BIGSdb Documentation

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Gene-by-gene population annotation and analysis

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

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

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

Concepts and terms

1.1 BIGSdb

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

1.2 Loci

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

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

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

1.3 Alleles

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

When a specific allele of a locus is identified within the sequence data of an isolate record, the allele designation, i.e. identifier, is associated with the isolate record. This efficiently stores the sequence variation found within an isolate. Two isolates with the same allele designation for a locus have identical sequences at that locus. Once the sequence variation within a genome has been reduced to a series of allele designations, genomes can be efficiently compared by identifying which loci vary between them.

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

1.4 Schemes

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

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

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

1.5 Profiles

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

1.6 Sequence tags

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

- sequence bin id this identifies a particular contig
- locus name
- start position
- end position
- flag to indicate if sequence is reversed
- flag to indicate if sequence is complete and does not continue off the end of the contig

1.7 Sets

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

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

BIGSdb dependencies

2.1 Required packages

BIGSdb requires a number of software components to be installed:

2.1.1 Linux packages

- Apache2 web server with mod_perl2
- PostgreSQL database
- Perl 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.

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

- Config::Tiny Configuration file handling.
- Bio::Biblio This used to be part of BioPerl but will need to be installed separately if using BioPerl 1.6.920 or later.
- IO::String
- Data::UUID Globally unique identifer handling for preference storage.
- List::MoreUtils (version 0.28+).
- Time::Duration [optional] Used by Job Viewer to display elapsed time in rounded units.
- Excel::Writer::XLSX Used to export data in Excel format.
- Parallel::ForkManager Required for multi-threading autotagger and autodefiner scripts.
- Net::Oauth Required for REST authentication (this needs to be installed even if you are not using REST).
- Crypt::Eksblowfish::Bcrypt Used for password hashing.
- Mail::Sender [optional] Used to send E-mail messages by submission system.

2.1.3 Optional packages

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

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

Installation and configuration of BIGSdb

3.1 Software installation

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

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

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

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

- 2. Copy the bigsdb.pl and bigscurate.pl scripts to a subdirectory of your web server's cgi-bin directory. Make sure these are readable and executable by the web server daemon.
- Copy the contents of the lib directory to /usr/local/lib/BIGSdb/. Make sure you include the Plugins and Offline directories which are subdirectories of the main lib directory.
- Copy the contents of the javascript directory to a javascript directory within the web root tree, i.e. accessible from http://your_website/javascript/.
- 5. Copy the contents of the css directory to a css directory within the web root tree, i.e. accessible from http://your_website/css/.
- 6. Copy the contents of the fonts directory to a fonts directory within the web root tree, i.e. accessible from http://your_website/fonts/.
- 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/

pg_hba.conf

```
# Database administrative login by UNIX sockets
       all
local
                   postgres
                                                      ident map=mymap
# TYPE DATABASE
                   USER
                                CIDR-ADDRESS
                                                      METHOD
# "local" is for Unix domain socket connections only
local all
                 all
                                                      ident map=mymap
# IPv4 local connections:
                                127.0.0.1/32
                                                      md5
host
       all
                   all
# IPv6 local connections:
                   all
                                                     md5
host
       all
                                ::1/128
```

pg_ident.conf

# MAPNAME	SYSTEM-USERNAME	PG-USERNAME
тутар	postgres	postgres
тутар	webmaster	postgres
тутар	www-data	apache

mymap	bigsdb	bigsdb	
mymap	bigsdb	apache	

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

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

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

See Tuning Your PostgreSQL Server for more details.

Restart PostgreSQL after any changes, e.g.

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

3.3 Site-specific configuration

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

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

3.4 Setting up the offline job manager

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

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

sudo useradd -s /bin/sh bigsdb

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

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

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

psql ALTER ROLE bigsdb WITH PASSWORD 'bigsdb';

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

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

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

- 4. Copy the job_logging.conf file to the /etc/bigsdb directory.
- 5. Set the script to run frequently (preferably every minute) from CRON. Note that CRON does not like '.' in executable filenames, so either rename the script to 'bigsjobs' or create a symlink and call that from CRON, e.g.:

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

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

Add the following to /etc/crontab::

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

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

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

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

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

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

3.5 Setting up the submission system

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

 Create a writable submissions directory in the root of the web site called submissions, i.e. accessible from http://your_website/submissions. This is used for file uploads. The directory should be writable by the Apache web daemon (user 'www-data' on Debian/Ubuntu systems). 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 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.

3.6 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
```

3.7 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).

#Prevent prefs database getting too large
00 18 * * 0 postgres psql -c "DELETE FROM guid WHERE last_accessed < NOW() - INTERVAL '6 monthly of the second secon

3.8 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).

#Purge jobs older than 7 days from the jobs database. 00 5 * * * postgres psql -c "DELETE FROM jobs where (stop_time IS NOT NULL AND stop_time < now</pre>

3.9 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
```

3.10 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.

3.11 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.

3.11.1 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>
```

Database setup

There are two types of BIGSdb database:

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

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

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

4.1 Creating databases

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

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

```
sudo su postgres
```

then

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

Create an isolate database the same way:

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

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

psql bigsdb_test_isolates

and alter the isolate table::

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

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

4.2 Database-specific configuration

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

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

4.3 XML configuration attributes used in config.xml

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

4.3.1 Isolate database XML attributes

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

<db>

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

<system>

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.
- 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_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+).
- 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.
- default
 - Default value. This will be entered automatically in the web form but can be overridden.
- 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_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').
- 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'.
- 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_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'.
- 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'.
- 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 *seqbin filter*.
 - Example: seqbin_size_threshold="0.5,1,2,4".
- seq_export_limit
 - Overrides the sequence export limit (records x loci) in the Sequence Export plugin. Default: '1000000'.
- sets
 - Use sets: either 'yes' or 'no', default 'no'.
- set_id
 - Force the use of a specific set when accessing database via this XML configuration: Value is the name of the set.
- start_id
 - Defines the minimum record id to be used when uploading new isolate records. This can be useful when
 it is anticipated that two databases may be merged and it would be easier to do so if the id numbers in the
 two databases were different. Default: '1'.
- submissions
 - Enable automated submission system: either 'yes' or 'no', default 'no' (version 1.11+).
 - The curate_script and query_script paths should also be set, either in the bigsdb.conf file (for site-wide configuration) or within the system attribute of config.xml.
- tblastx_tagging
 - Sets whether tagging can be performed using TBLASTX: either 'yes' or 'no', default 'no'.
- user
 - Username for access to isolates database, default 'apache'.
- use_temp_scheme_table

- Sets whether entire schemes are imported in to the isolate database in to an indexed table rather than querying the seqdef scheme view for isolate results tables. Under some circumstances this can be considerably quicker than querying the seqdef scheme view (a few ms compared to >10s if the seqdef database contains multiple schemes with an uneven distribution of a large number of profiles so that the Postgres query planner picks a sequential rather than index scan). This scheme table can also be generated periodically using the update_scheme_cache.pl script to create a persistent cache. This is particularly useful for large schemes (>10000 profiles) but data will only be as fresh as the cache so ensure that the update script is run periodically.
- 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. The bigsdb.css stylesheet file should be located in this directory. 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 or date.
- comments * optional
 - Comments about the field. These will be displayed in the field description plugin and as tooltips within the curation interface.
- 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 types. Special values such as CURRENT_YEAR can be used.
- min
 - Minimum value for integer types.
- optlist
 - Sets if this field has a list of allowed values, default 'no'. Surround each option with an <option> tag.
- regex
 - Regular expression used to constrain field values, e.g. regex="^[A-Z].*\$" forces the first letter of the value to be capitalized.
- required
 - Sets if data is required for this field, 'yes' or 'no', default 'yes'.
- userfield
 - Select if you want this field to have its own dropdown filter box of users (populated from the users table): 'yes' or 'no', default 'no'.
- web
 - URL that will be used to hyperlink field values. If [?] is included in the URL, this will be substituted for the actual field value.

Special values

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

• CURRENT_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>

- 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_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.
- 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'.
- 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.
- materialized_views
 - Enable materialized views: either 'yes' or 'no', default 'no'.
- 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.
- 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'.
- 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.
- webroot
 - URL of web root, which can be relative or absolute. The bigsdb.css stylesheet file should be located in this directory. Default '/'.

4.4 User authentication

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

4.4.1 Apache authentication

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

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

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

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

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

4.4.2 Built-in authentication

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

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

When a user logs in, the server provides a random one-time session variable and the user is prompted to enter their username and password. The password is encrypted within the browser using a Javscript one-way hash algorithm, and this is combined with the session variable and hashed again. This hash is passed to the server. The server compares this hash with its own calculated hash of the stored encrypted password and session variable that it originally sent to the browser. Implementation is based on perl-md5-login.

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

4.5 Setting up the admin user

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

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

If you are using built-in authentication, set the password for this user using the *add_user.pl* script. This 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).

4.6 Updating PubMed citations

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

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

```
pubmlst_bigsdb_neisseria_isolatesrefspubmlst_bigsdb_neisseria_seqdefprofile_refs, sequence_refs, locus_refs
```

The script can be called as follows:

```
getrefs.pl getrefs.conf
```

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

Administrator's guide

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

5.1 Types of user

There are 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 priveleges from an account. They can also not raise the status of a user to admin level.
- modify_usergroups allowed to add or modify user groups and add users to these groups.

- set_user_passwords allowed to modify other users' passwords (if built-in authentication is in use).
- modify_loci allowed to add or modify loci.
- modify_schemes allowed to add or modify schemes.
- modify_sequences allowed to add sequences to the sequence bin (for isolate databases) or new allele definitions (for sequence definition databases).
- modify_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).

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

Database: Sp Users: Add 0 Isolates: Add	Query/u	pdate		ies) Curator	r's page (database)
gged in: Keith Jolley (keith). 🗭 Log ou	t Chan	ge password			
atabase curator's	inte	rface	- Neisser	ia Publ	MLST
🕜 Add, update or delet	te rec	ords			
Record type	Add	Batch Add	Update o	r delete	Comments
users	+	++	?		
user groups	+	++	?		Users can be members of these groups - use for setting access permissions.
user group members	+	++	?		Add users to groups for setting access permissions.
curator permissions			?		Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query brov batch u		
isolate field extended attribute values	+	++	?		Add values for additional isolate field attributes.
projects	+	++	?		Set up projects to which isolates can belong.
project members	+	++	?		Add isolates to projects.
isolate aliases	+	++	?		Add alternative names for isolates.
PubMed links	+	++	?		
allele designations		++	?		Allele designations can be set within the isolate table functions.
sequences		++	?		The sequence bin holds sequence contigs from any source.
accession number links	+	++	?		Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?		Set up experiments to which sequences in the bin can belong.
experiment sequences			?		Add links associating sequences to experiments.
sequence tags		scan	?		Tag regions of sequences within the sequence bin with locus information.
Database configurati Table		atch Add	Update or delete		Comments
100			6		
locus aliases	datab	ankscan	2		a server for losi. These was also be activitied user being additioni
		++	() ()		e names for loci. These can also be set when you batch add loci.
PCR reactions	++	++			o PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes					tide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
isolate field extended attributes	+	++	?	Define additio	anal attributes to associate with values of a particular isolate record field.

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



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

ogged III. Relat Solley (Relat). e	Log out Change pass	word		Help 🗹
et curator peri	nissions			
	Action Select			
Halkilahti, Jani	*			
Check the boxes for the req	uired permissions. U	Jsers with a sta	itus of 'subi	nitter' have a restricted list of allowed permissions that can be selected.
Dormission	Curato Clemence, Marianne		All/None	Update
modify users				
modify isolates	V			
		V		
modify projects				
modify projects				
modify projects modify sequences				
modify projects modify sequences tag sequences				
modify projects modify sequences tag sequences designate alleles modify usergroups set user passwords				
modify projects modify sequences tag sequences designate alleles modify usergroups set user passwords modify loci				
modify projects modify sequences tag sequences designate alleles modify usergroups set user passwords modify loci modify schemes				
modify projects modify sequences tag sequences designate alleles modify usergroups set user passwords modify loci modify schemes modify composites				
modify projects modify sequences tag sequences designate alleles modify usergroups set user passwords modify loci modify schemes modify composites modify field attributes				
modify projects modify sequences tag sequences designate alleles modify usergroups set user passwords modify loci modify schemes modify composites modify field attributes modify value attributes				
modify projects modify sequences tag sequences designate alleles modify usergroups set user passwords modify loci modify schemes modify composites modify field attributes modify value attributes modify probes				
modify projects modify sequences tag sequences designate alleles modify usergroups set user passwords modify loci modify schemes modify composites modify field attributes modify value attributes modify probes modify experiments				
modify projects modify sequences tag sequences designate alleles modify usergroups set user passwords modify loci modify schemes modify composites modify field attributes modify value attributes modify probes modify experiments delete all				
modify projects modify sequences tag sequences designate alleles modify usergroups set user passwords modify loci modify schemes modify composites modify field attributes modify value attributes modify probes modify experiments				

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.

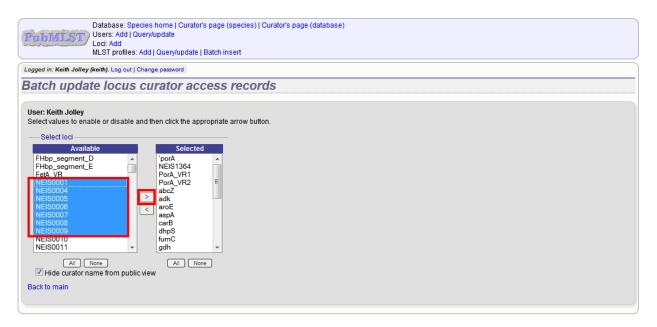
The easiest way to modify these lists is to use the batch update link next to 'locus curator control list' and 'scheme curator control list':

Users: Add Query/up Loci: Add MLST profiles: Add G	date		page (species) Curator's pa atch insert	
ogged in: Keith Jolley (keith). 🗭 Log out Chang	e passi	word		
atabase curator's inte	rfac	e - N	eisseria locus/s	equence definitions
	Tur	<i>·</i> · · ·		
Add, update or delete reco	ords Add	Batch	Update or delete	Comments
110.070	+	Add	?	
users user groups	+	++	2	Users can be members of these groups - use for setting access permissions.
user group members	+	++	2	Add users to groups for setting access permissions.
curator permissions	-		?	Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++	2	
scheme curator control list	+	++	guery batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	query batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++ FASTA	?	perme which culators can add or update sequences for particular rock.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	+	++	?	
Bexsero Antigen Sequence Typing (BAST) profiles	+	++	query browse list batch update	
MLST profiles	+	++	query browse list batch update	
rpIF species profiles	+	++	query browse list batch update	
		++		

Select the curator from the list:

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert
Logged in: Keith Jolley (keith). Log out Change password
Batch update locus curator access records
Select user The user status must also be set to curator for permissions to work. users: Jolley, Keith (keith) [Select]]

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



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

Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
		tabank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
cus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these databases when you query sequences or profiles in this database.
client database loci	+	++	?	Define loci that are used in client databases.
client database schemes	+	++	?	Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
cheme group scheme members	+	++	?	Defines which schemes belong to a group.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

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

Print/ILST Users: Add Query/update Isolates: Add Query/update Batch insert										
ogged in: Keith Jolley (keith). Log out Change password										
et user password										
User: Jolley, Keith (keith)										
New password: ••••••										
Retype password: ••••••										
Set password										

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

5.7 Setting the first user password

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

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

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

5.8 Enabling plugins

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

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

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

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
serverl	server2
localhost	server2

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

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

5.11 Improving performance

5.11.1 Use mod_perl

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

5.11.2 Cache scheme definitions within an isolate database

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

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

update_scheme_caches.pl -d pubmlst_bigsdb_neisseria_isolates

This script creates indexed tables within the isolate database called temp_scheme_X and temp_isolates_scheme_fields_1 (where X is the scheme_id). If these table aren't present, they are created as temporary tables every time a query is performed that requires a join against scheme definition data. This requires importing all profile definitions from the definitions database and determining scheme field values for all isolates. This may sound like it would be slow but caching only has a noticeable effect once you have >5000 profiles.

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

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

5.11.3 Use materialized views for scheme definitions

Because of the way BIGSdb allows any number of profile schemes to be set up, the data are stored in a normalised manner in multiple tables. A database view, e.g. scheme_1, is created that joins these tables so that they can be queried as you would a single table. A view, however, is only a pre-selected query rather than a physical table and you can not index columns on it to optimise query performance.

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

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

```
materialized_views="yes"
```

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

If you want an isolate database to benefit from this materialized view, make sure you put 'mv_scheme_X' (where X is the scheme id) in the dbase_table field (rather than 'scheme_X') when setting up the scheme in the isolate database configuration.

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

SELECT refresh_matview('mv_scheme_X');

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

5.11.4 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.

accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.			
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.			
experiment sequences			?	Add links associating sequences to experiments.			
sequence tags	S	can	?	Tag regions of sequences within the sequence bin with locus information.			
📂 Database configurati	on						
Table	Add B	atch Add	Update or delete	Comments			
loci	+ ++		?				
	databa	ank scan					
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.			
PCR reactions	+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.			
nucleotide probes	+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci			
isolate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.			
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.			
sequence attributes	+	++	?	Define attributes that can be set for contigs in the sequence bin.			
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.			
set loci	+	++	?	Add loci to sets.			
set schemes	+	++	?	Add schemes to sets.			
set metadata	+	++	?	Add metadata collection to sets.			
setview	+	++	?	Set database views linked to sets.			
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.			
scheme members	+	++	?	Defines which loci belong to a scheme.			
scheme fields	+	++	?	Defines which fields belong to a scheme.			
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.			
cheme group scheme members	+	++	?	Defines which schemes belong to a group.			
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.			
0.1							
the second s				log on or change an existing password.			
 Conliguration check - Chec 	ks data	ibase con	nectivity for loci an	d schemes and that required helper applications are properly installed.			

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

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



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>
  <option>death</option>
  </optlist>
</field>
```

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

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

isolates	-				
		++		wse list update	
isolate field extended attribute values	+	++	1	?	Add values for additional isolate field attributes.
projects	+	++	1	?	Set up projects to which isolates can belong.
project members	+	++	1	?	Add isolates to projects.
isolate aliases	+	++	1	?	Add alternative names for isolates.
PubMed links	+	++	1	?	
allele designations		++	1	?	Allele designations can be set within the isolate table functions.
sequences		++	1	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	1	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	1	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			1	?	Add links associating sequences to experiments.
sequence tags		scan	1	?	Tag regions of sequences within the sequence bin with locus information.
loci	+	++	Update or delete ?		Comments
	datal	bank scan			
	ualai	Jank Stan			
locus aliases	+	++	?	Add alternative na	ames for loci. These can also be set when you batch add loci.
			?		ames for loci. These can also be set when you batch add loci. CR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
locus aliases PCR reactions nucleotide probes	+	++		Set up in silico PC	
locus aliases PCR reactions nucleotide probes	+ +	++ ++	?	Set up <i>in silico</i> PO Define nucleotide	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
locus aliases PCR reactions nucleotide probes solate field extended attributes composite fields	+ + +	++ ++ ++	? ?	Set up <i>in silico</i> PC Define nucleotide Define additional	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.
locus aliases PCR reactions nucleotide probes solate field extended attributes	+ + + +	++ ++ ++	? ? ?	Set up <i>in silico</i> PC Define nucleotide Define additional Used to construct o	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field.
locus aliases PCR reactions nucleotide probes solate field extended attributes composite fields sequence attributes sets	+ + + + +	++ ++ ++ ++	? ? ? ?	Set up <i>in silico</i> PC Define nucleotide Define additional Used to construct o Define attributes th	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields.
locus aliases PCR reactions nucleotide probes solate field extended attributes composite fields sequence attributes sets set loci	+ + + + + + +	+++ +++ +++ +++ +++ +++ +++	? ? ? ? ?	Set up in silico PC Define nucleotide Define additional Used to construct of Define attributes th Sets describe a co Add loci to sets.	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci, probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci, attributes to associate with values of a particular isolate record field, composite fields consisting of fields from isolate, loci or scheme fields. hat can be set for contigs in the sequence bin. Illection of loci and schemes that can be treated like a stand-alone database.
locus aliases PCR reactions nucleotide probes solate field extended attributes composite fields sequence attributes sets set loci set loci set schemes	+ + + + + + + +	+++ +++ +++ +++ +++ +++ +++ +++	??????	Set up in silico PC Define nucleotide Define additional Used to construct of Define attributes th Sets describe a co Add loci to sets. Add schemes to se	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. hat can be set for contigs in the sequence bin. Illection of loci and schemes that can be treated like a stand-alone database.
locus aliases PCR reactions nucleotide probes solate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata	+ 1 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2 + 2	+++ +++ +++ +++ +++ +++ +++ +++ +++	???????????????????????????????????????	Set up in silico PC Define nucleotide Define additional Used to construct of Define attributes th Sets describe a co Add loci to sets. Add schemes to se Add metadata coll	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field. composite fields consisting of fields form isolate, loci or scheme fields. hat can be set for contigs in the sequence bin. Illection of loci and schemes that can be treated like a stand-alone database. ats. lection to sets.
locus aliases PCR reactions nucleotide probes solate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata set view	+ + + + + + + + +	+++ +++ +++ +++ +++ +++ +++ +++ +++	? ? ? ? ? ? ? ? ? ?	Set up in silico PC Define nucleotide Define additional Used to construct o Define attributes ti Sets describe a co Add loci to sets. Add schemes to se Add metadata coll Set database view	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. hat can be set for contigs in the sequence bin. Illection of loci and schemes that can be treated like a stand-alone database. ets. lection to sets. is linked to sets.
locus aliases PCR reactions nucleotide probes solate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata set view schemes	+ + + + + + + + +	+++ +++ +++ +++ +++ +++ +++ +++ +++	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico PC Define nucleotide Define additional Used to construct o Define attributes ti Sets describe a co Add loci to sets. Add schemes to se Add metadata coll Set database view Describes schemes	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. hat can be set for contigs in the sequence bin. Illection of loci and schemes that can be treated like a stand-alone database. lection to sets. s in liked to sets. s consisting of collections of loci, e.g. MLST.
locus aliases PCR reactions nucleotide probes solate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata set view schemes scheme members	+ + + + + + + + + +	+++ +++ +++ +++ +++ +++ +++ +++ +++ ++	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico PC Define nucleotide Define additional Used to construct d Define attributes th Sets describe a co Add loci to sets. Add schemes to se Add metadata coll Set database view Describes schemes Defines which loci	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci, probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci, attributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. hat can be set for contigs in the sequence bin. Illection of loci and schemes that can be treated like a stand-alone database. ets. lection to sets. Is linked to sets. Is consisting of collections of loci, e.g. MLST.
locus aliases PCR reactions nucleotide probes solate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata set view schemes schemes scheme members scheme fields	+ + + + + + + + + +	+++ +++ +++ +++ +++ +++ +++ +++ +++ ++	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico PC Define nudeotide Define additional Used to construct Define attributes ti Sets describe a co Add loci to sets. Add schemes to se Add metadata col Set database view Describes schemes Defines which field	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field. composite fields consisting of fields form isolate, loci or scheme fields. hat can be set for contigs in the sequence bin. Illection of loci and schemes that can be treated like a stand-alone database. ets. lection to sets. Is linked to sets. Is consisting of collections of loci, e.g. MLST. belong to a scheme. ds belong to a scheme.
locus aliases PCR reactions nucleotide probes solate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata set view schemes scheme fields scheme groups	+ + + + + + + + + +	+++ +++ +++ +++ +++ +++ +++ +++ +++ ++	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico PC Define nucleotide Define additional Used to construct o Define attributes ti Sets describe a co Add loci to sets. Add schemes to se Add netadata col Set database view Describes schemen Defines which fiel Describes groups i	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field. composite fields consisting of fields from isolate, loci or scheme fields. hat can be set for contigs in the sequence bin. Illection of loci and schemes that can be treated like a stand-alone database. ets. lection to sets. Is linked to sets. Is linked to sets. Is onsisting of collections of loci, e.g. MLST. I belong to a scheme. ds belong to a scheme. In to which schemes can belong - groups can also belong to other groups.
locus aliases PCR reactions nucleotide probes isolate field extended attributes composite fields sequence attributes sets set loci set schemes set metadata set view schemes scheme fields scheme groups cheme groups	+ + + + + + + + + +	+++ +++ +++ +++ +++ +++ +++ +++ +++ ++	? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ? ?	Set up in silico PC Define nucleotide Define additional Used to construct of Define attributes th Sets describe a co Add loci to sets. Add schemes to as Add metadata col Set database view Describes schemes Defines which field Defines which field Describes groups in Defines which schu	CR reactions. These can be used to filter genomes for tagging to specific repetitive loci. probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci. attributes to associate with values of a particular isolate record field. composite fields consisting of fields form isolate, loci or scheme fields. hat can be set for contigs in the sequence bin. Illection of loci and schemes that can be treated like a stand-alone database. ets. lection to sets. Is linked to sets. Is consisting of collections of loci, e.g. MLST. belong to a scheme. ds belong to a scheme.

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:

```
CREATE VIEW spneumoniae AS SELECT * FROM isolates WHERE species = 'Streptococcus pneumoniae';
GRANT SELECT ON spneumoniae TO apache;
```

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

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

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

5.12.5 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 Adding new loci

See also:

Loci (concept)

5.13.1 Sequence definition databases

Single locus

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

Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
		tabank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
ocus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of thes databases when you query sequences or profiles in this database.
client database loci	+	++	?	Define loci that are used in client databases.
lient database schemes	+	++	?	Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

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

- id The name of the locus.
 - Allowed: any value starting with a letter or underscore.
- data_type Describes whether the locus is defined by nucleotide or peptide sequence.
 - Allowed: DNA/peptide.
- allele_id_format The format for allele identifiers.
 - Allowed: integer/text.
- length_varies Sets whether alleles can vary in length.
 - Allowed: true/false.
- coding_sequence Sets whether the locus codes for a protein.
 - Allowed: true/false.
- formatted_name Name with HTML formatting (optional).
 - This allows you to add formatting such as bold, italic, underline and superscripting to locus names as they
 appear in the web interface.
 - Allowed: valid HTML.
- common_name The common name for the locus (optional).
 - Allowed: any value.
- formatted_common_name Common name with HTML formatting (optional).
 - Allowed: valid HTML.
- allele_id_regex Regular expression to enforce allele id naming (optional).
 - ^: the beginning of the string
 - \$:the end of the string
 - d: digit

- D: non-digit
- s: white space character
- S: non white space character
- w: alpha-numeric plus '_'
- .: any character
- *: 0 or more of previous character
- +: 1 or more of previous character
- e.g. ^Fd-d+\$ states that an allele name must begin with a F followed by a single digit, then a dash, then one or more digits, e.g. F1-12
- length Standard length of locus (required if length_varies is set to false.
 - Allowed: any integer.
- min_length Minimum length of locus (optional).
 - Allowed: any integer.
- max_length Maximum length of locus (optional).
 - Allowed: any integer (larger than the minimum length).
- orf Open reading frame of locus (optional).
 - 1-3 are the forward reading frame, 4-6 are the reverse reading frames.
 - Allowed: 1-6.
- genome_position The start position of the locus on a reference genome (optional).
 - Allowed: any integer.
- match_longest Specifies whether in a sequence query to only return the longest match (optional).
 - This is useful for some loci that can have some sequences shorter than others, e.g. peptide loci defining antigenic loops. This can lead to instances of one sequence being longer than another but otherwise being identical. In these cases, usually the longer sequence is the one that should be matched.
 - Allowed: true/false.
- full_name Full name of the locus (optional).
 - Allowed: any value.
- product Name of gene product (optional).
 - Allowed: Any value.
- description Description of the locus (optional).
 - Allowed: any value.
- aliases Alternative names for the locus (optional).
 - Enter each alias on a separate line in the text box.
 - Allowed: any value.
- pubmed_ids PubMed ids of publications describing the locus (optional).
 - Enter each PubMed id on a separate line in the text box.
 - Allowed: any integer.

- links Hyperlinks pointing to additional resources to display in the locus description (optional).
 - Enter each link on a separate line in the format with the URL first, followed by a | then the description (URLldescription).

Batch adding

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

Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	da	atabank		
		scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
locus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these
				databases when you query sequences or profiles in this database.
client database loci	+	++	?	Define loci that are used in client databases.
client database schemes	+	++	?	Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.
Set user password	k - Ch	ecks data	base connectiv	able them to log on or change an existing password. ity for loci and schemes and that required helper applications are properly installed.

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

1			
Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add			
MLST profiles: Add Query/update Batch insert			
Logged in: Keith Jolley (keith). Log out Change password			Toggle: i
Batch insert loci			
 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 (xisx format) 			
Desks is tok deligibed bod (include a field bonder line)	1 min m		
Paste in tab-delimited text (include a field header line).	Action		
	Reset	Submit	
Back			

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

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

5.13.2 Isolate databases

Single locus

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

Users: Add C Isolates: Add			atch insert		
ed in: Keith Jolley (keith). 🕒 Log ou	t Chang	e password			
tabase curator's	inte	rface	- Neisser	ia PubN	<i>ILST</i>
Add, update or delet	e reco	ords			
Record type	Add	Batch Add	Update (or delete	Comments
users	+	++		?	
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.
user group members	+	++		?	Add users to groups for setting access permissions.
curator permissions				?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++		wse list update	
solate field extended attribute values	+	++		?	Add values for additional isolate field attributes.
projects	+	++		?	Set up projects to which isolates can belong.
project members	+	++	?		Add isolates to projects.
isolate aliases	+	++		?	Add alternative names for isolates.
PubMed links	+	++		?	
allele designations		++		?	Allele designations can be set within the isolate table functions.
sequences		++		?	The sequence bin holds sequence contigs from any source.
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++		?	Set up experiments to which sequences in the bin can belong.
experiment sequences				?	Add links associating sequences to experiments.
sequence tags		scan		?	Tag regions of sequences within the sequence bin with locus information.
Database configurati		atch Add I	Indato or dolete		Comporte
loci	Add B	atch Add (Jpdate or delete ?		Comments
1001		ank scan	f .		
locus aliases	ualaba +	++	?	Add alternative	names for loci. These can also be set when you batch add loci.
PCR reactions	+	++	r		PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++			de probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
olate field extended attributes	+	++	2		al attributes to associate with values of a particular isolate record field.
composite fields	+		2		ct composite fields consisting of fields from isolate, loci or scheme fields.
composite lielus	+	++			ct composite fields consisting of fields from isolate, loci of scheme fields.

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

PUIDINLST Users: Add	Species home Curator Query/update es: Add Query/update	's page (species) Curator's page Batch insert	(database)	
Logged in: Keith Jolley (keith). 🕒 Log o	out Change password			Toggle: 🚯
Add new locus				
Please fill in the fields below - re	quired fields are marke	d with an exclamation mark (!).		
Record				Action
id:!				Reset Submit
data type:!	DNA 👻			
allele id format:	integer 👻 🕕			
length varies:!	🔘 true 🔘 false 🕕			
coding sequence:	🔍 true 🔘 false			
curator:!	Keith Jolley (keith)			
date entered:	2015-07-01			
datestamp:	2015-07-01			
formatted name:			0	
common name:			0	
formatted common name:			0	
allele id regex:			0	
length:				
min length:		÷ 0		
max length: orf:				
genome position:		÷ 0		
	🔿 true 🔘 false 🜖			
	◯ true ◯ false 0			
full name:				
lui name.				
product:				
description:				

- id The name of the locus
 - Allowed: any value starting with a letter or underscore.
- data_type Describes whether the locus is defined by nucleotide or peptide sequence.
 - Allowed: DNA/peptide.
- allele_id_format The format for allele identifiers.
 - Allowed: integer/text.
- length_varies Sets whether alleles can vary in length.
 - Allowed: true/false.
- coding_sequence Sets whether the locus codes for a protein.
 - Allowed: true/false.
- flag_table Set to true to specify that the sequence definition database contains an allele flag table (which is the case for BIGSdb version 1.4 onwards).
 - Allowed: true/false.
- isolate_display Sets how alleles for this locus are displayed in a detailed isolate record this can be overridden by user preference.
 - Allowed: allele only/sequence/hide.
- main_display Sets whether or not alleles for this locus are displayed in a main results table by default this can be overridden by user preference.

- Allowed: true/false.
- query_field Sets whether or not alleles for this locus can be used in queries by default this can be overridden by user preference.
 - Allowed: true/false.
- analysis Sets whether or not alleles for this locus can be used in analysis functions by default this can be overridden by user preference.
 - Allowed: true/false.
- formatted_name Name with HTML formatting (optional).
 - This allows you to add formatting such as bold, italic, underline and superscripting to locus names as they
 appear in the web interface.
 - Allowed: valid HTML.
- common_name The common name for the locus (optional).
 - Allowed: any value.
- formatted_common_name Common name with HTML formatting (optional).
 - Allowed: valid HTML.
- allele_id_regex Regular expression to enforce allele id naming.
 - ^: the beginning of the string
 - \$:the end of the string
 - d: digit
 - D: non-digit
 - s: white space character
 - S: non white space character
 - w: alpha-numeric plus '_'
 - .: any character
 - *: 0 or more of previous character
 - +: 1 or more of previous character
 - e.g. ^Fd-d+\$ states that an allele name must begin with a F followed by a single digit, then a dash, then one or more digits, e.g. F1-12
- length Standard length of locus (required if length_varies is set to false).
 - Allowed: any integer.
- orf Open reading frame of locus (optional). 1-3 are the forward reading frame, 4-6 are the reverse reading frames.
 - Allowed: 1-6.
- genome_position The start position of the locus on a reference genome.
 - Allowed: any integer.
- match_longest Only select the longest exact match when tagging/querying.

- This is useful for some loci that can have some sequences shorter than others, e.g. peptide loci defining antigenic loops. This can lead to instances of one sequence being longer than another but otherwise being identical. In these cases, usually the longer sequence is the one that should be matched.
- Allowed: true/false.
- reference_sequence Sequence used by the automated sequence comparison algorithms to identify sequences matching this locus. This is only used if a sequence definition database has not been set up for this locus.
- pcr_filter Set to true if this locus is further defined by genome filtering using in silico PCR.
 - Allowed: true/false.
- probe_filter Set to true if this locus is further defined by genome filtering using in silico hybdridization.
 - Allowed: true/false.
- dbase_name Name of database (system name).
 - Allowed: any text.
- dbase_host Resolved name of IP address of database host leave blank if running on the same machine as the isolate database.
 - Allowed: network address, e.g. 129.67.26.52 or zoo-oban.zoo.ox.ac.uk
- dbase_port Network port on which the sequence definition database server is listening leave blank unless using a non-standard port (5432).
 - Allowed: integer.
- dbase_user Name of user with permission to access the sequence definition database depending on the database configuration you may be able to leave this blank.
 - Allowed: any text (no spaces).
- dbase_password Password of database user again depending on the database configuration you may be able to leave this blank.
 - Allowed: any text (no spaces).
- dbase_table Table in the sequence definition database that contains allele sequences for this locus. If the definition database uses BIGSdb this will be 'sequences'.
 - Allowed: any text (no spaces).
- dbase_id_field Primary field in sequence database that defines allele. If the definition database uses BIGSdb this will be 'allele_id'.
 - Allowed: any text (no spaces).
- dbase_id2_field Secondary field in sequence database that defines alleles. If dbase_id_field uniquely defines alleles for this locus then this should be left blank. If the definition database uses BIGSdb this will be 'locus'.
 - Allowed: any text (no spaces).
- dbase_id2_value Secondary field value in sequence database that defines alleles. If dbase_id_field uniquely defines alleles for this locus then this should be left blank. If the definition database uses BIGSdb this will be the name of the locus used in the id field
 - Allowed: any text (no spaces).
- dbase_seq_field Field in sequence database containing allele sequence. If the definition database uses BIGSdb this will be 'sequence'.
 - Allowed: any text (no spaces).

- description_url The URL used to hyperlink to locus information in the isolate information page. This can either be a relative (e.g. /cgi-bin/...) or an absolute (containing http://) URL.
 - Allowed: any valid URL.
- url The URL used to hyperlink to information about the allele. This can either be a relative or absolute URL. If [?] (including the square brackets) is included then this will be substituted for the allele value in the resultant URL. To link to the appropriate allele info page on a corresponding seqdef database you would need something like /cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_neisseria_seqdef&page=alleleInfo&locus=abcZ&allele_id=[?].
 - Allowed: any valid URL.
- 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:

PTIDMLST / Users: Add	pecies home Curator Query/update d Query/update Batcl	r's page (species) Curator's page (c n insert	latabase)		
Logged in: Keith Jolley (keith). 🗭 Log o	ut Change password				Toggle: 🚯
Add new locus					Show tools
Please fill in the fields below - rec	quired fields are marke	ed with an exclamation mark (!).			
Record				Action	
id:!				Reset Submit	
data type:!	DNA 👻				
allele id format!	integer 👻 🕕				
length varies:!	🔘 true 🔘 false 🕦				
coding sequence:!					
	🖲 true 🔘 false 🚺	Seqdef database supports allele flags			
	allele only 👻 🕕				
	🔘 true 🔘 false 🚺				
	🔍 true 🔘 false 🚺				
	🔍 true 🔘 false 🕦				
	Keith Jolley (keith)				
date entered:					
datestamp:! formatted name:	2015-07-01		0		
common name:			0		
formatted common name:			0		
allele id regex:			0		
length:					
orf:	v ()				
genome position:		÷ 0			
match longest:	🔘 true 🔘 false 🕕				
reference sequence:					
			l h.	D	

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

PubMLST / Users: Add	pecies home Curator's page (species) Curator's page (data Query/update d Query/update Batch insert	abase)
Logged in: Keith Jolley (keith). 🔂 Log o	ut Change password	Toggle: 🕄
Add new locus		Hide tools
Please fill in the fields below - red	quired fields are marked with an exclamation mark (!).	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'
id: data type: allele id formati length varies: coding sequence: flag table: isolate display: main display: query field: analysis:	integer ● true ● false ● intue ○ false ● intue ○ false ● false <	in fields that include it.
datestamp: formatted name: common name: formatted common name: allele id regex iength: genome position: match longest		
reference sequence:		at O

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

allele id regex:		0	
length:	÷ 0		
orf:	v 0		
genome position:	÷ 0		
match longest:			
reference sequence:			
		. i	8
pcr filter:	🔿 true 🔘 false 🕦		
	○ true ○ false 0		
	pubmlst_bigsdb_neisseria_seqdef	Name of the database holding allele sequences	
dbase host:	public_bigedb_inclosend_bequer	IP address of database host	
dbase port:	() Network port accepting database	-	
dbase user:		0	
dbase password:		0	
dbase table:	sequences	Database table that holds sequence information for this locus	
dbase id field:		Primary field in sequence database that defines allele, e.g. 'allele	id'
dbase id2 field:		Secondary field that defines allele, e.g. 'locus'	-
	PUT LOCUS NAME HERE	Secondary field value, e.g. locus name	
dbase seq field:		Field in sequence database containing allele sequence	
	/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_ne		
	locus=PUT LOCUS NAME HERE	ibbeiin_bequeinpage ibbabinita	
		al j	Ð
url:	/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst ne	isseria seqdef&page=alleleInfo&	
	locus=PUT_LOCUS_NAME_HERE&allele_id=[?]	-	
		h.	Ð
submission template:	True Include column in isolate submission	template for this locus	
aliases:			
Action			

Complete the form and click 'Submit'.

Batch adding

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

ged in: Keith Jolley (keith). 🕪 Log o		ide password		
				NI 07
atabase curator's	; inte	erface -	· Neisseria Pul	DMLST
셠 🛛 Add, update or dele	ete rec	ords		
Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in th users table.
isolates	+	++	query browse list batch update	
isolate field extended attribute values	+	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences		++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.

Click the link to download an Excel template:

Profit MLST Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert				
Logged in: Keith Jolley (keith). Log out Change password				Toggle: i
Batch insert 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				
Download submission template (xisx format) Paste in tab-delimited text (include a field header line).	Action			
	Reset	Submit		
Back				

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 Defining locus extended attributes

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

To add extended attributes for a locus, click add (+) locus extended attributes in the sequence definition database curator's interface contents page.

user groups	+	++			Users can be members of these groups - use for setting access permissions.			
curator permissions				?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the user table.			
locus descriptions	+	++		?				
scheme curator control list	t +	++		query batch	Define which curators can add or update profiles for particular schemes.			
locus curator control list	+	++		query batch	Define which curators can add or update sequences for particular loci.			
sequences (all loci)	+	++ FASTA		?				
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.			
PubMed links (to sequences)	+	++		?				
MLST profiles	+	++	query	browse list batch update				
PubMed links (to profiles)	+	++		?				
	Add	Add	pdate or delete		Comments			
loci	+	++	?					
	data	abank						
	S	can						
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.				
ocus extended attributes	+	++	?		to associate with sequences of a particular locus.			
client databases	+	++	?		hat use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches n you query sequences or profiles in this database.			
client database loci	+	++	?	Define loci that are use				
lient database schemes	+	++	?		e used in client databases. You will need to add the appropriate loci to the client database loci table.			
client database fields linked to loci	+	++	?	Define fields in client d	atabase whose value can be displayed when isolate has matching allele.			
schemes	+	++	?		isting of collections of loci, e.g. MLST.			
scheme members	+	++	?	Defines which loci belo	-			
scheme fields	+	++	?	Defines which fields bel	•			
scheme groups	+	++	?		/hich schemes can belong - groups can also belong to other groups.			
scheme group scheme members	+	++	?	Defines which schemes	belong to a group.			
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.				
				-	or change an existing password. mes and that required helper applications are properly installed.			

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

PubMLST)	Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley	keith). @Log out Change password	Toggle: 🜖
Add new loo	cus extended attribute	
Please fill in the field	is below - required fields are marked with an exclamation mark (!).	
Record		— — Action — — — — — — — — — — — — — — — — — — —
locus:	•	Reset Submit
field:		
value format:!		
	◯ true	
	Keith Jolley (keith)	
datestamp:!	2015-07-01	
value regex: description:	U	
description.		
option list:		
	h	0
length:		
field order:	A V	

- locus Select locus from dropdown box.
 - Allowed: existing locus name.
- field Name of extended attributes.
 - Allowed: any value.
- value_format Data type of attribute.
 - Allowed: integer/text/boolean.
- required Specifies whether the attribute value but be defined when adding a new sequence.
 - Allowed: true/false.
- value_regex Regular expression to enforce allele id naming (optional).
 - ^: the beginning of the string
 - \$:the end of the string
 - d: digit
 - D: non-digit
 - s: white space character
 - S: non white space character
 - w: alpha-numeric plus '_'
 - .: any character
 - *: 0 or more of previous character
 - +: 1 or more of previous character

