BIGSdb Documentation

Release 1.19.0

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20 Database schema

Gene-by-gene population annotation and analysis

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

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

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

CHAPTER 1

Concepts and terms

1.1 BIGSdb

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

1.2 Loci

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

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

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

1.3 Alleles

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

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

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

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

1.4 Schemes

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

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

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

1.5 Profiles

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

1.6 Classification groups

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

1.7 Sequence tags

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

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

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

1.8 Sets

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

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

CHAPTER 2

BIGSdb dependencies

2.1 Required packages

BIGSdb requires a number of software components to be installed:

2.1.1 Linux packages

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

2.1.2 Perl modules

These are included with most Linux distributions.

• Archive::Zip - [required by PhyloTree plugin] - Used to upload to iTOL

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

2.1.3 Optional packages

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

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

CHAPTER 3

Installation and configuration of BIGSdb

3.1 Software installation

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

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

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

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

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

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

sudo su postgres

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

createuser apache

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

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

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

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

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

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

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

3.2 Configuring PostgreSQL

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

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

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

3.2.1 pg_hba.conf

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

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

3.2.2 pg_ident.conf

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

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

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

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

See Tuning Your PostgreSQL Server for more details.

Restart PostgreSQL after any changes, e.g.

/etc/init.d/postgresql restart

3.3 Setting global connection parameters

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

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

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

3.4 Site-specific configuration

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

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

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

3.5 Setting up the offline job manager

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

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

sudo useradd -s /bin/sh bigsdb

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

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

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

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

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

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

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

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

3.6 Setting up the submission system

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

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

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

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

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

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

3.7 Setting up a site-wide user database

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

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

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

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

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

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

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

→pubmlst_bigsdb_users
```

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

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

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

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

site_user_dbs=PubMLST|pubmlst_bigsdb_users

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

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

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

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

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

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

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

- Allow admin to merge user accounts.
- modify_users
 - Allow admin to edit user details.

e.g.

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

- 4. Specific *permissions can be set for curators* in individual databases:
 - import_site_users
 - This allows the curator to import site users in to the database.
 - modify_site_users
 - You may not wish to do this! It allows the curator of any database with this permission to change the details of a user that may be used on other databases on the site.
- 5. HTML header files can be defined for use when bigsdb.pl or bigscurate.pl are called withouth a database configuration, such as when a user is registering or modifying their user details. These files, site_header.html, site_footer.html, site_curate_header.html and site_curate_footer.html should be placed in the root directory of the web site.

3.8 Periodically delete temporary files

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

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

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

3.9 Prevent preference database getting too large

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

in /etc/crontab will remove the preferences for any user that has not accessed any database in the past 6 months (the script will run at 6pm every Sunday).

3.10 Purging old jobs from the jobs database

If you are running the offline job manager, the jobs database (default bigsdb_jobs) contains the parameters and output messages of these jobs. Job output files are only *usually kept on the server for 7 days* so there is no point keeping the database entries for longer than this. These can be purged with a daily cron job, e.g. set the following in /etc/crontab (the script will run at 5am every day).

3.11 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
```

3.12 Upgrading BIGSdb

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

psql -f isolatedb_v1.8.sql bigsdb_isolates

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

Minor version changes, e.g. 1.8.0 -> 1.8.1, have no modifications to the database structures. There will be changes to the Perl library modules and possibly to the contents of the Javascript directory, images directory and CSS files. The version number is stored with the bigsdb.pl script, so this should also be updated so that BIGSdb correctly reports its version.

3.13 Running the BIGSdb RESTful interface

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

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

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

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

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

resources

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

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

psql bigsdb_rest

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

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

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

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

Finally, add the database resources to the group:

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

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

./bigsrest.pl

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

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

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

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

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

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

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

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

sudo service bigsdb-rest start

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

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

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

sudo systemctl enable bigsdb-rest.service

It can also be manually started by calling:

sudo systemctl start bigsdb-rest.service

3.13.1 Proxying the API to use a standard web port

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

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

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

CHAPTER 4

Database setup

There are two types of BIGSdb database:

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

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

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

4.1 Creating databases

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

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

```
sudo su postgres
```

then

createdb bigsdb_test_seqdef
psql -f seqdef.sql bigsdb_test_seqdef

Create an isolate database the same way:

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

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

```
psql bigsdb_test_isolates
```

and alter the isolate table:

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

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

4.2 Database-specific configuration

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

- config.xml the database configuration file. Fields defined here correspond to fields in the isolate table of the database.
- banner.html optional file containing text that will appear as a banner within the database index pages. HTML markup can be used within this text.
- header.html HTML markup that is inserted at the top of all pages. This can be used to set up site-specific menubars and logos.
- footer.html HTML markup that is inserted at the bottom of all pages.
- curate_header.html HTML markup that is inserted at the top of all curator's interface pages.
- curate_footer.html HTML markup that is inserted at the bottom of all curator's interface pages.
- profile_submit.html HTML markup for text that is inserted in to the submission interface prior to profile submission finalization. This can be used to add specific instructions such as the requirement to make an isolate submission.
- allele_submit.html HTML markup for text that is inserted in to the submission interface prior to allele submission finalization. This can be used to add specific instructions such as the requirement to attach Sanger trace files.

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

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

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

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

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

4.3 XML configuration attributes used in config.xml

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

4.3.1 Isolate database XML attributes

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

<db>

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

<system>

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

- authentication
 - Method of authentication: either 'builtin' or 'apache'. See user authentication.
- db
 - Name of database on system.
- dbtype
 - Type of database: either 'isolates' or 'sequences'.
- description
 - Description of database used throughout interface.
- align_limit
 - Overrides the sequence export record alignment limit in the Sequence Export plugin. Default: '200'.
- all_plugins
 - Enable all appropriate plugins for database: either 'yes' or 'no', default 'no'.
- annotation
 - Semi-colon separated list of accession numbers with descriptions (separated by a l), eg. 'AL157959|Z2491;AM421808|FAM18;NC_002946|FA 1090;NC_011035|NCCP11945;NC_014752|020-06'. Currently used only by Genome Comparator plugin.
- cache_schemes
 - Enable automatic refreshing of scheme field caches when batch adding new isolates: either 'yes' or 'no', default 'no'.
 - See scheme caching.

- codon_usage_limit
 - Overrides the record limit for the Codon Usage plugin. Default: '500'.
- contig_analysis_limit
 - Overrides the isolate number limit for the Contig Export plugin. Default: '1000'.
- curate_config
 - The database configuration that should be used for curation if different from the current configuration. This is used when the submission system is being used so that curation links in the 'Manage submissions' pages for curators load the correct database configuration.
- curate_link
 - URL to curator's interface, which can be relative or absolute. This will be used to create a link in the public interface dropdown menu.
- curate_path_includes
 - Partial path of the bigscurate.pl script used to curate the database. See user authentication.
- curate_script
 - Relative web path to curation script. Default 'bigscurate.pl' (version 1.11+).
 - This is only needed if automated submissions are enabled. If bigscurate.pl is in a different directory from bigsdb.pl, you need to include the whole web path, e.g. /cgi-bin/private/bigsdb/bigscurate.pl.
- curator_home
 - URL of curator's index page, which can be relative or absolute. This will be used to add a link in the dropdown menu.
- curators_only
 - Set to 'yes' to prevent ordinary authenticated users having access to database configuration. This is only effective if read_access is set to 'authenticated_users'. This may be useful if you have different configurations for curation and querying with some data hidden in the configuration used by standard users. Default 'no'.
- daily_pending_submissions
 - Overrides the daily limit on pending submissions that a user can submit via the web submission system. Default: '15'.
- daily_rest_submissions_limit
 - Overrides the limit on number of submissions that can be made to the database via the RESTful interface. This is useful to prevent flooding of the submission system by aberrant scripts. Default: '100'.
- default_access
 - The default access to the database configuration, either 'allow' or 'deny'. If 'allow', then specific users can be denied access by creating a file called 'users.deny' containing usernames (one per line) in the configuration directory. If 'deny' then specific users can be allowed by creating a file called 'users.allow' containing usernames (one per line) in the configuration directory. See *default access*.
- default_private_records
 - The default number of private isolate records that a user can upload. The user account must have a status of either 'submitter', 'curator', or 'admin'. This value is used to set the private_quota field when creating a new user record (which can be overridden for individual users). Changing it will not affect the quotas of existing users. Default: '0'.

- default_seqdef_config
 - Isolate databases only: Name of the default seqdef database configuration used with this database. Used to automatically fill in details when adding new loci.
- default_seqdef_dbase
 - Isolate databases only: Name of the default seqdef database used with this database. Used to automatically fill in details when adding new loci.
- default_seqdef_script
 - Isolate databases only: URL of BIGSdb script running the seqdef database (default: '/cgibin/bigsdb/bigsdb.pl').
- export_limit
 - Overrides the default allowed number of data points (isolates x columns) to export. Default: '25000000'.
- fast_scan
 - Sets whether fast mode scanning is enabled via the web interface. This will scan all loci together, using exemplar sequences. In cases where multiple loci are being scanned this should be significantly faster than the standard locus-by-locus scan, but it will take longer for the first results to appear. *Allele exemplars* should be defined if you enable this option. Set to 'yes' to enable. Default: 'no'.
- fieldgroup1 fieldgroup10
 - Allows multiple fields to be queried as a group. Value should be the name of the group followed by a colon
 (:) followed by a comma-separated list of fields to group, e.g. identifiers:id,strain,other_name.
- genome_comparator_limit
 - Overrides the isolate number limit for the Genome Comparator plugin. Default: '1000'.
- genome_comparator_max_ref_loci
 - Overrides the limit on number of loci allowed in a reference genome. Default: '10000'.
- genome_comparator_recommended_schemes
 - Comma-separated list of recommended schemes to suggest to Genome Comparator users. If lots of schemes are defined, a user may be tempted to click 'All loci' and this may not be the best option. Populating this attribute, results in an additional list of preferred schemes that can be chosen.
- genome_comparator_threads
 - The number of threads to use for data gathering (BLAST, database queries) to populate data structure for Genome Comparator analysis. You should not set this to less than 2 as this will prevent job cancelling due to the way isolates are queued. Default: '2'.
- hide_unused_schemes
 - Sets whether a scheme is shown in a main results table if none of the isolates on that page have any data for the specific scheme: either 'yes' or 'no', default 'no'.
- host
 - Host name/IP address of machine hosting isolate database, default 'localhost'.
- job_priority
 - Integer with default job priority for offline jobs (default:5).
- job_quota
 - Integer with number of offline jobs that can be queued or currently running for this database.

- labelfield
 - Field that is used to describe record in isolate info page, default 'isolate'.
- locus_aliases
 - Display locus aliases and use them in dropdown lists by default: must be either 'yes' or 'no', default 'no'. This option can be overridden by a user preference.
- locus_superscript_prefix
 - Superscript the first letter of a locus name if it is immediately following by an underscore, e.g. f_abcZ would be displayed as fabcZ within the interface: must be either 'yes' or 'no', default 'no'. This can be used to designate gene fragments (or any other meaning you like).
- maindisplay_aliases
 - Default setting for whether isolates aliases are displayed in main results tables: either 'yes' or 'no', default 'no'. This setting can be overridden by individual user preferences.
- noshow
 - Comma-separated list of fields not to use in breakdown statistic plugins.
- no_publication_filter
 - Isolate databases only: Switches off display of publication filter in isolate query form by default: either 'yes' or 'no', default 'no'.
- only_sets
 - Don't allow option to view the 'whole database' only list sets that have been defined: either 'yes' or 'no', default 'no'.
- password
 - Password for access to isolates database, default 'remote'.
- port
 - Port number that the isolate host is listening on, default '5432'.
- privacy
 - Displays E-mail address for sender in isolate information page if set to 'no'. Default 'yes'.
- public_login
 - Optionally allow users to log in to a public database this is useful as any jobs will be associated with the user and their preferences will also be linked to the account. Set to 'no' to disable. Default 'yes'.
- query_script
 - Relative web path to bigsdb script. Default 'bigsdb.pl' (version 1.11+).
 - This is only needed if automated submissions are enabled. If bigsdb.pl is in a different directory from bigscurate.pl, you need to include the whole web path, e.g. /cgi-bin/bigsdb/bigsdb.pl.
- read_access
 - Describes who can view data: either 'public' for everybody or 'authenticated_users' for anybody who has been able to log in. Default 'public'.
- related_databases
 - Semi-colon separated list of links to related BIGSdb databases on the system. This should be in the form of database configuration name followed by a 'l' and the description, e.g. 'pubmlst_neisseria_seqdeflSequence and profile definitions'. This is used to populate the dropdown menu.

- remote_contigs
 - Optionally allow the use of remote contigs. These are stored in a remote BIGSdb database, accessible via the RESTful API. Set to 'yes' to enable.
- script_path_includes
 - Partial path of the bigsdb.pl script used to access the database. See user authentication.
- seqbin_size_threshold
 - Sets the size values in Mbp to enable for the sequin filter.
 - Example: seqbin_size_threshold="0.5,1,2,4".
- seq_export_limit
 - Overrides the sequence export limit (records x loci) in the Sequence Export plugin. Default: '1000000'.

• sets

- Use sets: either 'yes' or 'no', default 'no'.
- set_id
 - Force the use of a specific set when accessing database via this XML configuration: Value is the name of the set.
- start_id
 - Defines the minimum record id to be used when uploading new isolate records. This can be useful when
 it is anticipated that two databases may be merged and it would be easier to do so if the id numbers in the
 two databases were different. Default: '1'.
- submissions
 - Enable automated submission system: either 'yes' or 'no', default 'no' (version 1.11+).
 - The curate_script and query_script paths should also be set, either in the bigsdb.conf file (for site-wide configuration) or within the system attribute of config.xml.
- submissions_deleted_days
 - Overrides the default number of days before closed submissions are deleted from the system. Default: '90'.
- tblastx_tagging
 - Sets whether tagging can be performed using TBLASTX: either 'yes' or 'no', default 'no'.
- total_pending_submissions
 - Overrides the total limit on pending submissions that a user can submit via the web submission system. Default: '20'.
- user
 - Username for access to isolates database, default 'apache'.
- user_job_quota
 - Integer with number of offline jobs that can be queued or currently running for this database by any specific user - this parameter is only effective if users have to log in.
- user_projects
 - Sets whether authenticated users can create their own projects in order to group isolates: either 'yes' or 'no', default 'no'.

• view

- Database view containing isolate data, default 'isolates'.
- views
 - Comma-separated list of views of the isolate table defined in the database. This is used to set a view for a set.
- webroot
 - URL of web root, which can be relative or absolute. This is used to provide a hyperlinked item in the dropdown menu. Default '/'.

<field>

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

```
<field type="text" required="no" length="40" maindisplay="no"
web="http://somewebsite.com/cgi-bin/script.pl?id=[?]" optlist="yes">epidemiology
<optlist>
<option>carrier</option>
<option>healthy contact</option>
<option>sporadic case</option>
<option>endemic</option>
<option>epidemic</option>
<option>pandemic</option>
</optlist>
</field>
```

• type

- Data type: int, text, float, bool, or date.
- comments * optional
 - Comments about the field. These will be displayed in the field description plugin and as tooltips within the curation interface.
- curate_only
 - Set to 'yes' to hide field on an isolate information page in the standard interface. The field will be visible
 if the page is accessed via the curator's interface (version 1.10.0+).
- default
 - Default value. This will be entered automatically in the web form but can be overridden.
- dropdown
 - Select if you want this field to have its own dropdown filter box on the query page. If the field has an option list it will use the values in it, otherwise all values defined in the database will be included: 'yes' or 'no', default 'no'. This setting can be overridden by individual user preferences.
- length
 - Length of field, default 12.
- maindisplay
 - Sets if field is displayed in the main table after a database search, 'yes' or 'no', default 'yes'. This setting can be overridden by individual user preferences.
- max

- Maximum value for integer and date types. Special values such as CURRENT_YEAR and CUR-RENT_DATE can be used.
- min
 - Minimum value for integer and date types.
- no_curate
 - Setting this will hide the field in the curator interface and prevent it from being manually modified. This is
 useful for fields that are populated by automated scripts or database triggers. Can be 'yes' or 'no', default
 'no'.
- optlist
 - Sets if this field has a list of allowed values, default 'no'. Surround each option with an <option> tag.
- regex
 - Regular expression used to constrain field values, e.g. regex="^[A-Z].*\$" forces the first letter of the value to be capitalized.
- required
 - Sets if data is required for this field, 'yes' or 'no', default 'yes'.
- userfield
 - Select if you want this field to have its own dropdown filter box of users (populated from the users table):
 'yes' or 'no', default 'no'.

• web

- URL that will be used to hyperlink field values. If [?] is included in the URL, this will be substituted for the actual field value.

4.3.1.1 Special values

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

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

<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

Required attributes are in **bold**.

<db>

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

<system>

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

- authentication
 - Method of authentication: either 'builtin' or 'apache'. See user authentication.
- db
 - Name of database on system.
- dbtype
 - Type of database: either 'isolates' or 'sequences'.
- description
 - Description of database used throughout interface.
- align_limit
 - Overrides the sequence export record alignment limit in the Sequence Export plugin. Default: '200'.
- allele_comments
 - Enable comments on allele sequences: either 'yes' or 'no', default 'no'.
 - This is not enabled by default to discourage the practice of adding isolate information to allele definitions (this sort of information belongs in an isolate database).
- allele_flags
 - Enable flags to be set for alleles: either 'yes' or 'no', default 'no'.
- curate_config
 - The database configuration that should be used for curation if different from the current configuration. This is used when the submission system is being used so that curation links in the 'Manage submissions' pages for curators load the correct database configuration.
- curate_path_includes
 - Partial path of the bigscurate.pl script used to curate the database. See user authentication.
- curate_script
 - Relative web path to curation script. Default 'bigscurate.pl' (version 1.11+).
 - This is only needed if automated submissions are enabled. If bigscurate.pl is in a different directory from bigsdb.pl, you need to include the whole web path, e.g. /cgi-bin/private/bigsdb/bigscurate.pl.
- curator_home
 - URL of curator's index page, which can be relative or absolute. This will be used to add a link in the dropdown menu.
- curators_only
 - Set to 'yes' to prevent ordinary authenticated users having access to database configuration. This is only effective if read_access is set to 'authenticated_users'. This may be useful if you have different configurations for curation and querying with some data hidden in the configuration used by standard users. Default 'no'.
- daily_pending_submissions
 - Overrides the daily limit on pending submissions that a user can submit via the web submission system. Default: '15'.
- daily_rest_submissions_limit

- Overrides the limit on number of submissions that can be made to the database via the RESTful interface. This is useful to prevent flooding of the submission system by aberrant scripts. Default: '100'.
- diploid
 - Allow IUPAC 2-nuclotide ambiguity codes in allele definitions for use with diploid typing schemes: either 'yes' or 'no', default 'no'.
- disable_seq_downloads
 - Prevent users or curators from downloading all alleles for a locus (admins always can). 'yes' or 'no', default 'no'.
- exemplars
 - Use exemplar sequences in the BLAST caches used for the sequence query pages. This is useful on larger databases as it speeds up the query significantly. *Exemplar alleles MUST* be defined otherwise sequence queries will fail. 'yes' or 'no', default 'no'.
- isolate_database
 - The config name of the isolate database. This is used to provide a link to isolate submissions. You also need to set isolate_submissions="yes".
- · isolate_submissions
 - Set to yes to provide a link to isolate submissions. The isolate_database attribute also needs to be set. Default: 'no'.
- job_priority
 - Integer with default job priority for offline jobs (default:5).
- job_quota
 - Integer with number of offline jobs that can be queued or currently running for this database.
- profile_submissions
 - Enable profile submissions (automated submission system): either 'yes' or 'no', default 'no' (version 1.11+).
 - To enable, you will also need to set submissions="yes". By default, profile submissions are disabled since generally new profiles should be accompanied by representative isolate data, and the profile can be extracted from that.
- public_login
 - Optionally allow users to log in to a public database this is useful as any jobs will be associated with the user and their preferences will also be linked to the account. Set to 'no' to disable. Default 'yes'.
- query_script
 - Relative web path to bigsdb script. Default 'bigsdb.pl' (version 1.11+).
 - This is only needed if automated submissions are enabled. If bigsdb.pl is in a different directory from bigscurate.pl, you need to include the whole web path, e.g. /cgi-bin/bigsdb/bigsdb.pl.
- read_access
 - Describes who can view data: either 'public' for everybody, or 'authenticated_users' for anybody who has been able to log in. Default 'public'.
- related_databases

- Semi-colon separated list of links to related BIGSdb databases on the system. This should be in the form of database configuration name followed by a 'l' and the description, e.g. 'pubmlst_neisseria_isolateslIsolates'. This is used to populate the dropdown menu.
- script_path_includes
 - Partial path of the bigsdb.pl script used to access the database. See user authentication.
- seq_export_limit
 - Overrides the sequence export limit (records x loci) in the Sequence Export plugin. Default: '1000000'.

• sets

- Use sets: either 'yes' or 'no', default 'no'.
- set_id
 - Force the use of a specific set when accessing database via this XML configuration: Value is the name of the set.
- submissions
 - Enable automated submission system: either 'yes' or 'no', default 'no' (version 1.11+).
 - The curate_script and query_script paths should also be set, either in the bigsdb.conf file (for site-wide configuration) or within the system attribute of config.xml.
- submissions_deleted_days
 - Overrides the default number of days before closed submissions are deleted from the system. Default: '90'.
- total_pending_submissions
 - Overrides the total limit on pending submissions that a user can submit via the web submission system. Default: '20'.
- user_job_quota
 - Integer with number of offline jobs that can be queued or currently running for this database by any specific user this parameter is only effective if users have to log in.
- webroot
 - URL of web root, which can be relative or absolute. This is used to provide a hyperlinked item in the dropdown menu. Default '/'.

4.4 Over-riding global defaults set in bigsdb.conf

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

- query_script
 - Relative web path to bigsdb script.
- curate_script
 - Relative web path to curation script.
- prefs_db
 - The name of the preferences database.

- auth_db
 - The name of the authentication database.
- tmp_dir
 - Path to the web-accessible temporary directory.
- secure_tmp_dir
 - Path to the web-inaccessible (secure) temporary directory.
- ref_db
 - The name of the references database.

4.5 Over-riding values set in config.xml

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

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

4.6 User authentication

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

4.6.1 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'.

4.6.2 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'.

4.7 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 hashes the password and stores this within the authentication database. Other users can be added by the admin user from the curation interface accessible from http://your_website/cgi-bin/private/bigscurate.pl?db=test_db (or wherever you have located your bigscurate.pl script).

4.8 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 get_refs.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 refs
pubmlst_bigsdb_neisseria_seqdef profile_refs, sequence_refs, locus_refs
```

The script can be called as follows:

get_refs.pl getrefs.conf

Run either as the 'postgres' user or an account that is allowed to connect as the postgres user.

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

4.9 Configuring access to remote contigs

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

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

remote_contigs = "yes"

4.9.1 Setting up authentication

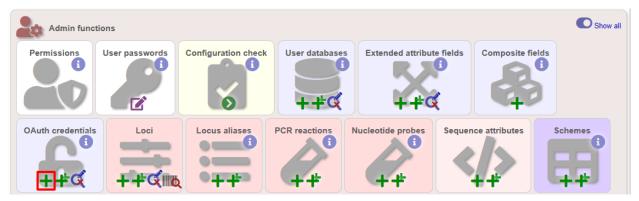
A client key for the BIGSdb remote contig manager needs to be generated. This can be done using the *cre-ate_client_credentials.pl* script, e.g.

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

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

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

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



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

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). @Log out Change password	Toggle: 🚯 🚍
Add new OAuth credentials	
Please fill in the fields below - required fields are marked with an exclamation mark (!). Record Action Action Consumer key:! RylqmtjBbSAkyyrZ5ZUyHzae Consumer secret! U6B_^%HJP9N^1Ax2wemPPkmqrt_J%m_rX6pkgkfdho access token! eHTH8jMXsnyhIUvJZFmDF7njI5I2QJsd access secret! QODGPqKoSgVcGwdlKBejufDsn4B1beX1 Curator:! Keith Jolley (keith) date entered:! 2017-11-23 datestamp:! 2017-11-23	Ē

4.9.2 Processing remote contigs

When remote contigs are first linked to a record, the sequences are downloaded in bulk (without their metadata). This allows the sequence lengths to be recorded as this is needed for various queries and outputs. The curator is then given an option to process the contigs, which involves downloading each contig individually to record metadata including the original designation and the sequence platform used. This may take a while so it may be preferable to perform this task offline. This can be done using the process_remote_contigs.pl script found in the scripts/automation directory. Options for using this script are shown below:

```
remote_contigs.pl --help
NAME
   process_remote_contigs.pl
   Download, check length and create checksum contigs stored as URIs
SYNOPSIS
   process_remote_contigs.pl --database NAME [options]
OPTIONS
--database NAME
   Database configuration name.
--exclude_isolates LIST
   Comma-separated list of isolate ids to ignore.
--exclude_projects LIST
   Comma-separated list of projects whose isolates will be excluded.
--help
   This help page.
--isolates LIST
   Comma-separated list of isolate ids to scan (ignored if -p used).
--isolate_list_file FILE
```

(continues on next page)

(continued from previous page)

```
File containing list of isolate ids (ignored if -i or -p used).
--min ID
Minimum isolate id.
--max ID
Maximum isolate id.
--projects LIST
Comma-separated list of project isolates to scan.
--quiet
Only display errors.
```

CHAPTER 5

Administrator's guide

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

5.1 Types of user

There are four types of user in BIGSdb:

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

5.2 User groups

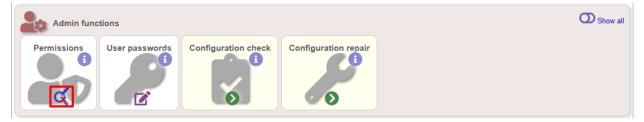
User groups allow submitter accounts to be grouped such that the submitter can edit isolates where the sender is either themselves or any member of a user group to which they belong.

5.3 Curator permissions

Individual permissions can be set for each curator:

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

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



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

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). [+Log out Change password	Help 🗗
Set curator permissions	
Select curator(s) Action Clark, Stephen (SClark) Select Clemence, Marianne (mclemence) Select Debech, Nadia (ndebech) Deghmane, Ala-Eddin (deghmane) Diallo, Kanny (kdiallo) Exley, Rachel (rexley) Feavers, Ian (ifeavers) Goodyer-Sait, Lily (lgoodyer) All None	

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

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

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

5.4 Locus and scheme permissions (sequence definition database)

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

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



Select the curator from the list:

Logged in: Keith Jolley (keith). C+Log out Change password Batch update locus curator access records
Batch update locus curator access records
users: Jolley, Keith (keith)

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

PubMLST Database home Curator home Contents
Logged in: Keith Jolley (keith). [+Log out Change password
Batch update locus curator access records
User: Keith Jolley Select values to enable or disable and then click the appropriate arrow button. Select loci VEIS0001 NEIS0005 NEIS0006 NEIS0006 NEIS007 NEIS0010 NEIS0010 NEIS0010 NEIS0010 NEIS0011 NEIS0012 NEIS0014 NEIS013 NEIS0014 NEIS014 NEIS014 NEIS014 NEIS014 NEIS014 NEIS014 NEIS014

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

5.5 Controlling access

5.5.1 Restricting particular configurations to specific user accounts

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

In the config.xml, add the following directive:

default_access="deny"

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

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

default_access="allow"

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

5.6 Setting user passwords

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

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



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

PubMLST Datab	ase home	Curator home	Contents		
Logged in: Keith Jolley (ke <i>ith).</i> 🗭 Log ou	t Change password			
Set user pas	ssword				
Passwords must be a	it least 8 chara	acters long.			
Passwords					Action
U	ser: Jolley, K	eith (keith)		•	Set password
	ord: ••••••				
Retype passwo	ord: ••••••	••			

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

5.7 Setting the first user password

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

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

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

5.8 Enabling plugins

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

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

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

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

BURST="yes"

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

5.9 Temporarily disabling database updates

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

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

5.9.1 Global

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

```
disable_updates=yes
```

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

disable_update_message=The server is currently undergoing maintenance.

5.9.2 Database-specific

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

```
<system

db="bigsdb_neisseria"

dbtype="isolates"

...

disable_updates="yes"

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

5.10 Host mapping

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

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

#Existing_host	Mapped_host
server1	server2
localhost	server2

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

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

5.11 Improving performance

5.11.1 Use mod_perl

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

5.11.2 Cache scheme definitions within an isolate database

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

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

update_scheme_caches.pl --database pubmlst_bigsdb_neisseria_isolates

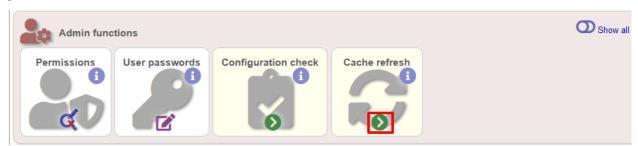
This script creates indexed tables within the isolate database called temp_scheme_X and temp_isolates_scheme_fields_1 (where X is the scheme_id). If these table aren't present, they are created as temporary tables every time a query is performed that requires a join against scheme definition data. This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

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

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

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

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



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

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

5.11.3 Use a ramdisk for the secure temporary directory

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

5.12 Dataset partitioning

5.12.1 Sets

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

See also:

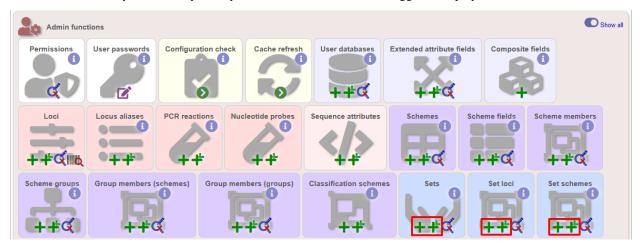
Sets (concept)

5.12.2 Configuration of sets

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

sets="yes"

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



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

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

PubMLST Database home Contents
Deg in Reisseria 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 Concess
Prease select: Whole database Curose Query database • Search or browse database • Main public projects • Set general options - including isolate table field handling. • Manage submissions • Manage submissions • Isolates: 46,731 • Search by combinations of loci (profiles) • Your projects • Set display and query options for locus, schemes or scheme fields. • Manage submissions • Isolates: 46,731 • Update history • About BIGSdb
Breakdown Breakdown Export Analysis Ocdon usage • Single field • Export dataset • Contigs • Codon usage • GrapeTree - Visualization of genomic relationships • Unique combinations • Sequences - XMFA / concatenated FASTA formats • Codon usage • GrapeTree - Visualization of genomic relationships • Scheme and alleles • Sequences - XMFA / concatenated FASTA formats • Description of database fields • Description of database fields • Niscellaneous • Description of database fields • Description of database fields • Wiscellaneous

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

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

set_id="1"

where the value is the name of the set.

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

5.12.3 Set 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>
</optlist>
</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.

Admin func	tions							C Show
Permissions	User passwords	Configuration ch	Cache refresh	User databases	Extended attribute fields	Composite fields		
Locus aliases	PCR reactions	PCR locus links	Nucleotide probes	Sequence attributes	Schemes	cheme fields Sche +++¢	erme members	
Scheme groups	Group members (schemes) Grou	p members (groups)	Classification schemer	s Sets	Set loci	et schemes	
Set metadata								

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'.

5.12.4 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:

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.

5.12.5 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>
```

5.13 Setting a site-wide users database

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

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



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

PubMLST Database	home Curator ho	ome Contents		
Logged in: Keith Jolley (keit	h). ⊕Log out Change pas	sword		Toggle: 🚺
Add new user	database			
	elow - required fields a	re marked with an exclamation mark (!).	+
Record				Action
id:	1	×		Reset Submit
name:	PubMLST	Site/domain name		
dbase name:!	pubmlst_bigsdb_users	3	Name of the database holding user data	
curator:	Keith Jolley (keith)			
datestamp:!	2016-12-16			
list order:				
auto registration:	🔘 true 🔘 false	Allow user to register themself for database	•	
dbase host:			IP address of database host	
dbase port:		🗧 🜖 Network port accepting database co	nnections	
dbase user:				
dbase password:)	
dbase user:			•	

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

5.14 Adding new loci

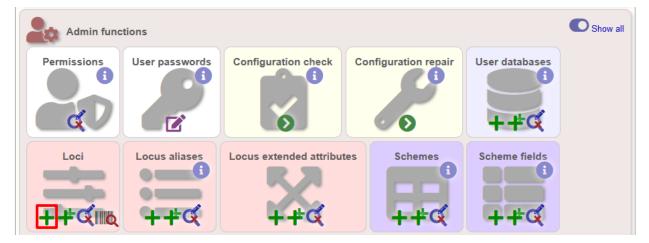
See also:

Loci (concept)

5.14.1 Sequence definition databases

5.14.1.1 Single locus

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



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

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

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

5.14.1.2 Batch adding

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

Admin func	tions				Show :
Permissions	User passwords	Configuration check	Configuration repair	User databases i ++¢	
	Locus aliases	Locus extended attribute	Schemes	Scheme fields	

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

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

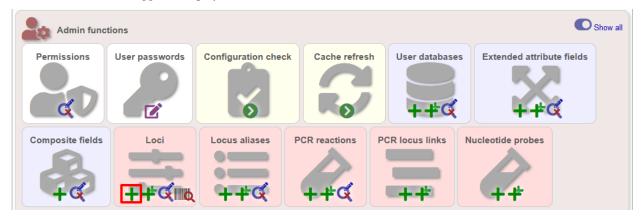
Fill in the spreadsheet using the fields described for *adding single loci*.

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

5.14.2 Isolate databases

5.14.2.1 Single locus

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



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

Logged in: Keith Jolley (keith). 🗭 Log o	out Change password				Toggle: 🚯 🗮
Add new locus					Show tools
Please fill in the fields below - re-	quired fields are marke	ed with an exclamation mark (!).		Action	+
id:!				Reset Submit	
data type:!	DNA 👻			- Court - Oubline	
allele id format!	integer 👻 🕕				
	🔘 true 🔘 false 🕕				
coding sequence:					
	allele only 👻 🕕				
main display:	🔘 true 🔘 false 🕕				
query field:	🖲 true 🔘 false 🚺				
analysis:	🖲 true 🔘 false 🚺				
curator:!	Keith Jolley (keith)				
date entered:!	2016-07-26				
datestamp:!	2016-07-26				
formatted name:			0		
common name:			0		
formatted common name:			0		
allele id regex:			0		
length:		♦ 1			
orf:	v 🚺				
genome position:		0			
match longest:	🔘 true 🔘 false 🜖				
reference sequence:					
				0	
	🔘 true 🔘 false 🜖	Do NOT set to true unless you define	PCR reactions linked to this locus.		
probe filter:	🔘 true 🔘 false 🜖	Do NOT set to true unless you define	probe sequences linked to this locus.		
dbase name:	pubmlst_bigsdb_neiss	seria_seqdef	Name of the database holding allele sequences		
dbase host:			 IP address of database host 		
dbase port:		🔹 🜖 Network port accepting database	connections		
dbase user:			0		
dbase password:			0		
dbase id:	PUT_LOCUS_NAME_H	HERE	Name of locus in seqdef database		

• id - The name of the locus

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

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

- description_url The URL used to hyperlink to locus information in the isolate information page. This can either be a relative (e.g. /cgi-bin/...) or an absolute (containing http://) URL.
 - Allowed: any valid URL.
- url The URL used to hyperlink to information about the allele. This can either be a relative or absolute URL. If [?] (including the square brackets) is included then this will be substituted for the allele value in the resultant URL. To link to the appropriate allele info page on a corresponding seqdef database you would need something like /cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_neisseria_seqdef&page=alleleInfo&locus=abcZ&allele_id=[?].
 - Allowed: any valid URL.
- submission_template Sets whether or not a column for this locus is included in the Excel submission template.
 - Allowed: true/false (default: false)

Using existing locus definition as a template

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

PubMLST Database home	Curator home Contents	
Logged in: Keith Jolley (keith). 🗭 Log ou	Change password	Toggle: 🜖 📃
Add new locus		Show tools
Record id:! data type:!		ľ
coding sequence:! isolate display:!	⊙ true	
query field:! analysis:!	● true	
datestamp:! ; formatted name: common name: formatted common name: allele id regex: length:		
complete cds: orf: genome position:	 ⊂ true ○ false ▼ ♥ 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'.

PubMLST	Database home	Curator home	Contents
Logged in: Keit	h Jolley (keith). 🗭 Log or	ut Change password	Toggle: 1) 📃
Add ne	w locus		Hide tools
	the fields below - requ id:! data type:! allele id format:! length varies:! coding sequence:! isolate display:! main display:! query field:! analysis:!	integer ▼ true ● false e true ● false allele only ▼ true ● false e true ● false e true ● false true ● false Keith Jolley (keith)	Copy configuration from NEIS0001 (lpxC) Copy All parameters will be copied except id, common name, reference sequence, genome position and length. The copied locus id will be substituted for 'PUT_LOCUS_NAME_HERE' in fields that include it.
	date entered.		
	formatted name:		
	common name:		
torm	atted common name: allele id regex:		
	length:		× v
	-	© true ◎ false	
	orf:	•	
	genome position:		
	match longest:	© true ◎ false	
	reference sequence:		

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

allele id regex:		0	
length:			
orf:			
genome position:			
match longest:			
reference sequence:			-
perfilter	☉ true .☉ false 1		0
	○ true ○ faise 1		
dbase host:	pubmlst_bigsdb_neisseria_seqdef	Name of the database holding allele sequences	
dbase port:			
dbase port. dbase user:			
dbase password:		0	
dbase table:			
dbase id field:		Database table that holds sequence information for this locus	-1- 14
dbase id2 field:		Primary field in sequence database that defines allele, e.g. 'alle	sie_id
	PUT_LOCUS_NAME_HERE	Secondary field that defines allele, e.g. 'locus'	
dbase idz value. dbase seq field:		Secondary field value, e.g. locus name	
	•	Field in sequence database containing allele sequence	_
description un.	/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_ne locus=PUT_LOCUS_NAME_HERE	isseria_seqdef&page=locusInfo&	
			0
uri:	<pre>/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_ne locus=PUT_LOCUS_NAME_HERE&allele_id=[?]</pre>	isseria_seqdef&page=alleleInfo&	
			0
submission template:	True Include column in isolate submission	template for this locus	
aliases:			
Action			

Complete the form and click 'Submit'.

5.14.2.2 Batch adding

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

Admin func	tions				C	Show
Permissions	User passwords	Configuration check	Cache refresh	User database	s Extended attribute fie	lds
Composite fields		Locus aliases	PCR reactions	PCR locus links	Nucleotide probes	

Click the link to download an Excel template:

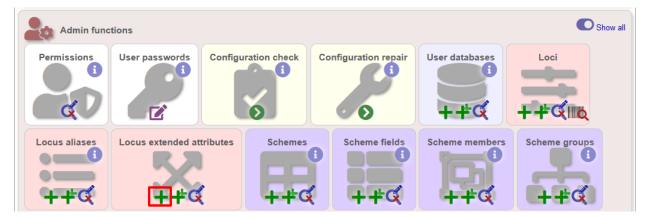
PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). C+Log out Change password		Toggle: 🚺 📃
Batch insert loci		
 This page allows you to upload locus data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order.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

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

5.15 Defining locus extended attributes

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

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



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

l in: Keith Jolley (keith). ➡Log out Change password			Toggle: 🕚
d new lo	cus extended attribute			
se fill in the field	below - required fields are marked with an exclam	nation mark (!).		
Record			Action	
locus:			Reset	ubmit
field:				
value format:!				
	🔿 true 🔘 false 🕓			
	● true ○ false			
	Keith Jolley (keith)			
datestamp:!	2018-06-18			
value regex: description:		0		
description.				
option list:				
			.4 🚯	
url:		6		
length:				
field order:	×			

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

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

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

5.16 Defining schemes

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

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

To set up a new scheme, you need to:

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

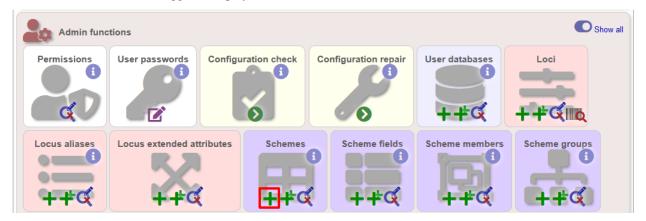
See also:

Schemes (concept)

5.16.1 Sequence definition databases

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

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



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

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

PubMLST Database I	home Curator home Contents	
Logged in: Keith Jolley (keith).	Log out Change password	Toggle: 🚯
Add new scher	ne	
Please fill in the fields below	v - required fields are marked with an exclamation mark (!).	
Record		_
id:!	1	
name:!	MLST 3	
curator:!	Keith Jolley (keith)	
datestamp:!	2018-06-18	
date entered:!	2018-06-18	
description:		
display order:		
	◯ true ◯ false 3 This is only relevant to schemes with primary key fields, e.g. MLST.	
disable:	\odot true \odot false Set to true to disable scheme. This can be overridden by user preference settings.	
no submissions:	🔿 true 🛇 false 💫 Set to true to prevent submission of profiles of this scheme via the automated submission syst	em.
flags:	experimental in development please cite unpublished Use CTRL/SHIFT click to select or deselect values	
PubMed ids:	h.	
links: (Format: URL description)		
Action Reset Submit		

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

Admin fund	ctions				Show all
Permissions	User passwords	Configuration check	Configuration repair	User databases	
Locus aliases	Locus extended attrib	Schemes	Scheme fields	Scheme members	Scheme groups

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

PubMLST Dat	abase home Curator hon	ne Contents			
Logged in: Keith Jolle	y (keith). 🗘 Log out Change password	1			Toggle: ()
Add new s	cheme member				
	at any modifications to the struct t allele designations, but any prof			al of all data from it. This i	s done to ensure data integrity.
Please fill in the fie	lds below - required fields are ma	ked with an exclam	ation mark (!). — Action ————		+
scheme id:!		•	Reset Submit		
locus:! curator:! datestamp:!	Keith Jolley (keith)				
field order:	1				

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

Admin fund	stions				Show all
Permissions	User passwords	uration check	Configuration repair	User databases ++¢¢	
Locus aliases	Locus extended attributes	Schemes +++¢	Scheme fields	Scheme members	Scheme groups

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

PubMLST Dat	tabase home	Curator home	Contents			
Logged in: Keith Jolle	ey (keith). 🗭 Log out	t Change password				Toggle: 🜖
Add new s	cheme fi	ield				
		ions to the structure ons, but any profiles			noval of all data from it. Thi	is is done to ensure data integrity.
	elds below - requi	red fields are marked	with an exclamati	on mark (!).		+
Record					Action	-
scheme id:!	MLST		-		Reset Submit	
field:	ST					
type:!	integer 👻					
primary key:!	◉ true ◯ false	e 🚹				
dropdown:!	🔘 true 🔘 false	ə 🚯				
curator:	Keith Jolley (ke	eith)				
datestamp:!	2018-06-18					
description:						
field order:	1	· · · · · · · · · · · · · · · · · · ·				
index:	© true © false	9 🚯				
value regex:				8		

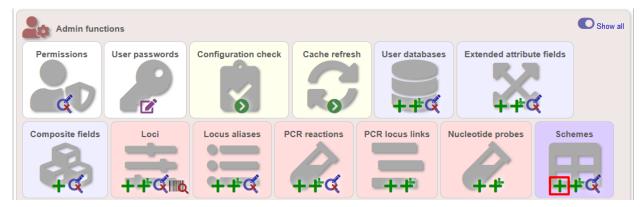
- scheme_id Dropdown box of scheme names.
 - Allowed: selection from list.
- field Field name.
 - Allowed: any value.
- type Format for values.
 - Allowed: text/integer/date.
- primary_key Set to true if field is the primary key. There can only be one primary key for a scheme.
 - Allowed: true/false.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

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

5.16.2 Isolate databases

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

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



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

Logged in: Keith Jolley (keith).	Dog out Change password		Toggle: 🚯 📃
Add new schen	ne		
	w - required fields are marked with an exclamation mark (!).	Action	+
name:! isolate display:! main display:! query field:! query status:! analysis:!		Action Reset Submit	
dbase name:	0		
dbase host:	0		
dbase port:	★ 0		
dbase user:	0		
dbase password:	0		
dbase id:			
display order:			
allow missing loci:	○ true ○ false ③ This is only relevant to schemes with primary key fields, e.g. MLST.		
	Citation required experimental in development unpublished Use CTRL/SHIFT dick to select or deselect values		
PubMed ids:			
links: (Format: URL description)			

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

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

5.17 Organizing schemes into hierarchical groups

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

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

	Joney (Kelui). 🗭 Log o	ut Change password					Help 🖍
ownloa	ad alle	le se	equences					
elect loci by	scheme A	Iphabeti	cal list All loci by s	scheme				
				g to scheme	es or groups of	chemes - clicking a group folder will displ	ay the loci for all s	chemes within the group and any subgrou
lick the node	es to expand	/collaps	е.					
4	Replicati	on and F	Repair					^
		replicat	ion					
		eotide e	xcision repair					
	Transcrip							
	🛄 Translati							
	Genomic isla							
	ineage Sch	emes						
-	Netabolism							
þ 🔊 N	 gonorrhoe 	ae AMR						
6 🔊 F	Plasmids							
— 🚛 🛄 Т	Typing							
	🔲 MLST							
								Ŧ
ILST								
		Allolos	Length (setting)	Min longth	Max longth	Ill name/product Curator(s)	Last updated	
abcZ			Fixed: 433 bp	433	434	O. Harrison, K. Jolley		
adk 🛃		651	Fixed: 465 bp	465	465	O. Harrison, K. Jolley		
aroE 🛃	DNA	929	Fixed: 490 bp	490	493	O. Harrison, K. Jolley	2018-06-11	
umC 🛃			Fixed: 465 bp	463	465	O. Harrison, K. Jolley		
gdh 🛓			Fixed: 501 bp	501	513	O. Harrison, K. Jolley		
	DNA		Fixed: 480 bp Fixed: 450 bp	480 447	503 450	O. Harrison, K. Jolley O. Harrison, K. Jolley		
pdhC 🚽	DNA							

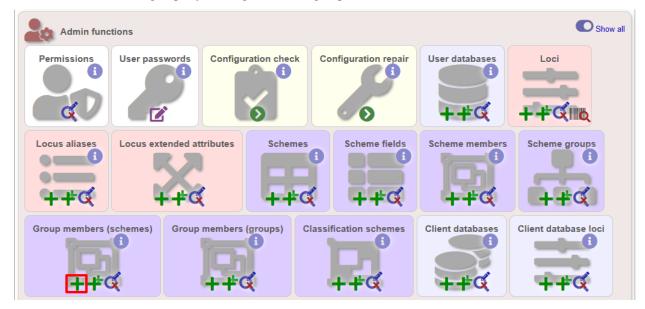
Scheme groups can be added in both the sequence definition and isolate databases. To add a new group, click the add (+) scheme group link on the curator's contents page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.

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

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

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

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



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

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

PubMLST Database home Curator home Co	ntents	
Logged in: Keith Jolley (keith). Hog out Change password		Toggle: 🜖 📃
Add new scheme group scheme	member	
Please fill in the fields below - required fields are marked with a Record group id:! Typing scheme id:! MLST curator:! Keith Jolley (keith) datestamp:! 2018-06-18	Action Reset Submit	ľ

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

5.18 Setting up client databases

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

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

Multiple client databases can be queried simultaneously.

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

Admin functions					C Shov
Permissions User pas	Sources Configuration	check Configuration	User datab		Locus aliases
Locus extended attributes	Schemes +++		Scheme ++ C	groups Group member Group member Group member Group member	ers (schemes)
Group members (groups)	Classification schemes	Client databases	Client database loci	Client database fields	Locus curators

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

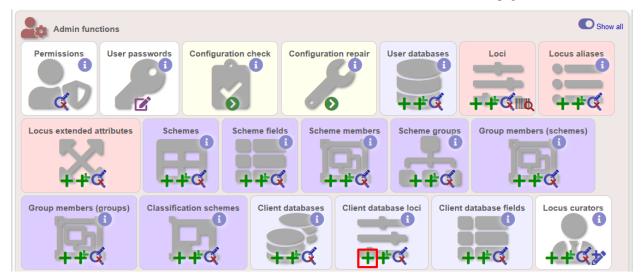
PubMLST Database	e home Curator home Con	tents	
Logged in: Keith Jolley (keith). 🕩 Log out Change password		Toggle: 🚯 📃
Add new clien	t database		
Please fill in the fields bel	ow - required fields are marked with an	n exclamation mark (l).	
Record		Action	
id:!	1	Reset Sub	mit 🔤
name:!	PubMLST isolates		
description:1	diversity of <u>Neisseria</u> spec database there is at least	tion of isolates that represent the total known ties. For every allelic profile in the profiles one corresponding isolate deposited here. Any o this database and consequently it should be noted a population sample.	
dbase name:!	pubmlst_bigsdb_neisseria_isolates	Name of the database holding isolate data	
dbase config name:!	pubmlst_neisseria_isolates	Name of the database configuration	
curator:	Keith Jolley (keith)		
datestamp:!	2018-06-19		
dbase host:		IP address of database host	
dbase port:	🕀 🚯 Network (oort accepting database connections	
dbase user:		0	
dbase password:		0	
dbase view:	isolates	View of isolates table to use	
url:	/cgi-bin/bigsdb/bigsdb.pl	Web URL to database script	

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

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

5.18.1 Look up isolates with given allele

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



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

PubMLST Databa	ase home Cu	irator home	Contents		
Logged in: Keith Jolley (ke	e <i>ith).</i> 🗭 Log out Cha	nge password			Toggle: 🜖 📃
Add new loc	us to clie	nt datab	ase definition		
Record client dbase id: locus: curator:	1) PubMLST isol abcZ Keith Jolley (ke 2018-06-19	ates 💌	with an exclamation mark (!).	Action Reset Submit	đ
lucus alias.			name that this locus is referred by in client database (if different)		

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



5.18.2 Look up isolates with a given scheme primary key

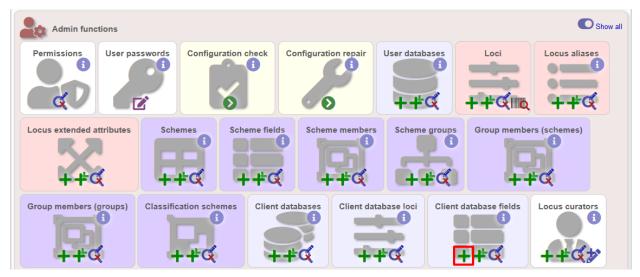
Setting this up is identical to setting up for alleles (see above) except you click on the add (+) client database schemes link and choose the scheme and client databases in the dropdown list boxes.

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

ST abcZ adk aroE fumC gdh pdhC pgm clonal complex 11 2 3 4 6 ST-11 complex sender: Paula Kriz, Paula Kriz and Keith Jolley curator: Keith Jolley, University of Oxford, UK date entered: 2001-02-07 client database	
11 2 3 4 3 8 4 6 ST-11 complex sender: Paula Kriz, Paula Kriz and Keith Jolley curator: Keith Jolley, University of Oxford, UK date entered: 2001-02-07 datestamp: 2009-11-11	e information for ST-11 (MLST)
curator: Keith Jolley, University of Oxford, UK date entered: 2001-02-07 datestamp: 2009-11-11	
date entered: 2001-02-07 datestamp: 2009-11-11	
datestamp: 2009-11-11	curator: Keith Jolley, University of Oxford, UK
	date entered: 2001-02-07
Client database	datestamp: 2009-11-11
onen auabase	ent database
PubMLST isolates: Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles data there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be not does not represent a population sample. 5433 isolates	there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should b

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

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



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

PubMLST Databa	se home Curator home Contents		
Logged in: Keith Jolley (ke	th). 🕩 Log out Change password		Toggle: 🜖
Add new loc	is to client database isolate field definition	n	
Record client dbase id:! locus:! isolate field:! curator:! datestamp:!	keith Jolley (keith)	Reset Submit	E

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

ged in: Keith Jolley (keith).	ELog out Change password Help E	3
lele informat	ion - penA: 9	
Provenance/met	ta data	
locus:	penA	
allele:	9	
sequence:	GACGGCGTTT TGCTGCCGGT CAGCTTTGAA AAACAGGCGG TTGCGCCGCA AGGCAAACGT ATATTTAAAG CATCGACCGC ACGTCAGGTG CGTCAGTTGA TGGTTTCTGT AACCGAACCT GGCGGTACGG GTACGGCGGG TGGCGGTAGAT GGTTTCGACG TCGGCGCAAA AACCGGTACG GCGCGTAAGT TGGTTAACGG TCGTTACGTC GATTACAAAC ACGTTGCCAC TTTCATCGGT TTTGCCCCGG CTAAAAATCC GCGGTGATT GTGGCGGTAA CCATTGACGA GCCGACTGCC AACGGTTACT ACGGCGGCGC AGTGACAGGT CCGGTCTTCA AACAAGTTAT GGGCGGTAGC CTGAACATCT TGGGCGTTTC TCCGACCAAA CCTCTGACCA AT	
length:	402	
status:	Sanger trace checked	
date entered:	2006-09-04	
datestamp:	2006-09-04	
sender:	Muhamed-Kheir Taha, National Reference Center for Meningococci, Institut Pasteur, France	
curator:	Keith Jolley, University of Oxford, UK	
mutation F504L:	yes	
mutation A510V:	yes	
mutation I515V:	yes	
mutation H541N:	yes	
mutation 1566V:	yes	
Publication (1)		
Heuberger S, Hoffma Stefanelli P, Thulin S	JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enríquez R, Fazio C, Frosch ann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczynska S, Tzanakaki G, Unemo M, Vogel U, Zarantonelli ML (2007). Target gene sequencing to characterize the penicillin G susceptibility of Neisseria crob Agents Chemother 51:2784-92	
Isolate database	2S	
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 dat there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be not does not represent a population sample. 494 isolates	
Linked data		
	>0.06 - 1 (intermediate) [n=92] PubMLST isolates	

5.19 Rule-based sequence queries

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

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

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

5.19.1 Example rule code

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

The code for this rule is as follows:

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

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5.19.1.1 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).

5.19.1.2 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

5.19.1.3 Adding descriptive text

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

5.20 Workflow for setting up a MLST scheme

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

Seqdef database

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

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

Isolate database

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

5.21 Automated assignment of scheme profiles

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

The script is run as follows:

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

A full list of options can be found by typing:

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

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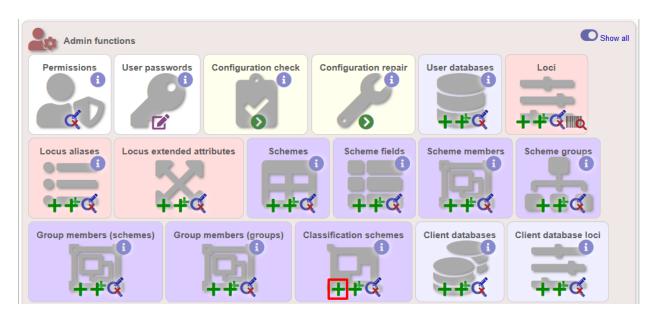
```
--exclude_projects LIST
   Comma-separated list of projects whose isolates will be excluded.
--ignore_multiple_hits
    Set allele designation to 'N' if there are multiple designations set for
    a locus. The default is to use the lowest allele value in the profile
    definition.
--isolates LIST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

5.22 Scheme profile clustering - setting up classification schemes

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

5.22.1 Defining classification scheme in sequence definition database

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



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

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

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

rather than

total loci - defined threshold

when an absolute threshold is used.

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

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

Press 'Submit' to create the classification scheme.

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

5.22.2 Defining classification scheme in isolate database

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

Admin fund	tions					C Sho
Permissions	User passwords	Configuration check	Cache refres	User databases	Extended attribute fields	Composite fields
Loci	Locus aliases	PCR reactions	CR locus links	Nucleotide probes	Sequence attributes	Schemes
Scheme fields	Scheme members	Scheme groups	Group members	s (schemes) Group	members (groups) Class	ification schemes

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

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

PubMLST Database hom	e Curator home Contents		
Logged in: Keith Jolley (keith). 🏵 Log	g out Change password		Toggle: 🜖 📃
Add new classific	cation scheme		
Please fill in the fields below - re 	quired fields are marked with an exclamation mark (!).	Action	ľ
id:!	2 .	Reset Submit	
scheme id:!	N. meningitidis cgMLST v1.0		
name:!	Nm_cgc_25		
inclusion threshold:	25 🚖 Maximum number of different alleles allowed between profile and at least one group member profile.		
use relative threshold:!	O true I false Calculate threshold using ratio of shared/present in both profiles in pairwise comparison.		
status:	experimental 💌		
curator:!	Keith Jolley (keith)		
datestamp:!	2018-06-19		
description:	Single linkage clustering with each group member having fewer than 25 allelic mismatches to at least one other member of the group. Missing loci are ignored in comparisons.		
seqdef cscheme id:	2 cscheme_id number defined in seqdef database		
display order:	A V		

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

5.22.3 Clustering

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

Currently only single-linkage clustering is supported.

The script is run as follows from the command line:

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

A full list of options can be found by typing:

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

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

generated and kept up-to-date.

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

	invasive (unspecified/other)			Potters Bar, UK	arus anu controis	,		
epidemiology:	endemic							
Publications (2)								
	, Urwin R, Russell JE, Bygra Clin Microbiol 37:3883-7 14		B, Maiden MC (1	999). Multilocus	sequence typing a	and antigen gen	e sequencing in the investigation of	f a meningococcal
	Bratcher HB, Harrison OB, Fe nods. <i>J Clin Microbiol</i> 50: 304		1aiden MC (2012).	Resolution of a	meningococcal di	sease outbreak	from whole-genome sequence dat	a with rapid Web-
Sequence bin								
contigs:	259	mean length:	8,245 bp	N90 c	ontig number:	63	N95 length (L95):	4,593
total length:	2,135,447 bp	N50 contig number:	18	NS	0 length (L90):	8,066	loci tagged:	2,180
max length:	130,716 bp	N50 length (L50):	38,364	N95 c	ontig number:	79	detailed breakdown:	Display
Similar isolates	(determined by classifi	cation schemes)						
Experimental schemes are	subject to change and are no	ot a stable part of the r	nomenclature.					
Classification scheme	Underlying scheme	Clustering method M	lismatch thresho	ld Status	Group			
	. meningitidis cgMLST v1.0	Single-linkage	200		group: 17 (841 is	olates)		
	. meningitidis cgMLST v1.0	Single-linkage	100	experimental	group: 38 (588 is	olates)		
	. meningitidis cgMLST v1.0	Single-linkage	50		group: 45 (4 iso			
Nm_cgc_25 N	. meningitidis cgMLST v1.0	Single-linkage	25	experimental	group: 45 (4 iso	lates)		
Schemes and lo	ci							
All loci	Navigate	and select schemes	within tree to disp	lay allele designa	ations			
Capsule								
	nation Processing							
Genetic mon	auon nocessing							

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

ged in: Keith Joll	ey (keith). 🗭 Log	out Chan	ge password								Hel	p 🗹	Toggle: 🤇
arch or	browse	e Neis	sseria PubMLS	ST database	9								
ter search crite	ria or leave bla	nk to brov	vse all records. Modify form	parameters to filter or	enter a list o	of values.							(
-Isolate prover	ance/phenoty	oe fields -		,	Allele design:	ations/schem	ne fields						
id	• =		✓ Enter value	+ 3 N	lm_cgc_25 gr	roup 👻	- •	45		+	6		
-Display/sort	ptions				Action —								
Order by:					Reset	Submit							
Display:	25 • record	ls per pag				Cubillit							
ecords returned - Your projects -	Click the hyp	erlinks for	detailed information.										
		erlinks for se record											
-Your projects - Select project	 Add the 	se record	s Isolate fie						MLST		typing anti		
Your projects - Select project	Add the liases court	se record Itry year	s Isolate fie disease	species) genogroup			clonal complex	PorA VR1	PorA VR2	FetA V	
Your projects elect project d isolate a 2 2837 M9	Add the liases cour //252508 Ui	se record Itry year (1997	s Isolate fie disease invasive (unspecified/other)	species Neisseria meningitidi	s C	genogroup	С	50	clonal complex ST-11 complex	PorA VR1 5-1	PorA VR2 10-4	FetA V F3-6	
Your projects Select project d isolate a 52 2837 M93 70 2840 M93	Add the Iiases cour //252508 UH //252535 UH	se record Itry year (1997 (1997	Isolate fie disease invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidi Neisseria meningitidi	s C s C) genogroup	C C	50 50	Clonal complex ST-11 complex ST-11 complex	PorA VR1 5-1 5-1	PorA VR2 10-4 10-4	FetA V F3-6 F3-6	
-Your projects Select project d isolate a 52 2837 M93 70 2840 M93	 Add the Iiases court I/252508 UF I/252535 UF I/252781 UF 	se record try year (1997 (1997 (1997	s Isolate fie disease invasive (unspecified/other)	species Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi	s C s C s C) genogroup	С	50 50 50	clonal complex ST-11 complex	PorA VR1 5-1	PorA VR2 10-4	FetA V F3-6	
Your projects Select project d isolate a 62 2837 M93 70 2840 M93 71 2844 M93 72 2847 M93	 Add the Iiases court I/252508 UH I/252535 UH I/252781 UH I/252943 UH 	se record try year (1997 (1997 (1997	s Isolate fie disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi	s C s C s C	genogroup	C C C	50 50 50	clonal complex ST-11 complex ST-11 complex ST-11 complex	PorA VR1 5-1 5-1 5-1	PorA VR2 10-4 10-4 10-4	FetA V F3-6 F3-6 F3-6	
Your projects jelect project d isolate a 52 2837 M97 70 2840 M97 71 2844 M97 72 2847 M97	 Add the Iiases court I/252508 UH I/252535 UH I/252781 UH I/252943 UH 	se record try year (1997 (1997 (1997	s Isolate fie disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi	s C s C s C) genogroup	C C C	50 50 50	clonal complex ST-11 complex ST-11 complex ST-11 complex	PorA VR1 5-1 5-1 5-1	PorA VR2 10-4 10-4 10-4	FetA V F3-6 F3-6 F3-6	
Your projects Select project d isolate a 52 2837 M93 70 2840 M93 71 2844 M93	 Add the liases court /252508 UH /252535 UH /252781 UH : 	se record try year (1997 (1997 (1997	s disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi	s C s C s C s C	genogroup	C C C	50 50 50 50	clonal complex ST-11 complex ST-11 complex ST-11 complex	PorA VR1 5-1 5-1 5-1	PorA VR2 10-4 10-4 10-4	FetA V F3-6 F3-6 F3-6	
Your projects select project 2 2837 M9 70 2840 M9 71 2844 M9 72 2847 M9 malysis tools	 Add the Iiases court /252508 UH /252781 UH /252781 UH : Fields Th 	se record try year (1997 (1997 (1997 (1997	Isolate fie disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) Combinations Polymor	species Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi Neisseria meningitidi	s C s C s C s C		C C C C Sequence bin	50 50 50 50	Clonal complex ST-11 complex ST-11 complex ST-11 complex ST-11 complex	PorA VR1 5-1 5-1 5-1	PorA VR2 10-4 10-4 10-4	FetA V F3-6 F3-6 F3-6	

5.23 Defining new loci based on annotated reference genome

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

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

Admin func	tions					C Show
Permissions	User passwords	Configuration che	Cache refre	User databases		Composite fields
	Locus aliases	PCR reactions	PCR locus links	Nucleotide probes	Sequence attributes	Schemes

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

Ξ

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

PubMLST	Database	home Curator home Contents	
Logged in: Keith	Jolley (keith	. (Log out Change password	=
Scan El	MBL/G	enbank record for loci	
	allows you to nter accessio	scan an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci. n number — — Primary identifier — — Action ——	
Accession:			
Download tabl	e: tab-delimit	ed text Excel format (suitable for batch upload of loci).	
Download allel	les: tab-delin	ited text Excel format (suitable for defining the first allele in the seqdef database).	
Annotation	n informati	on	
	accession	AM421808	
	version		
	type	dna	
		2194961	
		Neisseria meningitidis serogroup C FAM18 complete genome.	
	ling regions		
Coding see	quences		
Locus	Aliases	Product	Length
NMC0001	IpxC;	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924
	envA		
NMC0002	pilS1 pilS2	pilin (fragment) truncated pilin	291 366
NMC0003 NMC0004	fbp	peptidyl-prolyl cis-trans isomerase	330
NMC0005	inh	putative membrane protein	219
NMC0006		putative ritembare protein	954
NMC0007	metG	methionyl-tRNA synthetase	2058
NMC0008	glmS	qlucosaminefructose-6-phosphate aminotransferase [isomerizing]	1839
NMC0009	3	giocosanine indecese o prospinate animetara prospinate promotizante prospinate animetara	519
NMC0010	gna33	outer membrane lipoprotein Gna33 1	1326
NMC0011	3	putative integral membrane protein	840
NMC0012		putative lipoprotein	1167

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

PubMLST	Database I	nome Curator home Contents	
Logged in: Keith	Jolley (keith).	Log out Change password	Ξ
Scan El	MBL/Ge	nbank record for loci	
		can an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci.	
Accession:	nter accession AM421808	number Primary identifier Action © locus tag O gene name Submit	
		I text Excel format (suitable for batch upload of loci). ed text Excel format (suitable for defining the first allele in the seqdef database).	
Annotation	n informatio	n	
	accession:	AM421808	
	version:	1	
	type:	dna	
	length:	2194961	
		Neisseria meningitidis serogroup C FAM18 complete genome.	
	ling regions:		
Coding sec	quences		
Locus	Aliases	Product	Length
NMC0001	lpxC;	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924
	envA		
NMC0002	pilS1	pilin (fragment)	291
NMC0003	pilS2	truncated pilin	366
NMC0004 NMC0005	fbp	peptidyl-prolyl cis-trans isomerase	330
NMC0005 NMC0006		putative membrane protein putative glycerate dehydrogenase	219 954
NMC0006 NMC0007	metG	putative giycerate denydrogenase methionyl-tRNA synthetase	2058
NMC0007	glmS	glucosaminefructose-6-phosphate aminotransferase [isomerizing]	1839
NMC0009	gino	giucusanineructose-o-prosprate aninotransierase (isomenzing) putative lipoprotein	519
NMC0010	gna33	outer membrane lipoprotein Gna33 (3)	
111100010			1326
NMC0011	5	putative integral membrane protein	1326 840

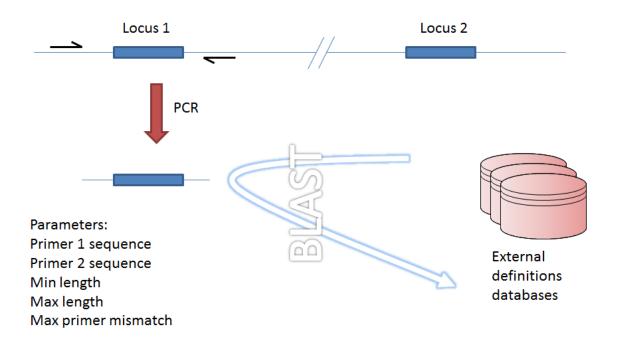
5.24 Genome filtering

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

5.24.1 Filtering by in silico PCR

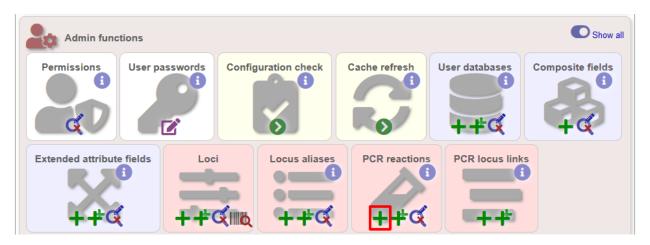
Provided a locus can be predicted to be specifically amplifed by a PCR reaction, the genome can be filtered to only look at regions predicted to fall within amplification products of one or more PCR reactions. Since this is *in silico* we don't need to worry about problems such as sequence secondary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

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



Locus 1 and locus 2 share allele pool

Fig. 1: Genome filtering by in silico PCR.

