man-Suen Chan. This version has been adapted for use as a plugin for the BIGSdb database software by Keith Jolley. BURST analysis can be used to: • Divide strains into groups according to their allelic profiles. • Count the number of Single Locus Variants (SLV), Double Locus Variants (DLV) and Satellites (SAT) for each sequence type (ST). • Identify the potential Ancestral Type (AT). These are shown with an asterisk next to their names in the results table. Graphic representations of BURST groups can be aved in SVG format. This is a vector image format that can be manipulated and scaled in drawing packages, including the freely available Inkscape. • Options Select scheme: MLST • Group definition: profiles match at in -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.

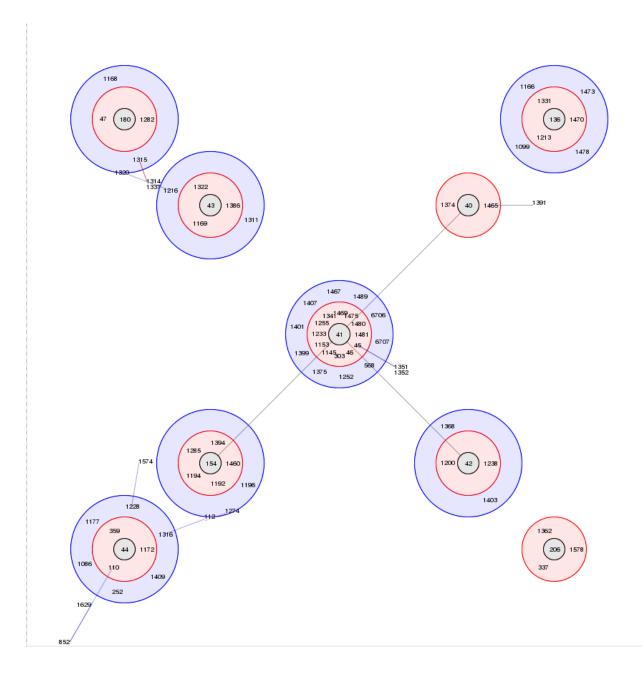
A series of tables will be displayed indicating the groups of profiles. Where one profile can be identified as a central genotype, i.e. the profile that has the greatest number of other profiles that are single locus variants (SLV), double locus variants (DLV) and so on, a graphical representation will be displayed. The central profile is indicated with an asterisk.



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.

group: 6									
ST	Frequency	SLV	DLV	SAT					
32*	2	3	2						
230	1	1	3	1					
484	1	0	3	2					
1015	1	1	4						
1100	1	1	2	2					
1148	1	0	4	1					
		1100 114	8						
	SVG file (right cli	ck to save	e)						

Groups can get very large, where linked profiles form sub-groups and an attempt is made to depict these.



# 11.9 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.

(PtrbMLST) Breakdown: Isolate	wse   Profile/ST   List fields   Scheme/alleles   Publications ome   Options   Profiles/sequences definitions   Database subn	vissions	
			in the profiles/sequence definition database there is at least one on sample.
Query database • Search database - advanced i • Browse database - peruse all • Search by combinations of loo • List query - find isolates by ma	records. • Set display a ci (profiles) - including partial matching.	ings options - including isolate table field handling and query options for locus, schemes or scheme fields.	i General information • Isolates: 29178 • Last updated: 2014-07-17 • Update history • About BICSdb
Breakdown     Single field     Two field     Unique combinations     Scheme and alleles     Publications     Sequence bin	Export dataset Contigs Sequences - XMFA / concatenated FASTA formats	Analysis Miscellar Codon usage • Presenceratisence status of loci • Genome comparator • BLAST	neous tion 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.

5 M00240227 6 M00282207	UK	2000	invocivo (unonocifio d/othor)							
	1.112		invasive (unspecified/other)	Neisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16	
7 7004 004 7	UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7 7891 B54; Z	054 Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	20	9	F3-1
8 M00242007	UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1102	ST-18 complex		14	
9 0021/84	Czech Republic	: 1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10 6748 B73; Z	073 Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11 129 B92; Z	092 Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12 0090/89	Czech Republic	: 1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13 139M B99; Z		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	X	117			14	
15 1	Germany	1999	carrier	Neisseria meningitidis	E	864				
16 2	Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17 3	Germany	1999	carrier	Neisseria meningitidis	w	174	ST-174 complex			
18 4	Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19 S3131 B213; Z	1213 Ghana		invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20 5	Germany	1999	carrier	Neisseria meningitidis		198	ST-198 complex			
21 6	Germany	1999	carrier	Neisseria meningitidis		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; Z	1227 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			