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

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

5.15 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)
```

5.15.1 Sequence definition databases

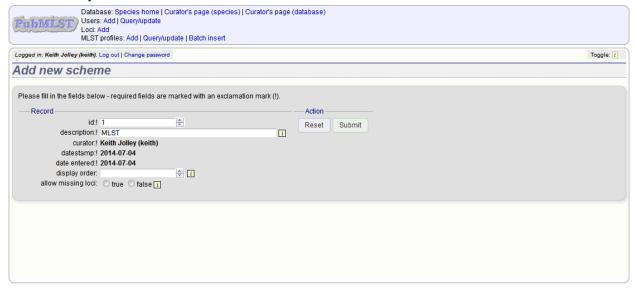
As with all configuration, tables can be populated using the batch interface (++) or one at a time (+). Details for the latter are described below:

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

				update	
PubMed links (to profile:	5) +	++		?	
🔎 Database con	figure	ation			
Database con	ngur	ation			
Table	Add	Batch Add	Update or delete	Comments	
loci	+	++	?		
	dat	abank			
	S	can			
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.	
locus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.	
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks and	
				searches of these databases when you query sequences or profiles in this database.	
client database loci	+	++	?	Define loci that are used in client databases.	
client database schemes	+	++	?	Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table.	
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.	
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.	
scheme members	+	++	?	Defines which loci belong to a scheme.	
scheme fields	+	++	?	Defines which fields belong to a scheme.	
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.	
cheme group scheme members	+	++	?	Defines which schemes belong to a group.	
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.	
	ck - Cl	hecks da	tabase conne	enable them to log on or change an existing password. ctivity for loci and schemes and that required helper applications are properly installed.	

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.



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

				update	
PubMed links (to profiles	s) +	++		?	
Database cont	figur	ation			
Table	Add	Batch Add	Update or delete	Comments	
loci	+	++	?		
		abank can			
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.	
locus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.	
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks and searches of these databases when you query sequences or profiles in this database.	
client database loci	+	++	?	Define loci that are used in client databases.	
client database schemes	+	++	?	Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci t	able.
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.	
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.	
scheme members	+	++	?	Defines which loci belong to a scheme.	
scheme fields	+	++	?	Defines which fields belong to a scheme.	
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.	
cheme group scheme members	+	++	?	Defines which schemes belong to a group.	
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.	
	ck - Cl	hecks da	tabase conne	enable them to log on or change an existing password. activity for loci and schemes and that required helper applications are properly installed.	

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

Database: Species home Curator's page (spec Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	ies) Curator's page (database)
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Add new scheme member	
Please be aware that any modifications to the structure of this schem profiles will have to be reloaded.	e will result in the removal of all data from it. This is done to ensure data integrity. This does not affect allele designations, but an
Please fill in the fields below - required fields are marked with an excl	lamation mark (!).
Record	— — Action — — — —
scheme id: MLST	Reset Submit
locus: abcZ	
curator:! Keith Jolley (keith) datestamp:! 2014-07-04	
field order: 1	

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

PubMed links (to profile	s) +	++		?	
Database con	figur	ation			
Table	Add	Batch Add	Update or delete	Comments	
loci	+	++	?		
	dat	abank			
	s	can			
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.	
locus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.	
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlinks and	
				searches of these databases when you query sequences or profiles in this database.	
client database loci	+	++	?	Define loci that are used in client databases.	
client database schemes	+	++	?	Define schemes that are used in dient databases. You will need to add the appropriate loci to the client database loci table.	
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.	
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.	
scheme members	+	++	?	Defines which loci belong to a scheme.	
scheme fields	+	++	?	Defines which fields belong to a scheme.	
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.	
cheme group scheme members	+	++	?	Defines which schemes belong to a group.	
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.	
	ck - Cl	hecks da	tabase conne	enable them to log on or change an existing password. ctivity for loci and schemes and that required helper applications are properly installed.	

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

PubMLST	Database: Species home Curator's page (species) Curato Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	ır's page (da	tabase)
Logged in: Keith Jolle	ey (keith). Log out Change password		Toggle: i
Add new s	cheme field		
Please be aware profiles will have t		in the remov	al of all data from it. This is done to ensure data integrity. This does not affect allele designations, but any
Please fill in the fi	elds below - required fields are marked with an exclamation ma	rk (!).	
Record		Action-	
scheme id:!	MLST -	Reset	Submit
field:			
	integer 👻		
	● true ◯ false <u>i</u>		
	🔿 true 🔘 false 👔		
	Keith Jolley (keith)		
datestamp: description:	2014-07-04		
field order:	the second se		
	True O false		
value regex:	_		

- 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

5.15.2 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.

		:	The sequence on holds sequence contrags from any source.
			Associate sequences with Genbank/EMBL accession number.
+	++		Set up experiments to which sequences in the bin can belong.
			Add links associating sequences to experiments.
s	can	?	Tag regions of sequences within the sequence bin with locus information.
ion			
Add	Batch Add	Update or delete	Comments
+	++	?	
datat	ank scan		
+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
+	++	?	Define additional attributes to associate with values of a particular isolate record field.
+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
+	++	?	Define attributes that can be set for contigs in the sequence bin.
+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.
+	++	?	Add loci to sets.
+	++	?	Add schemes to sets.
+	++	?	Add metadata collection to sets.
+	++	?	Set database views linked to sets.
+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
+	++	?	Defines which loci belong to a scheme.
+	++	?	Defines which fields belong to a scheme.
+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
+	++	?	Defines which schemes belong to a group.
+	++	?	Defines which scheme groups belong to a parent group.
	Add + + datat + + + + + + + + + + + + + + + + + +	+++	+ ++ ? scan ? scan ? Add Batch Add Update or delete + ++ * ++ + ++

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

ged in: Keith Jolley (keith). HLog out Change	password				Toggl
ld new scheme					
ease fill in the fields below - required field	s are marked with an excl	amation mark (!).			
Record			Action		
id:! 41			Reset	Submit	
description:		0			
isolate display:! 💿 true 🔘 false	9 🕕				
main display:! 💿 true 🔘 false	9 🕕				
query field:! 💿 true 🔘 false	3 ()				
query status:! 🔘 true 🔘 false	9 🕕				
analysis:! 💿 true 🔘 false	9 🕕				
curator:! Keith Jolley (keit	th)				
datestamp:! 2015-07-01					
date entered:! 2015-07-01					
dbase name:			0		
dbase host:		0			
dbase port:	÷ 1				
dbase user:		0			
dbase password:		0			
		6			
dbase table: display order:	× 0	•			

• id - Index number of scheme - the next available number will be entered automatically.

- Allowed: any positive integer.
- description Short description this is used in tables so make sure it's not too long.
 - Allowed: any text.
- isolate_display Sets whether or not fields for this scheme are displayed in a detailed isolate record this can be overridden by user preference.
 - Allowed: allele only/sequence/hide.
- main_display Sets whether or not fields for this scheme are displayed in a main results table by default this can be overridden by user preference.
 - Allowed: true/false.
- query_field Sets whether or not fields for this scheme can be used in queries by default this can be overridden by user preference.

- Allowed: true/false.

- query_status Sets whether a dropdown list box should be displayed in the query interface to filter results based on profile completion for this scheme this can be overridden by user preference.
 - Allowed: true/false.
- analysis Sets whether or not alleles for this locus can be used in analysis functions by default this can be overridden by user preference.
 - Allowed: true/false.
- dbase_name Name of seqdef database (system name) containing scheme profiles (optional).

- Allowed: any text.

- dbase_host Resolved name of IP address of database host leave blank if running on the same machine as the isolate database (optional).
 - Allowed: network address, e.g. 129.67.26.52 or zoo-oban.zoo.ox.ac.uk
- dbase_port Network port on which the sequence definition database server is listening leave blank unless using a non-standard port, 5432 (optional).
 - Allowed: integer.
- dbase_user Name of user with permission to access the sequence definition database depending on the database configuration you may be able to leave this blank (optional).
 - Allowed: any text (no spaces).
- dbase_password Password of database user again depending on the database configuration you may be able to leave this blank (optional).
 - Allowed: any text (no spaces).
- dbase_table Table in the sequence definition database that contains profiles for this scheme. If the definition database uses BIGSdb this will be 'scheme_X' where X is the scheme id number in the sequef database.

- Allowed: any text (no spaces).

- display_order Integer reflecting the display position for this scheme within the interface (optional).
 - Allowed: any integer.
- allow_missing_loci Allow profile definitions to contain '0' (locus missing) or 'N' (any allele).

5.16 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.

Main	LST	Downl	oad: A	ences Batch sequences Cor Ileles MLST profiles nts Home PorA FetA Optio	npare alleles Profile/ST Bato ns Isolate Database	ch profiles List Brow	se Query	
								Help 🗹
ownlo	oad a	allele	e se	quences				
	hu o ch o r			al list All loci by scheme				
				ails of loci belonging to schem ne nodes to expand/collapse.	es or groups of schemes - clic	king a group folder wil	I display the lo	ci for all schemes within the
roup and a	any subj	groups.	CIICK U	te nodes to expand/collapse.				
🛓 📗 All I	oci						~	
	Capsule							
- 🔺 🛄 (Genetic	Informat	ion Pro	ocessing				
4-1	🔲 Repli	cation a	nd Rej	pair				
	📗 D	NA repli	cation					
	📗 N	ucleotid	e excis	ion repair				
þ- (🔲 Trans	scription						
þ- /	🔲 Trans	ation						
- k- 🛄 I	Metaboli	sm					E	
- 👍 🛄 1	Typing							
- F	🔲 MLST	Г						
	Finet	yping an	tigens					
	🔲 Antig	en gene	s					
	🗍 eMLS	6T (20 lo	cus pa	artial genes)				
	👖 eMLS	6T (20 lo	cus wh	nole genes)				
k- 🛄 🤇	Other sc	hemes						
<u></u>	oci not	in scher	nes				T	
/LST								
1201								
Locus D					Full name/product	Curator(s)	Last updated	
adk 🚺	*	DNA		Fixed: 465 bp	test_full_name / test_product			
abcZ 🚯	÷	DNA		Variable: (432 min; 433 max)		O. Harrison, K. Jolley		
aroE 🕕	*	DNA		Fixed: 490 bp		O. Harrison, K. Jolley		
fumC 🕕	*	DNA		Fixed: 465 bp		O. Harrison	2013-01-23	
gdh 🕕	*	DNA		Fixed: 501 bp		O. Harrison	2013-01-22	
pdhC 🕕	ž	DNA		Fixed: 480 bp Fixed: 450 bp		O. Harrison O. Harrison	2013-01-21 2013-01-22	
pgm 🕕	-	DINA	075	Fixed, 400 pp		O. Hallison	2013-01-22	
ownload	table: tal	b-delimi	ted text	t Excel format				

Scheme groups can be added in both the sequence definition and isolate databases. To add a new group, click the add (+) scheme group link on the curator's contents page.

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

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). @Log out Change password	Toggle: 🚯
Add new scheme group	
Please fill in the fields below - required fields are marked with an exclamation mark (!). Record id: 1 name:! Typing curator.! Keith Jolley (keith) datestamp:! 2015-07-01 description:	_
display order: seq query: True false Action Reset Submit	

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

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

Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
		tabank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
locus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlin and searches of these databases when you query sequences or profiles in this database.
client database loci	+	++	?	Define loci that are used in client databases.
client database schemes	+	++	?	Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

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

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

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

5.17 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.

Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	dat	tabank		
	s	scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
locus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlin
				and searches of these databases when you query sequences or profiles in this database.
client database loci	+	++	?	Define loci that are used in client databases.
client database schemes	+	++	?	Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

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

User: Add [Ouerylupdate Batch insert Logged in: Keith Jolley (keith). Log out Change password Add new client database Please fill in the fields below - required fields are marked with an exclamation mark (!). Record Adianew: PubMLST isolates description! 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 mark be submitted to this database and consequently it should be noted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample. dbase nonted that it does not represent a population sample.		abase: Species home Curator's page (species) Curator's page (dat	abase)		
MLST profiles: Add Query/update Batch insert Logged in: Keith Jolley (Keith): Log out Change password Add new client database Please fill in the fields below - required fields are marked with an exclamation mark (I). Record id: 1 Record Action id: 1 Reset Submit description: Contains data for a collection of isolates that represent the total known diversity of Netseeria 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. 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! 2014.07-04 dbase host IP address of database hot					
Logged in: Keith Jolley (keith). Log out Change password To Add new client database Add new client database Please fill in the fields below - required fields are marked with an exclamation mark (!). Action Record Action id! Image: pubMLST isolates Action description! 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. dbase name! pubmlst_bigsdb_neisseria_isolates dbase config name! pubmlst_heisseria_isolates dtastamp! pubmlst_heisseria_isolates dtaste store I IP address of database host					
Add new client database Please fill in the fields below - required fields are marked with an exclamation mark (!). Record id! 1	MLO	i promes. Add I dderyrdpdate i Batch msert			
Please fill in the fields below - required fields are marked with an exclamation mark (!). Record id: name: PubMLST isolates description: 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. dbase name! pubmlst_bigsdb_neisseria_isolates Name of the database holding isolate data dbase config name! pubmlst_heisseria_isolates Name of the database configuration curator! Keith Jolley (keith) datestamp! 2014-07-04 I! IP address of database host	Logged in: Keith Jolley (keith)). Log out Change password			Toggle: i
Record Action idt Image: PubMLST isolates Reset description: 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. dbase name! pubmlst_bigsdb_neisseria_isolates Name of the database holding isolate data Name of the database configuration curator! dbase name! pubmlst_heisseria_isolates Name of the database configuration curator! dbase host I IP address of database host	Add new clien	t database			
idi Image: PubMLST isolates Reset Submit description: 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. Image:	Please fill in the fields be	low - required fields are marked with an exclamation mark (!).			
name:! PubMLST isolates description: 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. 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: dbase host	Record			Action	
name:! PubMLST isolates description: 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. 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: dbase host	id:	1		Beest Submit	
diversity of Neiszeria 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. dbase name: pubmist_bigsdb_neisseria_isolates	name:			Reset	
dbase config name:! pubmlst_neisseria_isolates Name of the database configuration curator:! Keith Jolley (keith) datestamp:! 2014-07-04 dbase host		diversity of <u>Neisseria</u> species. For every allel database there is at least one corresponding is isolate may be submitted to this database and c	tic profile in the profiles solate deposited here. Any consequently it should be		
curator:1 Keith Jolley (keith) datestamp:1 2014-07-04 dbase host I	dbase name:!	pubmlst_bigsdb_neisseria_isolates	Name of the database holding isolate data		
datestamp:1 2014-07-04 dbase host I IP address of database host	dbase config name:!	pubmlst_neisseria_isolates	Name of the database configuration		
dbase host					
dbase port					
			ns		
dbase user:					
dbase password:					
dbase view: isolates View of isolates table to use			ates table to use		
ufl: /cgi-bin/bigsdb/bigsdb.pl Web URL to database script	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 seqdef 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.

5.17.1 Look up isolates with given allele

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

Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	databank			
	5	scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
locus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlin
				and searches of these databases when you query sequences or profiles in this database.
client database loci	+	++	?	Define loci that are used in client databases.
client database schemes	+	++	?	Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
cheme group scheme members	+	++	?	Defines which schemes belong to a group.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

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 Us	tabase: Species home Curator's page (species) Cura ers: Add Query/update ci: Add ST profiles: Add Query/update Batch insert	itor's page (database)			
Logged in: Keith Jolley (keit	th). Log out Change password				Toggle: i
Add new locu	s to client database definition				
Please fill in the fields b	elow - required fields are marked with an exclamation m	nark (!).			
Record			Action —		
	1) PubMLST isolates 👻		Reset	Submit	
locus:					
curator:! K datestamp:! 2	Ceith Jolley (keith)				
locus alias:		name that this locus is referred by in client database (if different)			

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

rovenance/meta	data
locus:	abcZ
allele:	5
sequences:	ITTGATACCE TIGCCGAAGE TITGEGCGAA ATTCGCGATT TATTGCGCCE TTATCATCAT GICAGCCATE AGTIGGAAAA TGGTTCGAGT GAGGCTTIGI IGAAAGAGCT TAACGAATAG CAACTGAAA TCGAACCGA GGACGGCTGG AAGCTGGATG CGGCAGTCAA GCAGACTTIG GITGGCAGTG GATGGACAAA ATCGGCAACC TCTCCGGCGG ACAGAAAAA CGGTGTGCCC TAGGCGAGGC TIGGGTGAG AGACCTGATG TATTGCGTCG GACGAGCCG ACCAACATTI GGACATGA CGGGATTATI TGGCTGGAAA ATCGGCTAGA GGCAGCCTGG TIGTGATAC CCACGACCGC CGTTTTTGG ACAATATCGC CACGCGCATC GTCGAACTGG ATC
length:	433
status:	Sanger trace checked
date entered:	
datestamp:	2009-11-11
	Keith Jolley, University of Oxford, UK
curator:	Man-Suen Chan, University of Oxford (E-mail: man-suen.chan@paediatrics.ox.ac.uk)
rofiles containin	g this allele
MLST:	183 profiles
solate databases	

5.17.2 Look up isolates with a given scheme primary key

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

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



5.17.3 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.

Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
		tabank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
locus extended attributes	+	++	?	Define additional fields to associate with sequences of a particular locus.
client databases	+	++	?	Add isolate databases that use locus allele or scheme profile definitions defined in this database - this enables backlink and searches of these databases when you query sequences or profiles in this database.
client database loci	+	++	?	Define loci that are used in client databases.
client database schemes	+	++	?	Define schemes that are used in client databases. You will need to add the appropriate loci to the client database loci table.
client database fields linked to loci	+	++	?	Define fields in client database whose value can be displayed when isolate has matching allele.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
cheme group scheme members	+	++	?	Defines which schemes belong to a group.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

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.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add	
MLST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Add new locus to client database isolate field definition	
Please fill in the fields below - required fields are marked with an exclamation mark (!).	
Record Action	
client dbase id! 1) PubMLST isolates 👻 Reset Submit	
locus:1 penA	
isolate field: penicillin_range	
curator.! Keith Jolley (keith)	
datestamp:1 2014-07-04	
allele query: True Table Set to true to display field values when an allele query is done. 	

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

	nation - penA: 9
ovenance/met	a data
locus:	penA
allele:	9
sequences:	GACGECGTI IGCIGCCGGI CAGCITIGAA AAACAGGCGG IIGCGCCGCA AGGCAAACGI ATAITIAAAG CAICGACCGC ACGICAGGIG CGIGAGIIGA IGGITICIGI AAACGGAACCI GGCGGTACGG GTACGGCGGG IGCGGIAGII GGITICGACC ICGGCGCAAA AACCGGIAGG GCGCGIAAGI IGGITIACGG ICGIIACGI GAITACAAAC ACGIIGCCAC ITICAICGGI IIIGCCCCGG CIAAAAAICC GCGIGIGGAII GGGCGGIAA CCAIIGACGA GCCGACIGCA AACGGIIACI ACGGCGGCGI AGIGACAGGI CCGGICIICA AACAAGIIAI GGGCGGIAGC CIGAACAICI IGGGCGIIIC ICCGACCAAA CCICIGACCA AI
length:	402
status:	Sanger trace checked
date entered:	2006-09-04
datestamp:	2006-09-04
sender:	Muhamed-Kheir Taha, National Reference Center for Meningococci, Institut Pasteur, France
curator:	Keith Jolley, University of Oxford, UK (E-mail: keith.jolley@zoo.ox.ac.uk)
mutation F504L:	yes
mutation A510V:	yes
mutation I515V:	yes
mutation H541N:	yes
mutation I566V:	yes
ublication (1)	
Jolley KA, Kad	quez 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, lubowski 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 L (2007). Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis. Antimicrob Agents Chemother 51:2784-92
olate database	5
PubMLST isolates:	Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample. 141 isolates
aked data	
nked data	

5.18 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.

5.18.1 Example rule code

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

The code for this rule is as follows:

```
#Clinical identification rule
#Update job viewer status
update_status({stage=>'Scanning MLST loci'});
#Scan genome against all scheme 1 (MLST) loci
scan_scheme(1);
```