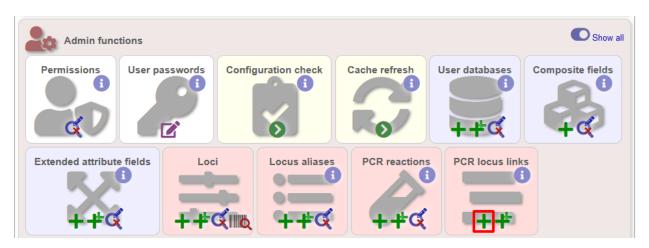


In the resulting web form you can enter values for your two primer sequences (which can be any length), the minimum and maximum lengths of reaction products you wish to consider and a value for the allowed number of mismatches per primer.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). C+Log out Change password	Toggle: 🚯 📃
Add new PCR reaction	
Please fill in the fields below - required fields are marked with an exclamation mark (!).	+
id: 2	E
description:	
primer1:	
primer2:1	
curator:! Keith Jolley (keith)	
datestamp: 2018-06-19	
min length: 🚔 Minimum length of product to return	
max length: 🚔 Maximum length of product to return	
max primer mismatch: 🚽 🕚 Maximum sequence mismatch per primer	
Action	
Reset Submit	

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

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



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

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

5.24.2 Filtering by in silico hybridization

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

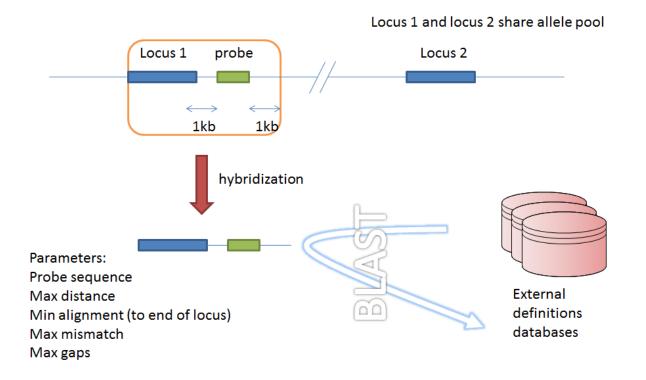
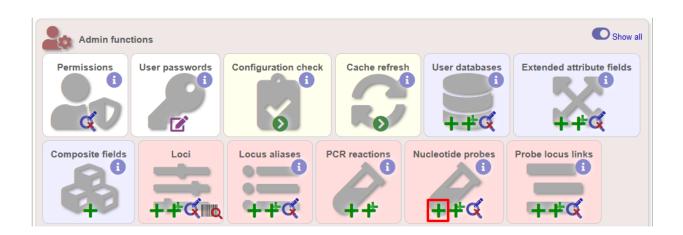
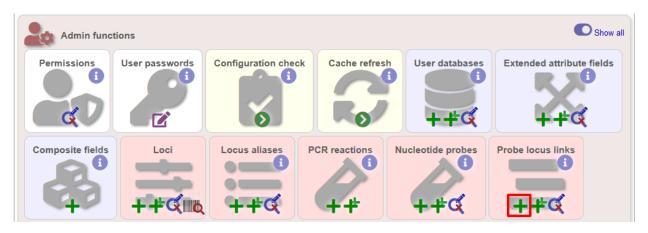


Fig. 2: Filtering by in silico hybridization

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



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



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

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

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

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

5.25 Setting locus genome positions

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

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

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

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

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

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

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

Click the 'Renumber' button:

gged in: Keitl	h Jolley (keith). 🗭	.og out Change pas	sword							Help 🗹	Toggle: 🕚	
equen	ce bin fo	r MC58										
ontig sun	nmary statistic	s										
	Contigs: 1											
	Length: 2,	272 360										
	Lengui: 2,	212,300										
Downlo	ad sequences (F	ASTA format)										
	bad sequences (i bad sequences wi		MBL form	at)								
• Downic	bad sequences wi	th annotations (E		ar)								
												_
equence	Sequencing method	Original designation	Length	Comments	Locus	Start	End	Direction	EMBL format	Artemis	Renumber	
equence 1	Sequencing method Sanger	Original designation	Length 2272360	Comments whole	Locus NEIS2139	Start 7	End 498	Direction ←	EMBL format	Artemis Artemis	Renumber	
	method								format	•	3	
	method			whole	NEIS2139	7	498	←	format	•	3	
	method			whole	NEIS2139 NEIS2140	7 502	498 897	$\begin{array}{c} \leftarrow \\ \leftarrow \\ \leftarrow \end{array}$	format	•	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141	7 502 918	498 897 2312	\downarrow \downarrow \downarrow	format	•	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142	7 502 918 2517	498 897 2312 3161	$\begin{array}{c} \downarrow \\ \downarrow $	format	•	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143	7 502 918 2517 3158	498 897 2312 3161 3511	↑ ↓ ↓ ↑ ↓ ↓ ↓	format	•	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2142 NEIS2143 NEIS2144	7 502 918 2517 3158 3635	498 897 2312 3161 3511 4117	+ + + + + + + + + + + + + + + + + + +	format	•	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2144	7 502 918 2517 3158 3635 4311	498 897 2312 3161 3511 4117 4961	↑ ↓ ↓ ↑ ↓ ↓ ↓	format	•	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2144 NEIS2145 NEIS2146	7 502 918 2517 3158 3635 4311 4958	498 897 2312 3161 3511 4117 4961 5875	$\begin{array}{c} \downarrow \\ \downarrow \\ \downarrow \\ \downarrow \\ \downarrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\$	format	•	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2144 NEIS2145 NEIS2146 NEIS2147	7 502 918 2517 3158 3635 4311 4958 5936	498 897 2312 3161 3511 4117 4961 5875 6214	$\begin{array}{c} \downarrow \\ \downarrow \\ \downarrow \\ \downarrow \\ \downarrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \uparrow \\ \downarrow \\ \downarrow$	format	•	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2145 NEIS2146 NEIS2146 NEIS2147 NEIS2148 (pgk) NEIS2149	7 502 918 2517 3158 3635 4311 4958 5936 6281	498 897 2312 3161 3511 4117 4961 5875 6214 7492	↓ ↓	format	•	3	
	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2145 NEIS2146 NEIS2147 NEIS2148 (pgk)	7 502 918 2517 3158 3635 4311 4958 5936 6281 7573	498 897 2312 3161 3511 4117 4961 5875 6214 7492 8826	$\begin{array}{c} \downarrow \downarrow$	format	•	3	
Sequence 1	method			whole	NEIS2139 NEIS2140 NEIS2141 NEIS2142 NEIS2143 NEIS2144 NEIS2145 NEIS2146 NEIS2147 NEIS2147 NEIS2148 (pgk) NEIS2149 tRNA-lys	7 502 918 2517 3158 3635 4311 4958 5936 6281 7573 9197	498 897 2312 3161 3511 4117 4961 5875 6214 7492 8826 9272	↓ ↓	format	•	3	

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

PubMLST Database home C	rator home Contents	
Logged in: Keith Jolley (keith). 🗭 Log out Chi	ge password	Ξ
Renumber locus gen	me positions based on tagged sequences	
You have selected to renumber the geno	ne positions set in the locus table based on the tagged sequences in sequence id#1.	
Option	Action	
Remove positions for loci not tagge	in this sequence Renumber	
The following designations will be made:		
Locus	nome position New genome position	
NEIS2139	7	
NEIS2140	502	
NEIS2141	918	
NEIS2142	2517	
NEIS2143	3158	
NEIS2144	3635	
NEIS2145	4311	
NEIS2146	4958	
NEIS2147	5936	
NEIS2148	6281	
NEIS2149	7573	
tRNA-lys	9197	
NEIS2150	9346	
NEIS2151	10350	
NEIS2152	10840	
NEIS2153	12174	
NEIS2979	13848	
NEIS0001	15221	
NEIS0210	17229	
NEISp0210	17232	
pilS	18127	

5.26 Defining composite fields

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

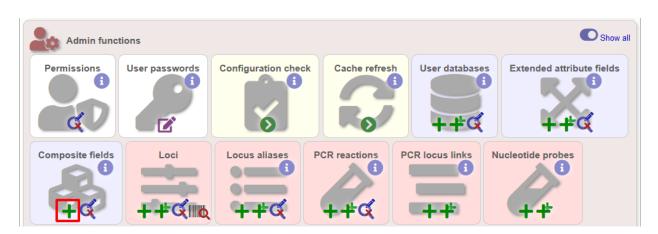
One example of a composite field is used in the Neisseria PubMLST database which has a strain designation composite field made up of serogroup, PorA VR1 and VR2, FetA VR, ST and clonal complex designations in the format:

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

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

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

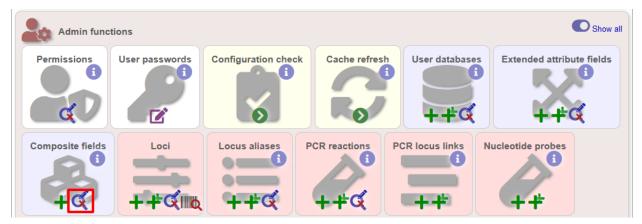
Composite fields can be added to the database by clicking the add (+) composite fields link on the curator's main page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



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

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

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



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

PubMLS	ST Da	tabase home	Curator ho	me Cont	ents	
Logged in: I	Keith Joll	ey (keith). 🗭 Log out	Change passwo	rd		
Jpda	te or	delete co	mposit	e field		
1 compos	ite field d	lefined.				
Delete	Update	field name	position after	main display	definition	missing data
×	ø	strain_designation	isolate	false	[capsule_group]: P1.[PorA_VR1].[PorA_VR2]: [FetA_VR]: ST-[scheme 1:ST] ([scheme 1:clonal_complex])	ND: P1.ND,ND: F-ND: ST- ND (-)

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

odate compos	ite field	l - strain	_designati	on					
Position/display									
position after: isolate		-							
, main display: ◯ true ◉ fa	lse								
Update									
field	empty value	ſ	egex	curator	datestamp	delete	edit	move	
apsule_group [isolate field]	ND		•	Keith Jolley		×		↑ ↓	
: P1.				Keith Jolley	2009-11-12	×		↑ ↓	- [
PorA_VR1 [locus]	ND			Keith Jolley	2009-11-12	×		↑ ↓	- <u>-</u>
,				Keith Jolley	2009-11-12	×		↑ 🗸	- <u>-</u>
PorA_VR2 [locus]	ND			Keith Jolley	2009-11-12	×		↑ ↓]
:				Keith Jolley	2009-11-12	×		↑ ↓	
FetA_VR [locus]	F-ND			Keith Jolley	2009-11-12	×		↑↓	.]
: ST-				Keith Jolley	2009-11-12	×		↑↓	•]
ST [MLST field]	ND			Keith Jolley	2009-11-12	×		↑]↓]
(Keith Jolley	2009-11-12	×		▲	•]
onal_complex [MLST field]	-	s/ST-(\S+)	complex.*/cc\$1/	-		×		▲	
)				Keith Jolley	2009-11-12	×		_+][↓	·
Add new field:									
text field:		+							
isolate field:		-+							
locus field:		•••	•						

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

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

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

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

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

5.27 Extended provenance attributes (lookup tables)

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

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

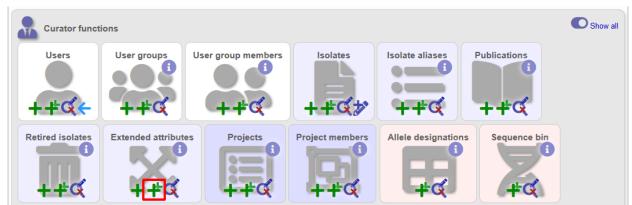


Fill in the web form with appropriate values. Required fields have an exclamation mark (!) next to them:

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

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

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



Download the Excel template:

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). De Log out Change password	Toggle: (1)
Batch insert isolate value extended attributes	
This page allows you to upload isolate field extended attribute value data as tab-delimited text or copied from a spreadsh • Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. • Download tab-delimited header for your spreadsheet - use 'Paste Special ^O Text' to paste the data. • Download submission template (xlsx format)	neet.
Paste in tab-delimited text (include a field header line).	Action
	Reset Submit

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

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

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

5.28 Sequence bin attributes

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

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

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

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

PubMLST D	atabase home	Curator home	Contents			
Logged in: Keith Jol	lley (keith). 🕩 Log out	Change password				Toggle: 🜖
Add new	sequence	attribute				
Record key type curator	r:! read_length 2:! integer 7:! Keith Jolley (ke 2:! 2018-06-19	ed fields are marked	with an exclam	ation mark (!). Action Reset	Submit	ľ

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

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

5.29 Checking external database configuration settings

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

Admin functions		O Show all
Permissions User passwords	Configuration check	

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

onfigurati	keith). 🔁 Log out Change password							
	on check - Neisseria	a PubN	ILST					
elper applicatio	ns							
Program	Path	Installed E	xecutable					
MBOSS infoalign	/usr/bin/infoalign	✓						
EMBOSS sixpack	/usr/bin/sixpack	~	~					
MBOSS stretcher	/usr/bin/stretcher	1	~					
blastn	/usr/local/ncbi-blast+/bin/blastn	~	~					
blastp	/usr/local/ncbi-blast+/bin/blastp	~						
blastx	/usr/local/ncbi-blast+/bin/blastx	~	~					
clustalw	/usr/bin/clustalw	~	~					
ipcress	/usr/bin/ipcress	~	~					
mafft	/usr/bin/mafft	 Image: A second s	×					
makeblastdb	/usr/local/ncbi-blast+/bin/makeblastdb	 Image: A second s	×					
mogrify	/usr/bin/mogrify	 ✓ 	~					
muscle	/usr/bin/muscle	~	✓					
maooro								
tblastx	/usr/local/ncbi-blast+/bin/tblastx	~	~					
tblastx	(only showing loci with poten	tial proble	ems - show a					
tblastx ocus databases Locus	(only showing loci with poten Database H	tial proble	ms - show a	Database accessib		y Sequences assigne	۵	
tblastx ocus databases Locus EIS0895 (parA) pu	: (only showing loci with poten Database H Ibmist_bigsdb_neisseria_seqdef zoo-a	tial proble ost Port berlour 5432	ems - show a Id field value NEIS0895	Database accessib	~	×	d	
tblastx ocus databases Locus EIS0895 (parA) pu EIS0903 (opaD) pu	(only showing loci with poten Database H Ibmlst_bigsdb_neisseria_seqdef zoo-a bmlst_bigsdb_neisseria_seqdef zoo-a	tial proble ost Port berlour 5432 berlour 5432	ms - show a Id field value NEIS0895 NEIS0903	Database accessib	*	×××	0	
tblastx ccus databases Locus EIS0895 (parA) pu EIS0903 (opaD) pu NEIS1454 pu	(only showing loci with poten Database H bmls_bigsdb_neisseria_seqdef zoo-a bimlst_bigsdb_neisseria_seqdef zoo-a bmlst_bigsdb_neisseria_seqdef zoo-a	tial proble ost Port berlour 5432 berlour 5432 berlour 5432	ms - show a Id field value NEIS0895 NEIS0903 NEIS1454	Database accessib	* * *	× × ×	đ	
tblastx ccus databases Locus EIS0895 (parA) pu EIS0903 (opaD) pu NEIS1454 pu EIS1551 (opaC) pu	(only showing loci with poten Database H bmlst_bigsdb_neisseria_seqdef zoo-a bmlst_bigsdb_neisseria_seqdef zoo-a bmlst_bigsdb_neisseria_seqdef zoo-a bmlst_bigsdb_neisseria_seqdef zoo-a	tial proble ost Port berlour 5432 berlour 5432 berlour 5432 berlour 5432	ems - show a ld field value NEIS0895 NEIS0903 NEIS1454 NEIS1551	Database accessib	* * * *	× × × ×	a	
tblastx cus databases Locus EIS0895 (parA) pr EIS08903 (opaD) pr NEIS1454 pr NEIS1551 (opaC) pr NEIS2013 pr	(only showing loci with poten Database H bmls_bigsdb_neisseria_seqdef zoo-a bimlst_bigsdb_neisseria_seqdef zoo-a bmlst_bigsdb_neisseria_seqdef zoo-a	tial proble ost Port beriour 5432 beriour 5432 beriour 5432 beriour 5432 beriour 5432	ms - show a d field value NEIS0895 NEIS0903 NEIS1454 NEIS1551 NEIS2013	Database accessib	* * *	× × ×	0	

Any problems will be highlighted with a red X.

5.30 Exporting table configurations

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

Admin func	tions						C Shov
Permissions	User passwords	Configuration chec	Cache refres	User databases	Extended attribute fie	Ids Composite fields	
	Locus aliases	PCR reactions	PCR locus links	Nucleotide probes	Sequence attributes	Schemes Sch	heme fields

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

PubMLST Database ho	ome Curator home Contents	
Logged in: Keith Jolley (keith). 🗭	Log out Change password	Toggle: 🚯 📃
Query schemes	for Neisseria PubMLST database	
-	eria below (or leave blank and submit to return all records).	
Search criteria	Display	_
id 💌 =	=	
- —⊽ Filter query by— isolate display:	Action	
main display:		
query field:		
query status:		
analysis:		
allow missing loci:		
curator:		
scheme:	I MLST	

Click the button 'Export configuration/data'.

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (Keith). (+Log out Change password	Toggle: 🕚	Ξ
Query schemes for Neisseria PubMLST database		
Please enter your search criteria below (or leave blank and submit to return all records).		
Search criteria		
id • = • Order by: id • ascending •		
Display: 25		
Filter query by Action		
isolate display: and the second seco		
query field:		
query status:		
analysis: 💽 0		
allow missing loci:		
scheme: MLST		
1 record returned.		
— Delete — Database configuration —		
Delete ALL Export configuration/data		
dbase dbase dbase isolate main guery guery display allow		
Delete Update id name dbase name dbase name dbase dbase dbase dbase disolate main query query analysis* display missing curator date loci	stamp	da ente
🗙 🥒 1 MLST pubmlst_bigsdb_neisseria_seqdef 1 🗹 🗹 🗹 1 🗋 Keith 2012	2-03-22 20	009-
Jolley		•
* Default values are displayed for this field. These may be overridden by user preference		

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

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

5.31 Authorizing third-party client software to access authenticated resources

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

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

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

(continues on next page)

(continued from previous page)

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

CHAPTER 6

Curator's guide

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



6.1 Adding new sender details

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

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

PubMLST Databas	se home Curator h	ome Contents	
Logged in: Keith Jolley (keit	th). 🕩 Log out Change pass	ord	Toggle: 🕚 📃
Database cur	ator's interfa	ce - Neisseria profile/sequence defir	nitions
Curator funct	tions		O Show all
Users	Sequences	MLST profiles	

Enter the user's details in to the form.

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

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

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

6.2 Adding new allele sequence definitions

6.2.1 Single allele

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

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

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

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

· Sanger trace checked

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

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

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

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

See also:

allele sequence flags

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

6.2.2 Batch adding multiple alleles

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

6.2.2.1 Upload using a spreadsheet

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

PubMLST	Database home	Curator home	Contents	
Logged in: Keith	h Jolley (keith). 🕩 Log ou	t Change password		Toggle: 🚺 📃
Databas	se curator's	interface	Neisseria profile/sequenc	e definitions
Cura	ator functions			O Show all
Use + +	seq CAC	uences M	ST profiles	

Download a template Excel file from the following page.

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

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

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

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

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

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

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

Logged in: Keith Jolley (keith). (PLog out] Change password Toggle: () Batch insert sequences This page allows you to upload allele sequence data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. If the locus uses integer allele ids you can leave the allele_id field blank and the next available number will be used. The status defines how the sequence was curated. Allowed values are: 'Sanger trace checked', 'WGS: manual extract (BIGSdb)', 'WGS: automated extra
 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 (BIGSdb)', 'WGS: automated extract (BIGSdb)', 'WGS: au
 Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. Fite locus uses integer allele ids you can leave the allele_id field blank and the next available number will be used. The status defines how the sequence was curated. Allowed values are: 'Sanger trace checked', 'WGS: manual extract (BIGSdb)', 'WGS: automated ex
Please select the sender from the list below: Jolley, Keith (keith) Value will be overridden if you include a sender field in your pasted data. Ignore existing or duplicate sequences
Ignore sequences containing non-nucleotide characters Image: Silently reject all sequences that are not complete reading frames - these must have a start and in-frame stop codon at the ends and no internal stop codons. Existing sequences are also ignored. Override sequence similarity check Paste in tab-delimited text (include a field header line). Action
locus allele_id status sequence abc2 MSS: automated extract (BIGSdb) ITTEGATACTGTTGCCCGAAGGTTGGSCGAAATCGCCGACGATTGCTGCGAAGGACGGCGGCGAGGACTGGGAAGGGCGGCGGGGAAATGGAGGGGGGGG

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

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

PubMLS	T D	atabase home	Curator hor	me Con	tents									
Logged in:	Keith Jo	l ey (keith). 🗭 Log out	Change passwor	ď								Help 🗹	Toggle: 🕻	
Batch	ins	ert sequei	nces											
Import	status													
Р	rimary	key	Р	Problem(s)										
locus: a	bcZ; alle	ele_id: 878 Sequend	ce contains non	nucleotide	(A C G T) charact	ers.								
Data to	be im	ported												
The follow	ving tab	le shows your data.	Any field with r	red text has	a problem and ne	eds to be checked.	Note: valid sequ	ence flags are	e display	ed with a	red backgrour	nd not red text.		
locus a	llele_id		sequer	псе		statu	IS	type_allele	sender	curator	date_entered	datestamp com	ments flag	S
abcZ	878	TTTGATACTGTTG	CCGAAGG	GCGAATTO	STCGAACTTGACC	WGS: automated e	extract (BIGSdb)		2	2	2018-06-07	2018-06-07		
abcZ	879	TTTGATACCGTTG	CCGAAGG	GCGGATTO	STCGAACTTGACC	WGS: automated e	extract (BIGSdb)		2	2	2018-06-07	2018-06-07		

6.2.2.2 Upload using a FASTA file

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

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

PubMLST Databas	se home Curator h	me Contents	
Logged in: Keith Jolley (kei	ith). 🍽 Log out Change passw	rd	Toggle: ()
Database cui	rat <mark>or's inter</mark> fa	e - Neisseria profile/sequence definition	S
Curator func	tions Sequences	MLST profiles	Show all

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

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

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

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

Click 'Check'.

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

PubMLST Database home Curato	r home Contents		
Logged in: Keith Jolley (keith). 🗣 Log out Change pa	ssword	Help 🗹	Toggle: 🚯
Batch insert sequences			
Sequence check			
Locus: abcZ			
Original designation Allele id Status	-Action		
isolate1 878 OK	Upload valid sequences		
isolate2 879 OK			

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

PubMLST	Databas	e home	Curator home	Contents				
Logged in: Keit	h Jolley (keith	h). (⇒ Log ou	ut Change password				Help 🗹	Toggle: 🚯 📒
Batch i	nsert s	eque	ences					
Sequence	check							
Locus: abcZ	!							
Original de	esignation A	Ilele id		Status	-	Action		
isola	ate1	878		OK		Upload valid sequences		
isola	ate2	879	Sequence contains no	n nucleotide (A C G T) charact	ters.	opioud valid sequences	J	

6.3 Updating and deleting allele sequence definitions

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

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

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

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

ubMLST Database home Curator home Contents
ogged in: Keith Jolley (keith). 🗘 Log out Change password Help 🗹 Toggle: 🕄
Query sequences for Neisseria profile/sequence definitions database
Some loci have additional fields which are not searchable from this general page. Search for these at the locus-specific query page. Use this page also for access to the sequence analysis or export plugins. Also note that some loci in this database have allele ids defined as text strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter you 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 + 0 Order by: locus v ascending v
Display: 25
locus: abcZ 💽 💽 Reset Submit
status:
type allele:
sender.
curator:
allele flag:

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

PubMLST Database home Curator home Contents									
Logged in: Keith Jolley (keith). Co out Change password							Help 🗗	Toggle: 🜖	Ξ
Query sequences for Neisseria prof	ile/sequ	ence def	inition	is dat	abase				
Some loci have additional fields which are not searchable from this ge analysis or export plugins. Also note that some loci in this database have allele ids defined as te your search to a locus that uses integer allele ids using the drop-dow	ext strings. Que n list.	ries using the '<'							
Please enter your search criteria below (or leave blank and submit to — Search criteria	return all record	-Display							
allele id v = v 4	+ 3	Order by:	ocus	√ a	scending 👻				
		Display:	25 🔻 reco	rds per pa	ge 🚯				
── ─ Filter query by		Action							
locus: abcZ	▼ 3	Reset Subr	nit						
status:									
type allele:									
sender:									
curator: allele flag:	▼ 3								
allele flag:									
1 record returned.									
Delete Database configuration Flags	_								
Delete ALL Export configuration/data Batch set									
Delete Update locus allele sequence	sequence	status	type allele	sender	curator	date	datestamp c	omments fla	ags
abcZ 4 TTTGATACCGTTGCC TTGCGAACTCGATC	length 433	Sanger trace checked		Keith Jolley	Man-Suen Chan	entered 2001-02-07	2009-11-11		

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

PubMLST Database	home Curator home Contents								
Logged in: Keith Jolley (keith). (+Log out Change password									
Delete allele se	quence								
You have chosen to delete t	the following record. Select 'Delete and Retire' to prevent the identifier being reused.								
locus:	abcZ								
allele id:	4								
sequence:	TITGATACCG TIGCCGAAGG TITIGGGCGAA ATICGIGAIT TAITGCGCCG TIAICAICAI GICAGCCAIG AGITGGAAAA IGGIICGAGI GAGGCIIIGI								
	TGAAAGAACT CAACGAATTG CAACTTGAAA TCGAAGCGAA GGACGGCTGG AAACTGGATG CGGCAGTCAA GCAGACTTTG GGGGAACTCG GTTTGCCCGGA								
	ANATGANANA ATCGGCNACC TTTCCGGCGG TCAGANANAG CGCGTCGCCT TGGCTCAGCC TGGGTGCAN ANGCCCGACG TATTGCTGCT GGACGAGCCG								
	ACCAACCATT TGGATATCGA CGCGATTATT TGGCTGGAAA ATCTGCTCAA AGCGTTTGAA GGCAGCTTGG TTGTGATTAC CCACGACCGC CGTTTTTTGG ACAATATCGC CACGCGGATT GTCGAACTCG ATC								
status:	Sanger trace checked								
type allele:									
	Keith Jolley								
	Man-Suen Chan								
date entered:	2001-02-07								
datestamp:	2009-11-11								
comments:									
Action									
Delete Delete and	Retire								

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

a m. Kerur Joney (Keru	h). €♦Log out Change password	Toggle:
date allele	sequence	
se fill in the fields bel	low - required fields are marked with an exclamation mark (!).	
Record		Action
locus:	abcZ	Reset Submit
allele id:	4	iteset Submit
sequence:!	TTTGATACCG TTGCCGAAGG TTTGGGCGAA ATTCGTGATT TATTGCGCCG TTATCATCAT GCACCCATG AGTTGGAAA TGGTTGGAGT GAAGCTTTGT TGAAAGAACT CAACGAATTG CAACTTGAAA TCGAACGGAA GGACGGCTGG AAACTGGATG CGGCAGTCAA CGAGACTTG GGGGAACTCG GTTTGCCGGA AAATGAAAAA	
status:!	Sanger trace checked -	
	Jolley, Keith (keith)	
	Keith Jolley (keith)	
date entered.	2001-02-07	
datestamp:!		
datestamp:!		
datestamp:!	2018-06-07	
datestamp:! type allele: comments:	2018-06-07 True false New allele searches can be constrained to use just type alleles in comparisons	a
datestamp:! type allele:	2018-06-07 True false New allele searches can be constrained to use just type alleles in comparisons	а
datestamp:! type allele: comments:	2018-06-07 True false New allele searches can be constrained to use just type alleles in comparisons atypical contains IS element frameshift internal stop codon Use Ctrl click to select/deselect multiple choices	.a
datestamp:! type allele: comments: Flags:	2018-06-07 True false New allele searches can be constrained to use just type alleles in comparisons atypical contains IS element frameshift internal stop codon Use Ctrl click to select/deselect multiple choices	
datestamp:! type allele: comments: Flags: PubMed ids:	2018-06-07 Itrue of false New allele searches can be constrained to use just type alleles in comparisons atypical contains IS element of downstream fusion frameshift internal stop codon Image: Use Ctrl click to select/deselect multiple choices	

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

6.4 Retiring allele identifiers

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

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

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

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

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

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

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

6.5 Updating locus descriptions

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

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

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

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

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

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

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

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

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

Click 'Submit'.

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

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

Fill in the form as needed:

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

• full_name

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

• product

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

• description

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

aliases

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

• Pubmed_ids

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

• Links

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

Click 'Submit' when finished.

6.6 Adding new scheme profile definitions

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

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



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

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

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

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

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

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

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

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

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (keith). 🕒 Log out Change password	Help 🗹	Toggle: 🚹
Batch insert MLST profiles		
 This page allows you to upload profiles as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. You can choose whether or not to include a ST field - if it is omitted, the next available ST will be used automatically. If however, y then you must also provide it for each profile record. Download tab-delimited header for your spreadsheet - use Paste Special Text to paste the data. Download submission template (xlsx format) Please paste in tab-delimited text (include a field header line) ebc2 adk excE fumC gdb pdbC pgm clonal complex 	you include it in the	e header line,
abcz adk aroE func gdh pdhC pgm clonal_complex 2 3 4 122 8 4 6		
Parameters Action Sender: Jolley, Keith (keith) Reset Submit Reset Submit Ignore previously defined profiles Ignore duplicate profiles Submit Submit Submit Submit Reset Submit Submit Submit Reset Submit <li< td=""><td></td><td></td></li<>		

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



6.7 Updating and deleting scheme profile definitions

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

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

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

PubMLST	Database h	ome	Curator h	nome	Contents										
Logged in: Keit	h Jolley (keith). 🖲	Log out C	Change pass	word									Help 🗹	Toggle	0 =
Query/เ	update p	rofile	es - Ne	eisse	eria pro	ofile/	/seq	uence d	lefi	inition	S				
Schemes															Modify form
Please selec	ct the scheme ye	ou would	like to quer	ry:											option
MLST			•	Select											_
Enter search	n criteria or leave	blank to	browse all	records.	Modify form p	paramet	ers to fil	ter or enter a li	ist of	values.					
Locus/s	cheme fields —							-Display/sort	optio	ins			Action		
													71011011		
ST	•	=	▼ 45	63		+) 🛛	Order by:	ST			g 🔻	Reset	Submit	
ST	•	=		63		+]	Order by:	ST			g 🔻		Submit	
ST 1 record retur		=	▼ 45	63		+) 🛛	Order by:	ST] •		Submit	
		=	▼ 45	63		+) 0	Order by:	ST			g •		Submit	
1 record retur	ned.	=	▼ 45	63		+)	Order by:	ST			g •		Submit	
1 record retur — Delete —	ned.	=	▼ 45	63		+) 0	Order by:	ST			g •		Submit	
1 record retur — Delete —	ned.		oE fumC g		C pgm clon 8 ST-		plex	Order by:	ST] •		Submit	

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

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

PubMLST Database	home Curator home Contents
Logged in: Keith Jolley (keith).	Log out Change password
Delete profile	
You have chosen to delete t	the following record. Select 'Delete and Retire' to prevent the identifier being reused.
scheme id:	1) MLST 4563 2
ST:	4563
abcZ :	2
adk :	7
aroE :	6
fumC :	
gdh :	
pdhC :	
pgm :	
clonal_complex :	S1-167 Complex Ana-Belen Ibarz-Pavon
	Keith Jolley
date entered:	
datestamp:	
-Action	
Delete Delete and	Retire

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

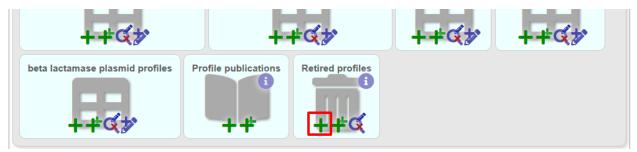
PubMLST Databa	se home Curator home Contents			
Logged in: Keith Jolley (ke	<i>ith</i>). ເ∳Log out Change password		Help 🖍	Toggle: 🚯 📃
Update profil	le			
Record		Action		
Update your record as	s required - required fields are marked with an exclamation mark (!):	Reset Submit		_0
ST: !	4563			
abcZ: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

6.8 Retiring scheme profile definitions

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

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

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



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

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

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

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

6.9 Adding isolate records

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

PubMLST Databas	se home Curator ho	me Contents									
Logged in: Keith Jolley (keith). G+Log out Change password											
Database curator's interface - Neisseria PubMLST											
Curator func	tions	O Show all									
Users	Isolates	Sequence bin	Sequence tags								

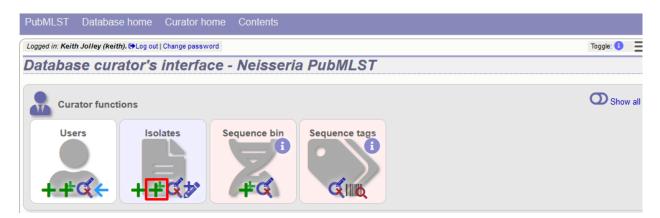
The next available id will be filled in automatically but you are free to change this. Fill in the individual fields. Required fields are listed first and are marked with an exclamation mark (!). Some fields may have drop-down list boxes of allowed values. You can also enter allele designations for any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

PubMLST Database home Curator home Contents													
Logged in: Keith Jolley (keith). 🗘 Log out Change password Toggle: ()													
Add new isolate													
Please fill in the fields below - required fields are marked with an exclamation mark (!).													
Isolate fields			Allele designations										
id:!	60465 🚔 🚯												
isolate:	_	6	6		abcZ	adk	MLST aroE fumC						
country:!	UK 👻	8			abcz	аак	aroE	iume					
species:!	Neisseria meningitidis		- 3		qdh	pdhC	pgm						
sender:!	Jolley, Keith (keith)			- 3	gun	pune	Pan						
	Keith Jolley (keith) 🚯												
	2018-06-07 🚯			Finetyping antigens									
	stamp: 2018-06-07 🚯				PorA VR1	PorA VR2	PorA VR3	FetA VR					
region:		0											
	2014				-Action								
epidemiological year:	6				Reset S	Submit							
age yr:													
age mth:													
sex:	- 0		_										
	meningitis	•	8										
source:	CSF 🔹 🕄												
epidemiology:	•												
serogroup:	B 🔻 🕄												
genogroup:	• •												
MLEE designation:	-												
serotype:													
sero subtype:													
ET no:													
penicillin:	6												
penicillin range:	•	6											

Press submit when finished.

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

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



Download a submission template in Excel format from the link.

PubMLST Database home Curato	r home Contents		
Logged in: Keith Jolley (keith). 🍽 Log out Change pa	ssword		Toggle: 🚺 📃
Batch insert isolates			
 Enter aliases (alternative names) for yo Enter references for your isolates as a You can also upload allele fields along a template for locus names). These will b You can choose whether or not to inclu 	Ind fields can be in any order. Optional field ur isolates as a semi-colon (;) separated li semi-colon (;) separated list of PubMed ids with the other isolate data - simply create a e added with a confirmed status and meth de an id number field - if it is omitted, the r <u>spread</u> sheet - use 'Paste Special ⊙ Text'	Is can be omitted if you wish. st. : (non-integer ids will be ignored). a new column with the locus name (see the 'allowed_lo od set as 'manual'. lext available id will be used automatically.	ci' tab in the Excel
Select sender	 Value will be overridden if you inc 	lude a sender field in your pasted data.	
Paste in tab-delimited text (include a field	d 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).

PubMLST Database home Curator home Contents
Logged in: Keith Jolley (keith). Change password Toggle: 1
Batch insert isolates
This page allows you to upload isolate data as tab-delimited text or copied from a spreadshet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. Enter aliases (alternative names) for your isolates as a semi-colon () separated list. Enter references for your isolates as a semi-colon () separated list of PubMed ids (non-integer ids will be ignored). You can also upload allele fields allong with the other isolate data - simply create a new column with the locus name (see the 'allowed_loci' tab in the Excel template for locus names). These will be added with a confirmed status and method set as 'manual'. You can choose whether or not to include an id number field - if it is omitted, the next available id will be used automatically. Download tab-delimited header for your spreadsheet - use 'Paste Special C Text to paste the data. Download submission template (dixx format) Please select the sender from the list below: Joley, Keth (keth) Value will be overridden if you include a sender field in your pasted data. Please select the sender form the list below: Joley, Keth (keth) Value will be overridden if you include a sender field in your pasted data. Please select the sender form the list below: Joley, Keth (keth) Value will be overridden if you include a sender field in your pasted data. Please select the sender form the list below: Joley, Keth (keth) Value will be overridden if you include a sender field in your pasted data. Please to tab-delimited text (include a field header line) Action Reset Submit Value will be overridden if you many and the decimate and available id your pasted data. Please select the sender form the list below: Joley, Keth (keth) Value will be overridden if you include a sender field in your pasted data. Please tab decimate text (include a fiel

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

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

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

PubMLST Data	base home	Curator	home Co	ontents								
Logged in: Keith Jolley	(keith). 🕩 Log out	Change pase	sword								Toggle: 🔇	
Batch inser	t isolate	S										
Import status												
Primary key			Problem(s)									
id: 60465 speci	es "Neisseria m	engitidis" is	not on the li	st of allowed val	ues for this field.							
Data to be impor	rted											
The following table sl	hows your data.	Any field w	ith red text h	as a problem ar	nd needs to be ch	ecked.						
	ses references			epidemiologio	cal_year_age_yr	age_mth			epidemiology			geno
60465 J323_2		UK	2014				meningitis	CSF		Neisseria mengitidis	В	
•	III											Þ

6.10 Updating and deleting single isolate records

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

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

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

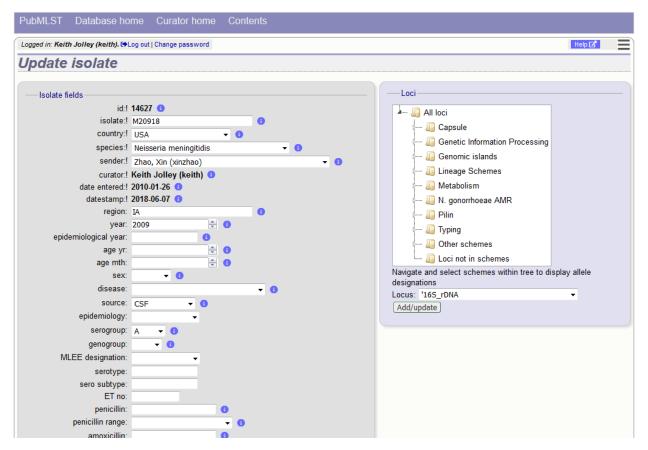
PubMLS	ST Da	atabase h	ome (Curato	r home	Contents									
Logged in:	Keith Jol	ley (keith). 🖨	Log out C	hange pa	ssword								Help 🗹	Toggle:	• =
Isolat	te qu	ery/up	odate												
Enter se	arch crite	eria or leave	blank to l	browse a	all records. N	Aodify form pa	arameters	to filte	er or enter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

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

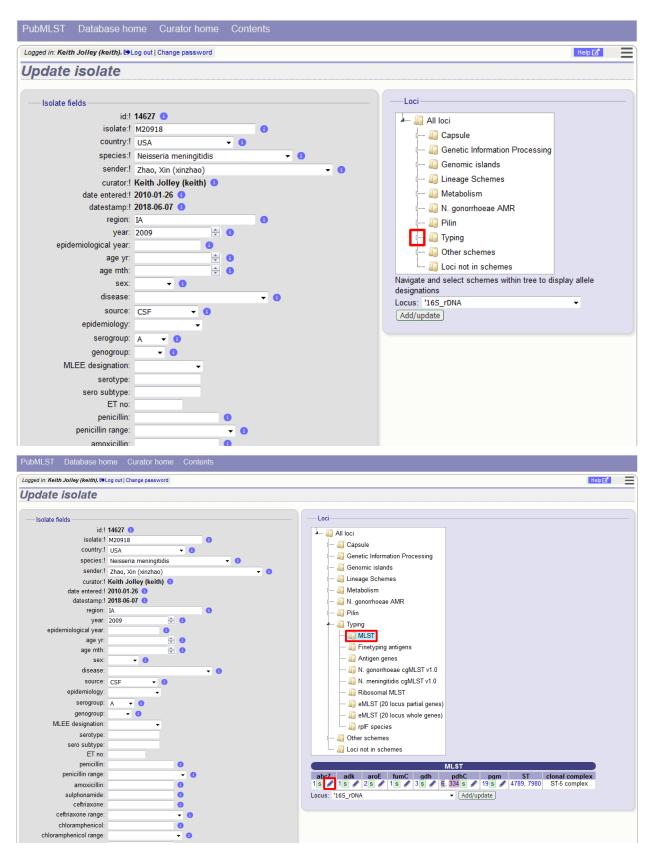
id: 14627 region: IA sender: Xin Zhao, Novartis (forme at US CDC) isolate: M20918 year: 2009 at US CDC) strain designation: A: P120,9: F3-1: source: CSF curator: Auto Tagger country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A datestamp: 2018-01-31	elete isolate	Log out Change password				Help 🗹
id: 14627 region: IA sender: Xin Zhao, Novartis (forme at US CDC) isolate: M20918 year: 2009 curator: Auto Tagger Strain designation: A: P120,9: F3-1: source: CSF curator: Auto Tagger country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A date stamp: 2018-01-31 Publication (1) Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display <th>elete isolate</th> <th></th> <th></th> <th></th> <th></th> <th></th>	elete isolate					
id: 14627 region: IA sender: Xin Zhao, Novartis (forme at US CDC) isolate: M20918 year: 2009 curator: Auto Tagger Strain designation: A: P120,9: F3-1: source: CSF curator: Auto Tagger country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A date stamp: 2018-01-31 Publication (1) Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display <th></th> <th>-</th> <th>elete and Retire' to prevent t</th> <th>he isolate id being reused.</th> <th></th> <th></th>		-	elete and Retire' to prevent t	he isolate id being reused.		
isolate: M20918 year: 2009 at US CDC) strain designation: A: P1.20.9: F3-1: source: CSF curator: Auto Tagger ST-4789,7980 (cc5) species: Neisseria meningitidis update history: 63 updates show details country: USA serogroup: A date entered: 2010-01-26 continent: Noth America capsule group: A datestamp: 2018-01-31 Publication (1) - - datestamp: 2018-01-31 Publication (1) - - - datestamp: 2018-01-31 Sequence bin - - - - - - Contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display	Provenance/met	a data				
strain designation: A: P1.20,9; F3.1: source: CSF curator: Auto Tagger strain designation: A: P1.20,9; F3.1: source: CSF update history: @3 updates show details country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A datestamp: 2018-01-31 Publication (1) . . Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90); 456 detailed breakdown: Display	id:	14627	region:	IA	sender:	Xin Zhao, Novartis (forme
Start 789,7980 (cc5) species: Neisseria meningitidis update history: (B3 updates show details country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A date entered: 2018-01-31 Publication (1) • Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display	isolate:	M20918	year:	2009		at US CDC)
country: USA serogroup: A date entered: 2010-01-26 continent: North America capsule group: A datestamp: 2018-01-31 Publication (1) • Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display	strain designation:	A: P1.20,9: F3-1:	source:	CSF	curator:	Auto Tagger
continent: North America capsule group: A datestamp: 2018-01-31 Publication (1) • Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display		ST-4789,7980 (cc5)	species:	Neisseria meningitidis	update history:	63 updates show details
Publication (1) • Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hare BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display	country:	USA	serogroup:	Α	date entered:	2010-01-26
 Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. <i>Bioinformatics</i> 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display 	continent:	North America	capsule group:	A	datestamp:	2018-01-31
 Kislyuk AO, Katz LS, Agrawal S, Hagen MS, Conley AB, Jayaraman P, Nelakuditi V, Humphrey JC, Sammons SA, Govil D, Mair RD, Tatti KM, Tondella ML, Hard BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. <i>Bioinformatics</i> 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display 	Publication (1)					
BH, Mayer LW, Jordan IK (2010). A computational genomics pipeline for prokaryotic sequencing projects. Bioinformatics 26:1819-26 18 isolates Sequence bin contigs: 2,046 N50 contig number: 510 N95 contig number: 1,633 total length: 1,717,803 bp N50 length (L50): 1,155 N95 length (L95): 324 max length: 5,436 bp N90 contig number: 1,414 loci tagged: 1,518 mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display		Amount C. Hanna MC. Cau	alau AR, Jawasanan D, Malali		A Cavil D Mais DD T	HI I/M Tandalla MI Llass
contigs:2,046N50 contig number:510N95 contig number:1,633total length:1,717,803 bpN50 length (L50):1,155N95 length (L95):324max length:5,436 bpN90 contig number:1,414loci tagged:1,518mean length:840 bpN90 length (L90):456detailed breakdown:Display	· · · · · · · · · · · · · · · · · · ·					
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total length:1,717,803 bpN50 length (L50):1,155N95 length (L95):324max length:5,436 bpN90 contig number:1,414loci tagged:1,518mean length:840 bpN90 length (L90):456detailed breakdown:Display						
total length:1,717,803 bpN50 length (L50):1,155N95 length (L95):324max length:5,436 bpN90 contig number:1,414loci tagged:1,518mean length:840 bpN90 length (L90):456detailed breakdown:Display	Sequence bin					
max length:5,436 bpN90 contig number:1,414loci tagged:1,518mean length:840 bpN90 length (L90):456detailed breakdown:Display		2 0/6	N50 contig number:	510	N95 contig number:	1 633
mean length: 840 bp N90 length (L90): 456 detailed breakdown: Display	contigs:				0	1 - Contract - Contrac
	contigs: total length:	1,717,803 bp	N50 length (L50):	1,155	N95 length (L95):	324
Action	contigs: total length: max length:	1,717,803 bp 5,436 bp	N50 length (L50): N90 contig number:	1,155 1,414	N95 length (L95): loci tagged:	324 1,518
	contigs: total length: max length:	1,717,803 bp 5,436 bp	N50 length (L50): N90 contig number:	1,155 1,414	N95 length (L95): loci tagged:	324 1,518

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

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



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



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

'Add/update'.

PubMLST Database ho	ome Curator home Conte	ents		
Logged in: Keith Jolley (keith). 🕩	Log out Change password			Help 🛃
Update isolate				
- Isolate fields id:! isolate:! country:! species:! sender:! curator:! date entered:!	Neisseria meningitidis Zhao, Xin (xinzhao) Keith Jolley (keith) © 2010-01-26 © 2018-06-07 © IA 2009 * © © © © © © © © © © © © © ©	6 - 0 - 0 - 0	Loci All loci Capsule Genetic Information Processing Genomic islands Lineage Schemes Metabolism N. gonorrhoeae AMR Pilin Typing Other schemes Loci not in schemes Navigate and select schemes within tree to display a Locus abcz	allele designations Add/update
serotype: sero subtype:				

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

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

6.11 Batch updating multiple isolate records

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

PubMLST Database	home Curator home Contents			
Logged in: Keith Jolley (keith)	ALST Database home Curator home Contents Tim: Keith Jolley (keith). (HLog out) Change password Toggle: • = rabase curator's interface - Neisseria PubMLST Curator functions Image: • • Curator functions Sequence bin Sequence tags • • Users Isolates Sequence tags • • •			
Database cura	tor's interface - Neisseria PubMLST			
	Isolates Sequence bin Sequence tags	Show all		

Prepare your update data in 3 columns in a spreadsheet:

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

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

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

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

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

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

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

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

ubMLST	Database ho	ome Curato	r home Contents					
ogged in: Keith	h Jolley (keith). 🗭	Log out Change pa	assword				Help 🛛	
Batch is	solate up	odate						
changes, pre	ss your browser	s back button.		this is what you intend and then	press 'Upload	ď. If you do not wish	to make these	
Transaction			lue(s) currently in datab					
1	100 serogroup		С	update field with new value				
2	101 serogroup	В	С	update field with new value				
Action	3-1							
-Action-	_							
Upload								
	•							

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

example using country and isolate name.

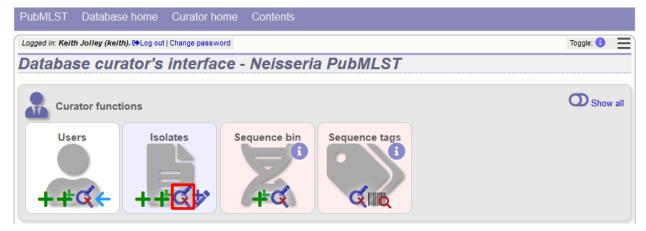
So, for example, to update the serogroups of isolates CN100 and CN103, both from the UK, select the appropriate primary and secondary fields and prepare the data as follows:

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

6.12 Deleting multiple isolate records

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

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



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

PubMLST Datab	ase hoi	ne Curator	home Contents			
Logged in: Keith Jolley (k	e <i>ith).</i> 🔂	og out Change pas	sword		Help 🗗 T	oggle: 🚯
solate quer	y/up	date				
Enter search criteria o	r leave b	ank to browse a	ll records. Modify form pa	rameters to fil	ilter or enter a list of values.	Mo
-Isolate provenance	e/phenoty	/pe fields			Display/sort options	for
Combine with: AND	-				Order by: id ascending	opti
date entered	-	- •	2014-03-18	+ 6	Display: 25 - records per page 3	_
curator (surname)	•	- •	Jolley			
					Action	
					Reset Submit	
3 records returned. Clic	k the hy	perlinks for detai	led information.			
	-Tag sca	anning Dro	jects			
		_	·			
Delete ALL	Sca	n Seleo	ct project	• L	Link	
Delete Update Seq	uence b	in New versior	id isolate aliases		Isolate fields 🛈 Finetyping and	
×	<u>±</u>	+	28787 M22296	USA	ear disease species serogroup genogroup capsule group PorA VRI PorA VR Neisseria meningitidis 5-1 / 2-81 /	Z FETA VR
×	1	÷	28788 M22553	USA	Neisseria meningitidis 5-2 / 10-96	
X	+	+	28789 M22568	USA	Neisseria meningitidis 7-2 4-39	+
	-		20100 11122000		The second	

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

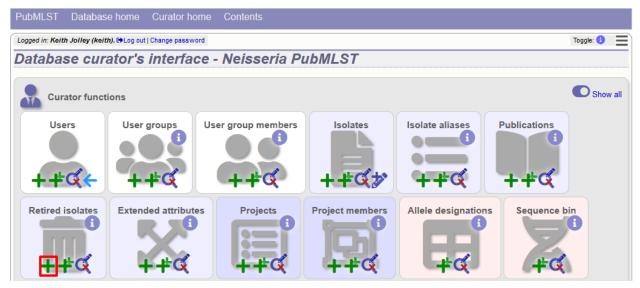
You will have a final chance to change your mind:

Click 'Confirm deletion!'.

6.13 Retiring isolate identifiers

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

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



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

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

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

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

6.14 Setting alternative names for isolates (aliases)

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

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

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

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

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

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

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). [0]Log out Change password	Toggle: 🚯 📃
Batch insert isolate aliases	
This page allows you to upload isolate alias data as tab-delimited text or copied from a spreadsheet. 9. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. 9. Deveload ab-delimited header for your spreadsheet - use 'Paste Special Q Text to paste the data. 9. Deveload submission template (disk format) 9. Deste nab-delimited text (include a field header line). 1. Spreadsheet - use 'Paste Special Q Text to paste the data. 1. Spreadsheet - use 'Paste Special Q Text to paste the data. 2. Spreadsheet - use 'Paste Special Q Text to paste the data. 2. Spreadsheet - use 'Paste Special Q Text to paste the data. 2. Spreadsheet - use 'Paste Special Q Text to paste the data. 2. Spreadsheet - use 'Paste Special Q Text to paste the data. 2. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use 'Paste Special Q Text to paste the data. 3. Spreadsheet - use '	Action Reset Submit
Back	

A confirmation page will be displayed.

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

Click 'import data'.

6.15 Linking isolate records to publications

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

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

PubMLST Databas	e home Curator he	ome Contents				
Logged in: Keith Jolley (keith). 🔁 Log out Change password						
Database cura	ator's interfa	ce - Neisseria Pu	bMLST			
Curator funct	User groups	User group members	Isolates	Isolate aliases	Publications i	Show all

Open the Excel template by clicking the link.

PubMLST Database home Curator home Contents		
Logged in: Keith Jolley (Keith). 🗘 Log out Change password		Toggle: ()
Batch insert refs		
This page allows you to upload PubMed link data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. Download tab-delimited header for your spreadsheet - use Paste Special	Action Reset Submit	

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

PubMLST Database home Curator home Contents					
Logged in: Keith Jolley (keith). [+Log out Change password	ogged in: Keith Jolley (keith). 🕩 Log out Change password Toggle: 🕚 📃				
Batch insert refs					
This page allows you to upload PubMed link data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. Download tab-delimited header for your spreadsheet - use 'Paste Special ^O Text' to paste the data. Download submission template (xlsx format) Paste in tab-delimited text (include a field header line). Isolate_idpubmed_id 616017517841 616217517841 896826515523	Action Reset Submit				

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

6.16 Uploading sequence contigs linked to an isolate record

6.16.1 Select isolate from drop-down list

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



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

Paste sequence contigs in FASTA format in to the form.

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). [+Log out Change password	Toggle: 🕦
Upload sequences	
This page allows you to upload sequence data for a specified isolate record in FASTA format. If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any ot FASTA file. This allows data for multiple isolates to be uploaded. <i>Please note that you can reach this page for a specific isolate by querying isolates and then clicking 'Upload' within th</i> Please fill in the following fields - required fields are marked with an exclamation mark (I).	A
Paste in sequences in FASTA format: ACCGTCARAATCGGTCGGCATCGATGAATCGATACCGCGCGAAAACAAATTTCTTGGATT TCGCCGTGGTCGTTGTCGTGATGAAGCGGTGAAGGCGGACGAGTGGTTTTAAACAGG CCGGAAGGGCGTGGAAGAATGAAATCCTTCTGTCGAATACACGAATCACAGAGG GGAATGCGCCACAAAATCGCGGCCGTTTCTGTCGAATACACGAATCACGAATGAGGG GAAATCCGCACCAAAATCGGGCATCACCGAACGGCAGTTGTGCGCCCTTTTGCGGCCTT CGTCAACGGAAGCGACTGGGCTTTTTGCGCGCATTCGCGCCGCTGTGCGCCCTT CGTCAACGGAAGCCAACAGCCGGCGTTCCCCCGCCGTGTGCGCCCCTTT CGTCAACGGAAGCCAACGGCGCGTTCCCCCCGCCGTGTGCGCCCCGACGCCCTT CGCATCGCGGCGCGACGCACCGCGCCGTTCCTCGCGAAGCGCCCCTTATCCAA GGCCATCGGGCGCGGCAACACGCCGCCGCTTCCCCGCGCACCGCCCTTATCCA GGCCATCGGGCGCTGGCTCCACGCCTCCTCCGGAAGCGCCCCGGACCGCCTT CGACTGCGGCGCTGGCTCCACGCCTCCTCCGGAAGCGCCCCGGACCGCCTT CGACTGCGGCCGTGGCTCCACGCCTCCTCGGAACGCGCCGGACCGCCTT CGACTGCGGCCGTGTGCCCCCCATCCCGGAACGCGCCGGACGCGCTT CGACTGCGGCCGTGTGCGCCCATCCCGGAACCGGCGGAAGCGGTCGGGGGGACGGCCTT CGCGGGGGGGAGCGAAGCAACGCGCCCGAACGCGCCGGAACGGCTT CGGCGGCGGTGGAGCAAGCAACGATCCGGGCCGCAAAGTTGCCGCGCTT CGACGCCCTATCCCGTTAAGCCAACAAAATTGCGCCGCCGAACGCTTCTCGGGC CGGGGGGGAAGCACTCCGGTTCCCTCGGAATGCCCCCTTATCCGGAC CGCGACGCCGGTGGCTCCCGCTTAGCCACAAGGAATCGGCGCCCGGATGCCCCTT CGACGCCCACCGCGTTACCCGGTTCCCTCGGAATGCGCCCCTTATCCGGGC CGGGGGGGAAGCACTAAGCAACAAAATTCCGCCGCAAGGTGCTTCCGGG CGGGGGGAAGCACTAAGCAACAAAATTCCGCCGCAAGGTGCTTCCGGGC CGGGGGGGAACCAATAATTCCGCCGCAAAGTACCGGGTCGCTCGGC CGGACGCCACGACGATACCGGTTCCCTCGCACTAACGGGTACCTCTAAGGTG CGACACCAACAACTAAACCGATTCCAAAGGAACGTTCCTAAGGTG CGACGCACCAACAATAATTCCGCTCTAATTCCATTCCAAGGTG CGAGGCGTGGAACCAATCCGGTTCCCTCCACGCGCGGGAATCCGGTTCCTGCGCCTTG CGACGCACCAACAACTAAAATTTGCCATTAAAATTTTGCTATTAAATACAGTGATTCCACGGTGCCTTGG CGAGGTGGAACCAATAAATTTGCAACTCAAAGGAACCGGTCCTCTGCGGCCTTG CGACGCCACCGACTAAACGATAAATTTGCCATTAAAACCGGTTCCTTGGGGCCGGGGAATCCGGTTCCTGCGCCTTG CGACGCACCAACGACTAAAACTTAACCCGCTCAAAGGCCACGGCGGGAATCCGGTTCCTGGCCCTTG CGACGCACCAACGCATTAAAAATTTGGAACCAACAAAAATTTGCAACGGGGGGAACCGGGTCGTCGGCCCTTG CGACACCACAACGCATTAAAAATTTGGACACAAAAATTTCCTTCAAGGCGGGGGAACCGGTTCCTGGCCCTTG CGCACCACGCACAACGACAAAAAATTTGGACACAACGCGCGAACCGGTCGCCGCGCGGCGGCGGCGGCGGCGGCG	Attributes isolate id: ! 2 isoley, Keth (keth) method: run id: assembly id: Options Options Options Attributes Alternatively upload FASTA file or enter Genbank accession Select FASTA file: Browse No file selected. Action Reset Submit

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

MLST Database home Curator home	e Contents		
ed in: Keith Jolley (keith). 🗣 Log out Change password			Toggle: 🚯
load sequences			
The following sequences will be entered.		SummaryAction	
Original designation	Sequence length Comments	Number of contigs: 364 Upload	
180062 NODE_116_length_5370_cov_18.338547	5408	Minimum length: 100	
180063 NODE_267_length_64_cov_54.562500	102	Maximum length: 50093	
180064 NODE_1024_length_456_cov_16.434210	494	Total length: 2069108	
180065 NODE_367_length_3545_cov_22.858955	3583	Mean length: 5684	
180066 NODE_361_length_87_cov_17.862068	125	N50 contig number: 44	
180067 NODE_1617_length_297_cov_11.111111	335	N50 contig length (L50): 15404	
180068 NODE_909_length_95_cov_9.073684	133	N90 contig number: 146	
180069 NODE_699_length_98_cov_110.918365	136	N90 contig length (L50): 3907	
180070 NODE_553_length_84_cov_47.964287	122	N95 contig number: 180	
180071 NODE_182_length_6772_cov_19.882162	6810	N95 contig length (L50): 2305	
180072 NODE_928_length_347_cov_35.201729	385	1495 contig length (LSU): 2305	
180073 NODE_19_length_12542_cov_19.259449	12580		
180074 NODE_60_length_5125_cov_18.960781	5163		
180075 NODE_168_length_7439_cov_17.615808	7477		
180076 NODE_1041_length_109_cov_27.752293	147		
180077 NODE_71_length_2120_cov_19.594339	2158		
180078 NODE_318_length_1827_cov_15.821566	1865		
180079 NODE_207_length_6398_cov_19.577681	6436		
180080 NODE_162_length_13775_cov_18.618221	13813		
180081 NODE_664_length_160_cov_35.068748	198		
180082 NODE_56_length_9475_cov_20.244328	9513		
180083 NODE_356_length_297_cov_41.383839	335		
180084 NODE_778_length_582_cov_42.140892	620		
180085 NODE_137_length_10168_cov_16.055567	10206		
180086 NODE_1102_length_82_cov_43.329269	120		

6.16.2 Select from isolate query

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

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



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

PubMLST Database home Curat	tor home Contents				
Logged in: Keith Jolley (keith). 🗭 Log out Change p	password				Help 🗹 🛛 Toggle: 🜖
Isolate query/update					
Enter search criteria or leave blank to browse	e all records. Modify form para				Modify
Isolate provenance/phenotype fields		Display/sort options		Action	form option
isolate 👻 =	✓ fam18	+ Order by: id	✓ ascent	ding 👻 Reset	Submit
		Display: 25 🔻 r	cords per page 3		
1 record returned. Click the hyperlink for detail	iled information.				
Delete Tag scanningF	Projects				
Delete ALL Scan Se	elect project	▼ Link			
But I Sequence New		Isolate fields		MLST	Finetyping antigens
	id isolate aliases	country year disease	species serogroup genogroup grou		PorA PorA FetA VR1 VR2 VR
× 🖉 🚨 🕂 🤅	698 FAM18 NIBSC_3076;	USA 1983 invasive	Neisseria C C	11 ST-11	5 🖋 2 🖋 F1-30
	Z4259	(unspecified/other)	meningitidis	complex	1

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

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). 🗘 Log out Change password	Toggle: ()
Upload sequences	
This page allows you to upload sequence data for a specified isolate record in FASTA format. If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any or FASTA file. This allows data for multiple isolates to be uploaded. Please note that you can reach this page for a specific isolate by querying isolates and then clicking 'Upload' within i	A
Please fill in the following fields - required fields are marked with an exclamation mark (!).	
Pease in sequences in FASTA format:	Attributes isolate id: [698) FAM18 sender: ! Select sender method: run id: assembly id: Options Options Optionsert sequences shorter than 25 bps. Link to experiment: Alternatively upload FASTA file or enter Genbank accession Select FASTA file Browse No file selected. Reset Submit

6.16.3 Upload options

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

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

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

6.17 Batch uploading sequence contigs linked to multiple isolate records

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

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

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

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

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

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

jea in: Ke i	ith Jolley	y (keith). 🗭 L	og out Cha	nge password				Тодо	gle: 🚯
tch (uplo	ad se	quen	ce assen	nblies to r	nultiple	solate records		
								_	
ease uplo	ad the a	assembly c	ontig files	for each isolate r	ecord.				
emove row	id	isolate	current se contigs	equence bin sta total size (bp		upload status			
	61222	JB_21292	-	-	JB_21292.fasta	×			
	61223	JB_21293	-	-	JB_21293.fasta	×		_	
	61224	JB 21294	-	-	JB 21294.fasta	×			
	01224	00_21204	-		JD_21234.10310	•			
Remove)	-	-		JD_21234.18388	Ŷ			
Remove ASTA file Contig) es left to assemb	– o upload. bly files——			_		. Individual filesize is limited to 6	54 MB. You can upload up to 64 MB in or	ne go
Remove ASTA file Contig Please up) es left to assemb pload co	o upload. bly files ntig assemi	blies with t	he filenames as	_	cated in the table	. Individual filesize is limited to 6	64 MB. You can upload up to 64 MB in or	ne go
Remove ASTA file Contig Please up) es left to assemb pload co	o upload. bly files ntig assemi	blies with t	he filenames as	you specified (indic	cated in the table	. Individual filesize is limited to 6	54 MB. You can upload up to 64 MB in or	ne go
Remove ASTA file Contig Please up) es left to assemb pload co	o upload. bly files ntig assemi	blies with t	he filenames as	you specified (indic	cated in the table	. Individual filesize is limited to 6	64 MB. You can upload up to 64 MB in or	ne go
Remove ASTA file Contig Please up) es left to assemb pload co	o upload. bly files ntig assemi	blies with t	he filenames as	you specified (indic	cated in the table	. Individual filesize is limited to 6	34 MB. You can upload up to 64 MB in or	ne go
Remove ASTA file Contig Please up) es left to assemb pload co	o upload. bly files ntig assemi	blies with t	the filenames as	you specified (indic size of the upload	cated in the table can be larger.		64 MB. You can upload up to 64 MB in or	ine go
Remove ASTA file Contig Please up) es left to assemb pload co	o upload. bly files ntig assemi	blies with t	the filenames as	you specified (indic size of the upload	cated in the table can be larger.	. Individual filesize is limited to 6	64 MB. You can upload up to 64 MB in or	ne go
Remove ASTA file Contig Please up) es left to assemb pload co	o upload. bly files ntig assemi	blies with t	the filenames as	you specified (indic size of the upload	cated in the table can be larger.		54 MB. You can upload up to 64 MB in or	ne go
Remove ASTA file Contig Please up) es left to assemb pload co	o upload. bly files ntig assemi	blies with t	the filenames as	you specified (indic size of the upload	cated in the table can be larger.		54 MB. You can upload up to 64 MB in or	ne go

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

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

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

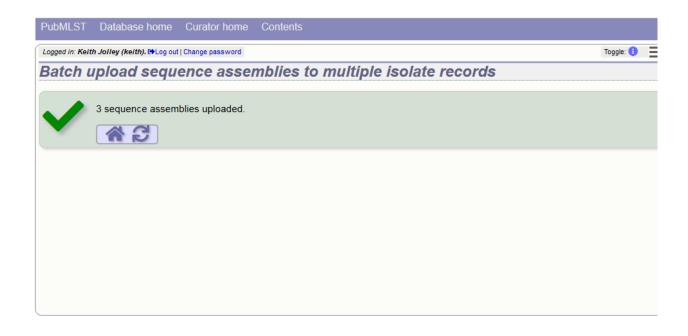
The files will be checked and a table will be displayed showing the total sequence size and number of contigs found. Select the data sender and, optionally the sequencing method from the dropdown lists. Then click 'Upload validated contigs'.

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

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

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

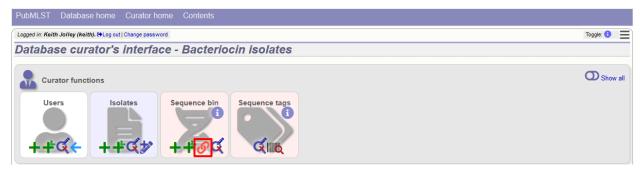
A confirmation message will be displayed after clicking the Upload button.



6.18 Linking remote contigs to isolate records

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

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



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

Press submit.

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

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



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

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

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

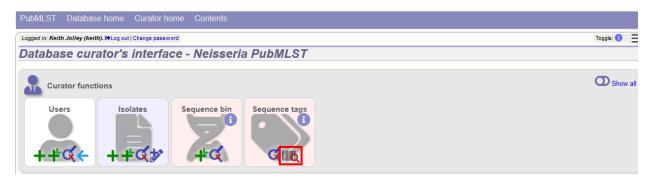


Alternatively, this step can be *performed offline automatically*.

6.19 Automated web-based sequence tagging

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

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



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

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

PubMLST Database home Curator home Contents	
Logged in: Keith Jolley (keith). @Log out Change password	Help 🕑 Toggle: 🚯 💻
Sequence tag scan Please select the required isolate ids and loci for sequence scanning - use Ctrl or Shift to make multiple selections. In addition to selecting individual loc the appropriate scheme description. By default, loci are only scanned for an isolate when no allele designation has been made or sequence tagged. You selecting the appropriate options. Isolates Lod \$195 \$3131 \$155 r0NA \$235 rRNA \$165 r0NA \$235 rRNA \$255 [old version] \$311 10 \$225 rRNA \$255 [old version] \$262 (NEIS1015) \$262 (NEIS1029) \$264 (NEIS1279) \$313 (33) \$64 (255 [old version] \$67 (S56 [11) All None Paste list All None Paste list All None Paste list Restrict included sequences by Sequence method: \$0 Project: \$0	i, you can choose to include all loci defined in schemes by selecting
Action Reset Scan	

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

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

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

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

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

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

PUDMLS1 Database nome Curator nome Contents	
Logged in: Keith Jolley (keith). (HLog out Change password	Help 🕼 Toggle: 🚯 💻
Sequence tag scan	
Please select the required isolate ids and loci for sequence scanning - use Cht or Shift to make multiple selections. In addition to selecting individual loci, yo the appropriate options. Isolates Loci 19) \$3131 1 23) 24 165_CNNA 30) 14 235_RNA 30) 14 abc2 33) 26 Exercise All R - in 46) 255 (Jold version] acce (NEIS1229) 3642 (NEIS12727) acnA (NEIS1727) acnA (NEIS1249) adh((NEIS1241) adh (NEIS1249) adh((NEIS1241) adh (NEIS1241) All None Paste list	

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

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

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

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

See also:

Sequence tag flags

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

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

by batch uploading to sequence definition database.

See also:

Offline curation tools

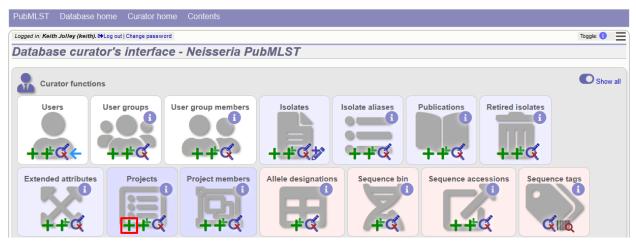
Automated offline sequence tagging

6.20 Projects

6.20.1 Creating the project

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

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



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

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

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

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

There are a further two option flags:

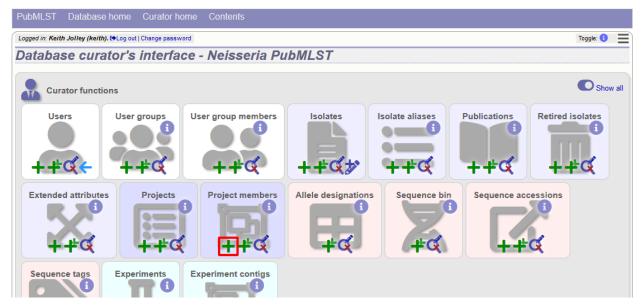
- private Setting this makes the project a private *user project*. You will be set as the project owner and will be the only user able to access it by default. You can add additional users or user groups who will be able to access and update the project data later.
- no_quota If set, isolates added to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

Click 'Submit'.

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

6.20.2 Explicitly adding isolates to a project

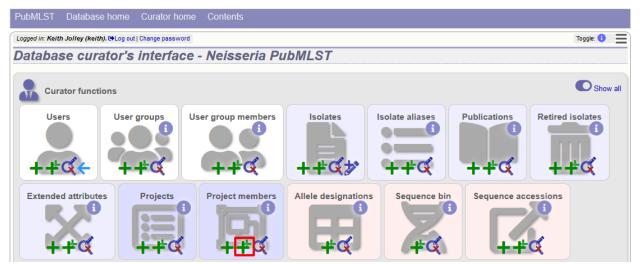
Explicitly adding isolates to the project can be done individually or in batch mode. To add individually, click the add (+) project member link on the curator's main page. This function is normally hidden, so you may need to click the 'Show all' toggle to display it.



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

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

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



Download an Excel submission template:

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

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

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

6.21 Isolate record versioning

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

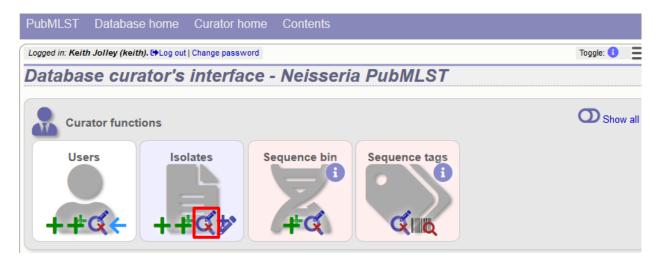
By default, old versions of the record are not returned from queries. Most query pages have a checkbox to 'Include old record versions' to override this.

Links to different versions are displayed within an isolate record:

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

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

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

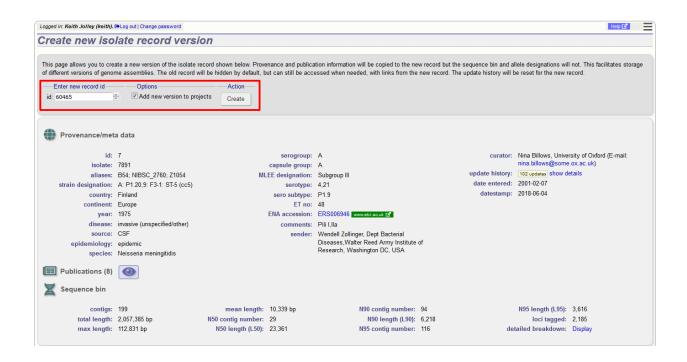


Click the 'create' new version link next to the isolate record:

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

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

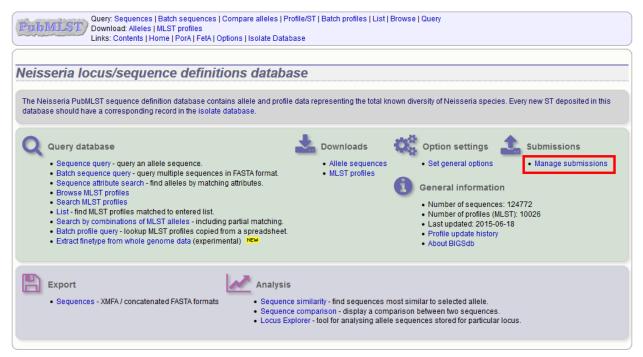
Click the 'Create' button.



CHAPTER 7

Curating submitted data

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



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

.ogged in: Keith Jolley (keith). 🗭 Lo	out Change password			
lanage submiss	ons			
Submit new data				
Data submitted here will go in	o a queue for handling by a curator or by an automated scr	ot. You will be able to track the s	tatus of any submission.	
Submission type:				
 alleles 				
 MLST profiles 				
New allele sequence su	bmissions waiting for curation			
Your account is authorized to h	andle the following submissions:			
Submission id	Submitted Updated Submitter Locu	Sequences		
BIGSdb_20150623074942_3	862_84622 2015-06-23 2015-06-23 Joe Bloggs NEIS00			
Return to index page				

7.1 Alleles

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

PTDMLST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
Logged in: Keith Jolley (keith). I#Log out Change password Hel	р 🗗
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
alleles MLST profiles	
New allele sequence submissions waiting for curation	
Your account is authorized to handle the following submissions:	
Submission id Submitted Updated Submitter Locus Sequences BIGSdb_20150709132553_20864_89729 2015-07-09 2015-07-09 Joe Bloggs NEIS0001 (lpxC) 3	
Return to index page	

You will see a summary section that describes details about how the sequences were obtained. There should also be link here to download all the sequences in FASTA format.

gged III. Kenn Solley (ken	h). 🕪 Log out Change password					He
urate submi	ssion					
ubmission: BIGSd	b_20150709132553_20864_897	29				
- Summary						
submitter: datestamp:		IdentifierLengthUK322924UK323924UK347924	Sequence АГССТССАААGААСТІСССС АСАГСАGАААТТСІССАТАА АГССТССАААGААСТІТССС АСАГСАGААСТІСІССАТАА АГССТССАААGAACTITССС АСАГСАGAAATTСІССАТАА	Complete CDS	Status pending v pending v	Assigned allele Curate Curate
locus: sequences:	status: pending locus: NEIS0001 (lpxC) ances: 3 2 lology: Illumina	Batch curate Messages	Archive Archive Archive and any supp	orting files:		Update
read length: coverage: assembly: assembly software:	20-49x de novo	Message: Appe	Download Tab			

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

ed in: Keith Jolley (keit	h). I Log out Change password					He
ırate submi	ssion					
ubmission: BIGSd —Summary—	b_20150709132553_20864_897	29 — Sequences —				
type: submitter: datestamp: status:	alleles Joe Bloggs, University of Oxford, UK 2015-07-09 pending NEIS0001 (IpxC)	Identifier Length UK322 924 UK323 924 UK347 924 Batch curate	Sequence АГССТБСАААGААСТІССВС АСАГСАБАААТІБІСБАТАР АГССТБСАААGААСТІТБЕС АСАГСАБААСТІБІББАТАР АГССТБСАААGААСТІТБЕС АСАГСАБАААТІБІББАТАР	Complete CDS	Status pending v pending v	Assigned allele Curate Curate Curate Update
sequences: technology: read length: coverage: assembly: assembly software:	3 mi Illumina 100-199 20-49x de novo	Messages Message: Apper	Archive Archive of submission and any supp Download	orting files:		

7.1.1 Individual allele curation

Individual sequences can be curated singly by clicking the 'Curate' links next to the sequence in the table. If you have supporting data attached to the submission, e.g. Sanger trace files then you may need to assess the submission based on the policy of the database.

ged in: Keith Jolley (keith). DLog out Change password							He
ırate submission							
ubmission: BIGSdb_20150709132553_20864_897							
- Summary	Sequence			S	Complete CDC	Status	Anningstallala
type: alleles	Identifier Lo		ATGCTGCAAAGAACTT	Sequence	Complete CDS	pending -	Assigned allele
submitter: Joe Bloggs, University of Oxford, UK				TGGC ACATCAGAACTTGTGGATAA		pending v	Curate
datestamp: 2015-07-09				TGGC ACATCAGAAATTGTGGATAA		pending +	
status: pending					•	pending +	
locus: NEIS0001 (lpxC)	Batch cura	ate					Update
sequences: 3 🕞	— Messages	s		Archive			
technology: Illumina	-			Archive of submission and any supp	orting files:		
read length: 100-199				- · · · ·			
coverage: 20-49x				Download TAR			
assembly: de novo	Message:	Appen	d Send now				

Clicking this link takes you to the curation interface *single sequence upload page*. The upload form will be filled with details from the submission. You may wish to manually change the status from the dropdown list of values.