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   Breakdown: Isolate fields   Scheme/ Links: Contents   Home   Options   F	alleles   Publications	ns   Database submissions	
			Toggle: i
Codon usage analysis			
			atabase containing sequences, or with sequences tagged, can be included. It is important to note that ng frame 1). Partial sequnces from the sequence bin will not be analysed. Please check the loci that you
	clude in identifier — –	-Loci	- Schemes
1 yea 2 epi 3 age 4 age 5 d 6 d sou	Intry E ion E r demiological year a yr e mth t ease	165_DNA  165_RNA (SSU_RNA) 235_RNA abc2 abc2 (NEIS1015) accf2 (NEIS1015) accf2 (NEIS1279) acA(NEIS1727) acnA (NEIS1727) acnA (NEIS1729) All Nore Pastelist	Control C
Sequence retrieval		Codons	Action
If both allele designations and tagged sequences exist for a locus, choose how you want these handled: [	7	Select codon order:	Submit
existion a locus, choose now you want these nancieu. [	<i>L</i>	alphabetical	
Use sequences tagged from the bin		C or G ending codons first	
O Use allele sequence retrieved from external databa	ISe		
☑ Do not include sequences with problem flagged (de	efined alleles will still be us	ed)	

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.

Period         Search         Browse         Profile/ST List           Breakdown: Solate Field         Schemelaleles         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

ob status viewer	
tatus Job id: BIGSdb_13269_1405586315_76138	
submit time;         2014-07-17 09-38:35           Status;         finished           Status;         finished <th></th>	
Total times 26 seconds output • Absolute frequency of codon usage by isolate	
Absolute frequency of codon usage by locus     Relative synonymous codon usage (RSCU) by isolate     Relative synonymous codon usage (RSCU) by locus     Tar file containing output files	

# 11.10 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.

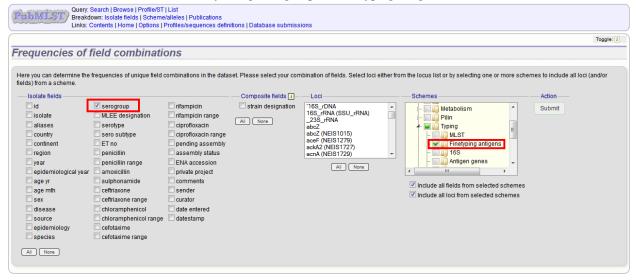
The function can be selected by clicking the 'Unique combinations' link in the Breakdown section of the main contents page. This will run the analysis on the entire database.

Pub	Query: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publicat Links: Contents   Home   Options   Profiles/sequence		
Neis	seria PubMLST database		
	eisseria PubMLST database contains data for a collection of isolate ponding isolate deposited here. Any isolate may be submitted to th		b. For every allelic profile in the profiles/sequence definition database there is at least one not represent a population sample.
Q	Query database • Search database - advanced queries. • Browse database - peruse all records. • Search by combinations of loci (profiles) - including partial mate • List query - find isolates by matching a field to an entered list.	Option settings  Set general options - including isolate table  Set display and query options for locus, sch ching.	
<b></b>	Breakdown Single field Two field Unique combinations Scheme and alleles Publications Sequence bin Export Export Export Export Contigs Sequences - XMFA / concater	Analysis  Codon usage  Presence/absence status of Genome comparator BLAST	Miscellaneous     Description of database fields floci

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.

6 M00	0240227		UK	2000	invasive (unspecified/other)	Naissaria maningitidia	В	1100	ST-32 complex/ET-5 complex	7	16	
7			UK		invasive (unspecified/other)	~	W	1101	ST-32 complex	'	10	
	7891	B54; Z1054	Finland		invasive (unspecified/other)		A	5	ST-5 complex/subgroup III	20	9	F3-1
0 1000	242007	854,21054	UK		invasive (unspecified/other)		B	1102	ST-18 complex	20	14	1.01
9 00	021/84				invasive (unspecified/other)		w	114	ST-22 complex		14	
	6748	B73; Z1073	Canada		invasive (unspecified/other)	~	A	1	ST-1 complex/subaroup I/II	18-1	3	F5-1
	129	B92; Z1092	Germany		invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
	090/89	032,21032			invasive (unspecified/other)		В	1015	ST-32 complex/ET-5 complex	7	16	13-0
	139M	B99: Z1099		1968	invasive (unspecified/uner)	Neisseria meningitidis	A	1	ST-1 complex/subaroup I/I	5-2	10	E5-1
	120/95	D33, 21033			invasive (unspecified/other)		X	117	or reomplex subgroup in	52	14	131
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 S	3131	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 S	\$4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	В	930	ST-334 complex			

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



Click submit. When the analysis has completed you will see a table showing the unique combinations of the selected fields along with the frequency and percentage of the combination.