```
#Update job viewer status
update_status({percent_complete=>30, stage=>'Scanning PorA and FetA VRs'});
#Scan genome against the PorA VR and FetA VR loci
scan_locus($_) foreach qw(PorA_VR1 PorA_VR2 FetA_VR);
Add text to main output
append_html("<h1>Strain type</h1>");
#Set variables for the scanned results. These can be found in the
#$results->{'locus'} hashref
my %alleles;
$alleles{$_} = $results->{'locus'}->{$_} // 'ND' foreach qw(PorA_VR1 PorA_VR2);
$alleles{'FetA_VR'} = $results->{'locus'}->{'FetA_VR'} // 'F-ND';
#Scheme field values are automatically determined if a complete
#profile is available. These are stored in the $results->{'scheme'} hashref
my $st = $results->{'scheme'}->{1}->{'ST'} // 'ND';
append_html("P1.$alleles{'PorA_VR1'}, $alleles{'PorA_VR2'}; $alleles{'FetA_VR'}; ST-$st ");
#Reformat clonal complex using a regular expression, e.g.
#'ST-11 clonal complex/ET-37 complex' gets rewritten to 'cc11'
my $cc = $results->{'scheme'}->{1}->{'clonal_complex'} // '-';
$cc =~ s/ST-(\S+) complex.*/cc$1/;
append_html("($cc)");
if ($st eq 'ND') {
 append_html("ST not defined. If individual MLST loci have been found "
  . "they will be displayed below:");
 #The get_scheme_html function automatically formats output for a scheme.
 #Select whether to display in a table rather than a list, list all loci, and/or list fields.
 append_html(get_scheme_html(1, {table=>1, loci=>1, fields=>0}));
}
#Antibiotic resistance
update_status({percent_complete=>80, stage=>'Scanning penA and rpoB'});
scan_locus($_) foreach qw(penA rpoB);
if (defined $results->{'locus'}->{'penA'} || defined $results->{'locus'}->{'rpoB'} ){
 append html("<h1>Antibiotic resistance</h1>");
 if (defined $results->{'locus'}->{'penA'}){
   append_html("<i>penA</i> allele: $results->{'locus'}->{'penA'}");
    #If a client isolate database has been defined and values have been defined in
    #the client_dbase_loci_fields table, the values for a field in the isolate database can be
    #retrieved based on isolates that have a particular allele designated.
    #The min_percentage attribute states that only values that are represented by at least that
    #proportion of all isolates that had a value set are returned (null values are ignored).
   my $range = get_client_field(1, 'penA', 'penicillin_range', {min_percentage => 75});
   append_html(" (penicillin MIC: $range->[0]->{'penicillin_range'})") if @$range;
   append_html("");
  }
 if (defined $results->{'locus'}->{'rpoB'}){
   append_html("<i>rpoB</i> allele: $results->{'locus'}->{'rpoB'}");
   my $range = get_client_field(1, 'rpoB', 'rifampicin_range', {min_percentage => 75});
   append_html(" (rifampicin MIC: $range->[0]->{'rifampicin_range'})") if @$range;
    append_html("");
  }
```

append_html("");

Rule files

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

Linking to the rule query

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

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

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

Adding descriptive text

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

5.19 Workflow for setting up a MLST scheme

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

Seqdef database

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

Isolate database

- 1. Create the same loci with the following additional parameters (example locus 'atpD')
- dbase_name: seqdef_db
- dbase_table: sequences
- dbase_id_field: allele_id
- dbase_id2_field: locus

- dbase_id_value: atpD
- dbase_seq_field: sequence
- url: something like /cgi-bin/bigsdb/bigsdb.pl?db=seqdef_db&page=alleleInfo&locus=atpD&allele_id=[?]
- 2. Create scheme 'MLST' with:
- dbase_name: seqdef_db
- dbase_table: scheme_1 (or whatever the id of your seqdef scheme is)
- 3. Add scheme_field ST as before
- 4. Add loci as scheme_members

5.20 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.

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

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

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert
Logged in: Keith Jolley (keith). Log out Change password
Scan EMBL/Genbank record for loci
This function allows you to scan an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci. Please enter accession number Primary identifier Accession: AM421808 Image: Comparison of the setting of the set

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

PubMI	ST/U	atabase: Species home Curator's page (species) Curator's page (database) sers: Add Query/update olates: Add Query/update Batch insert	
Logged in: Keit	h Jolley (ke	ith). Log out Change password	
Scan El	MBL/C	Genbank record for loci	
This function	allows yo	u to scan an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci.	
Please	enter acce	ssion number — Primary identifier – Action —	
Accession	AM42180	08 ● locus tag Submit	
		limited text Excel format (suitable for batch upload of loci). lelimited text Excel format (suitable for defining the first allele in the seqdef database).	
des	cession: version: type: length: cription: regions:	AM421808 1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975	
Locus	Aliases	Product	Length
NMC0001	IpxC; envA	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924
NMC0002	pilS1	pilin (fragment)	291
NMC0003	pilS2	truncated pilin	366
NMC0004	fbp	nontidul proble dia trans in programs	330
NMC0005		peptidyl-prolyl cis-trans isomerase	
NMC0006		putative membrane protein	219
NMC0007	metG	putative membrane protein putative glycerate dehydrogenase	954
NMC0008	glmS	putative membrane protein putative glycerate dehydrogenase methionyl-tRNA synthetase	954 2058
NMC0009		putative membrane protein putative glycerate dehydrogenase methionyl-tRNA synthetase glucosaminefructose-6-phosphate aminotransferase [isomerizing]	954 2058 1839
NMC0010		putative membrane protein putative glycerate dehydrogenase methionyl-IRNA synthetase glucosamine—fructose-6-phosphate aminotransferase [isomerizing] putative lipoprotein	954 2058 1839 519
NIMCORAL	gna33	putative membrane protein putative glycerate dehydrogenase methionyl-tRNA synthetase glucosaminefructose-6-phosphate aminotransferase [isomerizing] putative lipoprotein outer membrane lipoprotein Gna33 []	954 2058 1839 519 1326
NMC0011	gna33	putative membrane protein putative glycerate dehydrogenase methionyl-IRNA synthetase glucosaminefructose-6-phosphate aminotransferase [isomerizing] putative lipoprotein outer membrane lipoprotein Gna33 [] putative integral membrane protein	954 2058 1839 519 1326 840
NMC0012	gna33	putative membrane protein putative glycerate dehydrogenase methionyl-IRNA synthetase glucosamine-fructose-6-phosphate aminotransferase [isomerizing] putative lipoprotein outer membrane lipoprotein putative integral membrane protein putative lipoprotein	954 2058 1839 519 1326 840 1167
	gna33 phnA	putative membrane protein putative glycerate dehydrogenase methionyl-IRNA synthetase glucosaminefructose-6-phosphate aminotransferase [isomerizing] putative lipoprotein outer membrane lipoprotein Gna33 [] putative integral membrane protein	954 2058 1839 519 1326 840

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

gged in: Keit	h Jolley (ke	(ff). Log out Change password	
can El	MBL/C	Genbank record for loci	
This function	allows yo	u to scan an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci.	
Plasea	anter acce	ssion number — — Primary identifier – — Action —	
Accession:			
ownload tab	ole: tab-de	imited text Excel format (suitable for batch upload of loci).	
ownload all	eles: tab-c	elimited text Excel format (suitable for defining the first allele in the seqdef database).	
nnotatio	n Inform	ation	
ac	cession:	AM421808	
	version:	1	
	version: type:		
	type:		
	type: length:	dna	
des	type: length:	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome.	
des	type: length: cription:	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome.	
des coding	type: length: cription: regions:	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975	
des coding oding se	type: length: ccription: regions: equence	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S	Leng
des coding oding se Locus	type: length: cription: regions:	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S Product	_
des coding oding se Locus	type: length: cription: regions: equence Aliases	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S	_
des coding oding se Locus NMC0001	type: length: cription: regions: equence Aliases lpxC;	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S Product	924
des coding oding se Locus NMC0001 NMC0002	type: length: cription: regions: equence Aliases lpxC; envA	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S Product UDP-3-O-[3-hydroxymyristoy]] N-acetylglucosmine deacetylase	924 291
des coding oding se Locus NMC0001 NMC0002 NMC0003 NMC0004	type: length: ccription: regions: equence Aliases lpxC; envA pilS1	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S Product UDP-3-O-[3-hydroxymyristoy]] N-acetylglucosmine deacetylase pillin (fragment)	924 29 36 33
des coding oding se Locus NMC0001 NMC0002 NMC0002 NMC0003 NMC0004 NMC0005	type: length: ccription: regions: equence Aliases lpxC; envA pilS1 pilS2	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S Product UDP-3-O-[3-hydroxymyristoy] N-acetylglucosmine deacetylase UDP-3-O-[3-hydroxymyristoy] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin peptidyl-protyl cis-trans isomerase putative membrane protein	924 297 360 330 219
des coding oding se Locus NMC0001 NMC0002 NMC0003 NMC0003 NMC0005 NMC0006	type: length: ccription: regions: equence Aliases lpxC; envA pilS1 pilS2	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S Product UDP-3-O-[3-hydroxymyristoy]] N-acetylglucosmine deacetylase UDP-3-O-[3-hydroxymyristoy]] N-acetylglucosmine deacetylase pilin (fragment) truncated pilin putative glycerate dehydrogenase	924 291 360 330 219 954
des coding se coding se co	type: length: cription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S	924 291 360 219 954 205
des coding oding se Locus NMC0001 NMC0002 NMC0003 NMC0004 NMC0005 NMC0006 NMC0006 NMC0008	type: length: ccription: regions: equence lpxC; envA piIS1 piIS2 fbp	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S	924 291 366 330 219 954 205 183
des coding se oding se NMC0001 NMC0003 NMC0003 NMC0005 NMC0006 NMC0006 NMC0008 NMC0009	type: length: ccription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG glmS	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S Product UDP-3-O-[3-hydroxymyristoy[] N-acetylglucosmine deacetylase UDP-3-O-[3-hydroxymyristoy[] N-acetylglucosmine deacetylase IDD IDD IDD IDD IDD IDD IDD IDD IDD IDD	924 291 360 219 954 205 183 519
des coding se coding se Locus NMC0001 NMC0002 NMC0003 NMC0005 NMC0005 NMC0007 NMC0008 NMC0008 NMC0008 NMC00010	type: length: cription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 s Product UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase pilitin (fragment) truncated pilin truncated pilin utative glycerate dehydrogenase methionyl-tRNA synthetase glucosamine-fructose-6-phosphate aminotransferase [isomerizing] putative [ipoprotein putative [ipoprotein Gna33 []	924 291 366 330 219 954 205 183 519 132
des coding se coding se locus NMC0001 NMC0005 NMC0006 NMC0006 NMC0008 NMC0008 NMC0009 NMC0000 NMC0011	type: length: ccription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG glmS	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S	Leng 924 291 366 330 219 954 205 183 519 132 840
des coding se coding se coding se NMC0001 NMC0002 NMC0005 NMC0006 NMC0006 NMC0008 NMC0008 NMC0010 NMC0012	type: length: ccription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG glmS	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S	924 291 360 330 219 954 205 183 519 132 840 116
des coding se coding se NMC0001 NMC0002 NMC0003 NMC0005 NMC0005 NMC0005 NMC0005 NMC0009 NMC00010 NMC0011 NMC0011 NMC0013	type: length: ccription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG glmS gna33	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S Product UDP-3-O-[3-hydroxymyristoy[] N-acetylglucosmine deacetylase UDP-3-O-[3-hydroxymyristoy[] N-acetylglucosmine deacetylase plilin (fragment) truncated pilin truncated pilin putative lipoprotein putative lipoprotein Gna33 [] putative lipoprotein putative lipoprotein possible membrane protein	92- 29- 36- 33- 205- 183- 51- 132 84- 116- 126
des coding Coding se	type: length: ccription: regions: equence Aliases lpxC; envA pilS1 pilS2 fbp metG glmS	dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome. 1975 S	924 291 360 219 954 205 183 519 132 840 116 126 330

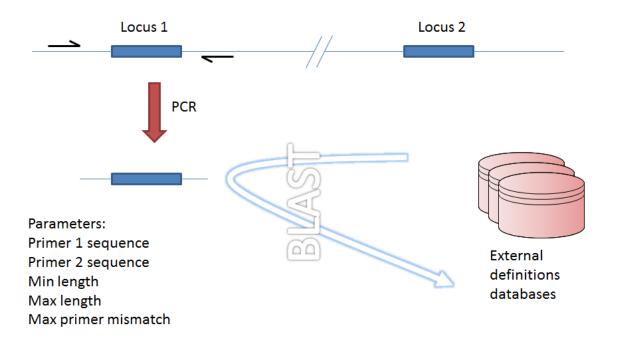
5.21 Genome filtering

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.

5.21.1 Filtering by in silico PCR

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

To define a PCR reaction that can be linked to a locus definition, click the add (+) PCR reaction link on the curator's main page.



Locus 1 and locus 2 share allele pool

Fig. 5.1: Genome filtering by in silico PCR.

allele designations sequences	+	+	?	Allele designations can be set within the isolate table functions.		
sequences				Andre designations dan be set main the isolate table fanatoris.		
	+		?	The sequence bin holds sequence contigs from any source.		
accession number links	+ +	+	?	Associate sequences with Genbank/EMBL accession number.		
experiments -	+ +	+	?	Set up experiments to which sequences in the bin can belong.		
experiment sequences			?	Add links associating sequences to experiments.		
sequence tags	scan		?	Tag regions of sequences within the sequence bin with locus information.		
Database configurati	ion					
Table A	dd 🗆 🚽 –	tch dd	Update or delete	Comments		
1001		++	?			
-	latabank					
Tocus anasos		++	?	Add alternative names for loci. These can also be set when you batch add loci.		
PCR reactions	+ •	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.		
nucleotide probes	+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.		
olate field extended attributes	+ ·	++	?	Define additional attributes to associate with values of a particular isolate record field.		
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.		
sequence attributes	+ ·	++	?	Define attributes that can be set for contigs in the sequence bin.		
sets	+ ·	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.		
set loci	+ ·	++	?	Add loci to sets.		
set schemes	+ ·	++	?	Add schemes to sets.		
set metadata	+ ·	++	?	Add metadata collection to sets.		
setview	+ ·	++	?	Set database views linked to sets.		
schemes	+ -	++	?	Describes schemes consisting of collections of loci, e.g. MLST.		
scheme members	+ -	++	?	Defines which loci belong to a scheme.		
scheme fields	+ ·	++	?	Defines which fields belong to a scheme.		
scheme groups	+ ·	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.		
scheme group scheme members	+ ·	++	?	Defines which schemes belong to a group.		
cheme group group members	+ •	++	?	Defines which scheme groups belong to a parent group.		
				n to log on or change an existing password. ci and schemes and that required helper applications are properly installed.		

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) Users:	se: Species home Curator's page (species) Curator's page (database) Add Query/update s: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). 🗭	Log out Change password	Toggle: 🚯
Add new PCR re	eaction	
Please fill in the fields below	required fields are marked with an exclamation mark (!).	
Record		
id:!		
description:		
primer1:		
primer2:		
aurata al		
	Keith Jolley (keith) 2015-07-01	
min length:		
max length:		
max primer mismatch:	▼ ① 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.

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

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

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

5.21.2 Filtering by in silico hybridization

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

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

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

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

- probe_id Dropdown list of probe names.
 - Allowed: selection from list.
- locus Dropdown list of loci.
 - Allowed: selection from list.
- max_distance Minimum distance of probe from end of locus.

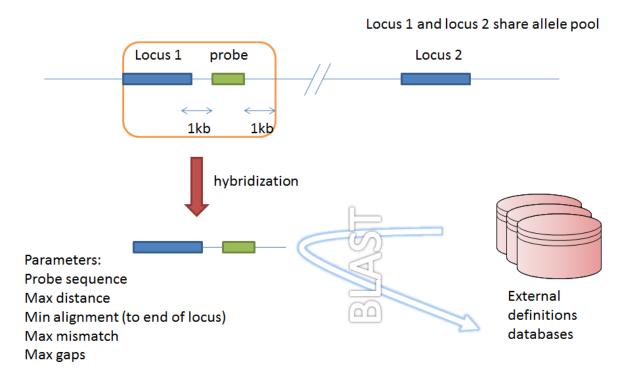


Fig. 5.2: Filtering by in silico hybridization

- 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.

5.22 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.

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

Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

experiments experiment sequences			2	Set up experiments to which sequences in the bin can belong. Add links associating sequences to experiments.
			?	
sequence tags	3	can	f	Tag regions of sequences within the sequence bin with locus information.
Database configura	tion			
Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	datal	bank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
PCR reactions	+	++	?	Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
PCR locus links	+	++		Link a locus to an in silico PCR reaction.
nucleotide probes	+	++	?	Define nucleotide probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.
probe locus links	+	++		Link a locus to an in silico hybridization reaction.
plate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes	+	++	?	Define attributes that can be set for contigs in the sequence bin.
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.
set loci	+	++	?	Add loci to sets.
setschemes	+	++	?	Add schemes to sets.
set metadata	+	++	?	Add metadata collection to sets.
setview	+	++	?	Set database views linked to sets.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
heme group group members	+	++	2	Defines which scheme groups belong to a parent group.

Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

Prrial/ILST Database: Species home | Curator's page (species) | Curator's page (database) Users: Add | Query/update Isolates: Add | Query/update | Batch insert

Logged in: Keith Jolley (keith). DLog out | Change password

Database curator's interface - Neisseria PubMLST

Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query browse list batch update	
solate field extended attribute values	+	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences		++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	2	Set up experiments to which sequences in the bin can belong.

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

Publ	MLS.	💟 Users: A	se: Specie: Add Query : Add Que	//upda	ite			es) C	urator's p	age (database)									
Logged in	: Keith Jo	ley (keith). Lo	g out Char	ige pa	sword								Toggle: i	Field	help: id					▼ Go
Isola	te qu	ery/up	date																	
—Isol	ate prove	nance/phen	otype field	s —						-Display/sort	options									Modify
isola	ate	•	=	•	MC58	3		-	• 1	Order by:	id			→ asc asc asc asc asc asc asc asc asc	ending	•				form
										Display:	25 👻 recor	ds p	er page 👔							options
Dele	set S returned	ubmit Click the hy Tag sc Sca	anning –	— Pi	ed infor ojects – ect proje				•	Link										
		Sequence	New					solate	fields 👔				MLST		ping an		test	tes		Loci
Delete	Update	bin	version	id	isolate	aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1	PorA VR2	FetA VR		PorA VR1	PorA VR2	'test9
delete	update	upload	create	240	MC58	Z7176	UK	1983		Neisseria meningitidis	В	74	ST-32 complex/ET-5 complex	7 update	16-2 update	F1-5 update	1	7 update	16-2 update	add

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

species: Neisseria meningitidis update history: 137 updates show details
Publications (4)
Bennett JS, Bentley SD, Vernikos GS, Quail MA, Cherevach I, White B, Parkhill J, Maiden MC (2010). Independent evolution of the core and accessory gene sets in the genus Neisseria: insights gained from the genome of Neisseria lactamica isolate 020-06. BMC Genomics 11:652 79 isolates
Bennett JS, Jolley KA, Earle SG, Corton C, Bentley SD, Parkhill J, Maiden MC (2012). A genomic approach to bacterial taxonomy: an examination and proposed reclassification of species within the genus Neisseria. Microbiology 158:1570-80 <u>55 isolates</u>
Stabler RA, Marsden GL, Witney AA, Li Y, Bentley SD, Tang CM, Hinds J (2005). Identification of pathogen-specific genes through microarray analysis of pathogenic and commensal Neisseria species. Microbiology 151:2907-22 https://doi.org Stabler RA, Marsden GL, Witney AA, Li Y, Bentley SD, Tang CM, Hinds J (2005). Identification of pathogen-specific genes through microarray analysis of pathogenic and commensal Neisseria species. Microbiology 151:2907-22 doi:10.100
• Tettelin H, Saunders NJ, Heidelberg J, Jeffries AC, Nelson KE, Eisen JA, Ketchum KA, Hood DW, Peden JF, Dodson RJ, Nelson WC, Gwinn ML, DeBoy R, Peterson JD, Hickey EK, Haft DH, Salzberg SL, White O, Fleischmann RD, Dougherty BA, Mason T, Ciecko A, Parksey DS, Blair E, Cittone H, Clark EB, Cotton MD, Utterback TR, Khouri H, Qin H, Vamathevan J, Gill J, Scarlato V, Masignani V, Pizza M, Grandi G, Sun L, Smith HO, Fraser CM, Moxon ER, Rappuoli R, Venter JC (2000). Complete genome sequence of Neisseria meningitidis serogroup B strain MC58. Science 287:1809-15 [] isolate]
Sequence bin
contigs: 1 detailed breakdown: Display length: 2272360 bp loci tagged: 1283
Schemes and loci
All loci Capsule Ca

Click the 'Renumber' button:

ogged in: Ke	ith Jolley (keith). Lo	g out Change	e password												Toggle:
equer	nce bin fo	r MC58	3												
ontig su	mmary statist	cs													
• Num	ber of contigs: 1														
	th: 2272360														
• Dow	nload sequences	(FASTA form	hat)												
	nload sequences			3L format)											
	Comunation	Original			fleat	604					_		EMDI-	Antomic	Descention
equence	Sequencing method d	Original esignation	Length	Comments	float test	SRA accession	test attribute	test test date int	Locus	Start	End	Direction	EMBL format	Artemis i	Renumber
1	Sanger		2272360	whole		account		date int	NEIS2140	502	897	←	EMBL	Artemis	Renumber
				genome					NEIS2141	918	2312	←			
									NEIS2142	2517	3161	←			
									NEIS2143	3158	3511	←			
									NEIS2144	3635	4117	\rightarrow			
									NEIS2145	4311	4961	\rightarrow			
									NEIS2146	4958	5875	\rightarrow			
									NEIS2147	5936	6214	\rightarrow			
									NEIS2148	6281	7492	←			
									(pgk)						
									NEIS2149	7573	8826	←			
									NEIS2150	9346	10317	←			
									NEIS2150 NEIS2151	9346 10350	10317 10811	\leftarrow			
									NEIS2151 NEIS2152						
									NEIS2151	10350	10811	←			

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

PubMLST		ate	ies) Curator's page (database)
Logged in: Keith Jolle	e y (keith) . Log out Change pa	ssword	
Ponumbor	locus denom	nositions ha	sed on tagged sequences
Nenumber	iocus genom		Seu oli layyeu sequellees
You have selected	I to renumber the genome	positions set in the locus	table based on the tagged sequences in sequence id#1.
Option		Actio	
	itions for loci not tagged in		
- itemove pos	allona for foci not tagged in	Ren	umber
The following desi	ignations will be made:		
	-		
	sting genome position 🗢		
NEIS2140	2181973	502	
NEIS2141	2182389	918	
NEIS2142	2183899	2517	
NEIS2143	2184552	3158	
NEIS2144	2185029	3635	
NEIS2145	2185705	4311	
NEIS2146	2186352	4958	
NEIS2147	2187330	5936	
NEIS2148	2187675	6281	
NEIS2149	2188934	7573	
NEIS2150	2190551	9346	
NEIS2151	2191558	10350	
NEIS2152	2192048	10840	
NEIS2153	2193382	12174	
NEIS0001	1261	15221	
NEIS0210	209923	17229	
pilS	3271	18127	
NEIS0004	4069	23904	
NEIS0005	4476	24311	
NEIS0007	5843	25679	

5.23 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.

Database configura	tion			
Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	datal	bank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
PCR reactions	+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		Define nucleotide probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.
olate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes	+	++		Define attributes that can be set for contigs in the sequence bin.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
heme group group members	+	++	?	Defines which scheme groups belong to a parent group.
				m to log on or change an existing password. ci and schemes and that required helper applications are properly installed.

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

PubMLST U	sers: Add Query/upd olates: Add Query/up	date Batch insert	or's page (database)		
Logged in: Keith Jolley (ke					Toggle: i
Add new con	nposite field	1			
	below - required fields strain_designations	s are marked with an exclamation m	ark (!). name of the field as it will appear in the web interface	Action Reset Submit	
position after:!		 field present in the isolate table 			
	○ true ● false Keith Jolley (keith) 2014-07-08	Sets whether to display field in isolate q	uery results table (can be overridden by user preference).		

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

Database configura	tion			
Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	data	bank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
PCR reactions	+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
olate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes	+	++		Define attributes that can be set for contigs in the sequence bin.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
cheme group group members	+	++	?	Defines which scheme groups belong to a parent group.
				n to log on or change an existing password. ci and schemes and that required helper applications are properly installed.

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

PubMLST	Database: Spec Users: Add Que Isolates: Add Q	ery/update		e (species) Curator's page (database) t	
Logged in: Keith Jolle	y (keith). Log out Ch	ange password	d		
Update or o	delete con	nposite	e field		
1 composite field de Delete Update	efined. field name	position after	main	definition	missing data
Delete Undate si	train_designation	isolate	display false	[serogroup]: P1.[PorA_VR1],[PorA_VR2]: [FetA_VR]: ST-[scheme 1:ST]	ND: P1.ND,ND: F-ND:
Delete Opdate of				([scheme 1:clonal_complex])	ST-ND (-)
				([scneme 1.cional_complex])	51-10 (-)

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.

Construction of the construction of the	dd Query/u Add Query	pdate /update Batch insert	
ogged in: Keith Jolley (keith). Log	out Change	password	
Ipdate composit	te field	- strain_designat	tion
position after: isolate		-	
main display: false 👻 curator: Keith Jolley			
datestamp: 2014-04-09		Update	
	empty value	regex	curator datestamp delete edit move
Serogroup [isolate field]	ND		Keith Jolley 2009-11-12 delete edit up down
: P1.			Keith Jolley 2009-11-12 delete edit up down
PorA_VR1 [locus]	ND		Keith Jolley 2009-11-12 delete edit up down
			Keith Jolley 2009-11-12 delete edit up down
PorA_VR2 [locus]	ND		Keith Jolley 2009-11-12 delete edit up down
:	E ND		Keith Jolley 2009-11-12 delete edit up down
FetA_VR [locus] ; ST-	F-ND		Keith Jolley 2009-11-12 delete edit up down
ST [MLST field]	ND		Keith Jolley 2009-11-12 delete edit up down Keith Jolley 2009-11-12 delete edit up down
or (MLST field)	ND		Keith Jolley 2009-11-12 delete edit up down Keith Jolley 2009-11-12 delete edit up down
clonal_complex [MLST field]	-	s/ST-(\S+) complex.*/cc\$1	L/ Keith Jolley 2009-11-12 delete edit up down
)		by bi ((b)) compilent y boyi	Keith Jolley 2009-11-12 delete edit up down
,			
Add new field:			
		Add new text field	
	•		
	•		
	curato	: Keith Jolley	
		: 2014-07-08	

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

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

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

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

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

5.24 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.

Database configura	tion			
Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	datal	bank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
PCR reactions	+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		Define nucleotide probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.
olate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes	+	++		Define attributes that can be set for contigs in the sequence bin.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
heme group group members	+	++	?	Defines which scheme groups belong to a parent group.
				m to log on or change an existing password. ci and schemes and that required helper applications are properly installed.

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).

Database: Spe Users: Add Q Isolates: Add	uery/up	date		Curator's page (database)
gged in: Keith Jolley (keith). 🗭 Log out	Change	e password		
atabase curator's	into	rfaco	Noissoria	PubMI ST
	IIICI	lace	- MEISSEITA	FUDMEST
Add, update or delete	e reco	ords		
Record type	Add	Batch Ad	ld Update or	delete Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query browse lis	t batch update
olate field extended attribute value	es +	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences		++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
	Add Ba		Update or delete	Comments
loci	+	++	?	
In such all second		ink scan		
locus aliases	+	++		alternative names for loci. These can also be set when you batch add loci.
PCR reactions	+	++		up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		ne nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
isolate field extended attributes	+	++		ne additional attributes to associate with values of a particular isolate record field.
composite fields	+			d to construct composite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes	+	++		ne attributes that can be set for contigs in the sequence bin.
schemes	+	++	2 Des	cribes schemes consisting of collections of loci, e.g. MLST.

Download the Excel template:

oggle: i

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'.

5.25 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.

S Database configura	ition			
Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	datat	bank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
PCR reactions	+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
olate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes	+	++		Define attributes that can be set for contigs in the sequence bin.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
cheme group group members	+	++	?	Defines which scheme groups belong to a parent group.
				m to log on or change an existing password. ci and schemes and that required helper applications are properly installed.

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

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

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change password	Toggle:
Batch insert sequences	
This page allows you to upload sequence data for a specified isolate record in FASTA format.	
If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any other iso FASTA file. This allows data for multiple isolates to be uploaded.	late table field that uniquely defines the isolate, can be named in the identifier rows of the
Please note that you can reach this page for a specific isolate by querying isolates and then clicking "Upload" within the isolate	ate table.
Please fill in the following fields - required fields are marked with an exclamation mark (!).	
Paste in sequences in FASTA format	Attributes
	isolate id: ! Read identifier from FASTA
	identifier field: id
	sender: !
	method:
	assembly id:
	read length:
	Options
	Don't insert sequences shorter than 250 👻 bps.
	Link to experiment:
	Alternatively upload FASTA file Action
	Select FASTA file: Reset Submit
	Browse No file selected.
Back	

5.26 Checking external database configuration settings

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

Table	Add	Batch Add	Update or delete	Comments			
loci	+	++	?				
	databank scan						
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.			
PCR reactions	+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.			
nucleotide probes	+	++		Define nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.			
olate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.			
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.			
sequence attributes	+	++		Define attributes that can be set for contigs in the sequence bin.			
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.			
scheme members	+	++	?	Defines which loci belong to a scheme.			
scheme fields	+	++	?	Defines which fields belong to a scheme.			
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.			
scheme group scheme members	+	++	?	Defines which schemes belong to a group.			
heme group group members	+	++	?	Defines which scheme groups belong to a parent group.			

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.

ged in: Keith Jolley	(keith). Log out Change password									
onfigurati	on check - Neisseria P	0.061/1	CT							
omgurau	on check - Neissena F	UDIVII	-21							
lelper applicati	ons									
Program		stalled [vecutat							
EMBOSS infoalign	/usr/bin/infoalign	ok	ok	лс						
EMBOSS sixpack	/usr/bin/sixpack	ok	ok							
EMBOSS stretcher	/usr/bin/stretcher	ok	ok							
blastn	/usr/local/ncbi-blast+/bin/blastn	ok	ok							
blastp	/usr/local/ncbi-blast+/bin/blastp	ok	ok							
blastx	/usr/local/ncbi-blast+/bin/blastx	ok	ok							
ipcress	/usr/bin/ipcress	ok	ok							
mafft	/usr/local/bin/mafft	ok	ok							
makeblastdb	/usr/local/ncbi-blast+/bin/makeblastdb	ok	ok							
mogrify	/usr/bin/mogrify	ok	ok							
muscle	/usr/bin/muscle	ok	ok							
tblastx	/usr/local/ncbi-blast+/bin/tblastx	ok	ok							
ocus database. Locus	Database	Host	Port		Secondary id field	Secondary id field valu	e Sequence field	Database accessible	Sequence query	
'16S rDNA	pubmlst_bigsdb_neisseria_seqdef				locus	'16S_rDNA	sequence	ok	ok	197
'porA	pubmlst_bigsdb_neisseria_seqdef				locus	'porA	sequence	ok	ok	164
'porB	pubmlst_bigsdb_neisseria_seqdef				locus	'porB	sequence	ok	ok	695
'rpIF	pubmlst_bigsdb_neisseria_seqdef				locus	'rpIF	sequence	ok	ok	109
BACT000001 (rps				sequences	locus	BACT000001	sequence	ok	ok	8189
BACT000002 (rps				sequences	locus	BACT000002	sequence	ok	ok	6567
BACT000003 (rps				sequences	locus	BACT000003	sequence	ok	ok	5965
BACT000004 (rps				sequences	locus	BACT000004	sequence	ok	ok	6195
BACT000005 (rps				sequences	locus	BACT000005	sequence	ok	ok	5707
BACT000006 (rps				sequences	locus	BACT000006	sequence	ok	ok	4918
BACT000007 (rps BACT000008 (rps		localhos		sequences	locus	BACT000007 BACT000008	sequence	ok ok	ok	5667 5260

Any problems will be highlighted with a red X.

5.27 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 '?' link (Update or delete) next to schemes in the curator's interface.

	tion			
Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	datat	ank scan		
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
PCR reactions	+	++		Set up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		Define nucleotide probes for <i>in silico</i> hybridization reaction to filter genomes for tagging to specific repetitive loci.
olate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes	+	++		Define attributes that can be set for contigs in the sequence bin.
schemes	+	++	?	Describes schemes consisting of collections of loci, e.g. MLST.
scheme members	+	++	?	Defines which loci belong to a scheme.
scheme fields	+	++	?	Defines which fields belong to a scheme.
scheme groups	+	++	?	Describes groups in to which schemes can belong - groups can also belong to other groups.
scheme group scheme members	+	++	?	Defines which schemes belong to a group.
cheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). @Log out Change password	Toggle: 🚯
Query schemes for Neisseria PubMLST database	
Please enter your search criteria below (or leave blank and submit to return all records). — Search criteria — Display — Disp	
id v = v + 6 Order by: id v ascending v	
Display: 25	
Filter query by- Action isolate display: Reset Submit query field: query status: query status:	

Click the button 'Export configuration/data'.

Database: Species home Curator's page (specie Users: Add Query/update Isolates: Add Query/update Batch insert	es) Cur	ator's p	oage (databa	ase)						
Logged in: Keith Jolley (keith). @Log out Change password										Toggle: 🚯
Query schemes for Neisseria PubMLS	T dat	taba	ise							
Please enter your search criteria below (or leave blank and submit to re	eturn all	records	s).							
Search criteria		— — D	Display —							
id 🗸 = 🗸	+ 1		Order by:			 asc 	ending	•		
			Display:	25 👻 re	ecords per	page (•			
		Action	ı——							
isolate display:		Reset	t Submi	it						
main display: query field:										
query field: 🔍 🕤 query status: 🔍 🕤										
analysis:										
allow missing loci: 📃 🕤										
curator:										
scheme: MLST	• 1									
1 record returned.										
Delete — Database configuration —										
Delete ALL Export configuration/data										
										allow
Delete Update (d) description dbase name	lbase dt host p	base port	dbase table	isolate display		query field*	query status*	analysis*	display order	missing c
Delete Update 1 MLST pubmlst_bigsdb_neisseria_seqdef			nv_scheme_		true	true	true	true	1	loci
The set of the se	reference	•			_					•

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.

scl	hemes				
	-			ase_name dbase_host dbase_port dbase_user dbase_password dbase_table bigsdb_neisseria_seqdef mv_scheme_1 1 1 1 1 1 1 2	e isolate_di 2012-03-22
scl	heme_memb	bers			
scl	heme_id	 lo	cus	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	
scl	heme_fiel	ds			
1	ST integ	ger	1	<pre>type primary_key description field_order url isolate_display main_ /cgi-bin/bigsdb/bigsdb.pl?page=profileInfo&db=pubmlst_neisseria_s text 0 2 1 1 1 1 2 2009-11-16</pre>	- 1 1 1

5.28 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/maintenace 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
   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).

Curator's guide

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

6.1 Adding new sender details

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

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

		e password		
tabase curator's int	ter	face -	Neisseria PubMLS	ST
🕤 Add, update or delete re	eco	rds		
Record type A	١dd	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query browse list batch update	
late field extended attribute values	+	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences		++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
Database configuration				
Database configuration				
			pdate or delete	Comments

Enter the user's details in to the form.

PubMLST Use	abase: Species home Curator's page (species) Curator's page (database) ers: Add Query/update d: Add 3T profiles: Add Query/update Batch insert			
Logged in: Keith Jolley (keith	h). @Log out Change password		Help 🖉	Toggle: 🚯
Add new user	,			
	elow - required fields are marked with an exclamation mark (!).	A still a		
Record	070	Action —		
	272	Reset	Submit	
user name:! surname:!				
first name:				
	joe.bloggs@zoo.ox.ac.uk			
affiliation:!	University of Oxford, UK			
status:!	user 🔻			
date entered:!	2015-06-18			
datestamp:!	2015-06-18			
	Keith Jolley (keith)			
submission emails:	○ true ○ false 1 Receive new submission E-mails			

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

Users: Add Query/update Loci: Add MLST profiles: Add Query/u	update	Batch inser	1	
ogged in: Keith Jolley (keith). 🕪Log out Change pass	vord			
atabase curator's interfac	:e -	Neisse	ria locus/sequen	ce definitions
			14 100040/00944011	
Add, update or delete records Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++	?	
scheme curator control list	+	++	guery batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	guery batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++ FASTA	?	
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	+	++	?	
Bexsero Antigen Sequence Typing (BAST) profiles	+	++	query browse list batch update	
MLST profiles	+	++	query browse list batch update	
rpIF species profiles	+	++	query browse list batch update	
PubMed links (to profiles)	+	++		

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

The status can either be:

- Sanger trace checked
- WGS: manual extract (BIGSdb)
- WGS: automated extract (BIGSdb)
- WGS: visually checked
- WGS: automatically checked
- unchecked

d new allele sequence ase fill in the fields below - required fields are marked with an exclamation mark (!). Record locus! abcZ allele id! 728 sequence! TTTGATACCGTTGCCGAAGGTTTGGCCGAAATTCGCGATTTATTGCGCCGTTATCATCATGTCAA GCACAATTCAGACGACGTTTTATTAAAGAACTCGACGAATTACAACTCGAAATCGAAGCGAAG TGGATGCGGCAGTCAAGCAGACTTTGGGCGAACTCGGTTGCCGGAAAACGAAAAAATCGGCAA CAGAAAAAGCGTGTCGCCTTGGCGCAGGCTTGGGTGCAGAAGCCCGACGTATTGCTGCTGGACG TTTGGATATTGACGCGATTATCTGGTTGGAAAACCTGCTCAAGGCGTTTGAAGGCAGCTTGGTC ATCGCCGTTTTTTTGGACAATATCGCCACGCGGATTGTCGAACTCGATC status! Sanger trace checked sender! Jolley, Keith (keith) curator! Keith Jolley (keith)	GGACGGC1 ACCTTTCC GAACCGAC	IGGAAGC CGGCGGT CCAACCA
ase fill in the fields below - required fields are marked with an exclamation mark (!). Record locus:! abcZ _ allele id:! 728 sequence:! TTTGATACCGTTGCCGAAGGTTTGGGCGAAATTCGCGATTATTGCGCCGTTATCATCATGTCAA GCACAATTCAGACGACGTTTTATTAAAAGAACTCAACGGAAAAACGAAAAAACGAAAAAACGGCAAG TGGATGCGGCAGTCAAGCAGACTTTGGGCGAACTCGGTTTGCCGGAAAACGAAAAAATCGGCAA CAGAAAAAGCGTGTCGCCTTGGCGCAGGCTTGGGGTGCAGAAGCCGACGAATTGCTGGTGCAAAGCGAGCTTGGTCGAAGCCGACGACTTGGTGGAAAACGAAAAAATCGGCAA CAGAAAAAGCGTGTCGCCTTGGCGCAGGCTTGGGGGGCAGAGCCGACGACGTTGGTCG TTGGGATATTGACGCGATTATCGGCTGGGGAAACCGAAGCCGGCGCGCGC	GGACGGC1 ACCTTTCC GAACCGAC	IGGAAGC CGGCGGT CCAACCA
locus:! abcZ allele id! 728 sequence! TTTGATACCGTTGCCGAAGGTTTGGGCGAAATTCGCGATTTATTGCGCCGTTATCATCATGTCAI GCACAATTCAGACGACGATCATTTTTTTAAAAGAAACTCAACGGAAATCGAAATCGAAACGAAAAAATCGGAAGC GCACAATTCAGACGACGTCAAGCAGACTTTGGGCGAAACCGAAAACGAAAAAATCGGCAAG CAGAAAAAGCGTGTCGCCTTGGCGCAGGCTTGGGTGCAGAAGCCCGACGTATTGCTGGTGCAA CAGAAAAAGCGTGTCGCCTTGGCGCCAGGCTTGGGTGCAAGACCCCGACGATTGCTGCTGGAAGCCGACGTTGGTCG TTTGGATATTGGACGAATTATCGCCACGCGGATTGTCGAAGCCGACGTTGGAGGCAGCTTGGTCG ATCGCCGTTTTTTGGACAATATCGCCACGCGGATTGTCGAACCCGACGT Status! Sanger trace checked	GGACGGC1 ACCTTTCC GAACCGAC	IGGAAGC CGGCGGT CCAACCA
locus:! abcZ allele id! 728 sequence! TTTGATACCGTTGCCGAAGGTTTGGGCGAAATTCGCGATTTATTGCGCCGTTATCATCATGTCAI GCACAATTCAGACGACGATCATTTTTTTAAAAGAAACTCAACGGAAATCGAAATCGAAACGAAAAAATCGGAAGC GCACAATTCAGACGACGTCAAGCAGACTTTGGGCGAAACCGAAAACGAAAAAATCGGCAAG CAGAAAAAGCGTGTCGCCTTGGCGCAGGCTTGGGTGCAGAAGCCCGACGTATTGCTGGTGCAA CAGAAAAAGCGTGTCGCCTTGGCGCCAGGCTTGGGTGCAAGACCCCGACGATTGCTGCTGGAAGCCGACGTTGGTCG TTTGGATATTGGACGAATTATCGCCACGCGGATTGTCGAAGCCGACGTTGGAGGCAGCTTGGTCG ATCGCCGTTTTTTGGACAATATCGCCACGCGGATTGTCGAACCCGACGT Status! Sanger trace checked	GGACGGC1 ACCTTTCC GAACCGAC	IGGAAGC CGGCGGT CCAACCA
locus:! abcZ allele id! 728 sequence:! TITGATACCGTTGCCGAAGGTTTGGGCGAAATTCGCGATTTATTGCGCCGTTATCATCATGTCAA GCACAATTCAGACGACGATTTATTAAAAGAACTCAACGAATTACAACTCGAAATCGAAGCGAAG TGGATGCGGCAGTCAAGCAGACTTTGGGCGAACTCGGGTGCGGAAAACGAAAAAAACGGCAAG CAGAAAAAGCGTGTGGCCAGGCATGGGTGGGAACACGGAAAACGAAAAAAACGGCAGGCA	GGACGGC1 ACCTTTCC GAACCGAC	IGGAAGC CGGCGGT CCAACCA
allele id.! 728 sequence:! TTTGATACCGTTGCCGAAGGTTTGGGCGAAATTCGCGATTATTGCGCCGTTATCATGTCATGCGCGAATTCAGACCGAAATCGAAATCGAAAGCGAAGCGAAGCGAAGCGAAGCGAAGCGGAGCGGCG	GGACGGC1 ACCTTTCC GAACCGAC	IGGAAGC CGGCGGT CCAACCA
sequence: TTTGATACCGTTGCCGAAGGTTTGGGCCGAAATTCGCGATTTATTGCGCCCGTTATCATCATGTCAGCGAAGCGGAAAACGGAAAACGGAAAACGGAGACGAC	GGACGGC1 ACCTTTCC GAACCGAC	IGGAAGC CGGCGGT CCAACCA
Status: Sanger trace checked	GGACGGC1 ACCTTTCC GAACCGAC	IGGAAGC CGGCGGT CCAACCA
sender: Jolley, Keith (keith)		
sender:! Jolley, Keith (keith)		
date entered: 2015-06-18		
datestamp:! 2015-06-18 comments:		
Flags: atypical contains IS element downstream fusion frameshift		
internal stop codon 🔻 Use Ctrl dick to select/deselect multiple choices		
PubMed ids:		
ENA ids:		
Genbank ids:		
Override sequence similarity check Override sequence length check		
- Action		

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

See also:

allele sequence flags

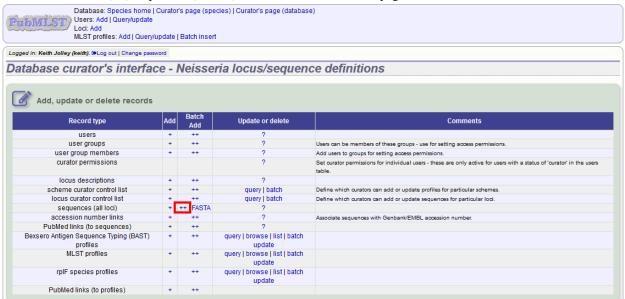
Sequences can also be associated with PubMed, ENA or Genbank id numbers by entering these as lists (one value per line) in the appropriate form box.

6.2.2 Batch adding multiple alleles

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

Upload using a spreadsheet

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



Download a template Excel file from the following page.

Prz12MILST Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Batch insert sequences	
 This page allows you to upload allele sequence data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. If the locus uses integer allele ids you can leave the allele_id field blank and the next available number will be used. The status defines how the sequence was curated. Allowed values are: 'Sanger trace checked', WGS: manual extract', Sequence flags can be added as a semi-colon (;) separated list Download tab-delimited header for your spreadsheet - use Paste special → text to paste the data. Download submission template (xlsx format) Please note, some loci have extended attributes which may be required. For affected loci please use the batch insert p Reload Please select the sender from the list below: Select sender Value will be overridden if you include a sender field in your pasted data. 	
✓ 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 code sequences are also ignored. Override sequence similarity check	on at the ends and no internal stop codons. Existing
Paste in tab-delimited text (include a field header line).	Action Reset Submit

Fill in the spreadsheet. If the locus uses integer allele identifiers, the allele_id can be left blank and the next available number will be used automatically. Paste the entire sheet in to the web form and select the sender from the dropdown box.

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

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Batch insert sequences	
This page allows you to upload allele sequence data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. If the locus uses integer allele ids you can leave the allele_id field blank and the next available number will be used. The status defines how the sequence was curated. Allowed values are: "Sanger trace checked", WGS: manual extract Sequence flags can be added as a semi-colon (;) separated list Download tab-delimited header for your spreadsheet - use Paste special → text to paste the data. Download submission template (xlsx format) Please note, some loci have extended attributes which may be required. For affected loci please use the batch insert Reload page specific for locus: Select Reload Please select the sender from the list below: Jolley. Keith (keith) value will be overridden if you include a sender field in your pasted data. Gillony Reith (keith) value will be overridden if you include a sender field in your pasted data. Gillony Reith (keith) value will be overridden if you include a sender field in your pasted data. Override sequences containing non-nucleotide characters Silently reject all sequences that are not complete reading frames - these must have a start and in-frame stop cod sequences are also ignored. Override sequence similarity check Paste in tab-delimited text (include a field header tine).	page specific to that locus: don at the ends and no internal stop codons. Existing —Action————
locus allele_id sequence status comments flags abs2 IIIGAIACIGTIGCCGAAGGTIGGGCGAAATICGCGATITATIGCAACGITATCAICAIGCAGCCAAGGACGCCGAGGTIGGAGAAAAT GGILCGAGGCGAGCCIGGGGGGGGAGCCGACCGACGGAGGACGCCCGGGGGAGAAAAAGCGG GCGSIGAAGCCGGGGGGGGGGGGGGGGGGGGGGGGGGGGG	Reset Submit

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

Database: Species home Curator's page (species) Curator's page (database Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert)
Logged in: Keith Jolley (keith). Log out Change password	Toggle: \overline{i}
Batch insert sequences	
Import status	
Sender: Keith Jolley	
No obvious problems identified so far.	
Import data	
Data to be imported	
The following table shows your data. Any field with red text has a problem and needs to be checked.	Note: valid sequence flags are displayed with a red background not red text.
	ender curator date_entered datestamp comments flags
abcZ 688 TTTGATACTGTTGCCGAAGG GCGGATTGTCGAACTCGATC Sanger trace checked	2 2 2014-07-09 2014-07-09
abcZ 689 TTTGATACTGTTGCCGAAGC GCGGATTGTCGAACTCGATC Sanger trace checked	2 2 2014-07-09 2014-07-09

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

Publ	MLS	an		Curator's page (databa:	se)				
Logged in	: Keith Jo	Iley (keith). Log out Change pas	ssword						Toggle: i
Batc	h ins	ert sequences							
P	t statu: rimary k abcZ; all		Problem(s) on nucleotide (G A T C) char	acters.					
The foll		iported ble shows your data. Any field sequ	l with red text has a problem uence				-	e displayed with a re	 not red text.
abcZ	688	TTTGATACTGTTGCCGAAGG .	GCGGATTGTCGAACTCGAI		2	2		2014-07-09	
abcZ	689	TTTGATACTGTTGCCGAAGC .	GCGGATTGTCGAACTCGAI	C Sanger trace checked	2	2	2014-07-09	2014-07-09	

Upload using a FASTA file

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

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

Users: Add Query/update Loci: Add MLST profiles: Add Query/u			ecies) Curator's page (databas t	e)
gged in: Keith Jolley (keith). DLog out Change passw	vord			
atabase curator's interfac	I	Neisse	ria locus/sequen	ce definitions
	- I	101000	na locus/scquen	
Add, update or delete records Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++	?	
scheme curator control list	+	++	query batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	query batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++ FASTA	?	
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	+	++	?	
Bexsero Antigen Sequence Typing (BAST) profiles	+	++	query browse list batch update	
MLST profiles	+	++	query browse list batch update	
rpIF species profiles	+	++	query browse list batch update	

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

PubML	Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert
Logged in: Keith	Jolley (keith). Log out Change password Toggle: 1
Batch in	sert sequences
(loci with integ	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 ger ids only). Do not include the locus name in the identifier in the FASTA file. nat you can not use this page to upload sequences for loci with extended attributes.
locus:	
	Sanger trace checked 🗸
sender:!	Jolley, Keith (keith)
(FASTA):!	>isolate1 ITTGATACTGTTGCCGAAGGTTTGGGCGAAATTCGCGATTTATTGCAACGTTATCATCAT GTCAGCCATGGAGTCGGAAGGACGGCCGAAGGGCGGCGGCGGCGGCGGCGGCGG
sequences	all sequences that are not complete reading frames - these must have a start and in-frame stop codon at the ends and no internal stop codons. Existing are also ignored. e sequence similarity check xt available id (only for loci with integer ids)

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'.

Publ/LST Users: Add Query/up	ome Curator's page (species) Curator's page (database) odate Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change	password	Toggle: i
Batch insert sequences	;	
Sequence check Original designation Allele id Status isolate1 688 OK isolate2 689 OK	Action Upload valid sequences	

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

PubMLST	Users: Ad Loci: Add	: Species home Curator's page (species) Curator's page Id Query/update files: Add Query/update Batch insert	(database)			
Logged in: Keith Jolley (Logged in: Keith Jolley (keith). Log out Change password Toggle					
Batch insert	sequ	iences				
Sequence check Original designation isolate1 isolate2		Status OK Sequence contains non nucleotide (G A T C) characters.	Action Upload valid sequences			

6.3 Updating and deleting allele sequence definitions

Note: You cannot update the sequence of an allele definition. This is for reasons of data integrity since an allele may

form part of a scheme profile and be referred to in multiple databases. If you really need to change a sequence, you will have to remove the allele definition and then re-add it. 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 query (?) sequences (all loci) link - if only a few loci are defined with permission for the current user to curate then they will be listed individually and the specific locus query links can also be used.

Database: Species home Curator's page (species) Curator's page (database) Pri 17 MILST Loc: Add MLST profiles: Add Query/update Batch insert				
Logged in: Keith Jolley (keith). DLog out Change passw	ord			
Database curator's interfac	e -	Neisse	ria locus/sequen	ce definitions
Add, update or delete records				
Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++	?	
scheme curator control list	+	++	query batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	query batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++ FASTA	?	
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	+	++	?	
Bexsero Antigen Sequence Typing (BAST) profiles	+	++	query browse list batch update	
MLST profiles	+	++	query browse list batch update	
rpIF species profiles	+	++	query browse list batch update	
PubMed links (to profiles)	+	++		

Either search for specific attributes in the search form, or leave it blank and click 'Submit' to return all alleles. For a specific allele, select the locus in the filter and enter the allele number in the allele_id field.

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	gle: 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 export plugins. Also note that some loci in this database have allele ids defined as text strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter your search to a locus that uses integer allele ids using the drop-down list.	
Please enter your search criteria below (or leave blank and submit to return all records).	
Search criteria Display	
allele id v = v 4 + i Order by: locus v ascending v	
Display: 25 records per page 7	
Filter query by Action	
locus: abcZ Reset Submit	
status:	
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.

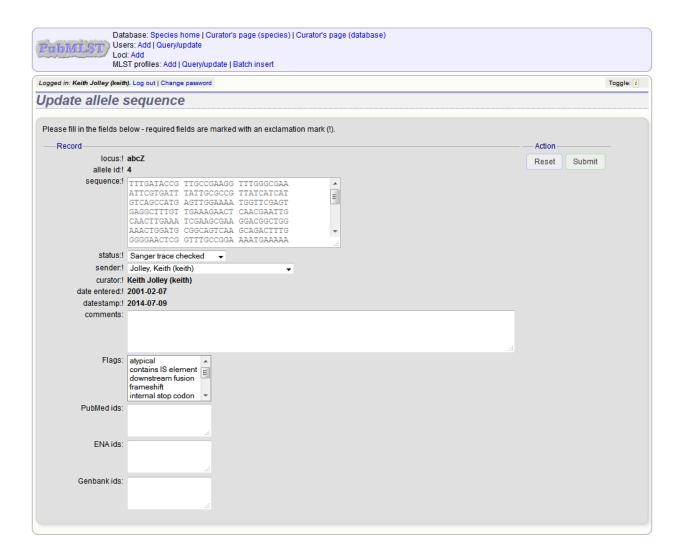
Database: Species home Curator's page (species Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	s) Curator's page (database)
Logged in: Keith Jolley (keith). Log out Change password	Toggle: [
Query sequences for Neisseria locus/se	equence definitions database
Some loci have additional fields which are not searchable from this gen	eral 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 uses integer allele ids using the drop-down list.	strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter your search to a locus that
Please enter your search criteria below (or leave blank and submit to ref	um all records).
Search criteria	Display
allele id 🔹 = 🔹 4	+ I Order by: locus v ascending v Display: 25 v records per page I
Filter query by locus: abcZ vI status: v sender: vI curator: vI allele flag: v	Action Reset Submit
1 record returned.	
Delete Database configuration Flags Delete ALL Export configuration/data Batch set	
Delete Update locus allele id sequence Delete Update abc2 4 TITEATACCETTECC TITEATACCETTECC	sequence length status sender curator date entered datestamp comments flags CGATC 433 Sanger trace checked Keith Jolley Man-Suen Chan 2001-02-07 2009-11-11

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

PubMLST L	Database: Species home Curator's page (species) Curator's page (database) PerthT/TLST Loc:: Add MLST profiles: Add Query/update Batch insert					
Logged in: Keith Jolley (ke	eith). Log out Change password					
Delete allele	sequence					
You have chosen to de	elete the following record:					
locus:	abcZ					
allele id:	4					
sequence:	ITIGATACCG ITGCCGAAGG ITIGGGCGAA AITCGIGAIT IAITGCGCCG ITAICAICAI GICAGCCAIG AGIIGGAAAA IGGIICGAGI GAGGCIIIGI IGAAGAACI CAACGAAIIG CAACIGAA ICGAAGCGAA GGACGGCIGG AAACIGGAIG CGGCAGICA GCAGCAIIG GGGGAACICG GIIGGCGGA AAAIGAAAA AICGGCAACC ITICGGGGG ICAGAAAAA CGGCIGCCI IGGCIACGA IIGGGIGCAA AAGCCCGACG IAITGCIGCIG GACGAGCCG ACCAACCAII IGGAIAICGA CGCGAIIAII IGGCIGGAAA AICIGCICAA AGCGIIIGAA GGCAGCIIG IIGIGAIIAC CCACGACCG CIIIIIIGG ACAAIAICCC CACGGGGAI GICGAACIGG AIC					
status:	Sanger trace checked					
sender:	Keith Jolley					
curator:	Man-Suen Chan					
date entered:	2001-02-07					
datestamp:	2009-11-11					
comments:						
Delete!						

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

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



6.4 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 next to 'locus descriptions'. 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 next to 'locus descriptions' 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).

Users: Add Query/update Loci: Add MLST profiles: Add Query/u	update	Batch inser	t	
ged in: Keith Jolley (keith). 🗭 Log out Change passv	vord			
atabase curator's interfac	:e -	Neisse	ria locus/sequen	ce definitions
Add, update or delete records Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
locus descriptions	+	++	?	
scheme curator control list	+	++	guery batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	query batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++ FASTA	?	
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	+	++	?	
Bexsero Antigen Sequence Typing (BAST) profiles	+	++	query browse list batch update	
MLST profiles	+	++	query browse list batch update	
rpIF species profiles	+	++	query browse list batch	
			update	

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

Database: Species home Curator's page (species) Curato Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	r's page (database)
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Query locus descriptions for Neisseria locus	s/sequence definitions database
Please enter your search criteria below (or leave blank and submit to return all rec Search criteria locus = NEIS0620 + {	Display Order by: locus ▼ ascending ▼ Display: 25 ▼ records per page [i]
Action Action Reset Submit	

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Query locus descriptions for Neisseria locus/sequence definitions database	
Please enter your search criteria below (or leave blank and submit to return all records). Search criteria locus	

Click 'Submit'.

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Query locus descriptions for Neisseria locus/sequence definitions database	
Please enter your search criteria below (or leave blank and submit to return all records).	
— Search criteria — — — — — — — — Display — — — — — — — — — — — — — — — — — — —	
locus v = v + i Order by: locus v ascending v Display: 25 v records per page i	
Filter query by Action Iocus: NEIS0620 (maeA) VEIS0620 (maeA) VEI	
1 record returned.	
— Delete — Database configuration —	
Delete ALL Export configuration/data	
Delete Update locus full name product description curator datestamp Delete Update VEIS0620 malate oxidoreductase (EC 1.1.1.38) Final step in TCA cycle producing oxaloacetate. Keith Jolley 2010-10-28	

Fill in the form as needed:

PubMLST Users	ase: Species home Curator's page (species) Curator's page (database) : Add Query/update Add profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith).	Log out Change password	Toggle: i
Update locus d	escription	
Please fill in the fields belo	w - required fields are marked with an exclamation mark (!).	
Record		Action
	NEIS0620	Reset Submit
	Keith Jolley (keith)	
datestamp:!	2014-11-04	
full name:	a.	
	malate oxidoreductase (EC 1.1.1.38)	
description:	Final step in TCA cycle producing oxaloacetate.	
	NMA0870 NMB0671 NMC0620	
PubMed ids:	14917678 .:!	
links: (Format: URL description)	http://www.enzyme-database.org /guery.php?ec=1.1.1.38 EC 1.1.1.38 	

• 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.

6.5 Adding new scheme profile definitions

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

To add a single profile you can click the add (+) profiles link next to the scheme name (e.g. MLST):

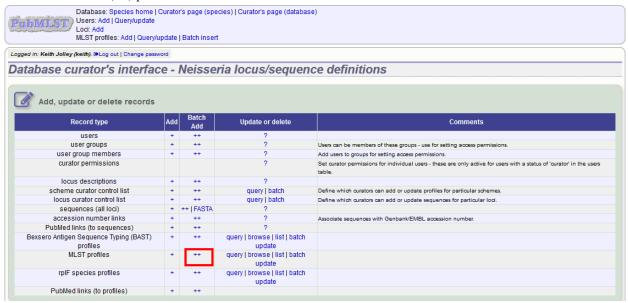
Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert						
ogged in: Keith Jolley (keith). 🗭 Log out Change passv	vord					
Database curator's interfac	e -	Neisse	ria locus/sequen	ce definitions		
	I	TCIOOC	na locus/sequent			
Add, update or delete records	Add	Batch Add	Update or delete	Comments		
users	+	++	?			
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.		
user group members	+	++	?	Add users to groups for setting access permissions.		
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.		
locus descriptions	+	++	?			
scheme curator control list	+	++	guery batch	Define which curators can add or update profiles for particular schemes.		
locus curator control list	+	++	guery batch	Define which curators can add or update sequences for particular loci.		
sequences (all loci)	+	++ FASTA	?			
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.		
PubMed links (to sequences)	+	++	?			
Bexsero Antigen Sequence Typing (BAST) profiles	+	++	query browse list batch update			
MLST profiles	+	**	query browse list batch update			
rpIF species profiles	+	++	query browse list batch update			
PubMed links (to profiles)	+	++				

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 U	atabase: Species home C sers: Add Query/update oci: Add _ST profiles: Add Query/up	Curator's page (species) Curato pdate Batch insert	r's page (database)	
Logged in: Keith Jolley (ke	ith). Log out Change password	đ		Toggle: i
Add new MLS	ST profile			
Please fill in the fields	below - required fields are	marked with an exclamation ma	rk (!).	
	10880	J.		
abcZ: !				
adk: !				
aroE: !	4			
fumC: !				
gdh: !	8			
pdhC: !	8 4			
pgm: !	6			
sender: !				
clonal_complex:				
curator: !	Keith Jolley (keith)			
date_entered: !	2014-07-10			
datestamp: !	2014-07-10			
PubMed ids:				
Action				
Reset Subr	it			

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:



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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Batch insert MLST profiles	
This page allows you to upload profiles as tab-delimited text or copied from a spreadsheet.	
 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 include it in the header line, then you also provide it for each profile record. 	ı must
 Download tab-delimited header for your spreadsheet - use Paste special → text to paste the data. Download submission template (xisx format) 	
Please paste in tab-delimited text (include a field header line)	

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

Database: Species home Curator's page (species) Curator's page (database Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert)
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Batch insert MLST profiles	
This page allows you to upload profiles as tab-delimited text or copied from a spreadsheet.	
 Field header names must be included and fields can be in any order. Optional fields can be o You can choose whether or not to include a ST field - if it is omitted, the next available ST will t you must also provide it for each profile record. Download tab-delimited header for your spreadsheet - use Paste special → text to paste the other states and the special and the sp	e used automatically. If however, you include it in the header line, then
Download submission template (xisx format) Please paste in tab-delimited text (include a field header line)	
Abd2 adk acc fumc gdh pdhc pgm clonal_comp	lex
Parameters Action Action	
Sender: Jolley, Keith (keith) Value will be overridden if you include a sender field in your pasted data.	
Ignore duplicate profiles	
Back	

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

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

6.6 Updating and deleting scheme profile definitions

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/lupdate Loc: Add MLST profiles: Add Query/lupdate Batch insert						
ed in: Keith Jolley (keith). 🕩 Log out Change pass	vord					
tabase curator's interfac	e -	Neisse	ria locus/sequen	ce definitions		
	~~	TTCIOOC	ind roodd/ocquein			
Add, update or delete records	Add	Batch Add	Update or delete	Comments		
users	+	++	?			
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.		
user group members	+	++	?	Add users to groups for setting access permissions.		
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.		
locus descriptions	+	++	?			
scheme curator control list	+	++	guery batch	Define which curators can add or update profiles for particular schemes.		
locus curator control list	+	++	query batch	Define which curators can add or update sequences for particular loci.		
sequences (all loci)	+	++ FASTA	?			
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.		
PubMed links (to sequences)	+	++	?			
Bexsero Antigen Sequence Typing (BAST) profiles	+	++	query browse list batch update			
MLST profiles	+	++	query browse list batch update			
rpIF species profiles	+	++	query browse list batch update			

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Query/update profiles - Neisseria locus/sequence definitions	
Schemes Please select the scheme you would like to query: MLST Select	
Locus/scheme fields Display/sort options ST • • • 4563 Filter query by Action clonal complex: • i Reset Submit	
1 record returned. Delete Delete ALL Delete Update ST abcZ adk aroE fumC gdh pdhC pgm clonal complex Delete Update 4563 2 7 6 13 9 18 8 ST-167 complex	

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

For deletion of a single record, the full record will be displayed. Confirm deletion by clicking 'Delete!'.

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

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

PubMLST L	Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert gged in: Keith Jolley (keith): Log out Change password Toggle: [4]											
Logged in: Keith Jolley (k	eith). Log out Change password		Toggle: i									
Update profi	le											
Record		Action										
Update your record a	as required - required fields are marked with an exclamation mark (!):	Reset Submit										
ST: !	4563											
abcZ: !	2											
adk: !												
aroE: !	6											
fumC: !												
gdh: !												
pdhC: !	18											
pgm: !												
	ST-167 complex											
	Ibarz-Pavon, Ana-Belen (aibarz) 👻											
date_entered: !	Keith Jolley (keith)											
datestamp: !												
PubMed ids:												

6.7 Adding isolate records

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

Add, update or delete record Record type Add Ba Users + user groups + user groups +	atch Add Update	e or delete	Comments
Record type Add Ba users + user groups +	atch Add Update		Comments
Record type Add Ba users + user groups +	atch Add Update		Comments
users + user groups +	++		Comments
user groups +			
		?	
user group members +	++	? Use	ers can be members of these groups - use for setting access permissions.
	++	? Add	d users to groups for setting access permissions.
curator permissions		? Set	t curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates +	++ query browse	list batch update	
olate field extended attribute values +	++	? Add	d values for additional isolate field attributes.
projects +	++	? Set	t up projects to which isolates can belong.
project members +	++	? Add	d isolates to projects.
isolate aliases +	++	? Add	d alternative names for isolates.
PubMed links +	++	?	
allele designations	++	? Alle	ele designations can be set within the isolate table functions.
sequences	++	? The	e sequence bin holds sequence contigs from any source.
accession number links +	++	? Ass	sociate sequences with Genbank/EMBL accession number.
experiments +	++	? Set	t up experiments to which sequences in the bin can belong.
experiment sequences		? Ado	d links associating sequences to experiments.
sequence tags so	can	? Tag	g regions of sequences within the sequence bin with locus information.

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.

PuliMLST / Users: A	se: Species home Curator's pa Add Query/update : Add Query/update Batch inse		s) Curator's page ((database)				
Logged in: Keith Jolley (keith). Lo	g out Change password							Toggle: i
Add new isolate								
Please fill in the fields below	- required fields are marked wit	n an exclar	mation mark (!).					
Isolate fields				Allele design	nations			
id:!	30457 🚔 🚺							
isolate:						MLST		
country:	UK	i		abcZ	adk	aroE	fumC	
species:!	Neisseria meningitidis		▼ i	ub of				
sender:!	Jolley, Keith (keith)		▼ [gdh	pdhC	pgm		
curator:!	Keith Jolley (keith) 👔							
	2014-07-10 i				Fin	etyping antig	ens	
	2014-07-10 <u>i</u>							
region:		İ		PorA VR1	PorA VR2	FetA VR		
year:								
epidemiological year:	i			Action				
age yr: age mth:				Reset S	Submit			
age mur. sex:	↓ i							
	▼ [] meningitis		1					
source:		▼ [i]					
epidemiology:	•							
serogroup:								
MLEE designation:								
serotype: sero subtype:								
ET no:								
penicillin:	i							
penicillin range:	i							
amoxicillin:	i							
sulphonamide:	i							
ceftriaxone:								

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

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

isolates + + plate field extended attribute values + + projects + + project members + + isolate aliases + + extreme + + isolate aliases + +	be members of these groups - use for setting access permissions. to groups for setting access permissions. r permissions for individual users - these are only active for users with a status of 'curator' in the users table. is for additional isolate field attributes. jects to which isolates can belong. tes to projects.	4 - k	snang	e password			
Add, update or delete records Record type Add Batch Add Update or delete Comments users + ++ ? Users can be members of these groups - use for setting access permissions. user groups + ++ ? Add users to groups for setting access permissions. user group members + + ? Add users to groups for setting access permissions. curator permissions ? Set curator permissions for individual users - these are only active for users with a status of 'curator' in the user isolates late field extended attribute values ++ ? Add values for additional isolate field attributes. projects ++ ? Add values for additional isolates an belong. projects ++ ? Add isolates to projects. isolate aliases + ? Add alternative names for isolates.	be members of these groups - use for setting access permissions. to groups for setting access permissions. r permissions for individual users - these are only active for users with a status of 'curator' in the users table. is for additional isolate field attributes. jects to which isolates can belong. tes to projects.		-	ufo o o	Najaaari		۲.
Record type Add Batch Add Update or delete Comments users + ++ ? Users can be members of these groups - use for setting access permissions. user group members + + ? Add users to groups for setting access permissions. user group members + + ? Add users to groups for setting access permissions. curator permissions ? Set curator permissions for individual users - these are only active for users with a status of 'curator' in the user isolates + + ? Add values for additional isolate field attributes. projects + + ? Add values for additional isolates an belong. projects + + ? Add isolates and points. isolate aliases + + ? Add isolates to projects.	be members of these groups - use for setting access permissions. to groups for setting access permissions. r permissions for individual users - these are only active for users with a status of 'curator' in the users table. is for additional isolate field attributes. jects to which isolates can belong. tes to projects.	tabase curator's in	ne	rrace	- Neisseri	a Pudmls	
Record type Add Batch Add Update or delete Comments users + ++ ? Users can be members of these groups - use for setting access permissions. user group members + + ? Add users to groups for setting access permissions. user group members + + ? Add users to groups for setting access permissions. curator permissions ? Set curator permissions for individual users - these are only active for users with a status of 'curator' in the user isolates isolates + + ? Add values for additional isolate field attributes. projects + + ? Set up rojects to which isolates an belong. projects + + ? Add values for additional isolates field attributes. projects + + ? Add values for additive names for isolates.	be members of these groups - use for setting access permissions. to groups for setting access permissions. r permissions for individual users - these are only active for users with a status of 'curator' in the users table. is for additional isolate field attributes. jects to which isolates can belong. tes to projects.						
Record type Add Batch Add Update or delete Comments users + ++ ? Users can be members of these groups - use for setting access permissions. user group members + + ? Add users to groups for setting access permissions. user group members + + ? Add users to groups for setting access permissions. curator permissions ? Set curator permissions for individual users - these are only active for users with a status of 'curator' in the user isolates isolates + + ? Add values for additional isolate field attributes. projects + + ? Set up rojects to which isolates an belong. projects + + ? Add values for additional isolates field attributes. projects + + ? Add values for additive names for isolates.	be members of these groups - use for setting access permissions. to groups for setting access permissions. r permissions for individual users - these are only active for users with a status of 'curator' in the users table. is for additional isolate field attributes. jects to which isolates can belong. tes to projects.						
users + ++ ? user groups + ++ ? Users can be members of these groups - use for setting access permissions. user group members + ++ ? Add users to groups for setting access permissions. user group permissions - ? Set curator permissions for individual users - these are only active for users with a status of 'curator' in the user isolates user field extended attribute values + ++ ? Add values for additional isolate field attributes. projects + ++ ? Add values for additional isolate field attributes. projects + ++ ? Add values for additional isolate field attributes. projects + ++ ? Add values for additional isolate field attributes. isolate aliases + ++ ? Add values for projects.	be members of these groups - use for setting access permissions. to groups for setting access permissions. r permissions for individual users - these are only active for users with a status of 'curator' in the users table. is for additional isolate field attributes. jects to which isolates can belong. tes to projects.	Add, update or delete	reco	ords			
users + ++ ? user groups + ++ ? Users can be members of these groups - use for setting access permissions. user group members + ++ ? Add users to groups for setting access permissions. curator permissions - ? Set curator permissions for individual users - these are only active for users with a status of 'curator' in the user isolates isolates + ++ ? Add values for additional isolate field attributes. projects + ++ ? Add values for additional isolate field attributes. projects + ++ ? Add values for additional isolate field attributes. projects + ++ ? Add values for additional isolate field attributes. isolate aliases + + ? Add values for projects.	to groups for setting access permissions. or permissions for individual users - these are only active for users with a status of 'ourator' in the users table. es for additional isolate field attributes. a before to which isolates can belong. tes to projects.	Record type	Add	Batch Ad	ld Update	e or delete	Comments