PubMLST Use	abase: Species home Curator's page (species) Curator's page (database) ers: Add Query/update i: Add ST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith	h). @Log out Change password Help E	🚹 Toggle: 🚯
Add new allele	e sequence	
Please fill in the fields be	elow - required fields are marked with an exclamation mark (!).	
	NEIS0001 -	
allele id:	210	
sequence:	ATGCTGCAAAGAACTTCGGCGAAATCCATCAGCGTTACCGGAGTCGGCCTGCATTCCGGCGAACGGGTCGC ACCCTGCACCCCGCGCCTGAAAACAGCGGGATTTCCTTCC	LACAA CCGTC = CACCC LAAAG CGCCG +
status:!	unchecked 👻	
sender:!	Bloggs, Joe (jbloggs)	
	Keith Jolley (keith)	
date entered:!		
datestamp:! comments:	2015-07-09	
comments:		
Flags:	atypical contains IS element downstream fusion	

Clicking 'Submit' from this form will define the new allele and add it to the database. A link on the confirmation page will take you back to the submission management page.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). Hog out Change password	Help 🗗	Toggle: 🜖
Add new allele sequence		
Sequence NEIS0001 (lpxC): 210 added!		
Add another Return to submission Back to main page		

You will find that the status of the newly assigned sequence has changed in the summary table. The assigned value and status are determined on display and should always reflect the live database values.

gged in: Keith Jolley (kei	h). @Log out Change password					Hel
urate submi	ssion					
Submission: BIGSc	lb_20150709132553_20864_8972	29 Sequences				
type: submitter: datestamp: status;	pending NEIS0001 (IpxC) 3 हाउ	Identifier Length UK322 924 UK323 924 UK347 924 Batch curate Messages	Sequence ATGCTGCAAAGAACTTCGGC ACATCAGAAATTGTGGATAA ATGCTGCAAAGAACTTGGC ACATCAGAAATTGTGGATAA ATGCTGCAAAGAACTTTGGC ACATCAGAAATTGTGGATAA	*	Status assigned pending • pending •	Assigned allele 210 Curate Curate Update

7.1.2 Batch allele curation

Often, you will want to batch upload submitted sequences. This can be done by clicking the 'Batch curate' button.

Note: Batch curation is only available for loci that do not have extended attributes defined. Entries for these loci

require additional values set for these additional fields and so need to be handled individually.

PUDMLST / Dov	ery: Sequences Batch sequences Co vnload: Alleles MLST profiles cs: Contents Home PorA FetA Optic			s List Browse Query			
ogged in: Keith Jolley (keith). Hog out Change password						Help 🗹
curate submis	ssion						
Submission: BIGSd	b_20150709132553_20864_8972	29					
		Sequences					
type:	alleles	Identifier Leng		Sequence	Complete CDS	Status	Assigned allele
submitter:	Joe Bloggs, University of Oxford, UK	UK322 924 UK323 924		TGGC ACATCAGAAATIGIGGATAA	*	assigned	210
datestamp:	2015-07-09	UK347 924		TGGC ACATCAGAAATTGTGGATAA		pending -	
status:	pending		1		•	pending +	
locus:	NEIS0001 (IpxC)	Batch curate	1				Update
sequences:	3 PAS	—Messages —		Archive			
technology:	Illumina			Archive of submission and any supp	orting files:		
read length:				Download 🛺			
coverage:	20-49x			Download TAR			
assembly:	de novo	Message: App	oend Send now				
assembly software:	Velvet						

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

The upload form will be filled with details from the submission. You may wish to manually change the status from the dropdown list of values.

PubML	Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert
Logged in: Keith	Jolley (keith). (bLog out Change password Toggle: ()
Batch in	sert sequences
only). Do not i	ows you to upload allele sequence data in FASTA format. The identifiers in the FASTA file will be used unless you select the option to use the next available id (loci with integer ids nclude the locus name in the identifier in the FASTA file. nat you can not use this page to upload sequences for loci with extended attributes.
	NEIS0001 (IpxC) V
	unchecked •
	Blogs, Joe (iblogs)
sequence (FASTA):!	
♥ Use ne — Action — Reset	xt available id (only for loci with integer ids)

Click 'Check' on this form will perform some standard checks before allowing you to upload the sequences.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert				
Logged in: Keith Jolley (keith). @Log out Change password	lelp 🖉	Toggle: 🜖		
Batch insert sequences				
Sequence check Original designation Allele id UK323 211 UK347 212 OK OK				

A link on the confirmation page will take you back to the submission management page.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). (DeLog out Change password	Help 🖉	Toggle: 🚯
Batch insert sequences		
Upload succeeded.		
Return to submission Upload more Back to main page		

The status of the sequences should reflect their newly assigned status.

PuthILST Download: Alleles I Links: Contents Ho	me PorA FetA Options Isolate Database				
Logged in: Keith Jolley (keith). Hog out Chan	ge password				Help 🖾
Curate submission					
Submission: BIGSdb_2015070913	Sequences				
type: alleles submitter: Joe Bloggs, Uni datestamp: 2015-07-09 status: pending locus: NEIS0001 (IpxC sequences: 3 2 2 technology: Illumina read length: 100-199 coverage: 20-49x assembly: de novo assembly software: Velvet	versity of Oxford, UK UK323 924 AT UK347 924 AT Messages	Sequence GEGIGCAAAGAACITGEGC ACAICAGAAAITGIGGATAA GEGIGCAAAGAACITGEGC ACAICAGAAAITGIGGATAA GEGIGCAAAGAACITIGEC ACAICAGAAAITGIGGATAA Archive of submission and any supp Download R	***	Status Assigned allele assigned 210 assigned 211 assigned 212 - Action Close submission	

7.1.3 Rejecting sequences

Sometimes you may need to reject all, or some of, the sequences in a submission. You can do this by changing the value in the status dropdown box next to each sequence. Click 'Update' to make the change.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database						
Logged in: Keith Jolley (keith). DeLog out Change password		Help 🖉				
Curate submission						
Submission: BIGSdb_20150709132553_20	0864_89729 Sequences					
type: alieles submitte: Joe Bloggs, University of C datestamp: 2015-07-09 status: pending outcome: accepted - data uploaded locus: NEIS0001 (lpxC) sequences: 3 Jack technology: Illumina read length: 100-199 coverage: 20-49x assembly: de novo assembly software: Velvet	Identifier Length Sequence Complete CDS Status Assigned allele Wdord, UK UK322 924 ATGCTGCAAAGAACTTCGGC ACATCAGAAATTGTGGATAA rejected rejected <td< td=""><td></td></td<>					

7.1.4 Requesting additonal information

You can send a message to the submitter by entering it in the Messages box and clicking 'Send now'. This will append a message to the submission and send an update to the submitter so that they can respond.

7.1.5 Closing the submission

You can add a message to the submitter by entering it in the message box and clicking 'Append'. Once sequences have all been either assigned or rejected, the 'Close submission' button will be displayed. Click this to close the submission. The submitter will be notified of their submission status.

PubMLST Do	ery: Sequences Batch sequences Co wnload: Alleles MLST profiles iks: Contents Home PorA FetA Optic			T Batch prof	iles List B	rowse Que	ery						
Logged in: Keith Jolley (kei	th). @Log out Change password												Help 🗗
Curate submi	ssion												
Submission: BIGS	ib_20150709132553_20864_897	29											
Summary													
type:	alleles	Identifier Leng			Sequ				mplete CDS	Status	6	Assigned allele	
	Joe Bloggs, University of Oxford, UK	UK322 924					SAAATTGTGGA1		×	rejected			
	2015-07-09	UK323 924					GAACTTGTGGA		×	rejected			
	pending	UK347 924	4 A16	LIGCAAAGAA	CITIGGC	. ACAICA	AAATTGTGGA	AAL	~	rejected	•		
	NEIS0001 (lpxC)											Update	
sequences:	3 745	— Messages —								ive			
technology:		Timesta	amp	User		Me	ssage		Archive	e of subm	issio	n and any suppo	rting files:
read length:		2015-07-09 12			ey These se			01 allel	es				-
coverage:									Downl	oad TAR			
assembly:	de novo												
assembly software:	Velvet								Actio	on —		-	
					Me	essage: /	Append Se	end nov	/ Clos	e submis	sion		

7.2 Profiles

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

Ouery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
Logged in: Keith Jolley (keith). (Hog out Change password	elp 🗗
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
alleles MLST profiles	
New allelic profile submissions waiting for curation	
Your account is authorized to handle the following submissions:	
Submission id Submitted Updated Submitter Scheme Profiles BIGSdb_20150709134405_4219_35535 2015-07-09 2015-07-09 Joe Bloggs MLST 3	
Return to index page	

You will see a table summarizing the profiles in the submission and their current status.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database												
Logged in: Keith Jolley (keith). In Log out Change password		Help 🗗										
Curate submission												
Submission: BIG Sdb_20150709134405_4219_38 — Summary	Profiles Identifier adk abc2 arcE fumC gdh phC pgm Status Assisted and	Messages Curate Curate Curate Update Message: Append Send now										

7.2.1 Individual profile curation

Individual profiles can be curated singly by clicking the 'Curate' links next to the profile in the table.

Printing Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database													
Logged in: Keith Jolley (keith). I Log out Change password													Help 🖉
Curate submission													
Submission: BIGSdb_20150709134405_4219_3553 — Summary type: profiles submitter: Joe Bloggs, University of Oxford, UK datestamp: 2015-07-09 status: pending	5 Profiles Identifier UK32 UK33 UK34 Batch c	adk 43 7 76	abcZ 2 56 3	aroE 12 4 5	fumC 32 3 3	gdh 32 2 87	pdhC 3 12 43	pgm 2 12 34	Status pending pending pending	- -	Assigned ST Curate Curate Curate Update		
Messages Archive Archive of submissi			orting	files:							Opulae		

Clicking this link takes you to the curation interface *single profile upload page*. The upload form will be filled with details from the submission.

PubMLST U	Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert											
Logged in: Keith Jolley (ke	ith). ⊕Log out Change passw	ord		Help 🗹	Toggle: 🚺							
Add new MLS	ST profile											
~												
Please fill in the fields	below - required fields are	marked with an exclamation	mark (!).									
Record												
	10056											
adk: !												
abcZ: !												
aroE: !	12											
fumC: !	32 🜲											
gdh: !	32											
pdhC: !	3											
pgm: !	2											
sender: !	Bloggs, Joe (jbloggs)	~										
clonal_complex:												
	Keith Jolley (keith)											
date_entered: !												
datestamp: !	2015-07-09											
PubMed ids:												
- Action												
Reset Subn	nit											

Clicking 'Submit' from this form will define the new profile and add it to the database. A link on the confirmation page will take you back to the submission management page.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). @Log out Change password	Help 🖓	Toggle: 🚯
Add new MLST profile		
ST-10056 added! Return to submission Add another Back to main page		

You will find that the status of the newly assigned profile has changed in the summary table. The assigned value and status are determined on display and should always reflect the live database values.

Putili/LST Download: Alleles Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
Logged in: Keith Jolley (keith). (Hog out Change password											Help 🖉
Curate submission											
Submission: BIGSdb_20150709134405_4219_35538 — Summary type: profiles submitter: Joe Bloggs, University of Oxford, UK datestamp: 2015-07-09 status: pending	5 Profiles Identifier UK32 UK33 UK34 Batch c	adk 43 7 76	abcZ 2 56 3	aroE 12 4 5	fumC 32 3 3	gdh 32 2 87	pdhC 3 12 43	pgm 2 12 34	Status assigned pending ↓ pending ↓	Assigned ST 10056 Curate Curate Update	
Messages Append Send now	on and any	suppo	orting	îles:							

7.2.2 Batch profile curation

Often, you will want to batch upload submitted profiles. This can be done by clicking the 'Batch curate' button.

Lin	wnload: Alleles MLST profiles ks: Contents Home PorA FetA Opt h). G+Log out Change password	ons Isolate	e Data	base								Help 🗗
Curate submi	ssion											
— Summary type: submitter: datestamp:	b_20150709134405_4219_3553 profiles Joe Bloggs, University of Oxford, UK 2015-07-09 pending	5 Profiles Identifier UK32 UK33 UK34 Batch ci	adk 43 7 76	abcZ 2 56 3	aroE 12 4 5	fumC 32 3 3	gdh 32 2 87	pdhC 3 12 43	pgm 2 12 34	Status assigne pending pending	Curate]
Messages Message: Append	Archive Archive of submissi Download	on and any	suppo	rting f	iles:							

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

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

PubM		sers: Add 0 oci: Add	ecies home Query/updat :: Add Quer	e		ies) Curator's pag	e (database)	
Logged in: W	(ke	ith). 🕩Log ou	t Change pa	ssword			Help 🗹 🛛 Toggle:	0
Batch	insert l	MLST	profile	s				
• Fie • Yo it f	eld header na u can choose or each profil	ames must l e whether or e record. delimited he	be included r not to inclu ader for you	and fields (de a ST fiel Ir spreadsh	an be in any d - if it is omi		ds can be omitted if you wish. ble ST will be used automatically. If however, you include it in the header line, then you must also provi	de
— Pleas adk 7 76	e paste in tal abcZ 56 3	b-delimited aroE 4 5	text (include fumC 3 3	e a field hea gdh 2 87	der line) — pdhC 12 43	pgm 12 34	Parameters Sender: Bloggs. Joe (jbloggs) Value will be overridden if you include a sender field in your pasted data. Ignore duplicate profiles Action Reset Submit	
Back								

After upload, a link on the confirmation page leads back to the submission management page.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). In Log out Change password	Help 🗹	Toggle: 🚯
Batch insert MLST profiles		
Database updated ok		
Return to submission Back to main page		

The status of the profiles should reflect their newly assigned status.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database													
Logged in: Keith Jolley (keit	th). @Log out Change password											Help	3
Curate submi	ssion												
— Summary type: submitter: datestamp:	Ib_20150709134405_4219_35534 profiles Joe Bloggs, University of Oxford, UK 2015-07-09 pending	Profiles	adk 43 7 76 ges	abcZ 2 56 3	12 4 5	fumC 32 3 3	32 2 87	3 12 43 Arct Dov	2 12 34 archive nive o wnloa	Status A assigned assigned assigned f submission d assigned submission	10056 10057 10058		s:

7.2.3 Rejecting profiles

Sometimes you may need to reject all, or some of, the profiles in the submission. This may be because isolate data had not been made available, against the policy of the database. You can do this by changing the value in the status dropdown box next to each profile. Click 'Update' to make the change.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database														
Logged in: Keith Jolley (keit	h). I Log out Change password													Help 🗹
Curate submi	ssion													
— Summary — type: submitter: datestamp: status:	Ib_20150709134405_4219_35533 profiles Joe Bloggs, University of Oxford, UK 2015-07-09 pending accepted - data uploaded	5 Profiles Identifier UK32 UK33 UK34 Batch c Message	adk 43 7 76 urate ges	abcZ 2 56 3	12 4 5	fumC 32 3 3 3	32 2 87	3 12 43 — A Arct	2 12 34 rchive	rejected rejected rejected	* * *	Assigned ST Curate Curate Update	ing files:	

7.2.4 Requesting additonal information

You can send a message to the submitter by entering it in the Messages box and clicking 'Send now'. This will append a message to the submission and send an update to the submitter so that they can respond.

7.2.5 Closing the submission

You can add a message to the submitter by entering it in the message box and clicking 'Append'. Once profiles have all been either assigned or rejected, the 'Close submission' button will be displayed. Click this to close the submission. The submitter will be notified of their submission status.

Query: Sequences Batch sequences Co Download: Alleles MLST profiles Links: Contents Home PorA FetA Optic				ST B	atch p	rofiles	s Lis	t Brov	wse Query					
Logged in: Keith Jolley (keith). HLog out Change password														Help 🖉
Curate submission														
Submission: BIGSdb_20150709134405_4219_35538 — Summary	Profiles Identifier UK32 UK33 UK34		abcZ 2 56 3	aroE 12 4 5	fumC 32 3 3	gdh 32 2 87	pdhC 3 12 43	pgm 2 12 34	Status rejected rejected rejected Archive	•	igned ST Update			
Timestamp User		essag							Archive of	subm	ission and	any suppo	rting files:	
2015-07-09 12:55:23+00 Keith Jolley You need to submit so	me repres		e isol sage:		lata fo bend	1	e prof end n	a	Download — Action – Close s		sion			

7.3 Isolates

Clicking the appropriate submission on the 'Manage submissions' page.

Output Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). IDLog out Change password	Help 🖉
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
• isolates	
Pending submissions	
You have submitted the following submissions that are pending curation:	
Submission id Updated Type Details	
BIGSdb_20150709121747_1342_99624 2015-07-09 2015-07-09 isolates 2 isolates	
Return to index page	

You will see a table summarizing the submission.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
ogged in: Keith Jolley (keith). III-Log out Change password	Help 🖓
Curate submission	
Submission: BIGSdb 20150709121747 1342 99624	
type: isolates	
submitter: Joe Bloggs, University of Oxford, UK	
datestamp: 2015-07-09	
status: pending	
Isolates	
isolate country disease source species serogroup adk arcE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2 UK322 UK meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2	
UK322 UK meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2 UK325 UK septicaemia CSF Neisseria meningitidis B 2 3 4 3 18 4 6 F1-5 5-1 2	
Batch curate Record status: pending v Update	
Messages Archive Archive	
Archive of submission and any supporting files:	
Download 🔜	
Message: Append Send now	

Click the 'Batch curate' button.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). III Log out Change password	Help 🖉
Curate submission	
Submission: BIGSdb_20150709121747_1342_99624 — Summary type: isolates submitter: Joe Bloggs, University of Oxford, UK datestamp: 2015-07-09 status: pending	
Isolates	
isolate country disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2 UK322 UK meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2	
UK322 OK interimination separatemia utoru versiena meningituto B 2 3 4 3 6 4 6 F1-5 5-1 2	
Batch curate Record status: pending 👻 Update	
Messages Append Send now	

This will take you to the batch isolate upload page in the curators' interface.

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

PubMLST / Users: Ad	: Species home Curator's Id Query/update Add Query/update Batch in		's page (database)		
Logged in: Keith Jolley (keith). 🕩 Lo	g out Change password				Toggle: 🜖
Batch insert isola	ntes				
Enter aliases (alternati Enter references for you You can also upload al locus names). These v You can choose wheth Download tab-delimite Download submission Please select the sender from Bloggs, Joe (jbloggs)	ust be included and fields c: ve names) for your isolates : ur isolates as a semi-colon iele fields along with the oth vill be added with a confirme er or not to include an id nun d header for your spreadshe template (xlsx format) the list below:	an be in any order. Optio as a semi-colon (;) sepa ;) separated list of Publ er isolate data - simply of d status and method se heer field - if it is omitted et - use 'Paste Special 4 overridden if you include a	nal fields can be omitte rated list Med ids (non-integer id reate a new column w it as 'manual'. , the next available id w O Text' to paste the data	s will be ignored). ith the locus name (; vill be used automat a.	see the 'allowed_loci' tab in the Excel template for iically. — Action —————
isolate country year			-	adk	Reset Submit
aroE fumC gdh UK233 UK 201		FetA_VR PorA_VE septicaemia	<pre>X1 PorA_V CSF Neisse</pre>		
meningitidis B	2 3	4 3	8 4	6	
F1-5 5 2 UK322 UK 201	4 meningitis	blood Neisser	ria meningitidis	в	
2 3 17	3 8	4 6	F1-5 5	2-1	
Back					

Click submit to check and then import if there are no errors.

After upload, a link on the confirmation page leads back to the submission management page.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). DeLog out Change password	Toggle: 🚯
Batch insert isolates	
Database updated ok Return to submission Back to main page	

Note: Depending on the database policy, definitions of new scheme profiles, e.g. for MLST, may require submission

of representative isolate records. Where this is the case, the curator will need to extract the new profile from the submitted record. The tab-delimited isolate text file can be downloaded from the archive of supporting files linked to the submission and used directly for *batch adding new profiles*. Alternatively, the curator could use the *Export functionality* of the database to generate the file required for batch profile definition after upload of the isolate data.

7.3.1 Requesting additonal information

You can send a message to the submitter by entering it in the Messages box and clicking 'Send now'. This will append a message to the submission and send an update to the submitter so that they can respond.

7.3.2 Closing the submission

You can add a message to the submitter by entering it in the message box and clicking 'Append'. Change the record status to either 'accepted' or 'rejected' depending on whether you have accepted the submission. Click 'Update'.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). I+Log out Change password	Help 🖉
Curate submission	
Submission: BIGSdb 20150709121747 1342 99624	
Summary	
type: isolates	
submitter: Joe Bloggs, University of Oxford, UK datestamp: 2015-07-09	
status: pending	
- Isolates	
isolate country disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1	
UK322 UK meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 UK325 UK septicaemia CSF Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5	2
Batch curate Record status: accepted ~	Update
	opulae
Messages	
Archive of submission and any supporting files:	
Download 🔜	
Message: Append Send now	

The 'Close submission' button will now appear. Click this to close the submission. The submitter will be notified of their submission status.

Prt17MJLST Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). IHLog out Change password	Help 🖓
Curate submission	
Submission: BIGSdb 20150709121747 1342 99624	
Summary	
type: isolates	
submitter: Joe Bloggs, University of Oxford, UK	
datestamp: 2015-07-09	
status: pending	
- Isolates	
isolate country disease source species serogroup abcZ adk are fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2	
UK322 UK meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2	
UK325 UK septicaemia CSF Neisseria meningitidis B 2 3 4 3 18 4 6 F1-5 5-1 2	
Record status: accepted 🗸 Update	
Messages — Archive — Archive — Action —	
Active of submission and any supporting lites. Close submission	
Download The	
Message: Append Send now	
Message. Append Send now	

CHAPTER 8

Offline curation tools

8.1 Automated offline sequence tagging

Sequence tagging is the process of identifying alleles by scanning the sequence bin linked to an isolate record. Loci need to be defined in an external sequence definition database that contains the sequences for known alleles. The tagging function uses BLAST to identify sequences and will tag the specific sequence region with locus information and an allele designation if a matching allele is identified by reference to an external database.

There is a script called 'autotag.pl' in the BIGSdb package. This can be used to tag genome sequences from the command line.

Before autotag.pl can be run for the first time, a log file needs to be created. This can be created if it doesn't already exist with the following:

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

The autotag.pl script should be installed in /usr/local/bin. It is run as follows:

autotag.pl --database <database configuration>

where <database configuration> is the name used for the argument 'db' when using the BIGSdb application.

If you have multiple processor cores available, use the –threads option to set the number of jobs to run in parallel. Isolates for scanning will be split among the threads.

The script must be run by a user that can both write to the log file and access the databases, e.g. the 'bigsdb' user (see 'Setting up the offline job manager').

A full list of options can be found by typing:

```
autotag.pl --help
NAME
autotag.pl - BIGSdb automated allele tagger
```

(continues on next page)

```
SYNOPSIS
   autotag.pl -- database NAME [options]
OPTIONS
-0, --missing
   Marks missing loci as provisional allele 0. Sets default word size to 15.
-d, --database NAME
   Database configuration name.
-e, --exemplar
   Only use alleles with the 'exemplar' flag set in BLAST searches to identify
   locus within genome. Specific allele is then identified using a database
   lookup. This may be quicker than using all alleles for the BLAST search,
   but will be at the expense of sensitivity. If no exemplar alleles are set
   for a locus then all alleles will be used. Sets default word size to 15.
-f --fast
    Perform single BLAST query against all selected loci together. This will
   take longer to return any results but the overall scan should finish
   quicker. This method will also use more memory - this can be used with
    --exemplar to mitigate against this.
-h, --help
   This help page.
-i, --isolates LIST
   Comma-separated list of isolate ids to scan (ignored if -p used).
--isolate_list_file FILE
   File containing list of isolate ids (ignored if -i or -p used).
-I, --exclude_isolates LIST
   Comma-separated list of isolate ids to ignore.
-l, --loci LIST
   Comma-separated list of loci to scan (ignored if -s used).
-L, --exclude_loci LIST
   Comma-separated list of loci to exclude
-m, --min_size SIZE
   Minimum size of seqbin (bp) - limit search to isolates with at least this
   much sequence.
-n, --new_only
   New (previously untagged) isolates only. Combine with --new_max_alleles
   if required.
--new_max_alleles ALLELES
   Set the maximum number of alleles that can be designated or sequences
   tagged before an isolate is not considered new when using the --new_only
   option.
-o, --order
   Order so that isolates last tagged the longest time ago get scanned first
```

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(continued from previous page)

```
(ignored if -r used).
--only_already_tagged
   Only check loci that already have a tag present (but no allele designation).
   This must be combined with the --already_tagged option or no loci will
   match. This option is used to perform a catch-up scan where a curator has
   previously tagged sequence regions prior to alleles being defined, without
   the need to scan all missing loci.
-p, --projects LIST
   Comma-separated list of project isolates to scan.
-P, --exclude_projects LIST
   Comma-separated list of projects whose isolates will be excluded.
-q, --quiet
   Only error messages displayed.
-r, --random
   Shuffle order of isolate ids to scan.
--reuse blast
   Reuse the BLAST database for every isolate (when running --fast option).
   All loci will be scanned rather than just those missing from an isolate.
   Consequently, this may be slower if isolates have already been scanned,
   and for the first isolate scanned by a thread. On larger schemes, such as
   wgMLST, or when isolates have not been previously scanned, setting up the
   BLAST database can take a significant amount of time, so this may be
   quicker. This option is always selected if --new_only is used.
-R, --locus_regex REGEX
   Regex for locus names.
-s, --schemes LIST
   Comma-separated list of scheme loci to scan.
-t, --time MINS
   Stop after t minutes.
--threads THREADS
   Maximum number of threads to use.
-T, --already_tagged
   Scan even when sequence tagged (no designation).
-v, --view VIEW
    Isolate database view (overrides value set in config.xml).
-w, --word_size SIZE
   BLASTN word size.
-x, --min ID
   Minimum isolate id.
-y, --max ID
   Maximum isolate id.
```

8.2 Defining exemplar alleles

Exemplar alleles are a subset of the total number of alleles defined for a locus that encompass the known diversity within a specified identity threshold. They can be used to speed up *autotagging* as the BLAST queries are performed against exemplars to identify the locus region in the genome followed by a direct database lookup of the sequence found to identify the exact allele found. This is usually combined with the autotagger –fast option.

Once exemplars have been defined you may also wish to set the fast_scan="yes" option in the config.xml file. This enables their use for scanning within the web curators' interface.

There is a script called 'find_exemplars.pl' in the BIGSdb scripts/maintenance directory.

A full list of options can be found by typing:

```
find_exemplars.pl --help
NAME
    find_exemplars.pl - Identify and mark exemplar alleles for use
   by tagging functions
SYNOPSIS
   find_exemplars.pl --database NAME [options]
OPTIONS
--database NAME
   Database configuration name.
--datatype DNA|peptide
   Only define exemplars for specified data type (DNA or peptide)
--exclude_loci LIST
    Comma-separated list of loci to exclude
--help
   This help page.
--loci LIST
   Comma-separated list of loci to scan (ignored {f if} -s used).
--locus_regex REGEX
   Regex for locus names.
--schemes LIST
   Comma-separated list of scheme loci to scan.
--update
   Update exemplar flags in database.
--variation DISSIMILARITY
   Value for percentage identity variation that exemplar alleles
    cover (smaller value will result in more exemplars). Default: 10.
```

8.3 Automated offline allele definition

There is a script called 'scannew.pl' in the BIGSdb scripts/automation directory. This can be used to identify new alleles from the command line. This can (optionally) upload these to a sequence definition database.

Before scannew.pl can be run for the first time, a log file needs to be created. This can be created if it doesn't already exist with the following:

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

The autotag.pl script should be installed in /usr/local/bin. It is run as follows:

```
scannew.pl --database <database configuration>
```

where <database configuration> is the name used for the argument 'db' when using the BIGSdb application.

If you have multiple processor cores available, use the –threads option to set the number of jobs to run in parallel. Loci for scanning will be split among the threads.

The script must be run by a user that can both write to the log file and access the databases, e.g. the 'bigsdb' user (see 'Setting up the offline job manager').

A full list of options can be found by typing:

```
scannew.pl --help
NAME
 scannew.pl - BIGSdb automated allele definer
SYNOPSIS
 scannew.pl --database NAME [options]
OPTIONS
-a, --assign
   Assign new alleles in definitions database.
--allow_frameshift
   Allow sequences to contain a frameshift so that the length is not a
   multiple of 3, or an internal stop codon. To be used with
    --coding_sequences option to allow automated curation of pseudogenes.
   New alleles assigned will be flagged either 'frameshift' or 'internal stop
   codon' if appropriate. Essentially, combining these two options only
   checks that the sequence starts with a start codon and ends with a stop
   codon.
--allow_subsequences
   Allow definition of sub- or super-sequences. By default these will not
   be assigned.
-A, --alignment INT
   Percentage alignment (default: 100).
-B, --identity INT
   Percentage identity (default: 99).
-c, --coding_sequences
   Only return complete coding sequences.
```

(continues on next page)

```
-d, --database NAME
   Database configuration name.
-h, --help
   This help page.
-i, --isolates LIST
   Comma-separated list of isolate ids to scan (ignored if -p used).
--isolate_list_file FILE
   File containing list of isolate ids (ignored if -i or -p used).
-I, --exclude_isolates LIST
   Comma-separated list of isolate ids to ignore.
-l, --loci LIST
   Comma-separated list of loci to scan (ignored if -s used).
-L, --exclude_loci LIST
   Comma-separated list of loci to exclude.
-m, --min_size SIZE
   Minimum size of seqbin (bp) - limit search to isolates with at least this
   much sequence.
-n, --new_only
   New (previously untagged) isolates only.
-o, --order
   Order so that isolates last tagged the longest time ago get scanned first
    (ignored if -r used).
-p, --projects LIST
   Comma-separated list of project isolates to scan.
-P, --exclude_projects LIST
   Comma-separated list of projects whose isolates will be excluded.
-r, --random
   Shuffle order of isolate ids to scan.
-R, --locus_regex REGEX
   Regex for locus names.
-s, --schemes LIST
   Comma-separated list of scheme loci to scan.
-t, --time MINS
   Stop after t minutes.
--threads THREADS
   Maximum number of threads to use.
--type_alleles
   Only use alleles with the 'type_allele' flag set to identify locus.
   If a partial match is found then a full database lookup will be performed
```

(continues on next page)

(continued from previous page)

```
to identify any known alleles. Using this option will constrain the search
space so that allele definitions don't become more variable over time. Note
that you must have at least one allele defined as a type allele for a locus
if you use this option otherwise you will not find any matches!
-T, --already_tagged
Scan even when sequence tagged (no designation).
-v, --view VIEW
Isolate database view (overrides value set in config.xml).
-w, --word_size SIZE
BLASTN word size.
-x, --min ID
Minimum isolate id.
-y, --max ID
Maximum isolate id.
```

8.4 Cleanly interrupting offline curation

Sometimes you may wish to stop running autotagger or allele autodefiner jobs as they can be run for a long time and as CRON jobs. If these are running in single threaded mode, the easiest way is to simply send a kill signal to the process, i.e. identify the process id using 'top', e.g. 23232 and then

```
kill 23232
```

The scripts should respond to this signal within a couple of seconds, clean up all their temporary files and write the history log (where appropriate). Do not use 'kill -9' as this will terminate the processes immediately and not allow them to clean up.

If these scripts are running using multiple threads, then you need to cleanly kill each of these. The simplest way to terminate all autotagger jobs is to type

```
pkill autotag
```

The parent process will wait for all forked processes to cleanly terminate and then exit itself.

Similarly, to terminate all allele autodefiner jobs, type

pkill scannew

8.5 Uploading contigs from the command line

There is a script called upload_contigs.pl in the BIGSdb scripts/maintenance directory. This can be used to upload contigs from a local FASTA file for a specified isolate record.

The upload_contigs.pl script should be installed in /usr/local/bin. It is run as follows:

```
upload_contigs.pl --database <NAME> --isolate <ID> --file <FILE>
--curator <ID> --sender <ID>
```

The script must be run by a user who has the appropriate database permissions and the local configuration settings should be modified to match the database user account to be used. The default setting uses the 'apache' user which is used by the BIGSdb web interface.

A full list of options can be found by typing:

```
upload_contigs.pl --help
NAME
    upload_contigs.pl - Upload contigs to BIGSdb isolate database
SYNOPSIS
   upload_contigs.pl --database NAME --isolate ID --file FILE
         --curator ID --sender ID [options]
OPTIONS
-a, --append
   Upload contigs even {\tt if} isolate already has sequences {\tt in} the bin.
-c, --curator ID
   Curator id number.
-d, --database NAME
   Database configuration name.
-f, --file FILE
   Full path and filename of contig file.
-h, --help
   This help page.
-i, --isolate ID
    Isolate id of record to upload to.
-m, --method METHOD
   Method, e.g. 'Illumina', default 'unknown'.
--min_length LENGTH
   Exclude contigs with length less than value.
-s, --sender ID
    Sender id number.
```

CHAPTER 9

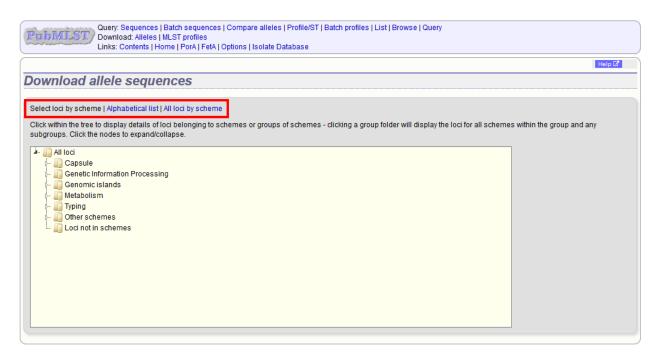
Definition downloads

The sequence definition database defines alleles, i.e. links an allele identifier to a sequence. It also defines scheme, e.g. MLST, profiles.

9.1 Allele sequence definitions

Click the 'Allele sequences' link in the 'Downloads' section. Depending on the database, you may see either a hierarchical scheme tree or a table of loci. You can choose to display links either by scheme using the scheme tree, as an alphabetical list or a page of all schemes, by selecting the appropriate link at the top of the page.

9.1.1 Scheme tree



You can drill down through the tree by clicking branch nodes. Clicking the labels of internal nodes will display tables of all schemes belonging to that scheme group. Clicking the labels of terminal nodes will display that single scheme table.

elect loci by scheme Aphabetical list All loci by scheme lick within the tree to display details of loci belonging to schemes or groups of schemes - dicking a group folder will display the loci for all schemes within the group and any abgroups. Click the nodes to expand/collapse.															Help 🗹
 All loci Capsule Genetic Information Processing Genomic islands Metabolism Trping Finetyping antigens Finetyping antigens Finetyping antigens Genus Capsule Multiple Statistics Multiple Statistics<th>ownl</th><th>oad a</th><th>allele</th><th>seq</th><th>uences</th><th>•</th><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th>	ownl	oad a	allele	seq	uences	•									
All loci Capsule Ca	elect loci	i by schen	me Alpha	ibetica	list All loci	y scheme									
Image: Capsule Capsule Image: Capsule Genetic Information Processing Image: Capsule Metabolism Image: Capsule Image: Capsule Image: Capsule Imag						nging to schemes o	or groups of schemes	- clicking a gro	up folder will	display the	loci for all	schemes	within the <u>c</u>	roup and	any
		Capsule Genetic I Genomic Metabolis	Informatio c islands	n Proc	essing										
		MLST Finety PIFs Antige MLS MLS MLS Other sch Loci not i	yping anti species en genes BT (20 locu BT (20 locu eningitidis hemes in schemo	us part us who s cgML es	le genes) ST v1.0										
	LST 0ccus	MLST Finety PIFs Antige MLS MLS Other sch Loci not i	yping anti species en genes 3T (20 loct 3T (20 loct eningitidis hemes in scheme d Type Al	us part us who s cgML es	le genes) ST v1.0	Full name/product			-						
bcZ 🚯 📥 DNA 728 Fixed: 433 bp O. Harrison, K. Jolley 2015-06-22	LST 0.0CUS [0.0CUS [0.0CUS]	MLST Finety	yping anti species en genes ST (20 loct ST (20 loct eningitidis hemes in scheme d Type Al DNA	us part us who s cgML es lleles 728 F	le genes) ST v1.0 Length Fixed: 433 bp	Full name/product	O. Harrison, K. Jolle	2015-06-22	-						
bcZ 0 ± DNA 728 Fixed: 433 bp O. Harrison, K. Jolley 2015-06-22 dk 0 ± DNA 501 Fixed: 465 bp O. Harrison, K. Jolley 2015-06-08	LST occus (bcZ () adk ()	MLST Finety profession Antige MLS MLS MLS N. me Other sct Loci not i Download 2 2	yping anti- species en genes ST (20 loca ST (20 loca eningitidis hemes in scheme DNA DNA	us part us who s cgML es lleles 728 501	le genes) ST v1.0 Euength Fixed: 433 bp Fixed: 465 bp	Full name/product	O. Harrison, K. Jolle O. Harrison, K. Jolle	2015-06-22 2015-06-08							
bcZ 0 ± DNA 728 Fixed: 433 bp O. Harrison, K. Jolley 2015-06-22 adk 0 ± DNA 501 Fixed: 465 bp O. Harrison, K. Jolley 2015-06-08 roE 0 ± DNA 775 Fixed: 490 bp O. Harrison, K. Jolley 2015-06-22	LST occus (bcZ () adk () roE ()	MLST Finety Finety Finety Finety Finety Finety Antige MLS Finety N. me Other sct Loci not i	yping anti- species en genes ST (20 loct ST (20 loct eningitidis hemes in scheme DNA DNA DNA	us part us who s cgML es leles 728 f 501 f 775 f	Length Fixed: 433 bp Fixed: 465 bp Fixed: 490 bp	Full name/product	O. Harrison, K. Jolle O. Harrison, K. Jolle O. Harrison, K. Jolle	y 2015-06-22 y 2015-06-08 y 2015-06-22							
bcZ 0 ± DNA 728 Fixed: 433 bp O. Harrison, K. Jolley 2015-06-22 adk 0 ± DNA 501 Fixed: 465 bp O. Harrison, K. Jolley 2015-06-08 roE 0 ± DNA 775 Fixed: 490 bp O. Harrison, K. Jolley 2015-06-22 mC 0 ± DNA 732 Fixed: 456 bp O. Harrison, K. Jolley 2015-06-02	LST 	MLST Finety Finety Finety Finety Finety Finety Finety MLS Finety Other sch Loci not i Download	yping anti- species en genes ST (20 loc: ST (20 loc: eningitidis hemes in scheme DNA DNA DNA DNA	us part us who s cgMLs es lleles 728 F 501 F 775 F 775 F	Length ST v1.0 Fixed: 433 bp Fixed: 465 bp Fixed: 465 bp Fixed: 465 bp	Full name/product	O. Harrison, K. Jolle O. Harrison, K. Jolle O. Harrison, K. Jolle O. Harrison, K. Jolle	y 2015-06-22 y 2015-06-08 y 2015-06-22 y 2015-06-02							
bcZ 0 ± DNA 728 Fixed: 433 bp O. Harrison, K. Jolley 2015-06-22 adk 0 ± DNA 501 Fixed: 465 bp O. Harrison, K. Jolley 2015-06-08 roE 0 ± DNA 775 Fixed: 490 bp O. Harrison, K. Jolley 2015-06-22	LST 	MLST Finety Files Antige MLS MLS MLS N. me Other sci Loci not i	yping anti- species en genes ST (20 loca ST (20 loca eningitidis hemes in schemu DNA DNA DNA DNA DNA DNA	us part us who s cgMLs es 101 F 728 F 501 F 775 F 732 F	Length ST v1.0 Eixed: 433 bp Fixed: 443 bp Fixed: 445 bp Fixed: 465 bp Fixed: 465 bp	Full name/product	O. Harrison, K. Jolle O. Harrison, K. Jolle O. Harrison, K. Jolle O. Harrison, K. Jolle O. Harrison, K. Jolle	y 2015-06-22 y 2015-06-08 y 2015-06-02 y 2015-06-02 y 2015-06-11							

Click the download link for the required locus

Locus	Download	Туре	Alleles	Length	Full name/product	Curator(s)	Last updated
abcZ 🚺	*	DNA	728	Fixed: 433 bp		O. Harrison, K. Jolley	2015-06-22
adk 🕦	*	DNA	501	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-08
aroE 🕕	*	DNA	775	Fixed: 490 bp		O. Harrison, K. Jolley	2015-06-22
fumC 🚺	*	DNA	732	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-02
gdh 🚺	*	DNA	732	Fixed: 501 bp		O. Harrison, K. Jolley	2015-06-11
pdhC 🚺	*	DNA	747	Fixed: 480 bp		O. Harrison, K. Jolley	2015-06-25
pgm 🕕	*	DNA	749	Fixed: 450 bp		O. Harrison, K. Jolley	2015-06-22

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

>fumC_1 GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG

(continues on next page)

	(continued from previous page)
ACCATCGGTATGGCGGGCGCGCGGGGCAATTTCGAGCTGAACGTCTATATGCCCGTCATC	
GCCTACAACCTCTTGCAATCCATCCGCCTGTTGGGCGACGCGTGCAACAGCTTCAACGAA	
CACTGCGCCGTCGGCATTGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC	
CTGATGCTCGTTACCGCGTTAAACCGCAAAATCGGTTACGAAAAC	
>fumC_2	
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG	
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGG	
TTGGGCGAAATCAAAATCCCCGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC	
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT	
ACCATCGGCATGGCGGGCGCGCCGGGCGAATTTCGAGCTGAACGTCTATATGCCCGTTATC	
GCCTACAACCTCTTGCAATCCATCCGCCTCTTGGGCGACGCGTGCAACAGCTTCAACGAA	
CACTGCGCCATCGGCATCGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC	
CTGATGCTCGTTACCGCGTTAAACCGCAAAATCGGTTACGAAAAC	
>fumC_3	
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG	
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGG	
TTGGGCGAAATCAAAATCCCCGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC	
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT	
ACCATCGGCATGGCGGGCGGCGGCGGCGGCGAATTTCGAGCTGAACGTCTATATGCCCGTTATC	
GCCTACAACCTCTTGCAATCCATCCGCCTGTTGGGCGACGCGTGCAACAGCTTCAACGAA	
CACTGCGCCGTCGGCATCGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC	
CTGATGCTGGTTACTGCGTTAAAACCGTAAAATCGGCTACGAAAAC	

9.1.2 Alphabetical list

Loci can be displayed in an alphabetical list. Loci will be grouped in to tables by initial letter. If common names are set for loci, they will be listed by both primary and common names.

	ownload: /			PorA FetA Options Isolate Dat	abase		
							Help
ownload al	lele se	ane	ence	25			
omnoud un		-yu		.0			
alastiasi ku ashasa	LAlphohat	ical list	LAILLOS	i bu a dhama			
elect loci by scheme	Alphabet	ICal list	[All loc	a by scheme			
Locus	Download	Type	Alleles	Length	Full name/product	Curator(s)	Last updated
ArsR [NEIS1769] ()	*	DNA	70	Variable: No limits set	ArsR family transcriptional regulator		2015-03-18
AsnC [NEIS1566] ()	±	DNA	160	Variable: No limits set	transcription regulator AsnC		2015-05-20
abcZ 🕕	±	DNA	728	Fixed: 433 bp		O. Harrison, K. Jolley	2015-06-22
abcZ [NEIS1015] 🕕	*	DNA	493	Variable: No limits set	ABC transporter ATP-binding protein		2015-05-19
aceF [NEIS1279] 🕕	٠.	DNA	477	Variable: (1563 min; 1641 max)	dihydrolipoamide acetyltransferase (EC 2.3.1.12)		2015-05-19
ackA2 [NEIS1727] 0	±	DNA	408	Variable: No limits set	acetate kinase		2015-05-20
acnA [NEIS1729] 🕕	±	DNA	527	Variable: No limits set	aconitate hydratase 1 (EC 4.2.1.3)		2015-05-20
acnB [NEIS1492] 1	<u>له</u>	DNA	476	Variable: No limits set	aconitate hydratase 2 (EC 4.2.1.3)		2015-05-19
adhA [NEIS0486] ()	±	DNA	614	Variable: No limits set	alcohol dehydrogenase		2015-05-17
adhC [NEIS1241] 🕕	<u>*</u>	DNA	239	Variable: No limits set	alcohol dehydrogenase		2015-05-20
adk 🕕	±	DNA	501	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-08
adk [NEIS0767] ()	*	DNA	208	Variable: No limits set	adenylate kinase		2015-05-18
aldA [NEIS1942] ()	±	DNA	447	Variable: No limits set	aldehyde dehydrogenase		2015-05-20
aniA [NEIS1549] 🕕		DNA	0	Variable: No limits set	nitrite reductase, major outer membrane copper-containing protein		
anmK [NEIS1788] 🕕	*	DNA	480	Variable: No limits set	anhydro-N-acetylmuramic acid kinase	A. Jamet	2015-05-20
apaH [NEIS0610] 🕕	±	DNA	116	Variable: No limits set	diadenosine tetraphosphatase		2015-05-17
argH [NEIS0580] 🕕	±	DNA	433	Variable: No limits set	argininosuccinate lyase		2015-05-18
aroE 🜖	*	DNA	775	Fixed: 490 bp		O. Harrison, K. Jolley	2015-06-22
aroE [NEIS1810] 🕕	٠.	DNA	305	Variable: No limits set	shikimate dehydrogenase		2015-05-21
aspA 🕕	±	DNA	189	Fixed: 432 bp		K. Jolley	2015-04-21
aspA [NEIS1185] 🕕	±	DNA	501	Variable: No limits set	aspartate ammonia-lyase		2015-05-20
atIA [NEIS2274] 1	<u>*</u>	DNA	18	Variable: No limits set	atlA / peptidoglycan transglycosylase	O. Harrison	2014-12-10
autA [NEIS1859] 1	*	DNA	242	Variable: No limits set	autotransporter A		2015-05-20

Click the download links for the required locus.

9.1.3 All loci by scheme

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

										Hel
										nei
wnload a	allele	sequ	ence	es e						
lect loci by sche	me į Alpha	abetical lis	t All loc	i by scheme						
LST										
ocus Downloa		leles I	Length	Full name/product	Curator(s)	Last upd	lated			
bcZ 🕕 📩	DNA		d: 433 b). Harrison, K. Jolley					
adk 🚯 📩			d: 465 b). Harrison, K. Jolley					
roE 🕕 👎	DNA		d: 490 b). Harrison, K. Jolley					
mC 🚺 📩	DNA	732 Fixe	d: 465 b	p C). Harrison, K. Jolley	2015-06	5-02			
jdh 🚯 土	DNA	732 Fixe	ed: 501 b	p O). Harrison, K. Jolley	2015-06	5-11			
dhC 🚺 🛛 📩	DNA	747 Fixe	ed: 480 b	p C). Harrison, K. Jolley	2015-06	6-25			
gm 🕕 🛛 📩	DNA	749 Fixe	ed: 450 b	p C). Harrison, K. Jolley	2015-06	5-22			
orA VR1 0	nload Ty per	pe Allele otide 264 otide 735 otide 581	4 Varia 5 Varia	Length Full ble: No limits set PorAv ble: No limits set PorAv ble: No limits set	variable region 1 K variable region 2 K	C Jolley	Last updated 2015-06-16 2015-06-16 2015-06-26			
IF species										
ocus Download			ength	Full name/proc		r(s) Last				
olF 🚯 🕹	DNA 1	23 Fixed	i: 413 bp	50S ribosomal protein	L6 (partial) E. Wate	dins 201	5-01-30			
)P-heptose b	iosynth	ocic								
n -neptose b	losyntii	6313								
Locus	Down	load Type	Alleles	Length		Full name	/product	Aliases	Curator(s)	Last updated
IEIS0769 (hIdA)			244	Variable: No limits set				NMB0825; NMC0769; rfaE	C. Kahler	2015-05-18
IEIS0773 (hldD)	0 1	DNA		Variable: No limits set			otose epimerase	NMB0828; NMC0773	C. Kahler	2015-05-17
					Distance base Diller	ate e e 1 7	the state of the s	NIMP00000 NIM00044	O Kables	0045 05 00
EIS2014 (gmhB)			216	Variable: No limits set				NMB2033; NMC2014	C. Kahler	2015-05-20
	0 1	DNA	206	Variable: No limits set Variable: No limits set Variable: No limits set	D-beta-D-heptos	e-1-phosp	oispnospnate pnospnatase ohate adenylyltransferase osphate isomerase	NMB2033, NMC2014 NMB2076; NMC2055 NMB2090; NMC2070	C. Kahler	2015-05-20 2015-05-21 2015-05-21

Click the green download links for the required locus.

9.1.4 Download locus table

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

	Genomi Metabol Typing MLS Fine Fine Anti <u>c</u> ML: ML: N. m Other so	ic island: lism typing an species gen gene ST (20 lo ST (20 lo	tigens s cus pa cus wi lis cgM	urtial genes) nole genes) ILST v1.0						
MLST	ownloa	d Type	Allolos	Length	Full name/product Curator(s)	Last updated				
abcZ 1	±	DNA	728	Fixed: 433 bp	O. Harrison, K. Jolley					
adk 🕕	*	DNA	501	Fixed: 465 bp	O. Harrison, K. Jolley					
aroE 🕕	±	DNA	775	Fixed: 490 bp	O. Harrison, K. Jolley	2015-06-22				
fumC 🕕	±	DNA	732	Fixed: 465 bp	O. Harrison, K. Jolley	2015-06-02				
gdh 🕕	*	DNA	732	Fixed: 501 bp	O. Harrison, K. Jolley	2015-06-11				
pdhC 🕕	±.	DNA	747	Fixed: 480 bp	O. Harrison, K. Jolley	2015-06-25				
pgm 🕦	*	DNA	749	Fixed: 450 bp	O. Harrison, K. Jolley	2015-06-22				
Download	table ta	ab-delimi	ted tex	t Excel format]					

9.2 Scheme profile definitions

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home Options PubMLST.org Isolate Database										
Campylobacter locus/sequence definitions database										
The Campylobacter PubMLST sequence definition database contains allele and profile data representing the total kno database should have a corresponding record in the isolate database.	wn diversity of C. jejuni and C. coli. Every new ST deposited in this									
Query database Sequence query - query an allele sequence. Batch profile query - query multiple sequences in FASTA format. Search by combinations of MLST profiles copied from a spreadsheet. 	Option settings Submissions • Set general options • Manage submissions General information • Number of sequences: 412175 • Number of profiles (MLST): 7841 • Last updated: 2015-06-17 • Profile update history • About BIGSdb									
Export Sequences - XMFA / concatenated FASTA formats Analysis Sequence similarity - find sequences most sin Sequence comparison - display a comparison Locus Explorer - tool for analysing allele sequence 	n between two sequences.									

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

Profit/UST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Toggle: ()
Neisseria locus/sequence definitions database
The Neisseria PubMLST sequence definition database contains allele and profile data representing the total known diversity of Neisseria species. Every new ST deposited in this database should have a corresponding record in the isolate database.
 Query database Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Batch sequence atribute search - find alleles by matching attributes. Browse profiles Search profiles Search profile matched to entered list. Search profile query - lookup profiles copied from a spreadsheat. Extract finetype from whole genome data
 Export Sequences - XMFA / concatenated FASTA formats Analysis Sequence similarity - find sequences most similar to selected allele. Sequence comparison - display a comparison between two sequences. Locus Explorer - tool for analysing allele sequences stored for particular locus.

Profiles will be downloaded in tab-delimited format, e.g.

ST	abcZ	adk	aroE	fumC	gdh	pdhC	pgm	clonal_complex
1	1	3	1	1	1	1	3	ST-1 complex/subgroup I/
⇔II								
2	1	3	4	7	1	1	3	ST-1 complex/subgroup I/
∽II								
3	1	3	1	1	1	23	13	ST-1 complex/subgroup I/
⇔II			_				_	
4	1	3	3	1	4	2	3	ST-4 complex/subgroup IV
5	1	1	2	1	3	2	3	ST-5 complex/subgroup_
⇔III	-							
6	1	1	2	1	3	2	11	ST-5 complex/subgroup_
∽III	-							
7	1	1	2	1	3	2	19	ST-5 complex/subgroup_
∽III	-							
8	2	3	7	2	8	5	2	ST-8 complex/Cluster A4
9	2	3	8	10	8	5	2	ST-8 complex/Cluster A4
10	2	3	4	2	8	15	2	ST-8 complex/Cluster A4
11	2	3	4	3	8	4	6	ST-11 complex/ET-37
⇔con	nplex							
12	4	3	2	16	8	11	20	
13	4	10	15	7	8	11	1	ST-269 complex
14	4	1	15	7	8	11	1	ST-269 complex

CHAPTER 10

Data records

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

10.1 Isolate records

An Isolate record page displays everything known about an isolate.

PubMLST/B	reakdown: Isolate fie	se Profile/ST List ads 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 M		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 Meningococc	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 update history: 103 updates show details					
epidemiological year:			2012-02-15			
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						
b- 🛄 Pilin						
See In Typing						
Other schen Loci not in se						

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

10.1.1 Projects

Projects This isolate is a member of the following projects:	
MRF Meningococcus Genome Library	_
The MRF Meningococcus Genome Library is a collaboration between Public Health England, The Wellcome Trust Sanger Institute and the University of Oxford, funded by the Meningitis Research Foundation.	Ś
Use of the MRF Genome Library data must be cited in any publication or presentation making use of it.	Meningitis Research Foundation

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

10.1.2 Provenance metadata

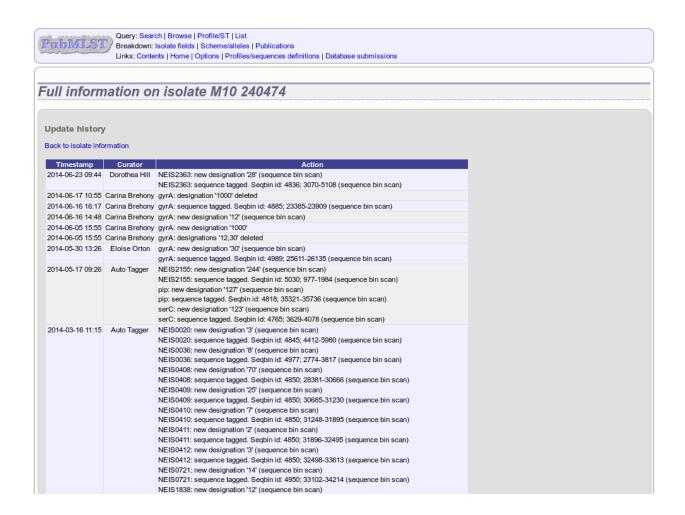
```
id: 18968
                                                                                               species: Neisseria meningitidis
            isolate: M10 240474
                                                                                            serogroup: B
                                                                                        ENA accession: ERR086224 → www.ebi.ac.uk
  strain designation: B: P1.19-1,15-11: F3-9: ST-269 (cc269)
          country: UK
                                                                                               sender: Dorothea Hill
          continent: Europe
                                                                                               curator: Dorothea Hill, University of Oxford, UK (E-mail:
                                                                                                       dorothea.hill@zoo.ox.ac.uk)
            region: South East
             year: 2010
                                                                                         update history: 103 updates show details
epidemiological year: 07/2010-06/2011
                                                                                          date entered: 2012-02-15
                                                                                            datestamp: 2014-06-23
           disease: invasive (unspecified/other)
```

This section includes:

Provenance/meta data

- provenance fields
- · housekeeping data
 - who sent the isolate
 - who last curated
 - record creation times
 - last update times
 - links to update history

The update link displays page with exact times of who and when updated the record.



10.1.3 Publications

Publications (8) show/hide

- Bennett JS, Jolley KA, Sparling PF, Saunders NJ, Hart CA, Feavers IM, Maiden MC (2007). Species status of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from multilocus sequence typing. BMC Biol 5:35 576 isolates
- Didelot X, Urwin R, Maiden MC, Falush D (2009). Genealogical typing of Neisseria meningitidis. Microbiology 155:3176-86 [93 isolates]
- Jolley KA, Sun L, Moxon ER, Maiden MC (2004). Dam inactivation in Neisseria meningitidis: prevalence among diverse hyperinvasive lineages. BMC Microbiol 4:34 et isolates
- Jolley KA, Wilson DJ, Kriz P, McVean G, Maiden MC (2005). The influence of mutation, recombination, population history, and selection on patterns of genetic diversity in Neisseria meningitidis. Mol Biol Evol 22:562-9 [378 isolates]
- Maiden MC, Bygraves JA, Feil E, Morelli G, Russell JE, Urwin R, Zhang Q, Zhou J, Zurth K, Caugant DA, Feavers IM, Achtman M, Spratt BG (1998). Multilocus sequence typing: a portable approach to the identification of clones within populations of pathogenic microorganisms. Proc Natl Acad Sci U S A 95:3140-5 107 isolates
- Thompson EA, Feavers IM, Maiden MC (2003). Antigenic diversity of meningococcal enterobactin receptor FetA, a vaccine component. Microbiology 149:1849-58 [107 isolates]
- Urwin R, Russell JE, Thompson EA, Holmes EC, Feavers IM, Maiden MC (2004). Distribution of surface protein variants among hyperinvasive meningococci: implications for vaccine design. Infect Immun 72:5955-62 [78 isolates]
- Wang JF, Caugant DA, Li X, Hu X, Poolman JT, Crowe BA, Achtman M (1992). Clonal and antigenic analysis of serogroup A Neisseria meningitidis with particular reference to epidemiological features of epidemic meningitis in the People's Republic of China. Infect Immun 60:5267-82 [47] isolates]

This section includes full citation for papers linked to the isolate record. Each citation has a button that will return a dataset of all isolates linked to the paper.

If there are five or more references they will be hidden by default to avoid cluttering the page too much. Click the 'Show/hide' button to display them in this case.

10.1.4 Sequence bin summary

Sequence bin			
contigs:	275	N90:	6405
total length:	2195045 bp	N95:	3513
max length:	109859 bp	loci tagged:	1611
mean length:	7982 bp	detailed breakdown:	Display
N50:	34308		

This section contains basic statistics describing the sequence bin. Clicking the 'Display' button navigates to the *sequence bin record*.

10.1.5 Scheme and locus data

A hierarchical tree displays available schemes. Click within internal nodes to expand them.

Schemes and loci	
🛓 🛄 All loci	Navigate and select schemes within tree to display allele designations
⊳. 📗 Capsule	
- 💭 Genetic Information Processing	
🗁 🌆 Metabolism	
🗁 🚛 Pilin	
🗁 🌆 Typing	
Other schemes	
🕼 Loci not in schemes	

Clicking any terminal node will display data available for a scheme or group of schemes.

Schemes and loci									
Genetic Information Processing					М	LST			
Pilin Typing MLST 	abcZ 4 S	adk 10 S	aroE 15 S	fumC 9S	gdh 8 S	pdhC 11 S	9S	ST 269	clonal complex ST-269 complex

Click an allele number within the scheme profile, will display the appropriate *allele definition record*. Clicking the green 'S' link will display the appropriate *sequence tag record*.

10.2 Allele definition records

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



If the allele is a member of a scheme profile, e.g. MLST, this will be listed. In this case, there will be a button to display all profiles of that scheme that contain the allele.

Similarly, if a *client database* has been setup for the database and the allele has been identified in an isolate, there will be a button to display all isolates that have that allele.

10.3 Sequence tag records

EIS0346 alle	ele sequen	ice: id-1	8968										
ontig position													
sequence bin id:	4956				length:	744							
contig length:	22993			огі	ientation:	forward							
start:	13864			с	omplete:	yes							
end:	14607				method:	Illumina							
equence													
ACTGTACGC GGCGCAC	GGC TTCAGCATTG	CGGGCAGGCG	GAAAAACTAT	TACCGTACAG	CCGACGGI	TAA AACCGAAGA	GCCGTCTTAA	TGGAGAAAAT	ATGTTAAGCG	CGCGCTACCT	CCACCTGCAC	GAAGCCTTGG 0	GTTTGGGCCC
ATGTGGTTG AAGCGGGG	GAG CCGTCGTCCT	GCCGTCCGCA	ACATTGCCGG	AAAGCCCGAC	ACAAATCO		AAACCGTCCT	CAGCATTCCG	CAGCGTCCGT	CCGAACAGCA	TACCGGTCAG	GCACGGCTCA #	
STGTTGGAA ACAACCG						000 0000144410							
		CAAACCCGCG	CCTGAAACCG		GICCGGC	GTT TCAGACGGC	A TCGCCCCCGT						
ATGGTTTAC GGGCAAC	TGT TCCACGGAAA	CAAACCCGCG AGCGGGTGTC	CCTGAAACCG CTGCTCGACA	ATATACTCAA	GTCCGGCC	GTT TCAGACGGC. GGG CTCGATGCC	A TCGCCCCCGT G CCTATGTCCA	CAAAACCTGT	TGGGTGAAAA	CCGCCGCCGT	CGGCAACCCG	ATGCCGTCTG #	AAGCGGCAAT
GCAAATGCG CTGGAAC	CTGT TCCACGGAAA	CAAACCCGCG AGCGGGTGTC ACTCGACGGC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC	ATATACTCAA CCGCCGTCCT	GTCCGGCC AGCCGTAC GTTCCTCC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA	CAAAACCTGT ACGGCAGGCG	TGGGTGAAAA ATGATTGAAA	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
	CTGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC	ATATACTCAA CCGCCGTCCT	GTCCGGCC AGCCGTAC GTTCCTCC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA	CAAAACCTGT ACGGCAGGCG	TGGGTGAAAA ATGATTGAAA	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAAATGCG CTGGAAC SCCCGGCTG TTGCGCC CAAAATGAC CGATTTC	CTGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC	ATATACTCAA CCGCCGTCCT	GTCCGGCC AGCCGTAC GTTCCTCC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA	CAAAACCTGT ACGGCAGGCG	TGGGTGAAAA ATGATTGAAA	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAAATGCG CTGGAACA	CTGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC	ATATACTCAA CCGCCGTCCT	GTCCGGCC AGCCGTAC GTTCCTCC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA	CAAAACCTGT ACGGCAGGCG	TGGGTGAAAA ATGATTGAAA	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAAATGCG CTGGAAC SCCCGGCTG TTGCGCC CAAAATGAC CGATTTC	CTGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC	ATATACTCAA CCGCCGTCCT	GTCCGGCC AGCCGTAC GTTCCTCC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA	CAAAACCTGT ACGGCAGGCG	TGGGTGAAAA ATGATTGAAA	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAAATGCG CTGGAAC SCCCGGCTG TTGCGCC CAAAATGAC CGATTTC ranslation	TGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA CCGC CAAGATTTCC	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC TTAAATTCTC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC CCTC	ATATACTCAA CCGCCGTCCT TCAAGCAGCT	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT GTC TTGGCGCAA	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA G GCGGCGGCAG	CAAAACCTGT ACGGCAGGCG TTGAAGCGCG	TGGGTGAAAA ATGATTGAAA CCGCACGGGG	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
ECAAATGCG CTGGAAC SCCCGGCTG TTGCGCC CAAAATGAC CGATTCC ranslation H C T	R R T A S	A L R A	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC CCTC	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC	GTT TCAGACGGC GGG CTCGATGCO GGA CAGGCGTTT GTC TTGGCGCAA	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA G GCGGCGGCAG M P S *	W R K	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAAATGCG CTGGAAC SCCCGGCTG TTGCCCCC CAAAATGAC CGATTCC Tanslation H C T T V R	TGT TCCACGGAAA CAAA CCGCCCGCGA CAAC CCGAACTCAA CCGC CAAGATTTCC	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCCGCGCC TTAAATTCTC	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC CCTC	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P	GTCCGGCG AGCCGTAG GTTCCTCC CAAACGTC	GTT TCAGACGGC GGG CTCGATGCC GGA CAGGCGTTT GTC TTGGCGCAA T V K P K R X N R 1	A TCGCCCCCGT G CCTATGTCCA G TCAAACCGGA G GCGGCGGCAG M P S R C R L	WRK NGEN	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAAATGCG CTGGAAC CCCGGCTG TTGGGCCI CAAATGAC CGATTCC ranslation H C T T V R L Y J 1 CACTGTAC	TGT TCCACGGAAA CCGCCCGCGA CAAC CCGAACTCAA CCGC CAAGATTTCC R R T A S & G A R L (A A H G F CCGCGCCACGCTT(CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCGCGCC TTAAATTCTC A L R J Q H C G S I A G CAGCATTGCGGG	CCTGAAACCG CTGCTCGACA TGCCGCGCGAC TGGCAGACGC CCTC A G G K Q A E K R R K 1 5CAGGCGGAAAJ	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATTACCG	GTCCGGCG AGCCGTAG GTTCCTCC CAAACGTC CAAACGTC Y S R T A D TACAGCCGJ	STT TCAGACGEC GGG CTCGATGCC GGA CAGGCGTTT STC TTGGCGCAA I V K P K R M R I G K T E ACGGTAAAACCGA	A TCGCCCCGT G CTATATGTCA G TCAAACCGGA G CGGCGGGAG M P S R C R L D A V L D A V L	CAAAACCIGI ACGGCAGGGG IIGAAGCGCG W R K N G E N M E K I AAIGGAGAAAA	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 I 100	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAAATGCG CTGGAAC CCCGGCTG TTGGGCCI CAAATGAC CGATTCC ranslation H C T T V R L Y J 1 CACTGTAC	TGT TCCACGGAAA CAAA CCGCCGCGA CAAC CCGAAACTCAA CCGC CAAGATTTCC R R T A S & G A R L (A A H G F	CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCGCGCC TTAAATTCTC A L R J Q H C G S I A G CAGCATTGCGGG	CCTGAAACCG CTGCTCGACA TGCCGCGCGAC TGGCAGACGC CCTC A G G K Q A E K R R K 1 5CAGGCGGAAAJ	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATTACCG	GTCCGGCG AGCCGTAG GTTCCTCC CAAACGTC CAAACGTC Y S R T A D TACAGCCGJ	STT TCAGACGEC GGG CTCGATGCC GGA CAGGCGTTT STC TTGGCGCAA I V K P K R M R I G K T E ACGGTAAAACCGA	A TCGCCCCGT G CTATATGTCA G TCAAACCGGA G CGGCGGGAG M P S R C R L D A V L D A V L	CAAAACCIGI ACGGCAGGGG IIGAAGCGCG W R K N G E N M E K I AAIGGAGAAAA	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 I 100	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAAATGCG CTGGAAC SCCCGGCTG TTGCGCCC SAAATGAC CGATTCC ranslation H C T T V R L Y J 1 CACTGTAC 	TGT TCCACGGAAA CAAA COGCCCCCA AAC CCGAACATCAA CCGC CAAGATTCC R R T A S & G A R L (A A H G F GCGGCGCCACGCCTT 	CAAACCCGCG AGCGGGTGTC AGCCGCGCGCC TIAAATICTC A L R J Q H C G S I A G CAGCATTGCGGG	CCTGAAACCG CTGCTCGACA TGCCCCGCAC TGGCAGACGC CCTC A G G K Q A E K R R K 1 SCAGGCGGAAA	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATTACCG :!:	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC Y S R T A D TACAGCCGJ	STT TCAGACGEC SGG CTCGATGCC GGA CAGGCGCTT STC TIGGCGCAA I V K P K R N R I G K T E ACGGTAAAACCGA -:!	A TCGCCCCCGT S CTATATCCA S TCAAACCGA G CCGCCGCCAG A V S A C R L D A V L GATGCCGTCTT 	CAAAACCIGI ACGGCAGGGG TIGAAGCGCG N G K N M E K I AAIGGAGAAAA 	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 I 100 I	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAATEGC CTGEAAC SCCCEGECTS TIECCCCC CAAATEGC CEATTCC Tanslation H C T T V R L Y 1 1 CACTETAC 	TGT TCCACGGAAA CCGCCCGCGA CAAC CCGAACTCAA CCGC CAAGATTTCC R R T A S & G A R L (A A H G F CCGCGCCACGCTT(CAAACCCGCG AGCGGGTGTC ACTCGACGGC AGCCGCGCC TTAAATTCTC A L R J Q H C G S I A G S I A G S I A G P A R S	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGCCGCGCAC CCTC A G G K Q A E K R R K 1 SCAGGCGGAAAA : L G F (ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATTACCG ::: S P D V	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC Y S R T A D TACAGCCG7 V E A	STT TCAGACGEC SGG CTCGATGCC SGC CAGCGCTT STC TIGGCGCAA I V K P K R N R 1 G K T E G S R R	M P S M P S CCBACGGCGGCAG M P S CCBCCGCGCGCAG A V L D A V L D A V L P A V R	CAAAACCTGT ACGGCAGGGG TTGAAGCGCG N G E N M E K I AATGGAGAAAA : N I A G	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 I 100 F1	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
SCAATEGC CTGEAALC SCCGCCTG TIGCCCCC SAAATGC CATTCC ranslation H C T T V R L Y J 1 CACTGTAC 	TIGT ICCACGGAAA CAA COGGCCGCGA AAC COGACACTCAA COGC CAAGAITICC R R T A S R G A R L (A A H G F COGGCGCACAGGGCTT 	CAAACCCGCG AGCGGGTGTC AGTCGACGGC AGCCGCGCGC TTAATTCTC A L R J Q H C G S I A G CAGCATTGCGGC CAGCATTGCGGC CAGCATTGCGGC L H E J	CCTGAAACCG CTGCTCGACA TGCCGCGCAC TGGCAGACGC CCTC A G G K Q A E K R R K 1 5CAGGCGGAAA L G F (A L G L	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y R AACTATTACCG ::: G P D V G P M W	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC Y S R T A D TACAGCCGJ V E A L L K H	TI TCAGAGGGC GGG CTCGATGCO GGA CAGGCGTTI GTC TIGGCGCAA R R K R K R R R R R R R R R R R R R R	A TCGCCCCCGT S CTATATCCCA S TCAALCCGA G CGGCGGCAG A V R AGAIGCCGTCTT P A V R L P S A	CAAAACCTGT ACGGCAGGGG TTGAAGCGCG M R K N G E N M E K I AATGGAGAAA 	TGGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 I 100 F1	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAATEGC CTGGAAC SECCEGETG TIEGCECC TANATEGC CEATTCC TANSIATION H C T T V R L Y J 1 CACTEGTAC U K H M L S C S A 101 ATETTAAG	TRET TCCAGGGAAA CAA CCGACCGGA AC CCGAAGATTAC CGC CAAGATTAC CGC CAAGATTAC CGC CAAGATTAC A A H G F GCGCGCCACGCGACGGCTA 	CAAACCCECG AGCGGGTGTC ACTCGACGGC AGCCGCGCCC TITAATICTC A L R J Q H C G S I A G C AGCATTGCGGG C CAGCATTGCGGG L H E J I C T K ACCTGCACGGAAC	CCTGALACCE CTGCTCGACA TGGCCGCACA TGGCCGCACA TGGCAGAACGC CCTC A G G K Q A E K R R K 1 CCAGCGGAALA :L G F (A L G L P W V W SCCTTGGGTTT	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATACA G P M W A R C GGCCCGATGT	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC Y S R T A D TACAGCCGJ V E A L K H G * S GGTGAAGC	TI V K P K GG CICGAIGCO GG CACGCGITI SIC TIGGCGCAA C K P K C K R K C K R K C G K R R C G R R R G A V V G E P S CGGGGARCCCICG	A TORECCECTET S CCTAIGICCA S TCAAACCGAA S CCACCGACAG A C R L D A V L AGAIGCCGICTI P A V R L P S A S C R P L P S A C R P C R C C C R C C C R C	CANAACCIGT ACGGCAGGGG TIGAAGGGGG N G E N M E K I AATGGAGAAA 	TGGGTGAAAA ATGATGAAA CCCCACGGGG Y F1 F2 F3 T 100 I F1 E F2 F3 G 200	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAATEGC CTGGAAC SECCEGETG TIEGCECC TANATEGC CEATTCC TANSIATION H C T T V R L Y J 1 CACTEGTAC U K H M L S C S A 101 ATETTAAG	THET TECACEGEAAA TAAA COSGOCEGEGA TAAC COSGACECEAA COSEC CAAGAITICE R A R T A S R G A R L C A A H G F GEGEGEGECACEGECTT 	CAAACCCECG AGCGGGTGTC ACTCGACGGC AGCCGCGCCC TITAATICTC A L R J Q H C G S I A G C AGCATTGCGGG C CAGCATTGCGGG L H E J I C T K ACCTGCACGGAAC	CCTGALACCE CTGCTCGACA TGGCCGCACA TGGCCGCACA TGGCAGAACGC CCTC A G G K Q A E K R R K 1 CCAGCGGAALA :L G F (A L G L P W V W SCCTTGGGTTT	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T I T V L L P N Y Y R AACTATACA G P M W A R C GGCCCGATGT	GTCCGGCC AGCCGTAC GTTCCTCC CAAACGTC Y S R T A D TACAGCCGJ V E A L K H G * S GGTGAAGC	TI V K P K GG CICGAIGCO GG CACGCGITI SIC TIGGCGCAA C K P K C K R K C K R K C G K R R C G R R R G A V V G E P S CGGGGARCCCICG	A TORECCECTET CCTATGTCCA TCAAACCGGA GCGGCGGGAG A C R L D A V L AGAIGCCGTCTT P A V R L P S A C R P C R C C R C C R C	CANAACCIGT ACGGCAGGGG TIGAAGGGGG N G E N M E K I AATGGAGAAA 	TGGGTGAAAA ATGATGAAA CCCCACGGGG Y F1 F2 F3 T 100 I F1 E F2 F3 G 200	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAATEGC CTGEAAC CCCCCCCT TECCCCC CAAATEGC CATTCC TANATEGC CATTCC T V R L Y J 1 CACTETAC V K I M L S C A 101 ATETTACC	TIGT ICCACGGAAA CAA COGGCCGCCA AC COGACACTCAA COGC CAAGAITICC R R T A S & G A R L (A A H G F CGGGCGCACGGGCTT R A L P P A R A T S : CGGGGGCACCTCCC 	CAACCOGGS AGCGGGTGTC AGCCGGGGC AGCCCGGGCC TTAAATTCTC Q H C G S I A G CAGCATTCCGGC P A R S L H E J T C T K ACCTGCAGGARG	CCTGAAACGC CTGCTCGACA TGCCCGCACA TGCCCGCACA CCTC A G G K Q A E K R R K 1 CCGCCGAAA CCGCGCGAAA CCGCGCGAAA CCGCGCGAAA CCGCGCGAAA CCGCGCGAAA CCGCGCGAAA CCGCGCGAAA CCGCGCGAAA CCGCGCGCAAA CCGCGCGCAAA CCGCGCGCAAA CCGCGCGCAAA CCGCGCGCAAA CCGCGCGCAAA CCGCGCGCAAA CCGCGCGCG	ATATACTCAA CCGCCGTCCT TCAAGCAGCT T L L P N Y Y R AACTATTACCG S P D V G P M W 3GGCCCGATGT :	GTCCGGCC AGCCGTA GTCCTCC CAAACGTC Y S R T A D TACAGCCG V E A G S GGTGAAGC 	I V K P K G C A CAGCGTIT STC TIGGCGCAA I V K P K R N R I G K T E CGGTAAAACCGA CGGTAAAACCGA G E P S CGGGGGAGCCGTCG I I I	M P S CCRIGCCCCGT CCRAGCCGA CCRCGCGCGCGCA CCRCGCGCGCGCA ACCRL D A V L MARIGCCGTCT P A V R L P S A C R L P A V R L P S A C R L CCRCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGCGCG	CAAAACCIGT ACGGCAGGCG ITGAAGCGCG N G E N M E K I AAATGGGAAAA N I A G T L P CAACATIGCCG	TGGGTGAJAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 T 100 I F1 E F2 F3 S 200 I	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC
CAATEGE CTGEAAC CCCGECTG TIECECCC ANATEGE CEATTCC Tanslation H C T T V R L Y J 1 CACTGTAC 	TRET TCCAGGGAAA CAA CCGACCGGA AC CCGAAGATTAC CGC CAAGATTAC CGC CAAGATTAC CGC CAAGATTAC A A H G F GCGCGCCACGCGACGGCTA 	CAACCOSCG AGCOGGTGTC AGCCOGGCC THAATTCTC AGCCCGCGCC THAATTCTC A L R J Q H C G S I A G S I A G CAGCATTCCCGG -:	CCTGALACCE CTGCTGGCA TGGCCGGACA TGGCCGGACA TGGCAGACGC CCTC A G G K K R R K 1 CCASCGGALA :	I I I V L L P V L L P N Y Y R ARCTATIACG G P M W A R C S A A	GTCCGGCC AGCCGTAC GTTCCTCC AAACGTC Y S R T A D TACAGCCGS V E A G S G S S V R	T V K P K G C C G A C G C G C C G A C G C G C G C	A TOBOCCOCOT S CCTAIGTOCA S CCTAIGTOCA S TCAAACCOBA S CC R L D A V L BARICCOGTCIT P A V R L P S A S C R P COCTECCOTCOC 	CAAAACCIGT ACGGCAGGCG IIGAAGCGCG N G E N M E K I AAIGGAGAAAA 	TGGTGAAAA ATGATTGAAA CCGCACGGGG Y F1 F2 F3 T 100 I F1 F1 F1 F1	CCGCCGCCGT CTTTGTGCGC	CGGCAACCCG	ATGCCGTCTG A	AAGCGGCAAT ICGACCATCC

A sequence tag record displays information about the location within a contig of a region associated with a locus. The nucleotide sequence will be displayed along with upstream and downstream flanking sequence. The length of these flanking sequences can be modified within the *general options*.