						Τος
quen	cies of f	ield col	mbinat	ions		
nber of uni	que combinatio	ons: 2939				
nercentar	e may add un	to more than	100% if you	have celecter	Loci or scheme t	fields with multiple values for an isolate.
					Percentage 🗢	
B W	7-2 5	4	F1-5 F1-1	625 513	5.65 4.64	
B	19	15	F1-1 F5-1	385	3.48	
c	5	2	F3-6	283	2.56	
-	18-10	43	F3-14	281	2.54	
В	7	16	F3-3	252	2.28	
c	5-1	10-8	F3-6	222	2.01	
в	22	9	F5-12	171	1.55	
В	22	14	F5-5	167	1.51	
Α	5-2	10	F3-5	135	1.22	
в	19-1	15-11	F5-1	107	0.97	
Y	5-1	10-1	F4-1	96	0.87	
-	5	2	F1-1	93	0.84	
Y	5-2	10-1	F4-1	79	0.71	
С	5	2	F5-8	79	0.71	
W	18-1	3	F4-1	77	0.70	
В	22-1	14	F4-1	77	0.70	
С	5	2	F3-3	76	0.69	
B	18-1 5-1	3	F1-5 F5-8	72 69	0.65	
Y B	5-1	2-2	F5-8 F1-14	69	0.62	
В	7-2	15	F1-14 F1-5	61	0.55	
	1-2	13-2	F (-5	56	0.55	

The table can be downloaded in tab-delimited text or Excel formats by clicking hte links at the bottom of the page.

					0.01
в	19	13-2	F5-1	1	0.01
В	12.1	13.1	F3-29	1	0.01
NG	7-2	16-126	F3-3	1	0.01
в	7-2	30	F5-1	1	0.01
в	7	30-3	F1-14	1	0.01
В	5-1	10-10	F3-16	1	0.01
-	7-2	30-3	F1-7	1	0.01
С	5-2	10	F1-7	1	0.01
NG	18-1	3	F1-34	1	0.01
NG	22	14-6	F4-2	1	0.01
в	7-2	4	F1-88	1	0.01
NG	5-1	10-62	F1-3	1	0.01
Y	12-3	4	F4-1	1	0.01
NG	7-2	16	F1-104	1	0.01
Х	12-1	16-52	F3-9	1	0.01
NG	18-4	35-34	F4-1	1	0.01
	oad as tab-del oad in Excel fo				

# 11.11 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.

12 13 14 15	6748 129 0090/89 139M	B73; Z1073 B92; Z1092	Canada Germany		invasive (unspecified/other) invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
13 14 15	0090/89	B92; Z1092		1964	invasive (unspecified/other)	Naicearia maningitidie						
12 13 14 15 16			One of Description			Nelssena meningiuuis	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
14 15	139M		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
15		B99; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
16	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
	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			
irea Ai	nalysis: 🔳	S: Two Fi URST Code Nataset Cont	ons Presence/At			alleles Publications	Sequence	bin	Tag status			

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

Prink/LST         Ouery: Search   Profile/ST   List           Breakdown: Solate fields   Schemeralicities   Publications         Database submissions           Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions	
Polymorphic site analysis	Toggle: i
This tool will analyse the polymorphic sites in the selected locus for the current isolate dataset. If more than 50 sequences have been selected, the job will be run by the offline job manager which may take a few minutes (or longer depending on the queue). This is because sequences may have gaps in them and consequently need to be aligned which is a processor and memory-intensive operation. Loci Options Action 165 rRNA (SSU rRNA) 165 rRNA (S	

Click 'Analyse'.

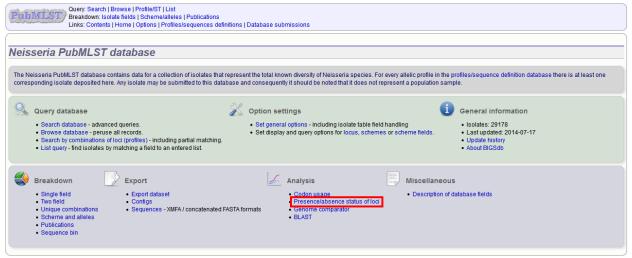
A schematic of the locus is generated showing the polymorphic sites. A full description of this can be found in the *Locus Explorer polymorphic site analysis* section.