user group members + +++ ? Add users to groups for setting access permissions. curator permissions ? Set curator permissions for individual users - these are only active for users with a status of 'curator' in the user' isolates + +++ ? Add values for additional isolate field attributes. projects + ++ ? Add values for additional isolate field attributes. projects + ++ ? Add values for additional isolate field attributes. projects + ++ ? Add values for projects to which isolates can belong. project atlases + + ? Add attermative names for isolates.	to groups for setting access permissions. or permissions for individual users - these are only active for users with a status of 'ourator' in the users table. es for additional isolate field attributes. a before to which isolates can belong. tes to projects.		+				
user group members + +++ ? Add users to groups for setting access permissions. curator permissions ? ? Seturator permissions for individual users - these are only active for users with a status of 'curator' in the user isolates + +++ ? Seturator permissions for individual users - these are only active for users with a status of 'curator' in the user projects + ++ ? Add values for additional isolate field attributes. projects + ++ ? Set up rojects to which isolates can belong. projects + ++ ? Add values to projects. isolate allases + + ? Add atternative names for isolates.	or permissions for individual users - these are only active for users with a status of 'curator' in the users table. It is for additional isolate field attributes. Jjects to which isolates can belong. Les to projects.	user groups	+	++		?	Users can be members of these groups - use for setting access permissions.
isolates +++ query browse list batch update late field extended attribute values + + projects + + project members + + isolate aliases + + ? Add values for additional isolate field attributes. biolate aliases + +	s for additional isolate field attributes.		+	++		?	Add users to groups for setting access permissions.
Idlet field extended attribute values + + ? Add values for additional isolate field attributes. projects + + ? Set up projects to which isolates can belong. project members + + ? Add isolates to projects. Isolate allases + + ? Add attribute names for isolates.	ojects to which isolates can belong. Les to projects.	curator permissions				?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
projects + +++ ? Set up projects to which isolates can belong. project members + +++ ? Add isolates to projects. isolate aliases + +++ ? Add alternative names for isolates.	ojects to which isolates can belong. Les to projects.	isolates	+	++	query browse	list batch update	
project members + ++ ? Add isolates to projects. isolate aliases + ++ ? Add isolates to projects.	tes to projects.	late field extended attribute values	; +	++		?	Add values for additional isolate field attributes.
Isolate aliases + ++ ? Add alternative names for isolates.		projects	+	++		?	Set up projects to which isolates can belong.
	native names for isolates.	project members	+	++		?	Add isolates to projects.
PubMed links + ++ 2		isolate aliases	+	++		?	Add alternative names for isolates.
T domed mins		PubMed links	+	++		?	
allele designations ++ ? Allele designations can be set within the isolate table functions.	ignations can be set within the isolate table functions.	allele designations		++		?	Allele designations can be set within the isolate table functions.
SEQUENCES ++ ? The sequence bin holds sequence contigs from any source.	ance bin holds sequence contigs from any source.	sequences		++		?	The sequence bin holds sequence contigs from any source.
accession number links + ++ ? Associate sequences with Genbank/EMBL accession number.	sequences with Genbank/EMBL accession number.	accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
experiments + ++ ? Set up experiments to which sequences in the bin can belong.		experiments	+	++		?	Set up experiments to which sequences in the bin can belong.
experiment sequences ? Add links associating sequences to experiments.		experiment sequences				?	Add links associating sequences to experiments.
Sequence taos Scan ? Tag regions of sequences within the sequence bin with locus information.	periments to which sequences in the bin can belong.	sequence tags		scan		?	Tag regions of sequences within the sequence bin with locus information.
	periments to which sequences in the bin can belong.						
accession number links + ++ ? Associate sequences with Genbank/EMBL accession number.	sequences with Genbank/EMBL accession number.	accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
experiments + ++ ? Set up experiments to which sequences in the bin can belong.		experiments	+	++		?	Set up experiments to which sequences in the bin can belong.
experiment sequences ? Add links associating sequences to experiments.		experiment sequences				?	Add links associating sequences to experiments.
SEQUENCE tags SCAN ? Tag regions of sequences within the sequence bin with locus information.	periments to which sequences in the bin can belong.	sequence tags		scan		?	Tag regions of sequences within the sequence bin with locus information.
	periments to which sequences in the bin can belong. associating sequences to experiments.						
	periments to which sequences in the bin can belong. associating sequences to experiments.						
	periments to which sequences in the bin can belong. associating sequences to experiments.						
	periments to which sequences in the bin can belong. associating sequences to experiments.	Database configuration	۱. I				
Catabase configuration	periments to which sequences in the bin can belong. associating sequences to experiments.		_				
Catabase configuration	periments to which sequences in the bin can belong. associating sequences to experiments. ns of sequences within the sequence bin with locus information.	Table A	dd Ba	atch Add	Update or delete		Comments
	periments to which sequences in the bin can belong. associating sequences to experiments. ns of sequences within the sequence bin with locus information.	loci -	F I	++	?		
Database configuration Table Add Batch Add Update or delete Comments	periments to which sequences in the bin can belong. associating sequences to experiments. ns of sequences within the sequence bin with locus information.	d	ataba	ink scan			
Database configuration Table Add Batch Add Update or delete Comments	periments to which sequences in the bin can belong. associating sequences to experiments. ns of sequences within the sequence bin with locus information.	locus aliasos	+	++	? /	Add alternative names	s for loci. These can also be set when you batch add loci.
Database configuration Table Add Batch Add Update or delete Comments loci + ++ ? databank scan ?	periments to which sequences in the bin can belong. associating sequences to experiments. ns of sequences within the sequence bin with locus information. Comments						· · · · · · · · · · · · · · · · · · ·
Table Add Batch Add Update or delete Comments loci + ++ ? databank scan ?	periments to which sequences in the bin can belong. associating sequences to experiments. associating sequences to experiments. associating sequences within the sequence bin with locus information. Comments These can also be set when you batch add loci.		1				

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert										
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i									
Batch insert isolates										
This page allows you to upload isolate data as tab-delimited text or copied from a spreadsheet.										
 Field header names must be included and fields can be in any order. Optication to be called a status and the procession of the pr										
Download tab-delimited header for your spreadsheet - use Paste special → text to paste the data. Download submission template (xlsx format) Please select the sender from the list below:										
Select sender Value will be overridden if you include a sender field in your pasted data.										
Paste in tab-delimited text (include a field header line).	Action									
	Reset Submit									

Download a submission template in Excel format from the link.

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 / Users: Add Qu	ies home Curator's page (s ery/update luery/update Batch insert	species) Curator's	page (database)						
Logged in: Keith Jolley (keith). Log out Ch	nange password					Toggle: i				
Batch insert isolates										
 This page allows you to upload isolate data as tab-delimited text or copied from a spreadsheet. Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. Enter aliases (alternative names) for your isolates as a semi-colon (;) separated list. Enter references for your isolates as a semi-colon (;) separated list of PubMed ids (non integer ids will be ignored). You can also upload allele fields along with the other isolate data - simply create a new column with the locus name. 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 → text to paste the data. Download submission template (xlsx format) 										
Please select the sender from the lis	t below:									
Jolley, Keith (keith)	✓ Value will be override	den if you include a se	nder field in your p	asted data.						
— Paste in tab-delimited text (inclue	de a field header line).				Action					
isolate aliases reference age_rr age_mth sex MLFE_designation penicillin_range Ctftrlaxong_range Ctftrlaxong_range Ctftrlaxong_range private_project comments pdm J392_1 meningitis and septicaen B	disease source epi secotype set amoxicillin sul chloramphenicol chl rifampicin rif pending_assembly abcZ add UK 201	demiology phonamide phonamide pramphenicol ampicin_range assembly assembly assembly	ceftriaxone range <u>ce</u> f	egreup icillin etaxime roflexacin _accession _gdhC _male	Reset Submit					

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

Database: Species home C Users: Add Query/update Isolates: Add Query/update	urator's page (species) Curator's Batch insert	page (database)		
Logged in: Keith Jolley (keith). Log out Change password				Toggle: i
Batch insert isolates				
Import status				
Sender: Keith Jolley				
No obvious problems identified so far.				
Import data				
Data to be imported				
The following table shows your data. Any field with	red text has a problem and needs	to be checked.		
id isolate aliases references country reg			source epidemiology species	serogroup MLEE_desig
30457 J392_1 UK	2014	12 male meningitis and septicaemia	CSF Neisseria meningitidi	
< <u> </u>				Þ

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

Prrh/TLST Users: Add Query/update Isolates: Add Query/update Batch insert												
Logged in: Keith Jolley (keith). Log out Change password To	ggle: i											
Batch insert isolates												
Import status												
Primary key Problem(s)												
id: 30457 species 'Neisseria meningtidis' is not on the list of allowed values for this field.												
Data to be imported												
The following table shows your data. Any field with red text has a problem and needs to be checked.												
id isolate aliases references country region year epidemiological_year age_yr age_mth sex disease source epidemiology species serogroup MLEE	desia											
30457 J392_1 UK 2014 12 male meningitis CSF Neisseria B												
and meningtidis septicaemia												
<	•											

6.8 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.

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

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.

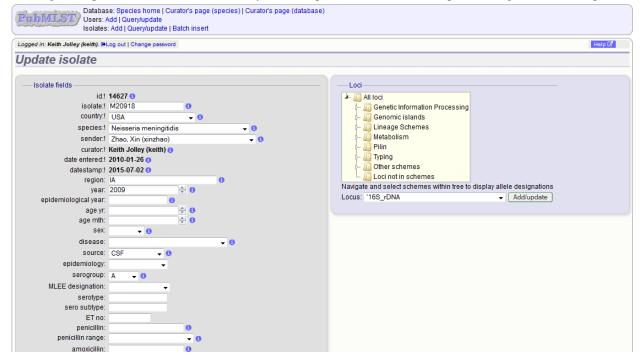
gged in	: Keith Jo	lley (keith). L	.og out Cł	nange pa	ssword					То	ggle: i Fie	ld help: id			-	G
ola	te qu	ery/uµ	odate													
-Iso	late prove	enance/phe	enotype fie	elds —				—— c	Display/sort optic	ons						lod
Comb	oine with:	AND 👻							Order by: id			•	ascend	ding 👻		
cou	ntry	-	=	•	- USA		+ [i	Display: 25	- records per	r page 👔				0	
yea	r	•	=	•	2009											
— Acti	ion —															
Per	not C	ubmit														
Res	set S	Submit														
recor	ds return	ed. Click th	e hyperlin	ks for d	etailed inforn	nation.										
Dale																
	ata	Tog	conning	D	ninete											
	ete	Ē	scanning	_	rojects —											
	ete ete ALL	Ē	canning can	_	rojects ect project			▼ L	ink							
		Ē		_				• L	ink							
		Ē		_											F	in
Dele	ete ALL	Ē	can	_			Iso	↓ L				Seqbin		MLST	í	an
Dele		S	can	_		aliases	Iso country	late field		species	serogroup	size (hn)	ST	MLST clonal complex		an
Dele elete	ete ALL	Sequence	New version	Sel	ect project	aliases	1	late field	s i	Neisseria	serogroup B	size (hn)	ST 7301	cional complex ST-32	a PorA	an
Dele elete	update	Sequence bin	New version	Sel	ect project isolate	aliases	country	late field year	s i			size (bp)		clonal complex ST-32 complex/ET-5	e PorA VR1	an
Dele elete lelete	Update	Sequence bin upload	New version create	Sel id 12674	ect project isolate M18700	aliases	country USA	late field year 2009	s i	Neisseria meningitidis	В	size (bp) O	7301	cional complex ST-32	PorA VR1 add	ar
Dele elete lelete	update	Sequence bin	New version create	Sel	ect project isolate	aliases	country	late field year	s i	Neisseria		size (bp)		clonal complex ST-32 complex/ET-5	e PorA VR1	an
Dele elete lelete lelete	Update	Sequence bin upload	New version create create	Sel id 12674	ect project isolate M18700	aliases	country USA	late field year 2009	s i	Neisseria meningitidis Neisseria	В	size (bp) O	7301	clonal complex ST-32 complex/ET-5	PorA VR1 add	an
Dele elete lelete lelete	update update update update	Sequence bin upload upload upload	New version create create create	id 12674 12675 12676	isolate M18700 M18701 M18725		Country USA USA USA	ate field year 2009 2009 2009	s 🛿	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	B	size (bp) 0 0 0	7301 7302 7303	clonal complex ST-32 complex/ET-5	e PorA VR1 add	an
Dele elete lelete lelete	Update Update update update	Sequence bin upload upload	New version create create create	Sel id 12674 12675	isolate M18700	aliases	Country USA USA	late field year 2009 2009	s i	Neisseria meningitidis Neisseria meningitidis Neisseria neningitidis Neisseria	В	size (bp) O	7301 7302	clonal complex ST-32 complex/ET-5	e PorA VR1 add	an
Delete delete delete delete delete	Update Update Update Update Update	Sequence bin upload upload upload upload	New version create create create create	Sel id 12674 12675 12676 13090	ect project isolate M18700 M18701 M18725 M19024		Country USA USA USA USA	ate field year 2009 2009 2009 2009	s 🛿	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	size (bp) 0 0 0 0	7301 7302 7303 7575	clonal complex ST-32 complex/ET-5 complex	PorA VR1 add add add add	
Delete delete delete delete delete	update update update update	Sequence bin upload upload upload	New version create create create create	id 12674 12675 12676	isolate M18700 M18701 M18725		Country USA USA USA	ate field year 2009 2009 2009	s 🛿	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria	B	size (bp) 0 0 0	7301 7302 7303 7575 4789,	Clonal complex ST-32 complex/ET-5 complex	add add add add add	
Delete delete delete delete delete	Update Update Update Update Update	Sequence bin upload upload upload upload	New version create create create create	Sel id 12674 12675 12676 13090	ect project isolate M18700 M18701 M18725 M19024		Country USA USA USA USA	ate field year 2009 2009 2009 2009	s 🛿	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB	size (bp) 0 0 0 0	7301 7302 7303 7575 4789,	clonal complex ST-32 complex/ET-5 complex	add add add add add	

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

(PubMLST) U	Isolates: Add Query/update Batch insert										
Logged in: Keith Jolley (ke	eith). Log out Change password										
Delete isolate	6										
You have selected to d	You have selected to delete the following record:										
Provenance/meta	data										
id:	14627	source:	CSF	update history:	26 updates show details						
isolate:	M20918	species:	Neisseria meningitidis	date entered:	2010-01-26						
strain designation:	A: P1.20,9: F3-1: ST-4789,7980	serogroup:	A	datestamp:	2014-06-17						
	(cc5)	sender:	Xin Zhao, Novartis (formerly at US								
country:			CDC)								
region:	North America	curator:	Carina Brehony, University of Oxford, UK (E-mail:								
year:			carina.brehony@zoo.ox.ac.uk)								
your.	2003										
Publication (1)											
			iditi V, Humphrey JC, Sammons SA, Govi ncing projects. <i>Bioinformatics</i> 26:1819-26		, Tondella ML, Harcourt BH, Mayer LW,						
Sequence bin											
contigs:	2049	N90:	456								
total length:	1718070 bp	N95:	324								
max length:	5436 bp	loci tagged:	979								
mean length:	839 bp	detailed breakdown:	Display								
N50:	1155										
Action											
Delete											

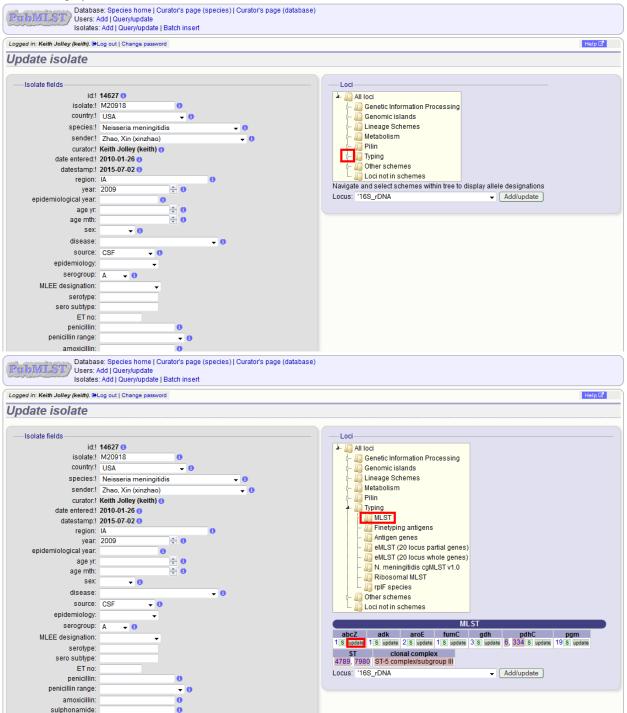
Pressing 'Delete' from this record page confirms the deletion.

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/Users:	se: Species home Curator's page (species) Curator's page (database) Add Query/update s: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). 🕏	Log out Change password	Help 🗹
Update isolate		
isolate: country: species: sender: curator: date entered: datestamp: region:	Neisseria meningitidis Chao, Xin (xinzhao) Chao, Xin (xinzhao) Chao, Xin (xinzhao) Chao,	Loc All loc Genetic Information Processing Genomic Islands Hetabolism Hetabolism Difference Difference Navigate and select schemes within tree to display allele designations Navigate and select schemes within tree to display allele designations Locus: abcZ Add/update
penicillin range: amoxicillin: sulphonamide:	• 0 0	

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

(PubMLST) U	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 (ke	eith). Log out Change password								
Update abcZ	allele for isolate 146	27							
Provenance/meta	a data	Locus: abcZ							
id:	14627	Add new allele designation							
isolate:	M20918	Please fill in the fields below - required fields are marked with an exclamation mark (!).							
strain designation:	A: P1.20,9: F3-1: ST-4789,7980								
	(cc5)	Record							
country:		isolate id: 14627							
region:		locus: abcZ							
	2009	allele id:1 5							
source:		sender: Jolley, Keith (keith)							
	Neisseria meningitidis	status: confirmed -							
serogroup:	A Xin Zhao	method: manual							
		curator:! Keith Jolley (keith)							
	Carina Brehony	datestamp:1 2014-07-10 date entered:1 2014-07-10							
	26 updates show details	comments:							
date entered:									
datestamp:	2014-06-17	Action							
Update other loci	:	Reset Submit							
Locus: abcZ	✓ Add/update	Existing designations							
		Update Delete allele id sender status method comments Update Delete 1 Xin Zhao confirmed manual							

6.9 Batch updating multiple isolate records

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

Database: Spe Users: Add Qu Isolates: Add Q	iery/u	pdate	tor's page (species) Curator's pa itch insert	age (database)
ogged in: Keith Jolley (keith). 🕒 Log out	Chang	ge password		
atabase curator's i	nte	rface	Neisseria PubMI	ST
		Tuve	iteleocenti i upini	
🕜 Add, update or delete	reco	ords		
Record type	Add	Batch Ad	d Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query browse list batch upda	ate
olate field extended attribute value	s +	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences		++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
Database configuratio		otob Addil	Indate or delete	Compute
loci	аа в +	atch Add t	2	Comments
		ank scan	(
locus aliases	+	++	? Add alternative nar	mes for loci. These can also be set when you batch add loci.
	+	++		R reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
	+	++		ttributes to associate with values of a particular isolate record field.

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'.

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

Problem Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert
Logged in: Keith Jolley (keith). Log out Change password
Batch isolate update
The following changes will be made to the database. Please check that this is what you intend and then press 'Upload'. If you do not wish to make these changes, press your
browser's back button.
Transaction id Field New value Value(s) currently in database Action
1 100 serogroup B C update field with new value
2 101 serogroup B C update field with new value
Action
Upload
Back to main page

You can also use a secondary selection field such that a combination of two fields uniquely defines the isolate, for example using country and isolate name.

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

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

6.10 Deleting multiple isolate records

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

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

Database: Spec Users: Add Qu Isolates: Add C	ery/up	date	tor's page (species) Curator's pa tch insert	ge (database)
gged in: Keith Jolley (keith). 🕒 Log out	Change	e password		
atabase curator's i	ntei	rface -	Neisseria PubML	ST
	1001	lave		
Add, update or delete	reco	rde		
Record type		Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
isolates	+	++	query browse list batch updat	te
olate field extended attribute values	s +	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences		++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
Database configuration				
			pdate or delete	Comments
100	+ lataba	++ nk scan	?	
	+	++	? Add alternative nam	es for loci. These can also be set when you batch add loci.
PCR reactions	+	++		reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		robes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
isolate field extended attributes	+	++		tributes to associate with values of a particular isolate record field.

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

Publ	VILST	💟 Users: /	se: Specie Add Quer : Add Qu	y/updat	e		(species) C	Curator	s page (databas)	e)								
Logged in:	Keith Jol	lley (keith). 🕩	Log out Ch	nange pa	ssword						Help 🗹	Toggle: 🚯 🛛	Field help:	id				- Co
solat	te qu	ery/up	date															
—Isol	ate prove	enance/pher	otype field	ds —					— Display/sort	options								Modify
Comb	ine with:	AND 👻							Order by:	id				asce	nding 👻			form
date	entered	-	=		2014-03	-17		+ 🚺	Display:	25 👻 records	per page 🕦							option
cura	tor (surna	ame) 👻	=	•	Jolley													
-Acti	on ——																	
Res	-	ubmit																
Res	et	ubmit																
3 records	returne	d. Click the h	yperlinks	for deta	iled infor	mation.												
Dala		Teere		D														
Dele	1	_	anning-		jects													
Dele	te ALL	Sci	an	Sele	ct project			•	Link									
_																		
_	_							lacia	te fields						MLST	Finate		linens
Delete	Undate	Sequence	New									- Seqbin	Contigs			PorA	ping an PorA	FetA
Delete	opuuto	bin	version	id	isolate	aliases	country	year	disease	species	serogrou	Jp size (bp)	Contago	ST	clonal complex	VR1	VR2	VR
delete	update	upload	create	28783	0012/14		Czech	2014	carrier	Neisseria	a W	0	0	10733		5-2	10-1	F5-8
							Republic			meningitid						update	update	update
delete	update	upload	create	28784	0014/14			2014	carrier	Neisseria		0	0	35	ST-35 complex	22-1	14	F4-1
delete		in the set	and the	00705	0045444		Republic	0044	laura di sa	meningitid				40704	07.4444	update	update	update
aelete	update	upload	create	28785	0015/14		Czech Republic	2014	invasive (unspecified/oth	Neisseria (er) meningitid		0	0	10734	ST-41/44 complex/Lineage 3	22-1 update	14 update	F5-2 update
							Republic		(unspecified/ou	ier) meningiud	10				complex clifeage 3	update	update	update

You will have a final chance to change your mind:

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

Click 'Confirm deletion!'.

6.11 Uploading sequence contigs linked to isolate records

6.11.1 Select isolate from drop-down list

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

Users: Add C Isolates: Add			Batch insert		
ed in: Keith Jolley (keith). 🗭 Log ou	t Char	nge password	i .		
tabase curator's	inte	erface	- Neisser	ia PubN	ILST
🕜 Add, update or delet	e rec	ords			
Record type	Ado	i Batch Add	Update	or delete	Comments
users	+	++		?	
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.
user group members	+	++		?	Add users to groups for setting access permissions.
curator permissions				?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the use table.
isolates	+	++		owse list update	
isolate field extended attribute values	+	++		?	Add values for additional isolate field attributes.
projects	+	++		?	Set up projects to which isolates can belong.
project members	+	++		?	Add isolates to projects.
isolate aliases	+	++		?	Add alternative names for isolates.
PubMed links	+	++		?	
allele designations		++		?	Allele designations can be set within the isolate table functions.
sequences		++		?	The sequence bin holds sequence contigs from any source.
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++		?	Set up experiments to which sequences in the bin can belong.
experiment sequences				?	Add links associating sequences to experiments.
sequence tags		scan		?	Tag regions of sequences within the sequence bin with locus information.
Database configurati Table		Batch Add	Update or delete		Comments
loci	Auu I	++	2		<u>comments</u>
1001		ank scan			
locus aliases	ualai	++	2	Add alternative	names for loci. These can also be set when you batch add loci.
	-		r	Add alternative	names for rou. These can also be set when you batch add rou.
PCR reactions	+	++		Set up in eiliee	PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.

Select the isolate that you wish to link the sequence to from the dropdown list box. You also need to enter the person who sent the data. Optionally, you can add the sequencing method used.

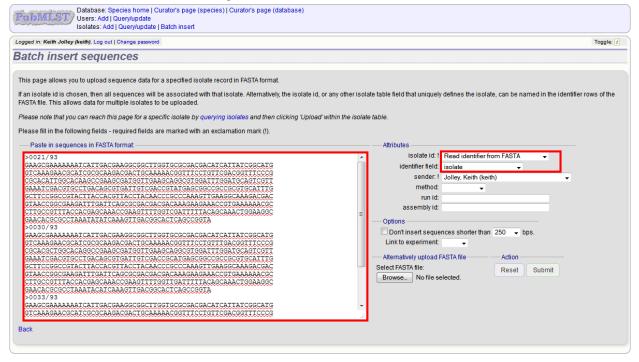
Paste sequence contigs in FASTA format in to the form.

PTIDULST Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change password	Toggle: [i]
Batch insert sequences	
This page allows you to upload sequence data for a specified isolate record in FASTA format.	
If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any other isola FASTA file. This allows data for multiple isolates to be uploaded.	
Please note that you can reach this page for a specific isolate by querying isolates and then clicking "Upload" within the isolate Please fill in the following fields - required fields are marked with an exclamation mark (!).	e lacile.
Paste in sequences in FASTA format	Attributes
TTTAATTCTAAAATATATTTTTTTCAAAGTTACTCATATTTAGTTAG	isolate id: 1 2) 120M identifier field: id sender: 1 Jolley, Keith (keith) method: un id: assembly id: Options Options Don't insert sequences shorter than 250 bps. Link to experiment Alternatively upload FASTA file Action Select FASTA file: Browse No file selected.

gged in: Keith Jolley (keith). Log out Change password			Toggl
atch insert sequences			
e following sequences will be entered.			
Original designation	equence length Comm	nents the feature of the offe	
180426 NODE_1211_length_26135_cov_16.536217	26167	Number of contigs: 359 Minimum length: 265	
180427 NODE_619_length_1208_cov_9.455298	1240	Minimum length: 205 Maximum length: 33563	
180428 NODE_655_length_1534_cov_15.418513	1566	Maximum length: 33503 Total length: 2059411	
180429 NODE_675_length_1548_cov_17.753876	1580	Mean length: 5736	
180430 NODE_31_length_8390_cov_14.525030	8422	• N50: 10581	
180431 NODE_254_length_2721_cov_18.400587	2753	 N90: 3126 	
180432 NODE_262_length_1955_cov_8.388747	1987	• N95: 1863	
180433 NODE_252_length_30791_cov_15.767627	30823		
180434 NODE_189_length_536_cov_31.078358	568	Upload	
180435 NODE_716_length_511_cov_12.113503	543		
180436 NODE_465_length_13739_cov_15.131669	13771		
180437 NODE_38_length_15888_cov_17.174660	15920		
180438 NODE_778_length_2398_cov_8.673060	2430		
180439 NODE_1765_length_657_cov_8.754947	689		
180440 NODE_729_length_255_cov_13.007843	287		
180441 NODE_52_length_16337_cov_17.192997	16369		
180442 NODE_190_length_652_cov_116.434052	684		
180443 NODE_95_length_3094_cov_14.927279 180444 NODE_770_length_5072_cov_12.878943	3126		
180444INODE_//0_length_5072_cov_12.878943 180445INODE 263 length 1223 cov 10.451349	5104 1255		
180446 NODE_203_length_1223_cov_10.451349 180446 NODE_181_length_4496_cov_14.635231	4528		
180446[NODE_181_length_4496_cov_14.635231 180447[NODE_558 length_4436_cov_14.670198	4528		
180448 NODE_1179_length_917_cov_13.504908	949		
180449 NODE_1779_length_4033_cov_15.608480	4065		
180449NODE_227_length_2435_cov_12.223409	2467		
180451INODE 54 length 790 cov 9.398734	822		
180452 NODE 146 length 12761 cov 14.578794	12793		
180453 NODE 11 length 16414 cov 13.733703	16446		
180454 NODE 386 length 3699 cov 13.323060	3731		
180455 NODE 215 length 395 cov 4.250633	427		

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

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



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

PrrhTATLSTP Users: Add Query/update Isolates: Add Query/update Batch insert							
Logged in: Ke	Logged in: Keith Jolley (keith). Log out Change password						
Batch i	Batch insert sequences						
BIGSdb id	ng sequences will be en Identifier field (isolate)	Sequence length Co	omments Status	Upload			
938 944	0021/93	465 465	Will upload Will upload				
944	0033/93	465	Will upload				

6.11.2 Select from isolate query

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

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

ged in: Keith Jolley (keith). (HLog out atabase curator's					
	inte				
		rface	- Neisser	ia PubN	ILST
🛃 Add, update or delet	e reco	ords			
Record type	Add	Batch Add	Update	or delete	Comments
users	+	++		?	
user groups	+	++		?	Users can be members of these groups - use for setting access permissions.
user group members	+	++		?	Add users to groups for setting access permissions.
curator permissions				?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users
					table.
isolates	+	++		owse list update	
isolate field extended attribute values	+	++		?	Add values for additional isolate field attributes.
projects	+	++		?	Set up projects to which isolates can belong.
project members	+	++		?	Add isolates to projects.
isolate aliases	+	++		?	Add alternative names for isolates.
PubMed links	+	++		?	
allele designations		++		?	Allele designations can be set within the isolate table functions.
sequences		++		?	The sequence bin holds sequence contigs from any source.
accession number links	+	++		?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++		?	Set up experiments to which sequences in the bin can belong.
experiment sequences				?	Add links associating sequences to experiments.
sequence tags		scan		?	Tag regions of sequences within the sequence bin with locus information.
🚩 Database configuratio	on				
-					
			Update or delete		Comments
loci	+	++	?		
		ank scan			
locus aliases	+	++	?		names for loci. These can also be set when you batch add loci.
PCR reactions	+	++		Set up in silico	PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++			

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert									
Logged in: Keith Jolley (keith). 🕏 Log out Change password Help 🗹 Toggle: 🚯 Field help: id 🗸 🕞									
Isolate query/update									
	elds		options			Modify			
isolate 👻 =	✓ FAM18	+ 1 Order by:	id		- ascending				
		Display:	25 👻 records per page	0		options			
Action Reset Submit 1 record returned. Click the hyperlink for detailed information. Delete — Tag scanning — Projects Delete ALL Scan Select project Link									
Delete Update Sequence New		Isolate fields 🛈		Seqbin Contigs	MLST	Finetyping antigens			
benete opulate bin version	id isolate aliases	country year disease	species serogroup		ST clonal complex	PorA PorA FetA VR1 VR2 VR			
delete update upload create	698 FAM18 NIBSC_3076; Z4259	USA 1983 invasive (unspecified/other)	Neisseria C meningitidis	2194961 1	11 ST-11 complex/ET-37 complex	5 2 F1-30 update update			

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

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

6.11.3 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.

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert	
Logged in: Keith Jolley (keith). Log out Change password	Toggle: i
Batch insert sequences	
This page allows you to upload sequence data for a specified isolate record in FASTA format. If an isolate id is chosen, then all sequences will be associated with that isolate. Alternatively, the isolate id, or any other iso rows of the FASTA file. This allows data for multiple isolates to be uploaded.	olate table field that uniquely defines the isolate, can be named in the identifier
Please note that you can reach this page for a specific isolate by guerying isolates and then clicking 'Upload' within the isolates	ate table.
Please fill in the following fields - required fields are marked with an exclamation mark (!).	
— Paste in sequences in FASTA format:	Attributes isolate id: ! Read identifier from FASTA • identifier field: id • method: • run id: assembly id: Options Options Options Options Atternatively upload FASTA file Action Select FASTA file: Browse. No file selected.
Back	

6.12 Automated web-based sequence tagging

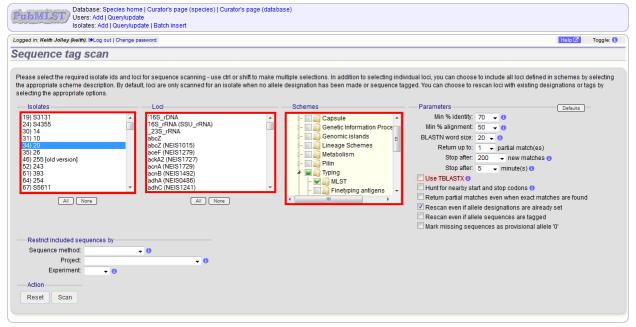
Sequence tagging, or tag-scanning, is the process of identifying alleles by scanning the sequence bin linked to an isolate record. Defined loci can either have a single reference sequence, that is defined in the locus table, or they can be linked to an external database that contains the sequences for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

isolates + ++ query browse list batch update	delete Comments Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
Add, update or delete records Record type Add Batch Add Update or delete Comments users + ++ ? Users can be members of these groups - use for setting access permissions. user group members + ++ ? Add users to groups for setting access permissions. curator permissions - ? Set curator permissions for individual users - these are only active for users with a status of 'curator' in the user's curator permissions. isolates + ++ ? Add values for additional isolate field attributes. projects + ++ ? Add values for additional isolates is on belong. project members + ++ ? Add values for additional isolates an belong. project members + ++ ? Add values for isolates. PubMed links + + ? Add alternative names for isolates. PubMed links +++ ? Add alternative names for isolate. PubMed links +++ ? Allele designations can be set within the isolate table functions. sequences +++ ? Allele designations can be set within the isolate table functions. <th>delete Comments Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.</th>	delete Comments Users can be members of these groups - use for setting access permissions. Add users to groups for setting access permissions. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table. Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
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Control	
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allele designations ++ ? Allele designations can be set within the isolate table functions. sequences ++ ? The sequence bin holds sequence contigs from any source.	
Sequences ++ ? The sequence bin holds sequence contigs from any source.	
SEQUENCES ++ ? The sequence bin holds sequence contigs from any source.	Allele designations can be set within the isolate table functions.
experiments + ++ ? Set up experiments to which sequences in the bin can belong.	
experiment sequences ? Add links associating sequences to experiments.	Set up experiments to which sequences in the bin can belong.
Sequence tags Scan ? Tag regions of sequences within the sequence bin with locus information.	
	Add links associating sequences to experiments.

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

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



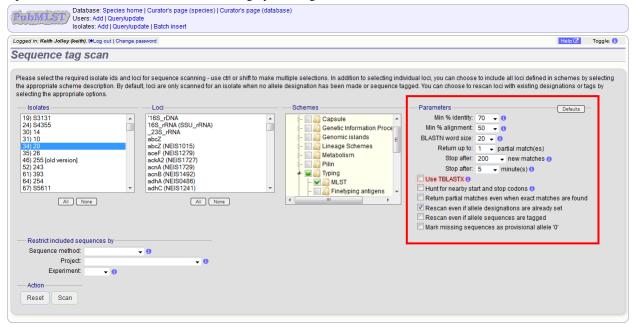
Choose your scan parameters. Lowering the value for BLASTN word size will increase the sensitivity of the search at the expense of time. Using TBLASTX is more sensitive but also much slower. TBLASTX can only be used to identify the sequence region rather than a specific allele (since it will only match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

By default, for each isolate only loci that have not had either an allele designation made or a sequence region scanned

will be scanned again. To rescan in these cases, select either or both the following:

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

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



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

olate	Match	Locus	Allele	% identity	Alignment length	Allele lengt	1 E-value	Sequence bin id	Start	End	Predicted star	Predicted end	Orientation	Designate allele	Tag sequence	Flag 🚯	
	exact		1	100.00	433	433	0.0	182791	7064		7064	7496 extract -	←		V		•
4) 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	33066	32577	33066 extract -	←	V	V		-
4) 20	exact	fumC	1	100.00	465	465	0.0	182815	19783	20247	19783	20247 extract -	\rightarrow		V		-
4) 20	exact	gdh	1	100.00	501	501	0.0	182852	7516	8016	7516	8016 extract -	\rightarrow	V	V		-
4) 20	exact	pdhC	1	100.00	480	480	0.0	182819	13868	14347	13868	14347 extract -	\rightarrow	V	V		-
4) 20	exact	pgm	3	100.00	450	450	0.0	182831	24559	25008	24559	25008 extract -	\rightarrow		V		-
Actio		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

6.13 Projects

6.13.1 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.

tabase curator's int	ter			
*		face -	Neisseria PubMLS	ST
2				
🐔 Add, update or delete re	eco	rds		
Depend tune		Batch Add	Update or delete	Comments
Record type A users	400	Batch Add	0 Opuale of delete	Comments
user groups	+	++	2	Users can be members of these groups - use for setting access permissions.
user group members	+	++	2	Add users to groups for setting access permissions.
curator permissions			2	Set curator permissions for individual users - these are only active for users with a status of 'curator' in the users table.
	+	++	query browse list batch update	
late field extended attribute values		++	2	Add values for additional isolate field attributes.
	+	++	2	Set up projects to which isolates can belong.
projects projects	+	++	2	Add isolates to projects.
isolate aliases	+	++	2	Add alternative names for isolates.
	+	++	2	
allele designations		++	2	Allele designations can be set within the isolate table functions.
sequences		++	2	The sequence bin holds sequence contigs from any source.
	+	++	2	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
Database configuration				
Database configuration				
Table Add	l Ba	tch Add U	pdate or delete	Comments
loci +		++	?	
dat	abai	nk scan		
locus aliases +		++	? Add alternative name	es for loci. These can also be set when you batch add loci.
Tocus allases •		++	Set up in silico PCR r	· · · · · · · · · · · · · · · · · · ·
Tocus allases				

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.

Click 'Submit'.

PubMLST / Use	abase: Species home Curator's page (species) Curator's page (database) rs: Add Query/update ates: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). @Log out Change password		Toggle: 🚯
Add new proje	ect description		
	low - required fields are marked with an exclamation mark (!).		
		Action	
id:!		Reset Submit	
	MRF Meningococcus Genome Library 0 Keith Jolley (keith)		
datestamp:!			
	<pre><div style="float:right; padding: 0 2em"><img <br="" src="/images/mrf 20.gif"/>alt="MRF" style="border: 1px solid #a0000; background:white" /></div> <div>The MRF Meningccoccus Genome Library is a collaboration between Public Health England, the Scottish Haemophilus, Legionella, Meningcoccus and Pneumccoccus Reference (SHLMPR) Laboratory, The Wellcome Trust Sanger Institute and the University of Oxford, funded by the Meningitis Research</div></pre>		
	● true ○ false ● ● true ○ false ●		

6.13.2 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.

ged in: Keith Jolley (keith). @Log ou Mabase curator's		ige password		
tabase curator's	2000			
	inte	erface -	Neisseria Pu	bMLST
🖌 Add, update or delet	te rec	ords		
Record type	Add	Batch Add	Update or delete	Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set curator permissions for individual users - these are only active for users with a status of 'curator' in th users table.
isolates	+	++	query browse list batch update	
isolate field extended attribute values	+	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences		++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
Database configurati				
Table	Add I	Batch Add U	pdate or delete	Comments
loci	+	++	?	
	datat	bank scan		
locus aliases	+	++	? Add alterr	native names for loci. These can also be set when you batch add loci.
PCR reactions	+	++	Set up in	silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++	Define nu	cleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
nucleolide probes				

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'.

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

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

	t Cha	nge password			
tabase curator's			Noissor	io Dub	MIST
llabase curator s	IIIU	enace	· Neissen	ia rup	IMLS I
💦 Add, update or delet	o ro	cords			
	ere	0105			
Record type	Add	Batch Add	Update or	delete	Comments
users	+	++	?		
user groups	+	++	?		Users can be members of these groups - use for setting access permissions.
user group members	+	++	?		Add users to groups for setting access permissions.
curator permissions			?		Set curator permissions for individual users - these are only active for users with a status of 'curator' in th users table.
isolates	+	++	query brow batch up		
isolate field extended attribute values	+	++	?		Add values for additional isolate field attributes.
projects	+	++	?		Set up projects to which isolates can belong.
project members	+	++	?		Add isolates to projects.
isolate aliases	+	++	?		Add alternative names for isolates.
PubMed links	+	++	?		
allele designations		++	?		Allele designations can be set within the isolate table functions.
sequences		++	?		The sequence bin holds sequence contigs from any source.
accession number links	+	++	?		Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?		Set up experiments to which sequences in the bin can belong.
experiment sequences			?		Add links associating sequences to experiments.
sequence tags		scan	?		Tag regions of sequences within the sequence bin with locus information.
•					
🚩 Database configurati	on				
-		Detek A tabl			On more and a
Table			Jpdate or delete		Comments
loci	+	++	?		
		bank scan	-		
locus aliases	+	++			ive names for loci. These can also be set when you batch add loci.
PCR reactions	+	++			ico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		Define nucle	otide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
solate field extended attributes	+	++	2		ional attributes to associate with values of a particular isolate record field.

Download an Excel submission template:

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Isolates: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). Log out Change password	1	Foggle: i
Batch insert project members		
This page allows you to upload project member data as tab-delimited text or copied from a spreadsheet. • Field header names must be included and fields can be in any order. Optional fields can be omitted if you wish. • 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).	Action Reset Submit	
Back		

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

PubMLST / Us	atabase: Species home Curator's page (species) Curator's page sers: Add Query/update olates: Add Query/update Batch insert	(database)
Logged in: Keith Jolley (kei	ith). Log out Change password	Toggle: i
Batch insert p	project members	
 Field header na Download tab-d Download subn 	o upload project member data as tab-delimited text or copied from imes must be included and fields can be in any order. Optional fiel felimited header for your spreadsheet - use Paste special \rightarrow text to hission template (xlsx format)	s can be omitted if you wish. paste the data.
	ited text (include a field header line).	— Action
project_id	isolate_id	Reset Submit

6.14 Isolate record versioning

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

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

Links to different versions are displayed within an isolate record:

(PubMLST) B	tuery: Search Browse Profile/S reakdown: Isolate fields Schen inks: Contents Home Options		ase submissions		
Full informat	ion on isolate 5				
Provenance/meta	ı data				
id:	21	source:	throat swab	update history:	1 update show details
isolate:	5	epidemiology:	endemic	date entered:	2014-06-30
strain designation:	NG: P1.ND,ND: F-ND: ST-ND (-		Neisseria meningitidis	datestamp:	2014-06-30
	Germany	serogroup:			
continent:	· · · · · · · · · · · · · · · · · · ·		Bavarian carriage study		
region: year:	Volkach	sender:	Ulrich Vogel, Univerity of Wuerzburg, Wuerzburg, Germany		
age yr:		curator:	Keith Jolley, University of Oxford, UK (E-mail:		
disease:			keith.jolley@zoo.ox.ac.uk)		
Versions					
More than one version	of this isolate record exist.				
Older versions:	20				
Publication (1)					
Claus H, Maide 822 isolates	en MC, Wilson DJ, McCarthy ND,	Jolley KA, Urwin R, Hessler F, Frosch M	, Vogel U (2005). Genetic analysis of meningococci o	carried by children a	nd young adults. <i>J Infect Dis</i> 191:1 263-71
Schemes and loc	i				
🗏 🏭 No loci availab	le for analysis.				

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:

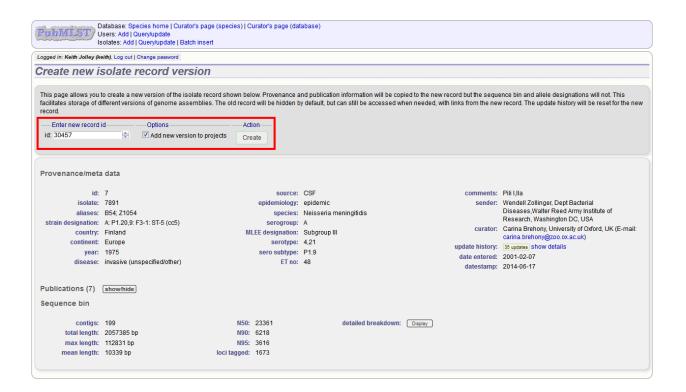
Users: Add C			atch insert	
ged in: Keith Jolley (keith). 🕩Log ou	it Char	nge password		
tabase curator's	inte	erface	- Neisser	PubMI ST
	mic	Indoc	- Meisser	
Add, update or delet	te rec	ords		
Record type	Add	Batch Add	Update or	elete Comments
users	+	++	?	
user groups	+	++	?	Users can be members of these groups - use for setting access permissions.
user group members	+	++	?	Add users to groups for setting access permissions.
curator permissions			?	Set ourator permissions for individual users - these are only active for users with a status of 'curator' in users table.
isolates	+	++	query brow batch up	
isolate field extended attribute values	+	++	?	Add values for additional isolate field attributes.
projects	+	++	?	Set up projects to which isolates can belong.
project members	+	++	?	Add isolates to projects.
isolate aliases	+	++	?	Add alternative names for isolates.
PubMed links	+	++	?	
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences		++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.
Database configurati		Batch Add	Update or delete ?	Comments
loci			Y	
locus aliases	datat	bank scan	2	di alternative annua far lasi. These can also be estudian vev batch add lasi
	+	++	() () () () () () () () () ()	dd alternative names for loci. These can also be set when you batch add loci.
PCR reactions	++	++		et up in silico PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes			0	efine nucleotide probes for in silico hybridization reaction to filter genomes for tagging to specific repetitive loci.
solate field extended attributes	+	++	?	efine additional attributes to associate with values of a particular isolate record field.

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

PubMLST	🕖 Users: Add	d Query/upd	ate	Batch inser		l curator s page	(ualabase)										
Logged in: Keith Joll	ey (keith). 🗭Log	out Change	passw	rord									Togg	le: 🜖 Field help: id			-
Browse Ne	eisseria	PubMl	LS	T datab	ase												
	d ascending 25 v record	ds per page (0		•	Action Browse all re	cords										
36583 records retu Delete Delete ALL Page: 1 2 3	Tag scan Scan	ning P Se	rojec lect p	cts project		information. Link		late f	elds n					MLST	Fine	typing anti	2000
Delete Update	Sequence bin	New version	n id i	isolate		liases	country	vear		disease	species	serogroup	ST	cional complex	PorA VR1		
delete update	upload	create	1	A4/M1027		2803; Z1001	USA				Neisseria meningitidis		4	ST-4 complex/subgroup IV	5-2 update		F1-5 update
delete update	upload	create	2			C 2822; Z1035	Pakistan				Neisseria meningitidis		1	ST-1 complex/subgroup I/II	5-2 update		F5-1 update
delete update	upload	create	3	M00242905			UK	2000	invasive (u	Inspecified/other)	Neisseria meningitidis	в	1099		19 update	15 update	add
delete update	upload	create	4	M1027	B43; NIBS	C_3076; Z1043	USA	1937	invasive (u	Inspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	add	add	add
delete update	upload	create	5	M00240227			UK	2000	invasive (u	Inspecified/other)	Neisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7 update	16 update	add
delete update	upload	create	6	M00282207			UK	2000	invasive (u	unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex	add	add	add
delete update	upload	create	7	7891	B54; NIBS	C_2760; Z1054	Finland	1975	invasive (u	Inspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	20 update	9 update	F3-1 update
delete update	upload	create	8	M00242007			UK	2000	invasive (u	Inspecified/other)	Neisseria meningitidis	В	1102	ST-18 complex	add	14 update	add
delete update	upload	create	9	0021/84			Czech Republic	1984	invasive (u	Inspecified/other)	Neisseria meningitidis	W	114	ST-22 complex	add	add	add
doloto undoto	unload	croate	10	6740	D72- NIDO	0 0704-74070	Conodo	1071	invocivo (r	inconcified/other)	Noiceoria moningitidia	Α	4	QT 1 complex/cubaroup I/II	10.1	2 undete	EE 1 Junior

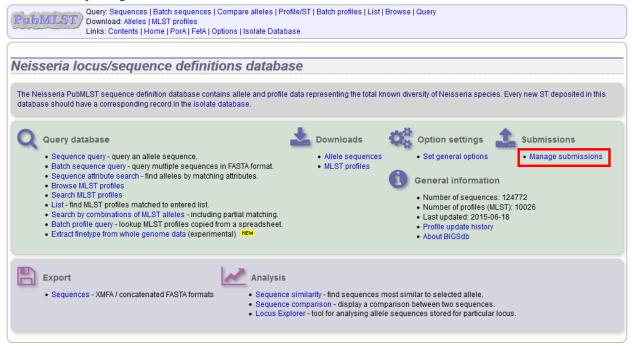
The isolate record will be displayed. The suggested id number for the new record will be displayed - you can change this. By default, the new record will also be added to any projects that the old record is a member of. Uncheck the 'Add new version to projects' checkbox to prevent this.

Click the 'Create' button.



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	g out Change password			
lanage submiss	ions			
O u han it a suu da ta				
Submit new data				
Data submitted here will go in	to a queue for handling by a curator or by an autom	nated script. You will be abl	le to track the status of any submission.	
Submission type:				
allelesMLST profiles				
New allele sequence su	bmissions waiting for curation			
Your account is authorized to h	andle the following submissions:			
Submission id	Submitted Updated Submitter	Locus Sequences		
BIGSdb_20150623074942_3	1862_84622 2015-06-23 2015-06-23 Joe Bloggs			
Return to index page				

7.1 Alleles

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

ed in: Keith Jolley (keit	h). @Log out Change password							
ırate submi	ssion							
ubmission: BIGSd	b 20150623074942 31862 846	22						
- Summary			es—					
		Identifier	Length	1	Sequence	Complete CDS	Status	Assigned allele
	alleles	UK322	924	ATGCTGCAAAGA	ACTTTGGC ACATCAGAAATTGTGGATAA	~	pending 👻	Curate
	Joe Bloggs, University of Oxford, UK	UK323	924	ATGCTGGAAAGA	ACTITIGGC ACATCAGAACTIGIGGATAA	✓	pending 👻	Curate
datestamp:	2015-06-23 pending	UK347	924	ATGCTGCAAAGA	ACTTTGGC ACATCAGAAATTCTGGATAA	✓	pending 👻	Curate
	accepted - data uploaded	Batch cu	rate					Update
	NEIS0001				Archive			
	3 745	— Message	85		Archive of submission and any supportin	a filoa:		
					Archive of submission and any support	ig mes.		
technology:					Download TAR			
read length:								
coverage: assembly:				Add message				
assembly:	de novo							

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

PTIDMLST / Download: A	Cuery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database									
Logged in: Keith Jolley (keith). 🔂 Log o	out Change password									
Curate submission	1									
Submission: BIGSdb_2015 — Summary		Sequences								
type: alleles submitter: Joe Blog datestamp: 2015-06 status: pending outcome: accepte	ggs, University of Oxford, UK -23	dentifier Leng UK322 924 UK323 924 UK347 924 Batch curate	4 ATGCTGCAAAGAA 4 ATGCTGGAAAGAA	Sequence ACTTGGC ACATCAGAAATTGTGGATAA CTTTGGC ACATCAGAACTTGTGGATAA ACTTGGC ACATCAGAAATTCTGGATAA	Complete CDS	Status pending v pending v pending v	Assigned allele Curate Curate Curate Update			
locus: NEIS00 sequences: 3 153 technology: Illumina read length: 100-195 coverage: 20-49x assembly: de novo assembly: software: Velvet	01	Messages —	.d Add message		ng 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.

Links: Contents Home PorA FetA Options Isolate Database ged In: Keiff Jolley (keiff). @Log out Change password									
urate submis	sion								
ubmission: BIGSdl — Summary—	b_20150623074942_31862_8462	22 — Sequences							
		Identifier Len	ngth		Sequence	Complete CDS	Status	Assigned allele	
type:		UK322 92	24 ATG	CTGCAAAGAA	ACTITIGGC ACATCAGAAATTGTGGA		pending 👻	Curate	
	Joe Bloggs, University of Oxford, UK	UK323 92	24 ATG	CTGGAAAGAA	ACTITIGGC ACATCAGAACTIGIGGA	'AA 🖌	pending 👻	Curate	
datestamp:		UK347 92	24 ATG	CTGCAAAGAA	CTTTGGC ACATCAGAAATTCTGGA	'AA 🗸	pending 👻	Curate	
status:		Batch curate	a					Update	
	accepted - data uploaded NEIS0001	Messages-			Archive				
sequences:	3 745			_	Archive of submission and any supp	orting files:			
technology:	Illumina								
read length:					Download TAR				
coverage:	20-49x		Add m	nessage					
coverage.									
assembly:									

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 will need to manually set the status from the dropdown list of values.

PubMLST Use	abase: Species home Curator's page (species) Curator's page (database) irs: Add Query/update i: Add 3T profiles: Add Query/update Batch insert			
Logged in: Keith Jolley (keith). IPLog out Change password		Help 🖉	Toggle: 🚺
Add new allele	e sequence			
	elow - required fields are marked with an exclamation mark (!).	Antion		
Recordlocusil	NEIS0001 V	Action		
allele id:1		Reset Submit		
sequence:!	ATGCTGCAAAGAACTTTGGCCAAATCCATCAGCGTTACCGGAGTCGGCCTGCATTCCGGCGAACGGGTCGCACTG ACCCTGCACCCCGCGCCTGAAAACAGCGGGATTTCCTTCC			
status:!	•			
sender:!	Bloggs, Joe (jbloggs)			
	Keith Jolley (keith)			
date entered:!				
datestamp:! comments:	2015-06-23			
	the state of the s			
riags.	atypical contains IS element downstream fusion			

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

Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert		
Logged in: Keith Jolley (keith). B+Log out Change password	Help 🗹	Toggle: 🚺
Add new allele sequence		
Sequence NEIS0001 (IpxC): 209 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.

Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database									
ogged in: Keith Jolley (keith). (#Log out Change password									
Curate submission									
Submission: BIGSdb_201506	23074942_31862_84622	2 — Sequences							
·		Identifier Len	nath	Sequenc	e	Complete CDS	Status	Assigned allele	
type: alleles					ACATCAGAAATTGTGGATAA		assigned	209	
	, University of Oxford, UK	UK323 92	24 🛛	ATGCTGGAAAGAACTTTGGC A	ACATCAGAACTTGTGGATAA	~	pending 👻	Curate	
datestamp: 2015-06-23	3	UK347 92	24 A	ATGCTGCAAAGAACTTTGGC A	ACATCAGAAATTCTGGATAA	~	pending 👻	Curate	
status: pending		Batch curate	e					Update	
locus: NEIS0001									
sequences: 3 FAS		-Messages-		Archive					
technology: Illumina				Archive of subr	nission and any supportir	ng files:			
read length: 100-199				Download TAR					
coverage: 20-49x			_						
assembly: de novo			Add	d message					
assembly software: Velvet									

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.

ged in: Keith Jolley (keith). @Log out Change password									
urate submi	ssion								
Submission: BIGS	1b 20150623074942 31862 846	22							
Summary									
· ·		Identifier Length	h Sequence	Complete CDS	Status	Assigned allele			
	alleles	UK322 924	ATGCTGCAAAGAACTTTGGC ACATCAGAAATTGTGGATAA		assigned	209			
	Joe Bloggs, University of Oxford, UK	UK323 924	ATGCTGGAAAGAACTTTGGC ACATCAGAACTTGTGGATAA	 Image: A set of the /li>	pending 👻	Curate			
	2015-06-23	UK347 924	ATGCTGCAAAGAACTTTGGC ACATCAGAAATTCTGGATAA	✓	pending 👻	Curate			
	pending	Batch curate				Update			
locus:	NEIS0001	Daton barato				opullo			
sequences:	3 FAS	— Messages —	Archive						
technology:	Illumina		Archive of submission and any supporti	ng files:					
read length:	100-199		Download TAR						
coverage:	20-49x								
			Add message						
assembly:	de novo								

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 will need to manually set the status from the dropdown list of values.

PubML	Database: Species home Curator's page (species) Curator's page (database) Users: Add Query/update Loci: Add MLST profiles: Add Query/update Batch insert	
Logged in: Keith	Jolley (keith). @Log out Change password Help 12 T	oggle: 📵
Batch in	sert sequences	
Do not include	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 id e the locus name in the identifier in the FASTA file. hat you can not use this page to upload sequences for loci with extended attributes. ameters	s only).
	NEIS0001 (IpxC) V	
status:!		
sender:!	Bloggs, Joe (jbloggs) 🗸	
sequence (FASTA):!	>UK323 ATGCTGGAAAGAACTTTGGCGAAATCCATCAGCGTTACCGGAGTCGGGCTGCATTCGGCG GAACGCGTCGGCGCGCGCGCGCGCAAAACAGCGGGGTTGCTTCCGCCGCG ACCGATTTGGACGCGCGACAAATCCAACCTGACCCCTTAITTGATCAACGAT ACCGCGCTTTCGTCCGCCATCGGCAACGGCGGCGGCGCGCCGCACGGACGACCGATCGAACAC ATTATGTCCGGCGTGTCCGCCATCGGCAACGGCGGTGATGAGCGGACGGCC GAAATCCCGATTATGGACGGCCCACTGGCACGGCTGGATGGA	
Override	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 ig le sequence similarity check xt available id (only for loci with integer ids) 	nored.

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

PubMLST	Users: Ad Loci: Add	d Query/upo	e Curator's page (species) Curator's page (database) te ry/update Batch insert		
Logged in: Keith Jolle	y (keith). 🕩Log	g out Change	assword	Hel	p 🖸 🛛 Toggle: 🚯
Batch inse	rt sequ	ences			
Sequence cher Original designati UK323 UK347		Status OK OK	Action Upload valid sequences		

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

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

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database										
Logged in: Keith Jolley (kei	th). @Log out Change password									
Curate submi	ssion									
Submission: BIGSo — Summary	lb_20150623074942_31862_8462	2 Sequence	es ——							
submitter: datestamp: status:	Illumina 100-199 20-49x de novo	UK323	924 924 924 s	ATGCTGCAAAGA ATGCTGGAAAGA	AACTTTGGC AACTTTGGC Archive	ACATCAGAAATTG ACATCAGAACTTG ACATCAGAAATTC ubmission and any	TGGATAA TGGATAA TGGATAA	*	DS Status As assigned assigned assigned Action Close submissio	209 210 211

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.

	DeLog out Change password							
urate submis	sion							
ubmission: BICSdb	20150623074942 31862 8465	20						
	_20150625074542_51662_646							
- Summary		Sequen						
type: a	lleles	Identifier UK322	Lengti 924		Sequence ACTITIGGC ACATCAGAAATTGTGGAT	Complete CDS	Status	Assigned allele
submitter: J	oe Bloggs, University of Oxford, UK	UK323	924	ATGCTGGAAAGA			rejected v	Curate
datestamp: 2	015-06-23	UK347	924		ACTITGGC ACATCAGAAATTCTGGAT	-	rejected +	Curate
status: p	ending	Batch cu				•	rojoolou v	
	ccepted - data uploaded	Batch cu	rate					Update
locus: N		Messag	es		Archive			
sequences: g	FAS	_			Archive of submission and any suppo	ting files:		
technology: I	lumina				Download TAR			
read length: 1	00-199				Download TAR			
coverage: 2	20-49x			Add message				
assembly: c	le novo							
	/elvet							

7.1.4 Closing the submission

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

Query: Sequences Batch s Download: Alleles MLST p Links: Contents Home Po	rofiles		s List Browse Query				
Logged in: Keith Jolley (keith). Hog out Change passe	vord						
Curate submission							
Submission: BIGSdb_20150623074942 Summary	_31862_84622	ces					
type: alleles	Identifier			Complete CDS	Status A	ssigned allele	
submitter: Joe Bloggs, University	UK322		ITGGC ACATCAGAAATTGTGGATAA	 ✓ 	rejected 👻		
datestamp: 2015-06-23	UK323		ITGGC ACATCAGAACTTGTGGATAA	 ✓ 	rejected 👻		
status: pending	UK347	924 ATGCTGCAAAGAACT	ITGGC ACATCAGAAATTCTGGATAA	 ✓ 	rejected 👻		
outcome: rejected - data not uploa	hahe					Update	
locus: NEIS0001							
_	Message				hive		
U 1772		estamp User	Message		e of submissio	n and any suppo	orting files:
technology: Illumina	2015-06-2	3 07:44:40+00 Keith Jolley	These sequences are not NEIS0001 a	Down	load TAR		
read length: 100-199							
coverage: 20-49x				Act	ion		
assembly: de novo							
assembly software: Velvet			Add mess	sage Clo	se submission		

7.2 Profiles

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Logged in: Keith Jolley (keith). @Log out Change password
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_20150623105542_5928_87752 2015-06-23 2015-06-23 Joe Bloggs MLST 3
Return to index page

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

	eny: Sequences Batch sequences Co wnload: Alleles MLST profiles ks: Contents Home PorA FetA Optic h). &Log out Change password					atch p	rofile	s List	t Brov	vse Query			
Curate submis	ssion												
— Summary	b_20150623105542_5928_87752 profiles Joe Bloggs, University of Oxford, UK 2015-06-23 pending	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 —	.d Add message
Archive Archive of submission Download	and any supporting files:												

7.2.1 Individual profile curation

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

Query: Sequences Batch sequences Co Download: Alleles MLST profiles Links: Contents Home PorA FetA Opti				latch p	rofile	s Lis	t Brov	vse Quer	/			
Logged in: Keith Jolley (keith). I Log out Change password												
Curate submission												
Submission: BIGSdb 20150623105542 5928 8775	2											
	- Profiles											
Summary	Identifier adk	abo7	aroF	fumC	adb	ndbC	nam	Status		Assigned ST		
type: profiles	UK32 43	2	12	32	32	3	2	pending		Curate		
submitter: Joe Bloggs, University of Oxford, UK	UK33 7	56	4	3	2	12	12	pending	_	Curate 3		
datestamp: 2015-06-23	UK34 76	3	5	3	87	43	34	pending	•	Curate 3		
status: pending	Batch curate									Update		
Archive of submission a	nd any supportin	a files	c									
		-										
Download TAR												
Add message												

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 L	Database: Species home Curator's page (species) Curator's page (database) Jsers: Add Query/update .oci: Add ILST profiles: Add Query/update Batch insert		
Logged in: Keith Jolley (ke	eith). I@Log out Change password	Help 🖉	Toggle: 🚯
Add new ML	ST profile		
Please fill in the fields	below - required fields are marked with an exclamation mark (!).		
Record			
ST: !	10024		
adk: !			
abcZ: !	2 4		
aroE: !	2 4 12 4 32 4 V		
fumC: !	32 *		
gdh: !	32		
pdhC: !	3 *		
pgm: !	2		
sender: !	Bloggs, Joe (jbloggs)		
clonal_complex:			
curator: !	Keith Jolley (keith)		
date_entered: !			
datestamp: !	2015-06-23		
PubMed ids:			
Action			
Reset Subr	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). DLog out Change password	Help 🖉	Toggle: 🚯
Add new MLST profile		
ST-10024 added!		
Return to submission Add another Back to main page		

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

Query: Sequences Batch sequences Co Download: Alleles MLST profiles Links: Contents Home PorA FetA Option					atch p	rofile	s List	Bro	wse Query			
Logged in: Keith Jolley (keith). Hog out Change password												
Curate submission												
Submission: BIGSdb_20150623105542_5928_8775;	2 — Profiles											
	Identifier		aba7	oroF	fumC	adb	ndhC	Dam	Status	Assigned ST	-	
type: profiles	UK32	43	2	12	32	32	3	pgin 2	assigned	10024		
submitter: Joe Bloggs, University of Oxford, UK	UK33	7	56	4	3	2	12	12	pending 👻	Curate		
datestamp: 2015-06-23	UK34	76	3	5	3	87	43	34	pending 👻	Curate 3		
status: pending	Batch cu	irate								Update		
Messages — Archive —												
Archive of submission a	nd any supp	orting	; files	:								
Download 🕞		-										
Add message												

7.2.2 Batch profile curation

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

Query: Sequences Batch sequences Co Download: Alleles MLST profiles Links: Contents Home PorA FetA Option				Batch p	orofile	s List	t Bro	wse Query		
Logged in: Keith Jolley (keith). Hog out Change password										
Curate submission										
Submission: BIOSdb 20150502105540 5000 0775	,									
Submission: BIGSdb_20150623105542_5928_8775										
Summary	Profiles									
type: profiles	Identifier a UK32 4			fumC 32	gdh 32	pdhC 3	pgm 2		Assigned ST 10024	
submitter: Joe Bloggs, University of Oxford, UK		32 56	12	32	2	12	12	assigned	Curate	
datestamp: 2015-06-23		6 3	5	3	87	43	34	pending +	Curate	
status: pending	Batch cura	te							Update	
Archive of submission a	nd any suppo	ting file	s:							
Download TAR										
AL DOWNOOD TAK										
Add message										

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		ers: Add C ci: Add	ecies home Query/update :: Add Quer	e		es) Curator's page	database)	
Logged in: M	eith Jolley (kei	th). 🕩 Log ou	t Change pa	ssword				Help 🗹 🛛 Toggle: 🚯
Batch	insert l	ILST	profile	S				
• Fie • Yo it f	eld header na u can choose or each profile ownload tab-d	mes must l whether or record. elimited he	be included r not to inclue ader for you	and fields c de a ST field r spreadshi	an be in any 1 - if it is omi	i from a spreadsheet order. Optional field tted, the next availab ste Special © Text to	s can be omitted if y e ST will be used a	ou wish. utomatically. If however, you include it in the header line, then you must also provide
	wnload subn				der line) —			- Parameters -
716as	abcZ 56 3	aroE 4 5	text (Include func 3 3	gdh 2 87	der inte, pdhC 12 43	pgm 12 34		Sender: Bloggs, Joe (jbloggs) Value will be overridden if you include a sender field in your pasted deta. 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). I+Log out Change password	Help 🖉	Toggle: 🜖
Batch insert MLST profiles		
Database updated ok		
Return to submission Back to main page		

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

Logged in: Keith Jolley (keit Curate submis	h). GeLog out Change password		
Submission: BIGSd — Summary—	b_20150623105542_5928_8775	2	Messages —————
submitter: datestamp:	profiles Joe Bloggs, University of Oxford, UK 2015-06-23 pending	Identifier adk abcZ aroE fumC gdh pdhC pgm Status Assigned ST UK32 43 2 12 32 3 2 assigned 10024 UK33 7 56 4 3 2 12 12 assigned 10025 UK34 76 3 5 3 87 43 34 assigned 10026	.d Add message
		Download TR	

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 (keith). 🖗 Log out Change password													
Curate submission													
— Summary — type:	Ib_20150623105542_5928_8775; profiles Joe Bloggs, University of Oxford, UK	Profile: Identifie UK32	r <mark>adk</mark> 43	2	12	32	32	3	2	rejected 👻	Assigned ST	Messages —	
datestamp: status:	2015-06-23 pending accepted - data uploaded	UK33 UK34 Batch of Archive of Download	subm	56 3 ission	4 5 and a	3 3 any su	2 87 Jpport		12 34	rejected • rejected •	Curate Curate Update	(.ii Add message

7.2.4 Closing the submission

You can add a message to the submitter by entering it in the message box and clicking 'Add message'. 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 Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database															
Logged in: Keith Jolley (keith). @Log out Change password															
Curate submi	ssion														
Submission: BIGSd	b_20150623105542_5928_8775	2													
		-Profiles											_		
type	profiles	ldentifier adk abcZ aroE fumC gdh pdhC pgm Status Assigned ST													
	Joe Bloggs, University of Oxford, UK	UK32	43	2	12	32	32	3	2	rejected					
datestamp:	2015-06-23	UK33 UK34	7	56 3	4	3	2 87	12 43	12 34	rejected rejected	_				
	pending	01104	10	Ŭ	Ŭ		07	40	04	rejected	•	Update			
outcome:	rejected - data not uploaded											Opuale			
		Messag	·												
			nesta 23 10:		+00	Use Keith I		You n	eed to	submits	me	Message representative	isolate da	ta for this n	rofiles
		2013 00	25 10.	42.00		i tonin o	oney	louin		Submit S	, inc i	representative	isolate de	na ior ano p	ionico.
															.a
														Add mes	sage
Archive	Action -		_												
Archive of submission	and any supporting files: Close s	ubmission													
Download TAR	Download 🔜														

7.3 Isolates

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

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications
Links: Contents Home Options Profiles/sequences definitions Database submissions
Logged in: Keith Jolley (keith). [+Log out Change password
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
New isolate submissions waiting for curation
Your account is authorized to handle the following submissions:
Submission id Submitted Updated Submitter Isolates
BIGSdb_20150623132929_11187_32555 2015-06-23 2015-06-23 Joe Bloggs 2
Return to index page

You will see a table summarizing the submission.

Publications Database submissions													
Logged in: Keith Jolley (keith). @Log out Change password													
Curate submission													
Submission: BIGSdb_20150623132929_111	87_32555												
type: isolates submitter: Joe Bloggs, University of Oxf	ord LIK												
datestamp: 2015-06-23	JIU, OK												
status: pending													
Isolates													
isolate country year disease		serogroup ab											
UK233 UK 2015 meningitis and septicaemia UK322 UK 2014 meningitis	CSF Neisseria meningitidis blood Neisseria meningitidis	B 2	3 4	3 8	4 6	F1-5 F1-5	5	2					
Batch curate						status: pe	-						
								opullo					
Messages Archive Archive													
Archive of subr	nission and any supporting files:												
Download TAR													
Add message													
Add message													

Click the 'Batch curate' button.

Publications Database submissions													
Logged in: Keith Jolley (keith). @Log out Change password													
urate submission													
Submission: BIGSdb 20150623132929 11187 32555													
Summary													
type: isolates													
submitter: Joe Bloggs, University of Oxford, UK													
datestamp: 2015-06-23 status: pending													
otatos, pending													
- Isolates													
isolate country year disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2													
UK233 UK 2015 meningitis and septicaemia CSF Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2 UK322 UK 2014 meningitis blood Neisseria meningitidis B 2 3 17 3 8 4 6 F1-5 5 2													
Batch curate Record status: pending VDB													
Messages Archive Archive													
Archive of submission and any supporting files:													
Download 🕞													
Add message													
nau moody.													

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.

PTIDITIST Users: Add Query/update Isolates: Add Query/update Batch insert													
Logged in: Keith Jolley (keith). Dog out	Change password			Toggle: 🚯									
Batch insert isolates	s												
 Enter aliases (alternative na Enter references for your iso You can also upload allele fi locus names). These will be You can choose whether or it 	e included and fields can be in any imes) for your isolates as a semi- olates as a semi-colon (.) separater ields along with the other isolate da a added with a confirmed status an not to include an id number field - if ader for your spreadsheet - use 'Par plate (xlsx format) ist below:	order. Optional fields can olon (;) separated list d list of PubMed ids (non- tat - simply create a new o d method set as 'manual' it is omitted, the next ava ste Special O Text' to past	nteger ids will be ignored). column with the locus name i lable id will be used automa e the data.	(see the 'allowed_loci' tab in the Excel template for attically.									
isolate country year aroE fumC gdh UK233 UK 2015 meningitidis B F1-5 5 2 UK322 UK 2014 2 3 17	-	s serogroup R PorA_VR1 emia CSF 3 8 Neisseria mening 6 F1-5	abcZ adk PorA_VR2 Neisseria 4 6 pitidis B 5 2-1	Reset Submit									
Back													

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

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



7.3.1 Closing the submission

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

Publ	Cuery: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions																
Logged in	.ogged in: Keith Jolley (keith). [+Log out Change password																
Curate submission																	
Submission: BIGSdb 20150623132929 11187 32555																	
	Summary																
	type: isolates submitter: Joe Bloggs, University of Oxford, UK																
				Joe Bloggs, Universit 2015-06-23	y of Oxford	1, UK											
				pending													
	lates																
isola UK2		ountry UK	year 2015	disease meningitis and	source CSF	species Neisseria	serogroup	abcZ 2	adk 3	aroE 4	fum(3	gdh 8	pdhC 4	pgm 6	FetA_VR F1-5	PorA_VR1 5	PorA_VR2 2
UNZ	55	UK	2013	septicaemia	001	meningitidis	0	2	5	-	5	Ů	-		11-5	5	2
UK3	22	UK	2014	meningitis	blood	Neisseria meningitidis	В	2	3	17	3	8	4	6	F1-5	5	2-1
Bat	ich ci	urate											R	ecord s	status: ad	ccepted 👻	Update
— Me	ssag	jes —			/e												
				Archive	ofsubmis	sion and any sup	porting files:										
				Downlo	ED he												
			Add me	essage													

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

Pul	Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions																
Logged	Logged in: Keith Jolley (keith). @Log out Change password																
Cura	Curate submission																
Subi	Submission: BIGSdb 20150623132929 11187 32555																
	Summary																
			type: i: ittor: I	solates loe Bloggs, Universit	v of Oxford	шк											
	(2015-06-23	y or Oxford	, or											
		sta	atus: p	ending													
	olate																
		s country	voar	disease	source	species	Serogroup	ahc7	adk	aroE	fum(adb	ndhC	nam			PorA VR2
	233	UK	2015	meningitis and septicaemia	CSF	Neisseria meningitidis	B	2	3	4	3	8	4	6	F1-5	5	2
UK	322	UK	2014	meningitis	blood	Neisseria meningitidis	В	2	3	17	3	8	4	6	F1-5	5	2-1
													Re	ecord s	status: ad	cepted 👻	Update
— N	essa	qes —		Archi	ve				Actio	n —							
		-		Archive	of submis	sion and any sup	porting files:	 Г 	Close	e subr	missio	n					
				Downlo	en De			- L				_					
				it.													
			Add me	essage													

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
SYNOPSIS
   autotag.pl --database NAME [options]
OPTIONS
-0, --missing
   Marks missing loci as provisional allele 0. Sets default word size to 15.
-d, --database NAME
```

```
Database configuration name.
-h, --help
   This help page.
-i, --isolates LIST
   Comma-separated list of isolate ids to scan (ignored if -p used).
--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.
-1, --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
    (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.
-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 Automated offline allele definition

There is a script called 'scannew.pl' in the BIGSdb scripts/automation directory. This can be used to identify new alleles from the command line. This can (optionally) upload these to a sequence definition database.

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

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

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

scannew.pl --database <database configuration>

where <database configuration> is the name used for the argument 'db' when using the BIGSdb application.

If you have multiple processor cores available, use the –threads option to set the number of jobs to run in parallel. Loci for scanning will be split among the threads.

The script must be run by a user that can both write to the log file and access the databases, e.g. the 'bigsdb' user (see 'Setting up the offline job manager').

A full list of options can be found by typing:

```
scannew.pl --help
NAME
scannew.pl - BIGSdb automated allele definer
SYNOPSIS
scannew.pl --database NAME [options]
```

```
OPTIONS
-a, --assign
    Assign new alleles in definitions database.
-A, --alignment INT
   Percentage alignment (default: 100).
-B, --identity INT
   Percentage identity (default: 99).
-c, --coding_sequences
   Only return complete coding sequences.
-d, --database NAME
   Database configuration name.
-h, --help
   This help page.
-i, --isolates LIST
    Comma-separated list of isolate ids to scan (ignored if -p used).
--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.

-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.
```

8.3 Cleanly interrupting offline curation

Sometimes you may wish to stop running autotagger or allele autodefiner jobs as they can be run for a long time and as CRON jobs. If these are running in single threaded mode, the easiest way is to simply send a kill signal to the process, i.e. identify the process id using 'top', e.g. 23232 and then

```
kill 23232
```

The scripts should respond to this signal within a couple of seconds, clean up all their temporary files and write the history log (where appropriate). Do not use 'kill -9' as this will terminate the processes immediately and not allow them to clean up.

If these scripts are running using multiple threads, then you need to cleanly kill each of these. The simplest way to 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

8.4 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 if isolate already has sequences 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'.
-s, --sender ID
    Sender id number.
```

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.

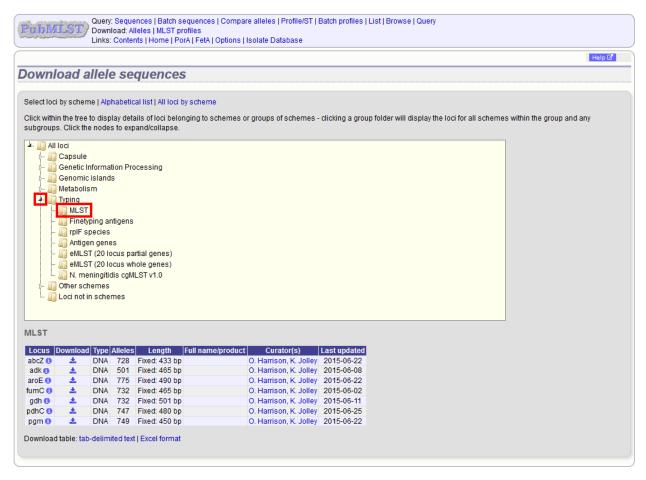
9.1 Allele sequence definitions

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.



Click the download link for the required locus

Locus	Download	Туре	Alleles	Length	Full name/product	Curator(s)	Last updated
abcZ 🕕	*	DNA	728	Fixed: 433 bp		O. Harrison, K. Jolley	2015-06-22
adk 🕦	<u>له</u>	DNA	501	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-08
aroE 🚺	*	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 📵	<u>له</u>	DNA	747	Fixed: 480 bp		O. Harrison, K. Jolley	2015-06-25
pgm 🕕	*	DNA	749	Fixed: 450 bp		O. Harrison, K. Jolley	2015-06-22

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

>fumC_1

GCCTACAACCTCTTGCAATCCATCCGCCTGTTGGGCGACGCGTGCAACAGCTTCAACGAA
CACTGCGCCGTCGGCATTGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC
CTGATGCTCGTTACCGCGTTAAACCGCAAAATCGGTTACGAAAAC
>fumC_2
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGG
TTGGGCGAAATCAAAATCCCCGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT
ACCATCGGCATGGCGGGCGCGCCGGGCAATTTCGAGCTGAACGTCTATATGCCCGTTATC
GCCTACAACCTCTTGCAATCCATCCGCCTCTTGGGCGACGCGTGCAACAGCTTCAACGAA
CACTGCGCCATCGGCATCGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC
CTGATGCTCGTTACCGCGTTAAACCGCAAAATCGGTTACGAAAAC
>fumC_3
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGG
TTGGGCGAAATCAAAATCCCCGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT
ACCATCGGCATGGCGGGCGCGCCGGGCAATTTCGAGCTGAACGTCTATATGCCCGTTATC
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.

Li	nks: Cont	ents H	lome I	PorA FetA Options Isolate Dat	tabase		
							He
ownload all	ele se	eaue	ence	25			
elect loci by scheme	Alphabol	lical list		i by achoma			
election by scheme	Alphabel	ucarnst	PAILIO	a by scheme			
Locus	Download		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] ()	٤.	DNA	477	Variable: (1563 min; 1641 max)	dihydrolipoamide acetyltransferase (EC 2.3.1.12)		2015-05-19
ackA2 [NEIS1727] 🕕	±	DNA	408	Variable: No limits set	acetate kinase		2015-05-20
acnA [NEIS1729] 🕕	±	DNA	527	Variable: No limits set	aconitate hydratase 1 (EC 4.2.1.3)		2015-05-20
acnB [NEIS1492] ()	±	DNA	476	Variable: No limits set	aconitate hydratase 2 (EC 4.2.1.3)		2015-05-19
adhA [NEIS0486] ()	±	DNA	614	Variable: No limits set	alcohol dehydrogenase		2015-05-17
adhC [NEIS1241] 🕦	±	DNA	239	Variable: No limits set	alcohol dehydrogenase		2015-05-20
adk 🕕	±	DNA	501	Fixed: 465 bp		O. Harrison, K. Jolley	2015-06-08
adk [NEIS0767] ()	*	DNA	208	Variable: No limits set	adenylate kinase		2015-05-18
aldA [NEIS1942] 🕕	*	DNA	447	Variable: No limits set	aldehyde dehydrogenase		2015-05-20
aniA [NEIS1549] 🕕		DNA	0	Variable: No limits set	nitrite reductase, major outer membrane copper-containing protein		
anmK [NEIS1788] 🕕	*	DNA	480	Variable: No limits set	anhydro-N-acetylmuramic acid kinase	A. Jamet	2015-05-20
apaH [NEIS0610] 🕦	±	DNA	116	Variable: No limits set	diadenosine tetraphosphatase		2015-05-17
argH [NEIS0580] 🕕	*	DNA	433	Variable: No limits set	argininosuccinate lyase		2015-05-18
aroE 🕕	*	DNA	775	Fixed: 490 bp		O. Harrison, K. Jolley	2015-06-22
aroE [NEIS1810] 🕕	*	DNA	305	Variable: No limits set	shikimate dehydrogenase		2015-05-21
aspA 🕕	±	DNA	189	Fixed: 432 bp		K. Jolley	2015-04-21
aspA [NEIS1185] 🕕	±	DNA	501	Variable: No limits set	aspartate ammonia-lyase		2015-05-20
atIA [NEIS2274] ()	<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.

PubM	LST	Down	load: Al	leles N	/LST pr					Batch pi	rofiles List Browse Query					
																Help 🗗
Downlo	oad a	allel	e se	quei	nces	5										
Select loci I	by scher	me Alp	habetic	al list /	All loci t	y scheme										
MLST																
IVILSI																
Locus D	ownload	d Type	Alleles	Len	igth	Full name/p	oroduct	Cura	tor(s)	Lastur	odated					
abcZ 🕕	*	DNA	728	Fixed: 4	433 bp		C). Harrisc	on, K. Jolle	y 2015-i	06-22					
adk 📵	*	DNA		Fixed: 4					on, K. Jolle							
aroE 🕕	±	DNA		Fixed: 4					on, K. Jolle							
fumC 📵	*	DNA	732	Fixed: 4					on, K. Jolle							
gdh 🕕	±	DNA	732	Fixed:					on, K. Jolle	-						
pdhC 🕕	*			Fixed: 4					on, K. Jolle							
pgm 🕕	*	DNA	749	Fixed: 4	450 bp		C). Harrisc	on, K. Jolle	y 2015-i	06-22					
Finetypin	Down	load	Type /			Length e: No limits :		l name/pr variable r			Last updated 2015-06-16					
PorA VR2	0 1	L p	eptide	735	Variable	e: No limits	set PorA	variable r	region 2	K. Jolley	2015-06-16					
FetA VR 👩) 2	e p	eptide	581	Variable	e: No limits	set		1	Feavers	2015-06-26					
rpIF spec		Type A	lleles	Leng	ıth	Full r	name/pro	duct	Curat	or(s) las	t updated					
rpIF 6						50S ribosom										
ADP-hept	tose b	iosynt	hesis													
		Dave	mload	Type Al	leles	Lengt	th			Full nam	e/product	Aliases	_	Curator(s)	Last updated	
Loc	us	Dow	moau													
Loc NEIS0769						ariable: No l			D-beta-D	heptose-	7-phosphate kinase	NMB0825; NMC0	769; rfaE	C. Kahler	2015-05-18	
	9 (hldA)	0	*	DNA :	244 V	_	limits set				7-phosphate kinase eptose epimerase	NMB0825; NMC0 NMB0828; NM			2015-05-18 2015-05-17	
NEIS0769	9 (hldA) 8 (hldD)	0	* *	DNA :	244 V 311 V	/ariable: No /ariable: No	limits set limits set		ADP-D-	beta-D h		NMB0828; NM	C0773		2015-05-17	
NEIS0769 NEIS0773	9 (hidA) 3 (hidD) (gmhB)	0 0 0	* * *	DNA CONA	244 V 311 V 216 V	/ariable: No /ariable: No	limits set limits set limits set	D-alpha	ADP-D- beta,D-He	beta-D h ptose 1,7	eptose epimerase	NMB0828; NM	C0773 C2014	C. Kahler C. Kahler	2015-05-17	

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.

🕨 🛄 G										
	Senetic In	nformati	ion Pro	cessing						
🕒 🗠 🛄 G	Genomic	islands								
👘 🖳 M	/letabolis	m								
👘 🧍 T	Typing									
- I F 🛽	MLST									
- 7	Finety	ping ant	tigens							
	rpIF sp	pecies	-							
	Antige	n genes	5							
- I L]	eMLS1	- T (20 loc	cus pa	rtial genes)						
				ole genes)						
	N. mei									
	Other sch	_	lo ogin	201110						
	_oci not ir									
			les							
···· 🚛 L										
🦓 L										
<u>aj</u> L										
MLST										
MLST		Tupo	Violos	Longth	Full name/product	Curator(e)	Last undated	 		
MLST	ownload				Full name/product	Curator(s)	Last updated			
MLST Locus Do abcZ ()	ownload	DNA	728	Fixed: 433 bp		O. Harrison, K. Jolley	2015-06-22			
MLST Locus Do abcZ () adk ()	ownload	DNA DNA	728 501	Fixed: 433 bp Fixed: 465 bp		O. Harrison, K. Jolley O. Harrison, K. Jolley	2015-06-22 2015-06-08			
MLST Locus Do abcZ () adk () aroE ()	ownload * *	DNA DNA DNA	728 501 775	Fixed: 433 bp Fixed: 465 bp Fixed: 490 bp		O. Harrison, K. Jolley O. Harrison, K. Jolley O. Harrison, K. Jolley	2015-06-22 2015-06-08 2015-06-22			
MLST Locus Do abcZ () adk () aroE () fumC ()	ownload * * * *	DNA DNA DNA	728 501 775 732	Fixed: 433 bp Fixed: 465 bp		O. Harrison, K. Jolley O. Harrison, K. Jolley	2015-06-22 2015-06-08 2015-06-22 2015-06-02]	
MLST Locus Do abcZ () adk () aroE ()	ownload ± ± ± ±	DNA DNA DNA DNA	728 501 775 732 732	Fixed: 433 bp Fixed: 465 bp Fixed: 490 bp Fixed: 465 bp		O. Harrison, K. Jolley O. Harrison, K. Jolley O. Harrison, K. Jolley O. Harrison, K. Jolley	2015-06-22 2015-06-08 2015-06-22 2015-06-02 2015-06-11			
MLST Locus Do abcZ () adk () aroE () fumC () gdh ()	ownload * * * * * *	DNA DNA DNA DNA DNA DNA	728 501 775 732 732 747	Fixed: 433 bp Fixed: 465 bp Fixed: 490 bp Fixed: 465 bp Fixed: 501 bp		O. Harrison, K. Jolley O. Harrison, K. Jolley O. Harrison, K. Jolley O. Harrison, K. Jolley O. Harrison, K. Jolley	2015-06-22 2015-06-08 2015-06-22 2015-06-02 2015-06-11 2015-06-25			

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 Brow Download: Alleles MLST profiles Links: Contents Home Options PubMLST.org Isolate Database	vse Query
Campylobacter locus/sequence definitions database The Campylobacter PubMLST sequence definition database contains allele and profile data representing the total kn database should have a corresponding record in the isolate database.	nown diversity of <i>C. jejuni</i> and <i>C. coli.</i> 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 attributes. Brows MLST profiles List - find MLST profiles matched to entered list. Search by combinations of MLST alleles - including partial matching. Batch profile query - lookup MLST profiles copied from a spreadsheet. 	Option settings Submissions • Set general options • Manage submissions General information • Mumber of sequences: 412175 • Number of profiles (MLST): 7841 • Last updated: 2015-06-17 • Profile update history • About BIGSdb
Export Sequences - XMFA / concatenated FASTA formats Sequence similarity - find sequences most a Sequence comparison - display a comparis Locus Explorer - tool for analysing allele sequence	son between two sequences.

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
Neisseria locus/sequence definitions database	Toggle: 🕄
The Neisseria PubMLST sequence definition database contains allele and profile data representing the total known diversity of Neisseria species. Every new ST deposited in the have a corresponding record in the isolate database.	is database should
Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching attributes. Browse profiles Submissi	eral options
Export Sequences - XMFA / concatenated FASTA formats Sequence similarity - find sequences most similar to selected allele. Sequence comparison - display a comparison between two sequences. Locus Explorer - tool for analysing allele sequences stored for particular locus.	

Profiles will be downloaded in tab-delimited format, e.g.

ST	abcZ	adk	aroE	fumC	gdh	pdhC	pgm	clonal_complex
1	1	3	1	1	1	1	3	ST-1 complex/subgroup I/II

2	1	3	4	7	1	1	3	ST-1 complex/subgroup I/II
3	1	3	1	1	1	23	13	ST-1 complex/subgroup I/II
4	1	3	3	1	4	2	3	ST-4 complex/subgroup IV
5	1	1	2	1	3	2	3	ST-5 complex/subgroup III
6	1	1	2	1	3	2	11	ST-5 complex/subgroup III
7	1	1	2	1	3	2	19	ST-5 complex/subgroup III
8	2	3	7	2	8	5	2	ST-8 complex/Cluster A4
9	2	3	8	10	8	5	2	ST-8 complex/Cluster A4
10	2	3	4	2	8	15	2	ST-8 complex/Cluster A4
11	2	3	4	3	8	4	6	ST-11 complex/ET-37 complex
12	4	3	2	16	8	11	20	
13	4	10	15	7	8	11	1	ST-269 complex
14	4	1	15	7	8	11	1	ST-269 complex

Data records

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

10.1 Isolate records

An Isolate record page displays everything known about an isolate.

	reakdown: Isolate fie	rse Profile/ST List alds Scheme/alleles Publications ne Options Profiles/sequences definition	s Database submissions							
Full informat	ion on iso	late M10 240474								
Projects										
This isolate is a member of the following projects:										
		MRF Menir	ngococcus Genome Library							
The MRF Meningococo Oxford, funded by the N		is a collaboration between Public Health E Foundation.	ngland, The Wellcome Trust Sar	nger Institute and the University of	À					
		be cited in any publication or presentation	making use of it.		Meningitis 🛃					
	,		Ū.		Research Foundation					
			899_MRF							
MRF-MGL isolates epi	years 2010/2011 to	2011/2012 excluding Northern Ireland								
	_	E&W	_genogroup_B_MRF							
All MRF Meningococcu	us Genome Library (genogroup B isolates from England and Wa								
	udine Marthana Inda	-1	MRF_no_NI							
All MRF genomes excl	uding Northern Irela	na								
Provenance/meta	data									
id:	18968		species:	Neisseria meningitidis						
id: isolate:	18968 M10 240474	72 0. 07 000 (+-000)	serogroup:	В						
id: isolate: strain designation:	18968 M10 240474 B: P1.19-1,15-11: F	^{-3-9:} ST-269 (cc269)	serogroup: ENA accession:	B ERR086224 → www.ebi.ac.uk						
id: isolate:	18968 M10 240474 B: P1.19-1,15-11: F UK	⁻ 3-9: ST-269 (cc269)	serogroup: ENA accession: sender:	В	(E-mail:					
id: isolate: strain designation: country: continent:	18968 M10 240474 B: P1.19-1,15-11: F UK	⁻ 3-9: ST-269 (cc269)	serogroup: ENA accession: sender: curator:	B ERR086224 → www.ebi.ec.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk)	(E-mail:					
id: isolate: strain designation: country: continent: region: year:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010	F3-9: ST-269 (cc269)	serogroup: ENA accession: sender: curator: update history:	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates_show details	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011		serogroup: ENA accession: sender: curator: update history: date entered:	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates_show details	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010		serogroup: ENA accession: sender: curator: update history: date entered:	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011		serogroup: ENA accession: sender: curator: update history: date entered:	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bln	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi	ied/other)	serogroup: ENA accession: sender: curator: update history: date entered: datestamp:	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi	ied/other) N90:	serogroup: ENA accession: sender: curator: update history: date entered:	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bin contigs:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi 275 2195045 bp	ied/other) N90:	serogroup: ENA accession: sender: curator: update history: date entered: datestamp: 6405 3513	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bin contigs: total length: max length: mean length:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi 275 2195045 bp 109859 bp 7982 bp	ied/other) N90: N95:	serogroup: ENA accession: sender: curator: update history: date entered: datestamp: 6405 3513	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bin contigs: total length: max length: mean length:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi 275 2195045 bp 109859 bp	ied/other) N90: N95: Ioci tagged:	ENA accession: ENA accession: sender: curator: update history: date entered: datestamp: 6405 3513 1611	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bin contigs: total length: max length: mean length: N50:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi 275 2195045 bp 109859 bp 7982 bp	ied/other) N90: N95: Ioci tagged:	ENA accession: ENA accession: sender: curator: update history: date entered: datestamp: 6405 3513 1611	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bin contigs: total length: max length: max length: N50:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi 275 2195045 bp 109859 bp 7982 bp	ied/other) N90: N95: loci tagged: detailed breakdown:	ENA accession: Sender: curator: update history: date entered: datestamp: 6405 3513 1611 Display	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bin contigs: total length: max length: max length: N50: Schemes and loci	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi 275 2195045 bp 109859 bp 7982 bp	ied/other) N90: N95: Ioci tagged:	ENA accession: Sender: curator: update history: date entered: datestamp: 6405 3513 1611 Display	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bin contigs: total length: max length: max length: N50:	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi 275 2195045 bp 109859 bp 7982 bp 34308	ied/other) N90: N95: loci tagged: detailed breakdown:	ENA accession: Sender: curator: update history: date entered: datestamp: 6405 3513 1611 Display	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bln contigs: total length: max length: max length: N50: Schemes and loci	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi 275 2195045 bp 109859 bp 7982 bp 34308	ied/other) N90: N95: loci tagged: detailed breakdown:	ENA accession: Sender: curator: update history: date entered: datestamp: 6405 3513 1611 Display	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bin contigs: total length: max length: max length: N50: Schemes and loci	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi 275 2195045 bp 109859 bp 7982 bp 34308	ied/other) N90: N95: loci tagged: detailed breakdown:	ENA accession: Sender: curator: update history: date entered: datestamp: 6405 3513 1611 Display	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					
id: isolate: strain designation: country: continent: region: year: epidemiological year: disease: Sequence bln contigs: total length: max length: max length: N50: Schemes and loci	18968 M10 240474 B: P1.19-1,15-11: F UK Europe South East 2010 07/2010-06/2011 invasive (unspecifi 275 2195045 bp 109859 bp 7982 bp 34308	ied/other) N90: N95: loci tagged: detailed breakdown:	ENA accession: Sender: curator: update history: date entered: datestamp: 6405 3513 1611 Display	B ERR086224 → www.ebi.ac.uk Dorothea Hill Dorothea Hill, University of Oxford, UK dorothea.hill@zoo.ox.ac.uk) 103 updates show details 2012-02-15	(E-mail:					

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

10.1.1 Projects



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

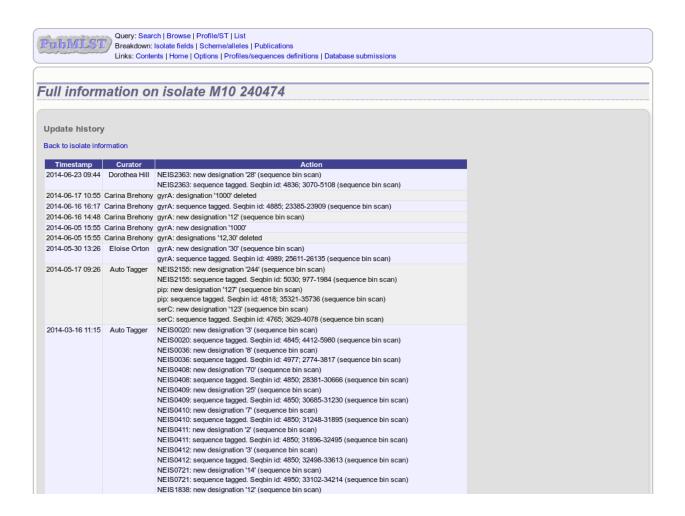
10.1.2 Provenance metadata

Provenance/meta	data		
id:	18968	species:	Neisseria meningitidis
isolate:	M10 240474	serogroup:	В
strain designation:	B: P1.19-1,15-11: F3-9: ST-269 (cc269)	ENA accession:	ERR086224 → www.ebi.ac.uk
country:	UK	sender:	Dorothea Hill
continent:	Europe	curator:	Dorothea Hill, University of Oxford, UK (E-mail:
region:	South East		dorothea.hill@zoo.ox.ac.uk)
year:	2010	update history:	103 updates show details
epidemiological year:	07/2010-06/2011	date entered:	2012-02-15
disease:	invasive (unspecified/other)	datestamp:	2014-06-23

This section includes:

- provenance fields
- · housekeeping data
 - who sent the isolate
 - who last curated
 - record creation times
 - last update times
 - links to update history

The update link displays page with exact times of who and when updated the record.



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 [578 isolates]
- Didelot X, Urwin R, Maiden MC, Falush D (2009). Genealogical typing of Neisseria meningitidis. Microbiology 155:3176-86 93 isolates
- Jolley KA, Sun L, Moxon ER, Maiden MC (2004). Dam inactivation in Neisseria meningitidis: prevalence among diverse hyperinvasive lineages. BMC Microbiol 4:34 [24 isolates]
- Jolley KA, Wilson DJ, Kriz P, McVean G, Maiden MC (2005). The influence of mutation, recombination, population history, and selection on patterns of genetic diversity in Neisseria meningitidis. Mol Biol Evol 22:562-9 [378 isolates]
- Maiden MC, Bygraves JA, Feil E, Morelli G, Russell JE, Unvin R, Zhang Q, Zhou J, Zurth K, Caugant DA, Feavers IM, Achtman M, Spratt BG (1998). Multilocus sequence typing: a portable approach to the identification of clones within populations of pathogenic microorganisms. Proc Natl Acad Sci U S A 95:3140-5 107 isolates
- Thompson EA, Feavers IM, Maiden MC (2003). Antigenic diversity of meningococcal enterobactin receptor FetA, a vaccine component. Microbiology 149:1849-58
 Torisolates
- Unvin 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 	 adk aroE 0 S 15 S	fumC 9S	gdh 8 S	pdhC 11 S	pgm 9 S	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.

	uery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query winkoad: Alleles MLST profiles
	Window Andrea International Andrea
Allolo inform	ation - abcZ: 2
Provenance/meta	data
locus:	abcZ i
allele:	2
	TITGATACCS TIGCCGAAGG TITGGGTGAA ATTCGCGATI TATTGCGCCG TIACCACCGC GICGGCCAIG AGTGGAAAA CGGTICGGGI GAGGCTITGI IGAAAGAACT CAACGAATAA CAACTIGAAA ICGAAGCGAA GGACGGCCTGS AAGCTGGAIG CGGCASICAA GCAGACTITG GGGGAACICG GITIGCCGGA AAACGAAAAA AICGGCAACC TITCCGGCGG ICAGAAAAAG CGTGICGCCI IGGCGAAGCCIAGA AGACCGGACCAA TATTGCIGCI GGACGAACCG ACCAACCATI IGGATAICGA CGCGAITAIT IGGCIGGAAA AICTGCICAA AGCGIIGAA GGCAGCIIGG IIGIGAIACC CACGACCGC CGIIIIIIGG ACAATAICGC CACGCGGAIT GICGAACICG AIC
length:	433
status:	Sanger trace checked
date entered:	2001-02-07
datestamp:	2009-11-11
sender:	Keith Jolley, University of Oxford, UK
curator:	Man-Suen Chan, University of Oxford (E-mail: man-suen.chan@paediatrics.ox.ac.uk)
Profiles containin	g this allele
MLST:	993 profiles
Isolate databases	
	Contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in the profiles database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample. [5041 isolates]

If the allele is a member of a scheme profile, e.g. MLST, this will be listed. In this case, there will be a button to display all profiles of that scheme that contain the allele.

Similarly, if a *client database* has been setup for the database and the allele has been identified in an isolate, there will be a button to display all isolates that have that allele.

10.3 Sequence tag records

PubMLST/B	uery: Search Browse Profile/S reakdown: Isolate fields Schem inks: Contents Home Options		base submissions							
IEIS0346 alle	ele sequence: id-	8968								
Contig position										
sequence bin id: contig length: start:		length: orientation: complete:	forward							
end:	14607	method	Illumina							
Sequence										
SATGIGGIIG AAGCGGG AGIGIIGGAA ACAACCO IAIGGIIIAC GGGCAAO CGCAAAIGCG CIGGAAO CGCCCGGCIG IIGCGCO	SGAG CCGTCGTCCT GCCGTCCGCJ SCCG TACATACGCG CAAACCCGCC CTGT TCCACGGAAA AGCGGGTGTC CAAA CCGCCCGCGA ACTCGACGG	 GANAAACTAT TACCETACAS CCEACE ACATTECCEG ANAGECCEAC ACANAT CCTEGAACEG ANAGECCTCT GTCCEG CEGCTCEACA ATATACTCAN AGECET TGECCEGCAC CCECCETCT GTTCCT TGECAGACEC TCAAGEAGECT CAACE CCTC 	CCGC CCGCAAAAGC CGTT TCAGACGGCA AGGG CTCGATGCCG CGGA CAGGCGTTTG	AAACCGTCCT C TCGCCCCCGT T CCTATGTCCA C TCAAACCGGA A	AGCATTCCG CCCGCCGCT AAAACCTGT CGGCAGGCG	CAGCGTCCGT TCGGGCATAA TGGGTGAAAA ATGATTGAAA	CCGAACAGCA CCAAACTIGC CCGCCGCCGT CTITGTGCGC	TACCGGTCAG (CGTTGTCAGC (CGGCAACCCG) CGGCCGCCCC ?	GCACGGCTCA : CIGIGICCGC (AIGCCGICIG : IICTICAICA :	AAACCATGAA CGACCGAGGA AAGCGGCAAT ICGACCATCC
Translation										
T V F L Y 1 CACTGTAC : V K M L S C Y J	R G A R L Q H C G A A H G F S I A (CGCGGCGCACGCGTCAGCATTCGCG 	A G G K T I I V Q P Q A E K L L P Y S R GCAGCGGAAAACTATTACCGTACAGCC 	R N R R D G K T E GACGGIAAAACCGAA : A G S R R R G A V V G E P S S	CRLN DAVLM GATGCCGTCTTAA 	EKI TGGAGAAAAT 	F2 F3 100 F1 F2 F3				
K P I S P K A R 201 AAAGCCCC	D T N P P A K A N T Q I R P Q K Q T H K S A R K S K SACACADATCCGCCCCGCADAAGCAD	R P Q H S A A S V R V L S I P Q R P S P S S A F R S V R P COCTOCTACGATICOGRACETCOCTOC -:	TAYRS EQHTG NSIPV GAACAGCATACCGGT	G T A Q Q A R L K R H G S I CAGGCACGGCTCA	N H E T M K K P * K AAACCATGAA					

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) Do	ery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query wnload: Alleles MLST profiles ks: Contents Home PorA FetA Options Isolate Database
Profile inform	ation for ST-11 (MLST)
ST abcZ adk ar	roE fumC gdh pdhC pgm clonal complex
11 2 3	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: 2	2009-11-11
Client database	
	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. (2009 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

-surrent mil	Links: Conte	Isolate fields Scheme/ ents Home Options P	Profiles/sequences de	innuons Database sub	missions						
											Toggle
equen	ce bin for N	/10 240474									
ontig sum	nmary statistics		Contig size	distribution	Cumulative cont	tig lengt	h				
 Total le Minimu Maximu Mean l σ lengt N50: 3 N90: 6 N95: 3 	6405		Click to enlarg	je oad lengths							
	load sequences (FAS load sequences with	STA format) annotations (EMBL form		oudrongino							
• Downl	load sequences with	annotations (EMBL form	mat)	-	Locus	Start	End	Direction	EMBL format	Artemis 🖬	
• Downl		annotations (EMBL forn Original de	mat) esignation	Length Comments	Locus NEIS1151	Start 488	End		EMBL format		
• Downl	load sequences with Sequencing method	annotations (EMBL form	mat) esignation	Length Comments				Direction	EMBL format	Artemis i Artemis	
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151	488	1144	← ←			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150	488 1141	1144 2913	←			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149	488 1141 3155	1144 2913 3733	$\begin{array}{c} \leftarrow \\ \leftarrow \\ \rightarrow \end{array}$			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149 NEIS1148	488 1141 3155 3896	1144 2913 3733 4513	$\begin{array}{c} \downarrow \\ \downarrow \\ \uparrow \\ \uparrow \end{array}$			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147	488 1141 3155 3896 4521	1144 2913 3733 4513 5384	1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1 +			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146	488 1141 3155 3896 4521 5397	1144 2913 3733 4513 5384 5831	1 + + + 1 1 + + + 1			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146 NEIS1145	488 1141 3155 3896 4521 5397 6141	1144 2913 3733 4513 5384 5831 6869	$\downarrow \downarrow \uparrow \uparrow \uparrow \downarrow \downarrow \uparrow$			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146 NEIS1145 NEIS1144 NEIS1143 NEIS1142	488 1141 3155 3896 4521 5397 6141 6892 8005 9288	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541	1 + + + + + + + + + + + + + + + + + + +			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146 NEIS1145 NEIS1144 NEIS1143	488 1141 3155 3896 4521 5397 6141 6892 8005 9288	1144 2913 3733 4513 5384 5831 6869 7923 8313	11111111			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146 NEIS1145 NEIS1144 NEIS1143 NEIS1142	488 1141 3155 3896 4521 5397 6141 6892 8005 9288	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241	11111111			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1147 NEIS1146 NEIS1145 NEIS1145 NEIS1144 NEIS1142 NEIS1142 NEIS1140	488 1141 3155 3896 4521 5397 6141 6892 8005 9288 10613	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241 12744	111111111			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149 NEIS1148 NEIS1146 NEIS1146 NEIS1145 NEIS1144 NEIS1143 NEIS1142 NEIS1140 NEIS1139	488 1141 3155 3896 4521 5397 6141 6892 8005 9288 10613 12391 12824	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241 12744	↓ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↓ ↓ ↓ ↓ ↓			
• Downl	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1150 NEIS1149 NEIS1149 NEIS1146 NEIS1146 NEIS1145 NEIS1143 NEIS1143 NEIS1142 NEIS1140 NEIS1139 NEIS1138	488 1141 3155 3896 4521 5397 6141 6892 8005 9288 10613 12391 12824	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241 12241 122744 14362 15046	4 4 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1			
Downl equence	load sequences with Sequencing method	annotations (EMBL forn Original de	mat) esignation	Length Comments	NEIS1151 NEIS1149 NEIS1149 NEIS1148 NEIS1147 NEIS1145 NEIS1144 NEIS1144 NEIS1144 NEIS1142 NEIS1140 NEIS1137	488 1141 3155 3896 4521 5397 6141 6892 8005 9288 10613 12391 12824 14426 15102	1144 2913 3733 4513 5384 5831 6869 7923 8313 10541 12241 12241 122744 14362 15046	L L L T T T T L T L L L T T			

A sequence bin record contains information about that contigs associated with an isolate record. This includes:

- Number of contigs
- Total length
- Minimum length
- Maximum length
- N50, N90 and N95 values
- Size distribution charts

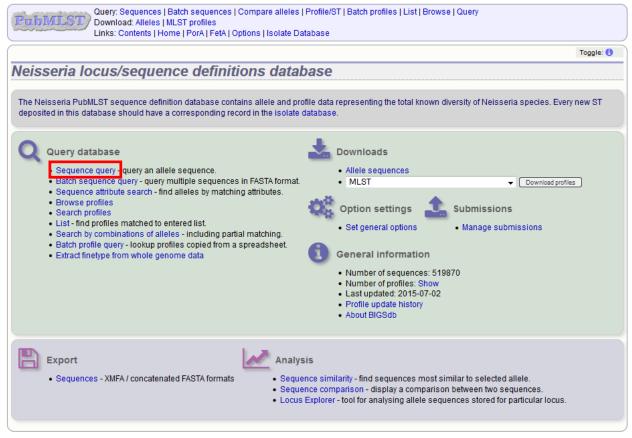
There are also links to download the contigs in FASTA or EMBL format.

Finally there is a table that shows the loci that are tagged on each contig. Individual contigs can also be downloaded in EMBL format.

Querying data

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'.

PubMLST Download: Alleles MLST profile	ences Compare alleles Profile/ST Batch profile s FetA Options Isolate Database	es List Browse Query	
Sequence query - Neisseria l	ocus/sequence definitions		
Please paste in your sequence to query against the c partial matches will be identified if an exact match is Please select locus/scheme All loci Enter query sequence (single or multiple contigs GACGCGGTGCGCGATGAAAAGTCAAAGTCAAAGTCATCAA CTTGTCAATGAAAAATCTCCTGCGCGGACAAATATAA CTTGTCAATGAAAAATCTACTGCGTGCGCGGACAAATATAA CTTGTCAATGAAAAATCTACTGCGTTGGCCGCGGACAAATATAA CTTGTCAATGAAAAAACCATTTTGCTTTGGGCGCGCGGGCG TTGAAAGGAACCACTTTGCCTTTGGGCACGGCGCGGGCG TTGAAAGGAACCACTTTTGCGCCATTGGGCGCGGGCG TTGAAAGGAACCACTTTTGCGCATTGGGCGGCGGGGG TTGAAAGGAACCACTTTTGGCCATTGGGCGGCGGGGG TTGAAAGGAACCACTTTTGGCCATTGGGCGGCGGGGGGGG	not found. You can query using either DNA or pept 		- they do not need to be trimmed. The nearest Action Reset Submit

If an exact match is found, this will be indicated along with the start position of the locus within your sequence.

Ouery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles Links: Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database Sequence query - Neisseria locus/sequence definitions	st Browse Query
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 so paste in the second	Alternatively upload FASTA file Action Select FASTA file: Reset Submit
1 exact match found. Translate query	
Allele Length Start position End position Flags Comments aroE: 8 490 136 625	

If only a partial match is found, the most similar allele is identified along with any nucleotide differences. The varying nucleotide positions are numbered both relative to the pasted in sequence and to the reference sequence. The start position of the locus within your sequence is also indicated.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database						
Sequence query - Neisseria locus/sequence definitions						
Please paste in your sequence to query against the database. Query sequences will be checked first partial matches will be identified if an exact match is not found. You can query using either DNA or properties of the properties of t		- they do not need to be trimmed. The nearest Action Reset Submit				
Translate query Closest match: aroE: 8 Show alignment Differences 2 differences found. [] 259T						

As an alternative to pasting a sequence in to the box, you can also choose to upload sequences in FASTA format by clicking the file browse button.

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

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.

Profit/UST Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database								
Sequence query - Neisseria locus/sequence definitions								
Please paste in your sequence to query against the database. Query sequences will be checked first for an exact match against the chosen (or all) loci - they do not need to be trimmed. The nearest partial matches will be identified if an exact match is not found. You can query using either DNA or peptide sequences.								
Please select locus/scheme								
MLST • locus •								
- Enter query sequence (single or multiple contigs up to whole genome in size) - Atternatively upload FASTA file - Action - Action								
>4758 NODE_192_length_1326_cov_47.828808 Select FASTA file: Reset Submit								
TAGAACAACAGCAATATICAAAGATTATCTGAAAGTCCGAGATTCTAGATTCCCGCTTTC GCGGGAATGACGAAAAGCAAGCCGTAGGTCGGATACTTGTATCCGACAAAAGCCTGCCAT								
CTCAAATAGCCGTCGGATTCGAGAATCCGACCTGCCAAACCGGGCGGCGGGGGCGCCGGCC								
GECAETTAGTACGCAAATCGAACAACAACAACAAAAAAGCCCCGATTCGGATTTTCCAAT CGGGCTTTTTTTGCGCCCGTTTTGTCATCCCGTGAAAATATCCGCATGACAAAAATATAGTG								
AATTAACAAAAATCAGGACCAAGGCCGACGCAGGCCGCAGCCGTACGGATAAGGCGTAAGG								
7 exact matches found.								
Allele Length Start position End position Flags Comments								
abc2:4 433 203051 203483								
adk: 10 465 938327 938791 aroE: 15 490 1775325 1775814								
alle: 19 490 1775253 177514 ImmC 9 465 1134240 1134704								
adh 8 501 961439 961939								
pdhC: 11 480 1341678 1342157								
pgm: 9 450 1416246 1416695								
MLST								
ST 269								
Cional complex ST-269 complex								

11.2 Searching for specific allele definitions

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

Query: Sequences Batch sequences Compare alleles Profile Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	
	Toggle: 🚯
Neisseria locus/sequence definitions database	2
The Neisseria PubMLST sequence definition database contains allele and profile dat deposited in this database should have a corresponding record in the isolate databa	
Q Query database	Downloads
Sequence query - query an allele sequence.	Allele sequences
Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching attributes. Browse profiles Search profiles List - find profiles matched to entered list. Search by combinations of alleles - including partial matching. Batch profile query - lookup profiles copied from a spreadsheet. Extract finetype from whole genome data	MLST Download profiles Download profiles Submissions Set general options Manage submissions General information Number of sequences: 519870 Number of profiles: Show Last updated: 2015-07-02 Profile update history About BIGSdb
Sequence co	milarity - find sequences most similar to selected allele. mparison - display a comparison between two sequences. er - tool for analysing 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.

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.													
locus v = v abcZ + ? Order by: locus v ascending v													
Display: 25													
Reset Submit													
Coolink													

Click submit.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Toggle: 1
uery sequences for Neisseria locus/sequence definitions database
ome 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 ugins. so 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
cus that uses integer allele ids using the drop-down list. ease 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 i
allele id • = • 5
E Filter query by Action Reset Submit
ecord returned. Click the hyperlink for detailed information.
bcus allele id sequence sequence length comments flags bcz 5 TTTGATACCETTGCC TCGTCGAACTCGATC 433

Click the hyperlinked results to display allele records.

PribMLST / Dow	ry: Sequences Batch sequences Compar /nload: Alleles MLST profiles :s: Contents Home PorA FetA Options I	are alleles Profile/ST Batch profiles List Browse Query Isolate Database
		Toggle: i
Query sequend	ces for Neisseria locus/	s/sequence definitions database
plugins.	-	s general page. Search for these at the locus-specific query page. Use this page also for access to the sequence analysis or export
	in this database have allele ids defined as te llele ids using the drop-down list.	text strings. Queries using the '<' or '>' modifiers will work alphabetically rather than numerically unless you filter your search to a
Please enter your search	criteria below (or leave blank and submit to	to return all records). Matching sequences will be returned and you will then be able to update their display and query settings.
		Display
Combine searches with	1: AND 👻	Order by: locus 👻 ascending 👻
	✓ = ✓ abcZ	+ i Display: 25 - records per page i
allele id 👻	• = • 5	
	Action	
	Reset Submit	
	Reset Submit	
1 record returned. Click the	e hyperlink for detailed information.	
locus allele id	sequence seque	uence length comments flags
		433

	ownload: Alleles MLST profiles inks: Contents Home PorA FetA Options Isolate Database
llele inform	ation - abcZ: 5
Provenance/meta	data
locus:	abcZ i
allele:	5
sequences:	TITGATACCS TIGCCGAAGS TITGGGCGAA ATICGCGATI TAITGCGCCS ITAICATCAI GICAGCCAIG AGTIGGAAAA TGGTICGAGI GAGGCITIGI TGAAAGAGCI TAACGAATIG CAACITGAAA TCGAAGCGAA GGACGGCIGG AAGCCIGGAIG CGGCGAGICAA GCAGACITIG GGICGAACIIG GITTGCCAGA AAACGAAAAA AICGGCAACC CGIGIGIGCC TAGCGCAGGC TIGGGIGCGG AAGCCIGAIG TAITGGIGCGGAACGG GACGGAACCG ACCAACCAIT IGGACATIGA CGCGAITAIT IGGCIGGAAA AICIGCITAA AGCGITIGAA GGCAGCCIGG IIGGAITAC CCACGACCGC CGITITIIGG ACAATAICGC CACCGCAIC GICGAACCG AIC
length:	433
status:	Sanger trace checked
date entered:	2001-02-07
datestamp:	2009-11-11
	Keith Jolley, University of Oxford, UK
curator:	Man-Suen Chan, University of Oxford (E-mail: man-suen.chan@paediatrics.ox.ac.uk)
Profiles containin	g this allele
MLST:	183 profiles
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.

Prr11//ILST Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database												
Toggle: [
Query sequences for Neisseria locus/sequence definitions database												
Some loci have additional fields which are not searchable from this general page. Search for these at the locus-specific guery 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 + ; Order by: locus • ascending •												
Display: 25 → records per page []												
locus: abcZ T i Reset Submit												
status:												
sender:												
curator:												
allele flag:												
9 records returned. Click the hyperlinks for detailed information.												
locus allele id sequence sequence length comments flags												
abcz 1 TITGATACTGTIGCC TIGICGAACICGATC 433												
abcz 2 TITGATACCGITGCC TIGICGAACTCGAIC 433												
abcz 3 TITGATACCGTIGCC TIGTIGAACTIGACC 433												
abcz 4 TITGATACCGTIGCC TIGTCGAACICGATC 433												
abcz 5 ITTGATACCGTTGCC TCGTCGAACTCGATC 433												
abcz 6 ITTGATACCGTTGCC TTGTCGAACCCGATC 433												
abcz 7 ITTGATACTGTTGCC TIGTCGAACICGATC 433												
abcz 8 TITGATACCGTIGCC TIGTCGAACTIGACC 433												
abcZ 9 TITGATACCGTIGCC TIGICGAACTCGATC 433												

11.2.1 Locus-specific attributes

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Toggie:
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 lage. 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
locus • = • • Order by: locus • ascending Display: 25 • records per page [i]
-> Filter query by Action Reset Submit

Pick the required locus from the dropdown box.

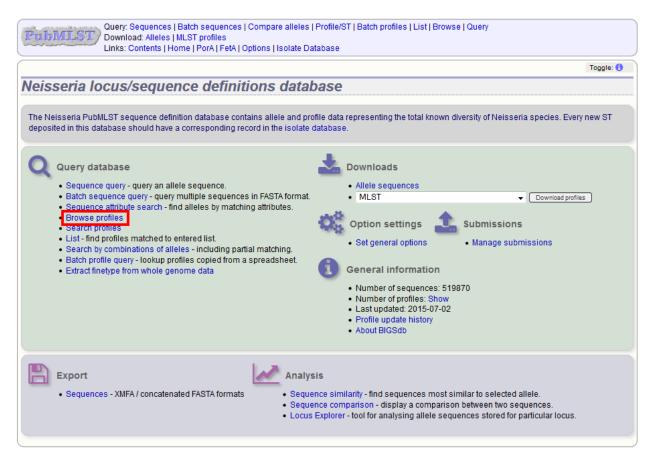
Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles I MLST profiles Links: Contents Home PorA FetA Options I solate Database												
		Toggle: i										
Query PorA VR2 sequences - Neisseria locus/sequence definitions database												
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 re	turn all records).											
Locus fields	Display	Filter query by										
allele id 🗸 = 🗸	+ i Order by: allele id • ascending											
	Display: 25 👻 records per page 👔	allele flag: 👻										
Action												
Reset Submit												

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

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															
													Toggle: i		
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 ente	er your s	earch criteria below (or leave	blank and submit to re	turn all records).											
— Locus f	ields —			——— Displa	ay				— — Filter q	lery by —					
family		▼ = ▼ 2		+ 👔 Ord	erby: a	llele id	-	ascending	 sta 	tus:		•			
				Dis	splay: 2	5 🗸	records per	page 👔	allele	flag:		-			
-Action -															
Reset	Sub	mit													
83 records r	eturned	(1 - 25 displayed). Click the h	vperlinks for detailed in	formation											
_			,,												
Page: 1	2 3	4 > Last													
	allele id		sequence length	comments		variant	old name		nAb1 reactivity		Ab2 reactivity	flags			
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 2-12	HEVLQTPQSQPTLVP	15 15		2	11									
PorA VR2	2-12	HFVQQIPKSQPTLVP			2	12		MNIAROADEA							
PorA VR2 PorA VR2	2-13	YFVQQTPQSQPTLVP HFVQQKLASKPTLVP	15 15		2	13 14	33	MN16C13F4	+						
PorA VR2 PorA VR2	2-14	HFVQQKLASKPILVP	15		2	14									
PorA VR2 PorA VR2	2-15	HFVQQKSISKPILVP	15		2	15	33a (33-1) 33b (33-2)								
PorA VR2 PorA VR2	2-10	HFVQQQPTSEPTLVP	15		2	17	330 (33-2) 33c (33-3)								
PorA VR2		HFVQQIPKSQPILVP	15		2	18	330 (33-3)								
PorA VR2		HEVOOTSOSOPTLVP	15		2	19									

11.3 Browsing scheme profile definitions

If a sequence definition database has schemes defined that include a primary key field, i.e. collections of loci that together create profiles, e.g. for MLST, click the link to 'Browse profiles'.



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

Pul	Mc	LS'	F / c	Down	load:	Alle	les N	ST profiles	
							-		Toggle: 👔
Bro	ws	e p	rof	ïles	5 -	Ca	mp	vlobacter locus/sequence definitions	
		e crite	rie					Action	
								Acion	
		er by:				•		Browse all records	
	Dire	ction:	asce	endin	g ,	•			
	Dis	splay:	25	• I	ecord	ds pe	er pag	I.	
	-	2 gInA						8 9 > Last clonal complex	
1	2	1	54	3	4	1	5	ST-21 complex	
2	4	7	51	4	1	7	1	ST-45 complex	
3	3	2	5	10	11	11	6	ST-49 complex	
4	10	11	16	7	10	5	7	ST-403 complex	
5	7	2	5	2	10	3	6	ST-353 complex	
6	63	34	27	33		5	7		
4	8	10	2	2	14	12	6	ST-354 complex	
8	2	1	1	3	2	1	6	ST-21 complex	
9 10	2	6 59	22 4	24 38	12 17	7	1	ST-508 complex ST-433 complex	
10	2 48	59	4	38 4		7	2 1	ST-45 complex	
12	40	1	5	2	11	3	6	ST-45 complex	
13	2	1	1	2	2	1	5	ST-21 complex	
	-				-	1.1			

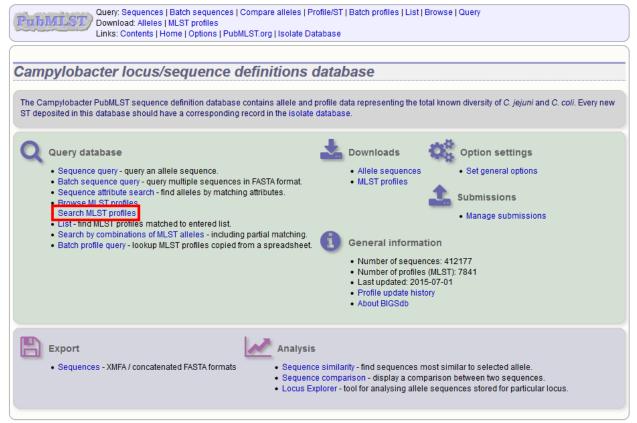
Clicking the hyperlink for any profile will display full information about the profile.