If the tag is for a DNA locus and it is marked as a coding sequence, the three-frame translation will also be displayed.

10.4 Profile records

(PubMLST) D	uery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query ownload: Alleles MLST profiles inks: Contents Home PorA FetA Options Isolate Database
Profile inform	nation for ST-11 (MLST)
ST abcZ adk at 11 2 3 3	aroE fumC gdh pdhC pgm clonal complex 4 3 8 4 6 ST-11 complex/ET-37 complex
sender:	Paula Kriz, Paula Kriz and Keith Jolley
curator:	Keith Jolley, University of Oxford, UK (E-mail: keith.jolley@zoo.ox.ac.uk)
date entered:	2001-02-07
datestamp:	2009-11-11
Client database	
PubMLST isolates:	Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample. 2809 isolates

A profile record displays information about a scheme, e.g. MLST, profile. Each allele number within the profile will be hyperlinked. Clicking these will take you to the appropriate *allele definition record*.

If a *client database* has been setup for the database and an isolate has the profile, there will be a button to display all isolates that have the profile.

10.5 Sequence bin records

PubMI	ST / Breakdown:	ch Browse Profile/ST List Isolate fields Scheme/alleles Publications ints Home Options Profiles/sequences de	finitions Database sub	missions						
										Toggle: i
Sequen	ce bin for N	110 240474								
Contig sur	nmary statistics	Contig size	distribution	Cumulative cont	tig lengt	n				
 Total Minim Maxin Mean σ leng N50: N90: N95: N95: Down 	6405 3513 Iload sequences (FAS	Click to enlarg	je oad lengths		-					
Sequence	Sequencing method	Original designation	Length Comments	Locus	Start	End	Direction	EMBL format	Artemis 👔	
4869	Illumina	NODE 90 length 109787 cov 40.983086		NEIS1151	488	1144	←	EMBL	Artemis	
				NEIS1150	1141	2913	←			
				NEIS1149	3155	3733	\rightarrow			
				NEIS1148	3896	4513	\rightarrow			
				NEIS1147	4521	5384	\rightarrow			
				NEIS1146	5397	5831	<u> </u>			
				NEIS1145	6141	6869	\rightarrow			
				NEIS1144	6892	7923	,			
				NEIS1143	8005	8313	÷			
				NEIS1142	9288	10541	~			
				NEIS1140	10613		÷			
				NEIS1139	12391		\rightarrow			
				NEIS1138	12824		\rightarrow			
				NEIS1137	14426		\rightarrow			
				NEIS1136	15102	15392	,			
				NEIS1135		16832	\rightarrow			
				NEIS1134	16825	17520	\rightarrow			

A sequence bin record contains information about that contigs associated with an isolate record. This includes:

- Number of contigs
- Total length
- Minimum length
- · Maximum length
- N50, N90 and N95 values
- Size distribution charts

There are also links to download the contigs in FASTA or EMBL format.

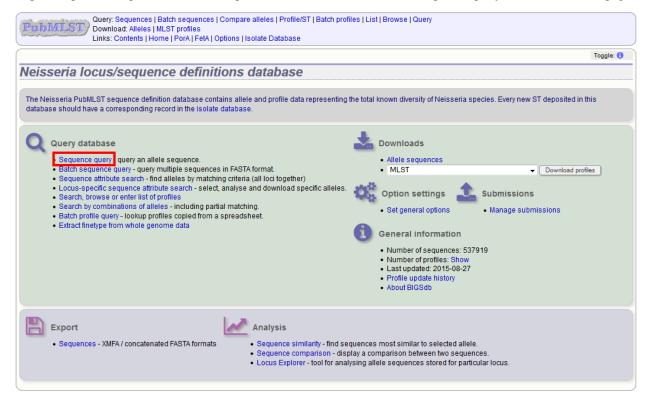
Finally there is a table that shows the loci that are tagged on each contig. Individual contigs can also be downloaded in EMBL format.

CHAPTER 11

Querying data

11.1 Querying sequences to determine allele identity

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



Paste your sequence in to the box - there is no need to trim. Normally, you can leave the locus setting on 'All loci' - the software should identify the correct locus based on your sequence. Sometimes, it may be quicker, however, to

select the specific locus or scheme (e.g. MLST) that a locus belongs to.

Note: If the locus you are querying is a shorter version of another, e.g. an MLST fragment of a gene where the full length gene is also defined, you will need to select the specific locus or the scheme from the dropdown box. Leaving the selection on 'All loci' will return a match to the longer sequence in preference to the shorter one.

Click 'Submit'.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles L Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	ist Browse Query
Sequence query - Neisseria locus/sequence definitions	
Please paste in your sequence to query against the database. Query sequences will be checked first for an partial matches will be identified if an exact match is not found. You can query using either DNA or peptide s	
GACGCGGTGCGCGATGAAAAAGTCAAAGTCATCAAGTCATGAAGCCGCTGAACCGCTGAA TCTGTCAATGAAAATGTCGTGCGCGGGACAATATACCGCCGCCGAAAGGCATGAACGGCTAT CTTGAAGGAAATCAACTATCGGTTGSCCAACGACATCACGCAGTCAAAAACATTGCCAT TGAGSGCAAAACCATTTGCTTTGGCGGGGGGGGGGGGGGG	Select FASTA file: Reset Submit Browse_ No file selected.

If an exact match is found, this will be indicated along with the start position of the locus within your sequence.

Cuery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List 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 sequences partial matches will be identified if an exact match is not found. You can query using either DNA or peptide sequences must be applied to the provide sequence (single or multiple contigs up to whole genome in size) Enter query sequence (single or multiple contigs up to whole genome in size) SACSCGSTSCGCGATGAAAAAGTCAAAGTCATGAAGTCATGAAGCGCTGAACGGCGTAACGGCTAT CTTGAAGAAATGAACGACTATGSCGTGGCGGGGCGGCGGCGGCGGCGGCGGCGGCGGCGGCGG							
1 exact match found. Translate guery							
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.

PulpI/ILCT Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database						
Sequence query - Neisseria locus/sequence definitions						
Please paste in your sequence to query against the database. Query sequences will be checked first for an exact match against the chosen (or all) loci - th partial matches will be identified if an exact match is not found. You can query using either DNA or peptide sequences.	hey do not need to be trimmed. The nearest					
MLST Iocus Alternatively upload FASTA file Alternatively upload FASTA file	Action					
GACGCGGTGCGCGATGAAAAAGTCAAAGTCATCAAGTCATTGAAGCCGCTGACCGTCGAA TCTGTCAATGAAAAAGTCACGTCGCGCGGAAATATACCGCCGCCGAAAGGCATGAACGGCAT CTTGAAGAAAATGTCACTATCGGTTGGCCAACGACATCACGCAGGCGGAAAACATTGCCGT TGAGGCAAAAACCATTTGGCTTTGGCCGACGGCGGGGGGGG	Reset Submit					
Translate query Closest match: aroE: 8 Show alignment						
Differences 2 differences found. 👔						
²⁵⁹ T → ³³³ A ³³³ A → ⁴⁸⁸ G						
The locus start point is at position 136 of your query sequence.						

As an alternative to pasting a sequence in to the box, you can also choose to upload sequences in FASTA format by clicking the file browse button.

PubMLST / Download: Alleles MLST pr	equences Compare alleles Profile/ST Batch ; ofiles rA FetA Options Isolate Database	profiles List Browse Query	
Sequence query - Neisseria Please paste in your sequence to query against partial matches will be identified if an exact match	* he database. Query sequences will be checked i	first for an exact match against the chosen (or all) loci	- they do not need to be trimmed. The nearest
All loci Enter query sequence (single or multiple cor	Order results by - Iocus	Alternatively upload FASTA file Select FASTA file: Browse_ No file selected.	Action Reset Submit

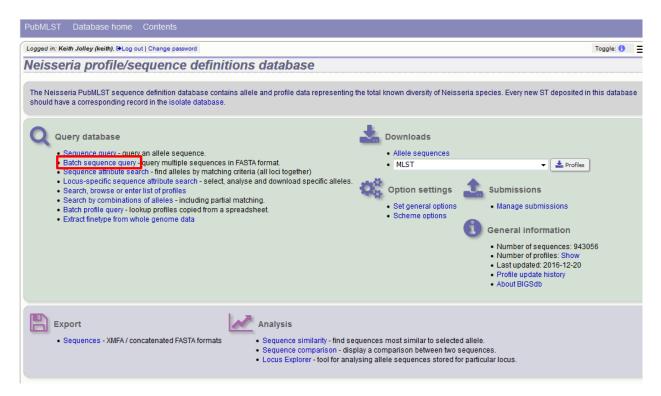
11.1.1 Querying whole genome data

The sequence query is not limited to single genes. You can also paste or upload whole genomes - these can be in multiple contigs. If you select a specific scheme from the dropdown box, all loci belonging to that scheme will be checked (although only exact matches are reported for a locus if one of the other loci has an exact match). If all loci are matched, scheme fields will also be returned if these are defined. This, for example, enables you to identify the MLST sequence type of a genome in one step.

Profile/ST Batch sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database										
Seauer	Sequence query - Neisseria locus/sequence definitions									
					ry sequences will be check can query using either DN/			ci - they do not need to be trimmed. The nearest		
Please	select	ocus/scheme		Order r	esults by-					
MLST				✓ locus	•					
— Enter q	uery se	quence (single	e or multiple co	ntigs up to whole g	enome in size)			Action		
>4758 1	NODE :	192 length	1326 cov	47.828808			Select FASTA file:	Reset Submit		
					CTAGATICCCGCIIIC GACAAAAGCCIGCCAI		Browse No file selected.			
CTCAAA	TAGCC	JTCGGATTCG	AGAATCCGAC	TGCCAAACCGGG	CGCGGACGCTCCGGCC					
					ATTCGGATTTTCCAAT TGACAAAAATATAGTG					
					AGATAGTACGGTAAGG	· ·				
7 exact mate	aboo fou	nd								
7 exact mate	ales lou	nu.								
				lags Comments						
abcZ: 4 adk: 10	433 465	203051 938327	203483 938791							
aroE: 15	490	1775325	1775814							
fumC: 9	465	1134240	1134704							
gdh: 8	501	961439	961939							
pdhC: 11	480	1341678	1342157							
pgm: 9	450	1416246	1416695							
MLST										
ST	2	59								
	cional complex ST-269 complex									

11.2 Querying multiple sequences to identify allele identities

You can also query mutiple sequences together. These should be in FASTA format. Click 'Batch sequence query' from the contents page.



Paste your sequences (FASTA format) in to the box. Select a specific locus, scheme or 'All loci'.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). @Log out Change password	3
Batch sequence query - Neisseria profile/sequence definition	ons
Please paste in your sequences to query against the database. Query sequences will be checked first for an extrimmed. The nearest partial matches will be identified if an exact match is not found. You can query using eith Please select locus/scheme Order results by MLST Incurs Incu	
CAAGECGAAAAAAATCATTGACGAAGGCGGCGTGGGGCGACGACGACGACATCATTATCGGCATGGTCAAAGAAC GCATCGGGCAAGACGACTGCAAAAACGGTTTCCTGTGGGTTTCCCGGCGACGGGCGACGGGCGA AGCGATGGGTGAAGCAGGCGIGGATTIGGATGCAGICGTTGAAGGACGGCGGACGAGGGGCGACGAGGGGCGACGAGGGCGACGA	Browse No file selected. Action Reset Submit

The best match will be displayed for each sequence in your file. If this isn't an exact match, the differences will be listed.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). [+Log out Change password
Batch sequence query - Neisseria profile/sequence definitions
Please paste in your sequences to query against the database. Query sequences will be checked first for an exact match against the chosen (or all) loci - they do not need to be trimmed. The nearest partial matches will be identified if an exact match is not found. You can query using either DNA or peptide sequences. Please select locus/schemeOrder results by
Sequence Results UIW_3 Exact match found; adk: 2 UEY_1 Partial match found; adk: 2: 2 differences found. ¹⁰⁸ T → ¹⁰⁸ A; ¹⁰⁷ T → ¹⁰⁷ A
DSH_1 Partial match found: adk: 10: 1 difference found. 286 G → 286 T
Text format. list table

11.3 Searching for specific allele definitions

There are two query pages available that allow searching for specific allele definitions. The first allows querying of all loci together by criteria that are common to all. The second is a locus-specific attribute query that can search on any extended attributes that may be defined for a locus. This locus- specific query also allows you to paste in lists of alleles for download or analysis.

11.3.1 General (all loci) sequence attribute search

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	iles List Browse Query
	Toggle: 🚯
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing database should have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in this
Query database • Sequence query - query multiple sequences in FASTA format. • Batch sequence query - query multiple sequences in FASTA format. • Sequence attribute search • Industry and alleles by matching criteria (all loci together) • Locus-specific sequence attribute search - select, analyse and download specific alleles. • Search, browse or enter list of profiles • Search by combinations of alleles - including partial matching. • Batch profile query - lookup profiles copied from a spreadsheet. • Extract finetype from whole genome data	 Downloads Allele sequences MLST Download profiles Option settings Submissions Set general options Manage submissions General information Number of profiles: 537919 Number of profiles: Show Last updated: 2015-08-27 Profile update history
Sequence comparison - disp	About BIGSdb quences most similar to selected allele. play a comparison between two sequences. ysing allele sequences stored for particular locus.

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

Designations can be queried using standard operators.

PULST Download: Al	nces Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query leles MLST profiles ts Home PorA FetA Options Isolate Database
	Toggle: i
Query sequences f	or Neisseria locus/sequence definitions database
Some loci have additional fields w plugins.	hich are not searchable from this general page. Search for these at the locus-specific query page. Use this page also for access to the sequence analysis or export
Also note that some loci in this dat locus that uses integer allele ids u	abase have allele ids defined as text strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter your search to a ising the drop-down list.
Please enter your search criteria b	elow (or leave blank and submit to return all records). Matching sequences will be returned and you will then be able to update their display and query settings.
Search criteria	Display
locus 🗸 =	abcZ + i i Order by: locus
	Display: 25 👻 records per page 👔
> Filter query by	Action
	Reset Submit

Click submit.

PubMLST / Dow	ry: Sequences Batch sequences /nload: Alleles MLST profiles s: Contents Home PorA FetA C	Compare alleles Profile/ST Batch	profiles List Browse Query	
LIIK	s. Contents [Home] FOIX [FEX] C	pitons fisolate Database		
				Toggle: i
Query sequen	ces for Neisseria lo	ocus/sequence defi	nitions database	
Some loci have additiona plugins.	I fields which are not searchable fr	om this general page. Search for th	ese at the <u>locus-specific query</u> page. Us	e this page also for access to the sequence analysis or export
	in this database have allele ids def llele ids using the drop-down list.	ined as text strings. Queries using t	ne '<' or '>' modifiers will work alphabetic	ally rather than numerically unless you filter your search to a
Please enter your search	criteria below (or leave blank and	submit to return all records). Matchir	g sequences will be returned and you w	vill then be able to update their display and query settings.
Search criteria		Display		
Combine searches with	n: AND 👻	Order b	Clocus - ascending -	•
locus	= → abcZ	+ i Displa	25 v records per page i	
allele id 🔹	• = • 5			
Filter query by	Action Reset Submit	Ī		
1 record returned. Click the	e hyperlink for detailed information			
locus allele id	sequence	sequence length comments fia	as	
	ACCGTTGCC TCGTCGAACTCGA			

Click the hyperlinked results to display allele records.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Toggle: [i]
Query sequences for Neisseria locus/sequence definitions database
Some loci have additional fields which are not searchable from this general page. Search for these at the locus-specific query page. Use this page also for access to the sequence analysis or export plugins.
Also note that some loci in this database have allele ids defined as text strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter your search to a locus that uses integer allele ids using the drop-down list.
Please enter your search criteria below (or leave blank and submit to return all records). Matching sequences will be returned and you will then be able to update their display and query settings.
- Search criteria - Display -
Combine searches with: AND - Order by: locus - ascending -
locus • = • abcZ + I Display: 25 • records per page [
allele id • = • 5
Filter query by Action Reset Submit
1 record returned. Click the hyperlink for detailed information.
locus allele id sequence sequence length comments flags abc2 5 TITGATACCGTTGCC TCGTCGAACTCGATC 433

Ilele inform	ation - abcZ: 5
Provenance/meta	data
locus	abcZ i
allele:	
	TITGATACCE TIGCCERAGE TITGEGEGEGA AITCECEGATI TATTEGECECE TIATCATCAI GICAGCCAIE AETTEGAAAA TEGTICEGAET GAEGETITEI TEAAAGAECT TAACGAATIE CAACTIGAA TEGAAECEAA GEAEGEGETEG AAGCTEGEATE CEGECAETA ECAEACTITE GETEGACITE GITIGECAEAAAAA AICEGECAACC ICTECEGEGE ACAGAAAAA CEISTIGECE TAGEGEGEGE TIGGETEGAE AAGCCIGAIE TATIGETEGT GEAEGAACTE GITEGECAIT GEACATIEA CEGEATAII IGECIGEAAA AICEGEAAAAA GECAECIGE TIGGETEAE AAGCCE CEITITITEG ACAAATACE CAECEGEAIE GICEAACTE GITEGECAIT GEACATIEA CEGEATAII IGECIGEAAA
length:	433
status:	Sanger trace checked
date entered:	2001-02-07
datestamp:	2009-11-11
sender:	Keith Jolley, University of Oxford, UK
curator:	Man-Suen Chan, University of Oxford (E-mail: man-suen.chan@paediatrics.ox.ac.uk)
Profiles containin	ig this allele
MLST:	183 profiles
Isolate databases	
PubMLST isolates:	Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample.

Various search criteria can also be selected by combining with filters. Click the filter heading to display these.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Toggle: i
Query sequences for Neisseria locus/sequence definitions database
Some loci have additional fields which are not searchable from this general page. Search for these at the locus-specific query page. Use this page also for access to the sequence analysis or export plugins.
Also note that some loci in this database have allele ids defined as text strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter your search to a locus that uses integer allele ids using the drop-down list.
Please enter your search criteria below (or leave blank and submit to return all records). Matching sequences will be returned and you will then be able to update their display and query settings.
Search criteria
allele id • < • 10 + i Order by: locus • ascending •
Display: 25
- Filter query by
sender:
curator:
allele flag:
9 records returned. Click the hyperlinks for detailed information.
a records returned. Crick the hyperinks for detailed information.
locus allele id sequence sequence length comments flags
abcZ 1 TITGATACTGTTGCC TITGTCGAACTCGATC 433
abcz 2 ITTGATACCGTTGCC TTGICGAACTCGATC 433
abcZ 3 ITTGATACCGITGCC TIGTIGAACTIGACC 433
abcz 4 ITIGATACCGITGCC TIGICGAACICGATC 433
abcZ 5 TITIGATACCGTIGCC TCGTCGAACTCGATC 433
abcZ 6 ITIGATACCGITGCC TIGICGAACTCGATC 433
abcz 7 TITGATACTGTTGCC TIGTCGAACTCGATC 433
abcz 8 ITTGATACCGITGCC TTGICGAACTIGACC 433
abcZ 9 TITGATACCGTTGCC TIGTCGAACTCGATC 433

11.3.2 Locus-specific sequence attribute search

Some loci have *extended attribute fields*. To query these, click 'Locus-specific sequence attribute search' on a sequence definition database contents page.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profile Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	iles List Browse Query
	Toggle: 🜖
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing database should have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in this
 Query database Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching criteria (all loci together) Locus-specific sequence attribute search. search, prove or enter rist or promes Search by combinations of alleles - including partial matching. Batch profile query - locup profiles copied from a spreadsheet. Extract finetype from whole genome data 	 Downloads Allele sequences MLST Download profiles Option settings Set general options Set general options Manage submissions Number of sequences: 537919 Number of profiles: Show Last updated: 2015-08-27 Profile update history About BIGSdb
Sequence comparison - dis	quences most similar to selected allele. play a comparison between two sequences. ysing allele sequences stored for particular locus.

Pick the required locus from the dropdown box.

PTTTTILLST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
Help 🗹	Toggle: 🚺
Query PorA VR2 sequences - Neisseria locus/sequence definitions database	
Locus PorA_VR2 Page will reload when changed • Further information is available for this locus. Please enter your search criteria below (or leave blank and submit to return all records).	Modify form options
Allele fields Display Action allele id • • Display: 25 • records per page •	

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

ित्तिय	LST)	Query: Sequences Batch se Download: Alleles MLST pr Links: Contents Home Po	ofiles		Batch pro	ofiles L	_ist Browse	Query				
											Help 🖉	Toggle: 🕄
Query	PorA	VR2 sequences	s - Neisseria	a locus/se	quen	ce d	efinitio	ons data	base			
Locus: Po	rA_VR2			when changed								Modi
• Furt	her inforr	mation is available for this loc	cus.									form
Please ent	er vour se	earch criteria below (or leave	blank and submit to re	eturn all records)								opuo
Allele fi	ields —			— Dis					Action			
family				+ 0 0	order by:	allele io	- I	 ascending 	 Reset 	Sut	omit	
					Display:	25 👻	records pe	r page 🕕				
Page: 1	2 3	1 - 25 displayed). Click the hy										
	allele id	sequence	sequence length	comments	_	variant	l old name		-		mAb2 reactivity f	lags
PorA VR2	2	HFVQQTPKSQPTLVP	15		2			MN16C13F4	+	AF202	-	
PorA VR2	2-1	HFVQQPPKSQPTLVP	15		2	1	2b	MN16C13F4	-	AF202	+	
PorA VR2	2-10	HFVQQAPQSQSTLVP	15		2	10						
PorA VR2	2-11	HFVLQTPQSQPTLVP	15		2	11						
PorA VR2	2-12	HEVQQIPKSQPTLVP	15		2	12						
PorA VR2	2-13	YFVQQTPQSQPTLVP	15		2	13		MN16C13F4	+			
PorA VR2	2-14											
		HFVQQKLASKPTLVP	15		2	14	33					
PorA VR2		HFVQQKLASKPILVP	15		2	14 15	33 33a (33-1)					
PorA VR2 PorA VR2												

The query form can be modified by clicking the 'Modify form options' tab:

Profit MLST / Download: Alleles MLST profil	ences Compare alleles Profile/ es FetA Options Isolate Database		vse Query		
				Help 🗹	Toggle: 🚺
Query abcZ sequences - Neis	sseria locus/seque	ence definitions	database		
Locus: abcZ • Further information is available for this locus Please enter your search criteria below (or leave bla	 Page will reload when changed and submit to return all records 	5)			Modify form options
Allele fields		Order by: allele id	✓ ascending ✓ per page ①	Action Reset Submit	

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

PubMLST	Download: Alleles ML Links: Contents Hom	ne PorA FetA Options Isolate Databas		Help 🕑	Toggle: 🚺
		Page will reload when changed his locus. leave blank and submit to return all record (ds). — Display — Order by: allele id → ascending — Display: 25 → records per page ()	X Modify form parameters Click to add or remove additional que • • • Allele fields • • • Allele id list box • • • Filters	Modify form options

Close the form modification tab and you can now enter a list of allele ids for retrieval.

PUDMLST / Dow	nload: Alleles MLST p	equences Compare alleles Pr ofiles rA FetA Options Isolate Datat		List Browse Query	
				Help 🖉	Toggle: 🚯
Query abcZ se	quences - N	eisseria locus/sec	quence defini	tions database	
Locus: abcZ	n is available for this lo	 Page will reload when change 	ed		Modify
		blank and submit to return all re	aarda)		options
Allele fields			Allele id list	Display Order by: allele id ascending Tecords per page ● Action Reset Submit	

Various analysis and export options will be available for use on the retrieved sequences. These include FASTA output and *Locus Explorer* analysis.

Further information is available for this locus. Please enter your search criteria below (or leave blank and submit to return all records).											
Please enter your search crit	eria below (or leave blank and su	ibmit to return all rec	ords).		_						
Allele fields			— Allele id list — —	— — Display — — — — — — — — — — — — — — — — — — —							
allele id 🚽 =		+ 1	1	Order by: allele id 🗸 ascending 🗸							
		0	2	Display: 25 👻 records per page 🜖							
			3	Antion							
			5	Action							
				Reset Submit							
E records returned. Click the k	yperlinks for detailed information										
Stecords returned. Click the r	typerinings for detailed information	I.									
locus allele id	sequence	sequence length c	comments flags								
	GTTGCC TTGTCGAACTCGATC										
	GTTGCC TTGTCGAACTCGATC										
	STIGCC TIGIIGAACTIGACC										
	GTTGCC TTGTCGAACTCGATC										
abcZ 5 TTTGATACCO	GTTGCC TCGTCGAACTCGATC	433									
Analysis tools: Export: FASTA Table Analysis: Locus Explorer											

11.4 Browsing scheme profile definitions

If a sequence definition database has schemes defined that include a primary key field, i.e. collections of loci that together create profiles, e.g. for MLST, these can be browsed by clicking the link to 'Search, browse or enter list of profiles'.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch prof Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	iles List Browse Query
	Toggle: 🕄
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in this database should
Query database Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching criteria (all loci together) Louis spacific sequence attribute search - select, analyse and download specific alleles. Search, browse or enter list of profiles Search by combinations of alleles - including partial matching. Batch profile query - lookup profiles copied from a spreadsheet. Extract finetype from whole genome data	 Downloads Allele sequences MLST Download profiles Option settings Submissions Set general options Manage submissions General information Number of sequences: 537919 Number of sequences: 537919 Number of profiles: Show Last updated: 2015-08-27 Profile update history About BIGSdb
Sequence comparison - disp	quences most similar to selected allele. Day a comparison between two sequences. Iysing allele sequences stored for particular locus.

Leave query form fields blank (the display of these may vary depending on modification options set by the user). Choose the field to order the results by, the number of results per page to display, and click 'Submit'.

Pul	Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
	Toggle: 🚯											
Sea	Search or browse profiles - Neisseria locus/sequence definitions											
	caron or promot promot - recoocha robuo/ocquenoe dennitiono											
Enter	Enter search criteria or leave blank to browse all records. Modify form parameters to filter or enter a list of values.											
			eme f						— — Display/sort options — Action — Action			
S		sisui	entei		1			C.				
3				•	=		•		Reset Sublinit			
									Display: 25 🗸 records per page 🚺			
Brows	sing	all red	cords.									
40050					05 48		-	inte de la compania dan dan dan dan dan dari				
10050	brec	oras i	returni	ea (1 -	25 QI	spiaye	a). Ci	ick the hyperlinks for detailed in	niormauon.			
Page	: 1	2	3	4	5	6 7	8	9 > Last				
	_		_	_								
ST	adk	abcZ	aroE	fumC	adh	pdhC	pam	clonal complex				
1	3	1	1	1	1	1	3	ST-1 complex/subgroup I/II				
2	3	1	4	7	1	1	3	ST-1 complex/subgroup I/II				
3	3	1	1	1	1	23	13	ST-1 complex/subgroup I/II				
4	3	1	3	1	4	2	3	ST-4 complex/subgroup IV				
5	1	1	2	1	3	2	3	ST-5 complex/subgroup III				
6	1	1	2	1	3	2	11	ST-5 complex/subgroup III				
7	1	1	2	1	3	2	19	ST-5 complex/subgroup III				
8	3	2	7	2	8	5	2	ST-8 complex/Cluster A4				
9	3	2	8	10	8	5	2	ST-8 complex/Cluster A4				
10	3	2	4	2	8	15	2	ST-8 complex/Cluster A4				
11	3	2	4	3	8	4	6	ST-11 complex/ET-37 complex	X			
12	3	4	2	16	8	11	20					
10	10	4	15	7	0	44	4	ST 260 complex				

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Help 02
Profile information for ST-11 (MLST)
ST adk abcZ aroE fumC gdh pdhC pgm clonal complex 11 3 2 4 3 8 4 6 ST-11 complex/ET-37 complex
sender: Paula Kriz, Paula Kriz and Keith Jolley
curator: Keith Jolley, University of Oxford, UK (E-mail: keith.jolley@zoo.ox.ac.uk)
update history: 2 updates show details
date entered: 2001-02-07
datestamp: 2013-04-27
Client database
PubMLST isolates: Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample. 1133 isolates

11.5 Querying scheme profile definitions

Click the link to 'Search, browse of enter list of profiles'.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profile Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	files List Browse Query
	Toggle: 🜖
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in this database should
Query database • Sequence query - query an allele sequence. • Batch sequence query - query multiple sequences in FASTA format. • Sequence attribute search - Ind alleles by matching criteria (all loci together) • Locus spacific sequence attribute search - select, analyse and download specific alleles. • Search by combinations of alleles - including partial matching. • Batch profile query - lookup profiles copied from a spreadsheet. • Extract finetype from whole genome data	Downloads • Allele sequences • MLST Download profiles Option settings Submissions • Set general options • Manage submissions Image submissions • Mumber of sequences: 537919 • Number of sequences: 537919 • Number of profiles: Shrow • Last updated: 2015-08-27 • Profile update history • About BIGSdb • About BIGSdb
Sequence comparison - disp	quences most similar to selected allele. play a comparison between two sequences. lysing allele sequences stored for particular locus.

Enter the search criteria you wish to search on. You can add search criteria by clicking the '+' button in the 'Locus/scheme fields' section. These can be combined using 'AND' or 'OR'.

Pub	Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database												
										Toggle: 🚯			
Search or browse profiles - Neisseria locus/sequence definitions													
שלמוכון טו שוטאשב אוטוובא י ואבוששבוום וטבעש/שבעעבוובב עבוווונוטווש													
C	Enter search criteria or leave blank to browse all records. Modify form parameters to filter or enter a list of values.												
Enters	earc	ch crite	ina or	leave	Diank	to pro	wsea	all records. Modify form paramet	ers to filter or enter a list of values.	Modify			
Lo	cus/	schen	ne field	ds —					— Display/sort options — Action — Action	- form			
Com	bine	searc	hes w	ith: Al	ND .	-			Order by: ST 🗸 ascending 🗸 Reset Submit	options			
dat	e en	itered		• >	>		-	2013-02-01 +	O Display: 25				
ser	nder	(surna	ime)	• =	•		•	Jolley					
5051 re	cord	ls retu	med (*	1 - 25 (displa	aved). (Click	the hyperlinks for detailed inforn	nation.				
	_												
Page:	1	2	3 4	5	6][7]	8	9 > Last					
						pdhC		cional complex					
5001	-	12	12	352	9	18	9	OT 14/14					
5002 5003	5 5	2	9	9 143	9 5	6 119	8 18	ST-41/44 complex/Lineage 3					
5003	8	9	185	26	10	1	16	ST-18 complex					
5005	8	7	10	19	10	351	16	ST-18 complex					
5006	8	13	10	19	10	1	9	ST-18 complex					
5007	8	7	10	3	9	15	20	er to complex					
5008	7	12	381	91	5	21	16						
5009	8	187	10	116	10	15	20						
5010	8	7	10	17	10	1	9	ST-18 complex					
5011	3	7	72	26	10	1	16						

Each field can be queried using standard operators.

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

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: 🚯
Sear	ch	or	bro	ws	e p	rof	iles	- Neisseria lo	cus/s	eauence	e definitio	ns			
Enter s	earc	h crite	eria or	leave	blank	to bro	wsea	all records. Modify form par	rameters to	filter or enter a	list of values.				
			ne fielo					, , ,		-Display/sor				Action	Modify form
						_				Order by:		and the second line of	_		options
		searc tered	hes w	101. A		•		2013-02-01				→ ascending →	•	Reset Submit	
				_			_		+ 0	Display:	25 - records	per page 🕕			
sen	der	(surna	ime)	•	=		•	Jolley							
5051 re Page:							Click	the hyperlinks for detailed i	information	1.					
ет	adle	abo7	araF	fum(adb	pdhC	Dana	clonal complex	_						
5001	6	12	12	352	gun 9	18	9	cional complex	-						
5002	5	2	9	9	9	6	8	ST-41/44 complex/Lineag	le 3						
5003	5	9	6	143	5	119	18								
5004	8	7	185	26	10	1	16	ST-18 complex							
5005	8	7	10	19	10	351	16	ST-18 complex							
5006	8	13	10	19	10	1	9	ST-18 complex							
5007	8	7	10	3	9	15	20								

Other query options are available by clicking the 'Modify form options' tab.

PubMLST	/ Download: Allel	es MLST profiles	Compare alleles Profile ptions Isolate Database		Browse Query		
							Toggle: 🚯
Search or b	prowse pr	ofiles - Neiss	seria locus/se	quence defin	itions		
Enter search criteri	ia or leave blank to) browse all records. Mo	dify form parameters to fi	lter or enter a list of value	es.		Modif
— Locus/scheme	e fields			-Display/sort options —			form
ST	▼ =	•	+ 0	Order by: ST Display: 25 🗸 r	 ascending ecords per page () 	Reset Submit	option

For example, you can enter a list of attributes to query on by clicking the 'Show' button next to 'Attribute values list'.

Puisivitus Query: Sequences Batch sequences Compare alleles Profile/ST []] Batch profiles Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
Logged in: Keith Jolley (keith).	Log out Change password			Help 🗹	Toggle: 🚯						
Search or brow	se profiles - Neiss	eria profile/sequen	ce definitions								
Enter search criteria or leav	ve blank to browse all records. Mo	dify form parameters to filter or ente	a list of values.		Modify						
			ort options	×	form						
ST 🗸	= •	+ 0 Order	y: ST 👻 ascen	Modify form parameters	options						
		Displ	y: 25 ▼ records per page	Click to add or remove additional que • O Locus/scheme field va • O Attribute values list • O Filters							

A list box will appear within the page. Hide the form modification tab by clicking the 'X' in the corner or the purple tab again. Now you can choose the attribute to search on along with a list of values.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
										Toggle: 🚺	
Search or browse profiles - Neisseria locus/sequence definitions											
Ente	rse	arch c	riteria	or lea	ve bla	ink to b	rows	e all records. Modify form parameters	s to filter or enter a list of values.	Modify	
	Locu ST	is/sch	eme f		=			+ 0		form	
									1 2 3 4 Action Reset Submit		
4 rec	ords	return	ed. C	lick th	e hype	erlinks	for de	tailed information.			
ST	adk	abcZ	агоЕ	fum(gdh	pdhC	pgm	clonal complex			
1	3	1	1	1	1	1	3	ST-1 complex/subgroup I/II			
2	3	1	4	7	1	1	3	ST-1 complex/subgroup I/II			
3	3	1	1	1	1	23	13	ST-1 complex/subgroup I/II			
4	3	1	3	1	4	2	3	ST-4 complex/subgroup IV			
Ana	1	s too : BL : Se		ces							

List values will be combined with any other attributes entered in the query form allowing complex queries can be constructed.

You can also add filters to the form by again clicking the 'Modify form options' tab and selecting 'Filters'.

Query: Sequences Batch sequences Compare a Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Iso			Help IZ Toggle: 8
			neipter Toggie.
Search or browse profiles - Neisseria p	profile/sequence definitions		
Enter search criteria or leave blank to browse all records. Modify form particular search criteria or leave blank to browse all records. Modify form particular search criteria search criteri	Arameters to filter or enter a list of values. Attribute values list Field: ST 1 2 3 4 	• 🕒 Locus/s	Additional query terms: cheme field values values list

Available filters will vary depending on the database. These will be combined with other query criteria or lists of attributes.

Query: Sequences Batch sequences Co Download: Alleles MLST profiles Links: Contents Home PorA FetA Opti	ompare alleles Profile/ST Batch profiles List Browse ions Isolate Database	Query
		Toggle: 🕄
Search or browse profiles - Neisse	eria locus/sequence definitions	\$
Enter search criteria or leave blank to browse all records. Modil	fy form parameters to filter or enter a list of values. Attribute values list Field: ST I 2 3 4	Filters Modify form options Clonal complex: ST-4 complex/subgroup IV ● Display/sort options Action Order by: ST ◆ ascending ♥ Display: 25 ▼ records per page ●
1 record returned. Click the hyperlink for detailed information. ST adk abcZ aroE fumC gdh pdhC pgm clonal comp 4 3 1 3 1 4 2 3 ST-4 complex/sub Analysis tools: Export: Sequences Sequences Sequences		

11.6 Identifying allelic profile definitions

For schemes such as MLST you can query allelic combinations to identify the sequence type (or more generically, the primary key of the profile).

Click the 'Search by combinations of alleles' link from the sequence definition contents page.

PubMLST Database home Contents	
el Log in	Toggle: ()
Neisseria profile/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing the to corresponding record in the isolate database.	tal known diversity of Neisseria species. Every new ST deposited in this database should have a
Q Query database	Downloads Option settings
Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching criteria (all loci together)	Allele sequences MLST Scheme options Scheme options
 Locus-specific sequence attribute search - select, analyse and download specific alleles. Search, browse or enter list of profiles 	submissions
 Search by combinations of alleles - including partial matching. Batch profile query - lookup profiles copied from a spreadsheet. 	Manage submissions
Extract finetype from whole genome data	General information
	Number of sequences: 943149 Number of profiles: Show
	Last updated: 2016-12-20 Profile update history
	About BIGSdb
	ces most similar to selected allele. comparison between two sequences. allele sequences stored for particular locus.

If multiple schemes are defined in the database you should select the scheme you wish to check.

PubMLST Database home Contents			
● Log in	Help 🖉	Toggle: 🚯	Ξ
Search Neisseria profile/sequence definitions database by combinations of loci			
Schemes			
Please select the scheme you would like to query:			
MLST Select			
Please enter your allelic profile below. Blank loci will be ignored. Autofill profile			
abcZ adk aroE fumC gdh pdhC pgm ST: Autofill			
Options Display/sort options Action			
Search: Exact or nearest match Order by: ST ascending Reset Submit			
Display: 25 👻 records per page ()			

Enter a combination of allelic values (you can enter a partial profile if you wish).

PubMLST Database home Contents		
HD Log in	Help 🖉	Toggle: 🚯 📃
Search Neisseria profile/sequence definitions database by combinations of loci		
Schemes		
Please select the scheme you would like to query:		
MLST • Select		
Please enter your allelic profile below. Blank loci will be ignored. Autofill profile		
abcz ack arote numc gan panc pgm ST: Autofill 2 3 4 3 8 4 6		
Options — Display/sort options — Action —		
Search: Exact or nearest match 👻 Order by: ST 🗸 ascending 🗸 Reset Submit		
Display: 25 👻 records per page 🛙		

Alternatively, you can automatically populate a profile by entering a value for the scheme primary key field (e.g. ST) and clicking 'Autofill'.

PubMLST Database home Contents		
Logged in: Keith Jolley (keith). @Log out Change password	Help 🖉	Toggle: 🚯 📃
Search Neisseria profile/sequence definitions database by combinations of loci		
Schemes		
Please select the scheme you would like to query:		
MLST - Select		
Please enter your allelic profile below. Blank loci will be ignored. Autofill profile abcZ adk aroE fumC gdh pdhC pgm ST: 11 Autofill		
Options Display/sort options Action Action		
Search: Exact or nearest match Order by: ST ascending Reset Submit Reset Submit		

To find the closest or exact match, leave the search box on 'Exact or nearest match' and click 'Submit'. The best match will be displayed.

PubMLST Database home Contents		
Logged in: Keith Jolley (keith). @Log out Change password	Help 🖉	Toggle: 🚯 🗧
Search Neisseria profile/sequence definitions database by combinations of loci		
Schemes		
Please select the scheme you would like to query:		
MLST - Select		
abcZ adk aroE fumC gdh pdhC pgm ST: 11 Autofill 2 3 4 3 8 4 6 5 6 5 6		
2 3 4 3 8 4 6 Options Display/sort options Action Search: Exact or nearest match + Order by: ST ascending + Display: 25 records per page •		
Exact matches found (7 loci).		
1 record returned. Click the hyperlink for detailed information.		
ST abc2 adk aroE fumC gdh pdhC pgm clonal complex 11 2 3 4 6 ST-11 complexET-37 complex		
Analysis tools:		
Export Sequences		

Alternatively, if you wish to find all profiles that match the query profile by at least a set number of loci, select the appropriate value in the search dropdown box, e.g. '4 or more matches' will show related profiles that share at least 4 alleles with the query.

Logged	in: Ke	ith Jo	iley (k	eith). 🕩	Log ou	ut Cha	inge p	essword	Help 🗗	Toggle: 🚯	
Sea	rch	N	iss	eri.	a n	rofi	le/	sequence definitions database by combinations of loci			
ocu	UII				u p	1011	167				
Sche	emes	5									
Pleas	e sel	ect th	e sch	eme yo	ou wo	uld lik	e to q	uery:			
MI CT	-										
MLST	I							▼ Select			
		ente			· ·			ank loci will be ignored. Autofill profile			
8	abcZ	-	adk	_	aroE		fumC				
	2		3		4		3	8 4 6			
0	ption							Display/sort options Action			
	Sear	rch:	4 or n	nore m	natche	es	•	Order by: ST 🛛 🗣 ascending 👻 Reset Submit			
								Display: 25 🗸 records per page 🕦			
409 re	cords	retur	ned (*	1 - 25 (displa	wed), (Click	he hyperlinks for detailed information.			
	_										
Page:	1	2	3	4 5		7	8	9 > Last			
10	abcZ 2	adk 3	arot 4	fumC 2	gdh 8	pdhC 15	pgm 2	clonal complex ST-8 complex/Cluster A4			
11	2	3	4	3	8	4	6	ST-11 complex/ET-37 complex			
50	2	3	19	3	8	4	6	ST-11 complex/ET-37 complex			
51	2	3	4	23	8	6	6	ST-11 complex/ET-37 complex			
52	7	3	4	3	8	4	6	ST-11 complex/ET-37 complex			
67	2	3	4	24	8	4	6	ST-11 complex/ET-37 complex			
165	2	3	4	48	8	4	6	ST-11 complex/ET-37 complex			
166	2	3	6	3	3	58	6	ST-11 complex/ET-37 complex			
211	2	3	4	8	8	4	6	ST-11 complex/ET-37 complex			
214	2	3	4	3	48	4	6	ST-11 complex/ET-37 complex			
247	2	3	4	5	8	4	6	ST-11 complex/ET-37 complex			
285	8	3	4	3	51	5	6	ST-11 complex/ET-37 complex			

11.7 Batch profile queries

To lookup scheme definitions, e.g. the sequence type for multiple profiles, click 'Batch profile query' from the sequence definition contents page.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). (HLog out Change password Neisseria profile/sequence definitions database	Taggle: ()
The Neisseria PubMLST sequence definition database contains allele and profile data representing should have a corresponding record in the isolate database.	Downloads
 Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching criteria (all loci together) Locus-specific sequence attribute search - select, analyse and download specific alleles. Search, browse or enter list of profiles Search by combinations of alleles - including partial matching. Batch profile query - lookup profiles copied from a spreadsheet. Extract finetype from whole genome data 	 Allele sequences MLST MLST
Sequence comparison - display the s	equences most similar to selected allele. play a comparison between two sequences. lysing allele sequences stored for particular locus.

If multiple schemes are defined in the database you should select the scheme you wish to check.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). @Log out Change password	3
Batch profile query - Neisseria profile/sequence definitions	
Schemes	
Please select the scheme you would like to query:	
MLST Select	
whitespace. The first column should be an isolate identifier and the remaining columns should comprise the allele num data. Non-numerical characters will be stripped out of the query. — Paste in profiles	bers (show column order). Click here for example Action Reset Submit

Copy and paste data from a spreadsheet. The first column is the record identifier, and the remaining columns are the alleles for each locus in the standard locus order defined for the scheme. There are links to the column order which can be used as a header line for your spreadsheet and to example data.

Click submit after pasting in the data.

ed in: Keith Jolley										
tch profil	e query	/ - Neis	sseria	profile	/seque	ence de	efinitions	1		
hemes										
nemes										
ase select the sc	heme you wo	ould like to q	uery:							
				-						
ST			 Select 							
or allelic profiles	holow in tab	dolimited to	vt format usi		d pacto (for (avample dire	ctly from a onros	adebaat) Colum	and can be constated by any an	ount of whiteens
									nns can be separated by any an	
e first column sho	uld be an iso	late identifie							nns can be separated by any an nn order). Click here for exampl	
e first column sho aracters will be str	uld be an iso ripped out of	late identifie								
e first column sho	uld be an iso ripped out of	late identifie								
e first column sho aracters will be str	uld be an iso ripped out of	late identifie							nn order). Click here for example	
e first column sho aracters will be str Paste in profiles	uld be an iso ripped out of	olate identifie the query.	er and the re	maining co	lumns shou	ld comprise	the allele numb		nn order). Click here for example	
e first column sho aracters will be str -Paste in profiles .solate_6	uld be an iso ripped out of 3	olate identifie the query. 6	er and the re	maining co	lumns shou	ld comprise	the allele numbers		nn order). Click here for example	
e first column sho aracters will be str -Paste in profiles .solate_6 .solate_7 .solate_8	uld be an iso ipped out of 3 6	olate identifie the query. 6 6	er and the re 9 365	5 55	lumns shou 8 72	ld comprise	9 20		nn order). Click here for example	
e first column sho iracters will be str - Paste in profiles solate_6 solate_7	uld be an isc ripped out of 3 6 4	olate identifie the query. 6 6 3	9 365 5	5 55 4	8 72 315	ld comprise	9 20 8		nn order). Click here for example	
e first column sho rracters will be sh Paste in profiles solate 6 solate 7 solate 8 solate 9 solate 10	uld be an isc ripped out of 3 6 4 2	6 6 6 3 273	9 365 5 19	5 55 4 3	8 72 315 8	ld comprise 6 6 21 4	9 20 8 6		nn order). Click here for example	
e first column sho racters will be stu Paste in profiles solate_6 solate_7 solate_8 solate_9 solate_10 solate_11	uld be an isc ripped out of 3 6 4 2 2	olate identifie the query. 6 6 3 273 7	9 365 5 19 159	5 55 4 3 92	8 72 315 8 93	6 6 21 4 6	9 20 8 6 2		nn order). Click here for example	
e first column sho rracters will be str Paste in profiles solate_6 .solate_7 .solate_8 .solate_9 .solate_10 .solate_11 .solate_12	uld be an isc ripped out of 3 6 4 2 2 2 2	olate identifie the query. 6 6 3 273 7 5	9 365 5 19 159 12	5 55 4 3 92 143	8 72 315 8 93 29	6 6 21 4 6 285	9 20 8 6 2 7		nn order). Click here for example	
e first column sho aracters will be str -Paste in profiles .solate_6 .solate_7 .solate_8 .solate_9	uld be an isc ripped out of 3 6 4 2 2 2 2 6	olate identifie the query. 6 6 3 273 7 5 7	9 365 5 19 159 12 9	5 55 4 3 92 143 56	8 72 315 8 93 29 26	6 6 21 4 6 285 18	9 20 8 6 2 7 8		nn order). Click here for example	

A results table will be displayed.

		-y pice	uŋ. er	.og out	() Una	nge pas	sword				
atch p	rof	ïle	au	erv	- N	leis	ser	ia pi	rofile/sequence d	finitions	
Isolate	abo7	odk	aroE	fumC	adb	pdhC	Dam	ST	clonal complex		
isolate 1	8	3	5	4	yun 1	3	8	290	ST-32 complex/ET-5 complex		
isolate 2	2	3	4	86	8	110	118		ST-11 complex/ET-37 complex		
isolate 3	4	26	15	9	8	11	18	8381	ST-269 complex		
isolate_4	20	5	144	35	8	130	123	942	cr 200 dompiox		
isolate_5			13	5	9	6	9	3312	ST-41/44 complex/Lineage 3		
isolate 6	3	6	9	5	8	6	9	485	ST-41/44 complex/Lineage 3		
isolate 7	6	6	365	55	72	6	20	4053			
isolate 8	4	3	5	4	315	21	8	3770	ST-32 complex/ET-5 complex		
isolate 9	2	273	19	3	8	4	6	6070	ST-11 complex/ET-37 complex		
solate_10	2	7	159	92	93	6	2	10908			
isolate_11	2	5	12	143	29	285	7	4658			
solate_12	6	7	9	56	26	18	8	10620	ST-175 complex		
isolate_13	11	5	18	5	9	24	3	10202	ST-22 complex		
isolate_14	222	231	406	12	161	2	16	8927			
isolate_15	9	4	9	17	5	3	2	8977	ST-103 complex		

11.8 Investigating allele differences

11.8.1 Sequence similarity

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profile Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	les List Browse Query
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing t this database should have a corresponding record in the isolate database.	the total known diversity of Neisseria species. Every new ST deposited in
Query database • Sequence query - query an allele sequence. • Batch sequence query - query multiple sequences in FASTA format. • Sequence attribute search - find alleles by matching criteria (all locit together) • Locus-specific sequence attribute search - select, analyse and download specific alleles. • Search browse or enter list of MLST profiles • Search by combinations of MLST alleles - including partial matching. • Batch profile query - lookup MLST profiles copied from a spreadsheet. • Extract finetype from whole genome data	 Downloads Allele sequences MLST profiles Set general options Set general options Manage submissions General information Number of sequences: 124770 Number of profiles (MLST): 10058 Last updated: 2015-08-19 Profile update history About BIGSdb
Sequence comparison - disp	quences most similar to selected allele. Ilay a comparison between two sequences. ysing allele sequences stored for particular locus.

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Horn Port Alleles Port Alleles<
Find most similar alleles - Neisseria locus/sequence definitions
This page allows you to find the most similar sequences to a selected allele using BLAST.
Select parameters Action Locus: abcZ Allele: 5 Allele: 5 Submit Number of results: 10 - Image: Second

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

quences.

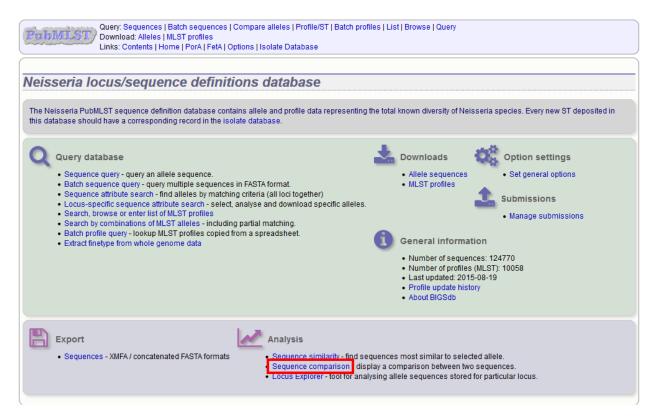
PTIDITIST Download: Alleles Batch sequences Compare alleles Profile/ST []] Batch profiles Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database											
Logged in: Ke	eith Jolley (ke	eith). 🕩Log ou	it Chan	ge password	Help 🗗						
Find m	ost sii	nilar a	llele	es - Nei	isseria profile/sequence definitions						
This page allows you to find the most similar sequences to a selected allele using BLAST.											
	·	s: abcZ		•	Reset Submit						
	Allel	e: 5									
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abcZ-5											
	% Identity	Nismatches	Gaps	Alianment	Compare						
	% Identity 99.77	Aismatches 1	Gaps 0	Alignment 433/433							
Allele			_		4						
Allele abcZ: 453	99.77	1	0	433/433							
Allele abcZ: 453 abcZ: 405	99.77 99.77	1 1	0	433/433 433/433	4호 4호 4호						
Allele abcZ: 453 abcZ: 405 abcZ: 404	99.77 99.77 99.77	1 1 1	0 0 0	433/433 433/433 433/433	[4월] [4월]						
Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213	99.77 99.77 99.77 99.77	1 1 1 1	0 0 0 0	433/433 433/433 433/433 433/433	4월 4월 4월 4월 4월						
Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166	99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1	0 0 0 0 0	433/433 433/433 433/433 433/433 433/433	42 42 42 42 42 43 44 43						
Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166 abcZ: 114	99.77 99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1 1 1	0 0 0 0 0 0 0	433/433 433/433 433/433 433/433 433/433 433/433	4월 4월 4월 4월 4월						
Allele abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166 abcZ: 114 abcZ: 103	99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1 1 1 1	0 0 0 0 0 0 0 0 0	433/433 433/433 433/433 433/433 433/433 433/433 433/433	4월 4월 4월 4월 4월 4월						

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

Query: Sequences Batch sequences Compare alleles 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 Action
Locus: abcZ ▼ Submit Allele #1: 5 Allele #2: 453
Nucleotide differences between abcZ: 5 and abcZ: 453
Identity: 99.77 % Show alignment
Differences: 1 300: $\mathbf{G} \rightarrow \mathbf{A}$

11.8.2 Sequence comparison

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



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 comp	arison - Neisseria locus/sequence definitions							
This tool allows you to select two alleles	and highlight the nucleotide differences between them.							
Select parameters Locus: abcZ Allele #1: 5 Allele #2: 8	Action Submit							

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

Prin MLST / Download: Alleles	Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query MLST profiles Iome PorA FetA Options Isolate Database								
Allele sequence comp	arison - Neisseria locus/sequence definitions								
This tool allows you to select two alleles and highlight the nucleotide differences between them.									
Select parameters Locus: abcZ Allele #1: 5 Allele #2: 8									
Nucleotide differences between	n abcZ: 5 and abcZ: 8								
Show alignment									
Differences: 41 $72: G \rightarrow T$ $78: A \rightarrow G$ $79: A \rightarrow C$ $81: T \rightarrow C$ $82: G \rightarrow A$ $83: G \rightarrow A$									
$87: G \rightarrow A$ $88: A \rightarrow G$ $89: G \rightarrow A$ $90: T \rightarrow C$ $93: G \rightarrow C$ $95: C \rightarrow T$									
99. $C \rightarrow I$ 99: $G \rightarrow A$ 102: $G \rightarrow A$									

See also:

Locus explorer plugin.

11.9 Browsing isolate data

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

Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions										
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample.										
Query database Search or browse database • Search by combinations of loci (profiles) • Projects - main projects defined in database.	Submissions Manage submissions Manage submissions General information Isolates: 35423 Last updated: 2015-08-27 Update history About BIGSdb									
Breakdown Export Analysis • Single field • Export dataset • Contigs • Unique combinations • Sequences - XMFA / concatenated FASTA formats • Codon usage • Publications • Sequence bin • Miscellaneous • Description of database fields • Description of database fields	oci									

Leave query form fields blank (the display of these may vary depending on modification options set by the user). Choose the field to order the results by, the number of results per page to display, and click 'Submit'.

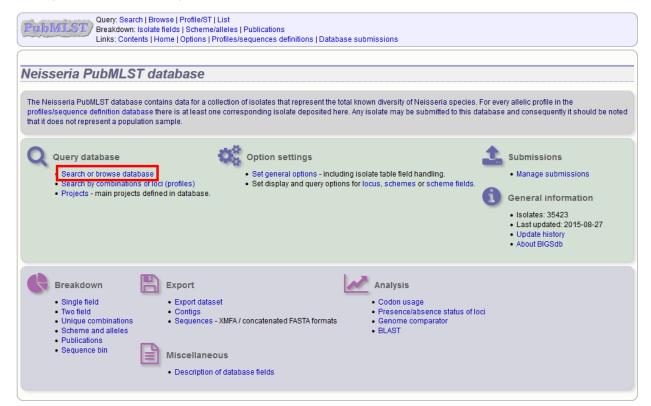
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a	arch or	browse Neisse	eria PubM	LS	r database)							
te	r search crite	ria or leave blank to browse	all records										
_	Isolate prove	nance/phenotype fields)ienlav/er	ort options				— — Acti	on	
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id	isolate	aliases	country	year	disease		species	serogroup	ST	MLST clonal complex	Finet PorA VR1		
_	isolate A4/M1027	aliases B1; NIBSC_2803; Z1001	country	year	disease	ed/other)	species Neisseria meningitidis	serogroup A	ST 4				
1 2	A4/M1027 120M		country USA Pakistan	year 1937 1967	disease invasive (unspecifi meningitis and sep	ticaemia	Neisseria meningitidis Neisseria meningitidis		4 1	clonal complex	PorA VR1	PorA VR2	FetA VR
1 2	A4/M1027	B1; NIBSC_2803; Z1001	Country USA Pakistan UK	year 1937 1967	disease invasive (unspecifi meningitis and sep	ticaemia	Neisseria meningitidis	A	4	clonal complex ST-4 complex/subgroup IV	PorA VR1 5-2	PorA VR2 10	FetA VR F1-5
1 2	A4/M1027 120M	B1; NIBSC_2803; Z1001	Country USA Pakistan UK USA	year 1937 1967 2000	disease invasive (unspecifi meningitis and sep invasive (unspecifi	oticaemia ed/other)	Neisseria meningitidis Neisseria meningitidis	A	4 1	clonal complex ST-4 complex/subgroup IV	PorA VR1 5-2 5-2	PorA VR2 10 10	FetA VR F1-5
1 2 3 4 5	A4/M1027 120M M00242905 M1027 M00240227	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	Country USA Pakistan UK USA UK	year 1937 1967 2000 1937 2000	disease invasive (unspecifi meningitis and sep invasive (unspecifi invasive (unspecifi invasive (unspecifi	oticaemia ed/other) ed/other) ed/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B	4 1099 4 1100	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-32 complex/ET-5 complex	PorA VR1 5-2 5-2 19	PorA VR2 10 10	FetA VR F1-5
1 2 3 4 5 6	A4/M1027 120M M00242905 M1027 M00240227 M00282207	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	Country USA Pakistan UK USA UK UK	year 1937 1967 2000 1937 2000 2000	disease invasive (unspecifi meningitis and sep invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi	ed/other) ed/other) ed/other) ed/other) ed/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B W	4 1099 4 1100 1101	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-32 complex/ET-5 complex ST-22 complex	PorA VR1 5-2 5-2 19	PorA VR2 10 10 15 16	FetA VR F1-5 F5-1
1 2 3 4 5 6 7	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035	Country USA Pakistan UK USA UK UK Finland	year 1937 1967 2000 1937 2000 2000 1975	disease invasive (unspecifi meningitis and sep invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi	ed/other) ed/other) ed/other) ed/other) ed/other) ed/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B A B W A	4 1099 4 1100 1101 5	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 ST-22 complex ST-5 complex/subgroup III	PorA VR1 5-2 5-2 19	PorA VR2 10 10 15 16 9	FetA VR F1-5
1 2 3 4 5 6 7	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043	Country USA Pakistan UK USA UK UK Finland UK	year 1937 1967 2000 1937 2000 2000 1975 2000	disease invasive (unspecifi meningitis and sep invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi	ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B A B W A B	4 1099 4 1100 1101 5 1102	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 ST-52 complex ST-5 complex/subgroup III ST-18 complex	PorA VR1 5-2 5-2 19 7	PorA VR2 10 10 15 16	FetA VR F1-5 F5-1
1 2 3 4 5 6 7	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054	country USA Pakistan UK USA UK UK Finland UK Czech Republic	year 1937 2000 1937 2000 2000 1975 2000 1975 2000 1984	disease invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi	ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other)	Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis	A B A B W A	4 1099 4 1100 1101 5	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-4 complex/subgroup IV ST-32 complex/ET-5 complex ST-22 complex/ST-22 complex ST-5 complex/subgroup III ST-18 complex ST-22 complex	PorA VR1 5-2 5-2 19 7	PorA VR2 10 10 15 16 9 14	FetA VR F1-5 F5-1 F3-1
1 2 3 4 5 6 7 8 9	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073	country USA Pakistan UK USA UK Finland UK Czech Republic Canada	year 1937 1967 2000 1937 2000 2000 1975 2000 1984 1971	disease invasive (unspecifi meningitis and seg- invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi	ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other)	Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis	A A B A B W A B	4 1099 4 1100 1101 5 1102	cional complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-4 complex/subgroup IV ST-32 complex/ET-5 complex ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-1 complex/subgroup I/I	PorA VR1 5-2 5-2 19 7 20 18-1	PorA VR2 10 10 15 16 9	FetA VR F1-5 F5-1
1 2 3 4 5 6 7 8 9 10 11	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748 129E	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054	country USA Pakistan UK USA UK Finland UK Czech Republic Canada Germany	year 1937 1967 2000 1937 2000 2000 1975 2000 1984 1971 1964	disease invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi	ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other)	Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A A	4 1099 4 1100 1101 5 1102 114 1 1	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 ST-52 complex/subgroup III ST-16 complex ST-22 complex ST-22 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	PorA VR1 5-2 19 7 20 18-1 5-2	PorA VR2 10 10 15 16 9 14 3 10	FetA VR F1-5 F5-1 F3-1
1 2 3 4 5 6 7 8 9 10 11 12	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748 129E 0090/89	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073 B92; NIBSC_2828; Z1092	country USA Pakistan UK USA UK Finland UK Czech Republic Germany Czech Republic	year 1937 1967 2000 1937 2000 2000 1975 2000 1984 1971 1964 1989	disease invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi	ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other)	Neisseria meningittäis Neisseria meningittäis Neisseria meningittäis Neisseria meningittäis Neisseria meningittäis Neisseria meningittäis Neisseria meningittäis Neisseria meningittäis Neisseria meningittäis Neisseria meningittäis	A B A B W A B W A A A B	4 1099 4 1100 1101 5 1102 114 1 1 1015	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-3 complex/subgroup IV ST-32 complex/ET-5 complex ST-22 complex/subgroup III ST-14 complex/subgroup /II ST-1 complex/subgroup /II ST-32 complex/subgroup /II	PorA VR1 5-2 5-2 19 7 20 18-1 5-2 7	PorA VR2 10 10 15 16 9 14 3 10 16	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6
1 2 3 4 5 6 7 8 9 10 11 12 13	A4/M1027 120M M00242905 M1027 M00240227 7891 M00282207 7891 M00242007 0021/84 6748 129E 0090/89 139M	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073	country USA Pakistan UK USA UK Finland UK Czech Republic Canada Germany Czech Republic Philippines	year 1937 1967 2000 1937 2000 2000 1975 2000 1975 2000 1984 1971 1964 1989 1968	disease invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi	ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other)	Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A A B A A	4 1099 4 1100 1101 5 1102 114 1 1 1015 1	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 ST-52 complex/subgroup III ST-16 complex ST-22 complex ST-22 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	PorA VR1 5-2 19 7 20 18-1 5-2	PorA VR2 10 10 15 16 9 9 14 3 10 16 10	FetA VR F1-5 F5-1 F3-1 F5-1
1 2 3 4 5 6 7 8 9 10 11 12 13	A4/M1027 120M M00242905 M1027 M00240227 M00282207 7891 M00242007 0021/84 6748 129E 0090/89	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073 B92; NIBSC_2828; Z1092	country USA Pakistan UK USA UK Finland UK Czech Republic Canada Germany Czech Republic Philippines	year 1937 1967 2000 1937 2000 2000 1975 2000 1975 2000 1984 1971 1964 1989 1968 1995	disease invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi	ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other)	Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A A B	4 1099 4 1100 1101 5 1102 114 1 1 1015 1 117	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-3 complex/subgroup IV ST-32 complex/ET-5 complex ST-22 complex/subgroup III ST-14 complex/subgroup /II ST-1 complex/subgroup /II ST-32 complex/subgroup /II	PorA VR1 5-2 5-2 19 7 20 18-1 5-2 7	PorA VR2 10 10 15 16 9 14 3 10 16	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6
2 3 4 5 6 7 8	A4/M1027 120M M00242905 M1027 M00240227 7891 M00282207 7891 M00242007 0021/84 6748 129E 0090/89 139M	B1; NIBSC_2803; Z1001 B35; NIBSC_2822; Z1035 B43; NIBSC_3076; Z1043 B54; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073 B92; NIBSC_2828; Z1092	country USA Pakistan UK USA UK Finland UK Czech Republic Canada Germany Czech Republic Philippines	year 1937 1967 2000 1937 2000 2000 1975 2000 1975 2000 1984 1971 1964 1989 1968	disease invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi invasive (unspecifi	ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other) ed/other)	Neisseria meningittidis Neisseria meningittidis	A B A B W A B W A A A B A A	4 1099 4 1100 1101 5 1102 114 1 1 1015 1	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup IV ST-3 complex/subgroup IV ST-32 complex/ET-5 complex ST-22 complex/subgroup III ST-14 complex/subgroup /II ST-1 complex/subgroup /II ST-32 complex/subgroup /II	PorA VR1 5-2 5-2 19 7 20 18-1 5-2 7	PorA VR2 10 10 15 16 9 9 14 3 10 16 10	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6

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

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2		B35; NIBSC 2822; Z1035	Pakistan		meningitis and septicaemia			4	ST-4 complex/subgroup I/I	5-2	10	F1-5 F5-1
	M00242905	000, NIDOO_2022, 21030	UK		invasive (unspecified/other)			1099	or r complex-subgroup I/II	19	15	1.0-1
4		B43; NIBSC 3076; Z1043	USA		invasive (unspecified/other)			4	ST-4 complex/subgroup IV	13	15	
5 N	M00240227	2.12, 1.1200_0010, 21040	UK		invasive (unspecified/other)				ST-32 complex/ET-5 complex	7	16	
6 N	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	s W	1101	ST-22 complex			
6 N		B54; NIBSC_2760; Z1054	UK Finland		invasive (unspecified/other) invasive (unspecified/other)	-		1101 5	ST-5 complex/subgroup III	20	9	F3-1
7		B54; NIBSC_2760; Z1054		1975		Neisseria meningitidis	s A			20	9 14	F3-1
7	7891	B54; NIBSC_2760; Z1054	Finland UK	1975 2000	invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis	a A a B	5	ST-5 complex/subgroup III	20		F3-1
7 8 N	7891 M00242007 0021/84 6748	B54; NIBSC_2760; Z1054 B73; NIBSC_2784; Z1073	Finland UK	1975 2000 1984	invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	s A B B W	5 1102	ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-1 complex/subgroup I/II	18-1		F3-1 F5-1
7 8 M 9 10 11	7891 M00242007 0021/84 6748 129E		Finland UK Czech Republic Canada Germany	1975 2000 1984 1971 1964	invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A B B B W A A A A A A A A A A A A A A	5 1102 114 1 1	ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	18-1 5-2	14	
7 8 9 10 11 12	7891 M00242007 0021/84 6748 129E 0090/89	B73; NIBSC_2784; Z1073 B92; NIBSC_2828; Z1092	Finland UK Czech Republic Canada Germany Czech Republic	1975 2000 1984 1971 1964 1989	invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A B B W A A A A A A A A A A A A A A A A	5 1102 114 1 1 1015	ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-32 complex/ET-5 complex	18-1 5-2 7	14 3 10 16	F5-1 F3-6
7 8 9 10 11 12 13	7891 M00242007 0021/84 6748 129E 0090/89 139M	B73; NIBSC_2784; Z1073	Finland UK Czech Republic Canada Germany Czech Republic Philippines	1975 2000 1984 1971 1964 1989 1968	invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	3 A 3 B 3 W 3 A 3 A 3 B 3 A	5 1102 114 1 1 1015 1	ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	18-1 5-2	14 3 10 16 10	F5-1
7 8 9 10 11 12 13 14	7891 M00242007 0021/84 6748 129E 0090/89 139M 0120/95	B73; NIBSC_2784; Z1073 B92; NIBSC_2828; Z1092	Finland UK Czech Republic Canada Germany Czech Republic Philippines Czech Republic	1975 2000 1984 1971 1964 1989 1968 1995	invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	3 A 3 B 4 W 5 A 5 A 5 A 5 A 5 A 3 A 3 A	5 1102 114 1 1 1015 1 117	ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-32 complex/ET-5 complex	18-1 5-2 7	14 3 10 16	F5-1 F3-6
7 8 9 10 11 12 13	7891 M00242007 0021/84 6748 129E 0090/89 139M	B73; NIBSC_2784; Z1073 B92; NIBSC_2828; Z1092	Finland UK Czech Republic Canada Germany Czech Republic Philippines	1975 2000 1984 1971 1964 1989 1968	invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	a A b B b W b A b A b A b A b A b A b A b A b A b A b A b A b A c A c A c A c A c A c A	5 1102 114 1 1 1015 1	ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-32 complex/ET-5 complex	18-1 5-2 7	14 3 10 16 10	F5-1 F3-6

11.10 Querying isolate data

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



To start with, only one provenance field search box is displayed but more can be added by clicking the '+' button (highlighted). These can be linked together by 'and' or 'or'.