																																	Toggi
olymo	rphio	: si	te a	naly	ysis	;																											
e colour co	toe roor	acont	the ne	rconto	an of a		that h	240.2	norticu	dor pu	clootide	at and	a nocit	ion Cli	ick onw	doro v	vithin t		100000	to drill	down	to all		and p	rofilo	inform	motion	n Tho	width	oftho	diento	v con br	altoro
ing to the o											cieoliud	ateau	i posit	.011. 011	CK allyv	niere w	//umru	ie sey	Jence		uown	to an	liele a	and pi	rome	mom	nauoi	n. me	wide	rorute	uispia	y can be	allere
alleles incl	uded in	analy	sis. 10	4 polyr	norphi	c sites	s foun	d.																									
y: <mark>0 - 10%</mark>	>10 - 20	8   >2	0 - 30	>30	- 40%	>40	- 50%	>50	60%	>60 -	70% >	70 - 809	>80	- 90%	>90 - 1	00%																	
1	10		20		30	)	4	0	5	50	6	0	70		80		90		100														
TTTC	ATAC <mark>C</mark> G				G <mark>CGAJ</mark> TA (				A T		CATCA		CCATG	A <mark>G</mark> TTG T	GAAAAC GC 1			AGG <mark>C</mark> T FCATC															
				_		-		÷.					•	- C				TC	-														
101 TGAA	110 AGAACT		120 AATTO		130 TGAA		14 AGCGA		15 (CCCT)		16 CTCCAT		170 GTCAA		180 CTV/CC	GCGAA	190	TTTGC	200														
A	G	TÖ	2	G	C CG		A	A	T	A	r aa	G	G	Ā		GA	T	C	A														
201	210		220		230		24		25		26		270		280	T	290		300														
AAAC	GAAAAA	ATCCO A	CAACC	TCC	GGCG	TCAG			TCCC T			CTTGGG	TGCAG A A		CGACGT T T		A C		CCC														
				•		A			÷.		÷								•														
301	310		320		330	G	34	0	35	50	36	0	370		380		390		400														
ACCA	ACCATT	TGGA				_	IGGAA	_	_		GTTTGA	AGGCAG	CTTGG C	TTGTC			CCGCC		TGG														
401	410		420		430			0		C				<b>•</b> •					1														
	TATCCC C T				ACTCO	ATC C																											
ucleotide					1	Ξ.																											
cleotide	nequ	ench		News	la a fist	_																											
sition 🔶 д	<b>≑</b> C <b>≑</b>	G ¢	T ≑  -		leotide		iG ≑	%T \$	%- ≑																								
9	0 25	0	5	0	8	3.33		16.67	'																								
	1 0	29	29		.33		96 67	96.67																									

## **11.12** Presence/absence

This plugin displays the status of loci for isolate records. It will shown whether a locus has been designated with an allele name, has a sequence tag, or both.

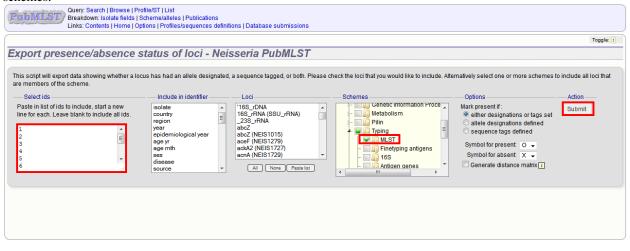
The function can be selected by clicking the 'Presence/absence status of loci' link in the 'Analysis' section of the main contents page.



Alternatively, it can be accessed following a query by clicking the 'Presence/Absence' 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.

5 1	00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16	
	100240227		UK		invasive (unspecified/other)		w	1101	ST-22 complex		10	
7	7891	B54; Z1054	Finland		invasive (unspecified/other)		A	5	ST-5 complex/subgroup III	20	9	F3-1
8 1	100242007		UK		invasive (unspecified/other)		В	1102	ST-18 complex		14	
9	0021/84		Czech Republic		invasive (unspecified/other)		W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89				invasive (unspecified/other)		В	1015		7	16	
13	139M	B99: Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95			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			
		elds Two Fi			Combinations Schemes/ Genome Comparator BL	alleles Publications	Sequence	bin 🗌	Tag status			

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.



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.

Partiliture Parties Profiles Provided Profiles Provided Profiles Provided Profiles Provided Profiles Provided Profiles Provided Profiles P	
	Toggle: i
Export presence/absence status of loci - Neisseria PubMLST	
This analysis has been submitted to the job queue.	
Follow the progress of this job and view the output.	

When complete, a single text file will have been generated.

Ouep: Search   Browse   Profile/ST   List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/sequences definitions   Database submissions
ob status viewer
tatus
Job Id: BIGSdb_31442_1405591304_69061 Submit time: 2014-07-17 11:01:44
Status: finished
Start time: 2014-07-17 11:01:44 Progress: 100%
Stop time:         2014-07-17 11:01:49           Total time:         4 seconds
Jutput
Main output file
ease note that job results will remain on the server for 7 days.