Querr Sequences | Botch sequences | Compare alleles | Brofile/CT | Botch profiles | List | B

(PubMLST) D	uery: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query ownload: Alleles MLST profiles Ins: Contents Home Options PubMLST.org Isolate Database
Profile inform	nation for ST-8 (MLST)
i iome miom	
STaspAglnA821	gltA glyA pgm tkt uncA clonal complex 1 3 2 1 6 ST-21 complex
sender:	Frances Colles
curator:	Frances Colles, University of Oxford, UK (E-mail: frances.colles@medawar.ox.ac.uk)
date entered:	2001-05-02
datestamp:	2001-05-02
Client database	
PubMLST isolates:	Contains data for a collection of isolates that represent the total known diversity of C. jejuni and C. coli. For every allelic profile in the profiles database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does not represent a population sample. (49 isolates)

11.4 Querying scheme profile definitions

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



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

													Toggle:
ar	ch	pro	file	s -	Cá	m	oylo	obacter loo	cus/seque	ence definitions			
-Lo	cus/s	chem	field	s —						Display/sort options			
		earch		_	ND.					Order by: ST	- ascendin		
	e ente		20 WI	• A		•	_	2014-02-01	(+)	Display: 25 - r		4 🔹	
				_				Cody	Ľ	Dispidy. 20 V	corus per page [7]		
ser	ider (s	urnar	ne)	•	-		-	Cody					
-Filt	ter qu	ery by						Acti	on				
		clonal	com	lex.				▼ I Res	et Submit				
									ouonit				
recol	rds re	humer	Clic	the	hyner	links	for de	tailed information					
recol	rds re	turnec	Clic	the	hyper	links	for de	tailed information.					
recol	rds re	turnec	. Clic	the	hyper	links	for de	tailed information.					
	rds re aspA				hyper pgm			tailed information.					
ST			gitA	glyA									
ST 117	aspA	ginA	gitA 65	glyA	pgm	tkt	uncA						
ST 117 162	aspA	ginA 66	gitA 65	g <mark>iyA</mark> 192	pgm 189	tkt 44	uncA 17	clonal complex					
ST 117 162 172	aspA 33 1	ginA 66 2	gitA 65 3	g <mark>iyA</mark> 192 539	pgm 189 5	tkt 44 9	uncA 17 3 384	clonal complex ST-42 complex					
ST 117 162 172 176	aspA 33 1	ginA 66 2 1	gltA 65 3 6 5	g <mark>iyA</mark> 192 539 3	pgm 189 5 2	tkt 44 9 1	uncA 17 3 384	Clonal complex ST-42 complex ST-21 complex					
ST 117 162 172 176 177	aspA 33 1 8 7	gInA 66 2 1 448	gltA 65 3 6 5	192 539 3 2 566	pgm 189 5 2 10	tkt 44 9 1 3	uncA 17 3 384 6 3	Clonal complex ST-42 complex ST-21 complex					
ST 117 162 172 176 177 178	aspA 33 1 8 7	gInA 66 2 1 448 21	gitA 65 3 6 5 2	192 539 3 2 566	pgm 189 5 2 10 11	tkt 44 9 1 3 37	uncA 17 3 384 6 3	Cional complex ST-42 complex ST-21 complex ST-353 complex					
ST 117 162 172 176 177 178 179	aspA 33 1 8 7 55 7	ginA 66 2 1 448 21 17	gltA 65 3 6 5 2 5 5 5	2 192 539 3 2 566 2 10	pgm 189 5 2 10 11 705	tkt 44 9 1 3 37 37	uncA 17 3 384 6 3 6	cional complex ST-42 complex ST-21 complex ST-353 complex ST-353 complex					
	aspA 33 1 8 7 55 7 3 79	ginA 66 2 1 448 21 17 495	gltA 65 3 6 5 2 5 5 5 420	2 566 2 10 372	pgm 189 5 2 10 11 705 11 20	tkt 44 9 1 3 37 3 68 1	uncA 17 3 384 6 3 6 6 6	cional complex ST-42 complex ST-21 complex ST-353 complex ST-353 complex					

Each field can be queried using standard operators.

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

Pub	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															
																Toggle: i
Sear	ch	pro	file	s.	Cá	amı	ovl	obacter lo	cus/sequenc	e defir	nitions					
ocui	011	pro					.,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	obuoter ro	ouorocquemo	e dem	naono					
Lo	Locus/scheme fields									Display/sort	options					
Com	bine s	earch	es w	ith: 🖌	ND ·	-				Order by:	ST	•	ascending	-		
dat	te ente	ered		-	>		-	2014-02-01	+ <u>i</u>	Display:	25 👻 re	cords pe	r page 👔			
sei	nder (:	surnar	ne)	-	=		-	Cody					_			
— Fil	ter au	ery by						Act	ion							
		clonal	com	plex:				▼ i Re	set Submit							
									Gubinit							
17 reco	rds re	turneo	I. Clic	ck the	hyper	rlinks	for de	etailed information.								
ST	aspA	qinA	qitA	qlyA	pgm	tkt	uncA	clonal complex								
7117		66		192			17									
7162	1	2		539	5	9	3	ST-42 complex								
7172		1	6	3	2	1	384									
7176		448 21	5	2 566	10 11	3 37	6 3	ST-353 complex								
7178	7	17	2	2	705	3	6	ST-353 complex								
7179	3	495	5	10	11	68	6	ST-49 complex								
7180	79	496	420	372		1	17									
7181	121	497		567		560										
7182	7	2	5	72	22	561	6									

11.5 Investigating allele differences

11.5.1 Sequence similarity

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

Tregel: 0 Verseseria 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 multiple sequences in FASTA format. Sequence attribute search - find alleles by matching attributes. Stows e profiles List - find profiles matched to entered list. Search profiles matched to entered list. Extract finetype from whole genome data Option settings List - find profiles copied from a spreadsheet. Extract finetype from whole genome data Mumber of profiles: Show Last updated: 2015-07-02. Profile update history Last updated: 2015-07-02. Profile update history Last updated: 2015-07-02. Profile update history Last update: 2015-07-02. Profile update: 2015-07-02. Profile update history Last update: 2015-07-02. Profile update: 2015-07-02. Profile update: 2015-07-02. Profile update history Last update: 2015-07-02. Profile update: 2015-07-02. Profile update: 2015-07-02. Last update: 2015-07-02. Profile update history Las	Query: Sequences Batch sequences Compare alleles Pr Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Datat	
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.		Toggle: 🚯
deposited in this database should have a corresponding record in the isolate database. Query database • Sequence query - query multiple sequences in FASTA format. • Sequence attribute search - find alleles by matching attributes. • Browse profiles • List - find profiles matched to entered list. • Search profile • List - find profiles matched to entered list. • Search profile guery - lookup profiles copied from a spreadsheet. • Extract finetype from whole genome data • Number of sequences: 519870 • Number of sequences: 519870 • Number of sequences: 519870 • Last update history • Sequences - XMFA / concatenated FASTA formats	Neisseria locus/sequence definitions databa	ise
 Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching attributes. Browse profiles Search profiles matched to entered list. Search profile query - lookup profiles copied from a spreadsheet. Extract finetype from whole genome data Search profiles: Show Number of sequences: 519870 Number of profiles: Show Show et al. Show Search profiles: Show Show Eligis at the state of the state		
Last updated: 2015-07-02 Profile update history About BIGSdb Analysis Sequences - XMFA / concatenated FASTA formats Sequence similarity find sequences most similar to selected allele. Sequence compansion - display a comparison between two sequences.	 Sequence query - query an allele sequence. Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching attributes. Browse profiles Search profiles List - find profiles matched to entered list. Search profile query - lookup profiles copied from a spreadsheet. 	 Allele sequences MLST Option settings Set general options Manage submissions General information Number of sequences: 519870
	Sequences - XMFA / concatenated FASTA formats Sequences -	Number of profiles: Show Last updated: 2015-07-02 Profile update history About BIGSdb e similarity find sequences most similar to selected allele. te comparison - display a comparison between two sequences.

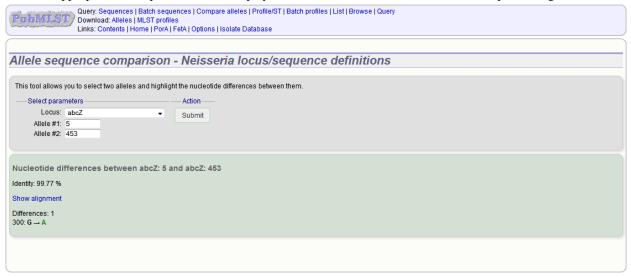
Enter the locus and allele identifier of the sequence to investigate and the number of nearest matches you'd like to see, then press submit.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Find most similar alleles - Neisseria locus/sequence definitions
This page allows you to find the most similar sequences to a selected allele using BLAST.
Select parameters
Locus: abcZ Reset Submit
Number of results: 10 -

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

	LI	inka. Conte	nts Ho	me fri on th						
ind m	ost sir	milar a	llele	es - Ne	isseria loo	us/seque	ence defi	nitions		
in a in	00000	initial d				uorocqu	unoe dem	maronio		
This page	allows you t	o find the m	nost sim	nilar sequen	ces to a selected	Illele using BLAS	ST.			
Select	parameters									
		s: abcZ			 Reset 	Submit				
	Allele	e: 5			Reser					
Num	ber of results	s: 10 👻								
abcZ-5										
	% Identity I	Mismatche	s Gaps	Alignment	Compare					
		Mismatche: 1	s Gaps 0	Alignment 433/433	Compare Compare abcZ:	657				
Allele										
Allele abcZ: 657	99.77	1	0	433/433	Compare abcZ:	453				
Allele abcZ: 657 abcZ: 453	99.77 99.77	1 1	0	433/433 433/433	Compare abcZ: Compare abcZ:	453 405				
Allele abcZ: 657 abcZ: 453 abcZ: 405	99.77 99.77 99.77	1 1 1	0 0 0	433/433 433/433 433/433	Compare abcZ: Compare abcZ: Compare abcZ:	453 405 404				
Allele abcZ: 657 abcZ: 453 abcZ: 405 abcZ: 404	99.77 99.77 99.77 99.77 99.77	1 1 1 1	0 0 0 0 0	433/433 433/433 433/433 433/433	Compare abcZ: Compare abcZ: Compare abcZ: Compare abcZ:	405 404 213				
Allele abcZ: 657 abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166	99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1	0 0 0 0	433/433 433/433 433/433 433/433 433/433	Compare abcZ: Compare abcZ: Compare abcZ: Compare abcZ: Compare abcZ:	453 405 404 213 166				
Allele abcZ: 657 abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213	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	433/433 433/433 433/433 433/433 433/433 433/433	Compare abcZ: Compare abcZ: Compare abcZ: Compare abcZ: Compare abcZ: Compare abcZ:	453 405 404 213 166 114				
Allele abcZ: 657 abcZ: 453 abcZ: 405 abcZ: 404 abcZ: 213 abcZ: 166 abcZ: 114	99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77 99.77	1 1 1 1 1 1 1 1 1	0 0 0 0 0 0 0	433/433 433/433 433/433 433/433 433/433 433/433 433/433	Compare abcZ: Compare abcZ: Compare abcZ: Compare abcZ: Compare abcZ: Compare abcZ: Compare abcZ:	453 405 404 213 166 114				

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



11.5.2 Sequence comparison

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database	List Browse Query
	Toggle: ()
Neisseria locus/sequence definitions database	
The Neisseria PubMLST sequence definition database contains allele and profile data representing the to deposited in this database should have a corresponding record in the isolate database.	tal known diversity of Neisseria species. Every new ST
Q Query database Downloads	
Sequence query - query an allele sequence. Allele sequence	s
 Batch sequence query - query multiple sequences in FASTA format. Sequence attribute search - find alleles by matching attributes. Browse profiles Search profiles List - find profiles matched to entered list. Search by combinations of alleles - including partial matching. Batch profile query - lookup profiles copied from a spreadsheet. Extract finetype from whole genome data MLST Option setting Set general option Number of sequences of the security of the securit	Manage submissions Manage submissions nation ences: 519870 les: Show 015-07-02
	ces most similar to selected allele. comparison between two sequences. allele sequences stored for particular locus.

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

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Allele sequence comparison - Neisseria locus/sequence definitions
This tool allows you to select two alleles and highlight the nucleotide differences between them.
Select parameters Action Locus: abcZ Allele #1: 5 Allele #2: 8

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

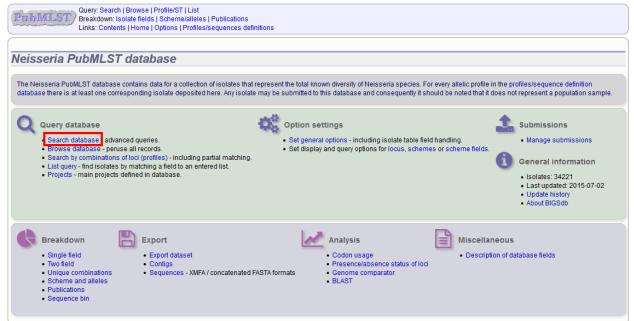


See also:

Locus explorer plugin.

11.6 Querying isolate data

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



To start with, only one provenance field search box is displayed but more can be added by clicking the '+' button (highlighted). These can be linked together by 'and' or 'or'.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definiti	ions Database submissions		
		Toggle: <i>i</i> Field help: id	▼ Go
Search Neisseria PubMLST database			
Isolate provenance/phenotype fields Combine with: AND ↓ country ↓ = ↓ USA ↓ 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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	MDL01A0601	USA	2001	meningitis	Neisseria meningitidis	Y	1378					
	MDL01A2447	USA		invasive (unspecified/other)	-	Y	1379	ST-23 complex/Cluster A3				
866	MD01227	USA	2001		Neisseria meningitidis		1624	ST-167 complex				
867	MDO1056	USA	2001		Neisseria meningitidis		1625					
868	MDO1066	USA	2001		Neisseria meningitidis		1626					
2281	M7089	USA		invasive (unspecified/other)		W		ST-11 complex/ET-37 complex	5	2		
2299		USA		invasive (unspecified/other)	-	W		ST-11 complex/ET-37 complex	5	2		
2316		USA		invasive (unspecified/other)	-	W	22	ST-22 complex	6	3		
2317		USA		invasive (unspecified/other)	-	W	22	ST-22 complex	6	3		
2322		USA		invasive (unspecified/other)	-	W	1065		6	3		
2323		USA		invasive (unspecified/other)		W	1286		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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34 49	41 M7085 99 MDL01A0601	USA USA	2000 2001	Isolate fields I disease invasive (unspecified/other) meningitis	Neisseria meningitidis Neisseria meningitidis	W Y	11 1378	clonal complex ST-11 complex/ET-37 complex ST-23 complex/Cluster A3			R
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34 49 50 86 86 86 228 229	M7085 99 MDL01A0601 00 MDL01A2447 66 MD01227 67 MD01056 58 MD01066 81 M7089 99 M7257	USA USA USA USA USA USA USA USA	2000 2001 2001 2001 2001 2001 2000 2000	Isolate fields [] disease invasive (unspecified/other) meningitis invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	W Y Y W	11 1378 1379 1624 1625 1626 11 11	cional complex ST-11 complex/ET-37 complex ST-23 complex/Cluster A3 ST-23 complex/Cluster A3 ST-167 complex ST-23 complex/Cluster A3 ST-269 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex	PorA VR1	PorA VR2 FetA V	R
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34 49 50 86 86 228 229 231	41 M7085 99 MDL01A0601 00 MDL01A2447 56 MD010227 77 MD01056 88 MD01066 81 M7089 99 M7257 16 M7084 22 M7092	USA USA USA USA USA USA USA USA	2000 2001 2001 2001 2001 2000 2000 2000	Isolate fields [2] disease Invasive (unspecified/other) meningitis invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis Neisseria meningilidis	W Y Y W W	11 1378 1379 1624 1625 1626 11 11 22	clonal complex ST-11 complex/ET-37 complex ST-23 complex/Cluster A3 ST-23 complex/Cluster A3 ST-167 complex/Cluster A3 ST-269 complex ST-11 complex/ET-37 complex ST-11 complex/ET-37 complex ST-22 complex	PorA VR1	PorA VR2 FetA V	R

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:

- Allele designations/scheme field values
 - Search by combination of allele designations and/or scheme fields e.g. ST, clonal complex information.
- Allele designation status
 - Search by whether allele designation status is confirmed or provisional.
- · Tagged sequence status
 - Search by whether tagged sequence data is available for a locus. You can also search by sequence flags.
- Filters
 - Various filters may be available, including
 - * Publications
 - * Projects
 - * MLST profile completion status
 - * Clonal complex
 - * Sequence bin size
 - * Inclusion/exclusion of old versions

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If the interface is modified, a button to 'Save options' becomes available within the tab. If this is clicked, the modified form will be displayed the next time you go to the query page.

11.6.1 Query by allele_designation/scheme field

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

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

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Designations can be queried using standard operators.

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

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

													Тс	oggle: <u>i</u> F	Field help: id	ł	-
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11.6.2 Query by allele designation status

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

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

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publicati Links: Contents Home Options Profiles/sequence			
(Toggle: i Field help: id 🗸 G	•
Search Neisseria PubMLST database			
Isolate provenance/phenotype fields	Display/sort options	Mod	ifv
id • = • Entervalue		form	
		Modify form parameters option	
Action		Click to add or remove additional query terms:	
Reset Submit		Show Allele designations/scheme field values	
		Show Allele designation status Show Tagged sequence status	
		Show Filters	

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

<u>נרת</u>	MILST	💟 Breal	kdown: Is	olate fi	se Profile/ST List elds Scheme/alleles F me Options Profiles/se		ns Database	e submissions				
									Toggle: <i>i</i> Field help: id			G G
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record	s returne	d. Click th	ie hyperli		detailed information.				ст	Finot	vning an	tigons
record: id	1			1	detailed information. solate fields 👔 disease	species	serogroup	ML ST	ST clonal complex	PorA	yping ant PorA VR2	FetA
id	1	aliases		l: year	solate fields 👔	species Neisseria meningitidis	serogroup B					
id 10735	isolate N 56/99	aliases	country	l: year 1999	solate fields 👔 disease invasive	Neisseria		ST	clonal complex	PorA VR1	PorA VR2	FetA VR
id	isolate N 56/99 8/00	aliases	country Norway	year 1999 2000	solate fields 1 disease invasive (unspecified/other) invasive	Neisseria meningitidis Neisseria	В	ST 45, <mark>2183, 4363, 9838</mark>	clonal complex ST-41/44 complex/Lineage 3, ST-41/44 complex/Lineage 3,	PorA VR1 5-1	PorA VR2 10-1	FetA VR F5-5
id 10735 10756	isolate N 56/99 8/00 10/00	aliases	country Norway Norway	year 1999 2000 2000	solate fields I disease invasive (unspecified/other) invasive (unspecified/other) invasive	Neisseria meningitidis Neisseria meningitidis Neisseria	B	ST 45, 2183, 4363, 9838 43, 1644, 2433, 4163	cional complex ST-41/44 complex/Lineage 3, ST-41/44 complex/Lineage 3, ST-213 complex ST-41/44 complex/Lineage 3,	PorA VR1 5-1 22	PorA VR2 10-1 14	FetA VR F5-5 F5-5
id 10735 10756 10758	isolate N 56/99 8/00 10/00	aliases	country Norway Norway Norway	year 1999 2000 2000 2000 2000 2000 2000 2000	solate fields [7] disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria	B B	ST 45, 2183, 4363, 9838 43, 1644, 2433, 4163 110, 1419, 1844, 6617	clonal complex ST-41/44 complex/Lineage 3, ST-41/44 complex/Lineage 3, ST-213 complex ST-41/44 complex/Lineage 3, ST-1157 complex	PorA VR1 5-1 22 21-7	PorA VR2 10-1 14 16	FetA VR F5-5 F5-5 F5-36
id 10735 10756 10758 10812	isolate N 56/99 8/00 10/00 64/00 Mk	aliases	country Norway Norway Norway Norway	year 1999 2000 2000 2000 1996	solate fields disease invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria	B B B	ST 45, 2183, 4363, 9838 43, 1644, 2433, 4163 110, 1419, 1844, 6617 146, 41, 303, 1788, 1823, 3142	cional complex ST-41/44 complex/Lineage 3, ST-41/44 complex/Lineage 3, ST-213 complex ST-41/44 complex/Lineage 3, ST-41/44 complex/Lineage 3	PorA VR1 5-1 22 21-7 7-2	PorA VR2 10-1 14 16 4	FetA VR F5-5 F5-5 F5-36 F1-5

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.

11.6.3 Query by tagged sequence status

Sequence tags identify the region of a contig within an isolate's sequence bin entries that correspond to a particular locus. The presence or absence of these tags can be queried as can whether or not the sequence has an a flag associated with. These flags designate specific characteristics of the sequences. Queries will be combined from the values entered in all form sections.

Make sure that the tagged sequences status fieldset is displayed by selecting it in the 'Modify form options' tab.

Pu	Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions								
						Toggle: i Field help: id	▼ Go		
Se	Search Neisseria PubMLST database								
_	Isolate provenance/ph	enotype fields –			Display/sort options		Modify		
	id 🔹	, =	 Enter value 	+ 1	Order by: id	[X]	form		
					Display: 25 👻 records per page	Modify form parameters	options		
	Action					Click to add or remove additional query terms:			
	Reset Submit					Show Allele designations/scheme field values			
						Show Allele designation status			
						Show Tagged sequence status			
						Show Filters			

Select a specific locus in the dropdown box (or alternatively 'any locus') and a status. Available status values are:

- untagged
 - The locus has not been tagged within the sequence bin.
- tagged
 - The locus has been tagged within the sequence bin.
- complete
 - The locus sequence is complete.
- incomplete
 - The locus sequence is incomplete normally because it continues beyond the end of a contig.
- flagged: any
 - The sequence for the locus has a flag set.
- flagged: none
 - The sequence for the locus does not have a flag set.
- flagged: <specific flag>
 - The sequence for the locus has the specific flag chosen.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions		
	Toggle: <i>i</i> Field help: id	▼ Go
Search Neisseria PubMLST database		
id • = • Entervalue (+) [Order by: id	✓ ascending ✓	Modify
Display: 25 records per page		form options
NEISUUU1 (lpxC) v Is flagged: internal stop codon v + i i Reset Submit		
1 record returned. Click the hyperlink for detailed information.		
Isolate fields 🔢 MLST Finetyping anti	gens	
id isolate aliases country year disease species serogroup ST clonal complex PorA VR1 PorA VR		
2077 153 alpha153 Germany 1999 carrier Neisseria meningitidis E 60 ST-60 complex 5 2	F1-7	
Analysis tools:		
Breakdown: Fields Two Field Codons Polymorphic sites Combinations Schemes/alleles Publications Sequence	a bin Tag status	
Analysis: Presence/Absence Genome Comparator BLAST		
Export: Dataset Contigs Sequences		

See also:

Sequence tag flags

11.6.4 Query filters

There are various filters that can additionally be applied to queries, or the filters can be applied solely on their own so that they filter the entire database.

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

(PubMLST) Bre	akdown: Isolate fi	se Profile/ST List elds Scheme/alleles Publi me Options Profiles/seque		s Database s	ubmissions		
						Toggle: i Field help: id	- Go
Search Neisse	eria PubM	LST database					
Isolate provenance/ id	phenotype fields -	✓ Enter value	+ <u>i</u>	— Display/sor Order by: Display:	id	[X] Modify form parameters	Modify form options
Action Reset Submit						Click to add or remove additional query terms: • Show Allele designations/scheme field values • Show Allele designation status • Show Tagged sequence status • Show 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*.

11.7 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. This can also be done in sequence definition databases if the scheme has a primary key field defined.

On the index page, click 'Search by combinations of loci (profiles)' for any defined scheme. Enter either a partial (any combination of loci) or complete profile.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in th database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it does	
 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 General information Isolates: 34221 Last updated: 2015-07-02 Update history About BIGSdb
Breakdown Export Analysis Miscellance • Single field • Export dataset • Contigs • Contigs • Description of • Unique combinations • Sequences - XMFA / concatenated FASTA formats • Codon usage • Description of • Publications • Sequence bin • Sequence for • Description of	pus of database fields

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

Query: Search Browse Profile/ST Breakdown: Isolate fields Scheme Links: Contents Home Options		
		Toggle: [
Search Neisseria PubMLST da	tabase by combinations of loci	
Schemes		
Please select the scheme you would like to query:		
MLST - S	elect	
Please enter your allelic profile below. Blank loci wil abcZ adk aroE fumC gdh		
	pdhC pgm ST:	Autofill
Filters	Options	- Display/sort options
Project:	i Search: Exact or nearest match	Order by: id ascending
Include old record versions		Display: 25 🗸 records per page 👔
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 submission	IS
	Toggle: []
Search Neisseria PubMLST database by combinations of lo	ci
Schemes	
Please select the scheme you would like to query:	
MLST Velect	
Please enter your allelic profile below. Blank loci will be ignored. — — Autofill profile by sear	ching remote database ——
abcZ adk aroE fumC gdh pdhC pgm ST: 2 3 4 3 8 4	Autofill
Filters Options	Display/sort options
Project:	Order by: id ascending
Include old record versions	Display: 25 🗸 records per page i
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.

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	
abcZ adk aroE fumC gdh pdhC pgm ST: 44 Autofill 9 6 9 9 6 9	
- Filters - Options - Display/sort options	
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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 datab	ISE
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Project: View Search: Exact or nearest match View Order by: id	
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Action	
Reset Submit	

Click 'Submit'.

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abcZ	adk aroE	fumC g	jdh	pdhC pgm	ST: 44		Autofill			
9	6 9	9	9	6 9						
- Filters				Options		-Display/	sort options			
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Reset Su ct matches fou records return ge: 1 2 3 id isolate 11 19 70 38	nd (7 loci). ed (1 - 25 display 3) 4) 5) > aliases	Last Country Germany Germany	Isolat year 1999 1999	e fields T disease carrier carrier	Neisseria meningitidis Neisseria meningitidis	serogroup B NG	MLST ST clonal complex 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3	PorA VR1	PorA VR2	FetA VR
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Reset St ct matches fou records return records return return ge: 1 2 id isolate 1 11 19 70 38 27 NG E30 74 99 132 92 99-132 99-132 132	aliases	Country Germany Germany Norway Canada Canada	Isolat year 1999 1999 1988 1999 1999	e fields 2 disease carrier carrier carrier invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup B NG B B B B B	MLST ST clonal complex 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3	PorA VR1 I	PorA VR2	FetA VR F1-7
Reset St act matches fou records return ge: 1 2 id isolate 41 19 70 38 127 NG E30 74 99 182 99-132 99-132 975 0069/93	aliases	Country Germany Germany Norway Canada Canada Czech Republic	Isolat year 1999 1999 1988 1999 1999 1993	e fields 👔 disease carrier carrier carrier invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup B NG B B B NG NG	MLST ST conplex 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3	PorA VR1	PorA VR2 16 14-4	FetA VR
Reset St act matches fou act matches fou act matches return act matches return ge: 1 2 id isolate 41 41 19 70 70 38 38 774 99 182 792 792 99-132 3057 3057 30503 3532	aliases Z4692 Z7184	Country Germany Germany Norway Canada Canada Czech Republic The Netherlands	Isolat year 1999 1999 1988 1999 1999 1993 1975	e fields disease carrier carrier carrier invasive (unspecified/other) invasive (unspecified/other) carrier	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup B NG B B B NG B B S B	MLST ST clonal complex 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3	PorA VR1 I 21 22	PorA VR2 16 14-4 4	FetA VR F1-7 F1-7
Reset Si act matches fou 9 records return 9 records return 9 records return 10 10 records return 12 3 14 19 70 38 127 NG E30 774 99 182 992 99-132 9975 0069/93	allases Z4692 Z7184	Country Germany Germany Norway Canada Canada Czech Republic	Isolat year 1999 1999 1988 1999 1999 1993 1975 1993	e fields 2 disease carrier carrier carrier invasive (unspecified/other) invasive (unspecified/other)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	serogroup B NG B B B NG NG	MLST ST conplex 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3 44 ST-41/44 complex/Lineage 3	PorA VR1 I	PorA VR2 16 14-4	FetA VR F1-7

11.8 Retrieving list of isolates or profiles

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

Click 'List query' on the main contents page.

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 doe	
 Query database Search database - advanced queries. Browse database - peruse all records. Search by combinations of loid (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 General information Isolates: 34221 Last updated: 2015-07-02 Update history About BIGSdb
Breakdown Export Analysis Miscellane • Single field • Export dataset • Contigs • Contigs • Contigs • Scheme and alleles • Sequences - XMFA / concatenated FASTA formats • Codon usage • Description • Sequence bin • Sequences - XMFA / concatenated FASTA formats • BLAST • Description	ous of database fields

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

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publicat Links: Contents Home Options Profiles/Sequence		omissions					
			Toggle: i	Field help: is	ł		▼ Go
Query Neisseria PubMLST database material Please select attribute isolate Enter your list of attribute values below (one per line) H44/76 MCSS alpha14 Act Re	ers clude old record versions	Display/so Order by Display	rt options : id	•	ascendi	ng 🔻	
4 records returned. Click the hyperlinks for detailed information.							
Isolate fields 1			MLST	Finet	ping antig	ens	
id isolate aliases country year disease	species	serogroup S		PorA VR1			
30 14 alpha14 Germany 1999 carrier	Neisseria meningitidis	NG 5	3 ST-53 complex	7	30-3	F5-5	
237 H44/76 44/76-3; Z3842 Norway 1976 invasive (unspecified/oth			2 ST-32 complex/ET-5 complex	7	16	F3-3	
240 MC58 Z7176 UK 1983	Neisseria meningitidis		4 ST-32 complex/ET-5 complex	7	16-2	F1-5	
20477 H44/76 44/76-3; Z3842 Norway 1976 invasive (unspecified/oth	er) Neisseria meningitidis	B 3	2 ST-32 complex/ET-5 complex	7	16	F3-3	
Analysis tools: Breakdown: Fields Two Field Codons Polymorphic sites Comb Analysis: BURST Presence/Absence Genome Comparator BLAS Export Dataset Contigs Sequences	inations Cohemes/alleles	Publications	Sequence bin Tag status				

11.9 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	
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 p 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 n	
 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 General information • Isolates: 34221 • Last updated: 2015-07-02 • Update history • About BIGSdb
Breakdown Export Analysis Miscellaneous • Single field • Export dataset • Configs • Condigs • Codon usage • Description of or • Unique combinations • Scheme and alleles • Sequences - XMFA / concatenated FASTA formats • Cadon usage • Description of or • Sequence bin • Sequence bin • Sequences - XMFA / concatenated FASTA formats • Description of or	

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

TIM CLUY	ST	Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissi	ons	
ublicat	tior	n breakdown of dataset		
	or: 🖌	Display NI authors Order by: number of isolates ↓ descending ↓ NI years ↓ Display: 25 ↓ records per page	Action —— Submit	
'age: <u>1</u> 2		d (1 - 25 displayed). Click the hyperlinks for detailed information.		
PubMed id Y	′ ear	Citation	Title	lsolates in database
17517841 2		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 2		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 2		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 2		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 2		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 2	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
18375809 2	8002	Russell JE. Urwin R. Grav SJ. Fox AJ. Feavers IM. Maiden MC (2008) Microbiology 154:	Molecular epidemiology of meningococcal disease in England and	223 ieolatee

These can be filtered by author and/or year, and the sort order changed.

ublica	tio	n breakdown of dataset		
	nor:	Jolley KA ▼ Order by: number of isolates ▼ descending ▼ Submit All years ▼ Display: 25 ▼ records per page		
PubMed	eturne Year	d. Click the hyperlinks for detailed information. Citation	Title	Isolates in database
	2007	Taha MK, Vázquez JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enriquez R, Fazio C, Frosch M, Heuberger S, Hoffmann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczynska A, Stefanelli P, Thulin S, Tzanakaki G, Unemo M, Vogel U, Zarantonelli ML (2007) Antimicrob Agents Chemother 51: 2784-92	Target gene sequencing to characterize the penicillin G susceptibility of 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	Query: 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 b Author: Year:			
13 records return	d. Click the hyperlinks for detailed information.		
PubMed id Year	Citation	Title	lsolates in database
17517841 2007	Taha MK, Vázquez JA, Hong E, Bennett DE, Bertrand S, Bukovski S, Cafferkey MT, Carion F, Christensen JJ, Diggle M, Edwards G, Enríquez R, Fazio C, Frosch M, Heuberger S, Hoffmann S, Jolley KA, Kadlubowski M, Kechrid A, Kesanopoulos K, Kriz P, Lambertsen L, Levenet I, Musilek M, Paragi M, Saguer A, Skoczynska A, Stefanelli P, Thulin S, Tzanakai G, Unemo M, Vogel U, Zarantonelli ML (2007) Antimicrob Agents Chemother 51 : 2784-92	Target gene sequencing to characterize the penicillin G susceptibility of Neisseria meningitidis.	1670 isolates
18815379 2008	Buckee CO, Jolley KA, Recker M, Penman B, Kriz P, Gupta S, Maiden MC (2008) Proc Natl Acad Sci U S A 105: 15082-7	Role of selection in the emergence of lineages and the evolution of virulence in Neisseria meningitidis.	1054 isolates
15776372 2005	Claus H, Maiden MC, Wilson DJ, McCarthy ND, Jolley KA, Urwin R, Hessler F, Frosch M, Vogel U (2005) J Infect Dis 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
11101585 2000	Iollev KA Kalmusova I Feil E L Gunta S Musilek M Kriz P Maiden MC (2000) I Clin Microbiol 38: 4492-8	Carried meningococci in the Czech Republic: a	017:

The abstract of the paper will be displayed (if available), along with all isolates linked to it.

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nn eC		ry (PubM	ed id: 178	2500								
ec	nett IS Ioli			2003	91)							
e	cies status seven loci l ilation gene species. A ecords retu	of Neisseria (leisseria MLS tic inferences nalysis of vari med (1 - 25 dia	onorrhoeae: e T scheme was to be made, in ation at a singl	evolution readil icludin le locus the hy	g direct comparisons with N.	nferences from multiloc isolates, providing a hig meningitidis and N. lact ns of identifying misclass	hly discrimir amica. Exan	natory	ng. typing method. In addition, th on of these data demonstrated I determining whether mixed (that allele	s were rar	ely shared amo
				1	solate fields 👔							
id	isolate	-8							MLST	Finet	ping antig	ens
		aliases	country	year	disease	species	serogroup	ST		Finet <u></u> PorA VR1		
1	A4/M1027	B1; Z1001	country USA	year			serogroup A	ST 4				
	A4/M1027 120M			year 1937	disease	Neisseria meningitidis			clonal complex	PorA VR1	PorA VR2	FetA VR
2		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	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	cional 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
2 7 10	120M 7891	B1; Z1001 B35; Z1035 B54; Z1054	USA Pakistan Finland	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	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 I/I 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	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	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	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 11 13 19	120M 7891 6748 129 139M	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099	USA Pakistan Finland Canada Germany Philippines	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	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/II ST-5 complex/subgroup I/II ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II ST-1 complex/subgroup I/II	PorA VR1 5-2 5-2 20 18-1 5-2 5-2 5-2	PorA VR2 10 10 9 3 10 10	FetA VR F1-5 F5-1 F3-1 F5-1 F3-6 F5-1
2 7 10 11 13 19 24	120M 7891 6748 129 139M \$3131	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 5 1 1 1 4	clonal complex ST-4 complex/subgroup IV ST-1 complex/subgroup I/I ST-5 complex/subgroup III ST-1 complex/subgroup I/I ST-1 complex/subgroup I/I 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	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)	Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis Neisseria meningitidis	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/II 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 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	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 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 5-1 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	120M 7891 6748 129 139M \$3131 \$4355 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 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 5-1 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 F5-1 F3-6 F5-1 F1-5 F3-1 F1-5 F1-7
2 7 10 11 13 19 24 31 34 35 46	120M 7891 6748 129 139M \$3131 \$4355 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 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 A A	4 5 1 1 4 5 4 1 4 4	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 IV ST-5 complex/subgroup IV ST-5 complex/subgroup IV ST-1 complex/subgroup IVI ST-1 complex/subgroup IVI	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 F5-1 F3-6 F5-1 F3-6 F5-1 F1-5 F3-1 F1-5 F1-7 F1-5
2 7 10 11 13 19 24 31 34 35 46 52	120M 7891 6748 129 339M S3131 S4355 10 20 26 255	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B275; 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 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	PorA VR2 10 10 9 3 10 10 13-1 9 13-1 10 13-1 10 13 13-1	FetA VR F1-5 F5-1 F3-1 F3-6 F5-1 F1-5 F3-1 F1-5 F3-1 F1-5 F1-7 F1-5 F1-5
2 7 10 11 13 19 24 31 34 35 46 52 61	120M 7891 6748 129 139M S3131 S4355 10 20 26 255 243 393	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B275; Z1276 B318; Z1388 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 5-2 200 18-1 5-2 5-2 7 5-1 7 5-2 7 7-2 7 7-2 7 5-2	PorA VR2 10 10 9 3 10 10 13-1 9 13-1 10 13-1 13 13-1 13 10	FetA VR F1-5 F5-1 F3-1 F3-1 F3-1 F3-1 F3-1 F1-5 F3-1 F1-5 F1-5 F1-5 F1-5 F1-5 F1-5 F1-5 F5-1
2 7 10 11 13 19 24 31 34 35 46 52	120M 7891 6748 129 339M S3131 S4355 10 20 26 255 243	B1; Z1001 B35; Z1035 B54; Z1054 B73; Z1073 B92; Z1092 B99; Z1099 B213; Z1213 B227; Z1227 B269; Z1269 B275; Z1275 B278; Z1278 B318; Z1318 B3362; Z1362	USA Pakistan Finland Canada Germany Philippines Ghana Denmark Burkina Faso Niger Burkina Faso Cameroon Greece Djibouti	year 1937 1967 1975 1971 1964 1968 1973 1974 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	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 20 18-1 5-2 5-2 7 5-2 7 5-1 7 5-2 7 5-2 7 7-2 7	PorA VR2 10 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 F3-6 F5-1 F1-5 F3-1 F1-5 F1-7 F1-5 F1-5 F1-5 F1-5

11.10 User-configurable options

The BIGSdb user interface is configurable in a number of ways. Choices made are remembered between sessions. If the database requires you to log on, the options are associated with your user account, whereas if it is a public database, that you haven't logged in to, the options are associated with a browser cookie so they will be remembered if you connect from the same computer (using the same browser).

Most options are set by clicking the 'Set general options' link on the database contents page. Most of the available options are visible for isolate databases, whereas sequence definition databases have fewer available.

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 not a submitted to 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 not a submitted to 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 not a submitted to 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 not a submitted to the database to the database to the database and consequently it should be noted that it does not a submitted to the database to the databas	
 Query database Search database - advanced queries. Browse database - peruse all records. Search by combinations of loci (profiles) - including partial matching. Stat query - find isolates by matching a field to an entered list. Projects - main projects defined in database. 	Submissions • Manage submissions General information • Isolates: 34221 • Last updated: 2015-07-02 • Update history • About BIGSdb
Breakdown Export Analysis Miscellaneou • Single field • Export dataset • Contigs • Codon usage • Description of • Unique combinations • Scheme and alleles • Sequences - XMFA / concatenated FASTA formats • Codon usage • Description of • Publications • Sequence bin • Sequence bin • BLAST • BLAST	

11.10.1 General options

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

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 dont 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. • Ceneral options • Lipslay 25 • lecords per page. Page bar position: top and bottom • Display 100 • nucleotides per line in sequence alignments. Display 100 • nucleotides of flanking sequence (where available). • Enable tooltips (teginner's mode). • Solate record display • Provenance field display • Our officer • Our officer • Conter al to defaults	ProhMUST Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
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 bary position: top and bottom Display 100 nucleotides per line in sequence alignments. Display 100 nucleotides per line in sequence alignments. Display 100 nucleotides per line in sequence (where available). Display locus aliases if set Stolate record display Provenance field display Ouery filters 		
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). Display 100 Page bar position: top and bottom Display 100 nucleotides of flanking sequence (where available).	Set database options	
Display 25 records per page. Page bar position: lop and bottom ~ Display 100 rucleotides per line in sequence alignments. Display 100 rucleotides of flanking sequence (where available). Ø Enable tootlips (beginner's mode). Set options > Main results table > Isolate record display > Provenance field display > Query filters		t
Page bar position: top and bottom Display 100 - nucleotides of flanking sequence alignments. Display 100 - nucleotides of flanking sequence (where available). Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases if set Image: Display locus aliases i	✓ General options	٦
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 Nain results table Isolate record display Provenance field display Provenance field display Query filters		
Display 100 v nucleotides of flanking sequence (where available). © Display focus aliases if set. © 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.		
Image: Construction of the set of t	Display 100 nucleotides of flanking sequence (where available).	
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.		
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.	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.	Main results table	
Ouery filters Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences.	 Isolate record display 	
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences.	Provenance field display	
Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences.	 Query filters 	
Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences.		
	Reset	
Reset all to defaults	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.

11.10.2 Main results table

The 'main results table' tab contains options for the display of paged results following a query.

Click the 'Main results table' header to display the tab.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
▼ General options
Display 25
➤ Main results table
Isolate record display
Provenance field display
► Query filters
Reset Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences. Reset all to defaults

The 'main results table' tab will scroll up.

Ouery: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/Sequences definitions Database submissions
Help 2"
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
General options
✓ Main results table
Hyperlink allele designations where possible. Display information about sequence bin records tagged with locus information (toottip). 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.

11.10.3 Isolate record display

The 'isolate record display' tab contains options for the display of a full isolate record.

Click the 'Isolate record display' tab to display the tab.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
- 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 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.

Cuery: Search Browse Profile/ST List Prr In MILST Readdown: Solar fields Scheme/alteles Publications Links: Contents Home Options Profiles/Sequences definitions Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
General options
► Main results table
✓ Isolate record display
Differentiate provisional allele designations. Display sender, curator and last updated details for allele designations (tooltip). Display information about sequence bin records tagged with locus information (tooltip). Display information about whether alleles have flags defined in sequence definition database (shown in sequence detail tooltip). Display 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.

11.10.4 Provenance field display

The 'provenance field display' tab contains checkboxes for fields to display in the main results table.

Click the 'Provenance field display' tab to display the tab.

Ouery: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Set database options
Here you can set options for your use of the website. Options are remembered between sessions and affect the current database (Neisseria PubMLST) only. If some of the options don't appear to set when you next go to a query page, try refreshing the page (Shift + Refresh) as some pages are cached by your browser.
▼ General options
Display 25 • records per page. Page bar position: top and bottom • Display 100 • nucleotides per line in sequence alignments. Display 100 • nucleotides of flanking sequence (where available). I bisplay locus aliases if set Enable tooltips (beginner's mode). Set options
Main results table
► Isolate record display
Provenance field display
Query filters
Reset
Click the reset button to remove all user settings for this database - this includes locus and scheme field preferences.
Reset all to defaults

The 'Provenance field display' tab will scroll up.

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 s hing the page (Shift + Refresh) as some pages		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 cettriaxone cettriaxone_range chloramphenicol chloramphenicol_range cefotaxime_range cefotaxime_range rifampicin_range ciprofloxacin	cus and scheme data can be made by performing a ciprofloxacin_range pending_assembly assembly_status ENA_accession private_project comments sender curator date_entered datestamp			
Query filters Reset Click the reset button to remove all user so Reset all to defaults	ettings for this database - this includes locus 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'.

11.10.5 Query filters

The 'query filters' tab contains checkboxes for provenance fields and scheme completion status. Checking these results in drop-down list box filters appearing in the query page *filters fieldset*.

Click the 'Query filters' tab to display the tab.

ProfixILST 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 'Query filters' tab will scroll up.

solate record display		
Provenance field display		
Query filters		
Select the fields for which you would like dropdow isolate country continent region year epidemiological_year age_yr age_yr age_mth sex disease source epidemiology species serogroup MLEE_designation serotype ET_no penicillin subtype ET_no penicillin subtype ET_no penicillin ceftriaxone_range chloramphenicol_range coltaxime_range coltaxime_range coltaxime_range coltaxime_range coltaxime_range coltaxime_range coltaxime_range coltaxime_range coltaxime_range coltaxime_range coltaxime_range coltaxime_range coltaxime_range coltoramphenicol_range coltoramphenicol_range coltoxacin_r	n lists containing known values on which to filter query results. These wi ENA_accession private_project comments sender curator date_entered datestamp MLST profile completion Finetyping antigens profile completion ADP-heptose biosynthesis profile completion ADP-heptose biosynthesis profile completion Antibiotic resistance profile completion Antibiotic resistance profile completion Capsule Region A - Serogroup A profile completion Capsule Region A - Serogroup D profile completion Capsule Region A - Serogroup Y profile completion Capsule Region D and D' profile completion NA replication profile completion NA replication profile completion NA replication profile completion NA replication profile completion Conocccal Genetic Island profile completion Gonocccal Genetic Island profile completion Kdo addition profile completion	Il be available in the filters section of the query interface. LOS alpha chain transferases profile completion LOS transport/export profile completion Lipid A biosynthesis: adyltransferases profile completion N. meningitdis profile completion N. meningitdis profile completion N. meningitdis profile completion Protein glycosylation profile completion Protein glycosylation profile completion Prinuis genes profile completion Printe metabolism profile completion Printe metabolism profile completion Printe metabolism profile completion Printe metabolism profile completion RNA polymerase profile completion Small regulatory RNAs profile completion UDP-GlcNAc synthesis profile completion UDP-GlcNAc synthesis profile completion WirB TASS profile completion WirB TASS profile completion MLST (20 locus partial genes) profile completion MLST (20 locus whole genes) profile completion Publications

A list of possible filters appears. Click any checkbox for a filter you would like to make available. Click 'Set options' when done. You can return to the default selection by clicking 'Default' followed by 'Set options'.

11.10.6 Modifying locus and scheme display options

Whether or not loci, schemes or scheme fields are displayed in result tables, isolate records, or within query dropdown boxes can all be set with default options when first defined. These attributes can, however, be overridden by a user, and these selections will be remembered between sessions.

The procedure to modify these attributes is the same for locus, schemes or scheme fields, so the steps for loci will be demonstrated only.

Click the appropriate link on the isolate contents page.

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. 	ptions - including isolate table field handling. ad query options for locus, schemes or scheme fields. General information - isolates: 34221 - Last updated: 2015-07-02 - Update history
Breakdown Export Analysis Miscellaneous • Single field • Export dataset • Contigs • Contigs • Contigs • Unique combinations • Scheme and alleles • Sequences - XMFA / concatenated FASTA formats • Codon usage • Description of database fields • Publications • Sequence bin • Sequence bin • Sequence bin • Export • Export	Codon usage • Description of database fields Presence/absence status of loci Genome comparator

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	
Togg	gle: 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	
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* guery field* analysis*	
abcZ DNA integer 433 false true 1 1176340 allele only false true true	
* Default values are displayed for this field. These may be overridden by user preference.	

Designations can be queried using standard operators.

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

uery			enta Frion	ne Options P	Profiles/sequer	ations nces defi	nitions Datab	ase submissions					
uery													Toggle: i
	y loci	for Neis	seria	PubML	ST data	base	è.						
Please e	enter your	search criteria	below (or	leave blank ar	nd submit to re	turn all r	ecords). Match	ing loci will be retu	med and you wi	ill then be ab	le to update	their display and query settings.	
Sea	rch criteria	a					— — Display						
id		▼ =		•		+	_	by: id	•	ascendin	g 👻		
							Disp	lay: 25 👻 reco	rds per page 🚺]			
—⊽ Fil	Iter query I	by-					Action						
		data type:	•				Reset Su	bmit					
	allele	id format:	-										
	len	gth varies:	v [
	coding s	sequence:											
		orf:	-										
	mate	ch longest:	v i										
		pcr filter:	v [
	р	orobe filter:	v [
		flag table:	- i	_									
		te display:		•									
		in display:	v i										
	C	query field:	– [
		analysis:	– i		_								
	- -	curator:		-									
		scheme: M	LST		•	1							
records	returned.	. Click the hype	rlinks for o	detailed inform	ation.								
Cust	omize —												
	options												
locus	options												
								on isolate display*		query field			
abcZ	DNA	integer	433	false	true	1	1176340	allele only	false	true	true		
adk	DNA DNA	integer	465	false	true	1	991951 2079469	allele only	false	true	true		
aroE fumC	DNA	integer integer	490 465	false false	true true	2	2079469	allele only allele only	false false	true true	true		
gdh	DNA	integer	501	false	true	1	1514394	allele only	false	true	true		
pdhC	DNA	integer	480	false	true	1	1453970	allele only	false	true	true		
pgm	DNA	integer	450	false	true	1	965481	allele only	false	true	true		
Default	values are	displayed for thi	s field. Thes	e may be overri	idden by user pr	eference.							

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

Cus	tomize											
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	
adk	DNA	integer	465	false	true	1	991951	allele only	false	true	true	
aroE	DNA	integer	490	false	true	2	2079469	allele only	false	true	true	
fumC	DNA	integer	465	false	true	1	1592943	allele only	false	true	true	
gdh	DNA	integer	501	false	true	1	1514394	allele only	false	true	true	
pdhC	DNA	integer	480	false	true	1	1453970	allele only	false	true	true	
pgm	DNA	integer	450	false	true	1	965481	allele only	false	true	true	

You can then choose to add or remove individual loci from the selection by clicking the appropriate checkboxes. At the bottom of the page are a number of attributes that you can change - clicking 'Change' will affect all selected loci.

Possible options for loci are:

• isolate_display - Sets how the locus is displayed within an isolate record:

- allele only display only identifier
- sequence display the full sequence
- hide don't show at all
- main_display Sets whether the locus is displayed in the main results table following a query.
- query_field Sets whether the locus appears in dropdown list boxes to be used within queries.
- analysis Sets whether the locus can be used in data analysis functions.