Profit/ILST Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions										
		Toggle: <i>i</i> Field help: id	▼ Go							
Search Neisseria PubMLST database										
Isolate provenance/phenotype fields Combine with: AND - country USA + I year - > 1999 Action Reset Submit	Display/sort options Order by: id Display: 25 ✔ records per page []	✓ ascending ✓	Modify form options							

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

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300 rec	cords returned (1 - 25 di	isplayed)	Click	the hyperlinks for detailed inf	ormation.							
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id	isolate	aliases	country	vear	disease	species	serogroup	ST	clonal complex		PorA VR2 Fe		
341	M7085		USA		invasive (unspecified/other)				ST-11 complex/ET-37 complex				
499	MDL01A0601		USA	2001	meningitis	Neisseria meningitidis		1378					
500	MDL01A2447		USA	2001	invasive (unspecified/other)	Neisseria meningitidis	Y	1379	ST-23 complex/Cluster A3				
866	MD01227		USA	2001		Neisseria meningitidis	1	1624	ST-167 complex				
867	MDO1056		USA	2001		Neisseria meningitidis	1	1625	ST-23 complex/Cluster A3				
868	MDO1066		USA	2001		Neisseria meningitidis	1	1626	ST-269 complex				
2281	M7089		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex	5	2		
2299	M7257		USA		invasive (unspecified/other)				ST-11 complex/ET-37 complex	5	2		
2316	M7086		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	22	ST-22 complex	6	3		
2317	M7084		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	22	ST-22 complex	6	3		
2322	M7092		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1065	ST-22 complex	6	3		
2323	M7100		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1286	ST-22 complex	6	3		
2324	M7259		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1066	ST-22 complex	6	3		

Each field can be queried using standard operators.

More search features are available by clicking the 'Modify form options' tab on the right-hand side of the screen.

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A tab will be displayed. Different options will be available here depending on the database. Queries will be combined from the values entered in all form sections. Possible options are:

- · Provenance fields
 - Search by combination of provenance field values, e.g. country, year, sender.
- Allele designations/scheme field values
 - Search by combination of allele designations and/or scheme fields e.g. ST, clonal complex information.
- Allele designation status
 - Search by whether allele designation status is confirmed or provisional.
- · Tagged sequence status
 - Search by whether tagged sequence data is available for a locus. You can also search by sequence flags.
- Attribute values list
 - Enter a list of values for any provenance field, locus, or scheme field.
- Filters
 - Various filters may be available, including
 - * Publications
 - * Projects
 - * MLST profile completion status
 - * Clonal complex
 - * Sequence bin size
 - * Inclusion/exclusion of old versions

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id • = • Enter value + 0	Modify form parameters options Click to add or remove additional query terms:
Order by: id ascending	Provenance fields
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If the interface is modified, a button to save options becomes available within the tab. If this is clicked, the modified form will be displayed the next time you go to the query page.

11.10.1 Query by allele designation/scheme field

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

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

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Designations can be queried using standard operators.

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

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

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id 341 2281	isolate alia M7085 M7089	ases country USA USA	year 2000 in 2000 in	Isolate fields () disease vasive (unspecified/other) vasive (unspecified/other)	Neisseria meningiti Neisseria meningiti	serogroup idis W idis W	5 ST 11 S 11 S	MLST clonal complex 3T-11 complex/ET-37 complex 3T-11 complex/ET-37 complex	PorA VR1	PorA VR2			
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id 341 2281 2299 19369 19371 19374	isolate alia M7085 M7089 M7257 M13519 M15141 M16917	ases country USA USA USA USA USA USA	year 2000 in 2000 in 2000 in 2005 in 2006 in 2007 in	Isolate fields disease disease vasive (unspecified/other) vasive (unspecified/other) vasive (unspecified/other) vasive (unspecified/other) vasive (unspecified/other) vasive (unspecified/other)	Neisseria meningiti Neisseria meningiti Neisseria meningiti Neisseria meningiti Neisseria meningiti Neisseria meningiti	serogroup idis W idis W idis W idis C idis C	ST 11 5 11 5 11 5 11 5 11 5 11 5	MLST clonal complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex	PorA VR1 5 5-1 5-1 5-1 5-1	PorA VR2 2 10-8 10-8 10-8	FetA VR F1-1		
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id 341 2281 2299 19369 19371 19374 19377 19379	isolate alia M7085 M7089 M7257 M13519 M15141 M16917	ases country USA USA USA USA USA USA USA	year 2000 in 2000 in 2005 in 2005 in 2006 in 2007 in 2008 in 2009 in	Isolate fields disease disease vasive (unspecified/other) vasive (unspecified/other) vasive (unspecified/other) vasive (unspecified/other) vasive (unspecified/other) vasive (unspecified/other)	Neisseria meningiti Neisseria meningiti Neisseria meningiti Neisseria meningiti Neisseria meningiti Neisseria meningiti Neisseria meningiti	serogroup idis W idis W idis W idis C idis C idis NG idis W idis W	ST 11 5 11 5 11 5 11 5 11 5 11 5 11 5 11	MLST clonal complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex	PorA VR1 5 5-1 5-1 5-1 5-1	PorA VR2 2 10-8 10-8 10-8	FetA VR F1-1		

11.10.2 Query by allele designation count

Queries can be combined with counts of the total number of designations or for individual loci.

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

Printifications Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	
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Search or browse Neisseria PubMLST database	
Enter search criteria or leave blank to browse all records. Modify form parameters to filter or enter a list of values.	Modify
	* form
id v = v Enter value + 0 Order by: id	Modify form parameters options
Display: 25 👻 records per page	Click to add or remove additional query terms:
Action	Provenance fields
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For example, to find all isolates that have designations at >1000 loci, select 'total designations > 1000', then click 'Submit'.

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1	A4/M1027	B1; NIBSC_2803; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	2069108	364	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; NIBSC_2822; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	2059411	359	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
7	7891	B54; NIBSC_2760; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	2057385	199	5	ST-5 complex/subgroup III	20	9	F3-1
10	6748	B73; NIBSC_2784; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	4241338	652	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129E	B92; NIBSC_2828; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	2072690	272	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
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You can also search for isolates where any isolate has a particular number of designations. Use the term 'any locus' to do this.

Finally, you can search for isolates with a specific number of designations at a specific locus.

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Additional search terms can be combined using the '+' button. Designation count queries will be combined with terms entered in other sections.

Note: Searches for 'all loci' with counts that include zero, e.g. 'count of any locus = 0' or with a '<' operator are not supported. This is because such searches have to identify every isolate for which one or more loci are missing. In databases with thousands of loci this can be a very expensive database query.

11.10.3 Query by allele designation status

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

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

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

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Provisional allele designations are marked within the results tables with a pink background. Any scheme field designations that depend on the allele in question, e.g. a MLST ST, will also be marked as provisional.

11.10.4 Query by sequence tag count

Queries can be combined with counts of the total number of tags or for individual loci.

Make sure that the tagged sequence counts fieldset is displayed by selecting it in the 'Modify form options' tab.

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For example, to find all isolates that have sequence tags at >1000 loci, select 'total tags > 1000', then click 'Submit'.

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2	120M	B35; NIBSC_2822; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	2059411	359	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
7	7891	B54; NIBSC_2760; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	2057385	199	5	ST-5 complex/subgroup III	20	9	F3-1
10	6748	B73; NIBSC_2784; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	4241338	652	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129E	B92; NIBSC_2828; 71092	Germany	1964	invasive (unspecified/other)	Neisseria	A	2072690	272	1	ST-1 complex/subgroup I/II	5-2	10	F3-6

You can also search for isolates where any isolate has a particular number of sequence tags. Use the term 'any locus' to do this.

Finally, you can search for isolates with a specific number of tags at a specific locus.

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Additional search terms can be combined using the '+' button. Sequence tag count queries will be combined with terms entered in other sections.

Note: Searches for 'all loci' with counts that include zero, e.g. 'count of any locus = 0' or with a '<' operator are not supported. This is because such searches have to identify every isolate for which one or more loci are not tagged. In databases with thousands of loci this can be a very expensive database query.

11.10.5 Query by tagged sequence status

Sequence tags identify the region of a contig within an isolate's sequence bin entries that correspond to a particular locus. The presence or absence of these tags can be queried as can whether or not the sequence has an a flag associated with. These flags designate specific characteristics of the sequences. Queries will be combined from the values entered in all form sections.

Make sure that the tagged sequences status fieldset is displayed by selecting it in the 'Modify form options' tab.

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Select a specific locus in the dropdown box (or alternatively 'any locus') and a status. Available status values are:

- untagged
 - The locus has not been tagged within the sequence bin.
- tagged
 - The locus has been tagged within the sequence bin.
- complete
 - The locus sequence is complete.
- incomplete
 - The locus sequence is incomplete normally because it continues beyond the end of a contig.
- flagged: any
 - The sequence for the locus has a flag set.
- flagged: none
 - The sequence for the locus does not have a flag set.
- flagged: <specific flag>
 - The sequence for the locus has the specific flag chosen.

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See also:

Sequence tag flags

11.10.6 Query by list of attributes

The query form can be modified with a list box in to which a list of values for a chosen attribute can be entered - this could be a list of ids, isolate names, alleles or scheme fields. This list will be combined with any other criteria or filter used on the page.

If the list box is not shown, add it by selecting it in the 'Modify form options' tab.

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Select the attribute to query and enter a list of values.

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2 120M B35; NIBSC_2822; Z1035 Pakistan 1967 meningitis and septicaemia Neisseria meningitidis A 1 ST-1 complex/subgroup I/II 5-2 10 F5-1 3 M00242905 UK 2000 invasive (unspecified/other) Neisseria meningitidis B 1099 19 15 4 M1027 B43; NIBSC_3076; Z1043 USA 1937 invasive (unspecified/other) Neisseria meningitidis A 4 ST-4 complex/subgroup I/I 5 5 M00240227 UK 2000 invasive (unspecified/other) Neisseria meningitidis B 1100 ST-32 complex/ET-5 complex 7 16 Analysis tools: Breakdown: Fields Two Field Combinations Polymorphic sites Schemes/alleles Publications Sequence bin Tag status Analysis: BURST Codons Presence/Absence Genome Comparator BLAST			
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4 M1027 B43; NIBSC_3076; Z1043 USA 1937 invasive (unspecified/other) Neisseria meningitidis A 4 ST-4 complex/subgroup IV 5 M00240227 UK 2000 invasive (unspecified/other) Neisseria meningitidis B 1100 ST-32 complex/ET-5 complex 7 16 Analysis tools: Breakdown: Fields Two Field Combinations Polymorphic sites Schemes/alleles Publications Sequence bin Tag status Analysis: BURST Codons Presence/Absence Genome Comparator BLAST			
5 M00240227 UK 2000 invasive (unspecified/other) Neisseria meningitidis B 1100 ST-32 complex/ET-5 complex 7 16 Analysis tools: Breakdown: Fields Two Field Combinations Polymorphic sites Schemes/alleles Publications Sequence bin Tag status Analysis: BURST Codons Presence/Absence Genome Comparator BLAST			
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Analysis: BURST Codons Presence/Absence Genome Comparator BLAST	Analysis tools:		
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Evnor: Dataset Contras Sequences	Export: Dataset Contigs Sequences		

11.10.7 Query filters

There are various filters that can additionally be applied to queries, or the filters can be applied solely on their own so that they filter the entire database.

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

Query: Search Profile/ST Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definition	s							
	Help 🗹 🛛 Toggle: 🚯 🖡	Field help: id 🔹 🖌 😡						
Search or browse Neisseria PubMLST database								
Enter search criteria or leave blank to browse all records. Modify form parameters to f	ilter or enter a list of values.	Modify						
	Display/sort options	form						
id → = → Enter value + 0	Order by: id	Modify form parameters options						
	Display: 25 👻 records per page 🜖	Click to add or remove additional query terms:						
		Provenance fields						
		Allele designations/scheme field values						
		Allele designation counts						
		Allele designation status						
		Co Tagged sequence counts						
		 Tagged sequence status 						
		Attribute values list						
		Filters						

The filters displayed will depend on the database and what has been defined within it. Common filters are:

• Publication - Select one or more publication that has been linked to isolate records.

- Project Select one or more project that isolates belong to.
- Profile completion This is commonly displayed for MLST schemes. Available options are:
 - complete All loci of the scheme have alleles designated.
 - incomplete One or more loci have not yet been designated.
 - partial The scheme is incomplete, but at least one locus has an allele designated.
 - started At least one locus has an allele designated. The scheme mat be complete or partial.
 - not started The scheme has no loci with alleles designated.
- Sequence bin Specify whether any sequence data has been associated with a record. Specific threshold values may be selected if these have been *set up for the database*.
- Provenance fields Dropdown list boxes of values for specific provenance fields may be present if set for the database. Users can choose to *add additional filters*.

11.11 Querying by allelic profile

If a scheme, such as MLST, has been defined for an isolate database it is possible to query the database against complete or partial allelic profiles. Even if no scheme is defined, queries can be made against all loci.

On the index page, click 'Search by combinations of loci (profiles)' for any defined scheme. Enter either a partial (any combination of loci) or complete profile.



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

Outp://www.search.jprofile/ST.jclist Breakdown: Isolate fields.jScheme/alleles.jPublications Links: Contents.jHome.jOptions.jProfiles/sequences definitions.jDatabase submiss	sions
	Toggle: i
Search Neisseria PubMLST database by combinations of	loci
Schemes	
Please select the scheme you would like to query:	
MLSI - Select	
-Please enter your allelic profile below. Blank loci will be ignored	searching remote database ——
abcZ adk aroE fumC gdh pdhC pgm ST:	Autofil
	Display/sort options
Project: vi Search: Exact or nearest match	
Include old record versions	Display: 25 🗸 records per page 👔
Action	
Reset Submit	

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

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
	Toggle: i
Search Neisseria PubMLST database by combinations of loci	
Schemes	
Please select the scheme you would like to query:	
MLST - Select	
<u></u>	
Please enter your allelic profile below. Blank loci will be ignored. — Autofill profile by searching remote database —	
abcZ adk aroE fumC gdh pdhC pgm ST: Autofill 2 3 4 3 8 4 Autofill Autofill	
Filters Options Display/sort options	
	scending 👻
Include old record versions Display: 25 records per page	
Action	
Reset Submit	

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

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

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

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

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

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
	Toggle: i
Search Neisseria PubMLST database by combinations of loci	
Schemes	
Please select the scheme you would like to query:	
MLST v Select	
Please enter your allelic profile below. Blank loci will be ignored. — Autofill profile by searching remote database —	
abcZ adk aroE fumC gdh pdhC pgm ST: 44 Autofill	
- Filters - Display/sort options - Display/so	
Project.	
Include old record versions Display: 25 🚽 records per page 👔	
Action	
Reset Submit	

Click 'Submit'.

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hemes											
ease select the s	scheme you wou	Id like to query:									
				_							
ILST			Selec	<u>*</u>							
-Please enter y	our allelic profile	below. Blank loci	will be	ignored	-Autofill profile by search	hing remote o	database ——				
abcZ a	dk aroE	fumC o	idh	pdhC pgm	ST: 44		Autofill				
9	6 9	9	9	6 9							
Filters				Options		Display/a	ort options				
Project					t or nearest match 👻						
	ecord versions			▼ i Search: Exact	t or nearest match 👻		ay: 25 → recor	ds per page 👔	•	 ascendi 	ing 👻
Action	_				tor nearest match 👻			ds per page i	•	 ascendi 	ing 🗸
Action	ecord versions			↓ Jeanul. Exact	tor nearest match 👻			ds per page i	ľ	- ascendi	ing 🔻
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Action Reset Sul	bmit			I Gealur. Exact	t or nearest match 👻			ds per page 👔	·	- ascena	ing 🔻
Action Reset Sul	bmit d (7 loci).	ed) Click the hype			t or nearest match 👻			ds per page 👔	·	- ascena	ing 🔻
Action Reset Sul	bmit d (7 loci).	ed). Click the hype		for detailed information.	t or nearest match			ds per page 👔		- ascena	ng 🔻
Action Reset Sul ct matches foun records returne	bmit d (7 loci). d (1 - 25 display	ed). Click the hype			Cor nearest match			ds per page 👔		ascena	ng v
Action Reset Sul ct matches foun records returne	bmit d (7 loci). d (1 - 25 display				Cor nearest match 👻			ds per page 👔		ascena	ng 🔻
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Action Reset Sul ct matches foun records returne ge: 1 2 3	bmit d (7 loci). d (1 - 25 display		rlinks	for detailed information.			v: 25 → recor	T	Finet	ping antig PorA VR2	ens
Action Reset Sul ct matches foun records returne ge: 1 2 3 d isolate	omit d (7 loci). d (1 - 25 display 4 5 >	Last	rlinks	for detailed information.		Displa	v: 25 → recor	T complex F	Finet	yping antig	ens
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Action Reset Sul ct matches foun records returne ge: 1 2 3 d isolate 11 19 0 38 27 NG E30	omit d (7 loci). d (1 - 25 display 4 5 >	Country Germany Germany Norway	rlinks solat year 1999 1999 1988	for detailed information. te fields 1 disease carrier carrier carrier	species Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis	Displa serogroup B NG B	MLS ST clonal (44 ST-41/44 com 44 ST-41/44 com	T complex p plex/Lineage 3 plex/Lineage 3	Finet	yping antig	ens
Action Reset Sul ct matches foun records returne pe: 1 2 3 d isolate h1 19 0 38 27 NG E30 74 99 182	d (7 loci). d (7 - 25 display 4 5 > aliases	Country Germany Germany Norway Canada	rlinks year 1999 1999 1988 1999	for detailed information. le fields [1] disease carrier carrier carrier invasive (unspecified/other)	species Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis	Displa serogroup B NG B B B	ML S ST clonal (44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com	T F complex F plex/Lineage 3 plex/Lineage 3 plex/Lineage 3 plex/Lineage 3	Finet, PorA VR1	yping antig PorA VR2	ens FetA VR
Action Reset Sul ct matches foun records returne ge: 1 2 3 d isolate 11 19 70 38 27 NG E30 74 99 182 99 182	d (7 loci). d (7 - 25 display 4 5 > aliases	Country Germany Germany Norway Canada Canada	rlinks year 1999 1998 1999 1988 1999	for detailed information. te fields 1 disease carrier carrier carrier invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	Displa serogroup B NG B B B B B B	ML S ST	T F complex F plex/Lineage 3 plex/Lineage 3 plex/Lineage 3 plex/Lineage 3	Finety PorA VR1 21	yping antig PorA VR2 16	ens FetA VR F1-7
Action Reset Sul ct matches foun records returne ge: 1 2 3 d isolate 11 19 0 38 27 NG E30 74 99 182 92 99-182 92 99-182 95 0069/93	d (7 loci). d (1 - 25 display 4 5 > aliases Z4692	Country Germany Germany Norway Canada Canada Czech Republic	rlinks year 1999 1988 1999 1988 1999 1999	for detailed information. le fields [1] disease carrier carrier carrier invasive (unspecified/other)	species Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis	Serogroup B NG B NG B NG	ML S ST clonal (44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com	T complex/Lineage 3 plex/Lineage 3 plex/Lineage 3 plex/Lineage 3 plex/Lineage 3 plex/Lineage 3	Finet, PorA VR1	yping antig PorA VR2 16 14-4	ens FetA VR
Action Reset Sul ct matches foun records returne ge: 1 2 3 id isolate 11 19 70 38 27 NG E30 74 99 182 92 99-132 75 0069/93 75 0069/93	d (7 loci). d (7 - 25 display 4 5 > aliases	Country Germany Germany Norway Canada Canada Czech Republic The Netherlands	rlinks year 1999 1988 1999 1988 1999 1993 1975	for detailed information. te fields [] disease carrier carrier carrier invasive (unspecified/other) invasive (unspecified/other) carrier	species Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis	Displa serogroup B NG B B B B B S B S B B S B S	ML S ST clonal (44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com	T plex/Lineage 3 plex/Lineage 3 plex/Lineage 3 plex/Lineage 3 plex/Lineage 3 plex/Lineage 3 plex/Lineage 3	Finet PorA VR1 21 22	yping antig PorA VR2 16 14-4 4	ens FetA VR F1-7 F1-7
Action Reset Sul ect matches foun records returne ge: 1 2 3 id isolate 41 19 70 38 127 NG E30 74 99 182 192 99 192 192 99 192	d (7 loci). d (1 - 25 display 4 5 > aliases Z4692	Country Germany Germany Norway Canada Canada Czech Republic	rlinks 1999 1999 1988 1999 1993 1999 1993	for detailed information. te fields 1 disease carrier carrier carrier invasive (unspecified/other) invasive (unspecified/other)	species Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis	Displa serogroup B NG B B B B B B B B B B B B B B B B B	ML S ST clonal (44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com 44 ST-41/44 com	T performance provided and a performance provided and a performance and a performanc	Finety PorA VR1 21	yping antig PorA VR2 16 14-4	ens FetA VR F1-7

11.12 Retrieving isolates by linked publication

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

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Neisseria PubMLST database	
The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it s sample.	
Query database Search or browse database Search by combinations of loci (profiles) Projects - main projects defined in database. Set display and query options for locus, schemes or scheme fields. 	Submissions • Manage submissions General information • Isolates: 35423 • Last updated: 2015-08-27 • Update history • About BIGSdb
Breakdown Export Analysis • Single field • Export dataset • Contigs • Unique combinations • Scheme and alleles • Sequences - XMFA / concatenated FASTA formats • Codon usage • Publications • Sequence bin • Sequence bin • BLAST	Miscellaneous Description of database fields

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

PubMLS	Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/Sequences definitions Database submiss	ions	
Publicati	on breakdown of dataset		
	by Display	Action	
	All authors Order by: number of isolates descending	Submit	
Year	All years Display: 25 records per page		
73 records return Page: 1 2	ared (1 - 25 displayed). Click the hyperlinks for detailed information.		
PubMed id Yea	r Citation	Title	Isolates in database
17517841 20	7 Taha MK, Vázquez JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enríquez R, Fazio C, Frosch M, Heuberger S, Hoffmann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczynska A, Stefanelli P, Thulin S, Tzanakaki G, Unemo M, Vogel U, Zarantonelli ML (2007) Antimicrob Agents Chemother 51: 2784-92	Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis.	1670 isolates
18815379 200	18 Buckee CO, Jolley KA, Recker M, Penman B, Kriz P, Gupta S, Maiden MC (2008) Proc Natl Acad Sci U S A 105: 15082-7	Role of selection in the emergence of lineages and the evolution of virulence in Neisseria meningitidis.	1054 isolates
15776372 20	15 Claus H, Maiden MC, Wilson DJ, McCarthy ND, Jolley KA, Urwin R, Hessler F, Frosch M, Vogel U (2005) J Infect Dis 191: 1263-71	Genetic analysis of meningococci carried by children and young adults.	822 isolates
15528708 200	4 Yazdankhah SP, Kriz P, Tzanakaki G, Kremastinou J, Kalmusova J, Musilek M, Alvestad T, Jolley KA, Wilson DJ, McCarthy ND, Caugant DA, Maiden MC (2004) J Clin Microbiol 42: 5146-53	Distribution of serogroups and genotypes among disease- associated and carried isolates of Neisseria meningitidis from the Czech Republic, Greece, and Norway.	667 isolates
17825091 200	17 Bennett JS, Jolley KA, Sparling PF, Saunders NJ, Hart CA, Feavers IM, Maiden MC (2007) BMC Biol 5: 35	Species status of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from multilocus sequence typing.	576 isolates
15537808 200	5 Jolley KA, Wilson DJ, Kriz P, McVean G, Maiden MC (2005) Mol Biol Evol 22: 562-9	The influence of mutation, recombination, population history, and selection on patterns of genetic diversity in Neisseria meningitidis.	378 isolates
18375809 20	8 Russell JE. Urwin R. Grav SJ. Fox AJ. Feavers IM. Maiden MC (2008) Microbiology 154:	Molecular epidemiology of meningococcal disease in England and	323 isolates

These can be filtered by author and/or year, and the sort order changed.

INIICa	ntio	n breakdown of dataset		
	hor:	Jolley KA		
records re PubMed	eturne	d. Click the hyperlinks for detailed information.		Isolates in
id	Year	Citation	Title	database
7517841	2007	Taha MK, Vázquez JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enríquez R, Fazio C, Frosch M, Heuberger S, Hoffmann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczynska A, Stefanelli P, Thulin S, Tzanakai G, Unemo M, Vogel U, Zarantonelli ML (2007) Antimicrob Agents Chemother 51: 2784-92	Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis.	1670 isolates
8815379	2008	Buckee CO, Jolley KA, Recker M, Penman B, Kriz P, Gupta S, Maiden MC (2008) Proc Natl Acad Sci U S A 105: 15082-7	Role of selection in the emergence of lineages and the evolution of virulence in Neisseria meningitidis.	1054 isolates
5776372	2005	Claus H, Maiden MC, Wilson DJ, McCarthy ND, Jolley KA, Urwin R, Hessler F, Frosch M, Vogel U (2005) J Infect Dis 191: 1263-71	Genetic analysis of meningococci carried by children and young adults.	822 isolates
5528708	2004	Yazdankhah SP, Kriz P, Tzanakaki G, Kremastinou J, Kalmusova J, Musilek M, Alvestad T, Jolley KA, Wilson DJ, McCarthy ND, Caugant DA, Maiden MC (2004) J Clin Microbiol 42: 5146-53	Distribution of serogroups and genotypes among disease-associated and carried isolates of Neisseria meningitidis from the Czech Republic, Greece, and Norway.	667 isolates
7825091	2007	Bennett JS, Jolley KA, Sparling PF, Saunders NJ, Hart CA, Feavers IM, Maiden MC (2007) BMC Biol 5: 35	Species status of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from	576 isolates
			multilocus sequence typing.	

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

PubMLST	Ouery: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions		
Publicatio	n breakdown of dataset		
— Filter query by Author: Year:			
13 records returne	I. Click the hyperlinks for detailed information.		
PubMed id Year	Citation	Title	Isolates in database
17517841 2007	Taha MK, Vázquez JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enríquez R, Fazio C, Frosch M, Heuberger S, Hoffmann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczynska A, Stefanelli P, Thulin S, Tzanakai G, Unemo M, Vogel U, Zarantonelli ML (2007) Antimicrob Agents Chemother 51 : 2784-92	Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis.	1670 isolates
18815379 2008	Buckee CO, Jolley KA, Recker M, Penman B, Kriz P, Gupta S, Malden MC (2008) Proc Natl Acad Sci U S A 105: 15082-7	Role of selection in the emergence of lineages and the evolution of virulence in Neisseria meningitidis.	1054 isolates
15776372 2005	Claus H, Maiden MC, Wilson DJ, McCarthy ND, Jolley KA, Urwin R, Hessler F, Frosch M, Vogel U (2005) J Infect Dis 191: 1263-71	Genetic analysis of meningococci carried by children and young adults.	822 isolates
15528708 2004	Yazdankhah SP, Kriz P, Tzanakaki G, Kremastinou J, Kalmusova J, Musilek M, Alvestad T, Jolley KA, Wilson DJ, McCarthy ND, Caugant DA, Maiden MC (2004) J Clin Microbiol 42: 5146-53	Distribution of serogroups and genotypes among disease-associated and carried isolates of Neisseria meningitidis from the Czech Republic, Greece, and Norway.	667 isolates
17825091 2007	Bennett JS, Jolley KA, Sparling PF, Saunders NJ, Hart CA, Feavers IM, Maiden MC (2007) BMC Biol 5: 35	Species status of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from multilocus sequence typing.	576 isolates
15537808 2005	Jolley KA, Wilson DJ, Kriz P, McVean G, Maiden MC (2005) Mol Biol Evol 22: 562-9	The influence of mutation, recombination, population history, and selection on patterns of genetic diversity in Neisseria meningitidis.	378 isolates
	Bennett JS, Griffiths DT, McCarthy ND, Sleeman KL, Jolley KA, Crook DW, Maiden MC (2005) Infect Immun 73: 2424-32	Genetic diversity and carriage dynamics of Neisseria lactamica in infants.	271 isolates
11101595 2000	Iolley KA Kalmusova I Feil E L Cupta S Musilek M Kriz P Maiden MC (2000) I Clin Microbiol 39: 4402-9	Carried meningococci in the Czech Republic: a	

The abstract of the paper will be displayed (if available), along with all isolates linked to it.

t			d in the ed id: 178	Nei	sseria PubMLS	T database						
nn		ry (PubM	ed id: 178			1 uutubuoc						
				2509	91)							
pu ree 6 re	seven loci h Ilation gene species. A ecords retu	leisseria MLS tic inferences nalysis of vari	T scheme was to be made, in ation at a singl splayed). Click	readil cludin e locu: the hy	g direct comparisons with N.	isolates, providing a hig meningitidis and N. lact ns of identifying misclas:	hly discrimi amica. Exan	natory	ny. typing method. In addition, th on of these data demonstrate I determining whether mixed (d that allele	s were rar	ely shared ar
id	isolate				solate fields 👔				MLST	Finety	ping antig	ens
	ISOluto	aliases	country	year	solate fields <mark>1</mark> disease	species	serogroup	ST		Finety PorA VR1		
1	A4/M1027	aliases B1; Z1001	country USA	year			serogroup A	ST 4				
			-	year 1937	disease	Neisseria meningitidis			clonal complex	PorA VR1	PorA VR2	FetA VR
2	A4/M1027	B1; Z1001	USA	year 1937 1967	disease invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis	A	4	clonal complex ST-4 complex/subgroup IV	PorA VR1 5-2	PorA VR2 10	FetA VR F1-5
2 7	A4/M1027 120M	B1; Z1001 B35; Z1035	USA Pakistan	year 1937 1967 1975	disease invasive (unspecified/other) meningitis and septicaemia	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A	4 1	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II	PorA VR1 5-2 5-2	PorA VR2 10 10	FetA VR F1-5 F5-1
1 2 7 10 11	A4/M1027 120M 7891	B1; Z1001 B35; Z1035 B54; Z1054	USA Pakistan Finland Canada	year 1937 1967 1975 1971	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A	4 1 5	cional complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-5 complex/subgroup III	PorA VR1 5-2 5-2 20	PorA VR2 10 10 9	FetA VR F1-5 F5-1 F3-1
2 7 10 11	A4/M1027 120M 7891 6748	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073	USA Pakistan Finland Canada Germany	year 1937 1967 1975 1971	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A	4 1 5 1	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-5 complex/subgroup III ST-1 complex/subgroup I/II	PorA VR1 5-2 5-2 20 18-1	PorA VR2 10 10 9 3	FetA VR F1-5 F5-1 F3-1 F5-1
2 7 10 11 13	A4/M1027 120M 7891 6748 129	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092	USA Pakistan Finland Canada Germany	year 1937 1967 1975 1971 1964 1968	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A	4 1 5 1 1	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I	PorA VR1 5-2 5-2 20 18-1 5-2	PorA VR2 10 10 9 3 10	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6
2 7 10	A4/M1027 120M 7891 6748 129 139M	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099	USA Pakistan Finland Canada Germany Philippines Ghana	year 1937 1967 1975 1971 1964 1968 1973	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A	4 1 5 1 1 1	cional complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I	PorA VR1 5-2 5-2 20 18-1 5-2 5-2 5-2	PorA VR2 10 10 9 3 10 10	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1
2 7 10 11 13 19	A4/M1027 120M 7891 6748 129 139M S3131	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227	USA Pakistan Finland Canada Germany Philippines Ghana Denmark	year 1937 1967 1975 1971 1964 1968 1973 1974	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A A	4 1 5 1 1 1 4	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup IV	PorA VR1 5-2 20 18-1 5-2 5-2 5-2 7	PorA VR2 10 9 3 10 10 10 13-1	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1 F1-5
2 7 10 11 13 19 24 31	A4/M1027 120M 7891 6748 129 139M S3131 S4355	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227	USA Pakistan Finland Canada Germany Philippines Ghana Denmark	year 1937 1967 1975 1971 1964 1968 1973 1974 1963	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A	4 5 1 1 1 4 5	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup III ST-5 complex/subgroup III ST-1 complex/subgroup I/II ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-5 complex/subgroup III	PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1	PorA VR2 10 10 9 3 10 10 13-1 9	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1 F1-5 F3-1
2 7 10 11 13 19 24 31 34	A4/M1027 120M 7891 6748 129 139M S3131 S4355 10	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269	USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso	year 1937 1967 1975 1971 1964 1968 1973 1974 1963 1963	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A	4 1 5 1 1 4 5 4	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-5 complex/subgroup I/I ST-4 complex/subgroup I/I	PorA VR1 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1 7	PorA VR2 10 10 9 3 10 10 13-1 9 13-1	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1 F1-5 F3-1 F1-5
2 7 10 11 13 19 24 31 34 35	A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 20	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B275; Z1278	USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger	year 1937 1967 1975 1971 1964 1968 1973 1974 1963 1963 1963	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A	4 5 1 1 4 5 4 1	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-5 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I	PorA VR1 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1 7 5-1 7 5-2	PorA VR2 10 10 9 3 10 10 13-1 9 13-1 10	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F1-5 F3-1 F1-5 F1-7
2 7 10 11 13 19 24 31 34 35 46	A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 20 26	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B275; Z1278	USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso	year 1937 1967 1975 1971 1964 1968 1973 1974 1963 1963 1963	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A A	4 1 5 1 1 4 5 4 1 4	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup III ST-5 complex/subgroup III ST-1 complex/subgroup I/II ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-5 complex/subgroup IV ST-5 complex/subgroup IV ST-1 complex/subgroup I/I ST-4 complex/subgroup I/I ST-4 complex/subgroup I/I	PorA VR1 5-2 20 18-1 5-2 5-2 7 5-1 7 5-1 7 5-2 7	PorA VR2 10 10 9 3 10 10 13-1 9 13-1 10 13	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1 F1-5 F3-1 F1-5 F1-7 F1-5
2 7 10 11 13 19 24	A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 20 26 255	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B276; Z1275 B278; Z1278 B318; Z1318	USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso Cameroon	year 1937 1967 1975 1971 1964 1968 1973 1974 1963 1963 1963 1966	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A A A	4 1 5 1 1 4 5 4 1 4 4 4	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-5 complex/subgroup IV ST-4 complex/subgroup IV	PorA VR1 5-2 20 18-1 5-2 5-2 7 5-2 7 5-1 7 5-1 7 5-2 7 7 7 2 5-2 7	PorA VR2 10 10 9 3 10 10 13-1 9 13-1 10 13-1 10 13 13-1	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F1-5 F3-1 F1-5 F1-7 F1-5 F1-5 F1-5 F1-5
2 7 10 11 13 19 24 31 34 35 46 52 61	A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 26 255 243 393	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B275; Z1278 B318; Z1318 B362; Z1362 B392; Z1392	USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Niger Burkina Faso Cameroon Greece	year 1937 1967 1975 1971 1964 1968 1973 1963 1963 1963 1966 1966 1968	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A A A A A	4 1 5 1 1 4 5 4 1 4 4 4 4 4 4 1	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup III ST-5 complex/subgroup III ST-1 complex/subgroup III ST-1 complex/subgroup IVI ST-4 complex/subgroup IVI ST-5 complex/subgroup IVI ST-4 complex/subgroup IVI	PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-1 7 5-1 7 5-2 7 7-2 7 7 5-2 7 5-2	PorA VR2 10 10 9 3 10 10 13-1 9 13-1 10 13 13-1 13 13-1 13 10	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F3-6 F3-1 F1-5 F3-1 F1-5 F1-7 F1-5 F1-5 F1-5 F1-5 F5-1
2 7 10 11 13 19 24 31 34 35 46 52	A4/M1027 120M 7891 6748 129 139M S3131 S4355 10 20 26 255 243	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B260; Z1269 B275; Z1275 B278; Z1278 B318; Z1318 B362; Z1362	USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Niger Burkina Faso Cameroon Greece Djibouti	year 1937 1967 1975 1971 1964 1968 1973 1963 1963 1963 1966 1966 1968 1966	disease invasive (unspecified/other) meningitis and septicaemia invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis	A A A A A A A A A A A A A A A A A	4 1 5 1 1 4 5 4 1 4 4 4 4 4	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup I/I ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I ST-4 complex/subgroup IV ST-5 complex/subgroup IV ST-4 complex/subgroup IV	PorA VR1 5-2 5-2 20 18-1 5-2 5-2 7 5-1 7 5-1 7 5-2 7 7 7-2 7	PorA VR2 10 9 3 10 10 13-1 10 13-1 10 13-1 13 13-1 13 13-1 13	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F1-5 F3-1 F1-5 F1-5 F1-5 F1-5 F1-5 F1-5

11.13 User-configurable options

The BIGSdb user interface is configurable in a number of ways. Choices made are remembered between sessions. If the database requires you to log on, the options are associated with your user account, whereas if it is a public database, that you haven't logged in to, the options are associated with a browser cookie so they will be remembered if you connect from the same computer (using the same browser).

Most options are set by clicking the 'Set general options' link on the database contents page. Most of the available options are visible for isolate databases, whereas sequence definition databases have fewer available.

Ouery: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample.
Query database Option settings Submissions • Search or browse database • Set general options - Including isolate table field handling. • Manage submissions • Projects - main projects defined in database. • Set display and query options for locus, schemes or scheme fields. • Manage submissions • Isolates: 35423 • Last updated: 2015-08-27 • Update history • About BIGSdb • About BIGSdb • About BIGSdb
Breakdown Export Analysis Miscellaneous • Single field • Export dataset • Codon usage • Codon usage • Two field • Contigs • Presence/absence status of loci • Description of database fields • Publications • Sequences • XMFA / concatenated FASTA formats • BLAST • Description of database fields

11.13.1 General options

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

Pro15///ILST Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions				
et database options				
* ere you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set hen 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.

11.13.2 Main results table

The 'main results table' tab contains options for the display of paged results following a query.

Click the 'Main results table' header to display the tab.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
▼ General options
Display 25 → records per page. Page bar position: top and bottom → Display 100 → nucleotides per line in sequence alignments. Display 100 → nucleotides of flanking sequence (where available). Image: Sequence 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.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Нер 2
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
General options
✓ Main results table
Hyperlink allele designations where possible. Jifferentiate provisional allele designations. Display information about sequence bin records tagged with locus information (tooltip). Display sequence bin size. Display contig count. Display publications. Set options
▶ Isolate record display
Provenance field display
Query filters
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences. Reset all to defaults

This tab allows the following options to be modified:

- Hyperlink allele designations Hyperlinks point to an information page about the particular allele definition. Depending on the locus, these may exist on a different website.
- Differentiate provisional allele designations Allele designations can be set as confirmed or provisional, usually depending on the method of assignment. Selecting this option will display provisional designations in a different colour to confirmed designations.
- Information about sequence bin records Creates a tooltip that displays details about sequence tags corresponding to a locus.
- Sequence bin records Displays a tooltip linking to the sequence tag if available.
- Sequence bin size Displays the size of the sum of all contigs associated with each isolate record.
- Contig count Displays the number of contigs associated with each isolate record.
- Publications Displays citations with links to PubMed for each record.

11.13.3 Isolate record display

The 'isolate record display' tab contains options for the display of a full isolate record.

Click the 'Isolate record display' tab to display the tab.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
- General options
Display 25 • records per page. Page bar position: top and bottom • Display 100 • nucleotides per line in sequence alignments. Display 100 • nucleotides of flanking sequence (where available). Ø Display locus aliases if set. Ø Enable tooltips (beginner's mode). Set options
Main results table
► Isolate record display
Provenance field display
Query filters
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences. Reset all to defaults

The 'Isolate record display' tab will scroll up.

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

This tab allows the following options to be modified:

• Differentiate provisional allele designations - Allele designations can be set as confirmed or provisional, usually depending on the method of assignment. Selecting this option will display provisional designations in a different colour to confirmed designations.

- Display sender, curator and last updated records Displays a tooltip containing sender information next to each allele designation.
- Sequence bin information Displays a tooltip with information about the position of the sequence if tagged within the sequence bin.
- Allele flags Displays information about whether alleles have flags defined in sequence definition databases.
- 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.

11.13.4 Provenance field display

The 'provenance field display' tab contains checkboxes for fields to display in the main results table.

Click the 'Provenance field display' tab to display the tab.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/Sequences definitions Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
General options
Display 25 • records per page. Page bar position: top and bottom • Display 100 • nucleotides per line in sequence alignments. Display 100 • nucleotides of flanking sequence (where available). Ø Display locus aliases if set Ø Enable tooltips (beginner's mode). Set options
Main results table
► Isolate record display
Provenance field display
► Query filters
Reset
Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences.
Reset all to defaults

The 'Provenance field display' tab will scroll up.

	se Profile/ST List elds Scheme/alleles Publications me Options Profiles/sequences definitions I	Database submissions	
Set database options			
	e website. Options are remembered between s hing the page (Shift + Refresh) as some page		a PubMLST) only. If some of the options don't appear to set
▶ General options			
▶ Main results table			
Isolate record display			
 Provenance field display 			
	and then selecting the 'Customize' option.	table following a query. Settings for displaying loc amoxicillin sulphonamide ceftriaxone chiramphenicol chiramphenicol chiramphenicol chiramphenicol cfotaxime cefotaxime cefotaxime rifampicin iffampicin_range ciprofloxacin	us and scheme data can be made by performing a ciprofloxacin_range pending_assembly assembly_status PhA_accession private_project comments sender curator date_entered datestamp
Query filters Reset Click the reset button to remove all user s Reset all to defaults	ettings for this database - this includes locus a	nd scheme field preferences.	

Some fields will be checked by default - these are defined during *database setup* (maindisplay option).

Check any fields that you wish to be displayed and then click 'Set options'. You can return to the default selection by clicking 'Default' followed by 'Set options'.

11.13.5 Query filters

The 'query filters' tab contains checkboxes for provenance fields and scheme completion status. Checking these results in drop-down list box filters appearing in the query page *filters fieldset*.

Click the 'Query filters' tab to display the tab.

ProbMLST 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 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 tootlips (beginner's mode). Set options
Main results table
► Isolate record display
Provenance field display
► Query filters
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences.

The 'Query filters' tab will scroll up.

Isolate record display		
Provenance field display		
Query filters		
Query filters Select the fields for which you would like dropdown isolate continent region year epidemiological_year age_mth sex disease source epidemiology species serogroup MLEE_designation serotype ET_no penicillin penicillin_range coftraxone coftraxone coftraxone coftraxone coftoramphenicol_range coftoraxim coftorample coftoraxim cofto	lists containing known values on which to filter query results. These will ENA_accession private_project comments sender curator date_entered datestamp VMLST profile completion 165 profile completion 165 profile completion Aminoacyl-tRNA biosynthesis profile completion Antipen genes profile completion Capsule Region A - Serogroup B profile completion Capsule Region A - Serogroup D profile completion Capsule Region A - Serogroup Y profile completion Capsule Region D and D' profile completion Capsule Region D and D' profile completion Capsule Region D and D' profile completion Capsule Region D profile completion Capsule Region D profile completion Capsule Region D profile completion Capsule Region Cand D' profile completion Capsule Region D profile completion Capsule Region Cand D' profile completion Capsule Region D profile completion Capsule Region D profile completion Capsule Region D profile completion Capsule Region Cand D' profile completion Capsule Region D profile completion Capsule Region D profile completion Capsule Region D profile completion Capsule Region Cand D' profile completion Capsule Region D profile completion Capsule Region Cand D' profile completion Capsule Region D profile complet	II be available in the filters section of the query interface. LOS alpha chain transferases profile completion LOS transport/export profile completion Lipid A biosynthesis: acyltransferases profile completion Lipid A biosynthesis: other profile completion N. meningitidis profile completion Nucleotide excision repair profile completion Protein glycosylation profile completion Protein glycosylation profile completion Prine metabolism profile completion RNA polymerase profile completion Small regulatory RNAs profile completion COP-ClcNAc synthesis profile completion UDP-GlcNAc synthesis profile completion UDP-GlcNAc synthesis profile completion WUDP-glucose and UDP-galactose biosynthesis profile completion MLST (20 locus whole genes) profile completion eMLST (20 locus whole genes) profile completion Pulis TaSS profile completion MLST (20 locus whole genes) profile completion Pulis TaSS profile completion MLST (20 locus whole genes) profile completion Pulis TaSS profile completion MLST (20 locus whole genes) profile completion Pulis TaSS profile completion MLST (20 locus whole genes) profile completion Pulications

A list of possible filters appears. Click any checkbox for a filter you would like to make available. Click 'Set options' when done. You can return to the default selection by clicking 'Default' followed by 'Set options'.

11.13.6 Modifying locus and scheme display options

Whether or not loci, schemes or scheme fields are displayed in result tables, isolate records, or within query dropdown boxes can all be set with default options when first defined. These attributes can, however, be overridden by a user, and these selections will be remembered between sessions.

The procedure to modify these attributes is the same for locus, schemes or scheme fields, so the steps for loci will be demonstrated only.

Click the appropriate link on the isolate contents page.

Ouery: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/Sequences definitions Database submissions
Neisseria PubMLST database
The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample.
Query database • Search or browse database • Search by combinations of loci (profiles) • Projects - main projects defined in database. • Definition of the search by combination of loci (profiles) • Projects - main projects defined in database. • Set display and query options for locus, schemes or scheme fields. • Set display and query options for locus, schemes or scheme fields. • Set display and query options for locus, schemes or scheme fields. • Set display and query options for locus, schemes or scheme fields. • Isolates: 35423 • Last update discord: • Update history • About BIGSdb
Breakdown Export Analysis Miscellaneous • Single field • Export dataset • Contigs • Codon usage • Description of database fields • Two field • Unique combinations • Sequences - XMFA / concatenated FASTA formats • Codon usage • Description of database fields • Publications • Sequence bin • Sequences - XMFA / concatenated FASTA formats • BLAST • Description of database fields

Either select the locus id by querying for it directly.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
	Toggle: i
Query loci for Neisseria PubMLST database	
Please enter your search criteria below (or leave blank and submit to return all records). Matching loci will be returned and you will then be able to update their display and query settings.	
— Search criteria — Display — Display	
id • = • abcZ + I 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	
abcZ DNA integer 433 false true 1 1176340 allele only false true true true *Default values are displayed for this field. These may be overridden by user preference.	

Designations can be queried using standard operators.

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

Publ	MLST	Breakdown	: Isolate fie		e/alleles Public		initions Data	base submissions					
													Toggle: i
Quer	y loci	for Neis	sseria	PubM	LST data	bas	e						
Please	enter your	search criteria	a below (or	leave blank	and submit to re	turn all	records). Matc	hing loci will be retur	ned and you w	ill then be ab	le to update	their display and query settings.	
— Sea	arch criteria	a					— — Displa	ıy					
id				•		+ [i Ord	er by: id	•	 ascending 	9 👻		
							Dis	play: 25 🗸 recor	ds per page 👔				
—⊽ F	ilter query	by-					Action						
		data type:	•				Reset S	ubmit					
		id format:											
		gth varies: sequence:	• i										
	county :		• •										
	mate	ch longest:	• • i										
		pcr filter:	- i										
	p	orobe filter:	▼ 1										
		flag table:	▼ i										
		te display:		•									
		in display:	▼ 1										
	C	query field:	• <u>i</u>										
		analysis: curator:	▼ 1		ī								
	<u> </u>	scheme: M	LST	•		i							
		outerne. M	201										
7			- Northeastern										
/ record:	s returned.	. Click the hype	eninks for o	setalled infor	mation.								
Cus	tomize												
locus	options												
id	data type	allele id forma	at length l	ength varies	coding sequer	ice orf	genome posi	tion isolate display*	main display*	* query field'	* analysis*		
abcZ	DNA	integer	433	false	true	1	1176340	allele only	false	true	true		
adk aroE	DNA DNA	integer integer	465 490	false false	true	1	991951 2079469	allele only allele only	false false	true	true true		
fumC	DNA	integer	465	false	true	1	1592943	allele only	false	true	true		
gdh	DNA	integer	501	false	true	1	1514394	allele only	false	true	true		
pdhC pgm	DNA DNA	integer integer	480 450	false false	true	1	1453970 965481	allele only allele only	false false	true	true		
		-			ridden by user pr			anele offiy	alse	aue	ude		

7 records returned. Click the hyperlinks for detailed information. Customize locus options id data type ele id forı at length length varies coding sequence orf ge olate display* uery field* analysis* ome posit in display* abc7 DNA integer 433 false true 1176340 allele only false true true adk DNA integer 465 false true 1 991951 allele only false true true aroE DNA 490 2 2079469 allele only false true integer false true true allele only integer fumC DNA 465 false true 1 1592943 false true true gdh DNA integer 501 false true 1514394 allele only false true true pdhC 1453970 DNA 480 allele only integer false false true true true integer DNA 450 false true 965481 allele only false true true pgm field. These * Default values a played for this nay be preference

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

You can then choose to add or remove individual loci from the selection by clicking the appropriate checkboxes. At the bottom of the page are a number of attributes that you can change - clicking 'Change' will affect all selected loci.

Possible options for loci are:

- isolate_display Sets how the locus is displayed within an isolate record:
 - allele only display only identifier
 - sequence display the full sequence
 - hide don't show at all
- main_display Sets whether the locus is displayed in the main results table following a query.
- query_field Sets whether the locus appears in dropdown list boxes to be used within queries.
- analysis Sets whether the locus can be used in data analysis functions.

Note: Settings for loci can be overridden by those set for schemes that they are members of. For example, if you set a locus to be displayed within a main results table, but that locus is a member of a scheme and you set that scheme not to be displayed, then the locus will not be shown. Conversely, if you set a scheme to be displayed, but set its member locus not to be shown, then that locus will not be displayed (but other loci and scheme fields may be, depending on their independent settings).

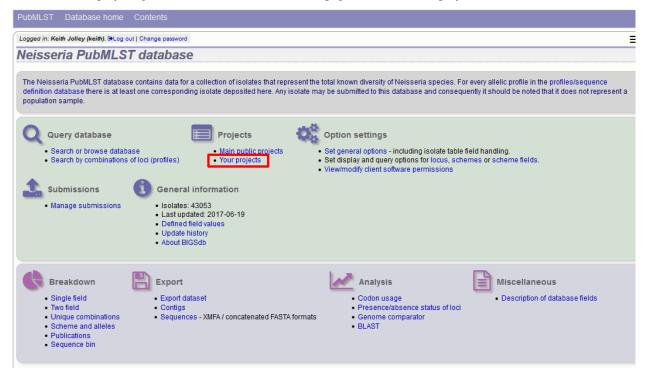
CHAPTER 12

User projects

If user projects are enabled, authenticated users are able to set up their own projects in order to group isolates for analysis. If private data and user quotas are enabled, these projects can include private records that can then be shared with other user accounts. Note, that simply adding a record to a user project does not make the record itself private.

Note: User projects can be enabled by an administrator by setting 'user_projects="yes" in the *config.xml* file for the database.

To create a new project, go to the isolate database contents page and click 'Your projects'.



Enter the name of your project (this must be unique on the system - you will be told if the name is already used). You can optionally include a description - if you do this, this will appear within *isolate records* when accessed from your account. Click 'Create'.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). (DLog out Change password
User projects
New private projects Projects allow you to group isolates so that you can analyse them easily together. Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an
isolate record page (only you and users you give access will see this).
New project
Name: UK group W ST-11 2016 Create
Description: Group W ST-11 isolates from the UK in 2016.
Existing projects
You do not own or are a member of any projects.
*

You can either add isolates to your project directly following a query or by manually editing a list of ids.

12.1 Adding isolates to a user project following a query

Perform an isolate database query. If you have set up a project, there will be a link in the results header box. Select your project and click 'Add these records'.

gged in	: Keith Jolle	ey (keith). 🔂	og out	Chang	ge password													He	elp 🖉	Toggi	le: 🚯
eard	ch or	brows	e N	eis	seria PubM	LST a	databas	9													
inter se	earch crite	ria or leave l	blank	to brov	vse all records. Modif	fy form pa	rameters to filt	er or enter a	list of values	B.											Мо
-Isol	late prover	ance/pheno	otype 1	fields -				Allele desig	nations/sch	eme field	s										for
Comb	ine with:	AND 👻						ST (MLST)	•	=		v 11	L				0				ot
cour	ntry	•	=		▼ UK		+ 0	Display/sort	ontiona							_	_	Actio			
sero	group	•	-		▼ W			Order by:													-
year		•	=		✓ 2016			Display:		aarda na		~					.enain	ng 🔻 Res	et	Submit	
								Dispidy.	23 v re	cords per	page	0									
Your JK gro	projects -	11 2016 🗸		dd the	se records	detailed i	nformation.														
- Your JK gro	projects - oup W ST	11 2016 🗸	A	dd thes	se records	detailed i	nformation.								MLS	Т			Finet	yping a	Intige
-Your JK gro	projects - pup W ST- 1 2 3	11 2016 🗸	A C	dd thes	se records	detailed i	nformation. species	serogroup	Seqbin size (bp)	Contigs	abcZ	adk a	aroE fu	IMC gd		1	ST	cional complex	Finet PorA VR1		Fet
- Your JK gro ge: [id	projects - bup W ST 1 2 3 isolate M16	11 2016 ↓ 4 5 aliases co	A I	dd thes	se records		species Neisseria	serogroup W		Contigs 257	abcZ 2	adk a	aroE fu 4	ımC gd 3 8	lh pdh	C pgm	ST 11	ST-11	PorA	PorA	Fet
- Your JK gro ge: [id	projects - oup W ST- 1 2 3 isolate	11 2016 ↓ 4 5 aliases co	A I	dd thes 7) > year	se records	source	species		size (bp)		abcz			-	lh pdh	C pgm			PorA VR1	PorA VR2	Fe
- Your JK gro ge: (id 2451	projects - oup W ST 1 2 3 isolate M16 240077 M16	11 2016 ↓ 4 5 aliases co	Ar C Untry JK	dd thes 7) > year	se records	source	species Neisseria meningitidis Neisseria		size (bp)		abcz			-	lh pdh 4	C pgm 6		ST-11 complex/ET-37 complex ST-11	PorA VR1	PorA VR2	Fet VI F1
- Your JK gro ge: (id 2451	projects – oup W ST- 1 2 3 isolate M16 240077	11 2016 ↓ 4 5 aliases co	Ar C Untry JK	dd the: 7 > year 2016	se records Last Isolate fields disease	source	species Neisseria meningitidis	w	size (bp) 2111799	257	2 2	3	4	3 8	lh pdh 4	C pgm 6	11	ST-11 complex/ET-37 complex	PorA VR1 5	PorA VR2 2	Fet VI F1
- Your JK gro ge: 1 id 2451 2475	projects - oup W ST- 1 2 3 isolate M16 240077 M16 240003 M16	11 2016 -	. A	dd the: 7 > year 2016	se records Last Isolate fields ① disease invasive (unspecified/other) invasive	source	species Neisseria meningitidis Neisseria meningitidis Neisseria	w	size (bp) 2111799	257	2 2	3	4	3 8	lh pdh 4	C pgm 6 6	11	ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-11	PorA VR1 5	PorA VR2 2	Fet VI F1-
Your UK gro age: 1 id 2451	projects - bup W ST- isolate M16 240077 M16 240003	11 2016 -	. A	dd the: 7 > year 2016 2016	se records Last Isolate fields disease invasive (unspecified/other)	source	species Neisseria meningitidis Neisseria meningitidis	w	size (bp) 2111799 2098168	257 222	2 2	3	4	3 8	lh pdh 4	C pgm 6 6	11	ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex	PorA VR1 5	PorA VR2 2 2	Fet VI F1-
- Your UK gro age: F	projects - oup W ST- 1 2 3 isolate M16 240077 M16 240003 M16	aliases co	Antry JK	dd the: 7 > year 2016 2016	se records Last Isolate fields ① disease invasive (unspecified/other) invasive	source	species Neisseria meningitidis Neisseria meningitidis Neisseria	w	size (bp) 2111799 2098168	257 222	2 2	3	4	3 8	h pdh 4 4 4 4	C pgm 6 6 6	11	ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37	PorA VR1 5	PorA VR2 2 2	

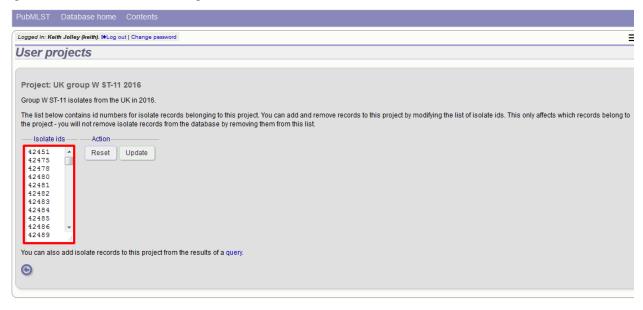
The records will be added to the project. Please note that it doesn't matter whether any of the records have been previously added.

12.2 Adding or removing isolates belonging to a user project by editing a list

From the user projects page, click the 'Add/remove records' link for the project that you wish to modify.

PUDMLST Database nome Contents
Logged in: Keith Jolley (keith). @Log out Change password
User projects
New private projects
Projects allow you to group isolates so that you can analyse them easily together.
Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an isolate record page (only you and users you give access will see this).
Name: Create
Description:
Your projects
Delete Add/remove records Modify users Project Description Administrator Isolates Browse
🗶 🥒 👑 UK group W ST-11 2016 Group W ST-11 isolates from the UK in 2016. 🕝 163 👔
You can also add isolates to projects from the results of a query.
Note that deleting a project will not delete its member isolates.
*

Edit the list of ids of records belonging to the list. You can copy and paste this list if you wish to prepare it in a spreadsheet or text editor. Click 'Update' when finished.



12.3 Accessing project isolates

To browse isolate records belonging to a project, go to the user projects page and click the 'Browse' link for the project.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). @Log out Change password
User projects
New private projects Projects allow you to group isolates so that you can analyse them easily together. Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an isolate record page (only you and users you give access will see this). New project Action Name: Create Description:
Your projects Delete Add/remove records Modify users Project Description Administrator Isolates Browse Image: Comparison of the second

Alternatively, you can select the project from the *projects filter* on the isolate query page. This would enable you to combine the project with additional search criteria

PubMLS	si Data	base h	ome	Conte	nts																
Logged in	: Keith Jolley	/ (keith).	€+Log out	Chang	e password														Help 🖉	Toggle	: 0 =
Searc	ch or b	orow	se N	eiss	seria PubN	ILST d	latabase														
Enter se	earch criteri	a or lea	ve blank	to brov	vse all records. Moo	lify form par	ameters to filte	r or enter a lis	st of values.												Modify
Isol	late provena	ance/ph	enotype	fields -			F	Filters													form
id		•	- =		- Enter value		+ 0	P	ublication:									¢	D		options
									Project:	1 selecte	ed				¢	0					
									T profiles:	✓ Chec				all	C	3					
								Clonal compl	· · ·	Irish N				nome	Libra ⁴						
								exsero OMV p		MRF											
							R	bosomal MLS		NI_E>											
								Sequ Include old	uence bin:	penA						1					
							Ľ			C rpoB											
	play/sort op							- Action		UK gr				Ibrary							
	Order by: id					•	ascending	Rese	t Subr	UK &	<u> </u>			11-20	3/14	-					
	Display: 2	5 v r	ecords (oer pag	e 🕕					•					۴						
163 reco	ords returne	d (1 - 25	5 display	ed). Cli	ck the hyperlinks fo	r detailed in	formation.														
-Your	r projects —																				
Select	t project		- A	dd thes	e records																
				-																	
Page:	1 2 3	46			Last																
					Isolate fields ()										MLS	т			Finet	/ping an	tigens
14	in alata da	lianan					anasian		Seqbin	Contigs	aba7								PorA		FetA
id		mases	country		disease	source	species	serogroup					roE fum		1			clonal complex	VR1	VR2	VR
42451	M16		UK	2016		sputum	Neisseria	W	2111799	257	2	3	4 3	8	4	6	11	ST-11	5	2	F1-1

Please note that you will only see your project in the filter list if you are logged in. As a private project, only you will see it.

12.4 Allowing other users to share your project

You can share a project that you own with any other user. In order to do this, you must know the username that they use to log in with. They will see the project in their own list of private projects and in the query interface projects filter.

From the user projects page, click the 'Modify users' link for the specified project:

PubMLST Database home Contents
Logged in: Keith Jolley (keith). [HLog out Change password
User projects
New private projects Projects allow you to group isolates so that you can analyse them easily together. Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an isolate record page (only you and users you give access will see this).
New project Action Name: Create Description:
Your projects
Delete Add/remove records Modify users Project Description Administrator Isolates Browse W group W ST-11 2016 Group W ST-11 isolates from the UK in 2016. Isolates to projects from the results of a query. You can also add isolates to projects from the results of a query. Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates Isolates
Note that deleting a project will not delete its member isolates.
*

Enter the username of the person you wish to share with and click 'Add user':

PubMLST Database home Contents
Logged in: Keith Jolley (keith). @Log out Change password
User projects
Project: UK group W ST-11 2016
Users
The following users have permission to access the project (either explicitly or through membership of a user group).
Users Action User Admin Add/Remove records Jolley, Keith (keith) Image: Control of the set of the
Enter username hbratcher You need to know the username or any user you wish to add.
•

If user groups are in use, you can also share your project with all members of a user group from the same page.

Once a user has been added, you can give them permission to administer (add other users, modify the description or delete) or add/remove records to the project:

PubMLST Database home Contents
Logged in: Keith Jolley (keith). (Honge password
User projects
Project: UK group W ST-11 2016 Users The following users have permission to access the project (either explicitly or through membership of a user group).
Users Admin Add/Remove records Remove User Bratcher, Holly (hbratcher) Users Jolley, Keith (keith) Image: Comparison of the second secon
Add user Action Enter username: hbratcher Add user You need to know the username of any user you wish to add. Add user
Θ

12.5 Deleting a user project

You can delete a project from the user projects page by clicking the 'Delete' link next to the project in question.

PubmLS1 Database nome Contents
Logged in: Keith Jolley (keith). @Log out Change password
User projects
New private projects
Projects allow you to group isolates so that you can analyse them easily together.
Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an isolate record page (only you and users you give access will see this).
New project Action Orreate Create
Your projects
Delete Add/remove records Modify users Project Description Administrator Isolates Browse X V W group W ST-11 2016 Group W ST-11 isolates from the UK in 2016. Iso Iso Iso You can also add isolates to projects from the results of a query. Iso Iso Iso Iso
Note that deleting a project will not delete its member isolates.
*

If the project contains any isolates you will be asked for confirmation. Click the 'Delete project' button.

PubMLST Database home Contents
Logged in: Keith Jolley (keith). @Log out Change password
User projects
This project contains 163 isolates. Please confirm that you wish to remove the project (the isolates in the project will not be deleted).
X Delete project
New private projects
Projects allow you to group isolates so that you can analyse them easily together.
Please enter the details for a new project. The project name needs to be unique on the system. A description is optional but only projects with descriptions will be displayed on an isolate record page (only you and users you give access will see this).
New project
Name: Create
Your projects
Delete Add/remove records Modify users Project Description Administrator Isolates Browse * * UK group W ST-11 2016 Group W ST-11 isolates from the UK in 2016. • 163 •
You can also add isolates to projects from the results of a query.
Note that deleting a project will not delete its member isolates.
*

If the project contains no isolates, the confirmation page is skipped and the project is removed immediately.

Note: Removing a project does not delete the isolate records belonging to it. A project is simply a means of grouping records.

CHAPTER 13

Private records

Users with a status of 'submitter', 'curator', or 'admin' can upload private isolate records that will be hidden from public view. A quota needs to be set for the user by an admin before they are able to do this.

13.1 Uploading private records

In order to upload private records, you need to make sure that you are logged in. If your account has a quota, there will be a menu item called 'Private data'. Click the 'Upload/manage records' link.



You will see an overview of your quota and links to upload and edit your records. Click the 'Upload private isolate records' link (assuming you have quota available).

PubMLST	Database	e home	Contents
Logged in: Keitt	h Jolley (keit	th). ເ∔Log o	ut Change password
Private I	record	ls	
Accounts have		or the nur	mber of private records that they can upload. Uploading of private data to some registered projects may not count against your quota.
	s (total): (
Records	(quota): (0	
	Quota:	100	
You can	upload: 1	100	
Cur	oad private ate		Cords

You will then be taken to a curator page that allows you to upload data copy and pasted from a spreadsheet. There is a link to an Excel template that you will need to use to prepare your data - this is the same template used if you were to submit your data to a curator.

PubMLST Database home Contents	
Logged in: Keith Jolley (keith). DeLog out Change password	Toggle: 🜖 📃
Batch insert isolates	
Private data upload These isolates will count against your quota of private data. Quota available: 100	ľ
 This page allows you to upload isolate data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. Enter aliases (alternative names) for your isolates as a semi-colon (;) separated list. Enter references for your isolates as a semi-colon (;) separated list of PubMed ids (non-integer ids will be ignored). You can also upload allele fields along with the other isolate data - simply create a new column with the locus name (see for locus names). These will be added with a confirmed status and method set as 'manual'. You can choose whether or not to include an id number field - if it is omitted, the next available id will be used automatical Download tab-delimited header for your spreadsheet - use 'Paste Special C Text' to paste the data. Download submission template (xlsx format) 	
Paste in tab-delimited text (include a field header line).	Action

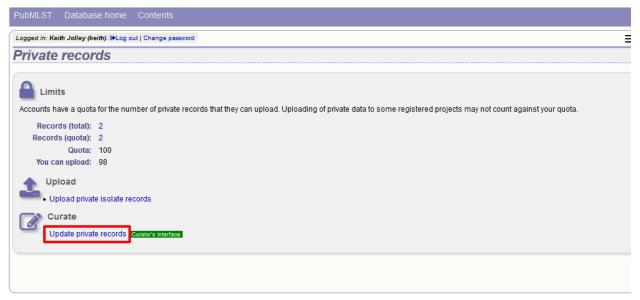
See batch adding isolate records for details of the upload process.

13.2 Modifying private records

Click the 'Upload/manage records' link on the contents page.

PubMLST Database home Co			
Logged in: Keith Jolley (keith). Dog out C	Change password		Ξ
Neisseria PubMLST o	database		
		known diversity of Neisseria species. For every allelic profile in th abase and consequently it should be noted that it does not repre	
Query database Search or browse database Search by combinations of to General information Isolates: 43172 Last updated: 2017-06-23 Defined field values Update history About BIGSdb	e • Main public projects • Set g loci (profiles) • Your projects • Set d	ion settings general options - including isolate table field handling. display and query options for locus, schemes or scheme fields. //modify client software permissions	Submissions Manage submissions Private data Upload/manage records
Breakdown - Single field - Two field - Two field - Unique combinations - Scheme and alleles - Publications - Sequence bin	Export Lataset • Contigs • Sequences - XMFA / concatenated FASTA formats	Analysis Codon usage Presence/absence status of loci Genome comparator BLAST Miscellanee Description of Description of	ous If database fields

Now click the 'Update private records' link. You will be taken to the *curators' interface*, where you will be able to use the standard curator tools.



Use the curators' interface to make any changes to your isolate records, including uploading genome data.

13.3 Sharing access to private records

If *user projects* are enabled on the database, you can share access to your private isolates by adding them in to a user project and then sharing this.

See user projects for more details.

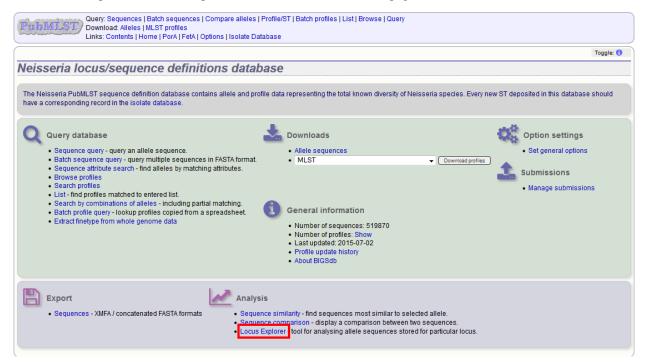
CHAPTER 14

Data analysis plugins

14.1 Locus explorer

The locus explorer is a sequence definition database plugin. It can create schematics showing the polymorphic sites within a locus, calculate the GC content and generate aligned translated sequences.

Click 'Locus Explorer' from the sequence definition database contents page.



14.1.1 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								
		Help 🖓						
Locus Explorer -	 Neisseria locus/sequence definitions 							
Please select locus for analy Locus adk Select sequences 1 2 3 4 5 6 4 None	Page will reload when changed Select analysis Polymorphic Sites - Display polymorphic site frequencies and sequence schematic Codon - Calculate G+C content and codon usage Translate - Translate DNA to peptide sequences	Action — Submit						

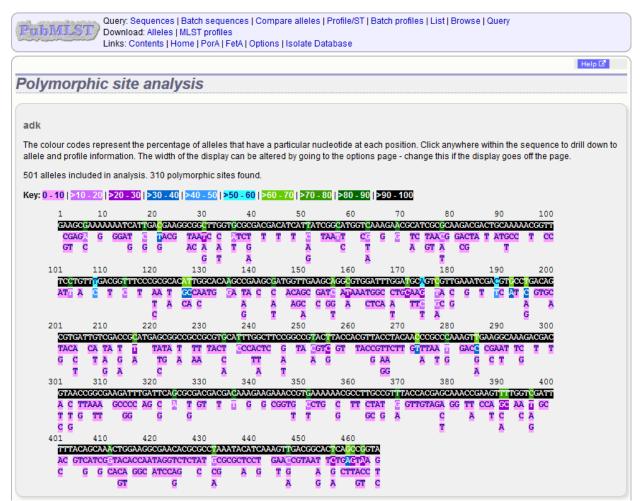
Select the alleles that you would like to include in the analysis. Variable length loci are limited to 2000 sequences or fewer since these need to be aligned. Select 'Polymorphic Sites' in the Analysis selection and click 'Submit'.

PubLST Downlo	Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query oad: Alleles MLST profiles Contents Home PorA FetA Options Isolate Database	
		Help 🗹
Locus Explorer	- Neisseria locus/sequence definitions	
Please select locus for anal		
Locus: adk	 Page will reload when changed 	
Select sequences 496 497 498 499 500 501 ▼ All None	 Select analysis Action Polymorphic Sites Display polymorphic site frequencies and sequence schematic Codon - Calculate G+C content and codon usage Translate - Translate DNA to peptide sequences 	

If an alignment is necessary, the job will be submitted to the job queue and the analysis performed. If no alignment is

necessary, then the analysis is shown immediately.

The first part of the page shows the schematic.



Clicking any of the sequence bases will calculate the exact frequencies of the different nucleotides at that position.

>40 - 50	<mark>>50 - 60</mark> <mark>></mark> 6	0 - 70 >70 - 8	0 >80 - 90 >9
30	40	50	60
GCGG <mark>C</mark> TTG	GT <mark>G</mark> CGCGACG	ACATCATTATC	GG <mark>C</mark> ATGGT <mark>C</mark> AAA(
TAA <mark>T</mark> C C	ATCT T	т т 🖸 т	AATT CG G
AC A A	TG	A	СТ
G T	A	G	A

te l	Explorer				Help 🛙
.~ 1				 	
lk po	osition 51				
	eles included in anal	veie			
ase I T	Number of alleles P 401	ercentage of alle 80.04	eles MLST profiles 11130 / 11407		
			(97.57%)		
С	98	19.56	275 / 11407 (2.41%)		
A	1 (adk-351)	0.20	1 / 11407 (0.01%)		
G	1 (adk-413)	0.20	1 / 11407 (0.01%)		

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

C	G				~					45.0			~		Т		A	G	
401	12/12/	410	amee	42	-	4 ACACGC	30	44		450		46							
						GTCTCT													
C				GGC			C CG			r G		GCT							
×			GT			G	A	•		A	G		GT						
cleotid	e fre	ane	ncie	25															
sition 🗢						lucleot													
	A ¢			T ≑		%A ≑			%T ≑	%- 🜩									
2	499	1	1	0	0		0.20												
3	498	0	2	1	0	99.40			0.20										
4	1	0	500	0	0	0.20		99.80											
5	0	500	1	0	0		99.80												
6	53	8	440	0	0	10.58	1.60	87.82											
9	499	0	2	0	0	99.60		0.40											
12	500	0	1	0	0	99.80		0.20											
13	500	0	1	0	0	99.80		0.20											
14	1	0	0	500	0	0.20			99.80										
15	0	488	1	12	0		97.41	0.20	2.40										
18	0	86	8	407	0		17.17	1.60	81.24										
21	0	315	1	185	0		62.87	0.20	36.93										
22	9	0	492	0	0	1.80		98.20											
23	500	1	0	0	0	99.80	0.20												
24	500	0	1	0	0	99.80		0.20											
27	3	488	0	10	0	0.60	97.41		2.00										
28	2	2	497	0	0	0.40	0.40	99.20											
29	2	0	499	0	0	0.40		99.60											
30	3	367	2	129	0	0.60	73.25	0.40	25.75										
31	0	11	0	490	0		2.20		97.80										
33	2	5	492	2	0	0.40	1.00	98.20	0.40										
33		0	445	3	0	10.58		88.82											
36	53	0	440	-	· ·														

See also:

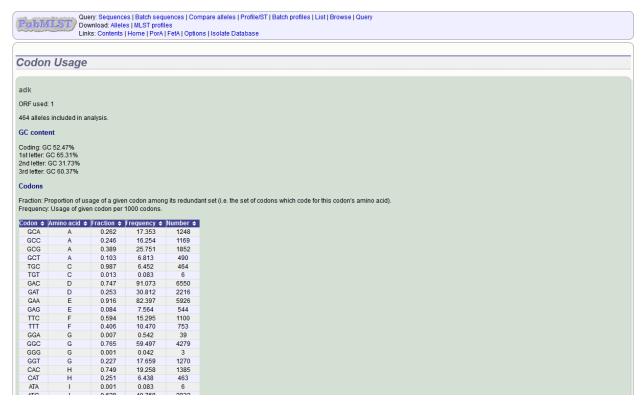
- Investigating allele differences.
- Polymorphism analysis following isolate query.