This is a tab-delimited text file that uses 'O' to represent presence and 'X' to represent a missing locus designation or tag.

id	pgm	adk	abcZ	pdhC	gdh	fumC	aroE
1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0
8	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0
10	0	0	0	0	0	0	0

#### 11.12.1 Options

There are a number of options that can be selected to modify the output.

— Options —	
Mark present if :	
either designation	s or tags set
Illele designation	s defined
🔘 sequence tags de	fined
Symbol for present:	0 🗸
Symbol for absent:	Χ 👻
Generate distance	matrix 👔

With these you can change the symbols used and whether designations, or tags, or both are counted.

You can also choose to generate a distance matrix based on presence/absence.

# 11.13 Tag status

The tag status plugin displays a graphical representation of the status of loci designations or tags for isolate data. It is accessed following a query by clicking the 'Tag status' button in the Breakdown section at the bottom of the results table.

ic		•	•	10		+	Order by: id Display: 25	✓ records	s per p	✓ ascending age i	•			1
-4	ction													
F	Reset S	Submit												
co	rds returne	d. Click the h	yperlinks for deta	ailed i	nformation.									
_										III of			_	
	isolate	aliases	country	ı vear	solate fields i dise		species	serogroup	ST	MLST clonal complex		yping antig PorA VR2		
	A4/M1027	B1: Z1001					Neisseria meningitidis		4	ST-4 complex/subgroup IV	5-2	10	F1-5	
		B35; Z1035					Neisseria meningitidis		1	ST-1 complex/subgroup I/II	5-2	10	F5-1	
N	00242905		UK	2000	invasive (unsp	pecified/other)	Neisseria meningitidis	В	1099		19	15		
	M1027	B43; Z1043	USA	1937	invasive (unsp	pecified/other)	Neisseria meningitidis	Α	4	ST-4 complex/subgroup IV				
N	00240227		UK	2000	invasive (unsp	pecified/other)	Neisseria meningitidis	В	1100	ST-32 complex/ET-5 complex	7	16		
N	00282207		UK	2000	invasive (unsp	pecified/other)	Neisseria meningitidis	W	1101	ST-22 complex				
		B54; Z1054					Neisseria meningitidis		5	ST-5 complex/subgroup III	20	9	F3-1	
	00242007						Neisseria meningitidis		1102	ST-18 complex		14		
	0021/84		Czech Republic	1984	invasive (unsp	pecified/other)	Neisseria meningitidis	W	114	ST-22 complex				
	lysis tool kdown: 🕞	S:	Field Polymor	phio cit	tes Combinati	ions Schome	es/alleles Publications	Sequence	hin	Tag status				
								Jesquence		100 310103				
	nalysis: B	SURST    Coo	dons Presence/	Absen	ce    Genome C	Comparator	BLAST							

#### Select the loci you would like to analyse.

PubliALSTD Breaken Florate lefter list use and the second	
	Toggle: i
Tag status	
Select schemes or groups of schemes within the tree. A breakdown of the individual loci belonging to these schemes will then be performed.	
In Capsule     Capsule	

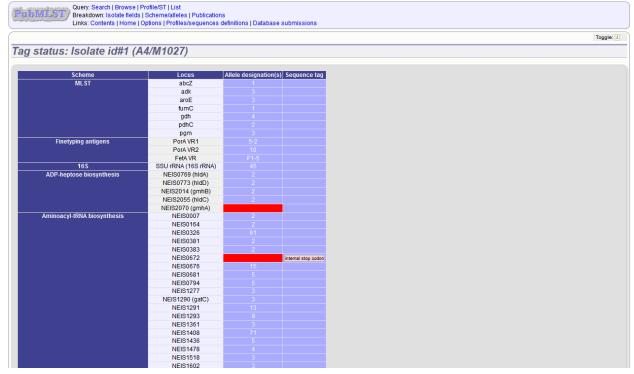
You should see a series of bars representing loci. The colour of these bars designates whether they have an allele designation only, a sequence tag only, both designations or tags, or whether they have flags set.

	Profile/ST   List   Scheme/alleles   Publications Dptions   Profiles/sequences defini	tions   Database submissions			
					Toggle: i
Tag status					
Select schemes or groups of schemes within II	roup A roup B	ral loci belonging to these scheme	s will then be performed.		
Bars represent loci by schemes arranged in aly Key Allele designated only   Sequence tagged only 2463 loci selected:			opear more than once in this gr	aphic. Click on the id hyperlink for a det	ailed breakdown for an isolate.
1 A4/M1027					
2 120M					
3 M00242905					
4 M1027					
5 M00240227					
6 M00282207					
8 M00242007					
9 0021/84					
•	III				•

Hovering the mouse over the bars will indicate the scheme represented.