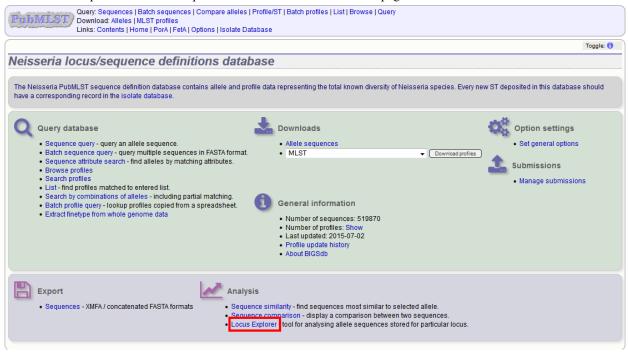
Note: Settings for loci can be overridden by those set for schemes that they are members of. For example, if you set a locus to be displayed within a main results table, but that locus is a member of a scheme and you set that scheme not to be displayed, then the locus will not be shown. Conversely, if you set a scheme to be displayed, but set its member locus not to be shown, then that locus will not be displayed (but other loci and scheme fields may be, depending on their independent settings).

Data analysis plugins

12.1 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.



12.1.1 Polymorphic site analysis

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

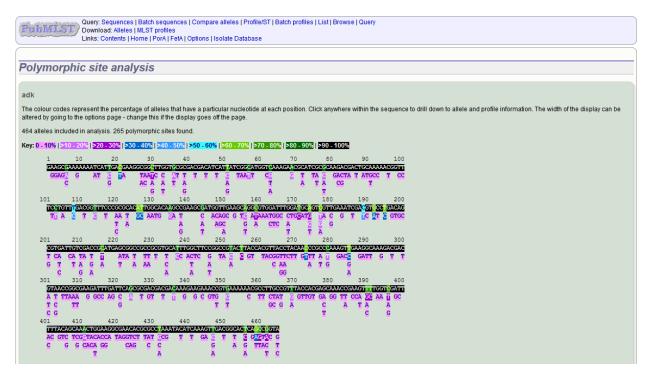
Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Locus Explorer - Neisseria locus/sequence definitions
Please select locus for analysis: Locus: adk - age will reload when changed Select sequences - Analysis functions Polymorphic site frequencies and sequence schematic Codon Calculate G+C content and codon usage Codon Calculate G+C content and codon usage Translate Translate DNA to peptide sequences

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

PTITINIST Owen: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Locus Explorer - Neisseria locus/sequence definitions
Please select locus for analysis:
Locus: adk Page will reload when changed
Select sequences Analysis functions 459 Polymorphic sites 461 Codon 463 Codon 464 Translate AN None

If an alignment is necessary, the job will be submitted to the job queue and the analysis performed. If no alignment is necessary, then the analysis is shown immediately.

The first part of the page shows the schematic.



Clicking any of the sequence bases will calculate the exact frequencies of the different nucleotides at that position.

40 -	50%	>50 -	60%	>60	- 70% >7	0 - 80%
	40		;	50	60)
GGT	'GCGCG	ACGA	CATC	ATTA	TCGGCAT(GTCAAA
С	AT T	Т	ТТ	C	TAATT	CG
A	ТА			Α		Т
Т	G			G		Α
Pub			es Batch seques MLST profile		npare alleles Profile/ST	Batch profiles List Bro
					ns Isolate Database	
Site	Explorer					
	osition 51 eles included in a	nalvsis				
Base	Number of alleles	Percentage				
С	370	79.7	(9	19 / 10883 97.57%)		
A	92	0.2	(2 / 10883 2.41%) / 10883		
G	(adk-351)	0.2	(0.01%) / 10883		
	(adk-413)			0.01%)		

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

•		••			4					
C	G									
401		410		42			30	44		450
									TCAAAC	
C			ACA			GTCT T CAG	C C	3 T	T GA	G
<u> </u>	g		T	00		CAG	Ă			A
lucleoti	de fre	que	encie	es 🛛						
						Nucleot	ido			
osition 🗢	Δ 🚖	∩		T 🔺		%A ≑		KC 🔺	%T \$	
2	463	0	1	0	0	99.78	70C V	0.22		
3	462	0	2	0	0	99.57		0.43		
4	1	0	463	0	0	0.22		99.78		
5	0	463	1	0	0		99.78			
6	52	7	405	0	0	11.21	1.51	87.28		
9	463	0	1	0	0	99.78		0.22		
14	1	0	0	463	0	0.22			99.78	
15	0	452	0	12	0		97.41		2.59	
18	0	76	7	381	0		16.38	1.51	82.11	
21	0	295	0	169	0		63.58		36.42	
22	8	0	456	0	0	1.72		98.28		
27	3	451	0	10	0		97.20		2.16	
28	2	1	461	0	0		0.22			
29	1	0	463	0	0	0.22		99.78		
30	3	341	1	119	0	0.65	73.49	0.22		
31	0	10	0	454	0		2.16		97.84	
33	2	5	455		0	0.43	1.08			
36	51	0	410			10.99		88.36		
37	0	463	0	1	0		99.78		0.22	

See also:

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

12.1.2 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
Locus Explorer - Neissena locus/sequence dennitions
Please select locus for analysis:
Locus: adk Page will reload when changed
Select sequences - Analysis functions 450 461 462 463 464 463 464 465 465 465 467 468 468 468 468 468 468 468 468

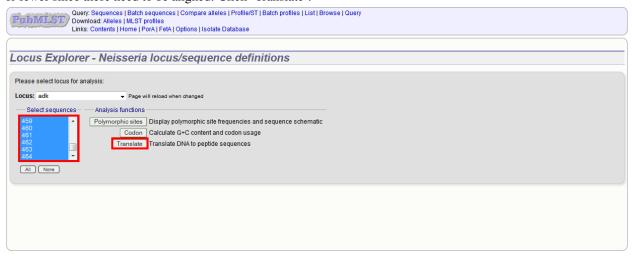
The GC content of the alleles will be determined and a table of the codon frequencies displayed.

Codon Usage adk ORF use1 1 464 alleles included in analysis. Gc ontent Coding (Co 52 47%) Stalleletr: CC 6531% And letter: CC 3173% Xit letter: CC 6531% Coding (So 22 47%) Stalletter: CC 6531% Coding (Annue, Coding 173%) Xit letter: CC 6531% Coding (Annue, Coding 174%) Stalletter: CC 6531% Coding (Annue, Coding 174%) Stalletter: CC 6531% Coding (Annue, Coding 174%) Stalletter: CC 6037% Coding (Annue, Coding 174%) Stalletter: CC 517%) Stalletter: CC 517% Stalletter: CC 517%) Stalletter: CC 517% Stalletter: CC 517%	Mdu	LST/Dc	iery: Sequence ownload: Allele hks: Contents	s MLST profil	les	
adk ORF used: 1 484 allelse included in analysis. GC ontent Coding: GC 52.47% Istelletr: GC 6531% And letter: GC 6031% Stelletr: GC 6531% And letter: GC 0037% Coding: GC 52.47% Istelletr: GC 0037% Coding: GC 52.47% Istelletr: GC 0037% Coding: GC 52.47% Istelletr: GC 0037% Coding: GM 100 mUltipation of Usage of a given codin among its redundant set (i.e. the set of codons which code for this codon's amino add). Frequency: Usage of given codon per 1000 codons. Coding: GM 100 mUltipation of Usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino add). Frequency: Usage of given codon per 1000 codons. GCG A 0.289 2.5.751 1852 GCG A 0.289 2.5.751 1852 GCG A 0.289 2.5.751 1852 GCG A 0.283 30.812 2.216 GAA D 0.027 30.812 2.216 GAA D 0.027 30.812 2.216 GAA D 0.044 7.593 5926 GAA E 0.916 82.397 <th>odon</th> <th>Usage</th> <th>2</th> <th></th> <th></th>	odon	Usage	2			
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State CG 63:31% 2nd letter: CC 60.37% Codons Fracton: Proportion of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid). requency: Usage of given codon per 1000 codons. Codon # Codo # Codon #	oding: GC	52.47%				
and letter: GC 60.37% Colons Fraction: Proportion of usage of a given codon among its redundant set (i.e. the set of codons which code for this codon's amino acid). Frequency: Usage of given codon per 1000 codons: Codo 4 0.262 17.353 1248 GCC A 0.389 25.751 1852 GCC C 0.987 6.452 464 TGC C 0.013 0.083 6 GAA E 0.016 82.397 5926 GAA E 0.016 82.397 5926 GAA GC 0.007 0.542 39 GCA GC <t< th=""><th>st letter: G</th><th>C 65.31%</th><th></th><th></th><th></th></t<>	st letter: G	C 65.31%				
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GAC D 0.747 91.073 6550 GAT D 0.253 30.812 2216 GAA E 0.916 82.397 5926 GAG E 0.084 7.564 544 TTC F 0.594 15.295 1100 TTT F 0.406 10.470 753 GGA G 0.007 0.542 39 GGC G 0.011 0.422 3 GGT G 0.227 17.659 1270 CAX H 0.749 19.258 1385 CAT H 0.251 6.438 463	odon ♦ A GCA GCC GCC GCG GCT	Usage of giv Amino acid + A A A A A A	 Fraction \$ 0.262 0.246 0.389 0.103 	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813	Number \$ 1248 1169 1852 490	
GAT D 0.253 30.812 2216 GAA E 0.916 82.397 5926 GAG E 0.084 7.564 544 TTC F 0.594 15.295 1100 TTT F 0.406 10.470 753 GGA G 0.007 0.542 39 GGC G 0.017 0.542 39 GGC G 0.012 3 3 GGT G 0.227 17.659 1270 CAZ H 0.749 19.258 1385 CAT H 0.251 6.438 463	odon 🔶 A GCA GCC GCC GCC GCT TGC	Usage of giv Amino acid 4 A A A A A C	en codon per 1 Fraction Colored Colo	1000 codons. Frequency ↓ 17.353 16.254 25.751 6.813 6.452	Number ≑ 1248 1169 1852 490 464	
GAA E 0.916 82.397 5926 GAG E 0.084 7.564 544 TTC F 0.594 15.295 1100 TTT F 0.406 10.470 753 GGA G 0.007 0.542 39 GGC G 0.765 59.497 4279 GGG G 0.001 0.042 3 GGT G 0.227 17.659 1270 CAC H 0.749 19.258 1385 CAT H 0.251 6.438 463	odon + A GCA GCC GCC GCC GCT TGC TGT	Usage of giv Amino acid 4 A A A A A C C C	en codon per 1 Fraction Colored Colo	1000 codons. Frequency ↓ 17.353 16.254 25.751 6.813 6.452 0.083	Number ¢ 1248 1169 1852 490 464 6	
GAG E 0.084 7.564 544 TTC F 0.594 15.295 1100 TTT F 0.406 10.470 753 GGA G 0.007 0.542 39 GGC G 0.765 59.497 4279 GGG G 0.010 0.042 3 GGT G 0.227 17.659 1270 CAC H 0.749 19.258 1385 CAT H 0.251 6.438 463	equency: odon + A GCA GCC GCG GCT TGC TGT GAC	Usage of giv Amino acid 4 A A A A C C C C D	en codon per 1 Fraction + 0.262 0.246 0.389 0.103 0.987 0.013 0.747	1000 codons. Frequency ◆ 17.353 16.254 25.751 6.813 6.452 0.083 91.073	Number 1248 1169 1852 490 464 6 6550	
TTC F 0.594 15.295 1100 TTT F 0.406 10.470 753 GGA G 0.007 0.542 39 GGC G 0.765 59.497 4279 GGG G 0.001 0.042 3 GGT G 0.227 17.659 1270 CAC H 0.749 19.258 1385 CAT H 0.251 6.438 463	equency: odon \$ A GCA GCC GCG GCT TGC TGT GAC GAT	Usage of giv Amino acid ¢ A A A A C C C C C D D D	en codon per 1 Fraction + 0.262 0.246 0.389 0.103 0.987 0.013 0.747	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.452 0.083 91.073 30.812	Number + 1248 1169 1852 490 464 6 6550 2216	
TTT F 0.406 10.470 753 GGA G 0.007 0.542 39 GGC G 0.755 59.497 4279 GGG G 0.001 0.042 3 GGT G 0.227 17.659 1270 CAC H 0.749 19.258 1385 CAT H 0.251 6.438 463	equency: odon \$ A GCA GCC GCG GCT TGC TGT GAC GAT	Usage of giv Amino acid ¢ A A A A C C C C D D D E	en codon per 1 Fraction + 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.452 0.083 91.073 30.812	Number + 1248 1169 1852 490 464 6 6550 2216	
GGA G 0.007 0.542 39 GGC G 0.765 59.497 4279 GGG G 0.011 0.042 3 GGT G 0.227 17.659 1270 CAC H 0.749 19.258 1385 CAT H 0.251 6.438 463	equency: odon \$ A GCA GCC GCG GCT TGC TGT GAC GAT GAA	Usage of giv Amino acid ¢ A A A A C C C C D D D E	en codon per 1 • Fraction	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397	Number + 1248 1169 1852 490 464 6 5550 2216 5926	
GGC G 0.765 59.497 4279 GGG G 0.001 0.042 3 GGT G 0.227 17.659 1270 CAC H 0.745 1385 CAT H 0.251 6.438 463	don + A GCA GCC GCG GCT TGC TGC TGT GAC GAT GAA GAG	Usage of giv Amino acid 4 A A A C C C D D E E E	en codon per 1 ► Fraction ← 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.084	1000 codons. Frequency ⇒ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564	Number 1248 1169 1852 490 464 6 6550 2216 5926 544	
GGG G 0.001 0.042 3 GGT G 0.227 17.559 1270 CAC H 0.749 19.258 1385 CAT H 0.251 6.438 463	equency: GCA GCC GCG GCT TGC TGT GAC GAT GAA GAA GAG TTC	Usage of giv Amino acid 4 A A A C C C D D D E E E F	en codon per 1 ► Fraction ← 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.084 0.594	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295	Number ◆ 1248 1169 1852 490 464 6 550 2216 5926 544 1100	
GGT G 0.227 17.659 1270 CAC H 0.749 19.258 1385 CAT H 0.251 6.438 463	requency: odon ↓ GCA GCC GAA GAG TTC TTT	Usage of giv Amino acid 4 A A A A C C C C D D D E E E F F	en codon per 1 Fraction ← 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.084 0.594 0.406	1000 codons. Frequency ◆ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470	Number ◆ 1248 1169 1852 490 464 6 6 5550 2216 5926 544 1100 753	
GGT G 0.227 17.659 1270 CAC H 0.749 19.258 1385 CAT H 0.251 6.438 463	odon ↓ / GCA GCC GCC GCC GCC GCC GCT TGC TGT GAC GAA GAG TTC TTT GGA GGA	Usage of giv Amino acid A A A A C C C C C D D E E E F F G	en codon per 1 Fraction Fraction Code Code Code Code Code Code Code Code	1000 codons. Frequency ◆ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.542	Number 1248 1169 1852 490 464 6 6550 2216 5926 544 1100 753 39	
CAC H 0.749 19.258 1385 CAT H 0.251 6.438 463	requency: odon \$ # GCA GCC GCC GCG GCT TGT GAC GAC GAC GAA GAG TTC TTT GGA GGC	Usage of giv Amino acid 4 A A A A C C C D D C C D D E E E F F F G G G	en codon per 1 Fraction ← 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.094 0.594 0.406 0.007 0.765	1000 codons. Frequency ◆ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.542 59.497	Number ↓ 1248 1169 1852 490 464 6 6550 2216 5926 544 1100 753 39 4279	
CAT H 0.251 6.438 463	requency: odon ◆ # GCA GCC GCG GCC GCG GCC GCG GCT TGT GAC GAT GAA GAG TTC TTT GGA GGC GGC GGA GGC GGA GGC GGG GGG	Usage of giv Amino acid A A A A A C C C C D D D E E E E F F G G G G	en codon per 1 > Fraction + 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.084 0.594 0.406 0.007 0.765 0.001	1000 codons. Frequency ◆ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.542 59.497 0.042	Number ◆ 1248 1169 1852 490 464 6 6550 2216 5926 544 1100 753 39 4279 3	
	equency: odon + / GCA GCC GCC GCT TGC TGT GAC GAC GAA GAG TTC TTT GGA GGG GGG GGG	Usage of giv Amino acid 4 A A A A A C C C D D D D D D D D C C D D C C C C	en codon per 1 > Fraction + 0.262 0.246 0.389 0.103 0.987 0.013 0.747 0.253 0.916 0.084 0.594 0.406 0.007 0.765 0.001 0.227	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.542 59.497 0.042 59.497 17.559	Number ♦ 1248 1169 1852 490 464 6 6 6550 2216 5926 544 1100 753 39 4279 3 1270	
	equency: odon + GCA GCC GCG GCT TGC TGC TGT GAC GAT GAA GAG TTT GGA GGG GGG GGT CAC	Usage of giv Imino acid 4 A A A A C C C C D D D E E F F G G G G H	en codon per 1	1000 codons. Frequency ♦ 17.353 16.254 25.751 6.813 6.452 0.083 91.073 30.812 82.397 7.564 15.295 10.470 0.470 0.447 0.042 17.659 19.258	Number ♦ 1248 1169 1852 490 464 6 6550 2216 5926 544 1100 753 39 4279 3 0 1270 31 85	

12.1.3 Aligned translations

If a DNA coding sequence locus is selected, an aligned translation can be produced.

Select the alleles that you would like to include in the analysis. Again, variable length loci are limited to 200 sequences or fewer since these need to be aligned. Click 'Translate'.



An aligned amino acid sequence will be displayed.

933 1	
134 1	L
35_1	T
36 1	
37 1	
137_1	
-	
139_1	
40_1	К.
41_1	
42_1	
43_1	
44_1	
45_1	
46_1	
47_1	
48_1	
149_1	
150_1	
151_1	
52_1	КТТ.
53_1	
54_1	IAT
155_1	
56_1	
57_1	G
58_1	
59_1	
60_1	<u>s</u>
61_1	
62_1	
63_1	
64_1	I
onsensus	eakkiidegglvrddiiigmvkeriaqddckngflfdgfprilaqaeamveagvdldavveidvpdsvivdrmsgrrvhlasgrtyhvtynppkvegkdd
	110 120 130 140 150
	:
_1	
_1	
_1	
_1	
_1	
5_1 5_1 7_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.

12.2 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 Nei database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and								
 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 Single field Wo field Unique combinations Scheme and alleles Publications Sequence bin Breakdown Export dataset Contigs Sequences - XMFA / concatenated FASTA formats Analysis Codon usage Presence/abs Genome com BLAST	Miscellaneous Description of database fields aparator							

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.

1						~						
5 M00240227		UK		invasive (unspecified/other)					ST-32 complex/ET-5 complex	7	16	
6 M00282207		UK		invasive (unspecified/other)				1101	ST-22 complex			
7 7891	B54; Z1054	Finland		invasive (unspecified/other)				5	ST-5 complex/subgroup III	20	9	F3-1
8 M00242007		UK		invasive (unspecified/other)				1102	ST-18 complex		14	
9 0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria	meningitid	is W	114	ST-22 complex			
10 6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria	meningitid	is A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11 129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria	meningitid	is A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12 0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria	meningitid	is B	1015	ST-32 complex/ET-5 complex	7	16	
13 139M	B99; Z1099	Philippines	1968		Neisseria	meningitid	is A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14 0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria	meningitid	is X	117			14	
15 1		Germany	1999	carrier	Neisseria	meningitid	is E	864				
16 2		Germany	1999	carrier	Neisseria	meningitid	is B	854	ST-18 complex			
17 3		Germany	1999	carrier	Neisseria	meningitid	is W	174	ST-174 complex			
18 4		Germany	1999	carrier	Neisseria	meningitid	is B	19	ST-18 complex			
19 S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria	meningitid	is A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20 5		Germany	1999	carrier	Neisseria	meningitid	is NG	198	ST-198 complex			
21 6		Germany	1999	carrier	Neisseria	meningitid	is NG	198	ST-198 complex			
22 7		Germany	1999	carrier	Neisseria	meningitid	is E	60	ST-60 complex			
23 8		Germany	1999	carrier	Neisseria	meningitid	is B	32	ST-32 complex/ET-5 complex			
24 S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria	meningitid	is A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25 9		Germany	1999	carrier	Neisseria	meningitid	is B	930	ST-334 complex			
	ields Two Fi	ence/Absence	Genome	norphic sites Combinations a Comparator BLAST	Schemes/	alleles F	Publications	Seque	nce bin) Teg status			

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

Prohitist Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Field breakdown of dataset
country continent region year epidemiological year age yr age mth sex disease source epidemiology species serogroup MLEE designation serotype sero subtype ET no peniciliin range amoxiciliin cettriaxone range chloramphenicol range cefotaxime range rifampicin range ciprofloxacin range
country
UK (7300 - 25.02%) Italy (334 - 1.11%) Czech Republic (2684 - 9.20%) Bigliun (362 - 1.24%) Word (368 - 1.26%) Proce (2047 - 7.02%) France (2047 - 7.02%) France (2047 - 7.02%) The Netherbards (1301 - 4.46%) Disk (486 - 1.56%) Usck (868 - 9.30%) Disk (486 - 1.56%) Disk (486 - 1.66%) Disk (486 - 1.56%) Disk (486 - 1.56%) Disk (486 - 1.56%) Disk (486 - 1.26%) Disk (486 - 1.56%) Disk (486 - 1.56%) Disk (486 - 1.56%) Disk (486 - 1.56%) Disk (486 - 1.56%) Disk (486 - 1.26%) Disk (486 - 1.56%) Disk (486 - 1.56%) Disk (486 - 1.56%)
Display table Tab-delimited text Excel format

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

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Field breakdown of dataset
country continent region year epidemiological year age yr age mth sex disease source epidemiology species serogroup MLEE designation serotype sero subtype ET no penicillin range amoxicillin ceftriaxone range chloramphenicol range cefotaxime range rifampicin range ciprofloxacin range
country
UK (7300 - 25.02%) all others (91 values) (3066 - 10.51%) Ceech Republic (2684 - 9.20%) Beiguin (368 - 1.26%) Warr (368 - 1.26%) Switch (368 - 1.26%) Cermany (2123 - 7.26%) Prance (2047 - 7.02%) Spain (1481 - 5.06%) Diana (405 - 1.36%) UbA (869 - 0.26%) Diana (405 - 1.56%) UbA (869 - 2.05%) Diana (768 - 2.70%) Ohma (768 - 2.70%) Norway (760 - 2.60%)
Display table Tab-delimited text Excel format

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

Users Search Browse (Profile/ST List Breakdown: Isolate fields (Scheme/alleles (Publications Links: Contents Home Options Profiles/Sequences definitions Database submissions									
LINK	s. Contents H	me Options Promes/sequence	delinitions Database submissions						
akdown by	country	,		Show					
alues.									
		Percentage 🗢							
UK	7300	25.02%							
Czech Republic	2684	9.20%							
Germany	2123	7.28%							
France	2047	7.02%							
Spain	1481	5.08%							
he 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.

PUDIALST Breakdown: Isolate fields Scheme-Alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Field breakdown of dataset
country continent region year epidemiological year age yr age mth sex disease source epidemiology species serogroup MLEE designation serotype sero subtype ET no penicillin range amoxicillin ceftriaxone range chloramphenicol range cefotaxime range rifampicin range ciprofloxacin range
country
UK (7300 - 25.02%) III others (91 values) (3066 - 10.51%) Izy (324 - 1.11%) Belgium (352 - 1.24%) Wger (368 - 9.20%) Wger (368 - 1.25%) Farmer (2123 - 7.28%) Belgium (352 - 1.24%) France (2047 - 7.02%) Spain (1481 - 5.08%) The Ideltration (3101 - 44.64) USA (688 - 3.05%) USA (688 - 3.05%) USA (689 - 3.05%) Chrina (789 - 2.70%) For (712 - 2.44%)
Display table Tab-delimited text Excel format

12.3 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
database there is at least one corresponding isolate deposited here. Any isolate m 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.	ay be submitted to this database and consequently it should be noted that it does not represent a population sample. Option settings Set general options - including isolate table field handling. 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 Publications Sequence bin	Analysis Codon usage Presence/absence status of loci Genome comparator BLAST Miscellaneous - Description of database fields

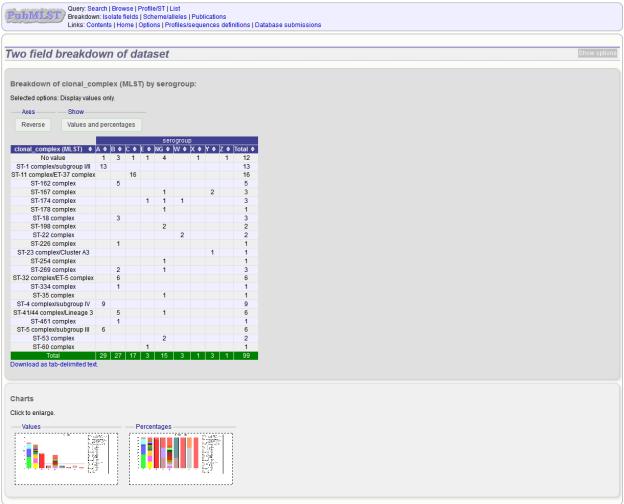
Alternatively, a two field breakdown can be displayed of the dataset returned from a query by clicking the 'Two field' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

M0 0	7891 0242007 0021/84	B54; Z1054			invasive (unspecified/other)	Neisseria meningitidis	w	1101	S1-22 complex			
9 0 10 11			Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	20	9	F3-1
10 11	021/84		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1102	ST-18 complex		14	
11			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
12 0	090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14 0	120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19 \$	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	в	32	ST-32 complex/ET-5 complex			
24 \$	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			

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

Query: Search Browse Profile/S Breakdown: Isolate fields Schen Links: Contents Home Options	ne/alleles Publications	Database submissions		
Two field breakdown of datase	et			Show options
Here you can create a table breaking down one field b Select fields Field 1: clonal complex (MLST) • Field 2: serogroup •	y another, e.g. breakdown of serc — Display — © values only C values and percentages C percentages only	group 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.



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.

12.4 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 definit	ions							
	present the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition nay 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. • Search 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 • Two field Contigs • Publications Sequences - XMFA / concatenated FAS	Analysis Codon usage Presence/absence status of loci Genome comparator BLAST • Description of database fields							

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

	A4/M1027	B1; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
3	M00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1099		19	15	
4	M1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV			
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	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	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	В	930	ST-334 complex			

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

PTTT51/41 31 Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Scheme field and allele breakdown of dataset	Show options
Select schemes or groups of schemes within the tree. A breakdown of the individual fields and loci belonging to these schemes will then be performed.	

Click 'Select'.

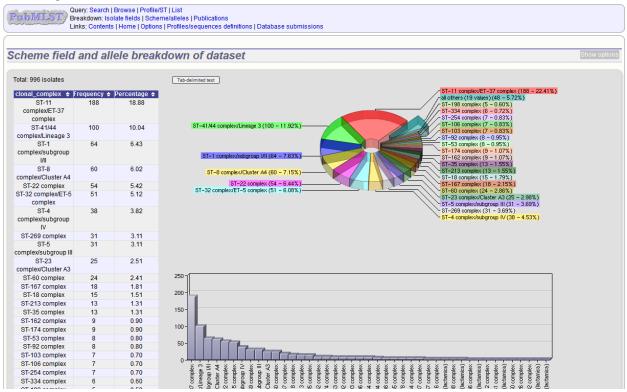
A table showing the number of unique values for each locus and scheme field will be displayed.

PubMLST	📝 Breakdowi		s Sche	me/alleles Put		ons Databa	ase submissions
Scheme fi	old and	allele h	roak	down of	datasa	t	Show options
							loci belonging to these schemes will then be performed.
All loci	osule netic Informatio abolism n ing	on Processing		* III •			
MLST	Fields				lieles		
Field name	Unique values	Analyse	Locus	A Unique alleles		Download	
ST	554	Breakdown	abcZ	64	Breakdown	Download	
clonal complex	43	Breakdown	adk	57	Breakdown	Download	
			aroE	80	Breakdown	Download	
			fumC gdh	85 79	Breakdown	Download	
			pdhC	83	Breakdown	Download Download	
			pgm	68	Breakdown	Download	

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

cheme fi	eld and	allele bi	reako	down of	dataset	t	Show option
elect schemes o	or groups of s	chemes within	the tree.	A breakdown o	of the individual	l fields and l	loci belonging to these schemes will then be performed.
🛓 🔲 🎧 All loci							
🚛 🔤 🚮 All IOCI	alla						
		on Processing					
- D Met		on rocessing					
- Dilir							
🛃 🔛 🛄 Typi	ng			-			
👍 🔛 🌆 Typi	ng			-			
🕴 🔛 🌆 Typi	ng			-			
🕂 🔛 🛄 Typi	ng			₹			
Select	ng			Ŧ			
🕂 🔛 🛄 Typi	ng w.or			•	lolos		
Select MLST	ng W OT Fields	s Analyse	Locus L		ieles Analyse	Download	
Select MLST	ng w.or		Locus L abcZ	T All Unique alleles 64		Download Download	
Select ALST Field name ST	ng Fields Unique values			Unique alleles	Analyse		
Select ALST Field name ST	ng Fields Unique values 554	Breakdown	abcZ	Unique alleles 64 (Analyse Breakdown	Download	
Select ALST Field name ST	ng Fields Unique values 554	Breakdown Breakdown	abcZ adk	Unique alleles 64 (57 (Analyse Breakdown Breakdown	Download Download	
Select ALST Field name ST	ng Fields Unique values 554	Breakdown Breakdown	abcZ adk aroE	Unique alleles 64 (57 (80 (Analyse Breakdown Breakdown Breakdown	Download Download Download	
Select MLST	ng Fields Unique values 554	Breakdown Breakdown	abcZ adk aroE fumC	Unique alleles 64 57 80 85	Analyse Breakdown Breakdown Breakdown Breakdown	Download Download Download Download	

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



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

cheme field	and all	ele breako	lown of dataset	
Total: 996 isolates			Tab-delimited text	-37 complex (188 - 22.41%
Clonal_complex ST-11 Complex/ET-37 Complex	requency ¢ 188	Percentage 18.88	- all others (19 value - 51-198 complex (1 - 51-334 complex (1 - 51-254 complex (1 - 51-254 complex (1	<pre>(48 - 5.72%) - 0.60%) - 0.72%) - 0.83%)</pre>
ST-41/44 complex/Lineage 3	100	10.04	ST-41/44 complex/Lineage 3 (100 - 11.92%) ST-41/44 complex/Lineage 3 (100 - 11.92%) ST-92 complex (1 ST-92 complex (1)	-0.83%)
ST-1 complex/subgroup I/II	64	6.43	ST-152 complex (8 ST-174 complex (9 ST-162 compl	- 0.95%) - 1.07%) - 1.07%)
ST-8 complex/Cluster A4	60	6.02	ST-8 complex/Cluster A4 (60 - 7.15%) ST-213 complex (15 ST-18 complex (15	3 - 1.55%) - 1.79%)
ST-22 complex	54	5.42	ST-22 complex (54 - 6.44%) ST-167 complex (
ST-32 complex/ET-5 complex	51	5.12		2.86%) ster A3 (25 - 2.98%) roup III (31 - 3.69%)
ST-4 complex/subgroup	38	3.82	ST-269 complex (

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.

PubMLS	📝 Breakdow		s Schei	me/alleles Put		ons Databa	base submissions	
Scheme fi	old and	allala b	rook	down of	dataca	4		Show options
Schemen	elu allu	allelen	Iean	uown oi	UdldSE	L		Show options
Select schemes	or groups of s	chemes within	the tree	. A breakdown	of the individu	al fields and	d loci belonging to these schemes will then be performed.	
All loci	osule netic Informati abolism n ing	on Processing		•				
MLST								
Field name	Fields Unique values	Analyse	Locus	A Unique alleles	lleles Analyse	Download		
ST	554	Breakdown	abcZ	64	Breakdown	Download		
clonal complex	43	Breakdown	adk	57	Breakdown	Download		
			aroE	80	Breakdown	Download]	
			fumC	85	Breakdown	Download		
			gdh	79	Breakdown	Download		
			pdhC pgm	83 68	Breakdown	Download Download		
			P g m		C	Costinidad		

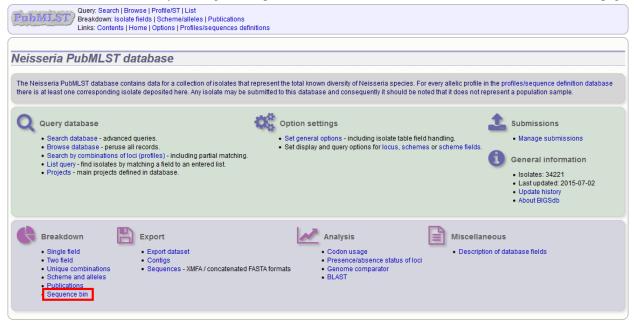
Sequences will be served in FASTA format in order of frequency.

>2
TTTGATACCGTTGCCGAAGGTTTGGGTGAAATTCGCGATTTATTGCGCCGTTACCACCGC
GTCGGCCATGAGTTGGAAAACGGTTCGGGTGAGGCTTTGTTGAAAGAACTCAACGAATTA
CAACTTGAAATCGAAGCGAAGGACGGCTGGAAGCTGGATGCGGCAGTCAAGCAGACTTTG
GGGGAACTCGGTTTGCCGGAAAACGAAAAAATCGGCAACCTTTCCGGCGGTCAGAAAAAG
CGTGTCGCCTTGGCGCAGGCTTGGGTGCAGAAGCCCGACGTATTGCTGCTGGACGAACCG
ACCAACCATTTGGATATCGACGCGATTATTTGGCTGGAAAATCTGCTCAAAGCGTTTGAA
GGCAGCTTGGTTGTGATTACCCACGACCGCCGTTTTTTGGACAATATCGCCACGCGGATT
GTCGAACTCGATC
>1
TTTGATACTGTTGCCGAAGGTTTGGGCGAAATTCGCGATTTATTGCGCCGTTATCATCAT
GTCAGCCATGAGTTGGAAAATGGTTCGAGTGAGGCCTTATTGAAAGAGCTCAACGAATTG
CAACTTGAGATCGAAGCGAAGGACGGCTGGAAGTTGGATGCGGCGGTGAAGCAGACTTTG
GGCGAACTCGGTTTGCCGGAAAACGAAAAAATCGGCAACCTCTCCGGCGGTCAGAAAAAG
CGCGTCGCCTTGGCGCAGGCTTGGGTGCAGAAGCCCGACGTATTGCTGCTCGATGAACCG
ACCAACCATTTGGACATCGACGCGATTATTTGGTTGGAAAACCTGCTCAAAGCGTTTGAA
GGCAGCCTGGTTGTGATTACCCACGACCGCCGTTTTTTGGACAATATCGCCACGCGGATT
GTCGAACTCGATC
>4

12.5 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.



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	120M	B35; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	А	1	SI-1 complex/subgroup I/II	5-2	10	F5-1
	M00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1099		19	15	
4	M1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex/subgroup IV			
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	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 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.

	s Scheme/alleles Publications Options Profiles/sequences de	finitions	Help	3
-				
All None Pastelist Filter by Sequence method: Project: Experiment • 0			• •	

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.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions									
	Help 🖉								
Breakdown of sequence bin contig properties									
tagged.									
oci ♦ % Loci ♦	Sequence +								
igeu taggeu									
1892 78.9	Display ->								
	Display ->								
	Display ->								
0 1 1 1 1	ci + % Loci + tagged + 892 78.9								

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 -
Download in tab-delimited text format Download in Excel format Click on the following charts to enlarge																		
Number	Number of contigs Total length Mean contig length Contig lengths																	
4	an: 225.4; σ:		-		n: 207276		T		an: 9357.0;	<u>σ: 1396.7</u>		all mean: 91	1111117111					

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

ri salar	ted: 2397																	
olate		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 -

12.6 Genome comparator

Genome Comparator is an optional plugin that can be enabled for specific databases. It is used to compare whole genome data of isolates within the database using either the database defined loci or the coding sequences of an annotated genome as the comparator.

Output is equivalent to a whole genome MLST profile, a distance matrix calculated based on allelic differences and a NeighborNet graph generated from this distance matrix.

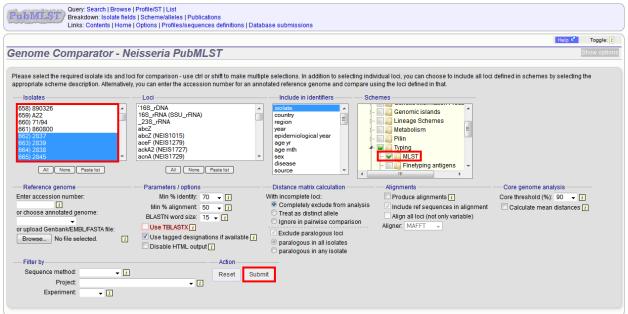
Genome Comparator can be accessed on databases where it is enabled from the contents page by clicking the 'Genome Comparator' link.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	
Neisseria PubMLST database The Neisseria PubMLST database contains data for a collection of isolates that represent the total known diversity of Neisseria species. For every allelic profile in t database there is at least one corresponding isolate deposited here. Any isolate may be submitted to this database and consequently it should be noted that it doe	
 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 General information • Isolates: 34221 • Last updated: 2015-07-02 • Update history • About BIGSdb
Breakdown Export Analysis Miscellane • Single field • Export dataset • Codin usage • Codon usage • Description • Unique combinations • Scheme and alleles • Sequences - XMFA / concatenated FASTA formats • Codon usage • Description • Scheme and alleles • Dublications • Sequence bin • BLAST • Description	eous n 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.

12.6.1 Analysis using defined loci

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



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.

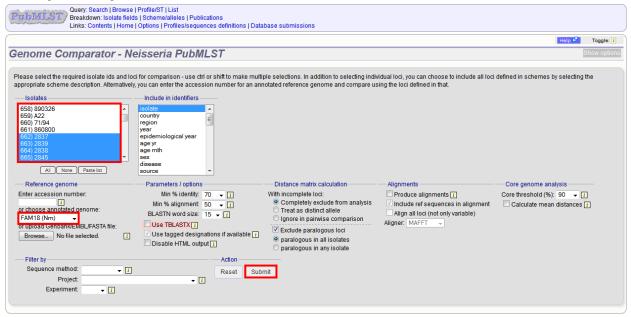
Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
	Toggle: i
Genome Comparator - Neisseria PubMLST	Show options
This analysis has been submitted to the job queue.	
Please be aware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

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

	Browse Profile/ST List					
	ate fields Scheme/alleles F Home Options Profiles/se		se submissions			
ob status viewer						
Status						
Job id: BIGSdb_27748_14054	410063_94241					
Submit time: 2014-07-15 08:41:03 Status: finished						
Start time: 2014-07-15 08:41:05 Progress: 100%						
Stop time: 2014-07-15 08:41:22 Total time: 17 seconds						
Dutput						
Analysis against defined loci						
llele numbers are used where these	e have been defined, otherwis	e sequences will be marked	as 'New#1, 'New#2' etc. I	lissing alleles are mark	ked as 'X'. Truncated alleles (located at end	of contig) are marked as 'T
Locus 644 (L93/4286) 662 (2837) (abcZ 2 2	663 (2839) 664 (2838) 665 (2 2 2	2845) 666 (2843) 667 (2842 2 2 2) 669 (2846) 670 (2840) 7 2	671 (2844) 672 (2847) 2 2	698 (FAM18)	
adk 3 3 aroE 4 19			3 3 4 19	3 3 19 19	3 4	
fumC 3 3 gdh 8 8	3 3 2 8 8 8		3 3 8 8	3 3 8 8	3 8	
pdhC 4 4 pgm 6 6	4 4 4 6 6 6	6 6			4 6	
oci with sequence differences	among isolates:					
ariable loci: 4						
Locus 644 (L93/4286) 662 (2837) 6 abcZ 2 2	663 (2839) 664 (2838) 665 (2845) 666 (2843) 667 (2842) 669 (2846) 670 (2840) 7 2	671 (2844) 672 (2847)	698 (FAM18)	
aroE 4 19 fumC 3 3	4 4 4 3 3 2		4 19 3 3	19 19 3 3	4	
pdhC 4 4	4 4 4	6 6	4 4	4 4	4	
latches: 3 Locus 644 (L93/4286) 662 (2837) 6 adk 3 3 gdh 8 8 pgm 6 6	663 (2839) 664 (2838) 665 (3 3 3 3 8 8 8 6 6 6 6	3 3 8 8 8) 669 (2846) 670 (2840) 3 3 8 8 6 6	671 (2844) 672 (2847) 3 3 8 8 6 6	698 (FAM18) 3 8 6	
Inique strains						
Jnique strains: 5						
Strain 1 Strain 2 Strain 3 544 (L93/4286) 662 (2837) 666 (284) 563 (2839) 670 (2840) 667 (284) 564 (2838) 671 (2844) 564 (2838) 571 (2844) 598 (FAM18) 672 (2847) 572 (2847) 572 (2847)	3) 665 (2845) 669 (2846)					
Text output file Excel format Distance matrix (Nexus format Splits graph (Neighbour-net, F		plitsTree. Distances between	taxa are calculated as th	e number of loci with dif	fferent allele sequences	
	(click to enlarge)	nd in Inkeenne er etherur der	graphics aditors			
Splits graph (Neighbour-net, S Locus presence frequency Locus presence frequency ch		ed in missage of other vector	graphics editors			
	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,					
Tar file containing output files	(click to enlarge)					
ease note that job results will remain						

12.6.2 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.



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.

PERDIALSET Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/Sequences definitions Database submissions																
ob stat	us viewer															
Status																
Submit time Status Start time Progress Stop time	BIGSdb_21911_1405410488_8452 2014-07-15 08:48:08 finished 2014-07-15 08:48:34 100% 2014-07-15 09:12:58 2014-07-15 09:12:58 24 minutes and 24 seconds															
Dutput																
Analysis by	reference genome															
accession version type length description	1 dna 2194961 Neisseria meningitidis serogroup C FAM18 complete genome.															
coding regio All loci	1975															
Each unique	allele is defined a number starting at 1. Missing alleles are marked as "	('. Truncated	i alleles (loc	ated at end o	f contig) are	marked a	as T.									
Locus	Product	Sequence length	Genome position	Reference genome	644 (L93/4286)	662 (2837)	663 (2830)	664 (2838)	665 (2845)	666 (2843)	667 (2942)	669 (2846)	670 (2840)	671 (2844)	672 (2847)	698 (FAM18
IpxC envA NMC0001	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924	1261	1	1	1	1	1	1	1	1	1	1	1	1	(0.400.00
piIS1 NMC0002	pilin (fragment)	291	3341				1									
NMC0002 pilS2	pilin (fragment) truncated pilin	291 366	3341 3675				1 2	1	1 2	1 2	1 2	1 2	1		1	
NMC0002 pilS2 NMC0003 fbp								1 2 2		1 2 2		1 2 T	1 2 2		1 2 2	
NMC0002 pilS2 NMC0003 fbp NMC0004	truncated pilin peptidyl-prolyl cis-trans isomerase	366 330	3675 4069				2		2	2	2	т			2	
NMC0002 pilS2 NMC0003 fbp NMC0004 NMC0005	truncaled pilin peptidyl-prolyl cis-trans isomerase putative membrane protein	366 330 219	3675 4069 4476	1			2 2 3	2	2 2 3	2	2 2 3	T 4	2	2 2 5	2	
NMC0002 pilS2 NMC0003 fbp NMC0004 NMC0005 NMC0006	truncated pilin peptidyl-prolyl cis-trans isomerase putative membrane protein putative glycerate dehydrogenase	366 330 219 954	3675 4069 4476 4816			2 2 3 2	2 2 3 2	2 3 2	2 2 3 2	2 3 2	2 2 3 2	T 4 2	2 3 2	2 2 5 2	2 3 2	
NMC0002 pilS2 NMC0003 fbp NMC0004 NMC0005 NMC0006 metG	truncaled pilin peptidyl-prolyl cis-trans isomerase putative membrane protein	366 330 219	3675 4069 4476	1			2 2 3	2	2 2 3	2	2 2 3	T 4	2	2 2 5	2	
NMC0002 pilS2 NMC0003 fbp NMC0004 NMC0005 NMC0006	truncated pilin peptidyl-prolyl cis-trans isomerase putative membrane protein putative glycerate dehydrogenase	366 330 219 954	3675 4069 4476 4816			2 2 3 2	2 2 3 2	2 3 2	2 2 3 2	2 3 2	2 2 3 2	T 4 2	2 3 2	2 2 5 2	2 3 2	

12.6.3 Include in identifiers fieldset

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

-Include in identifiers	
isolate	
country	
region	-
year	
epidemiological year	
age yr	
age mth	
sex	
disease	
source	Ŧ

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

12.6.4 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.

12.6.5 Parameters/options fieldset

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

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

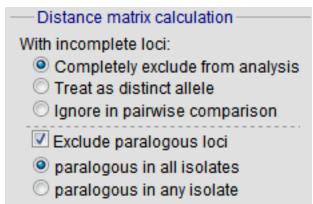
- Min % identity This sets the threshold identity that a matching sequence has to be in order to be considered (default: 70%). Only the best match is used.
- Min % alignment This sets the percentage of the length of reference allele sequence that the alignment has to cover in order to be considered (default: 50%).
- BLASTN word size This is the length of the initial identical match that BLAST requires before extending a match (default: 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.
- Use TBLASTX This compares the six-frame translation of your nucleotide query sequence against the sixframe translation of the contig sequences. Sequences will be classed as identical if they result in the same translated sequence even if the nucleotide sequence is different. This is significantly slower than using BLASTN.

Additionally, two other options are available in this fieldset:

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

12.6.6 Distance matrix calculation fieldset

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



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.

When paralogous loci are excluded, there are two further options:

- Exclude when paralogous in all isolates (default). Loci are only classed as paralogous when there are multiple hits in every genome (except if a genome is missing the locus entirely, in which case that genome is ignored in the calculation). This is generally the option that you will want to use with the default BLAST parameters since you can often expect multiple hits even when loci are not paralogous if you have used relaxed thresholds.
- Exclude when paralogous in any isolate. Unless you use stringent BLAST thresholds, this is likely to overestimate the number of paralogous loci, but may be useful if you are specifically looking for them.

12.6.7 Alignments fieldset

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

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

Available options are:

- Produce alignments Selecting this will produce the alignment files, as well as XMFA and FASTA outputs of aligned sequences. This will result in the analysis taking approximately twice as long to run.
- Include ref sequences in alignment When doing analysis using an annotated reference, selecting this will include the reference sequence in the alignment files.
- Align all loci By default, only loci that vary among the isolates are aligned. You may however wish to align all if you would like the resultant XMFA and FASTA files to include all coding sequences.
- Aligner There are currently two choices of alignment algorithm (provided they have both been installed)
 - MAFFT (default) This is the preferred option as it is significantly quicker than MUSCLE, uses less memory, and produces comparable results.

MUSCLE - This was originally the only choice. It is still included to enable previous analyses to be re-run
and compared but it is recommended that MAFFT issued otherwise.

12.6.8 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 👻	i
Calculate mean distances	i

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.

12.6.9 Filter fieldset

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

-Filter 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.

12.6.10 Understanding the output

Distance matrix

The distance matrix is simply a count of the number of loci that differ between each pair of isolates. It is generated in NEXUS format which can be used as the input file for SplitsTree. This can be used to generate NeighborNet, Split decomposition graphs and trees offline. If 200 isolates or fewer are included in the analysis, a Neighbor network is automatically generated from this distance matrix.

Unique strains

The table of unique strains is a list of isolates that are identical at every locus. Every isolate is likely to be classed as unique if a whole genome analysis is performed, but with a constrained set of loci, such as those for MLST, this will group isolates that are indistinguishable at that level of resolution.

12.7 **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 defin	litions
	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 Sequence bin	Analysis Codon usage Presence/absence status of loci BLAST ASTA formats Analysis Miscellaneous 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.

										depending on u		-	
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meni	ngitidis	В	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meni	ngitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meni	ngitidis	Α	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria meni	ngitidis	В	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meni	ngitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meni	ngitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meni	ngitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meni	ngitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meni	ngitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meni	ngitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meni	ngitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meni	ngitidis	В	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meni	ngitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meni	ngitidis	В	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meni	ngitidis	Α	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meni	ngitidis	NG	198	ST-198 complex			
21	6		Germany	1999	carrier	Neisseria meni	ngitidis	NG	198	ST-198 complex			
22	7		Germany	1999	carrier	Neisseria meni	ngitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meni	ngitidis	в	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meni	ngitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meni	ngitidis	в	930	ST-334 complex			
25												-	
	· _	elds Two Fi	eld Codons	Poly	morphic sites Combinations	Schemes/alleles	s Publ	lications	Seque	noe bin Tag status			
Bre	akdown: Fi	elds Two Fi		<u> </u>	e Comparator	Schemes/alleles	s Publ	lications	Seque	nce bin Tag status			
Bre	akdown: Fi Analysis: BL	elds Two Fi	ence/Absence	<u> </u>		Schemes/alleles	s Publ	lications	Seque	nce bin Tag status			

Select the isolate records to analyse - these will be pre-selected if you accessed the plugin following a query. Paste in a sequence to query - this be either a DNA or peptide sequence.

Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definit	tions Database submissions				
					Toggle: i
BLAST					
67) S5611 SCAASCCTSBATAAAATCSCCAAC 82) 11-004 94) (AL2229 90) CN100 120) F4698 120) F4698 128) F6124 160) 1014 CACTSCSCSTCSSCATCSAACCC	GCCGTTGCCGCTTCGGGCGCATTG GACAICCSCTGGCTGGCAAGCGGC AACGAGCGGGTTGTCCATCAIG ACCAIGGTGTGCTGCCAACAIGTCTC GSCAITTCGACTGAACAGCTCTAT CSCCTGTTGGGCGACGCGTCGACA GTACCGGAAAAAATCGACTATTTC	WAAACGCTGSCG ICGCSCTISCGGT ICGCSCTISCGGT ICGCSCTISCG ICGCCCGTIAIC ICGCCCGTAIC ICGCCCGAA	tide sequences can be quer 		
All None	CBIAAMAICUUCIACUAAAAC		source epidemiology	*	
Parameters	Options	Restrict included sequences by		Actio	in
BLASTN word size: 11 👻 👔	Show 0% matches in table	Sequence method:	▼ i	Res	et Submit
BLASTN scoring: reward:2; penalty:-3; gap open:5; gap extend:2 👻 🧵		Project:	-	▼ []	
Hits per isolate: 1 -		Experiment 🚽 👔]		
Flanking length (bp): 100 👻 👔					

Click submit.

A table of BLAST results will be displayed.