14.1.2 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'.

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 Formation in the sequence is and sequence schematic 461 Codon 463 Codon 464 Translate All None

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



14.1.3 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'.

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 450 Polymorphic sites Display polymorphic site frequencies and sequence schematic 451 Codon Calculate G+C content and codon usage 453 Translate Translate Ait None

An aligned amino acid sequence will be displayed.

433 I	5
434_1	
435_1	
436_1	
437_1	
438_1	
439_1	
440_1	К.
441_1	·
442 1	
443 1	
444 1	
445 1	
446 1	
447 1	
448_1	
449_1	
450_1	
451_1	
452_1	K
453_1	
454_1	
455_1	·
456_1	
457 1	
458 1	
459 1	
460 1	
461 1	
462 1	
463 1	
464_1	I LEAKIIDEGGUVRDDIIIGMVKERIADDDCKNGFLFDGFPRILAQAEAMVEAGVDLDAVVEIDVFDSVTUDMSGERVHLASGRIYHVTYNPPKVEGKDD
Consensus	FAKKIDEGED/KDDIIIGW/KEKIAQDD/KNGFDFDGFFKIDAQAEAN/EAG/DDDA/VEID/PDS/I/UKREGKK/DLAEGKIIN/INFFK/EGKDD
	110 120 130 140 150
	:::::::
1_1	
2_1	
3_1	
2_1 3_1 4_1	
5_1	······
6_1	·
7_1	
8 1	
-	

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

14.2 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.

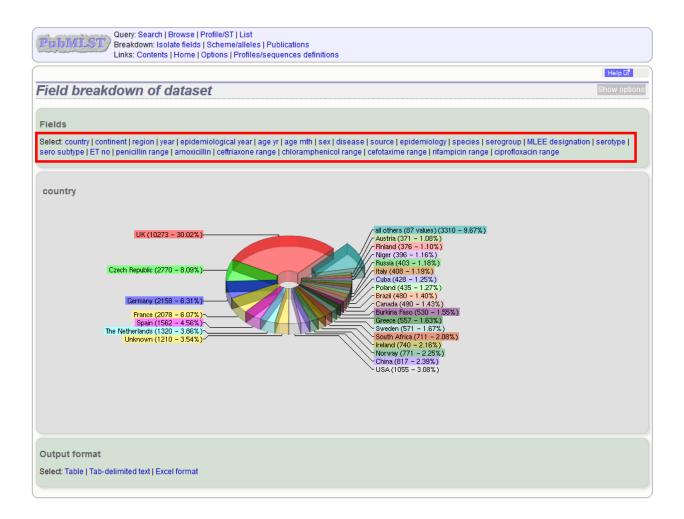
The breakdown function can be selected for the whole database by clicking the 'Single field' link in the Breakdown section of the main contents page.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neis	corio concise. For even allalia profile in the profiles/company definition
database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and i	
Query database • Search database - advanced queries. • Browse database - peruse all records. • Search by combinations of loci (profiles) - including partial matching. • List query - find isolates by matching a field to an entered list. • Projects - main projects defined in database.	g isolate table field handling. for locus, schemes or scheme fields.
Breakdown Export Analysis Single field • Export dataset • Contigs • Unique combinations • Sequences - XMFA / concatenated FASTA formats • Codon usage • Contigs • Sequence bin • BLAST	

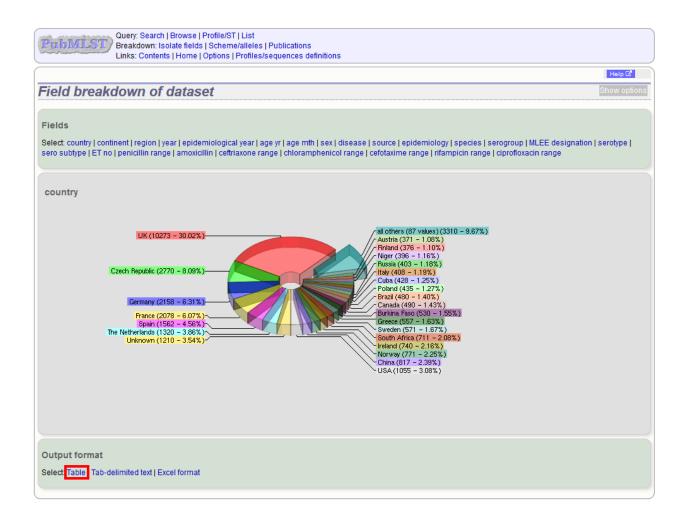
Alternatively, a breakdown can be displayed of the dataset returned from a query by clicking the 'Fields' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

6 M	100240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	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	s 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	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	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	в	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	s 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	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	B	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	s A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	B	930	ST-334 complex			

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

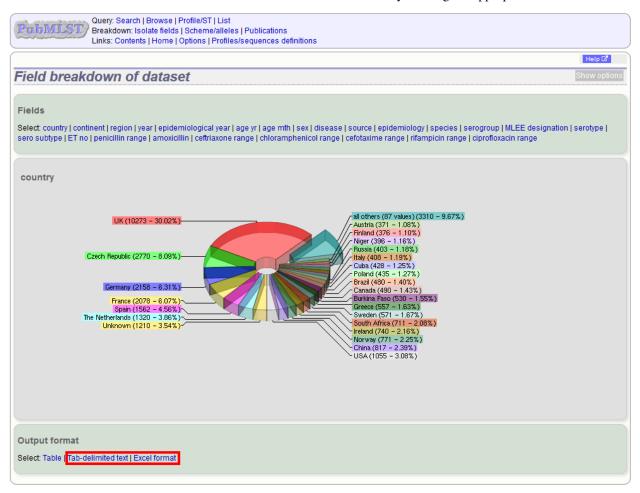


The values used to generate the chart can be displayed or extracted by clicking the 'Table' link at the bottom of the page.



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

akdown by	country		Show o
алиотту	country		
values.			
country 💠	Frequency 🔶	rcentage 🗢	
UK	7300	25.02%	
Czech Republic	2684	9.20%	
Germany	2123	7.28%	
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.

14.3 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.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definition	ons
	resent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition ay be submitted to this database and consequently it should be noted that it does not represent a population sample.
Query database • Search database - advanced queries. • Browse database - peruse all records. • Search by combinations of loci (profiles) - including partial matching. • List query - find isolates by matching a field to an entered list. • Projects - main projects defined in database.	 Option settings Set general options - including isolate table field handling. Set display and query options for locus, schemes or scheme fields. General information Isolates: 34221 Last updated: 2015-07-02 Update history About BIGSdb
Breakdown Single field Two field Onique combinations Scheme and alleles Publications Sequence bin	Analysis Codon usage Presence/absence status of loci Genome comparator BLAST Miscellaneous • Description of database fields

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

6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	S1-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	В	930	ST-334 complex			
Bre		elds Two Fi	noe/Absence		comparator BLAST	Schemes/alleles Pu	blications	Seque	nce bin Tag status			

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/SI Breakdown: Isolate fields Schem Links: Contents Home Options	e/alleles Publications	Database submissions		
Two field breakdown of datase	et			Show options
Here you can create a table breaking down one field by Select fields Field 1: clonal complex (MLST) Field 2: serogroup	another, e.g. breakdown of serce Display @ values only @ values and percentages @ percentages only	ogroup by year. — Calculate percentages by- @ dataset C row C column	Action Reset Submit	

Click submit. The breakdown will be displayed as a table. Bar charts will also be displayed provided the number of returned values for both fields are fewer than 30.

Two field breakdo				ption				ations ces defi	nitions
Two field breakdo									
	w	n o	f da	tas	set				
Breakdown of clonal_co	mpl	ex (I	/LST) by	sero	group	o :		
Selected options: Display value	es on	ıly.							
— Axes — Show —									
	dnar								
Reverse Values an	a per	centa	ges						
						ogroup			
						W \$			Total 🗢
No value	1	3	1	1	4		1	1	12
ST-1 complex/subgroup I/II ST-11 complex/ET-37 complex			16						13 16
ST-162 complex		5	10						5
ST-167 complex					1			2	3
ST-174 complex				1	1	1			3
ST-178 complex					1				1
ST-18 complex		3			0				3
ST-198 complex ST-22 complex					2	2			2
ST-226 complex		1				2			1
ST-23 complex/Cluster A3								1	1
ST-254 complex					1				1
ST-269 complex		2			1				3
ST-32 complex/ET-5 complex		6							6
ST-334 complex ST-35 complex		1			1				1
ST-4 complex/subgroup IV	8								8
ST-41/44 complex/Lineage 3		5			1				6
ST-461 complex		1							1
ST-5 complex/subgroup III	6								6
ST-53 complex					2				2
ST-60 complex		07		1	15	•			1
Total	28	27	17	3	15	3	1	3 1	98

The table values can be exported in a format suitable for copying in to a spreadsheet by clicking 'Download as tabdelimited text' underneath the table.

Note: The job will be submitted to the offline job queue if the query returns 10,000 or more isolates. In this case, the buttons to reverse the axes or to change whether values or percentages are shown will not be available.

14.4 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.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences defin	nitions
	represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition may be submitted to this database and consequently it should be noted that it does not represent a population sample.
Query database • Search database - advanced queries. • Browse database - peruse all records. • Search by combinations of loci (profiles) - including partial matching. • List query - find isolates by matching a field to an entered list. • Projects - main projects defined in database.	 Option settings Set general options - including isolate table field handling. Set display and query options for locus, schemes or scheme fields. General information Isolates: 34221 Last updated: 2015-07-02 Update history About BIGSdb
Breakdown Single field Two field Unique combinations Scheme and alleles Publications Sequence bin	Analysis Codon usage Presence/absence status of loci Genome comparator BLAST BLAST

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.

1	A4/M1027	B1; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitio	dis A	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitio	dis A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
3	M00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitio	dis B	1099		19	15	
4	M1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitio	dis A	4	ST-4 complex/subgroup IV			
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitio	dis B	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitio	dis W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitio	dis A	5	ST-5 complex/subgroup III	20	9	F3-1
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	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitio	dis A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitio	dis NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitio	dis NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitio	dis E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitio	dis B	32	ST-32 complex/ET-5 complex			
24	S4355	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			
Bre		elds Two Fi JRST Prese	eld Codons		norphic sites Combinations		Publications	Seque	nce bin Tag status			

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

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	
	Help 🖉
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.	
Select schemes	
Pilin Select MLST Select Image: Select Image: Select Image: Select Image: Select Image: Select Image: Select	

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

PubMLST	📝 Breakdov	vn: Isolate		neme/allele		ions es definitions	
							Help 🖓
Scheme fi	eld and	allele	e brea	kdow	n of da	ataset	Show options
Select schemes	or groups of s	schemes v	vithin the tr	ee. A break	down of the	e individual fields and loci belonging	to these schemes will then be performed.
	nes				A	ction —	
⊳- □ 0 G	enetic Inform enomic islan neage Schen etabolism	ds	essing		•		
	Fields			٨١	eles		
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ST	547	¢	abcZ	64	¢	(±)	
clonal complex	43	¢	adk	56	¢	1	
			aroE	80			
			fumC	83		<u>×</u>	
			gdh	77	¢		
			pdhC	82		<u>*</u>	
			pgm	68		<u></u>	

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

					Help 🖉
cheme fie	eld and a	llele brea	kdown o	f dataset	Show optio
elect schemes o	or groups of sch	emes within the tr	ee Abreakdown	n of the individual fields and loci belonging to these schem	nes will then he nerformed
—Select schem					
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ILST Field name	Fields Jnique values A 547	abcZ adk	Alleles hique alleles An 64 56 80	¢ <u>*</u>	
ILST Field name	Fields Jnique values A 547	abcZ adk aroE	Alleles nique alleles An 64 56 80 83		
ILST Field name	Fields Jnique values A 547	abcZ adk aroE fumC	Alleles nique alleles An 64 56 80 83 77	E ± E ± E ± E ±	

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

Cheme field and allele breakdown of dataset Frequency table Total: 985 isolates Conal_complex + Frequency + Percentage + ST-11 complex/ET-37 complex 186 18.88 ST-41/44 complex/Lineage 3 99 10.05 ST-1 complex/subgroup I/I 63 6.40 ST-8 complex/Cluster A4 60 6.09 ST-32 complex/Cluster A4 60 6.09 ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/subgroup I/I 31 3.15 ST-269 complex 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 24 2.44 ST-18 complex 18 1.83 ST-18 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22 ST-162 complex 9 0.91	Show option
Total: 985 isolates Clonal_complex ◆ Frequency ◆ Percentage ◆ ST-11 complex/ET-37 complex 186 18.88 ST-11 complex/Lineage 3 99 10.05 ST-1 complex/subgroup I/II 63 6.40 ST-8 complex/Cluster A4 60 6.09 ST-22 complex 53 5.38 ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/subgroup IV 37 3.76 ST-269 complex 31 3.15 ST-52 complex/Cluster A3 25 2.54 ST-60 complex 24 2.44 ST-167 complex 18 1.83 ST-18 complex 14 1.42 ST-213 complex 12 1.22	
Total: 985 isolates Clonal_complex ◆ Frequency ◆ Percentage ◆ ST-11 complex/ET-37 complex 186 18.88 ST-41/44 complex/Lineage 3 99 10.05 ST-1 complex/subgroup I/II 63 6.40 ST-8 complex/Cluster A4 60 6.09 ST-22 complex 53 5.38 ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/subgroup IV 37 3.76 ST-269 complex 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 24 2.44 ST-167 complex 18 1.83 ST-18 complex 14 1.42 ST-213 complex 12 1.22	
Total: 985 isolates Clonal_complex Frequency ◆ Percentage ◆ ST-11 complex/ET-37 complex 186 18.88 ST-11 complex/Lineage 3 99 10.05 ST-1 complex/subgroup I/II 63 6.40 ST-8 complex/Cluster A4 60 6.09 ST-22 complex 53 5.38 ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/subgroup IV 37 3.76 ST-269 complex 31 3.15 ST-52 complex/Cluster A3 25 2.54 ST-56 complex 18 1.83 ST-167 complex 18 1.83 ST-18 complex 14 1.42 ST-213 complex 12 1.22	
clonal_complex ◆ Frequency ◆ Percentage ◆ ST-11 complex/ET-37 complex 186 18.88 ST-41/44 complex/Lineage 3 99 10.05 ST-1 complex/subgroup I/II 63 6.40 ST-8 complex/Cluster A4 60 6.09 ST-22 complex 53 5.38 ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/subgroup IV 37 3.76 ST-269 complex 31 3.15 ST-50 complex/Cluster A3 25 2.54 ST-60 complex 18 1.83 ST-18 complex 14 1.42 ST-18 complex 13 1.32 ST-213 complex 12 1.22	
ST-11 complex/ET-37 complex 186 18.88 ST-41/44 complex/Lineage 3 99 10.05 ST-1 complex/subgroup I/II 63 6.40 ST-8 complex/Cluster A4 60 6.09 ST-32 complex 53 5.38 ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/subgroup I/V 37 3.76 ST-269 complex 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 18 1.83 ST-167 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22	
ST-41/44 complex/Lineage 3 99 10.05 ST-1 complex/subgroup I/II 63 6.40 ST-8 complex/Cluster A4 60 6.09 ST-22 complex 53 5.38 ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/subgroup I/V 37 3.76 ST-269 complex 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 18 1.83 ST-167 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22	
ST-1 complex/subgroup I/II 63 6.40 ST-8 complex/Cluster A4 60 6.09 ST-22 complex 53 5.38 ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/subgroup IV 37 3.76 ST-269 complex 31 3.15 ST-5 complex/subgroup III 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 18 1.83 ST-167 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22	
ST-8 complex/Cluster A4 60 6.09 ST-22 complex 53 5.38 ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/subgroup IV 37 3.76 ST-269 complex 31 3.15 ST-5 complex/subgroup III 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 18 1.83 ST-167 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22	
ST-22 complex 53 5.38 ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/Subgroup IV 37 3.76 ST-269 complex 31 3.15 ST-5 complex/Subgroup III 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 18 1.83 ST-167 complex 14 1.42 ST-213 complex 13 1.32 ST-213 complex 12 1.22	
ST-32 complex/ET-5 complex 51 5.18 ST-4 complex/subgroup IV 37 3.76 ST-269 complex 31 3.15 ST-5 complex/subgroup III 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 24 2.44 ST-167 complex 18 1.83 ST-18 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22	
ST-4 complex/subgroup IV 37 3.76 ST-269 complex 31 3.15 ST-5 complex/subgroup III 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 24 2.44 ST-167 complex 18 1.83 ST-18 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22	
ST-269 complex 31 3.15 ST-5 complex/subgroup III 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 24 2.44 ST-167 complex 18 1.83 ST-18 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22	
ST-5 complex/subgroup III 31 3.15 ST-23 complex/Cluster A3 25 2.54 ST-60 complex 24 2.44 ST-167 complex 18 1.83 ST-18 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22	
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ST-60 complex 24 2.44 ST-167 complex 18 1.83 ST-18 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22	
ST-167 complex 18 1.83 ST-18 complex 14 1.42 ST-213 complex 13 1.32 ST-35 complex 12 1.22	
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ST-213 complex 13 1.32 ST-35 complex 12 1.22	
ST-35 complex 12 1.22	
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01-102 complex 3 0.91	
ST-174 complex 9 0.91	
ST-53 complex 8 0.81	
ST-92 complex 8 0.81	
ST-106 complex 7 0.71	
ST-254 complex 7 0.71	
ST-103 complex 6 0.61	
ST-334 complex 6 0.61	
ST-198 complex 5 0.51	
ST-865 complex 5 0.51	
ST-178 complex 4 0.41	
ST-364 complex 4 0.41	
ST-37 complex 4 0.41	
ST-1157 complex 3 0.30	

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

OT-DD COMPLEX	0	0.01
ST-92 complex	8	0.81
ST-106 complex	7	0.71
ST-254 complex	7	0.71
ST-103 complex	6	0.61
ST-334 complex	6	0.61
ST-198 complex	5	0.51
ST-865 complex	5	0.51
ST-178 complex	4	0.41
ST-364 complex	4	0.41
ST-37 complex	4	0.41
ST-1157 complex	3	0.30
ST-116 complex	3	0.30
ST-1494 complex (lactamica)	3	0.30
ST-4240/6688 complex	3	0.30
ST-624 complex (lactamica)	3	0.30
ST-1136 complex	2	0.20
ST-1540 complex (lactamica)	2	0.20
ST-212 complex	2	0.20
ST-461 complex	2	0.20
ST-613 complex (lactamica)	2	0.20
	2	0.20
ST-750 complex		
ST-226 complex	1	0.10
ST-282 complex	1	0.10
ST-595 complex (lactamica)	1	0.10
ST-640 complex (lactamica)	1	0.10
Download: Tab-delimited tex		
Charts		
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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.

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	nd allele br	eakdown	of dataset	Show	options
Select schemes or groups performed.	of schemes within t	ne tree. A breakd	lown of the individual fi	elds and loci belonging to these schemes will the	n be
Select schemes					
🛓 📄 🎧 All loci			Select		
- 🔲 🌆 Capsule					
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- Lineage So					
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ST 547	🚯 abcZ				
clonal complex 43	🚯 adk	56			
	aroE	80			
	fumC	83			
	gdh				
	pdhC				
	pgm	68			

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

>2	
TTTGATACCGTTGCCGAAGGTTTGGGTGAAATTCGCGATTTATTGCGCCGTTACCACCGC	
GTCGGCCATGAGTTGGAAAACGGTTCGGGTGAGGCTTTGTTGAAAGAACTCAACGAATTA	
CAACTTGAAATCGAAGCGAAGGACGGCTGGAAGCTGGATGCGGCAGTCAAGCAGACTTTG	
GGGGAACTCGGTTTGCCGGAAAACGAAAAATCGGCAACCTTTCCGGCGGTCAGAAAAAG	
CGTGTCGCCTTGGCGCAGGCTTGGGTGCAGAAGCCCGACGTATTGCTGCTGGACGAACCG	
ACCAACCATTTGGATATCGACGCGATTATTTGGCTGGAAAATCTGCTCAAAGCGTTTGAA	
GGCAGCTTGGTTGTGATTACCCACGACCGCCGTTTTTTGGACAATATCGCCACGCGGATT	
GTCGAACTCGATC	
>1	
TTTGATACTGTTGCCGAAGGTTTGGGCGAAATTCGCGATTTATTGCGCCGTTATCATCAT	
GTCAGCCATGAGTTGGAAAATGGTTCGAGTGAGGCCTTATTGAAAGAGCTCAACGAATTG	
CAACTTGAGATCGAAGCGAAGGACGGCTGGAAGTTGGATGCGGCGGTGAAGCAGACTTTG	
GGCGAACTCGGTTTGCCGGAAAACGAAAAATCGGCAACCTCTCCGGCGGTCAGAAAAAG	
CGCGTCGCCTTGGCGCAGGCTTGGGTGCAGAAGCCCGACGTATTGCTGCTCGATGAACCG	
ACCAACCATTTGGACATCGACGCGATTATTTGGTTGGAAAACCTGCTCAAAGCGTTTGAA	
GGCAGCCTGGTTGTGATTACCCACGACCGCCGTTTTTTGGACAATATCGCCACGCGGATT	
GTCGAACTCGATC	
>4	
TTTGATACCGTTGCCGAAGGTTTGGGCGAAATTCGTGATTTATTGCGCCGTTATCATCAT	
GTCAGCCATGAGTTGGAAAATGGTTCGAGTGAGGCTTTGTTGAAAGAACTCAACGAATTG	
CAACTTGAAATCGAAGCGAAGGACGGCTGGAAACTGGATGCGGCAGTCAAGCAGACTTTG	
GGGGAACTCGGTTTGCCGGAAAATGAAAAAATCGGCAACCTTTCCGGCGGTCAGAAAAAG	
CGCGTCGCCTTGGCTCAGGCTTGGGTGCAAAAGCCCGACGTATTGCTGCTGGACGAGCCG	
	(continues on next page)