Note: Loci will be represented more than once if they are members of multiple selected schemes.

Clicking any of the isolate id hyperlinks navigates to a page that breaks down the exacty status for all loci of that isolate.



There is a column each for allele designations and sequence tags. If an allele designation is defined, the allele identifier is displayed. Cells shaded in blue show that the designation or tag is present, whereas red indicates thet they are absent.

# **Data export plugins**

# 12.1 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.

Query: Search  Brows   Profiles/T List Breakdown: Isolate fields   Scheme/alleles   Publications Links: Contents   Home   Options   Profiles/Sequences definitions   Database su	ubmissions
Neisseria PubMLST database	nown diversity of Neisseria species. For every allelic profile in the profiles/sequence definition database there is at least one
	0
Est query - Ind isolates by matching a field to an entered list.     Single field     Two field     Unique combinations     Scheme and alleles     Publications     Sequence bin	Analysis     Codon usage     Presencelabsence status of loci     Genome comparator     BLAST

Alternatively, you can export the recordsets of isolates returned from a database query by clicking the 'Dataset' button in the Export list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

				ls	olate fields 👔				MLST	Finet	yping antig	ens
id	isolate	aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1	PorA VR2	FetA VR
1	A4/M1027	B1; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; Z1035	Pakistan		meningitis and septicaemia		A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
3	M00242905		UK		invasive (unspecified/other)		В	1099		19	15	
4	M1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex/subgroup IV			
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975			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				invasive (unspecified/other)		W	114	ST-22 complex			
10	6748	B73; Z1073	Canada		invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic		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				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			invasive (unspecified/other)		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		ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)		Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			

#### Select the isolate fields and schemes to include.

							Toggle: i
Export dataset	taset in tab-delimited text, su	itable for importing into a	spreadsheet. Select which	fields you would li	ke included. Select loci either	from the locus list or by selecting one or more schemes to	include all
loci (and/or fields) from a sc locate fields V id V isolate allases continent region year epidemiological year age yt age mth sex	heme.	rifampicin rifampicin range diprofloxacin pending assembly assembly status ENA accession private project comments sender durator	Composite fields [	References references PubMed id Full citation	Loci 165.rDNA 165.rRNA (SSU_rRNA) _235_rRNA abc2 abc2 (NEIS1015) aceF (NEIS1279) aceF (NEIS1279) aceA (NEIS1727) aceA (NEIS1727) aceA (NEIS1729) All None	Schemes Generic information Proce Plin Plin Plin Finetyping antigens Antioen genes I include all fields from selected schemes I include all fields from selected schemes	
disease source epidemiology species	chloramphenicol     chloramphenicol range     cefotaxime     cefotaxime range	date entered	Options Childe locus commo Export allele numbers Use one row per field Include isolate field in Export full allele desi	s I 1 row (used only wi	th 'one row' option) ed only with 'one row' option)	Molecular weights Action C Export protein molecular weights GTG/TTG at start codes for methionine	]

Click Submit.

You can then download the data in tab-delimited text or Excel formats.

Ouery: Search   Browse   Profile/ST   List           Breakdown: Isolate fields   Scheme/alleles   Publications           Links: Contents   Home   Options   Profile/Sequences definitions   Database submissions	
	Toggle: i
Export dataset	
Please wait for processing to finish (do not refresh page).	
Output files being generated done	
Download: Text file   Excel file (right-click to save)	

### 12.1.1 Advanced options

Options	
Include locus common names	
Export allele numbers	
Use one row per field	
Include isolate field in row (used only with 'one row' option)	
Export full allele designation record (used only with 'one row' optic	on)

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.

### 12.1.2 Molecular weight calculation

The plugin can also calculate the predicted molecular weight of the gene product of any allele designated in the dataset.

Molecular weights

Export protein molecular weights

GTG/TTG at start codes for methionine

Click the 'Export protein molecular weight' checkbox. Additional columns (or rows depending on the output format) will be created to include the molecular weight data.

# 12.2 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.

Pub	Query: Search   Browse   Profile/ST   Li Breakdown: Isolate fields   Scheme/al Links: Contents   Home   Options   Pro			
Neis	seria PubMLST database			
		ection of isolates that represent the total known diversity of Neisseria specie s database and consequently it should be noted that it does not represent a	es. For every allelic profile in the profiles/sequence definition database there is at least one correspondin a population sample.	ng
Q	Query database	📈 Option settings	() General information	
	Search database - advanced queries.     Browse database - peruse all records.     Search by combinations of loc (profiles) - includi     List query - find isolates by matching a field to an			
	Breakdown Export	🖌 Analysis	Miscellaneous	
	Single field     Two field     Unique combinations     Scheme and alleles     Publications     Sequence bin	t - Codon usage Presence/absence status o GMFA / concatenated FASTA formats GMFA / concatenated FASTA formats BLAST	Description of database fields floci	

Alternatively, you can access this function by clicking the 'Sequences' button in the Export list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

	M1027	B43; 21043			Invasive (unspecified/other)		А	4	SI-4 complex/subgroup IV			
	M00240227				invasive (unspecified/other)		в		ST-32 complex/ET-5 complex	7	16	
6 1	M00282207				invasive (unspecified/other)		W	1101	ST-22 complex			
7	7891	B54; Z1054			invasive (unspecified/other)		A	5	ST-5 complex/subgroup III	20	9	F3-1
8 1	M00242007				invasive (unspecified/other)		в	1102	ST-18 complex		14	
9	0021/84				invasive (unspecified/other)		W	114	ST-22 complex			
10	6748	B73; Z1073			invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092			invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	в	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099		1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95						Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2			1999		Neisseria meningitidis	в	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4			1999		Neisseria meningitidis	в	19	ST-18 complex			
19		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			

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.

	ofile/ST   List Scheme/alleles   Publications ptions   Profiles/sequences defin	ittions   Database submissions			Toggle: i
identifiers, or DNA and peptide loci with genome	led Multi-FASTA (XMFA) format su sequences tagged, can be inclu	uitable for loading into third-party ap uded. Please check the loci that you	pplications, such as ClonalFrame. It will also produ	ce concatenated FASTA files. Only DNA loci that have a corresponding database or ore schemes to include all iod that are members of the scheme. If a sequence do the generate the output file.	
Select ids Paste in list of ids to include, start a new line for each. Leave blank to include all ids.	Include in identifier	Lod 1955_CNA 155_CRNA(SSU_RNA) 235_CRNA abb2 abb2 abb2 abb2 All None Pastelist All None Pastelist	Schemes Genetic information Proce Wetabolism Trping Trping Information antigens Information antigens In	Options     If both allel designations and tagged sequences     exist for a locus, choose how you want these handled [	Adion

#### 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.

Query: 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_29565_1405601815_9307           Submit time:         2014-07-17 13:56:55           Status:         finished           Start time:         2014-07-17 13:57:10           Progress:         100%           Stop time:         2014-07-17 13:57:23           Total time:         12 seconds
Output  XMFA output file (not aligned)  Concatenated FASTA (not aligned)  Tar file containing output files
Please note that job results will remain on the server for 7 days.

### 12.2.1 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
options
If both allele designations and tagged sequences
exist for a locus, choose how you want these handled:
existion a locus, choose now you want these handled.
Our of the sequences tagged from the bin
O Use allele sequence retrieved from external database
O Ose allele sequence retreved formexternal 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 🚽
I ranslate 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.

# 12.3 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.

Pub	MLST / Breakdown: Iso	Browse   Profile/ST   List olate fields   Scheme/alleles   Public s   Home   Options   Profiles/sequen		ubmissions		
The Ne		contains data for a collection of isola		nown diversity of Neisseria species. Fr consequently it should be noted that it		ofiles/sequence definition database there is at tion sample.
0,			<ul> <li>Set display</li> </ul>	ettings ral options - including isolate table fiel ay and query options for locus, schem		General information • Isolates: 29178 • Last updated: 2014-07-17 • Update history • About BIGSdb
	Breakdown • Single field • Two field • Unique combinations • Scheme and alleles • Publications • Sequence bin	Export • Export • Configs • Sequences - XMFA / concat	enated FASTA formats	Analysis • Codon usage • Presence/absence status of loci • Genome comparator • BLAST	Miscellaneous     Oescription of data	atabase 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.

5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria	meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria	meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria	meningitidis	A	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria	meningitidis	в	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria	meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria	meningitidis	A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria	meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria	meningitidis	в	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria	meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria	i meningitidis	X	117			14	
15	1		Germany	1999	carrier	Neisseria	i meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria	i meningitidis	в	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria	i meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria	meningitidis	в	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria	meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria	i meningitidis	s NG	198	ST-198 complex			
21			Germany	1999	carrier	Neisseria	meningitidis	s NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria	meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria	meningitidis	B	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria	meningitidis	A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria	meningitidis	в	930	ST-334 complex			
Br	_	s: elds Two Fi URST Coda			Combinations Schemes/	alleles I	Publications	Sequence I	oin 🗌	Tag status			

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.

	s   Profile/ST   List ds   Scheme/alleles   Publications e   Options   Profiles/sequences definitions   Database submiss	ions	
			Toggle: i
Contig analysis and exp	ort		
	which contigs are associated - use Ctrl or Shift to make multiple erlap then the total tagged length will be reported as being longe	selections. Please note that the total length of tagged sequence is calc er than it really is but it won't exceed the length of the contig.	ulated by adding up the length of all
Isolates	Options	Filter by	— — Action —
1) A4/M1027 2) 120M 7) 7891	Identify contigs with >= 0	Sequence method:	Reset Submit
10) 6748 11) 129 13) 139M		Experiment: 🚽 👔 Minimum length: 🚽 👔	
19) \$3131 24) \$4355 🔹			
All None			

#### At its simplest, press submit.

A table will be produced with download links. Clicking these will produce the contigs in FASTA format.