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ACCAACCATTTGGATATCGACGCGATTATTTGGCTGGAAAATCTGCTCAAAGCGTTTGAA
GGCAGCTTGGTTGTGATTACCCACGACCGCCGTTTTTTGGACAATATCGCCACGCGGATT
GTCGAACTCGATC
```

14.5 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.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences def	Initions
	t represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition database submitted to this database and consequently it should be noted that it does not represent a population sample.
Query database • Search database - advanced queries. • Browse database - peruse all records. • Search by combinations of loci (profiles) - including partial matching. • List query - find isolates by matching a field to an entered list. • Projects - main projects defined in database.	Option settings Submissions • Set general options - including isolate table field handling. • Manage submissions • Set display and query options for locus, schemes or scheme fields. • Manage submissions • Isolates: 34221 • Last updated: 2015-07-02 • Update history • About BIGSdb
Breakdown Single field Two field Unique combinations Scheme and alleles Bequence bin Export dataset Contigs Sequences - XMFA / concatenated	Analysis Codon usage • Codon usage • Presence/absence status of loci • FASTA formats • BLAST

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.

3 1	120M	B35; 21035	Pakistan		meningitis and septicaemia			1	SI-1 complex/subgroup I/II	5-2	10	F5-1
4	M00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1099		19	15	
-	M1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	s A	4	ST-4 complex/subgroup IV			
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в В	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	s W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis		5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	з В	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	s 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	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	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis		864				
16	2		Germany	1999	carrier	Neisseria meningitidis	в	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	s 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		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	в	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	s A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			

Select the isolate records to analyse - these will be pre-selected if you accessed the plugin following a query. You can also select loci and/or schemes which will be used to calculate the totals and percentages of loci designated and tagged. This may be useful as a guide to assembly quality if you use a scheme of core loci where a good assembly would be expected to include all member loci. To determine the total of all loci designated or tagged, click 'All loci' in the scheme tree.

There is also an option to determine the mean G+C content of the sequence bin of each isolate.

Click submit.

	Profile/ST List Scheme/alleles Publications Options Profiles/sequences definition	ns	
Breakdown of convence b			Help 🗹
Breakdown of sequence k	oin conug properues		
Please select the required isolate ids for comp	parison - use Ctrl or Shift to make mult	iple selections. Select loci/schemes to use for calculating pe	rcentage of alleles designated or tagged.
Isolates 64) 254 67) S5611 82) 11-004 84) IAL 2229 90 CN100 120) P4698 128) F6124 160) 1014	Loci 165_rDNA 165_rRNA (SSU_rRNA) _235_rRNA abcZ abcZ (NEIS1015) aceF (NEIS1279) ackA2 (NEIS1727) acnA (NEIS1729) All None Paste list	Schemes	Options ———— Calculate %GC
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.

<u>शित्तां ज</u> ्	LST	Query: Sear Breakdown: Links: Conte	Isolate fiel	ds Sc	heme/all	eles Put			s									
																		Help 🖉
Break	down	of sea	uence	bin	con	tia pr	ope	rties										
Please se	elect the rea	uired isolat	e ids for co	mparis	on - use	Ctrl or Sh	ift to ma	ake multir	ple selection:	s. Select I	oci/schemes	to use for	calculating	percentage of all	eles designate	d or tadded		
— Isolat				—Lo						-Scheme				- Options				
64) 254 67) 556 82) 11- 84) IAL 90) CN 120) F4 128) F6 160) 10 	All None	od:		169 _23 abc abc ace ack	S_rRNA Z Z (NEIS1 F (NEIS1 A2 (NEIS1 A (NEIS1	279) 1727)	e Pas	Action — Reset	-		Capsule		ion A · ion A · ion A · ion A ·	Calculate %	GC			
Loci selec Isolate id \$			Total	Min ¢	Max ¢	Mean ¢	σ \$	N50 contig number	iength	N90 contig number	length	N95 contig number	iengtn	Alleles designated	% Alleles designated \$	Loci tagged ≑	% Loci tagged ≑	Sequence ¢
64	254	251	2054183	257	69510	8184	9379	42	(L50) 15763	131	(L90) 4488	162	(L95) 2543	1817	75.8	1892	78.9	Display -
67	S5611	194	2084213	255	103457		14516		22332	94	6156	115	3531	1852	77.3	1898	79.2	Display -
82	11-004	258	2055227	251	47478	7966	8518	45	13854	139	4751	167	2921	1830	76.3	1886	78.7	Display -
84	IAL2229	188	2051679	256	96122	10914	13975	28	21515	93	6282	115	3629	1848	77.1	1896	79.1	Display -

You can choose to export the data in tab-delimited text or Excel formats by clicking the appropriate link at the bottom of the table.

67	S5611	194	2084213	255	103457	10744	14516	28	22332	94	6156	115	3531	1852	77.3	1898	79.2	Display -
82	11-004	258	2055227	251	47478	7966	8518	45	13854	139	4751	167	2921	1830	76.3	1886	78.7	Display -
84	IAL2229	188	2051679	256	96122	10914	13975	28	21515	93	6282	115	3629	1848	77.1	1896	79.1	Display 🛶
90	CN100	236	2118544	261	73069	8977	11101	36	19065	119	4570	149	2839	1848	77.1	1898	79.2	Display ->
• Do	ownload in ta ownload in E e following c	xcel format	t	t														
Number	Number of contigs Total length Mean contig length Contig lengths																	
Overall me	an: 225.4; σ:	32.5	Overa	ll mea	n: 207276	9.2; σ: 28	3828.2	Overall me	an: 9357.0	; o: 1396.7	Over	all mean: 91	196.0; σ: 11	481.9				
	Overall mean: 225.4; c; 32.5 Overall mean: 2072769.2; c; 28828.2 Overall mean: 9357.0; c; 1396.7 Overall mean: 9196.0; c; 11481.9																	
											Dow	nload length	IS					

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

ci seleci	ted: 2397																	
olate id 🔶	Isolate 🗢	Contigs 🗢	Total length \$	Min ¢	Max 🗢	Mean ¢		N50 contig number	× N50 contig length (L50)	N90 contig (number	N90 contig length (L90)	N95 contig number	N95 contig length (L95)	Alleles designated 🕈	% Alleles designated 🕈	Loci tagged \$	% Loci tagged ≑	Sequence bin
64	254	251	2054183	257	69510	8184	9379	42	15763	131	4488	162	2543	1817	75.8	1892	78.9	Display
67	S5611	194	2084213	255	103457	10744	14516	28	22332	94	6156	115	3531	1852	77.3	1898	79.2	Display
82	11-004	258	2055227	251	47478	7966	8518	45	13854	139	4751	167	2921	1830	76.3	1886	78.7	Display -
84	IAL2229	188	2051679	256	96122	10914	13975	28	21515	93	6282	115	3629	1848	77.1	1896	79.1	Display -
90	CN100	236	2118544	261	73069	8977	11101	36	19065	119	4570	149	2839	1848	77.1	1898	79.2	Display -

14.6 Genome comparator

Genome Comparator is an optional plugin that can be enabled for specific databases. It is used to compare whole genome data of isolates within the database using either the database defined loci or the coding sequences of an annotated genome as the comparator.

Output is equivalent to a whole genome MLST profile, a distance matrix calculated based on allelic differences and a NeighborNet graph generated from this distance matrix.

Genome Comparator can be accessed on databases where it is enabled from the contents page by clicking the 'Genome Comparator' link.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences defin	nitions
	represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition e may be submitted to this database and consequently it should be noted that it does not represent a population sample.
 Search database - advanced queries. Browse database - peruse all records. Search by combinations of loci (profiles) - including partial matching. List query - find isolates by matching a field to an entered list. Projects - main projects defined in database. 	 Set general options - including isolate table field handling. Set display and query options for locus, schemes or scheme fields. General information Isolates: 34221 Last updated: 2015-07-02 Update history About BIGSdb
Breakdown Export • Single field • Export dataset • Two field • Contigs • Unique combinations • Scheme and alleles • Publications • Sequences - XMFA / concatenated F	Analysis Codon usage Presence status of loci BLAST Analysis Miscellaneous • Description of database fields

Alternatively, it can be accessed following a query by clicking the 'Genome Comparator' button at the bottom of the results table. Isolates with sequence data returned in the query will be automatically selected within the Genome Comparator interface.

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

14.6.1 Analysis using defined loci

Select the isolate genomes that you wish to analyse. These will either be in a dropdown list or, if there are too many in the database, a text input where a list can be entered. You can also upload your own genomes for analysis - these should be either a single file in FASTA format (if you have just one genome), or a zip file containing multiple FASTA files. Select either the loci from the list or a set of schemes. Press submit.

Publics i Databa	ase nome Contents			
Logged in: Keith Jolley (k	keith). 🔁 Log out Change password			Help 🗹 🛛 Toggle: 🚯
Genome Cor	mparator - Neisseria Pub	MLST		
<u></u>				
			ons in list boxes. In addition to selecting individual loci, you o ence genome and compare using the loci defined in that.	can choose to include all loci defined in schemes by selecting
Isolates		Loci		
662 663 664 665	Optionally include data not in the database. Upload FASTA file (or <i>zip</i> file containing multiple FASTA files - one per genome): • Browse No file selected.	165_rDNA 165_rRNA (SSU_rRNA) 223_rRNA abc2 abc2 (NEIS1015) accF (NEIS1279) accA2 (NEIS1727) acnA (NEIS1729) All None Paste list	country region year epidemiological year age yr age mth sex disease source	N. gonorrhoeae AMR Pilin Pilin
Reference genon Enter accession nur or choose annotated or upload Genbank/ Browse No file	Imber: Min % identi Id genome: Min % alignmer BLASTN word siz	y: 70 v 0 With incomplete loci: t 50 v 0 Completely exclude	From analysis from analysis if include ref sequences in alignment ele Align all loci (not only variable) Aligner: MAFFT	Core genome analysis Core threshold (%): 90 → 0 Calculate mean distances 0
Sequence metho Proje Experime	ect:	Reset Submit		

The job will be submitted to the job queue and will start running shortly. Click the link to follow the job progress and view the output.



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

	Profile/ST List Scheme/alleles Publications Options Profiles/sequences defir	itions Database submissions		
- h - 4-4				
ob status viewer				
Status				
Job id: BIGSdb_27748_1405410063_ Submit time: 2014-07-15 08:41:03 Status: finished Start time: 2014-07-15 08:41:05	94241			
Progress: 100% Stop time: 2014-07-15 08:41:22 Total time: 17 seconds				
Dutput				
nalysis against defined loci				
				uncated alleles (located at end of contig) are marked as 'T'
ocus 644 (L93/4286) 662 (2837) 663 (283 abcZ 2 2 2 2	2 2 2	2 7 2	2 2 2	8)
adk 3 3 3 aroE 4 19 4		3 3 3 4 4 19	3 3 3 19 19 4	
fumC 3 3 3 gdh 8 8 8	3 24 23 8 8 8 8	23 3 3 8 8 8	3 3 3 8 8 8	
odhC 4 4 4 pgm 6 6 6	4 4 6 6 6 6	6 4 4 6 6 6	4 4 4 6 6 6	
oci with sequence differences among	isolates:			
riable loci: 4				
ocus 644 (1.93/4286) 662 (2837) 663 (283 abcz 2 2 2 aroE 4 19 4 umC 3 3 3 abcC 4 4 4	9) 664 (2838) 665 (2845) 666 (28 2 2 2 4 4 4 3 24 23 4 4 6	43) 667 (2842) 669 (2846) 670 (284 2 7 2 4 4 19 23 3 3 6 4 4	0) 671 (2844) 672 (2847) 698 (FAM1) 2 2 2 2 19 19 4 3 3 3 3 4 4 4	9
	4 4 0	0 4 4	4 4 4	•
xactly matching loci nese loci are identical in all isolates.				
atches: 3				
ocus 644 (L93/4286) 662 (2837) 663 (283 adk 3 3 3 gdh 8 8 8 pgm 6 6 6	9) 664 (2838) 665 (2845) 666 (28 3 3 3 8 8 8 6 6 6 6	43) 667 (2842) 669 (2846) 670 (284 3 3 3 8 8 8 6 6 6 6	0) 671 (2844) 672 (2847) 698 (FAM1) 3 3 3 8 8 8 6 6 6 6	9
nique strains				-
nique strains: 5				
Strain 1 Strain 2 Strain 3 Strain 4 144 (L93)4286) 662 (2837) 666 (2843) 665 (2833) 665 (2840) 667 (2840) 667 (2842) 54 (2838) 671 (2840) 667 (2842) 54 (2838) 671 (2840) 667 (2842) 54 (2838) 671 (2844) 54 (2838) 671 (2847) 58 (FAM18) 672 (2847) 54 (2837) 668 (2847) 56 (2847)				
Text output file Excel format Distance matrix (Nexus format) - Suitat Splits graph (Neighbour-net; PNG form		ances between taxa are calculated as	the number of loci with different allele	sequences
(Splits graph (Neighbour-net; SVG form Locus presence frequency Locus presence frequency chart (PNG	iat) - This can be edited in inkscape	or other vector graphics editors		
Tar file containing output files	click to enlarge)			
ease note that job results will remain on the :	server for 7 days.			

14.6.2 Analysis using annotated reference genome

Select the isolate genomes that you wish to analyse and then either enter a Genbank accession number for the reference genome, or select from the list of reference genomes (this list will only be present if the administrator has *set it up*). Selecting reference genomes will hide the locus and scheme selection forms.

PubMLST Databas	se home Contents				
Logged in: Keith Jolley (k	eith). 🔁 Log out Change password		Help 🗹	Toggle: 🚯	Ξ
Genome Con	nparator - Neisseria Pub	MLST			
		CTRL or SHIFT to make multiple selections in list boxes. In addition to selecting individual loci, you can choose to include all loci defined ccession number for an annotated reference genome and compare using the loci defined in that.	in scheme	s by selectin	ng
Isolates	User genomes	Include in identifiers			
662 663 664 665	Optionally include data not in the database. Upload FASTA file (or zip file containing multiple FASTA files - one per genome): Browse No file selected.	Bolate A Country E region E year e opdermological year age mth age mth sex disease age mth source T			
	ne ————————————————————————————————————				
Enter accession nur					
or choose annotated FAM18 (Nm) or upload Genbank/t Browse No file	BLASTN word size EMBL/FASTA file:	Trast as distinct allele			
Filter by Sequence metho Projec Experimer	ct:	Action Submit			

Output is similar to when comparing against defined loci, but this time every coding sequence in the annotated reference will be BLASTed against the selected genomes. Because allele designations are not defined, the allele found in the reference genome is designated allele 1, the next different sequence is allele 2 etc.

b stat	us viewer															
atus																
Job id	BIGSdb 21911 1405410488 8452															
	2014-07-15 08:48:08															
Status	finished															
Start time	2014-07-15 08:48:34															
Progress																
	2014-07-15 09:12:58															
Total time	24 minutes and 24 seconds															
Itput																
alysis by	reference genome															
accessior	AM421808															
version	1															
type	dna															
length	2194961															
description																
	Neisseria meningitidis serogroup C FAM18 complete genome.															
oding regio																
oding regio																
ding regio																
ding regio loci		X'. Truncated	alleles (loc	ated at end o	f contig) are	marked :	as T.									
ding regio loci ch unique	ns 1975 allele is defined a number starting at 1. Missing alleles are marked as '							664	665	666	667	669	670	671	672	60
ding regio loci ch unique Locus	ns 1975 allele is defined a number starting at 1. Missing alleles are marked as ' Product	Sequence length	Genome position	Reference genome	644 (L93/4286)	662	as 'T'. 663 (2839)	664 (2838)	665 (2845)	666 (2843)	667 (2842)	669 (2846)	670 (2840)	671 (2844)	672 (2847)	
ding regio loci ch unique Locus xC envA	ns 1975 allele is defined a number starting at 1. Missing alleles are marked as '	Sequence	Genome	Reference	644	662	663									(FAI
ding regio loci ch unique Locus (C envA IMC0001	ns 1975 allele is defined a number starting at 1. Missing alleles are marked as " Product UDP-3-O-(3-hydroxymyristoyl) N-acetylglucosmine deacetylase	Sequence length 924	Genome position 1261	Reference genome 1	644 (L93/4286) 1	662 (2837) 1	663 (2839) 1	(2838) 1	(2845) 1	(2843) 1	(2842) 1	(2846) 1	(2840) 1	(2844) 1	(2847) 1	(FAI
ding regio loci ch unique Locus xC envA IMC0001 pilS1	ns 1975 allele is defined a number starting at 1. Missing alleles are marked as ' Product	Sequence length	Genome position	Reference genome	644 (L93/4286)	662 (2837)	663 (2839)	(2838)	(2845)	(2843)	(2842)	(2846)	(2840)	(2844)	(2847)	(FAI
ding regio loci ch unique Locus (C envA IMC0001 pilS1 IMC0002	ns 1975 allele is defined a number starting at 1. Missing alleles are marked as " Product UDP-3-O-(3-hydroxymyristoyl) N-acetylglucosmine deacetylase	Sequence length 924	Genome position 1261	Reference genome 1	644 (L93/4286) 1	662 (2837) 1	663 (2839) 1	(2838) 1	(2845) 1	(2843) 1	(2842) 1	(2846) 1	(2840) 1	(2844) 1	(2847) 1	(FAI
ding regio loci ch unique Locus xC envA IMC0001 pilS1 IMC0002 pilS2 IMC0003	ns 1975 allele is defined a number starting at 1. Missing alleles are marked as ? Product UDP-3-O-[3-hydroxymyristoy] N-acetyfglucosmine deacetyfase pilin (fragment) truncated pilin	Sequence length 924 291 366	Genome position 1261 3341 3675	Reference genome 1 1 1	644 (L93/4286) 1 1 2	662 (2837) 1 1 2	663 (2839) 1 1 2	(2838) 1 1 2	(2845) 1 1 2	(2843) 1 1 2	(2842) 1 1 2	(2846) 1 1 2	(2840) 1 1 2	(2844) 1 1 2	(2847) 1 1 2	(FAN
ding regio loci ch unique Locus xC envA JMC0001 pilS1 JMC0002 pilS2 JMC0003 fbp	ns 1975 allele is defined a number starting at 1. Missing alleles are marked as ^r Product UDP-3-O-[3-hydroxymyristoy]] N-acetylglucosmine deacetylase pilin (fragment)	Sequence length 924 291	Genome position 1261 3341	Reference genome 1 1	644 (L93/4286) 1 1	662 (2837) 1 1	663 (2839) 1 1	(2838) 1 1	(2845) 1 1	(2843) 1 1	(2842) 1 1	(2846) 1 1	(2840) 1 1	(2844) 1 1	(2847) 1 1	(FAN
ding regio loci ch unique Locus xC envA MC0001 pilS1 MC0002 pilS2 MC0003 fbp MC0004	ns 1975 allele is defined a number starting at 1. Missing alleles are marked as ' Product UDP-3-O-[3-hydroxymyristoy] N-acetylglucosmine deacetylase pillin (tragment) truncated pillin peptidyl-prolyl cis-trans isomerase	Sequence length 924 291 366 330	Genome position 1261 3341 3675 4069	Reference genome 1 1 1 1 1	644 (L93/4286) 1 1 2 2	662 (2837) 1 1 2 2 2	663 (2839) 1 1 2 2	(2838) 1 2 2	(2845) 1 2 2	(2843) 1 2 2	(2842) 1 2 2	(2846) 1 1 2 T	(2840) 1 2 2	(2844) 1 2 2	(2847) 1 2 2	(FAN
ding regio loci ch unique Locus xC envA MC0001 pilS1 IMC0002 pilS2 IMC0003 fbp IMC0004 IMC0005	Ins 1975 allele is defined a number starting at 1. Missing alleles are marked as 7 Product UDP-3-O-[3-hydroxymyristoy] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin peptidyl-prolyl cis-trans isomerase putative membrane protein	Sequence length 924 291 366 330 219	Genome position 1261 3341 3675 4069 4476	Reference genome 1 1 1 1 1 1	644 (L93/4286) 1 1 2 2 2	662 (2837) 1 2 2 3	663 (2839) 1 2 2 3	(2838) 1 2 2 3	(2845) 1 2 2 3	(2843) 1 2 2 3	(2842) 1 2 2 3	(2846) 1 2 T 4	(2840) 1 2 2 3	(2844) 1 2 2 5	(2847) 1 2 2 3	(FAN
ding regio loci ch unique xC envA MC0001 pilS1 MC0002 pilS2 IMC0003 fbp IMC0004 IMC0004 IMC0004	ns 1975 allele is defined a number starting at 1. Missing alleles are marked as " Product UDP-3-O-[3-hydroxymyristoyi] N-acetylglucosmine deacetylase pillin (fragment) truncated pillin peptidyl-prolyl cis-trans isomerase putative membrane protein putative dycerate dehydrogenase	Sequence length 924 291 366 330 219 954	Genome position 1261 3341 3675 4069 4476 4816	Reference genome 1 1 1 1 1 1 1 1	644 (L93/4286) 1 2 2 2 2 2	662 (2837) 1 2 2 3 2	663 (2839) 1 2 2 3 2	(2838) 1 2 2 3 2	(2845) 1 2 2 3 2	(2843) 1 2 2 3 2	(2842) 1 2 2 3 2	(2846) 1 2 T 4 2	(2840) 1 2 2 3 2	(2844) 1 2 2 5 2	(2847) 1 2 2 3 2 2	
Ading regio I loci ch unique Locus XXC envA VMC0001 pilS1 VMC0002 pilS2 VMC0003	Ins 1975 allele is defined a number starting at 1. Missing alleles are marked as 7 Product UDP-3-O-[3-hydroxymyristoy] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin peptidyl-prolyl cis-trans isomerase putative membrane protein	Sequence length 924 291 366 330 219	Genome position 1261 3341 3675 4069 4476	Reference genome 1 1 1 1 1 1	644 (L93/4286) 1 1 2 2 2	662 (2837) 1 2 2 3	663 (2839) 1 2 2 3	(2838) 1 2 2 3	(2845) 1 2 2 3	(2843) 1 2 2 3	(2842) 1 2 2 3	(2846) 1 2 T 4	(2840) 1 2 2 3	(2844) 1 2 2 5	(2847) 1 2 2 3	699 (FAM 1 1 1 1 1 1

14.6.3 Include in identifiers fieldset

This selection box allows you to choose which isolate provenance fields will be included in the results table. This does not affect the output of the alignments as taxa names are limited in length by the alignment programs.

-Include in identifiers	
isolate	
country	=
region	=
year	
epidemiological year	
age yr	
age mth	
sex	
disease	
source	Ŧ

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

14.6.4 Reference genome fieldset

This section allows you to choose a reference genome to use as the source of comparator sequences.

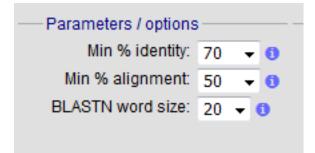
Reference genome Enter accession number: İ or choose annotated genome: FAM18 (Nm) or upload Genbank/EMBL/FASTA file: No file selected. Browse... i

There are three possibilities here:

- 1. Enter accession number Enter a Genbank accession number of an annotated reference and Genome Comparator will automatically retrieve this from Genbank.
- 2. Select from list The administrator may have selected some genomes to offer for comparison. If these are present, simply select from the list.
- 3. Upload genome Click 'Browse' and upload your own reference. This can either be in Genbank, EMBL or FASTA format. Ensure that the filename ends in the appropriate file extension (.gb, .embl, .fas) so that it is recognized.

14.6.5 Parameters/options fieldset

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



- Min % identity This sets the threshold identity that a matching sequence has to be in order to be considered (default: 70%). Only the best match is used.
- Min % alignment This sets the percentage of the length of reference allele sequence that the alignment has to cover in order to be considered (default: 50%).
- BLASTN word size This is the length of the initial identical match that BLAST requires before extending a match (default: 20). Increasing this value improves speed at the expense of sensitivity. The default value gives good results in most cases. The default setting used to be 15 but the new default of 20 is almost as good (there was 1 difference among 2000 loci in a test run) but the analysis runs twice as fast.

14.6.6 Distance matrix calculation fieldset

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

 Distance matrix calculation — — —
With incomplete loci:
Completely exclude from analysis
Treat as distinct allele
Ignore in pairwise comparison
Exclude paralogous loci

For incomplete loci, i.e. those that continue beyond the end of a contig so are incomplete you can:

- Completely exclude from analysis Any locus that is incomplete in at least one isolate will be removed from the analysis completely. Using this option means that if there is one bad genome with a lot of incomplete sequences in your analysis, a large proportion of the loci may not be used to calculate distances.
- Treat as a distinct allele This treats all incomplete sequences as a specific allele 'I'. This varies from any other allele, but all incomplete sequences will be treated as though they were identical.
- Ignore in pairwise comparison (default) This is probably the best option. In this case, incomplete alleles are only excluded from the analysis when comparing the particular isolate that has it. Other isolates with different alleles will be properly included. The effect of this option will be to shorten the distances of isolates with poorly sequenced genomes with the others.

Paralogous loci, i.e. those with multiple good matches, can be excluded from the analysis (default). This is the safest option since there is no guarantee that differences seen between isolates at paralogous loci are real if the alternative matches are equally good. NB: Loci are also only classed as paralogous when the alternative matches identify different sequences, otherwise multiple contigs of the same sequence region would result in false positives.

14.6.7 Alignments fieldset

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

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

Available options are:

- Produce alignments Selecting this will produce the alignment files, as well as XMFA and FASTA outputs of aligned sequences. This will result in the analysis taking longer to run.
- Include ref sequences in alignment When doing analysis using an annotated reference, selecting this will include the reference sequence in the alignment files.
- Align all loci By default, only loci that vary among the isolates are aligned. You may however wish to align all if you would like the resultant XMFA and FASTA files to include all coding sequences.
- Aligner There are currently two choices of alignment algorithm (provided they have both been installed)
 - MAFFT (default) This is the preferred option as it is significantly quicker than MUSCLE, uses less memory, and produces comparable results.
 - MUSCLE This was originally the only choice. It is still included to enable previous analyses to be re-run and compared but it is recommended that MAFFT is used otherwise.

14.6.8 Core genome analysis fieldset

This section enables you to modify the inclusion threshold used to calculate whether or not a locus is part of the core genome (of the dataset).

— Core genome analysis — — —
Core threshold (%): 90 👻 👔
Calculate mean distances 👔

The default setting of 90% means that a locus is counted as core if it appears within 90% or more of the genomes in the dataset.

There is also an option to calculate the mean distance among sequences of the loci. Selecting this will also select the option to produce alignments.

14.6.9 Filter fieldset

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

Sequence method:	▼ i	
Project:		▼ i
Experiment:	▼ į	

Available options are:

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

14.6.10 Understanding the output

14.6.10.1 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.

14.6.10.2 Unique strains

The table of unique strains is a list of isolates that are identical at every locus. Every isolate is likely to be classed as unique if a whole genome analysis is performed, but with a constrained set of loci, such as those for MLST, this will group isolates that are indistinguishable at that level of resolution.

14.7 **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.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic	
database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be note Query database • Search database - advanced queries. • Browse database - peruse all records. • Search by combinations of loci (profiles) - including partial matching. • List query - find isolates by matching a field to an entered list. • Projects - main projects defined in database.	Submissions • Manage submissions
	iscellaneous Description of database 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.

6 7 8 9	M00240227 M00282207		UK										
7 8 9					invasive (unspecified/other)	-		В		ST-32 complex/ET-5 complex	7	16	
9			UK		invasive (unspecified/other)	-		W	1101	ST-22 complex			
9	7891	B54; Z1054	Finland		invasive (unspecified/other)			A	5	ST-5 complex/subgroup III	20	9	F3-1
	M00242007		UK	2000	invasive (unspecified/other)	Neisseria mening	pitidis	В	1102	ST-18 complex		14	
10	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria mening	gitidis	W	114	ST-22 complex			
	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria mening	gitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria mening	gitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria mening	gitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria mening	pitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria mening	gitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria mening	gitidis	E	864				
16	2		Germany	1999	carrier	Neisseria mening	pitidis	в	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria mening	gitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria mening	pitidis	В	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria mening	pitidis	Α	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria mening	gitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria mening	pitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria mening	pitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria mening	gitidis	в	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria mening	pitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria mening	gitidis	В	930	ST-334 complex			
Brea	nalysis: BL	elds Two Fi	ence/Absence		norphic sites Combinations a Comparator BLAST	Schemes/alleles	Public	cations (Seque	rce bin Tag status			
		ataset Cont	igs 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.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Data	base submissions
	Toggle: i
BLAST	
Please select the required isolate ids to BLAST against (use ctrl or shift to make multiple set	ections) and paste in your query sequence. Nucleotide or peptide sequences can be queried.
64) 254 FAAGCCTTGSGCGSACGCGCGCGCGCGTG 67) 55611 GAAGCCTTGSGCGSACGCGCGCGCGCGCGCGGCGGCGGCGGCGGCGGCGGCGGC	SCIESCIESCIASCOSCCCSCIESCISSI region 3GGITICGICCATCATGCG3GSCAAAGTC year Figlemiological year ICGASCIGAACGICTATATGCCGGITATC age yr age yr
ParametersOption	
	w 0% matches in table Sequence method:
BLASTN scoring: reward:2; penalty:-3; gap open:5; gap extend:2 Hits per isolate: 1	Project.
Flanking length (bp): 100 Ţ □ Use TBLASTX Ţ	

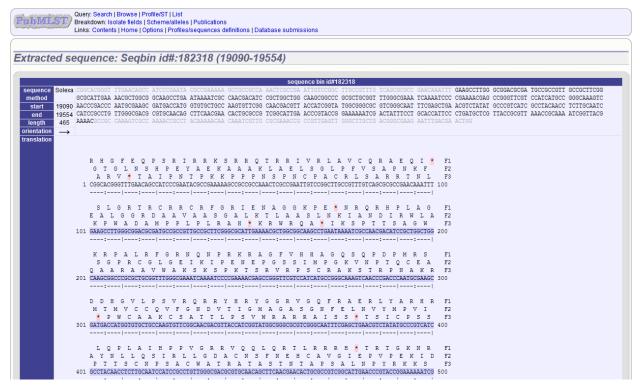
Click submit.

A table of BLAST results will be displayed.

457													т	oggle
	-													
ase sel	lect the requ	iired isolate id	s to BLAST ag	ainst (use ctr	l or shi	it to make n	nultiple sel	ections) and paste	in your qu	ery sequen	ce. Nucleotide or j	peptide sequences can be queried.		
Isolate	s		P	aste sequenc	e									
A4/M1 120M 7891 0) 6748 1) 129 3) 1391 9) S313 4) S43	M 3 31 55	None	GCA TTC AAC ACC GCC	AAGCCTGAA GGGCGAAAT CCCGACCCAA CATCGGCAT CTACAACCT CTGCGCCGT	TAAAA CAAAA ATGCG GGCGG CTTGC CGGCA	ICGCCAAC ICCCCGAA AAGCGAIG GCGCGICG AATCCAIC ICGAACCC	GACATCC AACGAGC ACCATGG GGCAATT CGCCTGT GTACCGG	CCGCTTCGGGCGC GCTGGCTGGCAAG CGGGTTCGTCCAT TGTGCTGCCAAGT TCGAGCTGAACGT TGGGCGACGGCG AAAAAATCGACTA TCGGCTACGAAAA	CGGCCCG CATGCCG GTTCGGC CTATATG CAACAGC TTTCCTG	CGCTGCG (GGCAAAG (AACGACG) (CCCGTTA) (TTCAACG)	GT IC IT IC AA	county region year epidemiological year age yr age mth sex disease source epidemiology *		
Param	neters						Option	15		Restrict inc	luded sequences	by	- Action	
		e: 11 👻 👔						w 0% matches in t		Sequence		-, ▼ []		
			penalty:-3; gap	open:5: gap	extend	2 - 🗊					Project:	- i		
	ts per isolat		penany. 5, gap	open.o, gap	CALCHIG					Eve	-	T T		
ate id	Isolate	% identity Alig	nment length	Mismatche	s Gaps	Seqbin id	Start	End	Drientatio	n E-value I	Bit score			
1	A4/M1027	98.49	465	7	0	180177	19444	19908 extract	\rightarrow	0.0	807			
2	120M 7891	98.49 98.49	465 465	7	0	180583 180965	4782 19869	5246 extract → 20333 extract →	←	0.0	807 807			
10	6748	98.49	465	7	0	180965	19869	20333 extract ->	\rightarrow	0.0	807			
10	129	98.49	465	7	0	181867	35889	36353 extract -	\rightarrow	0.0	807			
	139M	98.49	465	7	0	182004	36775	37239 extract ->	\rightarrow	0.0	807			
		98.49	465	7	0	182318	19090	19554 extract →	\rightarrow	0.0	807			
13	S3131				-	215673	4534	4998 extract -	é.		807			
13 19	S3131 S4355	98.49	465	7	0			4990 extract →		0.0				
13 19 24		98.49 97.42	465 465	7	0	8		4996 extract -	$\xrightarrow{\leftarrow}$	0.0	785			
13 19 24 30	S4355 14 10		465 465	12 7	-				•		785 807			
13 19 24 30 31 34	S4355 14 10 20	97.42 98.49 98.49	465 465 465	12 7 7	0	8 182380 182815	1363524 5559 19783	1363988 extract	\rightarrow \rightarrow \rightarrow	0.0 0.0 0.0	807 807			
13 19 24 30 31 34 35	S4355 14 10 20 26	97.42 98.49 98.49 98.49	465 465 465 465	12 7 7 7 7	0 0 0 0 0	8 182380 182815 182880	1363524 5559 19783 18879	1363988 extract	$ \begin{array}{c} \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow \\ \rightarrow \end{array} $	0.0 0.0 0.0 0.0	807 807 807			
13 19 24 30 31 34 35 46	\$4355 14 10 20 26 255	97.42 98.49 98.49 98.49 98.49 98.49	465 465 465 465 465	12 7 7 7 7 7	0 0 0 0 0	8 182380 182815 182880 183179	1363524 5559 19783 18879 4982	1363988 extract	. 1 1 1 1 L	0.0 0.0 0.0 0.0 0.0	807 807 807 807			
13 19 24 30 31 34 35 46 52	\$4355 14 10 20 26 255 243	97.42 98.49 98.49 98.49 98.49 98.49 98.49	465 465 465 465 465 465	12 7 7 7 7 7 7 7	0 0 0 0 0 0	8 182380 182815 182880 183179 183381	1363524 5559 19783 18879 4982 4532	1363988 extract	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0.0 0.0 0.0 0.0 0.0 0.0	807 807 807 807 807			
13 19 24 30 31 34 35 46 52 61	S4355 14 10 20 26 255 243 393	97.42 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49	465 465 465 465 465 465 465 465	12 7 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0	8 182380 182815 182880 183179 183381 183648	1363524 5559 19783 18879 4982 4532 7217	1363988 extract	. 1 1 1 1 4 1	0.0 0.0 0.0 0.0 0.0 0.0 0.0	807 807 807 807 807 807			
13 19 24 30 31 34 35 46 52 61 64	S4355 14 10 20 26 255 243 393 254	97.42 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49	465 465 465 465 465 465 465 465 465 465	12 7 7 7 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0	8 182380 182815 182880 183179 183381 183648 183818	1363524 5559 19783 18879 4982 4532 7217 4716	1363988 extract 6023 extract 20247 extract 19343 extract 5446 extract 4996 extract 7681 extract 5180 extract	. † † † † ↓ † ↓	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	807 807 807 807 807 807 807			
13 19 24 30 31 34 35 46 52 61 64 67	S4355 14 10 20 26 255 243 393 254 S5611	97.42 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49	465 465 465 465 465 465 465 465 465 465	12 7 7 7 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0 0 0 0 0	8 182380 182815 182880 183179 183381 183648 183818 184143	1363524 5559 19783 18879 4982 4532 7217 4716 4804	1363988 extract - 6023 extract - 20247 extract - 19343 extract - 5446 extract - 4996 extract - 5180 extract - 5180 extract - 5268 extract -	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	807 807 807 807 807 807 807 807			
13	S4355 14 10 20 26 255 243 393 254	97.42 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49	465 465 465 465 465 465 465 465 465 465	12 7 7 7 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0	8 182380 182815 182880 183179 183381 183648 183818	1363524 5559 19783 18879 4982 4532 7217 4716	1363988 extract 6023 extract 20247 extract 19343 extract 5446 extract 4996 extract 7681 extract 5180 extract	. † † † † ↓ † ↓	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	807 807 807 807 807 807 807			

Clicking any of the 'extract' buttons will display the matched sequence along with a translated sequence and flanking sequences.

181867	35889	36353 extract →	\rightarrow	0.0	807
182004	36775	37239 extract ->	\rightarrow	0.0	807
182318	19090	19554 extract ->	\rightarrow	0.0	807
215673	4534	4998 extract →	←	0.0	807
8	1363524	1363988 extract ->	\rightarrow	0.0	785
182380	5559	6023 extract →	\rightarrow	0.0	807
182815	19783	20247 extract ->	\rightarrow	0.0	807



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.

82 11-004	4 98.49	465	7	•	404007	40540				
		400	1	0	184297	19518	19982 extract -	\rightarrow	0.0	807
84 IAL222	9 98.49	465	7	0	184635	4530	4994 extract ->	←	0.0	807
90 CN10	0 98.49	465	7	0	184814	5350	5814 extract -	←	0.0	807

14.7.1 Include in results table fieldset

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

 Include in results table 	9—
country	
region	
year	-
epidemiological year	
age yr	
age mth	
sex	
disease	
source	
epidemiology	Ŧ

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

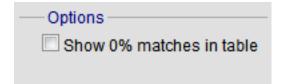
14.7.2 Parameters fieldset

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.

14.7.3 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.

14.7.4 Filter fieldset

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

-Restrict included sec	quences by	
Sequence method:	▼ [i	
Project:		▼ [i
Experiment:	▼ i	

Available options are:

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

14.8 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.

8 M00242007 UK 2000 Invasive (unspecified/other) Neisseria meningitidis B 1102 ST-18 complex 14 9 0021784 Czech Republic 1984 Invasive (unspecified/other) Neisseria meningitidis M 114 ST-22 complex 14 10 6748 B73; 21073 Canada 1971 Invasive (unspecified/other) Neisseria meningitidis A 1 ST-10 complex/subgroup //l 18-11 3 FE 11 129 B92; Z1092 Germany 1964 Invasive (unspecified/other) Neisseria meningitidis A 1 ST-10 complex/subgroup //l 18-1 3 12 0090/89 Czech Republic 1999 Invasive (unspecified/other) Neisseria meningitidis X 117 14 1 ST-10 complex/subgroup //l 5-2 10 FE 14 0120/95 Czech Republic 1995 Invasive (unspecified/other) Neisseria meningitidis X 117 14 14 14 15 1 Germ	6	M00282207		UK		invasive (unspecified/other)		W	1101	ST-22 complex			
9 0021/84 Czech Republic 194 invasive (unspecified/other) Neisseria meningitidis W 114 ST-22 complex C<	7		B54; Z1054							ST-5 complex/subgroup III	20		F3-1
10 6748 B73;21073 Canada 1971 invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup I/I 18-1 3 F5 11 129 B92;21092 Germany 1964 invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup I/I 5-2 10 F5 12 0090/08 Czech Republic 1999 invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup I/I 5-2 10 F5 13 139M B99;21099 Philippines 1986 Neisseria meningitidis A 1 ST-1 complex/subgroup I/I 5-2 10 F5 14 0120/95 Czech Republic 1999 carrier Neisseria meningitidis X 117 5-2 10 F5 16 2 Germany 1999 carrier Neisseria meningitidis W 174 ST-14 complex 14 12 14 12 14	8									ST-18 complex		14	
11 129 B92; Z1092 Germany 1964 invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup //II 5-2 10 F3 12 009/089 Czech Republic 1998 invasive (unspecified/other) Neisseria meningitidis B 1015 ST-32 complex/ET-5 complex 7 16 13 1398 B93; Z1099 Czech Republic 1995 invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup //II 5-2 10 F5 14 0120/055 Czech Republic 1995 invasive (unspecified/other) Neisseria meningitidis X 117 T1 5 14 14 14 15 1 Germany 1999 carrier Neisseria meningitidis B 854 ST-18 complex 14 18 4 Germany 1999 carrier Neisseria meningitidis M 174 ST-14 complex/subgroup I/V 7 13-1 F7 19 S3131 B213; Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningitidis </td <td>9</td> <td>0021/84</td> <td></td> <td>Czech Republic</td> <td>1984</td> <td>invasive (unspecified/other)</td> <td>Neisseria meningitidis</td> <td>W</td> <td>114</td> <td>ST-22 complex</td> <td></td> <td></td> <td></td>	9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
12 0090/09 Czech Republic 1998 (zoropie w/ET-5 complex T 7 16 13 139M B99, Z109 Philippines 1968 Neisseria meningitidis A 1 ST-1 complex/subgroup //l 5-2 10 F1 14 0120/95 Czech Republic 1995 Insseria meningitidis A 1 ST-1 complex/subgroup //l 5-2 10 F1 15 1 Germany 1999 carrier Neisseria meningitidis E 864 14 16 2 Germany 1999 carrier Neisseria meningitidis B 864 ST-18 complex 17 3 Germany 1999 carrier Neisseria meningitidis B 864 ST-18 complex 18 4 Germany 1999 carrier Neisseria meningitidis B 19 ST-18 complex ST-18 complex <td>10</td> <td>6748</td> <td>B73; Z1073</td> <td>Canada</td> <td>1971</td> <td>invasive (unspecified/other)</td> <td>Neisseria meningitidis</td> <td>Α</td> <td>1</td> <td>ST-1 complex/subgroup I/II</td> <td>18-1</td> <td>3</td> <td>F5-1</td>	10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
13 139M B99; Z1099 Philippines 1968 Neisseria meningitidis A 1 ST-1 complex/subgroup //II 5-2 10 F5 14 0120/95 Czech Republic 1995 invasive (unspecified/other) Neisseria meningitidis X 117 14 114 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 15	11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
14 0120/95 Czech Republic 1995 invasive (unspecified/other) Neisseria meningitidis X 117 14 14 15 1 Germany 1999 carrier Neisseria meningitidis E 864 57-18 14 16 2 Germany 1999 carrier Neisseria meningitidis B 854 ST-18 complex 14 17 3 Germany 1999 carrier Neisseria meningitidis B 854 ST-18 complex 14 18 4 Germany 1999 carrier Neisseria meningitidis A 4 ST-4 complex 14 19 S3131 B213; Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningitidis NG 198 ST-18 complex 14 20 5 Germany 1999 carrier Neisseria meningitidis NG 198 ST-182 complex 12-1 F1 21 6 Germany 1999 carrier Neisseria meningitidis NG 198 ST-182 complex 12-2 <t< td=""><td>12</td><td>0090/89</td><td></td><td>Czech Republic</td><td>1989</td><td>invasive (unspecified/other)</td><td>Neisseria meningitidis</td><td>в</td><td>1015</td><td>ST-32 complex/ET-5 complex</td><td>7</td><td>16</td><td></td></t<>	12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	в	1015	ST-32 complex/ET-5 complex	7	16	
15 1 Germany 1999 carrier Neisseria meningitidis E 864 ST-18 complex Image: State Stat	13	139M	B99; Z1099					A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
16 2 Germany 1999 carrier Neisseria meningitidis B 854 ST-18 complex ST-174 complex 17 3 Germany 1999 carrier Neisseria meningitidis W 174 ST-174 complex ST-174 complex 18 4 Germany 1999 carrier Neisseria meningitidis W 174 ST-174 complex ST-18 complex 19 S3131 B213, Z1213 Ghana 1973 imvasive (unspecified/other) Neisseria meningitidis A 4 ST-4 complex/subgroup IV 7 13-1 F1 20 5 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex 7 13-1 F1 21 6 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex 7 13-1 F1 22 7 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex 7 23 8 Germany 1999 carrier Neisseria meningitidis	14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
17 3 Germany 1999 carrier Neisseria meningitidis W 174 ST-174 complex V 174 18 4 Germany 1999 carrier Neisseria meningitidis B 19 ST-18 complex V 174 19 S3131 B213, Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningitidis A 4 ST-198 complex V 7 13.1 F 20 5 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex V 7 13.1 F 21 6 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex V V 7 13.1 F 22 7 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex V <	15			Germany		carrier							
18 4 Germany 1999 carrier Neisseria meningitidis B 19 ST-18 complex C 19 S3131 B213;Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningitidis A 4 ST-4 complex/subgroup IV 7 13-1 F1 20 5 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex V 2 7 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex V 2 2 7 Germany 1999 carrier Neisseria meningitidis E 60 ST-98 complex V 2 2 3 32 ST-323 complex/F-5 complex V 2 2 3 32 ST-32 complex/F-5 complex V 2 2 34 5 ST-5 complex/subgroup III 5-1 9 F3 24 S4355 B227;Z1227 Denmark 1974 invasive (unspecified/other) Neisseria meningitidis B 930 ST-34 complex V 4 51 9 5 53	16	2		Germany	1999	carrier	Neisseria meningitidis	в	854	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 20 5 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex F1 21 6 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex F1 22 7 Germany 1999 carrier Neisseria meningitidis E 60 ST-60 complex F1 23 8 Germany 1999 carrier Neisseria meningitidis E 60 ST-60 complex F1 24 S4355 B227;Z1227 Denmark 1974 invasive (unspecified/other) Neisseria meningitidis A 5 ST-50 complex/subgroup III 5-1 9 F3 25 9 Germany 1999 carrier Neisseria meningitidis B 930 ST-334 complex F1 9 F3	17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
20 5 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex 1 21 6 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex 1 22 7 Germany 1999 carrier Neisseria meningitidis E 60 ST-60 complex 1 23 8 Germany 1999 carrier Neisseria meningitidis B 32 ST-32 complex/E-5 complex 1 24 S4355 B227; Z1227 Denmark 1974 invasive (unspecified/other) Neisseria meningitidis A 5 ST-5 complex/subgroup III 5-1 9 F3 25 9 Germany 1999 carrier Neisseria meningitidis B 930 ST-334 complex 1	18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 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 E 60 ST-60 complex 24 S4355 B227;Z1227 Denmark 1974 invasive (unspecified/other) Neisseria meningitidis A 5 ST-5 complex/subgroup III 5-1 9 F3 25 9 Germany 1999 carrier Neisseria meningitidis B 930 ST-344 complex	19	S3131	B213; Z1213	Ghana		invasive (unspecified/other)	Neisseria meningitidis			ST-4 complex/subgroup IV	7	13-1	F1-5
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-50 complex/BUT-5 complex F3 25 9 Germany 1999 carrier Neisseria meningitidis B 930 ST-334 complex	20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
23 8 Germany 1999 carrier Neisseria meningitidis B 32 ST-32 Complex/ET-5 comple	21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
24 S4355 B227,Z1227 Denmark 1974 invasive (unspecified/other) Neisseria meningitidis A 5 ST-5 complex/subgroup III 5-1 9 F3 25 9 Germany 1999 carrier Neisseria meningitidis B 930 ST-334 complex	22	7		Germany		carrier	Neisseria meningitidis	E	60	ST-60 complex			
25 9 Germany 1999 carrier Neisseria meningitidis B 930 ST-334 complex	23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex			
	24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
Analysis tools:	25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			
reakdown: Fields Two Field Codons Polymorphic sites Combinations Schemes/alleles Publications Sequence bin Tag status Analysis: BURST Presence/Abence Genome Comparator BLAST Export Dataset Contigs Sequences	na	alysis tools akdown: Fie	elds Two Fi	eld Codons	Polyr	norphic sites							

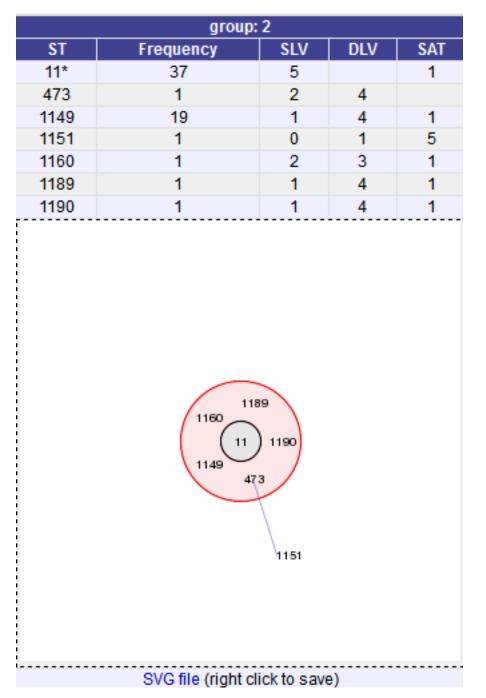
If there multiple schemes that can be analysed, these can then be selected along with the group definition.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
BURST analysis
This is the original BURST algorithm, developed by Ed Feil, first implemented by Man-Suen Chan. This version 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 SURGE 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 saved in SVG format. This is a vector image format that can be manipulated and scaled in drawing packages, including the freely available Inkscape. Options Select scheme: MLST Group definition: profiles match at m-2 © Shade 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.

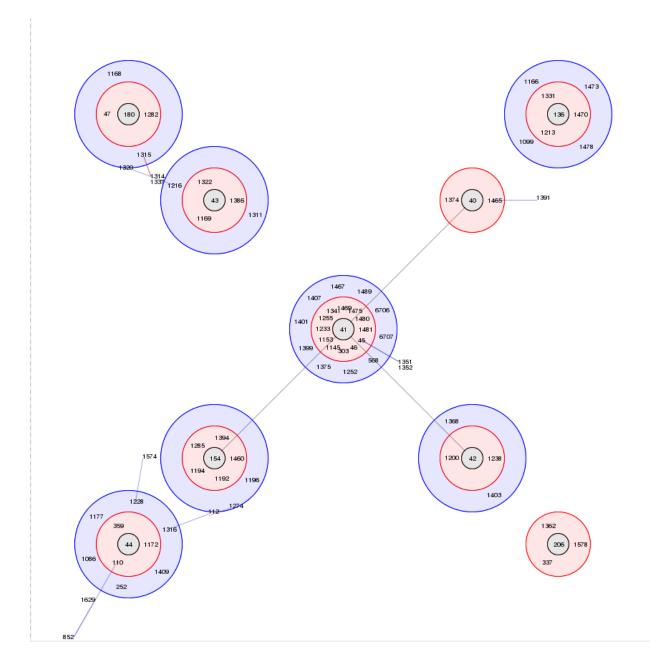
A series of tables will be displayed indicating the groups of profiles. Where one profile can be identified as a central genotype, i.e. the profile that has the greatest number of other profiles that are single locus variants (SLV), double locus variants (DLV) and so on, a graphical representation will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

ST Frequency 32* 2 230 1 484 1 1015 1 1100 1 1148 1	SLV 3 1	DLV 2	SAT
32* 2 230 1 484 1 1015 1 1100 1	3		
484 1 1015 1 1100 1	1	2	
1015 1 1100 1		3	1
1100 1	0	3	2
	1	4	
11/0 1	1	2	2
1140 1	0	4	1
SVG file (right of	1100 114		

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



14.9 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.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it	
Query database • Search database - advanced queries. • Browse database - peruse all records. • Search by combinations of loci (profiles) - including partial matching. • List query - find isolates by matching a field to an entered list. • Projects - main projects defined in database.	
Breakdown Export • Single field • Export dataset • Unique combinations • Contigs • Scheme and alleles • Sequences - XMFA / concatenated FASTA formats • Sequence bin • BLAST	Miscellaneous • Description of database fields

Alternatively, it can be accessed following a query by clicking the 'Codons' button in the Analysis list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

			UK	2000	invasive (unspecified/other)	Noiscoria moningitidie	В	1100	ST-32 complex/ET-5 complex	7	16	
	00240227		UK		invasive (unspecified/other)	-	W	1101	ST-32 complex ST-22 complex	'	10	
1	7891	B54; Z1054	Finland		invasive (unspecified/other)			5	ST-5 complex/subgroup III	20	9	F3-1
8 M	100242007	B54, Z1054	UK		invasive (unspecified/other)		AB	1102	ST-18 complex	20	14	P 3-1
	00242007				invasive (unspecified/other)		w	114	ST-22 complex		14	
	6748	B73; Z1073				-		114		40.4	2	F5-1
10		B73, 21073 B92: Z1092	Canada		invasive (unspecified/other)		A		ST-1 complex/subgroup I/II	18-1	3	F3-6
11	129	B92; 21092	Germany		invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	5-2	10	F3-0
	0090/89	D00 74000			invasive (unspecified/other)	-	В		ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099		1968	lana da constante de la la constante de la const	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
	0120/95				invasive (unspecified/other)		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			1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19		B213; Z1213	Ghana			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		ST-32 complex/ET-5 complex			
24		B227; Z1227	Denmark		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			

Enter the ids of the isolate records to analyse - these will be already entered if you accessed the plugin following a query. Select the loci you would like to analyse, either from the dropdown loci list, and/or by selecting one or more schemes.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publi Links: Contents Home Options Profiles/seque		
		Toggle: i
Codon usage analysis		
		database containing sequences, or with sequences tagged, can be included. It is important to note that ding frame 1). Partial sequences from the sequence bin will not be analysed. Please check the loci that you
	fier	Schemes
Paste in list of ids to include, start a new isolate line for each. Leave blank to include all ids. country region year epidemiological age yf age mth sex disease source		Genetic Information Proce
Sequence retrieval	Codons	— — Action —
If both allele designations and tagged sequences exist for a locus, choose how you want these handled: [] Use sequences tagged from the bin	Select codon order:	Submit
\odot Use allele sequence retrieved from external database		
☑ Do not include sequences with problem flagged (defined alleles	will still be used)	

Click submit. The job will be submitted to the queue and will start running shortly. Click the link to follow the job progress and view the output.

Public State fields Scheme/alleles Publications	
Links: Contents Home Options Profiles/sequences definitions Database submissions	
	Toggle: i
Codon usage analysis	
This analysis has been submitted to the job queue.	
Please be aware that this job may take some time depending on the number of sequences to analyse and how busy the server is.	
Follow the progress of this job and view the output.	

Four tab-delimited text files will be created.

- Absolute frequency of codon usage by isolate
- Absolute frequency of codon usage by locus
- Relative synonymous codon usage by isolate
- Relative synonymous codon usage by locus

Public Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profile/Sequences definitions Database submissions
Job status viewer
Status
Job id: BIGSdb_13269_1405586315_76138 Submit time: 2014/07-17 09:38:35 Status: Inished Start time: 2014/07-17 09:38:39 Progress: 100% Stop time: 2014/07-17 09:39:05 Total time: 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
Please note that job results will remain on the server for 7 days.

14.10 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.

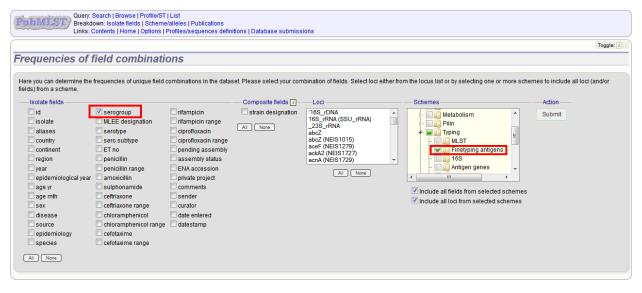
The function can be selected by clicking the 'Unique combinations' link in the Breakdown section of the main contents page. This will run the analysis on the entire database.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does Q Query database • Search database - pruse all records. • Search by combinations of loci (profiles) - including partial matching. • List query - find isolates by matching a field to an entered list. • Projects - main projects defined in database.	
 Breakdown Single field Two field Unique combinations Solumer and anteres Publications Sequence bin 	JS I database fields

Alternatively, it can be accessed following a query by clicking the 'Combinations' button in the Breakdown list at the bottom of the results table. This will run the analysis on the dataset returned from the query. Please note that the list of functions here may vary depending on the setup of the database.

6	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16	
	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	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	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			

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.

ubML	ST) Breakd		ields Schem	e/alleles Pul	blications Jences definition
requen	cies of f	field co	mbinat	ions	
-					
lumber of un	ique combinat	ions: 2939			
ne percentar	tes may add u	p to more tha	n 100% if you	have selected	d loci or scheme
		PorA VR2 \$	FetA VR ¢ F1-5	Frequency ¢ 625	Percentage \$
B	7-2 5	4	F1-5 F1-1	513	5.65 4.64
В	19	15	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
С	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
- Y	5 5-2	2 10-1	F1-1 F4-1	93 79	0.84
C	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
c	5	2	F3-3	76	0.69
В	18-1	3	F1-5	72	0.65
Y	5-1	2-2	F5-8	69	0.62
В	19	15	F1-14	61	0.55
В	7-2	13-2	F1-5	61	0.55
В	7-2	16	F3-3	56	0.51

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

в	12.1	13.1	F3-29	1	0.0
NG	7-2	16-126	F3-3	1	0.0
в	7-2	30	F5-1	1	0.0
в	7	30-3	F1-14	1	0.0
В	5-1	10-10	F3-16	1	0.0
-	7-2	30-3	F1-7	1	0.0
С	5-2	10	F1-7	1	0.0
NG	18-1	3	F1-34	1	0.0
NG	22	14-6	F4-2	1	0.0
в	7-2	4	F1-88	1	0.0
NG	5-1	10-62	F1-3	1	0.0
Y	12-3	4	F4-1	1	0.0
NG	7-2	16	F1-104	1	0.0
Х	12-1	16-52	F3-9	1	0.0
NG	18-4	35-34	E4-1	1	0.0

14.11 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.

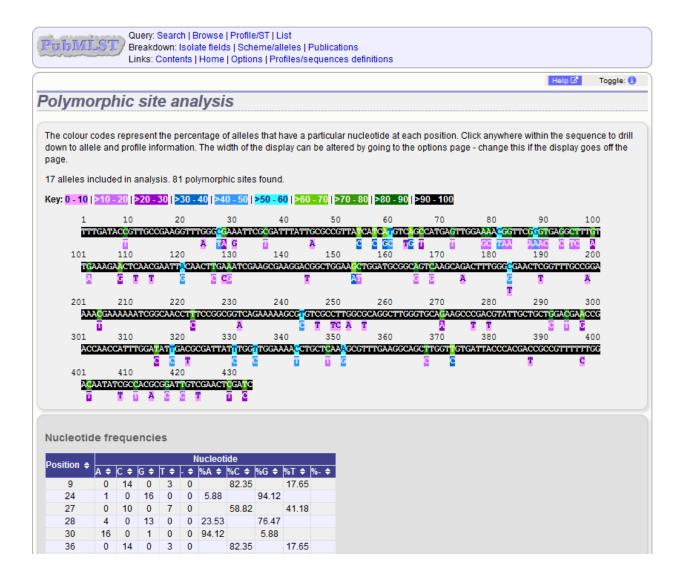
9 B92; Z1092 0/89 B99; Z1099 0/95	Germany Czech Republic Philippines		invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
9M B99; Z1099		1989		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
	Philippines		invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
0/95		1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
	Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
	Germany	1999	carrier	Neisseria meningitidis	E	864				
	Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
	Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
	Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
31 B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
	Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
	Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
	Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
	Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex			
855 B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
	Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			
		Germany Germany B213; Z1213 Ghana Germany Germany Germany Germany Germany	Germany 1999 Germany 1999 B1 B213;Z1213 Ghana 1973 Germany 1999 Germany 1999 Germany 1999 Germany 1999 Germany 1999 55 B227;Z1227 Demmark 1974	Germany 1999 carrier Germany 1999 carrier B213; Z1213 Ghana 1973 invasive (unspecified/other) Germany 1999 carrier S B227; Z1227 Demmark 1974 invasive (unspecified/other)	Germany 1999 carrier Neisseria meningildis Germany 1999 carrier Neisseria meningildis B213; Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningildis Germany 1999 carrier Neisseria meningildis S B227, Z1227 Denmark 1974 invasive (unspecified/other) Neisseria meningildis	Germany 1999 carrier Neisseria meningilidis W Germany 1999 carrier Neisseria meningilidis B 1 B213; Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningilidis B 31 B213; Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningilidis NG Germany 1999 carrier Neisseria meningilidis NG Germany 1999 carrier Neisseria meningilidis NG Germany 1999 carrier Neisseria meningilidis E Germany 1999 carrier Neisseria meningilidis B 55 B227; Z1227 Denmark 1974 invasive (unspecified/other) Neisseria meningilidis B	Germany 1999 carrier Neisseria meningitidis W 174 Germany 1999 carrier Neisseria meningitidis B 19 B213, Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningitidis A 4 Germany 1999 carrier Neisseria meningitidis NG 198 Germany 1999 carrier Neisseria meningitidis SE 60 Germany 1999 carrier Neisseria meningitidis SE 32 55 B227, Z1227 Denmark 1974 invasive (unspecified/other) Neisseria meningitidis A 5	Germany 1999 carrier Neisseria meningitidis W 174 957-174 complex Germany 1999 carrier Neisseria meningitidis B 19 ST-18 complex B1 B213; Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningitidis A 4 ST-4 complex/subgroup IV Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex Germany 1999 carrier Neisseria meningitidis NG 198 ST-196 complex Germany 1999 carrier Neisseria meningitidis E 60 ST-60 complex Germany 1999 carrier Neisseria meningitidis E 82 ST-32 complex/ET-5 complex/Subgroup IIV St B227; Z1227 Deman# 1974 invasive (unspecified/other) Neiss	Germany 1999 carrier Neisseria meninglidis W 174 97174 complex Germany 1999 carrier Neisseria meninglidis B 19 ST-174 complex B1 B213; Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meninglidis) A 4 ST-4 complex/subgroup IV 7 Germany 1999 carrier Neisseria meninglidis NG 198 ST-198 complex Germany 1999 carrier Neisseria meninglidis NG 198 ST-198 complex Germany 1999 carrier Neisseria meninglidis NG 198 ST-198 complex Germany 1999 carrier Neisseria meninglidis NG 198 ST-198 complex Germany 1999 carrier Neisseria meninglidis NG 198 ST-198 complex Germany 1999 carrier Neisseria meninglidis NG 32 ST-32 complex/ET-5 complex/ET-5 Germany 1999 carrier Neisseria meninglidis	Germany 1999 carrier Neisseria meningitidis W 174 ST-174 complex Germany 1999 carrier Neisseria meningitidis B 19 ST-18 complex B1 B213; Z1213 Ghana 1973 invasive (unspecified/other) Neisseria meningitidis A 4 ST-4 complex Subgroup IV 7 13-1 Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex - Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex - Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex - Germany 1999 carrier Neisseria meningitidis NG 198 ST-198 complex - Germany 1999 carrier Neisseria meningitidis E 60 ST-60 complex/subgroup III - Germany 1999 carrier Neisseria meningitidis A 5 ST-5 complex/subgroup II

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

Publicity Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profile/Sequences definitions Database submissions	
	Toggle: i
Polymorphic site analysis	
This tool will analyse the polymorphic sites in the selected locus for the current isolate dataset. If more than 50 sequences have been selected, the job will be run by the offline job manager which may take a few minutes (or longer depending on the queue). This is because sequences may have gaps in them and consequently need to be aligned which is a processor- and memory-intensive operation.	
Loci Options Action '16S_rDNA 16S_rRNA (SSU rRNA) If both allele designations and tagged sequences exist for a locus, choose how you want these handled. [] Analyse abc2 @ Use allele sequence retrieved from external database abc2 (NEIS1015) @ Use allele sequence retrieved from external database abc2 (NEIS1015) aoch2 (NEIS1272) ach42 (NEIS1727) @ Use sequences tagged from the bin ack42 (NEIS1727) @ Use sequences tagged from the bin ack42 (NEIS1727) @ Analyse single example of each unique sequence @ Exclude incomplete sequences	

Click 'Analyse'.

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



14.12 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.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences de	
	at represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition ate may be submitted to this database and consequently it should be noted that it does not represent a population sample.
Query database • Search database - advanced queries. • Browse database - peruse all records. • Search by combinations of loci (profiles) - including partial matching • List query - find isolates by matching a field to an entered list. • Projects - main projects defined in database.	Option settings Set general options - including isolate table field handling. Manage submissions • Set display and query options for locus, schemes or scheme fields. Manage submissions • Isolates: 34221 Isolates: 34221 • Last updated: 2015-07-02 Update history • About BIGSdb About BIGSdb
Breakdown Single field Two field Unique combinations Scheme and alleles Publications Sequence bin	d FASTA formats Analysis Codon usage Presence/absence status of loci Genome comparator BLAST

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.

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

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.

Cuery: Search Browse Pro Breakdown: Isolate fields S Links: Contents Home Opt Export presence/absence s This script will export data showing whether a loce are members of the scheme.	cheme/alleles Publications ions Profiles/sequences defini tatus of loci - Nei	sseria PubMLST	neck the loci that you would like to include. Alte	rnatively select one or more schemes to	Toggle: []
Select ids Paste in list of ids to include, start a new line for each. Leave blank to include all ids.	Include in identifier	Loci 165_rRNA (SSU_rRNA) 235_rRNA (SSU_rRNA) abc2 abc2 abc2 (NEIS1015) aceF (NEIS1729) achA2 (NEIS1727) achA2 (N	Schemes Genetic Information Proce Metabolism Plin Plin Finetyping antigens Anticen cenes	Options Mark present if : @ ether designations or tags set allele designations defined S sequence tags defined Symbol for present O • Symbol for absent X • C Generate distance matrix .	Action Submit

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.

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

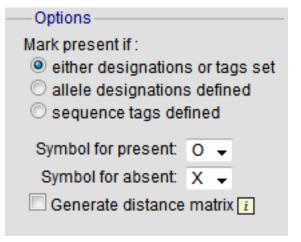
Ouery: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Job status viewer
Status
Job id: BicSdb_31442_1405591304_69061 Stubmit time: 2014-07-17 11:01:44 Stats: finished Stats: 2014-07-17 11:01:44 Progress: 1004 Stop time: 2014-07-17 11:01:49 Total time: 4 seconds
Please 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

14.12.1 Options

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



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.

14.13 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.

id	•	< •	10			+ i	Order by: id Display: 25	✓ record	s per p	✓ ascendin age i	g 👻			
Action Reset	Submit													
ecords return	ed. Click the h	perlinks for det												
d isolate	aliases	country	Is vear	solate field	ds 👔 disease		species	serogroup	ST	MLST clonal complex	Finet PorA VR1	ping anti		
1 A4/M1027	B1: Z1001	USA				(other) N	Veisseria meningitidis		4	ST-4 complex/subgroup IV	5-2	10	F1-5	
2 120M	B35; Z1035	Pakistan					veisseria meningitidis		1	ST-1 complex/subgroup I/I	5-2	10	F5-1	
3 M00242905		UK					veisseria meningitidis		1099		19	15		
4 M1027	B43; Z1043	USA	1937	invasive ((unspecified/	(other) N	veisseria meningitidis	A	4	ST-4 complex/subgroup IV				
5 M00240227	7	UK	2000	invasive ((unspecified/	/other) N	veisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16		
6 M00282207	7	UK	2000	invasive ((unspecified/	/other) N	veisseria meningitidis	W	1101	ST-22 complex				
7 7891	B54; Z1054	Finland	1975	invasive ((unspecified/	/other) N	veisseria meningitidis	A	5	ST-5 complex/subgroup III	20	9	F3-1	
	7	UK	2000	invasive ((unspecified/	/other) N	Veisseria meningitidis	в	1102	ST-18 complex		14		
8 M00242007		Creek Depublie	1004	1	(unenocified)	(other) N	Veisseria meningitidis	W	114	ST-22 complex				

Select the loci you would like to analyse.

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

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.

														Toggle:
ag status														
elect schemes or groups o	fschemes within	the tree. A brea	kdown of the indivi	dual loci belongin	g to these sche	mes will then be	e performed.							
- 📝 🛄 Capsule	igion A Region A - Serog Region A - Serog Region A - Serog	jroup A jroup B	•											
ars represent loci by schen	nes arranged in a	Iphabetical ord	er. If a locus appea	rs in more than o	ne scherne it wi	l appear more ti	nan once in this	graphic. Cli	ck on the id I	hyperlink fo	r a detailed	breakdown	n for an isol	ate.
ey lele designated only Seq 163 loci selected: 1 Isolate						l appear more ti	nan once in this	graphic. Cli	ck on the id I	hyperlink fo	r a detailed	breakdown	ı for an isol	ate.
ey lele designated only Seq 163 loci selected: 1 Isolate						I appear more t	nan once in this	graphic. Cli	ck on the id l	hyperlink fo	r a detailed	breakdown	n for an isol	ate.
ey ele designated only Seq 63 loci selected: Isolate A4/M1027						l appear more ti	nan once in this	graphic. Cli	ck on the id l	hyperlink fo	r a detailed	breakdown	n for an isol	ate.
ele designated only Seq 63 loci selected: Isolate A4/M1027 120M						l appear more ti	nan once in this	graphic. Cli	ck on the id l	hyperlink fo	r a detailed	breakdown	n for an isol	ate.
ele designated only Seq 63 loci selected: Isolate A4/M1027 120M M00242905						l appear more ti	nan once in this	: graphic. Cli	ck on the id l	hyperlink fo	r a detailed	breakdown	n for an isol	ate.
ey ele designated only Seq 63 loci selected: Isolate A4/M1027 120M M00242905 M1027						l appear more ti	nan once in this	graphic. Cli	ck on the id i	hyperlink fo	r a detailed	breakdown	n for an isol	ate.
ey ele designated only Seq 63 loci selected:						l appear more ti	nan once in this	graphic. Cli	ck on the id	hyperlink fo	r a detailed	breakdown	n for an isol	ate.
ey lete designated only Seq 63 loci selected: 1 20M 120M 1002422905 100242297 100240227 100240227						l appear more ti	nan once in this	graphic. Cli	ck on the id	hyperlink fo	r a detailed	breakdown	n for an isol	ate.
ey liele designated only Seq 463 loci selected: 1 A4/M1027 2 120M 3 M00242905 4 M1027 5 M00240227 5 M0024027 7 7891						appear more th	nan once in this	graphic. Cli	ck on the id	hyperlink fo	r a detailed	breakdown	n for an isol	ate.
1 A4/M1027 2 120M 3 M00242905 4 M1027 5 M00240227 6 M00282207						appear more th	nan once in this	graphic. Cli	ck on the id	hyperlink fo	r a detailed	breakdown	n for an isol	ate.

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 exact status for all loci of that isolate.

tus: Isolate id#1 (/	A/M1027)		
	1 4/11/1027)		
Scheme	Locus	Allele designation(s)	Sequence tag
MLST	abcZ	1	ooquonoo tug
mest.	adk	3	
	aroE	3	
	fumC	1	
	gdh	4	
	pdhC	2	
	pgm	3	
Finetyping antigens	PorA VR1	5-2	
r motyping anagono	PorA VR2	10	
	FetA VR	F1-5	
165	SSU rRNA (16S rRNA)	45	
ADP-heptose biosynthesis	NEIS0769 (hldA)	2	
	NEIS0773 (hldD)	2	
	NEIS2014 (gmhB)	2	
	NEIS2055 (hldC)	2	
	NEIS2070 (gmhA)		
minoacyl-tRNA biosynthesis	NEIS0007	2	
	NEIS0164	2	
	NEIS0326	61	
	NEIS0381	2	
	NEIS0383	2	
	NEIS0672		internal stop codon
	NEIS0676	15	
	NEIS0681	5	
	NEIS0794	5	
	NEIS1277	3	
	NEIS1290 (gatC)	3	
	NEIS1291	13	
	NEIS1293	9	
	NEIS1361	3	
	NEIS1408	71	
	NEIS1436	5	
	NEIS1478	4	
	NEIS1518	3	
	NEIS1602	3	

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.

14.14 GrapeTree

GrapeTree is a tool for generating and visualising minimum spanning trees. It has been developed to handle large datasets (in the region of 1000s of genomes) and works with 1000s of loci as used in cgMLST. It uses an improved minimum spanning algorithm that is better able to handle missing data than alternative algorithms and is able to produce publication quality outputs. Datasets can include metadata which allows nodes in the resultant tree to be coloured interactively.

GrapeTree can be accessed from the contents page by clicking the 'GrapeTree' link.

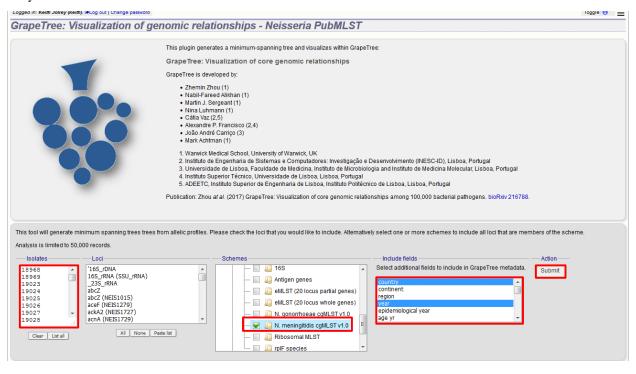
PubMLST Database home Contents	
	Ξ
Neisseria PubMLST database	
The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition database there is at leas corresponding 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.	t one
Q Query database 📰 Projects 👯 Option settings 🔔 Submissions	
Search or browse database Main public projects Search by combinations of loci (profiles) Your projects Set display and query options for locus, schemes or scheme fields.	
General information	
 Isolates: 44,865 Last updated: 2018-02-20 	
Defined field values Update history	
About BIGSdb	
Breakdown 🖺 Export Analysis C Third party tools	
Single field Export dataset Codon usage GrapeTree Visualization of genomic relationships Two field Contigs Presence/absence status of loci IDL - Phylogenetic trees with data overlays	
Unique combinations Sequences - XMFA / concatenated FASTA formats Scheme and alleles Scheme and a	
Publications Sequence bin Miscellaneous	
Description of database fields	

Alternatively, it can be accessed following a query by clicking the 'GrapeTree' button at the bottom of the results table. Isolates returned from the query will be automatically selected within the GrapeTree interface.

9024 M10 240480 9025 M10 240481 9026 M10 240482	UK 2010 invasive (unspecified/other) Neisseria meningitidis			7.0 1	1 3-12
		B 2267206	267 1194 ST-41/44 complex	7-2 4	F1-5
9026 M10 240482	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2194837	274 1831	22 9	F3-3
	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2184823	263 3754 ST-41/44 complex	7-2 4	F5-1
9027 M10 240484	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2168050	253 1097 ST-41/44 complex	17-1 23	F1-5
9028 M10 240485	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2193457	294 275 ST-269 complex	22 9	F5-12
9029 M10 240487	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2188678	241 1049 ST-269 complex	19-1 15-11	F5-1
9030 M10 240489	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2218969	275 461 ST-461 complex	19-2 13-1	F3-9
9031 M10 240490	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2175692	293 1161 ST-269 complex	22 9	F5-12
9032 M10 240498	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2154070	235 41 ST-41/44 complex	7-2 4	F1-5
9958 M10 240476	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2242902	284 9812 ST-213 complex	22 14	F5-5
9959 M10 240499	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2189734	198 275 ST-269 complex	22 9	F5-12
9960 M10 240500	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2197545	223 41 ST-41/44 complex	7-2 4	F1-5
9961 M10 240502	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2173298	188 340 ST-41/44 complex	7-2 4	F1-5
9962 M10 240503	UK 2010 invasive (unspecified/other) Neisseria meningitidis	Y 2101043	197 23 ST-23 complex	5-1 2-2	F1-96
9963 M10 240505	UK 2010 invasive (unspecified/other) Neisseria meningitidis	Y 2090713	189 1655 ST-23 complex	5-1 10-10	F4-1
9964 M10 240507	UK 2010 invasive (unspecified/other) Neisseria meningitidis	Y 2108738	170 183 ST-23 complex	21 16-5	deleted
9965 M10 240508	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2233910	196 1575	7-2 13-1	F1-7
9966 M10 240511	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2174583	219 4713	22 9	F5-12
9967 M10 240512	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2203751	205 41 ST-41/44 complex	7-1 1	F1-5
9968 M10 240514	UK 2010 invasive (unspecified/other) Neisseria meningitidis	W 2110464	160 11 ST-11 complex	5 2	F1-1
9969 M10 240515	UK 2010 invasive (unspecified/other) Neisseria meningitidis	B 2181841	205 269 ST-269 complex	5-1 2-2	F5-1
9970 M10 240520	UK 2010 invasive (unspecified/other) Neisseria meningitidis	Y 2095486	190 1655 ST-23 complex	5-1 10-1	F4-1

Select the isolates to include. The tree can be generated from allelic profiles of any selection of loci, or more conveniently, you can select a scheme in the Scheme selector to include all loci belonging to that scheme.

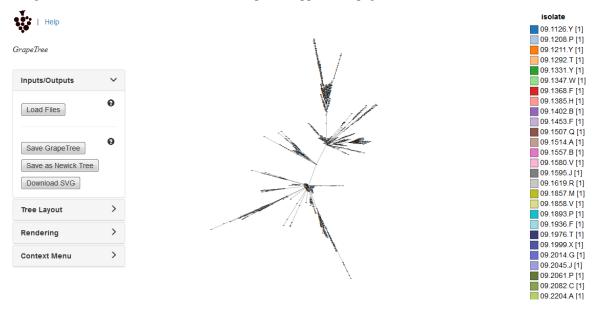
Additional fields can be selected to be included as metadata for use in colouring nodes - select any fields you wish to include. Multiple selections can be made by holding down shift or ctrl while selecting. Click 'Submit' to start the analysis.



Note: This analysis currently depends on allele designations having been defined within the database. It is not able to scan genomes itself (unlike Genome Comparator), so make sure that genomes have been tagged at the loci you wish to include before using GrapeTree.

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

PUDMLS1 Database nome Contents
Logged in: Keith Jolley (keith). (#Log out Change password
Job status viewer
Status
Job id: BIGSdb_141866_1519311802_19416
Submit time: 2018-02-22 15:03:22
Status: finished
Start time: 2018-02-22 15:03:42
Progress: 100%
Stop time: 2018-02-22 15:07:38
Total time: 3 minutes and 55 seconds
Output
Launch GrapeTree
Profiles (TSV format) (14.2 MB)
MS Tree (Newick format)
Metadata (TSV format) Tar file containing output files (only files <10MB included - download larger files separately)
tai me containing culputities (only ties < tomb included - download taiger ties separately)
Please note that job results will remain on the server for 7 days.

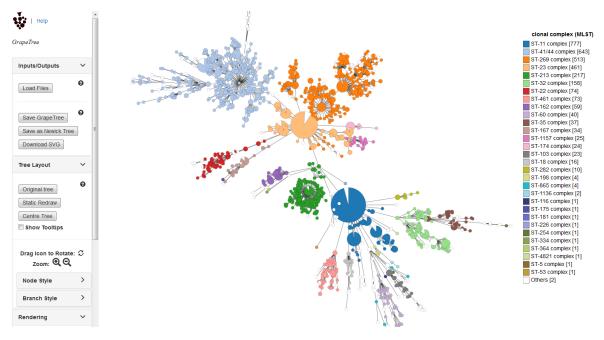


The generated tree will be rendered in the GrapeTree application page.

The image can be manipulated in various ways. These include modifying the tree layout, customising node labels and size, modifying branch lengths and collapsing branches. The image can be saved in SVG format which can be further edited in image publishing software such as Inkscape.

As an example, the default cgMLST tree (above) has been modified (below) as follows:

- Nodes coloured by clonal complex
- · Labels removed
- Branches collapsed where <=100 loci different
- Node size set to 200%
- Kurtosis (node size relative to number of isolates) set to 75%
- · Dynamic rendering allowed to run to fan out nodes



Full details can be found in the GrapeTree manual.

Note: GrapeTree has been described in the following preprint:

Z Zhou, NF Alikhan, MJ Sergeant, N Luhmann, C Vaz, AP Francisco, JA Carrico, M Achtman (2017) "GrapeTree: Visualization of core genomic relationships among 100,000 bacterial pathogens", bioRxiv 216788; doi: https://doi.org/10.1101/216788

CHAPTER 15

Data export plugins

15.1 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 Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions
Neisseria PubMLST database
The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample.
 Query database Search database - advanced queries. Browse database - peruse all records. Search by combinations of loci (profiles) - including partial matching. List query - find isolates by matching a field to an entered list. Projects - main projects defined in database. Submissions Manage submissions Isolate: 34218 Last updated: 2015-06-30 Update history About BIGSdb
Breakdown Export Analysis Miscellaneous • Single field • Codon usage • Codon usage • Description of database fields • Unique combinations • Sequences - XMFA / concatenated FASTA formats • Codon usage • Description of database fields • Publications • Sequence bin • Sequence bin • BLAST • Description of database fields

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	Finety	ping antig	ens
id	isolate	aliases		year	disease		serogroup	ST		PorA VR1		
1	A4/M1027	B1; Z1001	USA		invasive (unspecified/other)		Α	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; Z1035	Pakistan		meningitis and septicaemia		Α	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		invasive (unspecified/other)		Α	4	ST-4 complex/subgroup IV			
	M00240227		UK		invasive (unspecified/other)		в		ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)		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				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)		Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany		invasive (unspecified/other)		Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89				invasive (unspecified/other)		в		ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099		1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95				invasive (unspecified/other)	-	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2			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		B213; Z1213	Ghana		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			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		B227; Z1227			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.

PubMLST Breakd	Search Browse Profile/ST own: Isolate fields Scheme Contents Home Options	alleles Publications	itions Database submissi	ons		
						Toggle: i
Export dataset						
~						
This script will export the da loci (and/or fields) from a sc		uitable for importing into a	spreadsheet. Select which	ı fields you would lil	ke included. Select loci either fi	rom the locus list or by selecting one or more schemes to include all
				-References	Loci	Schemes
Id V isolate aliases V country continent region year epidemiological year age yr age mth esex	serogroup MLEE designation serotype ET no penicillin penicillin range amoxicillin sulphonamide ceftriaxone	Iffampicin Iffampicin range diprofloxacin oprofloxacin range pending assembly assembly status ENA accession private project comments sender curator	Strain designation	 references PubMed id Full citation 	1165_rDNA 165_rRNA (SSU_RNA) 223_rRNA abc2 abc2 (NEIS1015) acc42 (NEIS1727) acnA (NEIS1729) Al None	Genetic information Proce
disease	chloramphenicol	date entered	Options			Molecular weights — Action —
source	chloramphenicol range	datestamp	Include locus comm			Export protein molecular weights Submit
epidemiology	cefotaxime		Export allele number			GTG/TTG at start codes for methionine
species	cefotaxime range		Use one row per field Include isolate field i		th 'one row' ontion)	
All None					d only with 'one row' option)	

Click Submit.

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

Prohitist Ouery: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/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)	

15.1.1 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' option)

The options fieldset has the following options.

- Include locus common names any common name for the locus is displayed in parentheses following the primary name.
- Export allele numbers the allele designation is included for any locus included.
- Use one row per field this is an alternative output format where instead of each locus and field having a separate column, each field is export on a separate row.
- Include isolate field in row the name of the isolate is included as a separate column when exporting in 'one row per field' fomrmat.
- Export full allele designation record export sender, curator and datestamp information as separate rows when exporting allele designation data.

15.1.2 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.

15.2 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.

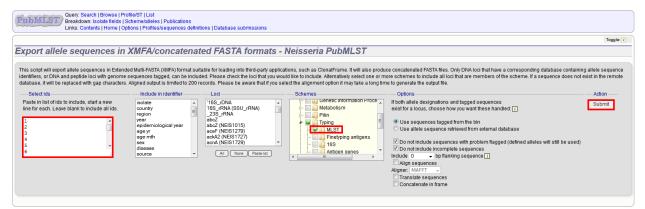
The sequence export function can be accessed by clicking the 'Sequences' link in the Export section of the contents page.



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.

00240227 00282207 7891					Neisseria meningitidis	A	4	SI-4 complex/subgroup IV			
				invasive (unspecified/other)		в		ST-32 complex/ET-5 complex	7	16	
7891				invasive (unspecified/other)		W	1101	ST-22 complex			
	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	20	9	F3-1
00242007				invasive (unspecified/other)		в	1102	ST-18 complex		14	
0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	в	1015	ST-32 complex/ET-5 complex	7	16	
139M	B99; Z1099				Neisseria meningitidis	Α	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	
1		Germany	1999	carrier	Neisseria meningitidis	E	864				
2		Germany	1999	carrier	Neisseria meningitidis	в	854	ST-18 complex			
3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
4		Germany	1999	carrier	Neisseria meningitidis	в	19	ST-18 complex			
S3131	B213; Z1213				Neisseria meningitidis	Α	4	ST-4 complex/subgroup IV	7	13-1	F1-5
5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
8		Germany	1999	carrier	Neisseria meningitidis	в	32	ST-32 complex/ET-5 complex			
S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			
	129 0090/89 139M 0120/95 1 2 3 4 \$3131 5 6 7 8 \$4355 9	129 B92; 21092 009089 1139M B99; 21099 012095 1 2 3 4 4 83131 B213; 21213 5 6 6 7 8 8 84355 B227; 21227	129 B92, Z1092 Germany 0009089 Czech Republic Czech Republic 139M B9, Z1099 Philippines 12095 Germany Germany 2 Germany Germany 3 Germany Germany 4 Germany Germany 5 Germany Germany 6 Germany Germany 7 Germany Germany 8 S227, Z1227 Germany 9 Germany Germany	129 B92, 21092 Cermany 1984 0090/89 Czech Republic 1989 139M B92, 21099 Philippines 1986 012095 Czech Republic 1995 1 1 Germany 1999 2 Germany 1999 3 Germany 1999 4 Germany 1999 4 Germany 1999 6 Germany 1999 5 Germany 1999 6 Germany 1999 6 Germany 1999 6 Germany 1999 6 Germany 1999 8 Germany 1999 8 S27, Z127 Demark 1944 Germany 1999	129 B92,21092 Germany 1964 Invasive (unspecified/other) 0009/089 Czech Republic 1989 Invasive (unspecified/other) 139M B9,21099 Philippines 1986 Invasive (unspecified/other) 12005 Czech Republic 1989 invasive (unspecified/other) 12005 Czech Republic 1989 invasive (unspecified/other) 12 Germany 1999 carrier 3 Germany 1999 carrier 4 Germany 1999 carrier 5 Germany 1999 carrier 6 Germany 1999 carrier 7 Germany 1999 carrier 8 Germany 1999 carrier 8 Germany 1999 carrier 8 Starter Germany 1999 carrier 9 Germany 1999 carrier 1999 carrier	129 B92, 21092 Germany 1984 Imvasive (unspecified/other) Neisseria meningitidis 0000/08 Czech Republic 1989 Invasive (unspecified/other) Neisseria meningitidis 1 Germany 1999 carrier Neisseria meningitidis 1 Germany 1999 carrier Neisseria meningitidis 3 Germany 1999 carrier Neisseria meningitidis 3 Germany 1999 carrier Neisseria meningitidis 3 Germany 1999 carrier Neisseria meningitidis 5 Germany 1999 carrier Neisseria meningitidis 5 Germany 1999 carrier Neisseria meningitidis 5 Germany 1999 carrier Neisseria meningitidis 6 Germany 1999 carrier Neisseria meningitidis 7 Germany 1999 carrier Neisseria meningitidis 8 B227, Z127 Dermark 1974 Invastve (unspecified/other) Neisseria meningitidis 9 Carrier Neisseria meningitidis Seria Meningitidis	129 B92, 21092 Germany 1964 Invasite (unspecified/other) Neisseria meningitidis A 0000/09 Szech Republic 1989 Invasite (unspecified/other) Neisseria meningitidis A 1 Germany 1999 carrier Neisseria meningitidis A 1 Germany 1999 carrier Neisseria meningitidis B 3 Germany 1999 carrier Neisseria meningitidis A 5 Germany 1999 carrier Neisseria meningitidis A 5 Germany 1999 carrier Neisseria meningitidis NG 6 Germany 1999 carrier Neisseria meningitidis NG 7 Germany 1999 carrier Neisseria meningitidis E 8 Germany 1999 carrier Neisseria meningitidis E 8 Germany 1999 carrier Neisseria meningitidis E<	129 B92, Z1092 Germany 1964 Invasive (unspecified/other) Neisseria meningitidis A 1 0090/89 Czech Republic 1989 Invasive (unspecified/other) Neisseria meningitidis A 1 139M B92, 2109 Philippines 1988 Invasive (unspecified/other) Neisseria meningitidis A 1 1 Germany 1999 carrier Neisseria meningitidis E 84 2 Germany 1999 carrier Neisseria meningitidis B 19 3 Germany 1999 carrier Neisseria meningitidis B 19 3 Germany 1999 carrier Neisseria meningitidis B 19 3111 B213, Z1213 Ghana 177 Invasive (unspecified/other) Neisseria meningitidis M 4 5 Germany 1999 carrier Neisseria meningitidis M 4 6 Germany 1999 carrier Neisseria meningitidis NG <td>129 B92,21092 Germany 1964 Invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /II 0000/09 B92,21092 Czech Republic 1989 Invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /II 139M B99,21099 Philippines 1986 Invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /II 12096 Czech Republic 1995 invasive (unspecified/other) Neisseria meningitidis E 864 2 Germany 1999 carrier Neisseria meningitidis W 174 ST-14 complex 3 Germany 1999 carrier Neisseria meningitidis W 174 ST-14 complex 4 Germany 1999 carrier Neisseria meningitidis A 4 ST-14 complex 5 Germany 1999 carrier Neisseria meningitidis A 4 ST-148 complex 5 Germany 1999</td> <td>129 B92,21092 Germary 1964 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 0000/09 Czech Republic 1989 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 0000/09 Philippines 1980 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 012005 Czech Republic 1995 invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 012005 Czech Republic 1995 carrier Neisseria meningitidis E 864 2 Germary 1999 carrier Neisseria meningitidis W 174 ST-14 complex 4 Germary 1999 carrier Neisseria meningitidis A 4 91 ST-14 complex 7 5 Germary 1999 carrier Neisseria meningitidis NG 198 ST-140 complex</td> <td>129 B92,21092 Germary 1964 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 10 0000/09 Czech Republic 1989 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 10 0000/09 Philippines 1980 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 10 012095 Czech Republic 1995 Invashe (unspecified/other) Neisseria meningitidis X 1 ST-1 complex/subgroup /III 5-2 10 1 Germary 1995 carrier Neisseria meningitidis K 1 ST-1 complex/subgroup /II 5-2 10 3 Germary 1999 carrier Neisseria meningitidis K 15-174 complex/subgroup /II 5-2 10 4 Germary 1999 carrier Neisseria meningitidis K 4 51-174 complex/subgroup /II 7</td>	129 B92,21092 Germany 1964 Invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /II 0000/09 B92,21092 Czech Republic 1989 Invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /II 139M B99,21099 Philippines 1986 Invasive (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /II 12096 Czech Republic 1995 invasive (unspecified/other) Neisseria meningitidis E 864 2 Germany 1999 carrier Neisseria meningitidis W 174 ST-14 complex 3 Germany 1999 carrier Neisseria meningitidis W 174 ST-14 complex 4 Germany 1999 carrier Neisseria meningitidis A 4 ST-14 complex 5 Germany 1999 carrier Neisseria meningitidis A 4 ST-148 complex 5 Germany 1999	129 B92,21092 Germary 1964 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 0000/09 Czech Republic 1989 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 0000/09 Philippines 1980 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 012005 Czech Republic 1995 invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 012005 Czech Republic 1995 carrier Neisseria meningitidis E 864 2 Germary 1999 carrier Neisseria meningitidis W 174 ST-14 complex 4 Germary 1999 carrier Neisseria meningitidis A 4 91 ST-14 complex 7 5 Germary 1999 carrier Neisseria meningitidis NG 198 ST-140 complex	129 B92,21092 Germary 1964 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 10 0000/09 Czech Republic 1989 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 10 0000/09 Philippines 1980 Invashe (unspecified/other) Neisseria meningitidis A 1 ST-1 complex/subgroup /III 5-2 10 012095 Czech Republic 1995 Invashe (unspecified/other) Neisseria meningitidis X 1 ST-1 complex/subgroup /III 5-2 10 1 Germary 1995 carrier Neisseria meningitidis K 1 ST-1 complex/subgroup /II 5-2 10 3 Germary 1999 carrier Neisseria meningitidis K 15-174 complex/subgroup /II 5-2 10 4 Germary 1999 carrier Neisseria meningitidis K 4 51-174 complex/subgroup /II 7

Select the isolate or profile records to analyse - these will be pre-selected if you accessed the plugin following a query. Select the loci to include either directly within the loci list and/or using the schemes tree.



Click submit.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
	Toggle: i
Export allele sequences in XMFA/concatenated FASTA formats - Neisseria PubMLST	
This analysis has been submitted to the job queue.	
Please be aware that this job may take a long time depending on the number of sequences to align and how busy the server is. Alignment of hundreds of sequences can take many hours!	
Follow the progress of this job and view the output.	
Please note that the % complete value will only update after the alignment of each locus.	

The job will be submitted to the job queue. Click the link to follow the progress and download the resulting files.

Sequences will be export in XMFA and FASTA file formats.

Putification 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: inished 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.					

15.2.1 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
If both allele designations and tagged sequences exist for a locus, choose how you want these handled: <i>i</i>
Use sequences tagged from the bin Use allele sequence retrieved from external database
 Do not include sequences with problem flagged (defined alleles will still be used) Do not include incomplete sequences Include 0 = bp flanking sequence i Align sequences Aligner: MAFFT Translate 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.

15.3 Profile export

You can export the allelic profiles for any indexed scheme (those containing a primary key field) defined in the sequence definition database.

The profile export function can be accessed by clicking the 'Profiles' link in the Export section of the contents page.

PubMLST Database home Contents	
+D Log in	Toggle: 🚯
Neisseria profile/sequence definitions database The Neisseria PubMLST sequence definition database contains allele and profile data representing record in the isolate database.	g the total known diversity of Neisseria species. Every newST deposited in this database should have a corresponding
Query database Sequence query - query an allele sequence or genome. Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching ordering (all loci together) Locus-specific sequence attribute search - select, analyse and download specific alleles. Search, trovese or enter list of profiles Search by combinations of alleles - induding partial matching. Batch profile query - lookup profiles copied from a spreadsheet. Extract finetype from whole genome data	 Downloads Allele sequences MLST MLST E Profiles Set general options Scheme options Submissions Manage submissions Number of sequences: 1135267 Number of profiles: Show Last updated: 2018-01-24 Profile update history About BIGSdb
Sequences - XMFA / concatenated FASTA formats Sequence comparison - di	d sequences most similar to selected allele. display a comparison between two sequences. analysing allele sequences stored for particular locus.

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

Ì			1			pdhC		
	1	3	4	1	1	1	3	ST-1 complex/subgroup //I ST-1 complex/subgroup //I
2	1	3	4	4	1	23	3 13	ST-1 complex/subgroup //i
3	1	3	3	4	4	23	3	ST-4 complex/subgroup IV
4 5	1	1	2	1	4	2	3	ST-5 complex/subgroup II
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		ST-11 complex/ET-37 complex
12	4	3	2	16	8	11	20	
13	4	10	15	7	8	11	1	ST-269 complex
14	4	1	15	7	8	11	1	ST-269 complex
15	13	3	16	1	3	11	9	ST-364 complex
16	15	9	9	13	8	19	15	ST-4240/6688 complex
17	8	3	13	1	11	12	4	
18	7	8	10	19	10	1	2	ST-18 complex
19	7	8	10	19	8	1	2	ST-18 complex
20	6	8	10	17	10	1	2	ST-18 complex
21	1	5	1	1	2	16	17	
22	11	5	18	8	11	24	21	ST-22 complex
23	10	5	18	9	11	9	17	ST-23 complex/Cluster A3
24 25	2	5	2	7	15	20	5	ST-750 complex
	6	5	2	12	6	13	14	

This will take you to a form with a list box in which the identifiers of the profile definitions you wish to include can be entered. Following a query, these values will be pre-entered. If the box is left empty then all profiles will be included.

PubMLST Database home Contents
10 Log in
Export allelic profiles - Neisseria profile/sequence definitions
Schemes
Please select the scheme you would like to query:
MLST
This script will export allelic profiles in tab-delimited text and Excel formats.
Select STs Adion
Paste in list of ids to include, start a new Submit
3 4
5 •

Click submit.

The export job will be submitted to the job queue.

PubMLST Database home Contents	
+9 Log in	Ξ
Job status viewer	
Status Job id: BIGSdb_012009_1516786630_99221 Submit time: 2018-01-24 09:37:10 Status: finished Statt time: 2018-01-24 09:37:24 Progress: 100% Stop time: 2018-01-24 09:37:36	
Total time: 12 seconds	
Output	
Output • Profiles - Tab-delimited text • Profiles - Excel format • Tar file containing output files	
Please note that job results will remain on the server for 7 days.	

The profiles will be exported in tab-delimited text and Excel formats.

15.4 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.

Output Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/Sequences definitions						
Neisseria PubMLST database						
	epresent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition may be submitted to this database and consequently it should be noted that it does not represent a population					
Query database • Search database - advanced queries. • Browse database - peruse all records. • Search by combinations of loci (profiles) - including partial matching. • List query - find isolates by matching a field to an entered list. • Projects - main projects defined in database.	 Option settings Set general options - including isolate table field handling. Set display and query options for locus, schemes or scheme fields. General information Isolates: 34218 Last update d:: 2015-06-30 Update history About BIGSdb 					
Breakdown Single field Two field Unique combinations Scheme and alleles Publications Sequence bin	Analysis Codon usage Presence/absence status of loci Genome comparator BLAST Miscellaneous • Description of database fields					

Alternatively, it can be accessed following a query by clicking the 'Contigs' button in the Export section at the bottom of the results table.

subgroup III 20 9 F3-1 mplex 14 subgroup I/II 18-1 3 F5-1 subgroup I/II 5-2 10 F3-6 EF-5 complex 7 16	ST-22 complex ST-5 complex/subgroup III ST-18 complex ST-22 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-32 complex/ET-5 complex	1101 5 1102 114 1 1 1	E	Neisseria meningi Neisseria meningi	e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other) e (unspecified/other)	1975 i 2000 i 1984 i	Finland UK	B54; Z1054	M00282207 7891	6 7
Implex 14 mplex 14 subgroup I/II 18-1 subgroup I/II 5-2 To F3-6 ET-5 complex 7 subgroup I/II 5-2 10 F5-1 subgroup I/II 5-2 10 F5-1	ST-18 complex ST-22 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	1102 114 1 1	E V	Neisseria meningi Neisseria meningi	e (unspecified/other) e (unspecified/other)	2000 i 1984 i	UK	B54; Z1054		7
mplex 3 F5-1 subgroup //II 18-1 3 F5-1 subgroup //II 5-2 10 F3-6 ET-5 complex 7 16 subgroup //I subgroup //II 5-2 10 F5-1	ST-22 complex ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	114 1 1	N /	Neisseria meningi	e (unspecified/other)	1984 i				
Subgroup I/II 18-1 3 F5-1 subgroup I/II 5-2 10 F3-6 ET-5 complex 7 16 subgroup I/II 5-2 10 F5-1	ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	1	1	-			Czech Republic		M00242007	8
subgroup I/II 5-2 10 F3-6 ET-5 complex 7 16	ST-1 complex/subgroup I/II	1		Neisseria meningi	e (unspecified/other)				0021/84	9
ET-5 complex 7 16 subgroup I/II 5-2 10 F5-1						1971 i	Canada	B73; Z1073	6748	10
subgroup I/II 5-2 10 F5-1	ST-32 complex/ET-5 complex			Neisseria meningi	e (unspecified/other)	1964 i	Germany	B92; Z1092	129	11
		1015	E	Neisseria meningi	e (unspecified/other)	1989 i	Czech Republic		0090/89	12
14	ST-1 complex/subgroup I/II	1	1	Neisseria meningi		1968	Philippines	B99; Z1099	139M	13
		117	3	Neisseria meningi	e (unspecified/other)	1995 i	Czech Republic		0120/95	14
		864	E	Neisseria meningi	carrier	1999	Germany		1	15
mplex	ST-18 complex	854	E	Neisseria meningi	carrier	1999	Germany		2	16
omplex	ST-174 complex	174	1	Neisseria meningi	carrier	1999	Germany		3	17
mplex	ST-18 complex	19	E	Neisseria meningi	carrier	1999	Germany		4	18
subgroup IV 7 13-1 F1-5	ST-4 complex/subgroup IV	4	1	Neisseria meningi	e (unspecified/other)	1973 i	Ghana	B213; Z1213	S3131	19
omplex	ST-198 complex	198	N	Neisseria meningi	carrier	1999	Germany		5	20
omplex	ST-198 complex	198	N	Neisseria meningi	carrier	1999	Germany		6	21
mplex	ST-60 complex	60	E	Neisseria meningi	carrier	1999	Germany		7	22
ET-5 complex	ST-32 complex/ET-5 complex	32	E	Neisseria meningi	carrier	1999	Germany		8	23
subgroup III 5-1 9 F3-1	ST-5 complex/subgroup III	5	1	Neisseria meningi	e (unspecified/other)	1974 i	Denmark	B227; Z1227	S4355	24
omplex	ST-334 complex	930	E	Neisseria meningi	carrier	1999	Germany		9	25
omplex mplex ET-5 complex subgroup III 5-1 9 F	ST-198 complex ST-60 complex ST-32 complex/ET-5 complex ST-5 complex/subgroup III	198 60 32 5	N E E	Neisseria meningi Neisseria meningi Neisseria meningi Neisseria meningi	carrier carrier carrier e (unspecified/other)	1999 1999 1999 1974 i	Germany Germany Germany Denmark		6 7 8 \$4355	1 2 3 4 5

Select the isolates for which you wish to export contig data for. If the export function was accessed following a query, isolates returned in the query will be pre-selected.

	Profile/ST List s Scheme/alleles Publications Options Profiles/sequences definitions			
			Help 🖓	Toggle: 🚯
Contig analysis and expo	ort			
	hich contigs are associated - use Ctrl or Shift to make multiple agged within the contig - if these loci overlap then the total tagge			
Isolates	Options	Filter by		
1) A4/M1027 2) 120M	Identify contigs with >= 0	Sequence method:	• 0	
7) 7891 10) 6748	FASTA header line: original designation 👻 🚺	Project: Experiment:	v ()	v 0
11) 129E		Minimum length:	- 0	
13) 139M 19) S3131	Action			
24) S4355 *	Reset Submit			

At its simplest, press submit.

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

			-Options				-Filter by			
) A4/M1027			Identify conti	gs with >= 0	 % of sequen 	ce untagged	Sequence metho	od:	- 0	
120M			FASTA head	er line: original	designation 👻	,	Proje	ect:		.
) 7891 0) 6748							Experime	nt 🚽 🖪	•	
1) 129E							Minimum leng		0	
3) 139M 9) S3131							-			
4) S4355		-	-Action							
			Reset	Submit						
L	All None									
ntigs with	>=0% sequ	ence lengt	h untagged							
		natching cont	tigs non-mate	hing contigs						
	Icontige 📤 🛏		load count \$							
⇒ isolate ≑	364	364 🛃	. 0							
A4/M1027		359 🔺	. 0							
	359									
A4/M1027	359 199	199 🛃	. 0							

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

	olates ——				Options				
	4/M1027			▲ Id	lentify contigs with >= 0	 % of sequence untagged 	Sequence method:	- (•
	20M /891			E F/	ASTA header line: original	designation 👻 🕕	Project:		
	6748						Experiment:	v 0	
	129E						Minimum length:	• 0	
	139M S3131				Action				
	S4355			-	Action				
		All None	٦ ۲		Reset Submit				
nt	igs with >	•=0% sec	juence le	ength ui	ntagged				
	-			-	ntagged				
	igs with > isolate ≑ c			contigs	non-matching contigs				
÷	-		matching	contigs	non-matching contigs				
÷	isolate 🗢 c	contigs 🗢	matching count 🔶 d	contigs lownload	non-matching contigs count \$ download				
÷	isolate	contigs \$ 364	matching count ¢ d 364	contigs lownload	non-matching contigs count 💠 download 0				

15.4.1 Filtering by tagged status of contigs

You can also export contigs based on the percentage of the sequence that has been tagged. This is useful to find sequences to target for gene discovery.

In order to export contigs where at least half the sequence has been tagged (and also the remaining contigs in a separate file), select '50' in the dropdown box for %untagged.

Options			
Identify contigs with	>= 50	🗸 % of seq	uence untagged
FASTA header line:	original	designation	▼ i

The resulting table has two download links for each isolate, one for contigs matching the condition, and one for contigs that don't match.

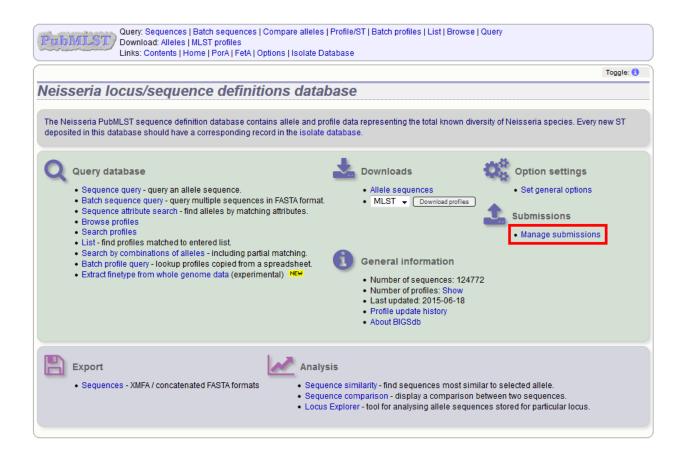
Con	Contigs with >=50% sequence length untagged									
id 🔺	icolato 🔺	contigs 🗢	matchin	g contigs	non-matcl	ning contigs				
iu 👻		conugs -	count 🔶	download	count 🔶	download				
1	A4/M1027	364	163	*	201	*				
2	120M	359	81	*	278	*				
7	7891	199	48	*	151	*				
10	6748	652	393	*	259	*				

CHAPTER 16

Submitting data using the submission system

The automated submission system allows users to submit data (new alleles, profiles, or isolates) to the database curators for assignment and upload to the database. The submission system is enabled on a per-database basis so will not always be available.

If the system is enabled, new submissions can be made by clicking the 'Manage submissions' link on the database front page.



16.1 Registering a user account

You must have an account for the appropriate database in order to use the submission system. On systems utilizing site-wide databases, such as PubMLST, this can be done automatically via the web. Other sites may require you to contact a curator to set this up.

16.2 Allele submission

New allele data can only be submitted from within the appropriate sequence definition database. Submissions consist of one or more new allele sequences for a single locus. You will need to create separate submissions for each locus - this is because different loci may be handled by different curators.

16.2.1 Start

Click the 'alleles' link under submission type on the submission management page.



16.2.2 Select the submission locus

Select the locus from the locus list box:

Query: Sequences Batch sequence Download: Alleles MLST profiles Links: Contents Home PorA Fet/		atch profiles List Browse Query	
Logged in: Keith Jolley (keith2). DLog out Change password			Help 🖉
Manage submissions			
Submit new alleles You need to make a separate submission for each locus any number of new sequences for a single locus as one Filter loci by scheme Filter Capsule Genetic Information Processing Metabolism Cher schemes Loci not in schemes	submission. Sequences should be		

The locus list may be very long in some databases. It may be possible to filter these to those belonging to specific schemes. If the scheme tree is shown, select the appropriate scheme, e.g. 'MLST' and click 'Filter'.

Query: Sequences Batch sequences C Download: Alleles MLST profiles Links: Contents Home PorA FetA Opt		ch profiles List Browse Query	
Logged in: Keith Jolley (keith). HLog out Change password			
Manage submissions			
Submit new alleles			
You need to make a separate submission for each locus for w number of new sequences for a single locus as one submiss			
Filter loci by scheme	Select locus		
Capsule	abcZ (NEIS1015) aceF (NEIS1279)	read length:! 100-199 👻	
Metabolism	acnA (NEIS1729) acnB (NEIS1492) adk	coverage:! 20-49x ↓ assembly:! de novo ↓	
- W L MLST	adk (NEIS0767) aroE	assembly software: Velvet	Action
- J J Finetyping antigens - J Antigen genes	aroE (NEIS1810) -	— FASTA or single sequence	Submit
- June and Contract (20 locus partial genes) - June and Contract (20 locus whole genes)			
- I Differences			

The locus list is now constrained making selection easier.

Query: Sequences Sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database			
Logged in: Keith Jolley (keith). Hog out Change password			
Manage submissions			
Submit new alleles You need to make a separate submission for each locus for with number of new sequences for a single locus as one submission Filter loci by scheme Filter loci by scheme Genetic Information Processing			

16.2.3 Enter details of sequencing method

There are a number of fields that must be filled in so that the curator knows how the sequence was obtained:

• technology - the sequncing platform used, allowed values are:

- 454

- Illumina
- Ion Torrent
- PacBio
- Oxford Nanopore
- Sanger
- Solexa
- SOLiD
- other
- unknown
- read length this is the length of sequencing reads. This is a required field for Illumina data, and not relevant to Sanger sequencing. Allowed values are:
 - <100
 - 100-199
 - 200-299
 - 300-499
 - >500
- coverage the mean number of reads covering each nucleotide position of the sequence. This is not relevant to Sanger sequencing, Allowed values are:
 - <20x
 - 20-49x
 - **-** 50-99x
 - >100x
- assembly the means of generating the submitted sequence from the sequencing reads. Allowed values are:
 - de novo
 - mapped
- assembly software this is a free text field where you should enter the name of the software used to generate the submitted sequence.

16.2.4 Paste in sequence(s)

Paste in the new variant sequences to the box. This can either be a stand- alone sequence or multiple sequences in FASTA format. The sequences must be trimmed to the start and end points of the loci - check existing allele definitions if in doubt. The submission is likely to be rejected if sequences are not trimmed. Click submit.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PortA Options Isolate Database			
Logged in: Keith Jolley (keith). HLog out Change password			
Manage submissions			
			nit any tion Ibmit

The system will perform some basic checks on the submitted sequences. If any of the sequences have been defined previously they must be removed from the submission before you can proceed. Curators do not want to waste their time dealing with previously defined sequences.

Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database		
Logged in: Keith Jolley (keith). It Log out Change password		
Manage submissions		
Error:		
Sequence 'NM432' has already been defined as abcZ-3.		
rew sequences for a single locus as one submission. Seque	which you have new alleles - this is because different loci may have different curators. You can submit any number of ences should be trimmed to the correct start/end sites for the selected locus. - Select locus - Sequence details - technology: Illumina - adk aroE fumC gdh pdC assembly: oftware: Veivet	
MLST Genes Ge	pgm FASTA or single sequence Action >NM322 Submit TTTGATACTGTCGCCGAAGGTTTGGGCGAA Submit ATTCGCATTATTGCGCCGTATCATCAT GTCAGCCATGAGTTGGAAAATGGTTCGAGT GAGGCCTTATGAAAGAGCTCAACGAATGG CAACTTGAGATCGAAGCGCAAGGACGGCTGG	

Assuming the preliminary checks have passed you will then be able to add additional information to your submission.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database		
Logged in: Keith Jolley (keith2). III-Log out Change password	Help 🖾	
Manage submissions		
Submission: BIGSdb_20150709114223_7557_43592 Sequences You are submitting the following abcZ sequences: Download Identifier Length Sequence NM322 433 TITGATACTGTTGCCGAACG GCGGATTGTCGAACTCGATC pending NM21 433 TITGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending NM21 433 TITGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending Lemail Action Updates will be sent to kajolley@gmail.com. Finalize submission! Image: Comporting files Finalize submission! Please upload any supporting files required for curation. Ensure that these are named unambiguously or the appropriate submission item. Individual filesize is limited to 32 MB. Browse No files selected. Upload files Messages	Sequence details technology! Illumina read length: 100-199 coverage: 20-49x assembly! de novo assembly software: Velvet	

16.2.5 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Append'.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database		
Logged in: Keith Jolley (keith2). @Log out Change password	Help 🗗	
Manage submissions		
Identifier Length Sequence Status Assigned allele coverage	! 100-199 ▼ ! 20-49x ▼ ! de novo ▼ ! Velvet	

The message will be attached. A curator may respond to the message and attach their own, with the full conversation becoming part of the submission record.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database		
Logged in: Keith Jolley (keith2). (+ Log out Change password		Help 🗹
Manage submissions		
Submission: BIG Sdb_20150709114223_7557_43592 Sequences You are submitting the following abcZ sequences: Download You are submitting the following abcZ sequences: Download Sequence Identifier Length Sequence Status Assigned allele NM322 433 TTTGATACTGTTGCCGAACG GCGGATTGTCGAACTCGATC pending NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending E-mail Action Finalize submission! Image: Description of the sent to kajolley@gmail.com Finalize submission!	Sequence details technology:! read length:! coverage:! assembly:! assembly software:!	100-199 ↓ 20-49x ↓ de novo ↓
 Supporting files Please upload any supporting files required for curation. Ensure that these are named unambiguously or a appropriate submission item. Individual filesize is limited to 32 MB. 	idd an explanatory note s	so that they can be linked to the
Browse No files selected. Upload files		
Timestamp User Message 2015-07-09 10:44:46+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.		
Message: Append		

16.2.6 Add supporting files

Some submissions will require the attachment of supporting files. This will depend on the policies of the individual databases. Sequences determined by Sanger sequencing should normally have forward and reverse trace files attached.

Files can be added to the submission by clicking the 'Browse' button in the 'Supporting files' section.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database		
Logged in: Keith Jolley (keith2). BLog out Change password		Help 🗹
Manage submissions		
Submission: BIG Sdb_20150709114223_7557_43592 Sequences You are submitting the following abcZ sequences: Download Image: Colspan="2">Sequence You are submitting the following abcZ sequences: Download Image: Colspan="2">Sequence Vou are submitting the following abcZ sequences: Download Image: Colspan="2">Sequence Vou are submitting the following abcZ sequences: Download Image: Colspan="2">Status Assigned allele NM322 433 TITGATACTGTTGCCGAACG GCGGATTGTCGAACTCGATC pending Mmage: Colspan="2">Mage: Colspan="2">Status Assigned allele NM21 433 TITGATACCGTTGCCGAACG GCGGATTGTCGAACTCGATC pending Email Action Updates will be sent to kajolley@gmail.com. Finalize submission! Finalize submission! Finalize submission!	Sequence details technology:! Illu read length:! 100 coverage:! 20- assembly!! de assembly software:! Velv	0-199 ↓ -49x ↓ novo ↓
Please upload any supporting files Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an explanatory note so that they can be linked to the appropriate submission item. Individual filesize is limited to 32 MB. Browse No files selected. Upload files Messages Timestamp User Message 2015-07-09 10:44:46+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates		

Select the file in the selection box, then click 'Upload files'.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database		
Logged in: Keith Jolley (keith2). (Change password		Help 🗗
Manage submissions		
Submission: BIG Sdb_20150709114223_7557_43592 Sequences You are submitting the following abcZ sequences: Download Email Vou are submitting the following abcZ sequences: Download Email Assigned allele NM322 433 TITGATACTGTTCCCGAACG CCGGATTGTCGAACTCGATC pending NM21 433 TITGATACCGTTGCCGAAGG CCGGATTGTCGAACTCGATC pending E-mail Action Enails ubmission updates Supporting files Supporting files	Sequence details technology:! read length:! coverage:! assembly:! assembly software:!	100-199 ↓ 20-49x ↓ de novo ↓
Supporting files Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an explanatory note so that they can be linked to the appropriate submission item. Individual filesize is limited to 32 MB. Browse abcZ.ace Upload files Messages Timestamp User Message 2015-07-09 10:44:46+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.		

The file will be uploaded and shown in a table.

Logged in: Keith Jolley (keith2). I@Log out Change password IMalp I2* Manage submissions Submission: BIG Sdb _20150709114223_7557_43592 Sequences Sequence details You are submitting the following abcZ sequences: Download technology! MM322 433 NM21 433 TITEGATACCETTECCGAACE ecceGATTETCGAACTCGATC NM21 433 TITEGATACCETTECCGAACE ecceGATTETCGAACTCGATC Updates will be sent to kajolley@gmail.com. Finalize submission! V E-mail Optates Supporting files Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an explanatory note so that they can be linked to the appropriate submission lem. Individual filesize is limited to 32 MB. BrowseNo files selected. Upload files
Submission: BIG Sdb_20150709114223_7557_43592 Sequences You are submitting the following abcZ sequences: Download regimered in the following abcZ sequences: Download regimered regimered in the sequences: Download regimered re
Sequences Sequences: Download Sequences: Download technology! Illumina read length: 100-199 read length: 100-199 coverage! 20-49x assembly! de novo
Filename Size Delete bclate selected files Delete selected files Messages Message 2015-07-09 10:44:46+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.

Files can be removed from the submission by checking the appropriate 'Delete' box and clicking 'Delete selected files'.

16.2.7 Finalize submission

Make sure the 'E-mail submission updates' box is checked if you wish to receive E-mail notification of the result of your submission. This setting is remembered between submissions.

Click 'Finalize submission!'.

PrrDMLST Query Sequences Batch sequences Compare alleles Profile/ST Batch profiles Li Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	st Browse Query
Logged in: Keith Jolley (keith2). @Log out Change password	Help 🖓
Manage submissions	
Submission: BIGSdb_20150709114223_7557_43592 	- Sequence details - E-mail
You are submitting the following abcZ sequences: Download 🔤	technology: Illumina VDpdates will be sent to kajolley@gmail.com. read length: 100-199 V VE-mail submission updates
Identifier Length Sequence Status Assigned allele NM322 433 TITGATACTGTTGCCGAACG GCGGATTGTCGAACTCGATC pending NM21 433 TITGATACCGTTGCCGAAGS GCGGATTGTCGAACTCGATC pending	coverage! 20-49x assembly:! de novo assembly: Velvet Finalize submission!
Supporting files	
Please upload any supporting files required for curation. Ensure that these are named unambiguously or 32 MB.	add an explanatory note so that they can be linked to the appropriate submission item. Individual filesize is limited to
Browse No files selected. Upload files	
Filename Size Delete abcZ.ace 1.7 MB	
Delete selected files	
Messages	
Timestamp User Message 2015-07-09 10:44:46+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.	
Message: Append	

Your submission will then be listed under 'Pending submissions' on your submission page.

Outry: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
Logged in: Keith Jolley (keith2). @Log out Change password	Help 🖉
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
alleles MLST profiles	
Pending submissions	
You have submitted the following submissions that are pending curation:	
Submission id Submitted Updated Type Details BIGSdb_20150709114223_7557_43592 2015-07-09 2015-07-09 alleles 2 abcZ sequences	
Return to index page	

16.3 Profile submission

16.3.1 Start

Note: Most MLST databases on PubMLST.org require you to submit an isolate record for each new ST that you wish to be defined. In these cases, you should add the isolate name to the id field of your profile submission and make a corresponding *isolate submission* containing the allelic profile.

Click the appropriate profiles link under submission type on the submission management page.

	10
Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Profile/ST Download: Alleles MLST profiles	Query
Links: Contents Home PorA FetA Options Isolate Database	
Links. Contents Home Fork Ferk Options Isolate Database	
ogged in: Keith Jolley (keith). @Log out Change password	
lanage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track th	e status of any submission.
Submission type:	
• alleles	
MLST profiles	
Return to index page	

Download the Excel submission template.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query: Sequences MLST profiles Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	ry
Logged in: Keith Jolley (keith). (+Log out Change password	
Manage submissions	
Submit new MLST profiles	
Paste in your profiles for assignment using the template available below.	
 Download tab-delimited header for your spreadsheet - use 'Paste Special Text' to paste the data. Download submission template (xlsx format) 	
Please paste in tab-delimited text (include a field header line)	Action
	Submit
ii.	

16.3.2 Paste in profile(s)

Fill in the template. The first column 'id' can be used to enter an identifier that is meaningful to you - it is used to report back the results but is not uploaded to the database. It can be left blank, or the entire column can be removed - in which case individual profiles will be identified by row number.

Copy and paste the entire contents of the submission worksheet. Click submit.

Ţ	LVIci v	LST/DC	ownload: Al	leles MLST	profiles		e alleles Pr solate Datab		h profiles List B	Browse Quen	у	
La	gged in: Kei	ith Jolley (kei	ith). ເ∔Log ou	t Change pa	ssword							
Μ	lanage	e subn	nissio	ns								
\$	Submit n	ew MLST	profiles									
F	Paste in you	ur profiles fo	or assignm	ent using the	e template a	vailable be	low.					
						eet - use 'Pa	aste Special	Text to pas	te the data.			
				nplate (xlsx f								
-	- Please	abcZ	adk	text (include	a field hea fumC		ndhC	nom			Action	
	14	8	5	aroE 32	2	gdh 6	pdhC 43	pgm 32			Submit	
		5 3	2	3 4	6 3	33 8	12 4	2 6				
										.::		

Some basic checks will be performed. These include whether the profile has already been assigned and whether each allele identifier exists. The submission cannot proceed if the checks fail.

Publ	ILST / D	ownload: All	nces Batch eles MLST its Home F	profiles			file/ST Batch profiles List Bro ase	owse Query	
Logged in	Keith Jolley (ke	ith). 🕩Log ou	t Change pas	sword					
Mana	ge subn	nissioi	าร						
Error:									
Row 3: I	Profile has alre	ady been de	efined as ST-	10018.					
Cubmi	t now ML CT	profiles							
	t new MLST		at using the	tomplate a	voiloble beli				
	your profiles fo	-	-				• Text to paste the data.		
	Download tab- Download subr				et-use Pa	ste Special (prext to paste the data.		
Ple	ase paste in tal	b-delimited	text (include	a field head	ler line) —				Action
id	abcZ 8	adk 5	aroE 32	fumC 2	gdh 6	pdhC 43	pgm 32		Submit
	5	7	3	6	33	12	2		
	3	2	4	3	8	4	6		

Provided the checks pass, you will then be able to add additional information to your submission

16.3.3 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Append'.

Query: Sequences Batch sequences Compare alleles Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Di	
Logged in: Keith Jolley (keith2). @Log out Change password	Help 🗹
Manage submissions	
Submission: BIGSdb_20150709115437_16625_11378 Profiles You are submitting the following MLST profiles: Download status Identifier adk abc2 aroE fumc gdh pdhC pgm Status Assigned ST Row 1 5 8 32 2 6 43 32 pending Row 2 7 5 3 6 33 12 2 pending	E-mail Action Dpdates will be sent to kajolley@gmail.com. Finalize submission! E-mail submission updates
Supporting files Please upload any supporting files required for curation. Ensure that these as submission item. Individual filesize is limited to 32 MB. Browse No files selected. Upload files Messages Corresponding isolate data has already been submitted (ids 43721-43722). 	are named unambiguously or add an explanatory note so that they can be linked to the appropriate

The message will be attached. A curator may respond to the message and attach their own, with the full conversation becoming part of the submission record.

Query: Sequences Batch sequences Compare alleles Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Di		
Logged in: Keith Jolley (keith2). @Log out Change password		Help 🖓
Manage submissions		
Submission: BIG Sdb_20150709115437_16625_11378 Profiles	─ E-mail Updates will be sent to kajolley@gmail.com. ♥ E-mail submission updates	Action Finalize submission!
Supporting files Please upload any supporting files required for curation. Ensure that these a submission item. Individual filesize is limited to 32 MB.	are named unambiguously or add an explanatory i	note so that they can be linked to the appropriate
Browse No files selected. Upload files		
Messages Timestamp User Me 2015-07-09 10:56:00+00 Keith Jolley Corresponding isolate data has alreed and the second seco	ssage ady been submitted (ids 43721-43722).	
	di Message: Append	

16.3.4 Add supporting files

Some submissions may require the attachment of supporting files. These files can be added to the submission by clicking the 'Browse' button in the 'Supporting files' section.

Select the file in the selection box, then click 'Upload files'.

16.3.5 Finalize submission

Make sure the 'E-mail submission updates' box is checked if you wish to receive E-mail notification of the result of your submission. This setting is remembered between sessions.

Click 'Finalize submission!'.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Logged in: Keith Jolley (keith2). Hog out Change password
Manage submissions
Submission: BIGSdb 20150709115437 16625 11378
You are submitting the following MLST profiles: Download
Identifier adk abcZ aroE fumC gdh pdhC pgm Status Assigned ST Row 1 5 8 32 2 6 43 32 pending
Row 2 7 5 3 6 33 12 2 pending
Supporting files
Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an explanatory note so that they can be linked to the appropriate submission item. Individual filesize is limited to 32 MB.
Browse No files selected. Upload files
Messages
Timestamp User Message 2015-07-09 10:56:00+00 Keith Jolley Corresponding isolate data has already been submitted (ids 43721-43722).
Message: Append
Message: Append

Your submission will then be listed under 'Pending submissions' on your submission page.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
Logged in: Keith Jolley (keith2). (>Log out Change password	Help 🖉
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
alleles MLST profiles	
Pending submissions	
You have submitted the following submissions that are pending curation:	
Submission id Submitted Updated Type Details BIGSdb_20150709115437_16625_11378 2015-07-09 2015-07-09 profiles 2 MLST profiles	
Return to index page	

16.4 Isolate submission

New isolate data can only be submitted from within the appropriate isolate database. You may be required to submit isolate data if you would like to get a new MLST sequence type defined, but this depends on individual database policy.

16.4.1 Start

Click the 'isolates' link under submission type on the submission management page.

Ouery: Search Profile/ST Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	
Logged in: Keith Jolley (keith). I Log out Change password	Help 🖉
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
isolates genomes (isolate records with associated assembly files)	
Return to index page	
Show closed submissions	

Download the Excel submission template.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). DLog out Change password	
Manage submissions	
Submit new isolates	
Paste in your isolates for addition to the database using the template available below.	
 Enter aliases (alternative names) for your isolates as a semi-colon (;) separated list. Enter references for your isolates as a semi-colon (;) separated list of PubMed ids. You can also upload additional allele fields along with the other isolate data - simply create a new column with the loc 	us name.
 Download tab-delimited header for your spreadsheet - use 'Paste Special O Text' to paste the data. Download submission template (xlsx format) 	
Please paste in tab-delimited text (include a field header line)	Action —
	Submit
h.	

16.4.2 Paste in isolate data

Fill in the template. Some fields are required and cannot be left blank. Check the 'Description of database fields' link on the database contents page to see a description of the fields and allowed values where these have been defined. Where allowed values have been set, the template will have dropdown boxes (although these require newer versions of Excel to work).

Some databases may have hundreds of loci defined, and most will not have a column in the template. You can add new columns for any loci that have been defined and for which you would like to include allelic information for. These locus names must be the primary locus identifier. A list of loci can be found in the 'allowed_loci' tab of the Excel submission template.

Copy and paste the entire contents of the submission worksheet. Click submit.

	eith Jolley (keit			ssword							
nag	e subm	ission	S								
bmit n	iew isolate	s									
ste in yo	ur isolates fo	r addition to	the datab	ase using t	he template	e available bel	ow.				
• Ente	er aliases (ali	ternative na	mes) for vo	our isolates	as a semi	-colon (;) sepa	rated list.				
 Enter 	er references	for your iso	lates as a	semi-color	(;) separat	ed list of Publ	led ids.				
• You	can also upl	oad addition	nal allele fi	elds along	with the oth	ier isolate dat	a - simply o	reate a new	column wi	th the lo	ocus name.
					eet - use 'F	aste Special (Text to p	aste the data	L		
• Dov	wnload subm	ission temp	late (xlsx f	ormat)							
Please	e paste in tab-	delimited te	ext (include	e a field hea	der line) –						1 - N
											- Action
.solat	e aliases	referen	ces	counti	y regio	n year	age yr	age mt	h sex	-	
liseas	e source	epidemi	ology	specie	es serog	roup	MLEE_C	age_mt lesignati	õn		Action
liseas eroty	e source pe	epidemi sero su	ology btype	specie ET no	es serog	roup illin	MLEE o	lesignati .llin_ran	õn		
liseas eroty moxic	e source pe illin	epidemi sero_su sulphon	ology btype amide	specie ET_no ceftri	penic penic	roup illin ceftria	MLEE o penici xone ra	lesignati .llin_ran unge	õn ge		
liseas eroty moxic hlora ifamp	e source pe illin mphenicol vicin	epidemi sero_su sulphon chloram rifampi	ology btype amide phenico cin_ran	specie ET_no ceftri 1_range ge	es serog penic Laxone cefot cipro	roup illin ceftria axime floxacin	MLEE o penici xone ra cefota ciproi	lesignati .llin_ran unge xime_ran loxacin_	õn ge ge range		
moxic infamp	e source pe illin mphenicol vicin g_assembl	epidemi sero_su sulphon chloram rifampi y	ology btype amide phenico cin_ran commen	specie ET_no ceftri 1_range ge ts	es serog penic Laxone cefot cipro abcZ	roup illin ceftria axime floxacin adk	MLEE o penici xone_ra cefota	lesignati .llin_ran unge xime_ran	õn ge ge		
eroty moxic hlora ifamp odhC	e source pe illin mphenicol vicin	epidemi sero_su sulphon chloram rifampi	ology btype amide phenico cin_ran commen PorA V	specie ET_no ceftri 1_range ge ts	es serog penic Laxone cefot cipro	roup illin ceftria axime floxacin adk	MLEE o penici xone ra cefota ciproi	lesignati .llin_ran unge xime_ran loxacin_	õn ge ge range		
eroty moxic hlora ifamp odhC K322	e source pe illin mphenicol vicin g_assembl	epidemi sero_su sulphon chloram rifampi y FetA_VR	ology btype amide phenico cin ran commen PorA V UK	specie ET_no ceftri 1_range ge ts	es serog penic Laxone cefot cipro abc2 PorA	roup illin ceftria axime floxacin adk VR2	MLEE o penici axone ra cefota ciproi aroE	lesignati .llin_ran unge xime_ran loxacin_	õn ge ge range		
eroty moxic hlora ifamp odhC K322	e source pe illin mphenicol icin g_assembl pgm	epidemi sero_su sulphon chloram rifampi y FetA_VR	ology btype amide phenico cin ran commen PorA V UK	specie ET_no ceftri 1_range ge ts R1	es serog penic Laxone cefot cipro abc2 PorA	roup illin ceftria axime floxacin adk VR2	MLEE o penici axone ra cefota ciproi aroE	lesignati .llin_ran unge vxime_ran loxacin fumC	õn ge ge range		
eroty moxic hlora ifamp odhC W322	e source pe illin mphenicol icin g_assembl pgm	epidemi sero_su sulphon chloram rifampi y FetA_VR	ology btype amide phenico cin ran commen PorA V UK	specie ET_no ceftri 1_range ge ts R1	es serog penic Laxone cefot cipro abc2 PorA	roup illin ceftria axime floxacin adk VR2	MLEE o penici axone ra cefota ciproi aroE	lesignati .llin_ran unge vxime_ran loxacin fumC	õn ge ge range	2	
iseas eroty moxic inlora ifamp endin odhC K322 ening W325	e source pe illin mphenicol icin g_assembl ggm ritis and 2	epidemi sero_su sulphon chlotam rifampi y FetA_VR septicae	ology btype amide phenico cin ran commen PorA V UK mia	specie ET_no ceftri j_range ge ts R1 blood 3	serog penic Laxone Cefot cipro abc2 PorA 2015	roup illin ceftrii axime floxacin adk vR2 Neisse: 4	MLEE o penici axone ra cefota ciprof aroE	lesignati llin_ran unge xime_ran loxacin fumC .ngitidis	õn ge range gdh	2	
iseas eroty moxic hlora ifamp odhC K322 eening	e source pe illin mphenicol icin g_assembl ggm ritis and 2	epidemi sero_su sulphon chloram rifampi Y FetA_VR septicae	ology btype amide phenico cin ran commen PorA_V UK mia 4	specie ET_no ceftri j_range ge ts R1 blood 3	s serog penic iaxone cefot cipro abc2 PorA 2015	roup illin ceftrii axime floxacin adk vR2 Neisse: 4	MLEE o penici axone ra cefota ciprof aroE	lesignati llin_ran unge xime_ran loxacin fumC .ngitidis	õn ge range gdh	2	
iseas eroty moxic inlora ifamp endin odhC K322 ening W325	e source pe illin mphenicol icin g_assembl ggm ritis and 2	epidemi sero_su sulphon chloram rifampi y FetA_VR septicae	ology btype amide phenico cin ran commen PorA_V UK mia 4	specie ET_no ceftri j_range ge ts R1 blood 3	serog penic Laxone Cefot cipro abc2 PorA 2015	roup illin ceftrii axime floxacin adk vR2 Neisse: 4	MLEE o penici axone ra cefota ciprof aroE	lesignati llin_ran unge xime_ran loxacin fumC .ngitidis	õn ge range gdh	2	
iseas eroty moxic inlora ifamp endin odhC K322 ening W325	e source pe illin mphenicol icin g_assembl ggm ritis and 2	epidemi sero_su sulphon chloram rifampi y FetA_VR septicae	ology btype amide phenico cin ran commen PorA_V UK mia 4	specie ET_no ceftri j_range ge ts R1 blood 3	serog penic Laxone Cefot cipro abc2 PorA 2015	roup illin ceftrii axime floxacin adk vR2 Neisse: 4	MLEE o penici axone ra cefota ciprof aroE	lesignati llin_ran unge xime_ran loxacin fumC .ngitidis	õn ge range gdh	2	

Some basic checks will be performed. These include checking all field values conform to allowed lists or data types. The submission cannot proceed if any checks fail.

	LII		olate fields	rofile/ST Li Scheme/all ptions Pro	leles Publ	lications ences definit	ions Data	base submis	ssions			
Logged in: Ke	eith Jolley (kei	th). ເ ≱Log out	Change pass	word								
Manag	e subn	nission	S									
Error:												
UK325 has	s problems -	species: 'Ne	isseria mei	ningitis' is n	ot on the lis	st of allowed	values for t	this field.				
Submit n	new isolate	95										
Paste in yo	our isolates fo	or addition to	the databa	se using the	e template	available bel	ow.					
 Ent 	er aliases (a er references I can also up	for your iso	lates as a s	emi-colon (;	;) separate	d list of Publ	Med ids.	reate a new (column wi	th the loc	cus name.	
	wnload tab-d wnload subn				et - use 'Pa	aste Special (D Text' to pa	aste the data				
riedst	e paste in tab	-delimited te	ext (include	a field head	er line) —						Action —	
isolat diseas seroty	e aliases se source pe	s referen epidemi sero_su	ces ology btype	country species ET_no	region serogr penici	oup 11in	MLEE_d penici	age_mth esignatic llin_rang	on		Action	
isolat diseas seroty amoxic chlora	e aliases se source pe cillin amphenicol	s referen epidemi sero_su sulphon L chloram	ces ology btype amide phenicol	country species ET_no ceftria _range	y region s serogr penici xone cefota	coup llin ceftria xime	MLEE_d penici axone_ra cefota	lesignatio llin_rang nge xime_rang	on ge			
isolat diseas seroty amoxic chlora rifamp	e aliases se source pe sillin mphenico picin	s referen epidemi sero_su sulphon L chloram rifampi	ces ology btype amide phenicol cin_rang	country species ET_no ceftria _range e	y region serogr penici xone cefota ciprof	coup Illin ceftria xime loxacin	MLEE_d penici axone_ra cefota ciprof	lesignatio llin_rang nge xime_rang loxacin_r	on ge ge range			
isolat diseas seroty amoxic chlora rifamp	e aliases se source pe cillin amphenicol	s referen epidemi sero_su sulphon chloram rifampi ly	ces ology btype amide phenicol	country species ET_no ceftria range e s	y region s serogr penici xone cefota	coup llin ceftria xime loxacin adk	MLEE_d penici axone_ra cefota	lesignatio llin_rang nge xime_rang	on ge			
isolat diseas seroty amoxic chlora rifamp pendin pdhC UK322	ce aliases se source pe cillin umphenico oicin ng_assembl	s referen epidemi sero_su sulphon chloram rifampi ly FetA_VR	ces ology btype amide phenicol cin_rang comment PorA_VF UK	country species ET_no ceftria range e s	y region serogr penici axone cefota ciprof abcZ PorA_V	coup ceftria xime Cloxacin adk R2	MLEE_d penici axone_ra cefota ciprof aroE	lesignatio llin_rang nge xime_rang loxacin_r	on ge ge range			
isolat diseas seroty amoxic chlora rifamp pendin pdhC UK322 mening B	e aliases se source pe sillin mphenico picin ng_assemb pgm	s referen epidemi sero_su sulphon chloram rifampi ly FetA_VR	es ology btype amide phenicol cin_rang comment PorA_VF UK mia	country species ET_no ceftria _range e s 1	region serogr penici uxone cefota ciprof abcZ PorA_V 2015	coup ceftria xime Cloxacin adk R2	MLEE_d penici axone_ra cefota ciprof aroE	lesignatio llin_rang nge xime_rang loxacin_r fumC	on ge ge range	2		
isolat diseas seroty amoxic chlora rifamp pendin pdhC UK322 mening	e aliases se source pe sillin mmphenico: bicin ng_assemb: pgm gitis and 2	s referen epidemi sero_su sulphon chloram rifampi ly FetA_VR septicae	ces ology btype amide phenicol cin_rang comment PorA_VR UK mia	country species ET_no ceftria range e s 1 blood	y region serogr penici axone cefota ciprof abcZ PorA_V 2015	coup Illin ceftria xime Cloxacin adk TR2 Neissen 4	MLEE_d penici axone_ra cefota ciprof aroE ria meni	lesignatic llin_ranç nge xime_ranç loxacin_i fumC ngitidis	on ge range gdh	2		
isolat diseas seroty amoxic chlora rifamp pendin pdhC UK322 mening B UK325 septic	e aliases se source pe sillin mmphenico: bicin ng_assemb: pgm gitis and 2	s referen epidemi sero_su sulphon chloram rifampi ly FetA_VR septicae	es ology btype amide phenicol cin_rang comment PorA_VF UK mia	country species ET_no ceftria range e s 1 blood	<pre>% region % serogr penici ixone cefota ciprof abc2 PorA_V 2015</pre>	coup Illin ceftria xime Cloxacin adk TR2 Neissen 4	MLEE_d penici axone_ra cefota ciprof aroE ria meni	lesignatic llin_ranç nge xime_ranç loxacin_i fumC ngitidis	on ge range gdh	2		

Provided the checks pass, you will then be able to add additional information to your submission.

16.4.3 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Append'.

	ing the following isolates: Dow							6		- the		F-44 1/D	Dent MD4	D 1/D2		
solate country JK322 UK	y disease meningitis and septicaemia	source		B	2 2	. adk	aroe 4	iumc 3	gan 8	panc. 4	pgm 6	FetA_VR F1-5	PorA_VR1 5	2		
JK325 UK	septicaemia	CSF	Neisseria meningitidis	В	2	3	4	3	18	4	6	F1-5	5-1	2		
E-mail			Action													
odates will be	sent to keith.jolley@zoo.ox.ac.u	ık. 🗍	Finalize submission!													
E-mail subm	nission updates															
Supporting file	•															
oupporting in															mission i	

The message will be attached. A curator may respond to the message and attach their own, with the full conversation becoming part of the submission record.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Schemelalleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). @Log out Change password	Help 🗗
Manage submissions	
Submission: BIGSdb_20150709121747_1342_99624	
You are submitting the following isolates: Download C31	
isolate country disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR	
UK322 UK meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5	2
UK325 UK septicaemia CSF Neisseria meningitidis B 2 3 4 3 18 4 6 F1-5 5-1	2
E-mail Action	
Updates will be sent to keith.jolley@zoo.ox.ac.uk. Finalize submission!	
IV E-mail submission updates	
Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an explanatory note so that they can be lin Individual filesize is limited to 32 MB.	ked to the appropriate submission item.
Browse No files selected. Upload files	
Messages	
Timestamp User Message 2015-07-09 11:19:12+00 Keith Jolley I think UK325 has a new MLST profile requiring definition of a new ST number. Thanks.	
Message: Append	

16.4.4 Add supporting files

You can add any files required to support the submission. You may, for example, wish to include a genome sequence for an isolate record (contigs in FASTA format). If you are doing this, make sure that the filename can be unambiguously linked to the appropriate isolate record and *add a message*.

Files can be added to the submission by clicking the 'Browse' button in the 'Supporting files' section.

Query: Search Browse Profile/S Breakdown: Isolate fields Scher Links: Contents Home Options	me/alleles Publications	tions Datab	ase subr	missions							
Logged in: Keith Jolley (keith). Dog out Change password											Help 🗗
Manage submissions											
Submission: BIGSdb_20150709121747_134 Isolates You are submitting the following isolates: Download	CST										
isolate country disease source UK322 UK meningitis and septicaemia bloo		serogroup a B	bcZ adk 2 3	aroE fum	C gdh 8	pdhC pgn 4 6	FetA_VR F1-5	PorA_VR1 5	PorA_VR2 2		
UK325 UK septicaemia CSF		В	2 3	4 3	18	4 6	F1-5	5-1	2		
E-mail Updates will be sent to keith.jolley@zoo.ox.ac.uk.	Action Finalize submission!										
Supporting files Please upload any supporting files required for cura Individual filesize is limited to 32 MB. Browse_ No files selected. Upload file Messages		amed unam	ibiguousl	y or add a	ı explar	atory note	so that the	y can be lin	ked to the app	propriate submis	ssion item.
Timestamp User 2015-07-09 11:19:12+00 Keith Jolley think UK325		essage Juiring defini	tion of a r	new ST nu	nber. T	hanks.					
				Messag	e: Ap	pend					

Select the file in the selection box, then click 'Upload files'.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). @Log out Change password	Help 🗹
Manage submissions	
Submission: BIGSdb 20150709121747 1342 99624	
You are submitting the following isolates: Download	
isolate country disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2 UK322 UK meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2	
UK325 UK septicaemia CSF Neisseria meningitidis B 2 3 4 3 18 4 6 F1-5 5-1 2	
— E-mail — Action — —	
Updates will be sent to keith.jolley@zoo.ox.ac.uk. Finalize submission!	
E-mail submission updates	
Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an explanatory note so that they can be linked to the appr Individual filesize is limited to 32 MB	opriate submission item.
BrowseUK325_genome_contigs.fas Upload files	
Messages	
Timestamp User Message	
2015-07-09 11:19:12+00 Keith Jolley I think UK325 has a new MLST profile requiring definition of a new ST number. Thanks.	
h.	
Message: Append	

The file will be uploaded and shown in a table.

Profit/ULST Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Logged in: Keith Jolley (keith). @Log out Change password Help [2]
Manage submissions
Submission: BIGSdb_20150709121747_1342_99624
You are submitting the following isolates: Download s
isolate country disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2
UK322 UK meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2 UK325 UK septicaemia CSF Neisseria meningitidis B 2 3 4 3 18 4 6 F1-5 5 2
E-mail Action
Updates will be sent to keith jolley@zoo.ox.ac.uk. Finalize submission!
V E-mail submission updates
Supporting files
Please upload any supporting files required for curation. Ensure that these are named unambiguously or add an explanatory note so that they can be linked to the appropriate submission item.
Individual filesize is limited to 32 MB.
Browse. No files selected. Upload files
Filename Size Delete
UK325_genome_contigs.fas 2 MB 📃
Delete selected files
Timestamp User Message
2015-07-09 11.19:12+00 Keith Jolley I think UK325 has a new MLST profile requiring definition of a new ST number. Thanks.
Message: Append

Files can be removed from the submission by checking the appropriate 'Delete' box and clicking 'Delete selected files'.

16.4.5 Finalize submission

Make sure the 'E-mail submission updates' box is checked if you wish to receive E-mail notification of the result of your submission. This setting is remembered between sessions.

Click 'Finalize submission!'.

Query: Search Browse Profile/ST Breakdown: Isolate fields Scheme Links: Contents Home Options f	alleles Publications	ions Databa	se sub	missio	ins						
Logged in: Keith Jolley (keith). In Log out Change password										He	p 🕑
Manage submissions											
Submission: BIGSdb 20150709121747 1342	99624										
											_
You are submitting the following isolates: Download c	SV										
isolate country disease source		erogroup at	o7 odl	aro F	fumC adb	ndbC	Dam	FotA VD			
isolate country disease source UK322 UK meningitis and septicaemia blood			cz au 2 3	4	3 8	punc 4	pgm 6	FetA_VR F1-5	5	2	
UK325 UK septicaemia CSF	Neisseria meningitidis	В	23	4	3 18	4	6	F1-5	5-1	2	
E-mail	Action										
Updates will be sent to keith.jolley@zoo.ox.ac.uk.	Finalize submission!										
E-mail submission updates											
Supporting files											
Please upload any supporting files required for curatio appropriate submission item. Individual filesize is limit		amed unaml	iguous	sly or ac	dd an expla	natory	note s	o that the	y can be link	ted to the	
Browse. No files selected. Unload files											
Browse No files selected. Upload files Filename Size Delete											
UK325_genome_contigs.fas 2 MB											
Delete selected files											
Messages											
Timestamp User	Me	ssage									
2015-07-09 11:19:12+00 Keith Jolley I think UK325 h	as a new MLST profile req	uiring definit	on of a	new ST	F number. 1	hanks					
				Mes	sage: Ap	pend					

Your submission will then be listed under 'Pending submissions' on your submission page.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). @Log out Change password	Help 🖉
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
isolates	
Pending submissions	
You have submitted the following submissions that are pending curation:	
Submission id Submitted Updated Type Details	
BIGSdb_20150709121747_1342_99624 2015-07-09 2015-07-09 isolates 2 isolates	
Return to index page	

16.5 Genome submission

Submitting genomes uses the same process as standard *isolate submission*. The only difference is that there are a couple of extra required fields in the submission table:

- assembly_filename this is the name of the FASTA file containing the assembly contigs. This must be uploaded as a supporting file you will not be able to finalize the submission until every isolate record has a matching contig file.
- sequence_method the sequencing technology used to generate the sequences. The allowed values are listed on the submission page.

To start the submission, click the 'genomes' link under submission type on the submission management page.

Putin/TLST Query: Search Profile/ST Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	
Logged in: Keith Jolley (keith). [9Log out Change password	Help 🖉
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
isolates genomes isolate records with associated assembly files)	
Return to index page	
Show closed submissions	

Then follow the steps for isolate submission, uploading the contigs files as supporting files.

16.6 Removing submissions from your notification list

Once a submission has been closed by a curator, the results will be displayed in your 'Manage submissions' area. You can remove submissions once you have noted the result by clicking the 'Remove' link.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
Logged in: Keith Jolley (keith2). (HLog out Change password	elp 🗗
Manage submissions	
Submit new data	
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.	
Submission type:	
• alleles • MLST profiles	
Recently closed submissions	
You have submitted the following submissions which are now closed:	
Submission id Submitted Updated Type Details Outcome Remove BIGSdb_20150714071515_10601_27668 2015-07-14 2015-07-14 alleles 3 NEIS0001 (lpxC) sequences Image: Comparison of the sequences </td <td></td>	
Return to index page	

Alternatively, submissions will be removed automatically a specified period of time after closure. By default, this time is 90 days, but this can vary depending on the site configuration.

CHAPTER 17

RESTful Application Programming Interface (API)

The REST API allows third-party applications to retrive data stored within BIGSdb databases or to send new submissions to database curators. To use the REST API, your application will make a HTTP request and parse the response. The response format is JSON (except for routes that request a FASTA or CSV file).

Access to protected resources, i.e. those requiring an account, can be accessed via the API using OAuth authentication.

17.1 Passing additional/optional parameters

If you are using a method called with GET, optional parameters can be passed as arguments to the query URL by adding a '?' followed by the first argument and its value (separated by a '='). Additional parameters are separated by a '&', e.g.

http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates?page=2&page_size=100

Methods called with POST require their arguments to be sent as JSON within the post body.

17.2 Paging using request headers

Paging of results can be selected using query parameters as described above. In this case, methods that support paging will include a paging object in the JSON response. This will contain links to the next page, last page etc.

The API also supports paging using request headers. The following request headers are supported:

- X-OFFSET
- X-PER-PAGE

e.g.

If either of these headers are used, the paging object is no longer returned as part of the JSON response. The response will include the following headers:

- X-OFFSET
- X-PER-PAGE
- X-TOTAL-PAGES

17.3 Resources

- GET / or /db List site resources
- *GET /db/{database}* List database resources
- *GET /db/{database}/classification_schemes* List classification schemes
- GET /db/{database}/classification_schemes/{classification_scheme_id} Retrieve classification scheme information and groups
- *GET /db/{database}/classification_schemes/{classification_scheme_id}/groups/{group_id}* List isolates belonging to a classification scheme group
- GET /db/{database}/loci List loci
- GET /db/{database}/loci/{locus} Retrieve locus record
- GET /db/{database}/loci/{locus}/alleles Retrieve list of alleles defined for a locus
- GET /db/{database}/loci/{locus}/alleles_fasta Download alleles in FASTA format
- GET /db/{database}/loci/{locus}/alleles/{allele_id} Retrieve full allele information
- POST /db/{database}/loci/{locus}/sequence Query sequence to identify allele
- POST /db/{database}/sequence Query sequence to identify allele without specifying locus
- GET /db/{database}/schemes List schemes
- *GET /db/{database}/schemes/{scheme_id}* Retrieve scheme information
- GET /db/{database}/schemes/{scheme_id}/loci Retrieve scheme loci
- GET /db/{database}/schemes/{scheme_id}/fields/{field} Retrieve information about scheme field
- GET /db/{database}/schemes/{scheme_id}/profiles List allelic profiles defined for scheme
- GET /db/{database}/scheme_id}/profiles_csv Download allelic profiles in CSV (tab-delimited) format
- GET /db/{database}/schemes/{scheme_id}/profiles/{profile_id} Retrieve allelic profile record
- *POST /db/{database}/scheme_id}/sequence* Query sequence to extract allele designations/fields for a scheme
- GET /db/{database}/isolates Retrieve list of isolate records
- POST /db/{database}/isolates/search Search isolate database
- GET /db/{database}/isolates/{isolate_id} Retrieve isolate record
- *GET /db/{database}/isolates/{isolate_id}/allele_designations* Retrieve list of allele designations
- GET /db/{database}/isolates/{isolate_id}/allele_designations/{locus} Retrieve full allele designation record
- *GET /db/{database}/isolates/{isolate_id}/allele_ids* Retrieve allele identifiers

- *GET /db/{database}/isolate_id}/schemes/{scheme_id}/allele_designations* Retrieve scheme allele designation records
- *GET /db/{database}/isolate_id}/schemes/{scheme_id}/allele_ids* Retrieve list of scheme allele identifiers
- GET /db/{database}/isolates/{isolate_id}/contigs Retrieve list of contigs
- GET /db/{database}/isolates/{isolate_id}/contigs_fasta Download contigs in FASTA format
- GET /db/{database}/isolates/{isolate_id}/history Retrieve isolate update history
- GET /db/{database}/contigs/{contig_id} Retrieve contig record
- GET /db/{database}/fields Retrieve list of isolate provenance field descriptions
- GET /db/{database}/fields/{field} Retrieve values set for a provenance field
- GET /db/{database}/users/{user_id} Retrieve user information
- GET /db/{database}/projects Retrieve list of projects
- *GET /db/{database}/projects/{project_id}* Retrieve project information
- GET /db/{database}/projects/{project_id}/isolates Retrieve list of isolates belonging to a project
- GET /db/{database}/submissions Retrieve list of submissions
- POST /db/{database}/submissions Create new submission
- GET /db/{database}/submissions/{submission_id} Retrieve submission record
- DELETE /db/{database}/submissions/{submission_id} Delete submission record
- GET /db/{database}/submissions/{submission_id}/messages Retrieve submission correspondence
- POST /db/{database}/submissions/{submission_id}/messages Add submission correspondence
- GET/db/{database}/submissions/{submission_id}/files retrieve list of supporting files uploaded for submission
- POST /db/{database}/submissions/{submission_id}/files Upload submission supporting file
- *GET /db/{database}/submissions/{submission_id}/files/{filename}* Download submission supporting file
- DELETE /db/{database}/submissions/{submission_id}/files/{filename} Delete submission supporting file

17.3.1 GET / or /db - List site resources

Required route parameters: None

Optional query parameters: None

Example request URI: http://rest.pubmlst.org/

Response: List of resource groupings (ordered by name). Groups may consist of paired databases for sequence definitions and isolate data, or any set of related resources. Each group contains:

- name [string] short name (usually a single word)
- description [string] fuller description
- databases [array] list of database objects, each consists of three key/value pairs:
 - name [string] name of database config
 - description [string] short description of resource
 - href [string] URI to access resource

17.3.2 GET /db/{database} - List database resources

These will vary depending on whether the resource is an isolate or a sequence definition database.

Required route parameter: database [string] - Database configuration name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates

Response: Object containing a subset of the following key/value pairs:

- *fields* [string] URI to isolate provenance field information
- isolates [string] URI to isolate records
- schemes [string] URI to list of schemes
- *loci* [string] URI to list of loci
- projects [string] URI to list of projects

17.3.3 GET /db/{database}/classification_schemes - List classification schemes

Required route parameter: database [string] - Database configuration name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/classification_schemes

Response: Object containing:

- records [int] Number of classification schemes.
- classification_schemes [array] List of URIs to classificaton schemes.

17.3.4 GET /db/{database}/classification_schemes/{classification_scheme_id} Retrieve classification scheme information and groups

Sequence definition databases only.

Required route parameters:

- database [string] Database configuration name
- classification_scheme_id [integer] Classification scheme id number

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/classification_schemes/1

Response: Object containing some or all of:

- id [integer] Classification scheme id
- name [text] Name of classification scheme
- · description [text] Description of classification scheme
- relative_threshold [boolean] True if a relative thresold is used
- inclusion_threshold [integer] The threshold for number of loci difference used to group
- groups [array] (sequence definition databases only) list of group objects consisting of:

- id [integer] group id
- profiles [array] list of URIs to profiles belonging to the group

17.3.5 GET /db/{database}/classification_schemes/{classification_scheme_id}/groups/{group_id - List isolates belonging to a classification scheme group

Isolate databases only.

Required route parameters:

- database [string] Database configuration name
- classification_scheme_id [integer] Classification scheme id number
- group_id [integer] Group id number

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/classification_schemes/4/groups/65

Response: Object containing of:

- records [integer] Number of isolates
- isolates [array] List of *URIs to isolate records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results
 - last URI to last page of results
 - return_all URI to page containing all results (paging disabled)

17.3.6 GET /db/{database}/loci - List loci

Required route parameter: database [string] - Database configuration name

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.
- alleles_added_after [date] Include only loci with alleles added after specified date (ISO 8601 format). Only recognized in sequence definition databases.
- alleles_updated_after [date] Include only loci with alleles last modified after specified date (ISO 8601 format). Only recognized in sequence definition databases.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci

Response: Object containing:

- records [integer] Number of loci
- loci [array] List of *URIs to defined locus records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results
 - last URI to last page of results
 - return_all URI to page containing all results (paging disabled)

Note: See also the *scheme specific version*, allowing filtering by date of last allele update for just the loci that are members of a scheme.

17.3.7 GET /db/{database}/loci/{locus} - Retrieve locus record

Provides information about a locus, including links to allele sequences (in seqdef databases).

Required route parameters:

- database [string] Database configuration name
- locus [string] Locus name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ

Response: Object containing a subset of the following key/value pairs:

- id [string] locus name
- data_type [string] 'DNA' or 'peptide'
- allele_id_format [string] 'integer' or 'text'
- allele_id_regex [string] regular expression constraining allele ids
- common_name [string]
- · aliases [array] list of alternative names of the locus
- length_varies [boolean]
- length [integer] length if alleles are of a fixed length
- coding_sequence [boolean]
- orf [integer] 1-6
- schemes [array] list of scheme objects, each consisting of:
 - scheme [string] URI to scheme information
 - description [string]

- min_length [integer] (seqdef databases) minimum length for variable length loci
- max_length [integer] (seqdef databases) maximum length for variable length loci
- alleles [string] (seqdef databases) URI to list of allele records
- alleles_fasta [string] (seqdef databases) URI to FASTA file of all alleles of locus
- curators [array] (seqdef databases) list of URIs to user records of curators of the locus
- publications [array] (seqdef databases) list of PubMed id numbers of papers describing the locus
- full_name [string] (seqdef databases)
- product [string] (seqdef databases)
- description [string] (seqdef databases)
- extended_attributes [array] (seqdef databases) list of extended attribute objects. Each consists of a subset of the following fields:
 - field [string] field name
 - value_format [string] 'integer', 'text', or 'boolean'
 - value_regex [string] regular expression constraining value
 - description [string] description of field
 - length [integer] maximum length of field
 - required [boolean]
 - allowed_values [array] list of allowed values
- genome_position [integer] (isolate databases)

17.3.8 GET /db/{database}/loci/{locus}/alleles - Retrieve list of alleles defined for a locus

Required route parameters:

- database [string] Database configuration name
- locus [string] Locus name

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.
- added_after [date] Include only alleles added after specified date (ISO 8601 format).
- updated_after [date] Include only alleles last modified after specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles

Response: Object containing:

- records [int] Number of alleles.
- last_updated [date] Latest allele addition/modification date (ISO 8601 format).
- alleles [array] List of *URIs to defined allele records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.

- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results
 - last URI to last page of results
 - return_all URI to page containing all results (paging disabled)

17.3.9 GET /db/{database}/loci/{locus}/alleles_fasta - Download alleles in FASTA format

Required route parameters:

- database [string] Database configuration name
- locus [string] Locus name

Optional parameters:

- added_after [date] Include only alleles added after specified date (ISO 8601 format).
- updated_after [date] Include only alleles last modified after specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles_fasta

Response: FASTA format file of allele sequences

17.3.10 GET /db/{database}/loci/{locus}/alleles/{allele_id} - Retrieve full allele information

Required route parameters:

- database [string] Database configuration name
- locus [string] Locus name
- allele_id [string] Allele identifier

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles/5

Response: Object containing the following key/value pairs:

- locus [string] URI to locus description
- allele_id [string] allele identifier
- sequence [string] sequence
- status [string] either 'Sanger trace checked', 'WGS: manual extract', 'WGS: automated extract', or 'unchecked'
- sender [string] URI to user details of sender
- curator [string] URI to user details of curator
- date_entered [string] record creation date (ISO 8601 format)
- datestamp [string] last updated date (ISO 8601 format)

17.3.11 POST /db/{database}/loci/{locus}/sequence - Query sequence to identify allele

Required route parameters:

- database [string] Database configuration name
- locus [string] Locus name

Required additional parameters (JSON-encoded in POST body):

• sequence [string] - Sequence string or base64-encoded FASTA file

Optional parameters (JSON-encoded in POST body):

- details [true/false] Return detailed exact match parameters
- base64 [true/false] Sequence is a base64-encoded FASTA file

Response: Object containing the following key/value pairs:

- exact_matches [array] list of match objects, each consisting of:
 - allele_id
 - href URI to allele record.

additionally if 'details' parameter passed:

- start start position on query
- end end position on query
- orientation forward/reverse
- length length of matched allele
- contig contig name if FASTA file is uploaded

If the locus is linked to field data in client isolate databases, there may also be an object called 'linked_data' containing values and frequencies of the field for the returned allele.

- best_match [object] consisting of key/value pairs (if no exact matches)
 - allele_id
 - href URI to allele record.
 - start start position on query (predicted taking account of allele length)
 - end end position on query (predicted taking account of allele length)
 - orientation forward/reverse
 - length length of matched allele
 - alignment length of BLAST alignment
 - mismatches number of mismatches
 - identity %identity of match
 - gaps number of gaps in alignment

17.3.12 POST /db/{database}/sequence - Query sequence to identify allele without specifying locus

Required route parameters:

• database [string] - Database configuration name

Required additional parameters (JSON-encoded in POST body):

• sequence [string] - Sequence string or base64-encoded FASTA file

Optional parameters (JSON-encoded in POST body):

- details [true/false] Return detailed exact match parameters
- base64 [true/false] Sequence is a base64-encoded FASTA file

Response:

- exact_matches [object] consisting of locus keys, each consisting of array of match objects consisting of:
 - allele_id
 - href URI to allele record.

additionally if 'details' parameter passed:

- start start position on query
- end end position on query
- orientation forward/reverse
- length length of matched allele
- contig contig name if FASTA file is uploaded

If the locus is linked to field data in client isolate databases, there may also be an object called 'linked_data' containing values and frequencies of the field for the returned allele.

Note: This method only supports exact matches. If no match is indicated for a specific locus, use the *locus-specific call* to identify the closest match.

17.3.13 GET /db/{database}/schemes - List schemes

Required route parameter: database [string] - Database configuration name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes

Response:

- records [integer] Number of schemes
- schemes [array] list of scheme objects, each containing:
 - scheme [string] URI to scheme information
 - description [string]

17.3.14 GET /db/{database}/schemes/{scheme_id} - Retrieve scheme information

Includes links to allelic profiles (in seqdef databases, if appropriate). Required route parameters:

- database [string] Database configuration name
- scheme_id [integer] Scheme id number

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1

Response: Object containing a subset of the following key/value pairs:

- id [integer]
- description [string]
- locus_count [integer] number of loci belonging to scheme
- loci [array] list of URIs to locus descriptions
- has_primary_key_field [boolean]
- fields [array] list of URIs to scheme field descriptions
- primary_key_field [string] URI to primary key field description
- profiles [string] URI to list of profile definitions (only seqdef databases)
- profiles_csv [string] URI to tab-delimited file of all scheme profiles
- curators [array] (seqdef databases) list of URIs to user records of curators of the scheme

17.3.15 GET /db/{database}/schemes/{scheme_id}/loci - Retrieve scheme loci

Required route parameters:

- database [string] Database configuration name
- scheme_id [integer] Scheme id number

Optional parameters:

- alleles_added_after [date] Include only loci with alleles added after specified date (ISO 8601 format). Only recognized in sequence definition databases.
- alleles_updated_after [date] Include only loci with alleles last modified after specified date (ISO 8601 format). Only recognized in sequence definition databases.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/loci

Response: Object containing:

- records [integer] Number of loci
- loci [array] List of URIs to defined locus records.

17.3.16 GET /db/{database}/schemes/{scheme_id}/fields/{field} - Retrieve information about scheme field

Required route parameters:

• database [string] - Database configuration name

- scheme_id [integer] Scheme id number
- field [string] Field name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/fields/ST

Response: Object containing the following key/value pairs:

- field [string] field name
- type [string] data type of field (integer or text)
- primary_key [boolean] true if field is the scheme primary key

17.3.17 GET /db/{database}/schemes/{scheme_id}/profiles - List allelic profiles defined for scheme

Required route parameters:

- database [string] Database configuration name
- scheme_id [integer] Scheme id

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.
- added_after [date] Include only profiles added after specified date (ISO 8601 format).
- updated_after [date] Include only profiles last modified after specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles

Response: Object containing:

- records [int] Number of profiles
- last_updated [date] Latest profile addition/modification date (ISO 8601 format).
- profiles [array] List of *URIs to defined profile records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results
 - last URI to last page of results
 - return_all URI to page containing all results (paging disabled)

Note: This method also supports content negotiation. If the request accepts header includes TSV or CSV, then the call is redirected to /*db*/{*database*}/schemes/{scheme_id}/profiles_csv.

17.3.18 GET /db/{database}/schemes/{scheme_id}/profiles_csv - Download allelic profiles in CSV (tab-delimited) format

Required route parameters:

- database [string] Database configuration name
- scheme_id [integer] Scheme id

Optional parameters:

- added_after [date] Include only profiles added after specified date (ISO 8601 format).
- updated_after [date] Include only profiles last modified after specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles_csv

Response: Tab-delimited text file of allelic profiles

17.3.19 GET /db/{database}/schemes/{scheme_id}/profiles/{profile_id} - Retrieve allelic profile record

Required route parameters:

- database [string] Database configuration name
- scheme_id [integer] Scheme id
- profile_id [string/integer] Profile id

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles/11

Response: Object containing the following key/value pairs:

- *primary_key_term* [string/integer] The field name is the primary key, e.g. ST. The value is the primary key value (primary_id used as an argument).
- alleles [object] list of URIs to allele descriptions
- *other_scheme_fields* [string/integer] Each scheme field will have its own value if defined. The field name is the name of the field.
- sender [string] URI to user details of sender
- curator [string] URI to user details of curator
- date_entered [string] record creation date (ISO 8601 format)
- datestamp [string] last updated date (ISO 8601 format)

17.3.20 POST /db/{database}/schemes/{scheme_id}/sequence - Query sequence to extract allele designations/fields for a scheme

Required route parameters:

- database [string] Database configuration name
- scheme_id [integer] Scheme id

Required additional parameters (JSON-encoded in POST body):

• sequence [string] - Sequence string or base64-encoded FASTA file

Optional parameters (JSON-encoded in POST body):

- · details [true/false] Return detailed exact match parameters
- base64 [true/false] Sequence is a base64-encoded FASTA file

Response: Object containing the following key/value pairs:

- exact_matches [array] list of match objects, each consisting of:
 - allele_id
 - href URI to allele record.

additionally if 'details' parameter passed:

- start start position on query
- end end position on query
- orientation forward/reverse
- length length of matched allele
- contig contig name if FASTA file is uploaded

If the locus is linked to field data in client isolate databases, there may also be an object called 'linked_data' containing values and frequencies of the field for the returned allele.

Example curl call to upload a FASTA file 'contigs.fasta' and extract MLST results from Neisseria database:

```
(echo -n '{"base64":true,"sequence": "'; base64 contigs.fasta; echo '"}') |
curl -s -H "Content-Type: application/json" -X POST "http://rest.pubmlst.org/db/
→pubmlst_neisseria_seqdef/schemes/1/sequence" -d @-
```

Note: This method only supports exact matches. If no match is indicated for a specific locus, use the *locus-specific call* to identify the closest match.

17.3.21 GET /db/{database}/isolates - Retrieve list of isolate records

Required route parameter: database [string] - Database configuration name

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.
- added_after [date] Include only isolates added after specified date (ISO 8601 format).
- updated_after [date] Include only isolates last modified after specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates

Response: Object containing:

- records [int] Number of isolates
- isolates [array] List of *URIs to isolate records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:

- previous URI to previous page of results
- next URI to next page of results
- first URI to first page of results
- last URI to last page of results
- return_all URI to page containing all results (paging disabled)

17.3.22 GET /db/{database}/isolates/{isolate_id} - Retrieve isolate record

Required route parameters:

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

Optional parameter:

· provenance_only [integer] - Set to non-zero value to only return provenance metadata

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1

Response: Object containing some or all of the following key/value pairs:

- provenance [object] set of key/value pairs. Keys are defined by calling the */fields route* route. The fields will vary by database but will always contain the following:
 - id [integer]
 - sender [string] URI to user details of sender
 - curator [string] URI to user details of curator
 - date_entered [string] record creation date (ISO 8601 format)
 - datestamp [string] last updated date (ISO 8601 format)
- publications [array] (seqdef databases) list of PubMed id numbers of papers that refer to the isolate
- sequence_bin [object] consists of the following key/value pairs:
 - contigs_fasta [string] URI to FASTA file containing all the contigs belonging to this isolate
 - contigs [string] URI to list of contig records
 - contig_count [integer] number of contigs
 - total_length [integer] total length of contigs
- allele_designations [object] consists of the following key/value pairs:
 - allele_ids URI to list of all allele_id values defined for the isolate
 - designation_count number of allele designations defined for the isolate
 - full_designations URI to list of full allele designation records
- schemes [array] list of scheme objects, each containing some of the following:
 - description [string] description of scheme
 - loci_designated_count [integer] number of loci within scheme that have an allele designated for this isolate.
 - allele_ids [string] URI to list of all allele_id values defined for this scheme for this isolate
 - full_designations [string] URI to list of full allele designation records for this isolate

- fields [object] consisting of key/value pairs where the key is the name of each scheme field
- classification_schemes [object] consisting of key/value pairs, where each key is the name of the classification scheme and the value is an object consisting of:
 - * href [string] URI to classification scheme description
 - * groups [array] list of group objects consisting of:
 - · group [integer] group id
 - · records [integer] number of isolates in group
 - · isolates [string] URI to classification group record containing URIs to member isolate records
- projects [array] list of project objects, each containing the following:
 - id [string] URI to project information
 - description [string] description of project
- history [string] URI to isolate history record
- new_version [string] URI to newer version of record
- old_version [string] URI to older version of record

17.3.23 GET /db/{database}/isolates/{isolate_id}/allele_designations - Retrieve list of allele designation records

Required route parameters:

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_designations

Response: Object containing:

- records [int] Number of allele designations
- allele_designations [array] List of *URIs to allele designation records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results
 - last URI to last page of results
 - return_all URI to page containing all results (paging disabled)

17.3.24 GET /db/{database}/isolates/{isolate_id}/allele_designations/{locus} - Retrieve full allele designation record

Required route parameters:

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier
- locus [string] Locus name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_designations/ BACT000065

Response: List of allele_designation objects (there may be multiple designations for the same locus), each containing:

- locus [string] URI to locus description
- allele_id [string]
- method [string] either 'manual' or 'automatic'
- status [string] either 'confirmed' or 'provisional'
- comments [string]
- sender [string] URI to user details of sender
- curator [string] URI to user details of curator
- datestamp [string] last updated date (ISO 8601 format)

17.3.25 GET /db/{database}/isolates/{isolate_id}/allele_ids - Retrieve allele identifiers

Required route parameters:

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_ids

Response: Object containing:

- records [int] Number of allele id objects
- allele_ids [array] List of allele id objects, each consisting of a key/value pair where the key is the locus name. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results

- last URI to last page of results
- return_all URI to page containing all results (paging disabled)

17.3.26 GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_designations - Retrieve scheme allele designation records

Required route parameters:

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier
- scheme_id [integer] Scheme identifier

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/schemes/1/allele_designations

Response:

- · records [int] Number of allele designation objects
- allele_designations [array] List of *allele designation objects* for each locus in the specified scheme that has been designated.

17.3.27 GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_ids -Retrieve list of scheme allele identifiers

Required route parameters:

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier
- scheme_id [integer] Scheme identifier

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/schemes/1/allele_ids

Response:

- records [int] Number of allele id objects
- allele_ids [array] List containing allele id objects for each locus in the specified scheme that has been designated. Each allele_id object contains a key which is the name of the locus with a value that may be either a string, integer or array of strings or integers (required where there are multiple designations for a locus). The data type depends on the allele_id_format set for the specific locus.

17.3.28 GET /db/{database}/isolates/{isolate_id}/contigs - Retrieve list of contigs

Required route parameters:

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/contigs

Response: Object containing:

- records [int] Number of contigs
- contigs [array] List of *URIs to contig records* Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results
 - last URI to last page of results
 - return_all URI to page containing all results (paging disabled)

17.3.29 GET /db/{database}/isolates/{isolate_id}/contigs_fasta - Download contigs in FASTA format

Required route parameters:

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

Optional parameter:

• header [string] - either 'original_designation' or 'id' (default is 'id'). This selects whether the FASTA header lines contain the originally uploaded FASTA headers or the sequence bin id numbers.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/contigs_fasta?header= original_designation

Response: FASTA format file of isolate contig sequences

17.3.30 GET /db/{database}/isolates/{isolate_id}/history - Retrieve isolate update history

Required route parameters:

- database [string] Database configuration name
- isolate_id [integer] Isolate identifier

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/history

Response: Object containing:

- records [int] Number of updayes
- contigs [array] List of update objects each consisting of the following key/value pairs:

- curator [string] URI to user details of curator
- timestamp [string] Time of update
- actions [array] List of update descriptions [strings]

17.3.31 POST /db/{database}/isolates/search - Search isolate database

Required route parameters:

• database [string] - Database configuration name

Optional parameters (appended to URI):

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Query parameters (JSON-encoded in POST body):

You must include at least one query parameter.

Flattened parameter names in the following forms are supported:

- field.{field} key/value pairs for provenance fields. Supported field names can be found by calling the */fields route*. The fields will vary by database.
- locus.{locus} key/value pairs of locus and its allele designation. Supported locus names can be found by calling the */loci route*.
- scheme.{scheme_id}.{scheme_field} key/value pairs of scheme fields and their values. Supported field names can be determined by following routes from the */schemes route*.

Parameters have to be flattened rather than using nested attributes to support passing via OAuth.

Example method call using curl: The following searches for *Neisseria* ST-11 isolates from Europe in 2015 (MLST is scheme#1 in this database).

```
curl -s -H "Content-Type: application/json" -X POST \
"http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/search" \
-d '{"field.continent":"europe", "field.year":2015, "scheme.1.ST":11}'
```

Response: Object containing:

- records [int] Number of isolates
- isolates [array] List of URIs to isolate records. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results
 - last URI to last page of results
 - return_all URI to page containing all results (paging disabled)

17.3.32 GET /db/{database}/contigs/{contig_id} - Retrieve contig record

Required route parameters:

- database [string] Database configuration name
- contig_id [integer] Contig identifier

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/contigs/180062

Response: Contig object consisting of the following key/value pairs:

- id [integer] contig identifier
- isolate_id [integer] isolate identifier
- sequence [string] contig sequence
- length [integer] length of contig sequence
- method [string] sequencing method
- sender [string] URI to user details of sender
- curator [string] URI to user details of curator
- date_entered [string] record creation date (ISO 8601 format)
- datestamp [string] last updated date (ISO 8601 format)
- loci [array] list of sequence tag objects consisting of:
 - locus [string] URI to locus description
 - locus_name [string]
 - start [integer]
 - end [integer]
 - direction [string] forward/reverse
 - complete [boolean] true/false

17.3.33 GET /db/{database}/fields - Retrieve list of isolate provenance field descriptions

Required route parameters:

• database [string] - Database configuration name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/fields

Response: Array of field objects, each consisting of some or all of the following key/value pairs:

- name [string] name of field
- type [string] data type (int, text, date, float)
- length [integer] maximum length of field
- required [boolean] true if field value is required
- min [integer] minimum value for integer values

- max [integer] maximum value for integer values
- regex [string] regular expression that constrains the allowed value of the field
- comments [string]
- · allowed values [array] list of allowed values for the field
- · values [string] URI to list of used field values

17.3.34 GET /db/{database}/fields/{field} - Retrieve values set for a provenance field

Required route parameters:

- database [string] Database configuration name
- field [string] Provenance metadata field name

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/fields/country

Response: Object containing:

- records [int] Number of values
- values [array] List of values used in isolate records. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results
 - last URI to last page of results
 - return_all URI to page containing all results (paging disabled)

17.3.35 GET /db/{database}/users/{user_id} - Retrieve user information

Users may be data submitters or curators.

Required route parameters:

- database [string] Database configuration name
- user_id [integer] User id number

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/users/2

Response: Object containing the following key/value pairs:

- id [integer] user id number
- first_name [string]

- surname [string]
- affiliation [string] institutional affiliation
- email [string] E-mail address

17.3.36 GET /db/{database}/projects - Retrieve list of projects

Required route parameter: database [string] - Database configuration name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/projects

Response:

- projects [array] List of project objects, each containing:
 - project [string] URI to project information
 - description [string]
 - isolate_count [integer] number of isolates in project

17.3.37 GET /db/{database}/projects/{project_id} - Retrieve project information

Required route parameters:

- database [string] Database configuration name
- project_id [integer] Project id number

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/projects/3

Response: Object containing a subset of the following key/value pairs:

- id [integer]
- description [string]
- isolates [string] URI to list of URIs of member isolate records.

17.3.38 GET /db/{database}/projects/{project_id}/isolates - Retrieve list of isolates belonging to a project

Required route parameter:

- database [string] Database configuration name
- project_id [integer] Project id number

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/projects/3/isolates

Response: Object containing:

- records [int] Number of isolates in the project
- isolates [array] List of URIs to isolate records. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results
 - last URI to last page of results
 - return_all URI to page containing all results (paging disabled)

17.3.39 GET /db/{database}/submissions - retrieve list of submissions

Required route parameter: database [string] - Database configuration name

Optional parameters:

- type [string] either 'alleles', 'profiles' or 'isolates'
- status [string] either 'closed' or 'pending'
- page [integer]
- page_size [integer]
- return_all [integer] Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/submissions

Response: Object containing:

- · records [int] Number of submissions
- submissions [array] List of URIs to submission records
- paging [object] Some or all of the following:
 - previous URI to previous page of results
 - next URI to next page of results
 - first URI to first page of results
 - last URI to last page of results
 - return_all URI to page containing all results (paging disabled)

17.3.40 POST /db/{database}/submissions - create new submission

Required route parameter: database [string] - Database configuration name

Required additional parameters (JSON-encoded in POST body):

- type [string] either:
 - alleles (sequence definition databases only)
 - profiles (sequence definition databases only)
 - isolates (isolate databases only)

- genomes (isolate databases only)

The following are required with the specified database type:

Allele submissions

- locus [string] name of locus
- technology [string] name of sequencing technology: either '454', 'Illumina', 'Ion Torrent', 'PacBio', 'Oxford Nanopore', 'Sanger', 'Solexa', 'SOLiD', or 'other'
- read_length [string] read length of sequencing: either '<100', '100-199', '200-299', '300-499', '>500', or any positive integer (only required for Illumina)
- coverage [string] mean coverage of sequencing: either '<20x', '20-49x', '50-99x', '>100x', or any positive integer (only required for Illumina)
- assembly [string] assembly method: either 'de novo' or 'mapped'
- software [string] name of assembly software
- sequences [string] either single raw sequence or multiple sequences in FASTA format

Profile submissions

- scheme_id [int] scheme id number
- profiles [string] tab-delimited profile data this should include a header line containing the name of each locus

Isolate submissions

• isolates [string] - tab-delimited isolate data - this should include a header line containing each field or locus included

Genome submissions

• isolates [string] - tab-delimited isolate data - this should include a header line containing each field or locus included as well as for 'assembly_filename' and 'sequence_method'. The 'sequence_method' should be either '454', 'Illumina', 'Ion Torrent', 'PacBio', 'Oxford Nanopore', 'Sanger', 'Solexa', 'SOLiD', or 'other'. Follow-ing submission, contig files should be uploaded with the same names as set for 'assembly_filename'. This can be done using the *file upload route*.

Optional parameters:

- message [string] correspondence to the curator
- email [int] set to 1 to enable E-mail updates (E-mails will be sent to the registered user account address).

Response: Object containing:

• submission - URI to submission record

For genome submissions, the response object will also contain:

- missing_files [array] List of filenames that need to be uploaded to complete the submission. These filenames are defined in the 'assembly_filename' field of the isolate record upload. The files should contain the contig assemblies.
- message [string] 'Please upload missing contig files to complete submission.'

17.3.41 GET /db/{database}/submissions/{submission_id} - Retrieve submission record

Required route parameters:

- database [string] Database configuration name
- submission_id [string] Submission id

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740

Response: Object containing some of the following:

- id [string] Submission id
- type [string] Either 'alleles', 'profiles', 'isolates'
- date_submitted [string] Submission date (ISO 8601 format)
- datestamp [string] Last updated date (ISO 8601 format)
- submitter [string] URI to user details of submitter
- curator [string] URI to user details of curator
- status [string] either 'started', 'pending', or 'closed'
- outcome [string] either 'good' (data uploaded), 'bad' (data rejected), or 'mixed' (parts of submission accepted)
- correspondence [array] List of correspondence objects in time order. Each contains:
 - user [string] URI to user details of user
 - timestamp [string]
 - message [string]

Allele submissions

- · locus [string] name of locus
- technology [string] name of sequencing technology: either '454', 'Illumina', 'Ion Torrent', 'PacBio', 'Oxford Nanopore', 'Sanger', 'Solexa', 'SOLiD', or 'other'
- read_length [string] read length of sequencing: either '<100', '100-199', '200-299', '300-499', '>500', or any positive integer (only required for Illumina)
- coverage [string] mean coverage of sequencing: either '<20x', '20-49x', '50-99x', '>100x', or any positive integer (only required for Illumina)
- assembly [string] assembly method: either 'de novo' or 'mapped'
- software [string] name of assembly software
- seqs [array] List of sequence objects each containing:
 - seq_id [string] Sequence identifier
 - assigned_id [string] Allele identifier if uploaded to the database (otherwise undefined)
 - status [string] Either 'pending', 'assigned', or 'rejected'
 - sequence [string]

Profile submissions

- scheme [string] URI to scheme information
- profiles [array] List of profile record objects. Each contains:
 - profile_id [string] Record identifier

- assigned_id [string] Profile identifier if uploaded to the database (otherwise undefined)
- status [string] Either 'pending', 'assigned', or 'rejected'
- designations [object] containing key/value pairs for each locus containing the allele identifier

Isolate submissions

• isolates [array] - List of isolate record objects. Each contains key/value pairs for included fields.

17.3.42 DELETE /db/{database}/submissions/{submission_id} - Delete submission record

You must be the owner and the record must be closed.

Required route parameters:

- database [string] Database configuration name
- submission_id [string] Submission id

Optional parameters: None

ExamplerequestURI:http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740

Response: message [string] - 'Submission deleted.'

17.3.43 GET /db/{database}/submissions/{submission_id}/messages - Retrieve submission correspondence

Required route parameters:

- database [string] Database configuration name
- submission_id [string] Submission id

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740/messages

Response: Array of correspondence objects in time order. Each contains:

- user [string] URI to user details of user
- timestamp [string]
- message [string]

17.3.44 POST /db/{database}/submissions/{submission_id}/messages - Add submission correspondence

Required route parameters:

- database [string] Database configuration name
- submission_id [string] Submission id

Required additional parameter (JSON-encoded in POST body):

• message [string] - Message text

Optional parameters: None

Response: message [string] - 'Message added.'

17.3.45 GET /db/{database}/submissions/{submission_id}/files - Retrieve list of supporting files uploaded for submission

Required route parameters:

- database [string] Database configuration name
- submission_id [string] Submission id

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_ 20151013081836_14559_14740/files

Response: Array of URIs to files

17.3.46 POST /db/{database}/submissions/{submission_id}/files - Upload submission supporting file

Required route parameters:

- database [string] Database configuration name
- submission_id [string] Submission id

Required additional parameters (JSON-encoded in POST body):

- filename [string] Name of file to store within submission
- upload [base64 encoded data] Raw file data

Optional parameters: None

Response: message [string] - 'File uploaded.'

17.3.47 GET /db/{database}/submissions/{submission_id}/files/{filename} - Download submission supporting file

Required route parameters:

- database [string] Database configuration name
- submission_id [string] Submission id
- filename [string] Name of file

Optional parameters: None

Response: File download

17.3.48 DELETE /db/{database}/submissions/{submission_id}/files/{filename} · Delete submission supporting file

Required route parameters:

- database [string] Database configuration name
- submission_id [string] Submission id
- filename [string] Name of file

Optional parameters: None

Response: message [string] - 'File deleted.'

17.4 Authentication

Protected resources, i.e. those requiring a user to log in, can be accessed via the API using OAuth (1.0A) authentication (see IETF RFC5849 for details). Third-party client software has to be registered with the BIGSdb site before they can access authenticated resources. The overall three-legged flow works as follows:

- 1. Developer signs up and gets a consumer key and consumer secret specific to their application.
- 2. Application gets a request token and directs user to authorization page on BIGSdb.
- 3. BIGSdb *asks user for authorization* for application to access specific resource using their credentials. A verifier code is provided.
- 4. The application exchanges the request token and OAuth verifier code for an *access token and secret* (these do not expire but may be revoked by the user or site admin).
- 5. Application uses access token/secret to request session token (this is valid for 12 hours).
- 6. All calls to *access protected resources* are signed using the session token/secret and consumer key/secret.

It is recommended that application developers use an OAuth library to generate and sign requests.

17.4.1 Developer sign up to get a consumer key

Application developers should apply to the site administrator of the site running BIGSdb. The administrator can *generate a key and secret* using a script - both of these will need to be used by the application to sign requests.

The client id is usually a 24 character alphanumeric string. The secret is usually a 42 character alphanumeric (including punctuation) string, e.g.

- client_id: efKXmqp2D0EB1MBkZaGC21Pf
- client_secret: F\$M)_+fQ2AFFB2YBDfF9fpHF^qSWJdmmN%L4Fxf5Gur3

17.4.2 Getting a request token

- Relative URL: /db/{database}/oauth/get_request_token
- Supported method: GET

The application uses the consumer key to obtain a request token. The request token is a temporary token used to initiate user authorization for the application and will expire in 60 minutes. The request needs to contain the following parameters and to be signed using the consumer secret:

- oauth_consumer_key
- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')

- oauth_signature
- oauth_timestamp (UNIX timestamp seconds since Jan 1 1970) this must be within 600 seconds of the current time.
- oauth_callback ('oob' for desktop applications)
- oauth_nonce (random string)
- oauth_version ('1.0')

If the application has been registered and has been granted permission to access the specific resource, a JSON response will be returned containing the following parameters:

- oauth_token
 - This is the request token. It is usually a 32 character alphanumeric string.
 - e.g. fKFm0WNhCfbEX8zQm6qhDA8K23FOWDGE
- oauth_token_secret
 - This is the secret associated with the request token. It is usually a 32 character alphanumeric string.
 - e.g. aZ0fncP7i5w5jlebdK5zyQ4vrRRVcdnv
- oauth_callback_confirmed
 - This parameter is always set to true.

17.4.3 Getting user authorization

Once a request token has been obtained, this can be used by the end user to grant permission to access a specific resource to the application. The application should direct the user to the client authorization page (authorizeClient) specific to a database within BIGSdb, e.g. http://pubmlst.org/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_neisseria_seqdef& page=authorizeClient&oauth_token=fKFm0WNhCfbEX8zQm6qhDA8K23FOWDGE

The user will be asked if they wish to grant access to the application on their behalf:

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home Options PubMLST.org Isolate Database			
Logged in: Keith Jolley (keith). Log out Change password			
Authorize client software to access your account			
Do you wish for the following application to access	data on your behalf?		
Application Resource	Action		
testApp version 1.0 Aeromonas locus/seque	nce definitions Cancel Authorize		
You will be able to revoke access for this application at any time.			

If they authorize the access, they will be presented with a verifier code. This should be entered in to the client application which will use this together with the request token to request an access token.

PubMLST)	Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home Options PubMLST.org Isolate Database	
Logged in: Keith Jolley (keith). Log out Change password		
Authorize cl	lient software to access your account	
	testApp version 1.0 to access Aeromonas locus/sequence definitions on your behalf. erification code when asked by testApp.	
Verification code: 20	qaMxNrP	
This code is valid for	r 60 minutes.	

The verifier code is valid for 60 minutes.

17.4.4 Getting an access token

- Relative URL: /db/{database}/oauth/get_access_token
- Supported method: GET

The application uses the request token, verifier code and its consumer key to obtain an access token. The access token does not expire but can be revoked by both the end user or the site administrator. The request needs to contain the following parameters and to be signed using the consumer secret and request token secret:

- oauth_consumer_key
- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_token (request token)
- oauth_timestamp (UNIX timestamp seconds since Jan 1 1970) this must be within 600 seconds of the current time.
- oauth_nonce (random string)
- oauth_version ('1.0')

If the application has been registered and has been granted permission to access the specific resource, a JSON response will be returned containing the following parameters:

- oauth_token
 - This is the access token. It is usually a 32 character alphanumeric string.
 - e.g. SDrC74ZV15SYSqY8IWZqrRxnyDnNGVFO
- oauth_token_secret
 - This is the secret associated with the access token. It is usually a 32 character alphanumeric string.
 - e.g. tYI2SPzgiO02IRVzW4JR1ez6Vvm4gVyv

17.4.5 Getting a session token

- Relative URL: /db/{database}/oauth/get_session_token
- Supported method: GET

The application uses the access token and its consumer key to obtain a session token. The session token is valid for 12 hours before it expires. The request needs to contain the following parameters and to be signed using the consumer secret and access token secret:

- oauth_consumer_key
- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_token (access token)
- oauth_timestamp (UNIX timestamp seconds since Jan 1 1970) this must be within 600 seconds of the current time.
- oauth_nonce (random string)
- oauth_version ('1.0')

If the application has been registered and has been granted permission to access the specific resource, a JSON response will be returned containing the following parameters:

- oauth_token
 - This is the session token. It is usually a 32 character alphanumeric string.
 - e.g. H8CjIS8Ikq6hwCUqUfF1l4pTaCY18Ljw
- oauth_token_secret
 - This is the secret associated with the session token. It is usually a 32 character alphanumeric string.
 - e.g. RfponbaNPO7tkZ2miHFISk0pMndePNfJ

17.4.6 Accessing protected resources

• Supported method: GET

The application uses the session token and its consumer key to access a protected resource. The request needs to contain the following parameters and to be signed using the consumer secret and session token secret:

- oauth_consumer_key
- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_token (session token)
- oauth_timestamp (UNIX timestamp seconds since Jan 1 1970) this must be within 600 seconds of the current time.
- oauth_nonce (random string)
- oauth_version ('1.0')

CHAPTER 18

Frequently asked questions (FAQs)

18.1 General

1. What is the minimum specification of hardware required to run BIGSdb?

The software will run on fairly modest hardware - a number of PubMLST mirrors have been set up on virtual machines with 1 processor core and 4 GB RAM. This should be considered an absolute minimum specification though. For an installation with only local users, the following minimum is recommended:

- 4 processor cores
- 16 GB RAM
- 50 GB partition for temporary files
- 100 GB partition for databases

As usual, the more RAM that is available the better. Ideally you would want enough RAM that the whole database(s) can reside in memory (an approximation is roughly twice the total size of your contigs), although this is not absolutely required.

Offline jobs, such as *Genome Comparator* will use multiple cores (depending on the settings in bigsdb.conf), so if you want to run multiple jobs in parallel then you may want more cores (and memory). Tagging of new genomes using the offline *autotagger* is usually run in multi-threaded mode so the more cores available the faster this will be.

As a comparison, the PubMLST site is run on two machines - separate web and database servers. All offline jobs and tagging of genomes is performed on the database server. These have the following specification:

- web server: 40 cores, 128GB RAM
- database server: 64 cores, 1TB RAM, 3TB RAID 10 local storage

2. Why might icons be missing when using Internet Explorer?

This can occur if you have Compatibility Mode enabled. BIGSdb generates valid HTML5 and Compatibility Mode should not be used. Please ensure this is not enabled in the Internet Explorer tools section.

18.2 Installation

1. BIGSdb is accumulating files in various temp directories - is this normal and how do I clean them out?

See: Periodically delete temporary files.

2. BIGSdb is complaining of an invalid script path - what does this mean?

In your database config.xml file system tag are two attributes - script_path_includes and curate_path_includes. These contain regexes that the web url to your script (bigsdb.pl and bigscurate.pl respectively) must match. This prevents somebody from accessing a private database using an instance of bigsdb.pl that is not in a protected directory if you're using apache authentication.

So, if you access the script from http://localhost/cgi-bin/bigsdb/bigsdb.pl then you can set script_path_includes to something like "/bigsdb/" (which is the default), or "/cgi-bin/" or just "/" if you don't care about this check.

18.3 Administration

1. How can I make some isolates public but not others?

The easiest way to do this is to set up two or more separate configuration directories that refer to the database. The URLs to access these will differ by the value of the 'db' attribute, which refers to the name of the configuration directory (in /etc/bigsdb/dbases/). The database view accessed by each of these configurations can be different as can the access restrictions.

Example:

We have a database 'bigsdb_test' that contains data, only some of which we wish to make publicly available. The isolates to make public are all members of a project. First we can make a view of the isolates table that contains only isolates within this project.

For isolates in project id 3, create a database view by logging in to psql as the postgresql user. We will name this view 'public'.:

```
sudo su postgres
psql bigsdb_test
CREATE VIEW public AS SELECT * FROM isolates WHERE id IN (SELECT isolate_id
FROM project_members WHERE project_id=3);
GRANT SELECT ON public TO apache;
```

Create a private configuration that can access everything in the database in /etc/bigsdb/dbases/test_private. This will be accessible from http://IP_ADDRESS/cgi-bin/bigsdb/bigsdb.pl?db=test_private.

The important attributes to set in the system tag of the config.xml file in this directory are::

```
view="isolates"
read_access="authenticated_users"
```

This means that anyone with an account can log in and view all the isolates (because the view is set to the isolates table).

Now create a public configuration in /etc/bigsdb/dbases/test_public. This will be accessible from http: //IP_ADDRESS/cgi-bin/bigsdb/bigsdb.pl?db=test_public. It is better to create a symlink to the private config.xml and then override the attributes that are different. So create a symlink to the private config file:

```
cd /etc/bigsdb/dbases/test_public
sudo ln -s ../test_private/config.xml .
```

You can now override the view and access settings. Within /etc/bigsdb/dbases/test_public, create a file called system.overrides and add the following:

```
view="public"
read_access="public"
```

See also Restricting particular configurations to specific user accounts.

CHAPTER 19

Appendix

19.1 Query operators

Various query forms have operators for use with field values. Available operators are:

- =
- Exact match (case-insensitive).
- contains
 - Match to a partial string (case-insensitive), e.g. searching for clonal complex 'contains' st-11 would return all STs belonging to the ST-11 complex.
- starts with
 - Match to values that start with the search term (case-insensitive).
- ends with
 - Match to values that end with the search term (case-sensitive).
- >
- Greater than the search term.
- >=
 - Greater than or equal the search term.

• <

- Less than the search term.
- <=
 - Less than or equal the search term.

• NOT

- Match to values that do not equal the search term (case-insensitive).

- NOT contain
 - Match to values that do not contain the search term (case-insensitive).

19.2 Sequence tag flags

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

- ambiguous read
 - Genome sequence contains ambiguous nucleotides in coding sequence.
- apparent misassembly
 - Sequence has a region of very high identity to existing allele in one region but looks completely different in another.
- atypical
 - Catch-all term for a sequence that is unusual compared to other alleles of locus.
- · contains IS element
 - Coding sequence is interrupted by insertion sequence.
- downstream fusion
 - No stop codon present resulting in translation continuing.
- frameshift
 - Frameshift in sequence relative to other alleles, not resulting in internal stop codon.
- indel
 - Insertion/deletion in sequence that is uncommon compared to other alleles.
- · internal stop codon
 - Frameshift in sequence relative to other alleles, resulting in internal stop codon.
- · no start codon
 - No apparent start codon in immediate vicinity of usual start.
- · no stop codon
 - No stop codon in immediate vicinity of usual stop.
- · phase variable: off
 - Coding sequence has a homopolymeric run with a frameshift resulting in a stop codon preventing complete translation.
- truncated
 - Coding sequence is unusually short resulting in a truncated protein (not the same as running off the end of a contig).
- · upstream fusion
 - No apparent start codon in immediate vicinity of usual start, likely due to a gene fusion (sequence is transcribed together with upstream coding sequence).

19.3 Allele sequence flags

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

- atypical
 - Catch-all term for a sequence that is unusual compared to other alleles of locus.
- · contains IS element
 - Coding sequence is interrupted by insertion sequence.
- downstream fusion
 - No stop codon present resulting in translation continuing.
- frameshift
 - Frameshift in sequence relative to other alleles, not resulting in internal stop codon.
- indel
 - Insertion/deletion in sequence that is uncommon compared to other alleles.
- internal stop codon
 - Frameshift in sequence relative to other alleles, resulting in internal stop codon.
- no start codon
 - No apparent start codon in immediate vicinity of usual start.
- no stop codon
 - No stop codon in immediate vicinity of usual stop.
- phase variable: off
 - Coding sequence has a homopolymeric run with a frameshift resulting in a stop codon preventing complete translation.
- truncated
 - Coding sequence is unusually short resulting in a truncated protein (not the same as running off the end of a contig).
- upstream fusion
 - No apparent start codon in immediate vicinity of usual start, likely due to a gene fusion (sequence is transcribed together with upstream coding sequence).

CHAPTER 20

Database schema

- Sequence definition database
- Isolate database

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