							То
ontig analysis a	nd export						
		s are associated - use Ctrl or Shift to make multiple e total tagged length will be reported as being longe				ed by addin	g up the leng
-Isolates	Options					Action -	
1) A4/M1027 2) 120M	-	ader line: original designation • []	Sequence method: Project:	▼ i	<b>▼</b> []	Reset	Submit
7) 7891 10) 6748					•		
				- II			
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11) 129 13) 139M				<ul> <li>↓ i</li> </ul>			
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11) 129 13) 139M 19) S3131	Ŧ						
11) 129 13) 139M 19) S3131 24) S4355	*						
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11) 129 13) 139M 19) 83131 24) 84355 All Nore ontigs with >=0% seque solate ♦ contigs ♦ n 1 A4/M1027 384 2 120M 359	natching contigs non-m unt ¢ download count	atching contigs					

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

Pu	bMLST	📝 Breakd	iown: Isolate		iT   List ne/alleles   Publications   Profiles/sequences definitions   Database submi:	ssions					
Cor	ntia an	alveie	and ex	vport						т	oggle: i
COI	illy and	aiysis	andex	tport							
loci t					igs are associated - use Ctrl or Shift to make multip the total tagged length will be reported as being lor				ed by addin — Action —	g up the len	gth of all
_	A4/M1027				contigs with >= 0 v % of sequence untagged	Sequence method:	<b>▼</b> [1]		Reset	Outerit	
2)			i i i i i i i i i i i i i i i i i i i	-	header line: original designation v 1	Project:	•	<b>-</b> i	Reset	Submit	
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	) 129 ) 139M					Minimum length:	<b>▼</b> [i				
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id 🜩	isolate 🗢	contigs 🖨			matching contigs nt  ✦   download						
1	A4/M1027	364	364		0						
2	120M	359	359		0						
7	7891	199 652	199		0						
10			652		U						
			b-delimited t								
	Batch dov	vnioad all d	contigs from s	selected Isola	tes (tar format)						

#### 12.3.1 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	juence untagged
FASTA header line:	ori	ginal	des	ignation	<b>▼</b> [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.

d 🗢 isolate 🗢	contine t	matchin	ig contigs	non-matching contigs		
	isolate 🗢	contigs 🗢	count 🗢	download	count 🔶	download
1	A4/M1027	364	175	Ļ	189	<b>_</b>
2	120M	359	99	Ļ	260	1
7	7891	199	56	Ļ	143	1
10	6748	652	423	Ļ	229	1

# Frequently asked questions (FAQs)

### **13.1 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.

### **13.2 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.

# Appendix

## 14.1 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.

• <

- Less than 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).

### 14.2 Sequence tag flags

Sequences tagged in the sequence bin can have features indicated by specific flags. The presence of these flags can be queried. These are a superset of *flags available for allele sequences*. Available flags are:

- ambiguous read
  - Genome sequence contains ambiguous nucleotides in coding sequence.

- apparent misassembly
  - Sequence has a region of very high identity to existing allele in one region but looks completely different in another.
- atypical
  - Catch-all term for a sequence that is unusual compared to other alleles of locus.
- · contains IS element
  - Coding sequence is interrupted by insertion sequence.
- · downstream fusion
  - No stop codon present resulting in translation continuing.
- frameshift
  - Frameshift in sequence relative to other alleles, not resulting in internal stop codon.
- 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.
- 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).

# 14.3 Allele sequence flags

Sequences can be flagged with specific attributes - these are searchable when doing a sequence attribute query. These are a subset of *flags available for tagged sequences*. These are mainly for use with whole genome MLST type data. Multiple flags can be selected by Ctrl-clicking the list. Available flags are:

- atypical
  - Catch-all term for a sequence that is unusual compared to other alleles of locus.
- · contains IS element
  - Coding sequence is interrupted by insertion sequence.
- downstream fusion
  - No stop codon present resulting in translation continuing.
- frameshift
  - Frameshift in sequence relative to other alleles, not resulting in internal stop codon.

- 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.
- 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).