													Toggle
AS	Т												
ase se	elect the requ	uired isolate	ids to BLAST ag	ainst (use ctr	l or shif	ft to make n	nultiple se	lections) and paste	in your qu	ery sequei	nce. Nucleotide	or peptide sequences can be queried.	
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Parar	meters						Optio	ns		Restrict in	cluded sequence	ces by	
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ate id 1 2 7 10 11 13 30 31 34 35 46 52	ng length (b) e TBLASTX [A4/M1027 120M 7891 6748 129 139M S3131 S4355 14 10 20 26 255 243	D) 100 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49	ignment length 465 465 465 465 465 465 465 465 465 465	7 7 7 7 7 7 7 12 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	180177 180583 180965 181186 181867 182004 182318 215673 8 182380 182815 182880 183179 183381	19444 4782 19869 19181 35889 36775 19090 4534 1363524 5559 19783 19879 4982 4532	19908 settest = 5246 settest = 20333 settest = 19645 settest = 37239 settest = 4998 settest = 18554 settest = 18588 settest = 20247 settest = 5446 settest = 54496 settest =	1 J T T T T T T T T T T J J	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	807 807 807 807 807 807 807 807 807 807		
late id 1 2 7 10 11 13 19 24 30 31 34 35 46 52 61	ng length (b) e TBLASTX [A4M1027 120M 7891 6748 129 139M S3131 S4355 14 10 20 26 255 243 393	 p): 100 identity A 98.49 	Ignment length 465 465 465 465 465 465 465 465 465 465	7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	180177 180583 180965 181186 181867 182044 182318 215673 8 182380 182815 182880 182815 182880 183179 183381 183648	19444 4782 19869 19181 35889 36775 19090 4534 1363524 5559 19783 18879 4982 4532 7217	19908 estract 5246 extract 19945 extract 36353 extract 37239 extract 19554 extract 4998 extract 20247 extract 20247 extract 19348 extract 4996 extract 4996 extract	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	807 807 807 807 807 807 807 807 807 807		
Elankii Us Us Us Us Us Us Us Us Us Us Us Us Us	ng length (b) e TBLASTX [A4/M1027 120M 7891 6748 129 139M S3131 S4355 14 10 20 26 255 243 393 254	p) 100 *5 identity A 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49	ignment length 465 465 465 465 465 465 465 465 465 465	7 7 7 7 7 7 7 12 7 7 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	180177 180583 180965 181186 181867 182004 182318 215673 8 182380 182815 182880 183815 183881	19444 4782 19869 19181 35889 36775 19090 4534 1363524 5559 19783 18879 4982 4532 7217 4716	19908 senset - 5246 senset - 2033 senset - 19945 senset - 37239 senset - 37239 senset - 19554 senset - 19638 senset - 106398 senset - 19349 senset - 4996 senset - 4966 senset - 7681 senset - 5180 senset - 5180 senset -	+++++++++++++++++++++++++++++++++++++++	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	807 807 807 807 807 807 807 807 807 807		
Elankii Us Us Us Us Us Us Us Us Us Us Us Us Us	ng length (b) e TBLASTX [A4M1027 120M 7891 6748 129 139M S3131 S4355 14 10 20 26 255 243 393 254 25611	p) 100 • identity A 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49	ignment length 465 465 465 465 465 465 465 465 465 465	7 7 7 7 7 7 7 12 7 7 7 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	180177 180583 180965 181186 181867 182004 182318 215673 8 182380 182815 182880 182815 182880 183179 183381 183648 183818 183818 183818	19444 4782 19869 19181 35889 36775 19090 4534 1363524 5559 19783 18879 4982 4532 7217 7217 4716 4804	19908 strat - 5246 strat - 19908 strat - 19965 strat - 3033 strat - 33723 strat - 34723 strat - 19554 strat - 4998 strat - 19554 strat - 19934 strat - 19343 strat - 5446 strat - 7681 strat - 7681 strat - 7681 strat - 5180 strat - 5180 strat - 5180 strat - 35888 strat -	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	807 807 807 807 807 807 807 807 807 807		
Flankii Us late id 2 7 10 11 13 19 24 30 31 34 35 46 52 61 64 67 82	ng length (b) e TBLASTX [A4/M1027 120M 7891 6748 129 139M S3131 S4355 14 10 20 26 255 243 393 254 S5611 11-004	p): 100 * identity A 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49	Ignment lengtil 465 465 465 465 465 465 465 465 465 465	7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7		180177 180583 180965 181186 181867 182004 182318 215673 8 182380 182815 182880 182815 182881 183818 183818 183483 1844297	19444 4782 19869 19181 35889 36775 19090 4534 1363524 5559 19783 18879 4982 4532 7217 4716 4804 19518	19908 strat	1 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	807 807 807 807 807 807 807 807 807 807		
Flankii Us late id 2 7 10 11 13 19 24 30 31 34 35 46 52 61 64 67	ng length (b) e TBLASTX [A4M1027 120M 7891 6748 129 139M S3131 S4355 14 10 20 26 255 243 393 254 25611	p) 100 • identity A 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49 98.49	ignment length 465 465 465 465 465 465 465 465 465 465	7 7 7 7 7 7 7 12 7 7 7 7 7 7 7 7 7 7	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	180177 180583 180965 181186 181867 182004 182318 215673 8 182380 182815 182880 182815 182880 183179 183381 183648 183818 183818 183818	19444 4782 19869 19181 35889 36775 19090 4534 1363524 5559 19783 18879 4982 4532 7217 7217 4716 4804	19908 strat - 5246 strat - 19908 strat - 19965 strat - 3033 strat - 33723 strat - 34723 strat - 19554 strat - 4998 strat - 19554 strat - 19934 strat - 19343 strat - 5446 strat - 7681 strat - 7681 strat - 7681 strat - 5180 strat - 5180 strat - 5180 strat - 35888 strat -	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	807 807 807 807 807 807 807 807 807 807		

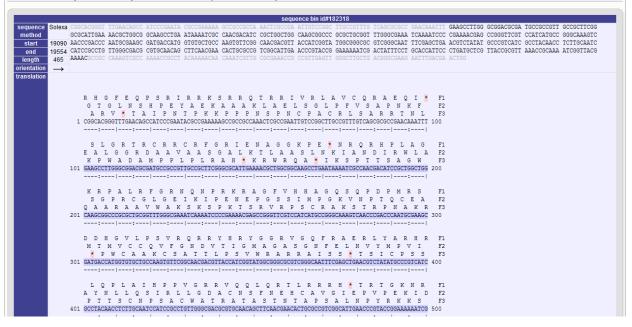
Clicking any of the 'extract' buttons will display the matched sequence along with a translated sequence and flanking sequences.

181867	35889	36353 extract →	\rightarrow	0.0	807
182004	36775	37239 extract ->	\rightarrow	0.0	807
182318	19090	19554 extract ->	\rightarrow	0.0	807
215673	4534	4998 extract →	←	0.0	807
8	1363524	1363988 extract ->	\rightarrow	0.0	785
182380	5559	6023 extract →	\rightarrow	0.0	807
182815	19783	20247 extract ->	\rightarrow	0.0	807

Query: Search | Browse | Profile/ST | List Breakdown: Isolate fields | Scheme/alleles | Publications

Links: Contents | Home | Options | Profiles/sequences definitions | Database submissions

Extracted sequence: Seqbin id#:182318 (19090-19554)



At the bottom of the results table are links to export the matching sequences in FASTA format, (optionall) including flanking sequences. You can also export the table in tab-delimited text or Excel formats.

07	53011	30.43	400	1	v	104143	4004	JZ00 extract ->	~	0.0	007
82	11-004	98.49	465	7	0	184297	19518	19982 extract -	\rightarrow	0.0	807
84	IAL2229	98.49	465	7	0	184635	4530	4994 extract -	←	0.0	807
90	CN100	98.49	465	7	0	184814	5350	5814 extract -	←	0.0	807

12.7.1 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 tabl 	е —
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.

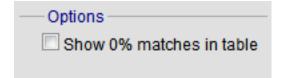
12.7.2 Parameters fieldset

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 👻 🚺
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.

12.7.3 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.

12.7.4 Filter fieldset

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

-Restrict included sec	nuences by	
100000000000000000000000000000000000000	44611666 83	
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.

12.8 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.

M	00282207		UK		invasive (unspecified/other)		W	1101	ST-22 complex			
8 M	7891	B54; Z1054	Finland		invasive (unspecified/other)		A	5	ST-5 complex/subgroup III	20	9	F3-1
	00242007		UK		invasive (unspecified/other)		В	1102	ST-18 complex		14	
9	0021/84				invasive (unspecified/other)		W	114	ST-22 complex			
0	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
2	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	в	1015	ST-32 complex/ET-5 complex	7	16	
3	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
4	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
6	2		Germany	1999	carrier	Neisseria meningitidis	в	854	ST-18 complex			
7	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
8	4		Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
9	S3131	B213; 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			
2	7		Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
3	8		Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			

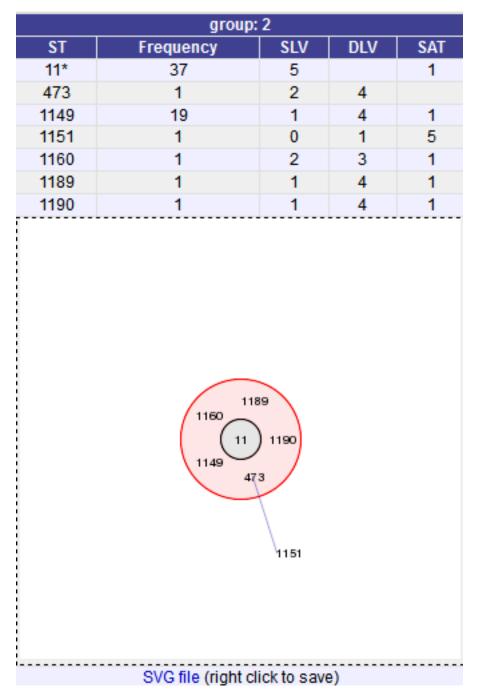
If there multiple schemes that can be analysed, these can then be selected along with the group definition.

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 ha BURST analysis can be used to: • Divide strains into groups according to their allelic profiles. • Count the number of Single Locus Variants (SLV), Double Locus Variants (DLV) and Satellities (SAT) for eac • Identify the potential Ancestral Type (AT). These are shown with an asterisk next to their names in the result Graphic representations of BURST groups can be saved in SVG format. This is a vector image format that can be Options Select scheme: MLST • Group definition: profiles match at n-2 • loci to any other member of the group [n = number of loci in scheme]. Ø Shade variant maps Hide variant names (useful for overview if names start to overlap)	h sequence type (ST). s table.

Modifying the group definition affects the size of groups and how they link together. By default, the definition is n-2 (where n is the number of loci), so for example on a 7 locus MLST scheme groups contain STs that match at 5 or more loci to any other member of the group.

Click Submit.

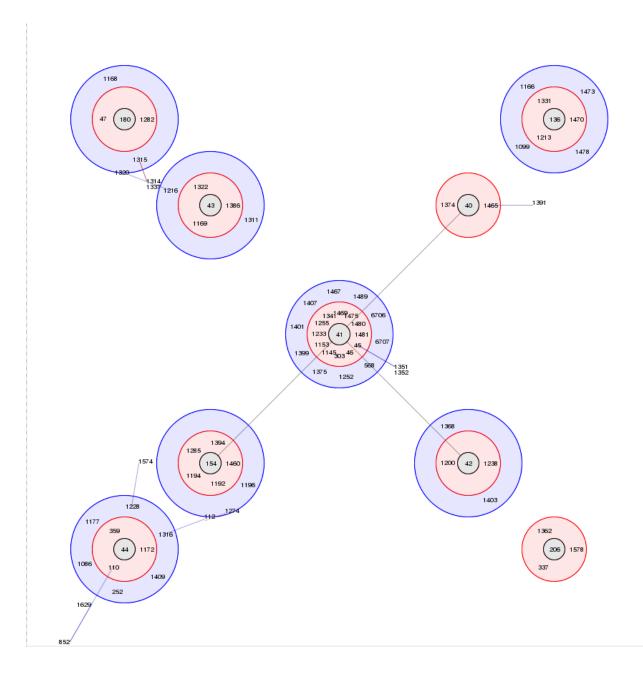
A series of tables will be displayed indicating the groups of profiles. Where one profile can be identified as a central genotype, i.e. the profile that has the greatest number of other profiles that are single locus variants (SLV), double locus variants (DLV) and so on, a graphical representation will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



SLV profiles that match the central profile are shown within a red circle surrounding the central profile. Most distant profiles (triple locus variants) may be linked with a line. Larger groups may additionally have DLV profiles. These are shown in a blue circle.

	group:	6		
ST	Frequency	SLV	DLV	SAT
32*	2	3	2	
230	1	1	3	1
484	1	0	3	2
1015	1	1	4	
1100	1	1	2	2
1148	1	0	4	1
	484	1100		
	230	114	8	

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



12.9 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	
	ent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition e submitted to this database and consequently it should be noted that it does not represent a population 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 update: 2015-07-02 • Update history • About BIGSdb
Breakdown Export • Single field Export dataset • Two field Contigs • 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 '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.

										Bon		
	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16	
5	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	В	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	В	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	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		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			
Ana	Ilysis tools	i: elds Two Fi	ield Polymorph	ic sites	Combinations Schemes/	alleles Publications	Sequence t	oin (Tag status			
Brea												
	_	JRST Code	ons Presence/Al	bsence	Genome Comparator BL	AST						
	nalysis: Bu	JRST Code		_	Genome Comparator BL	AST						

Enter the ids of the isolate records to analyse - these will be already entered if you accessed the plugin following a query. Select the loci you would like to analyse, either from the dropdown loci list, and/or by selecting one or more schemes.

Output Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Public Links: Contents Home Options Profiles/sequent			
			Toggle: i
Codon usage analysis			
		database containing sequences, or with sequences tagged, can be inclu ing frame 1). Partial sequnces from the sequence bin will not be analysed	
	ier — Loci —	Schemes	
Paste in list of ids to include, start a new isolate include all ids. country region year age of the start of	aceF (NEIS1279) ackA2 (NEIS1727) achA (NEIS1729) • All None Pastelist	Contract Information Proce Contract Information Contract Informatio	
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 Use allele sequence retrieved from external database	Select codon order:	Submit	
Ose allele sequences with problem flagged (defined alleles w	vill 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.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/allels 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

PtrisMJ_ST Breakdown: Isolate fields Scheme/alleles P Links: Contents Home Options Profiles/se	
Job status viewer	
Status Job id: BiGSdb_13269_1405586315_76138 Submit time: 2014-07-17 09:38:35 Status: finished Start time: 2014-07-17 09:38:39 Progress: toos. Stop time: 2014-07-17 09:38:05 Total time: 26 seconds Output Absolute frequency of codon usage by isolate Absolute frequency of codon usage by isolate Absolute frequency of codon usage by isolate Relative synonymous codon usage (RSCU) by isolate Relative synonymous codon usage (RSCU) by isolate Relative synonymous codon usage (RSCU) by isolate Tartific containing output files	
Please note that job results will remain on the server for 7 days.	

12.10 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.

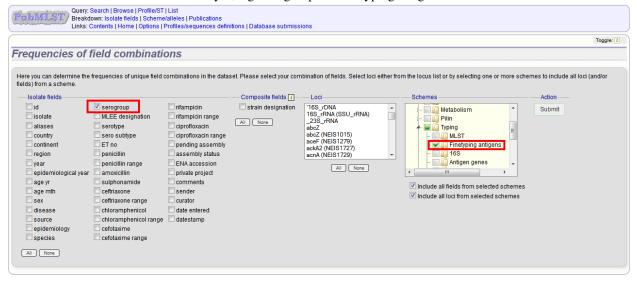
The function can be selected by clicking the 'Unique combinations' link in the Breakdown section of the main contents page. This will run the analysis on the entire database.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences defin	itions
	epresent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition may be submitted to this database and consequently it should be noted that it does not represent a population sample. Option settings • Set general options - including isolate table field handling. • Set display and query options for locus, schemes or scheme fields. • Isolates: 34221 • Last updated: 2015-07-02 • Update history • About BIGSdb
Breakdown Single field Won field Unique combinations Strieme and alteres Publications Sequence bin Export Export Export dataset Contigs Sequences - XMFA / concatenated Field Sequences - XMFA / concatenated Field Contigs Sequence bin Export Analysis Codon usage Presence/absence status of loci Genome comparator BLAST BLAST Miscellaneous Description of 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.

5 M0024 6 M0028 7 789 8 M0024 9 0021 10 674 11 12	82207 891 B54; Z1054 42007	UK UK Finland		invasive (unspecified/other)					7	10	
7 789 8 M0024 9 0021 10 674	891 B54; Z1054 42007		2000		-	В		ST-32 complex/ET-5 complex	(16	
8 M0024 9 0021 10 674	42007			invasive (unspecified/other)		W	1101	ST-22 complex			
9 0021 10 674				invasive (unspecified/other)		A	5	ST-5 complex/subgroup III	20	9	F3-1
10 674		UK		invasive (unspecified/other)		В	1102	ST-18 complex		14	
				invasive (unspecified/other)	~	W	114	ST-22 complex			
11 12		Canada		invasive (unspecified/other)	-	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
		Germany		invasive (unspecified/other)		A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
0090				invasive (unspecified/other)		В	1015	ST-32 complex/ET-5 complex	7	16	
13 139			1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14 0120	0/95			invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
15 1			1999		Neisseria meningitidis	E	864				
16 2	2	Germany	1999	carrier	Neisseria meningitidis	в	854	ST-18 complex			
17 3	3	Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18 4	4	Germany	1999	carrier	Neisseria meningitidis	В	19	ST-18 complex			
19 S31	131 B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20 5	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	7	Germany	1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23 8	8	Germany	1999	carrier	Neisseria meningitidis	В	32	ST-32 complex/ET-5 complex			
24 S43	355 B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25 9	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.

						Toggi
quen	cies of f	ïeld co	mbinat	ions		
mber of uni	ique combinatio	ons: 2939				
e nercentar	ies may add ur	to more that	n 100% if you	have selected	Lloci or scheme	fields with multiple values for an isolate.
					Percentage 🗢	
B W	7-2 5	4	F1-5 F1-1	625 513	5.65 4.64	
B	19	15	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	
A	5-2	10	F3-5	135	1.22	
в	19-1	15-11	F5-1	107	0.97	
Y	5-1	10-1	F4-1	96	0.87	
	5	2	F1-1	93	0.84	
Y	5-2	10-1	F4-1	79	0.71	
С	5	2	F5-8	79	0.71	
w	18-1	3	F4-1	77	0.70	
BC	22-1 5	14	F4-1 F3-3	77 76	0.70	
B	5	2	F3-3 F1-5	76	0.69	
Y	5-1	2-2	F1-5 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.

B NG B B B -	19 12.1 7-2 7-2 7 5-1 7-2 5-2	13-2 13.1 16-126 30 30-3 10-10 30-3	F5-1 F3-29 F3-3 F5-1 F1-14 F3-16	1 1 1 1 1 1	0.01 0.01 0.01 0.01 0.01
NG B B B -	7-2 7-2 7 5-1 7-2	16-126 30 30-3 10-10	F3-3 F5-1 F1-14 F3-16	1 1 1	0.01 0.01 0.01
B B B	7-2 7 5-1 7-2	30 30-3 10-10	F5-1 F1-14 F3-16	1	0.01
B B	7 5-1 7-2	30-3 10-10	F1-14 F3-16	1	0.01
B -	7-2	10-10	F3-16		
-	7-2			1	0.04
		30-3			0.01
	5-2		F1-7	1	0.01
С		10	F1-7	1	0.01
NG	18-1	3	F1-34	1	0.01
NG	22	14-6	F4-2	1	0.01
в	7-2	4	F1-88	1	0.01
NG	5-1	10-62	F1-3	1	0.01
Y	12-3	4	F4-1	1	0.01
NG	7-2	16	F1-104	1	0.01
Х	12-1	16-52	F3-9	1	0.01
NG	18-4	35-34	F4-1	1	0.01
	oad as tab-del oad in Excel fo				

12.11 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.

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			
irea		ields Two Fi		bsence		alleles Publications	Sequence	bin (Tag status			

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

PTITIALST Breakdown: Isolate fields [Schemeralisels Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Polymorphic site analysis	Toggle: i
This tool will analyse the polymorphic sites in the selected locus for the current isolate dataset. If more than 50 sequences have been selected, the job will be run by the offline job manager which may take a few minutes (or longer depending on the queue). This is because sequences may have gaps in them and consequently meet to be aligned which is a processor- and memory-intensive operation. Loci Options Action If both allele designations and tagged sequences exist for a locus, choose how you want these handled [] Analyse abc2 (NEIS1015) acc6 (NEIS1027) ach4 (NEIS1727) acn4 (NEIS1727) a	

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.

PubML					me/alleles s Profiles/		ons s definition:	s Databa	ise subr	nissions			
													Toggle: i
Polymoi	rphic s	site a	nalys	is									
he colour co joing to the op							nucleotide	at each po	osition. C	lick anywh	iere within	he sequei	nce to drill down to allele and profile information. The width of the display can be altered by
0 alleles incl	luded in ana	alysis. 104	polymor	phic sites	found.								
(ey: <mark>0 - 10%</mark>	>10 - 20%	>20 - 309	>30 - 4	0% >40 -	50% <mark>>50</mark>	- <mark>60%</mark> <mark>>6</mark>	0 - 70% >7	0 - 80% >	80 - 90%	>90 - 10	0%		
1	10	20		30	40	50	60		70	80	90		00
TTTG	ATACCGTTO		TTTGGG <mark>C</mark> (A T			A T	TATCATCAT		TGAGTT(GAAAACG GC TA		AGG <mark>C</mark> TTT GCATC	
101	110	120	_	30	140	150	160	1	.70	180	190	TC	00
	AGA <mark>A</mark> CTCAJ	ACGAATT <mark>G</mark>	CAACT <mark>T</mark> G7	AATCGAA	GCGAAGGA	CGGCTGGA	A <mark>GC</mark> TGGATG		AAGCAG	ACTTTGGG	GAACTCG	TTTGCCGG	GA
A	<u>G</u> T		GGC	G	AA	T	AT AA	G	A		GA T T	C A	
201	210	220		230	240	250	260 CCCCCACCC		270	280	290		00
		A		A G		T IC.		Å		T T		T G	*
301	310	320		330	340	350	360		370	380	390		00
401 ACAA	410 TATOGCCAC	420 GCC <mark>CATT</mark>	T GTCGAACT	130	GGAAAACC'		GCGTTTGAA	GGCAGC <mark>T</mark> T C	GGTTGT(C		ACGACCCCC T	C	<u></u>
lucleotide	frequen	cies											
			Nucleot	ide									
Position 🗢 🗚	¢ C ¢ G		¢ %A ≎	%C 🗢 %	G ≑ %T ≑								
9 12			0 3.33	83.33	16.67 96.67								
19	1 0 2	0 0	0 3 33	٩	6 67								

12.12 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.

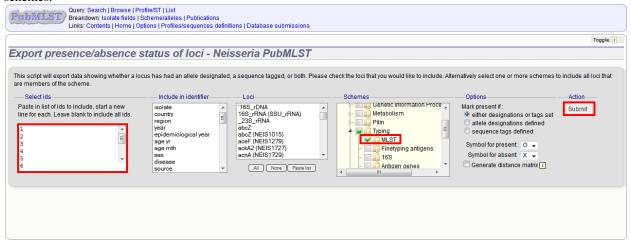
The function can be selected by clicking the 'Presence/absence status of loci' link in the 'Analysis' section of the main contents page.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences 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 not a submitted to the database and consequently it should be noted that it does not a submitted to the database and consequently it should be noted that it does not a submitted to the database and consequently it should be noted that it does not a submitted to the database and consequently it should be noted that it does not a submitted to the database and consequently it should be noted that it does not a submitted to the database and consequently it should be noted that it does not a submitted to the database and consequently it should be noted that it does not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the database and consequently it should be not a submitted to the datab	
 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 General information • Isolates: 34221 • Last updated: 2015-07-02 • Update history • About BIGSdb
Breakdown Export Analysis Miscellaneou • Single field • Export dataset • Contigs • Contigs • Description of • Unique combinations • Sequences - XMFA / concatenated FASTA formats • Codon usage • Description of • Publications • Sequence bin • Sequence / Presence/absence status of loci • Description of	-

Alternatively, it can be accessed following a query by clicking the 'Presence/Absence' button in the Analysis list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7		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		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		B213; Z1213	Ghana				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		B227; Z1227	Denmark				Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			
4		,	Denmark		invasive (unspecified/other)					5-1	9	F3-1
Bror	akdown: Fie	elds 🛛 Two Fi	eld Polymorph	ic sites	Combinations Schemes/	alleles Publications	Sequence	bin	Tag status			
Died												
	nalysis: BL	JRST Codo	ons Presence/Al	bsence	Genome Comparator BL	AST						
		JRST Codo		_	Genome Comparator BL	AST						

Enter the ids of the isolate records to analyse - these will be already entered if you accessed the plugin following a query. Select the loci you would like to analyse, either from the dropdown loci list, and/or by selecting one or more schemes.



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.

ProbMIST Brakdown Isolate Heids [Schemelandles 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.

Putpl/LIST Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profile/Sequences definitions Database submissions
Job status viewer
Status Job Id: BICSdb_31442_1405591304_69061 Submit time: 2014-07-17 11:01:44 Status: finished Status: 01:4-07-17 11:01:44 Progress: 100% Stop time: 2014-07-17 11:01:49 Total time: 4 seconds Output Main output file
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	

12.12.1 Options

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

-Options	
Mark present if :	
either designation	s or tags set
allele designation	s defined
🔘 sequence tags de	fined
Symbol for present:	0 -
Symbol for absent:	Х 🗸
Generate distance	matrix 👔

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

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

12.13 Tag status

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

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

Select the loci you would like to analyse.

Purinian Query: Search Browse Profiles/T 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.	
Capsule Cenetic Information Processing Output Will Cabsule Output Will Cabsule Output Will Cabsule Output Output	

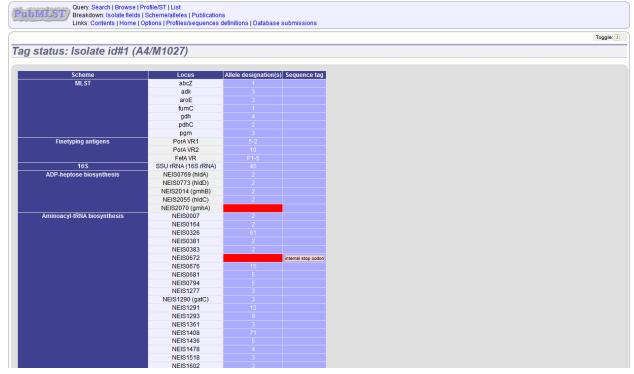
You should see a series of bars representing loci. The colour of these bars designates whether they have an allele designation only, a sequence tag only, both designations or tags, or whether they have flags set.

PTIDIALST Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
Toggle: [
ag status
Select schemes or groups of schemes within the tree. A breakdown of the individual loci belonging to these schemes will then be performed.
Capsule Capsule Region A Capsule Region A Capsule Region A - Serogroup A Capsule Region A - Serogroup B Capsule Region A - Serogroup B
III IV Select
Bars represent loci by schemes arranged in alphabetical order. If a locus appears in more than one scheme it will appear more than once in this graphic. Click on the id hyperlink for a detailed breakdown for an isolate.
Кеу
Allele designated only Sequence tagged only Allele designated + sequence tagged Flagged []
2463 loci selected:
Id Isolate
3 M00242905
4 M1027
5 M00240227
6 M00282207
8 M00242007
9 0021/84
<₽

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

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

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



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

Data export plugins

13.1 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. Set display and query options for locus, schemes or scheme fields. Projects - main projects defined in database. Submissions Isolates: 34218 Last updated: 2015-06-30 Update history Vision Barlow Control Vision Barlow Control
 Breakdown Single field Two field Unique combinations Scheme and aleles Publications Sequence bin

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

				ls	olate fields 👔				MLST	Finet	yping antig	jens
id	isolate	aliases	country	year	disease	species	serogroup) ST	clonal complex	PorA VR1	PorA VR2	FetA VR
1	A4/M1027	B1; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
3	M00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1099		19	15	
4	M1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	Α	4	ST-4 complex/subgroup IV			
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	в	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	в	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099		1968		Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95				invasive (unspecified/other)	Neisseria meningitidis	Х	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	в	854	ST-18 complex			
17	3			1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4			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			1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
22	7			1999	carrier	Neisseria meningitidis	E	60	ST-60 complex			
23	8		Germany	1999	carrier	Neisseria meningitidis	в		ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	Α	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			

Select the isolate fields and schemes to include.

	own: Isolate fields Scheme Contents Home Options I		tions Database submissio	ons			Toggle: i
Export dataset							
This script will export the da loci (and/or fields) from a sc lociate fields isolate aliases isolate isolate aliases icontinent region year epidemiological year age yr age mt sex		ittable for importing into a rifampicin range ciprofloxacin ciprofloxacin range pending assembly assembly status ENA accession private project comments sender curator	spreadsheet. Select which — Composite fields [] – – Strain designation All None	fields you would li References references 9 PubMed id Full citation	Loci Loci 16S_rDNA 16S_rDNA 16S_rANA (SAU_rRNA) 22S_rRNA (SAU_RAA abc2 22S_rRNA abc2 (NEIS1015) accF (NEIS1279) accA2 (NEIS1277) accA2 (NEIS1272) All None	from the locus list or by selecting one or more schemes to incl Schemes Genetic information Proce Fine Metabolism Metaboli	ude all
disease source epidemiology species	chloramphenicol chloramphenicol range cefotaxime cefotaxime range	date entered datestamp	Options Include locus commo Export allele numbers Use one row per field Include isolate field in Export full allele desig	s I 1 row (used only wi	th 'one row' option) cd only with 'one row' option)	Molecular weights Action Export protein molecular weights GTG/TTG at start codes for methionine	

Click Submit.

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

Prohitics Query 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	
Download: Text file Excel file (right-click to save)	

13.1.1 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.

13.1.2 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

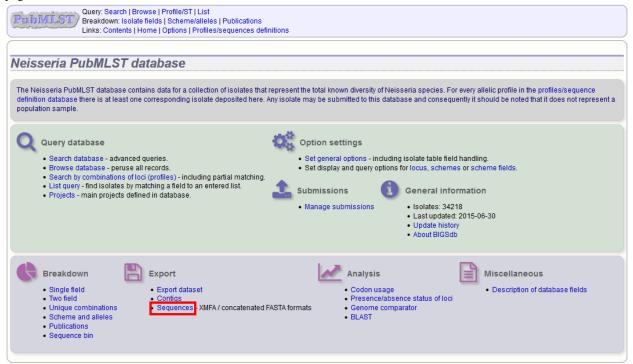
GTG/TTG at start codes for methionine

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.

13.2 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.

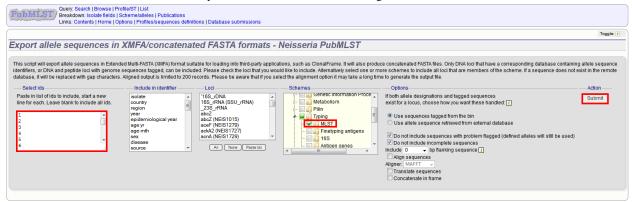
The sequence export function can be accessed by clicking the 'Sequences' link in the Export section of the contents page.



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.

5 1	M1027	B43; Z1043			invasive (unspecified/otner)		A	4	S1-4 complex/subgroup IV			
	M00240227				invasive (unspecified/other)		в		ST-32 complex/ET-5 complex	7	16	
6	M00282207				invasive (unspecified/other)		W	1101	ST-22 complex			
7	7891	B54; Z1054			invasive (unspecified/other)		Α	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007				invasive (unspecified/other)		в	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	Α	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
2	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	в	1015	ST-32 complex/ET-5 complex	7	16	
3	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	A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	в	930	ST-334 complex			

Select the isolate or profile records to analyse - these will be pre-selected if you accessed the plugin following a query. Select the loci to include either directly within the loci list and/or using the schemes tree.



Click submit.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
	Toggle: i
Export allele sequences in XMFA/concatenated FASTA formats - Neisseria PubMLST	
This analysis has been submitted to the job queue.	
Please be aware that this job may take a long time depending on the number of sequences to align and how busy the server is. Alignment of hundreds of sequences can take many hours!	
Follow the progress of this job and view the output.	
Please note that the % complete value will only update after the alignment of each locus.	

The job will be submitted to the job queue. Click the link to follow the progress and download the resulting files. Sequences will be export in XMFA and FASTA file formats.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions
ob status viewer
Job id: BIGSdb_29565_1405601815_9307 Submit time: 2014-07-17 13:56:55 Status: finished Start time: 2014-07-17 13:57:10 Progress: 100% Stop time: 2014-07-17 13:57:23 Total time: 12 seconds
XMFA output file (not aligned) Concatenated FASTA (not aligned) Tar file containing output files
lease note that job results will remain on the server for 7 days.

13.2.1 Aligning sequences

By default, sequences will be exported unaligned - this is very quick since no processing is required. You can choose to align the sequences by checking the 'Align sequences' checkbox.

Options
options
If both allele designations and tagged sequences
exist for a locus, choose how you want these handled: 👔
Our contract of the sequences tagged from the bin
Use allele sequence retrieved from external database
🔽 De net is slude as success with problem fleened (defined allalas will still be used)
Do not include sequences with problem flagged (defined alleles will still be used)
Do not include incomplete sequences
Include 0 – bp flanking sequence i
Align sequences
Aligner: MAFFT 👻
I ranslate sequences
Concatenate in frame

You can also choose to use MUSCLE or MAFFT as the aligner. MAFFT is the default choice and is usually much quicker than MUSCLE. Both produce comparable results.

13.3 Contig export

The contig export plugin can be accessed by clicking the 'Contigs' link in the Export section of the contents page of isolate databases.

Query: Search Browse Profile/ST List Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions	3
	sent the total known diversity of Neisseria species. For every allelic profile in the profiles/sequence definition 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 Submissions • Set general options - including isolate table field handling. • Manage submissions • Set display and query options for locus, schemes or scheme fields. • Manage submissions • General information • Isolates: 34218 • Last updated: 2015-06-30 • Update history • About BIGSdb • Manage submissions
Breakdown Single field Two field Unique combinations Scheme and alleles Publications Sequence bin Sequence bin	formats Analysis Codon usage Presence/absence status of loci Genome comparator BLAST

Alternatively, it can be accessed following a query by clicking the 'Contigs' button in the Export section at the bottom of the results table.

M			UK	2000	invasive (unspecified/other)	Neisseria meningitidis	s B	1100	ST-32 complex/ET-5 complex	7	16	
7	00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	s W	1101	ST-22 complex			
	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	s A	5	ST-5 complex/subgroup III	20	9	F3-1
B M	00242007		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			
0	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	s A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
1	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	s A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
2	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	в В	1015	ST-32 complex/ET-5 complex	7	16	
3	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	s A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
4	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	з Х	117			14	
5	1		Germany	1999	carrier	Neisseria meningitidis	s E	864				
6	2		Germany	1999	carrier	Neisseria meningitidis	в В	854	ST-18 complex			
7	3		Germany	1999	carrier	Neisseria meningitidis	s W	174	ST-174 complex			
8	4		Germany	1999	carrier	Neisseria meningitidis	в	19	ST-18 complex			
9	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	s A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
0	5		Germany	1999	carrier	Neisseria meningitidis	s NG	198	ST-198 complex			
1	6		Germany	1999	carrier	Neisseria meningitidis	s NG	198	ST-198 complex			
2	7		Germany	1999	carrier	Neisseria meningitidis	s E	60	ST-60 complex			
3	8		Germany	1999	carrier	Neisseria meningitidis	s B	32	ST-32 complex/ET-5 complex			
4	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	s A	5	ST-5 complex/subgroup III	5-1	9	F3-1
5	9		Germany	1999	carrier	Neisseria meningitidis	s B	930	ST-334 complex			

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 Is Scheme/alleles Publications Options Profiles/sequences definitions			
			Help 🖉	Toggle: 🚯
Contig analysis and expo	ort			
calculated by adding up the length of all loci t the length of the contig.	which contigs are associated - use Ctrl or Shift to make multiple lagged within the contig - if these loci overlap then the total tagge	ed length will be reported		
Isolates 1) A4/M1027 2) 120M 7) 7891 10) 6748 11) 129E 13) 139M 19) S3131 24) S4355 All None	Options Identify contigs with >= 0 • % of sequence untagged FASTA header line: original designation • 0 Action Reset Submit	Filter by Sequence method: Project Experiment Minimum length:	• 0 • 0 • 0	• 0

At its simplest, press submit.

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

-Isolates -			— — Op	otions	-Filter by		
) A4/M102	7	•	Iden	ntify contigs with >= 0 🗸 % of sequence untagged	Sequence method:	- 0	
) 120M			FAS	TA header line: original designation 👻 🕦	Project:		-
) 7891 0) 6748					Experiment:	• ()	
1) 129E					Minimum length:	• 0	
3) 139M						• •	
9) S3131			-Ac	tion ———			
		*		set Submit			
	All None	_		set Submit			
4) \$4355	All None	_		set Submit			
	All None	_		Submit			
	All None	_		Submit			
4) 84355		_	Re				
4) 84355		quence leng	Re gth unta	agged			
4) 84355 ntigs wi		quence leng	gth unta	agged on-matching contigs			
4) S4355 ntigs wi ≽ isolate	th >=0% sec ¢ contigs \$	quence leng matching co count \$ dow	gth unta ontigs n vnload c	agged on-matching contigs count 🔶 download			
4) S4355 ntigs wi isolate A4/M10	th >=0% sec contigs ¢ 27 364	quence leng matching co count + dow 364	gth unta ontigs n wnload c	agged on-matching contigs count + download 0			
4) S4355 ntigs wi isolate	th >=0% sec contigs ¢ 27 364	quence leng matching co count \$ dow	gth unta ontigs n vnload c	agged on-matching contigs count 🔶 download			

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

-Iso	olates ——			Op	otions	– – Filter by –		
1) A4	4/M1027		-	lden	ntify contigs with >= 0 🔍 🗸 % of sequence untagged	Sequence method:	• 0	
	20M 891			FAST	TA header line: original designation 👻 🕦	Project:		-
	6748					Experiment:	v 0	
	129E					Minimum length:	v ()	
I3) 1	139M							
(9) 5				A -4	B			
	S3131 S4355		-		tion			
	S3131 S4355		-					
	S3131 S4355	None	-	-				
	S3131 S4355	None)	-	-				
	S3131 S4355	JI None		-				
24) 8	83131 84355			Re	Submit			
24) 8	83131 84355	=0% sequ	ience len	Re:	agged			
4) s nti	\$3131 \$4355 igs with >	=0% sequ	lence len matching c	Re:	agged on-matching contigs			
4) s nti	83131 84355 igs with > solate ¢ c	=0% sequ ontigs \$	ience len matching c ount \$ dor	Res ngth unta contigs no wnload co	agged on-matching contigs ount + download			
4) s nti	83131 S4355 igs with > solate ¢ c A4/M1027	=0% sequ ontigs \$ c 364	uence len matching c ount \$ dor 364	Res rigth unta contigs no wnload co	agged on-matching contigs ount + download			
4) s nti	83131 84355 igs with > solate ¢ c	=0% sequ ontigs \$	ience len matching c ount \$ dor	Res ngth unta contigs no wnload co	agged on-matching contigs ount + download			

13.3.1 Filtering by tagged status of contigs

You can also export contigs based on the percentage of the sequence that has been tagged. This is useful to find sequences to target for gene discovery.

In order to export contigs where at least half the sequence has been tagged (and also the remaining contigs in a separate file), select '50' in the dropdown box for %untagged.

Options			
Identify contigs with	>= 50	🚽 % of seq	uence untagged
FASTA header line:	original	designation	▼ [i

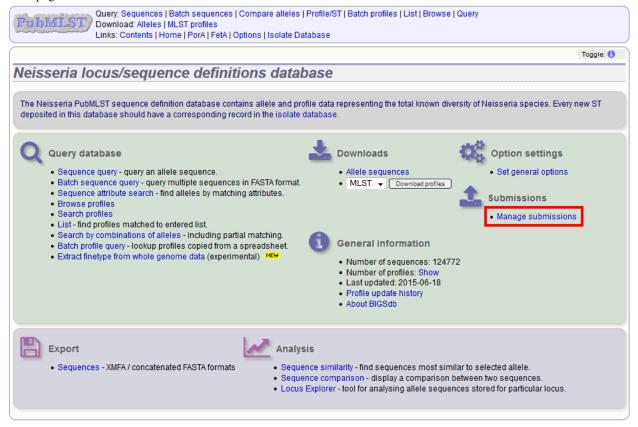
The resulting table has two download links for each isolate, one for contigs matching the condition, and one for contigs that don't match.

Con	tigs with	>=50% se	quence	length u	intagged	
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	<u>*</u>	259	*

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.



14.1 Registering a user account

You must have an account for the appropriate database in order to use the submission system. This will need to be set up by a curator, so contact them in the first instance.

14.2 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.

14.2.1 Start

Click the 'alleles' link under submission type on the submission management page.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database
Logged in: Keith Jolley (keith). (>Log out Change password
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
Return to index page

14.2.2 Select the submission locus

Select the locus from the locus list box:

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database Logged in: Keith Jolley (Keith). @Log out Change password			
Manage submissions			
You need to make a separate submission for each locus for number of new sequences for a single locus as one submis Filter loci by scheme Filter loci by scheme Filter Capsule Genetic Information Processing Hetabolism Conter schemes Loci not in schemes			d locus.

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 sequence Download: Alleles MLST profiles Links: Contents Home PorA Fet	ces Compare alleles Profile/ST Ba IA Options Isolate Database	tch 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 number of new sequences for a single locus as one sul Filter loci by scheme Filter loci by scheme Capsule Genetic Information Processing Metabolism Metabolism MLST MulsT MLST MulsT (20 locus partial genes) MLST (20 locus vhole genes) Contor schemes Loci not in schemes			d locus.

The locus list is now constrained making selection easier.

Profit MILST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database			
Logged in: Keith Jolley (keith). (+Log out Change password			
Manage submissions			
Capsule Capsule Capetic Information Processing Metabolism Typing			

14.2.3 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.

14.2.4 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 Download: Alleles MLST profiles Links: Contents Home PorA FetA Op	 ofile/ST Batch profiles List Browse Query pase
Logged in: Keith Jolley (keith). HLog out Change password	
Manage submissions	
	alleles - this is because different loci may have different curators. You can submit any build be trimmed to the correct start/end sites for the selected locus. Sequence details technology! Illumina read length! 100-199 coverage! 20-49x assembly! de novo assembly! de novo assembly! de novo assembly software! Velvet FASTA or single sequence Action Submit Submit

The system will perform some basic checks on the submitted sequences. If any of the sequences have been defined previously they must be removed from the submission before you can proceed. Curators do not want to waste their time dealing with previously defined sequences.

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). Dog out Change password			
Manage submissions			
Error: Sequence 'NM432' has already been defined as abcZ-3. Submit new alleles You need to make a separate submission for each locus for which new sequences for a single locus as one submission. Sequence Filter loci by scheme Filter loci by scheme Filter Capsule Genetic Information Processing Hetabolism Filter Dig Typing			
- Antigen genes - Antigen gene		>NM322 TTTGATACTGTCGCCGAAGGTTTGGGCGAA ATTCGCGATTATTGCGCCGTTATCATCAT GTCAGCCATGAGTTGGAAAATGGTTCGAGT GAGGCCTTATTGAAACAGCTCAACGAATTG - CAACTTGAGATCGAAGCGAAGGACGGCTGG	Submit

Assuming the preliminary checks have passed you will then be able to add additional information to your submission.

Putificities List Browse Query Download: Alleles MLST profiles List Browse Query Links: Contents Home PorA FetA Options Isolate Database List Browse Query			
Logged in: Keith Jolley (keith). (+Log out Change password			
Manage submissions			
Submission: BIGSdb 20150619110123 31937 75843			
You are submitting the following abcZ sequences: Download	technology:! Illumina		
	read length:! 100-199 👻		
Identifier Length Sequence Status Assigned allele	coverage: 20-49x -		
NM322 433 TTTGATACTGTCGCCGAAGG GCGGATTGTCGAACTCGATC pending NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending	assembly:! de novo 👻		
NM21 433 IIIBAIACCOIIBCCBARGO BCBBAIBICBARCICBAIC pending	assembly software: Velvet		
E-mail			
Updates will be sent to keith.jolley@zoo.ox.ac.uk. Finalize submission!			
Z 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.	and an explanatory note so that they can be linked to the		
Browse No files selected. Upload files			
Messages			
Add message			

14.2.5 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Add message'.

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		
Manage submissions		
Submission: BIGSdb 20150619110123 31937 75843		
Sequences	Sequence details	
You are submitting the following abcZ sequences: Download	technology: Illumina	
	read length: 100-199 👻	
Identifier Length Sequence Status Assigned allele NM322 433 TTTGATACTGTCGCCGAAGG GCGGATTGTCGAACTCGATC pending	coverage: 20-49x -	
NM21 433 TTTGATACCGTTGCCGAAGG GCGGATGTCGAACTCGATC pending	assembly:! de novo 👻	
	assembly software: Velvet	
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 curation. Ensure that these are named unambiguously or a	dd 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 —		
The sequence variant NM322 has		
been seen in 3 isolates.		
Add message		

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 (keith). HoLog out Change password		
Manage submissions		
Submission: BIG\$db_20150619110123_31937_75843		
Sequences	Sequence details	
You are submitting the following abcZ sequences: Download 🄜	technology:! Illumina 🗸	
Identifier Length Sequence Status Assigned allele	read length: 100-199 - coverage: 20-49x -	
NM322 433 TTTGATACTGTCGCCGAAGG GCGGATTGTCGAACTCGATC pending	assembly: de novo	
NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending	assembly software:! Velvet	
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 curation. Ensure that these are named unambiguously or a appropriate submission item. Individual filesize is limited to 32 MB.	add an explanatory note so that they can be linked to the	
Browse. No files selected. Upload files		
Browse No files selected. Upload files		
Messages		
Timestamp User Message 2015-06-19 10:10:04+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.		
Add message		

14.2.6 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.

Links: Contents Home PorA FetA Options Isolate Database			
Logged in: Keith Jolley (keith). @Log out Change password			
Manage submissions			
Submission: BIGSdb_20150619110123_31937_75843			
Sequences	Sequence details		
You are submitting the following abcZ sequences: Download 🔝	technology:!	Illumina 🗸	
Literational Automatical Status Assisted allala	read length:!		
Identifier Length Sequence Status Assigned allele NM322 433 TTTGATACTGTCGCCGAAGG GCGGATTGTCGAACTCGATC pending	-	20-49x 👻	
NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending	assembly software:	de novo 👻	
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 curation. Ensure that these are named unambiguously or	add an explanatory note :	so that they can be linked t	o the
appropriate submission item. Individual filesize is limited to 32 MB.			
Browse No files selected. Upload files			
Messages			
Timestamp User Message			
2015-06-19 10:10:04+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.			
Add message			

Select the file in the selection box, then click 'Upload files'.

Logged in: Keith Jolley (keith). IDLog out Change password		
Manage submissions		
Submission: BIGSdb 20150619110123 31937 75843		
	O a success dataila	
Sequences	Sequence details	
You are submitting the following abcZ sequences: Download ras	technology:	
Identifier Length Sequence Status Assigned allele	read length:!	
Identifier Length Sequence Status Assigned allele NM322 433 TTTGATACTGTCGCCGAAGG GCGGATTGTCGAACTCGATC pending	coverage:	
NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending		de novo 👻
	assembly software:!	Velvet
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 curation. Ensure that these are named unambiguously or appropriate submission item. Individual filesize is limited to 32 MB.	add an explanatory note s	so that they can be linked to the
appropriate submission tern, individual mesize is innited to 32 Mb.		
Browse abcZ.ace Upload files		
Messages		
Timestamp User Message		
2015-06-19 10:10:04+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.		
Add message		

The file will be uploaded and shown in a table.

เกิดเกลงร จนมากออางกอ	
Submission: BIGSdb_20150619110123_31937_75843	
Sequences	Sequence details
You are submitting the following abcZ sequences: Download ras	technology: Illumina
Identifier Length Sequence Status Assigned allele	read length: 100-199 V
NM322 433 TTTGATACTGTCGCCCGAAGG GCGGATTGTCGAACTCGATC pending	coverage:! 20-49x ▼ assembly:! de novo ▼
NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending	assembly software:! Velvet
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
appropriate submission item. Individual filesize is limited to 32 MB.	
Browse No files selected. Upload files	
Filename Size Delete	
abcZ.ace 1.7 MB	
Delete selected files	
Messages	
Timestamp User Message	
2015-06-19 10:10:04+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.	
Add message	

Files can be removed from the submission by checking the appropriate 'Delete' box and clicking 'Delete selected files'.

14.2.7 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!'.

ProbMILST 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). (+Log out Change password			
Manage submissions			
Submission: BIGSdb_20150619110123_31937_75843			
Sequences	Sequence details E-mail		
You are submitting the following abcZ sequences: Download ras	technology: Illumina Updates will be sent to keith.jolley@zoo.ox.ac.uk.		
Identifier Length Sequence Status Assigned allele	read length! 100-199 👻		
NM322 433 TTTGATACTGTCGCCGAAGG GCGGATTGTCGAACTCGATC pending	coverage: 1 20-49x - Action		
NM21 433 TTTGATACCGTTGCCGAAGG GCGGATTGTCGAACTCGATC pending	assembly software! Velvet Finalize submission!		
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 abcZ.ace 1.7 MB			
Delete selected files			
Messages			
Timestamp User Message 2015-06-19 10:10:04+00 Keith Jolley The sequence variant NM322 has been seen in 3 isolates.			
2015-06-19 10.10.04+00 Kein Joliey The sequence variant NM322 has been seen in 3 isolates.			
Add message			

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 (keith). [+Log out Change password
Manage submissions
Submit new data
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.
Submission type:
alleles MLST profiles
Pending submissions
You have submitted the following submissions that are pending curation:
Submission id Submitted Updated Type Details
BIGSdb_20150619110123_31937_75843 2015-06-19 2015-06-19 alleles 2 abcZ sequences
Return to index page

14.3 Profile submission

Even if the submission system has been enabled, submission of profiles has to be specifically enabled. Many databases require submission of representative isolate data for any new allelic profile for schemes such as MLST. In this case any new profiles can be readily extracted from the isoate data so profiles do not need to be submitted separately.

14.3.1 Start

Click the appropriate profiles link under submission type on the submission management page.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home Portions Isolate Database
Logged in: Keith Jolley (keith). DeLog out Change password
Manage submissions
Submit new data
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.
Submission type:
alleles MLST profiles
Return to index page

Download the Excel submission template.

Query: Sequences Compare alleles Profile/ST Batch profiles List Browse Query: Download: Alleles I MLST profiles List Browse Query: Sequences Query: Sequences Query: Sequences Query: Query: Sequences Query: Query: Sequences Query: Query:	
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
lh.	

14.3.2 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.

Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database						
Logged in: Keith Jolley (keith). @Log out Change password						
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 (xtsx format) Please paste in tab-delimited text (include a field header line) 1d abc2 adk arco2 func gdh pdhC pgm 3 2 4 3 8 4 6	Action Submit					

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.

P	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										
Log	Logged in: Keith Jolley (keith). @Log out Change password										
М	Manage submissions										
E	rror:										
R	ow 3: Profi	ile has alre	ady been d	efined as ST	-10018.						
		ew MLST	-								
P			-	ent using the							
				eader for you nplate (xlsx f		eet - use 'Pa	aste Special	Text to paste the transformed and the past of the p	ie data.		
_	-Please	paste in tal	b-delimited	text (include	a field hea	der 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

14.3.3 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Add message'.

PrrhL/LLST Query: Sequences Batch sequences Compare alleles Profile/ST Batch profiles List Browse Query Download: Alleles MLST profiles Links: Contents Home PorA FetA Options Isolate Database					
Logged in: Keith Jolley (keith). @Log out Change password					
Manage submissions					
Submission: BIGSdb_20150619135509_21808_97411 Profiles E-mail You are submitting the following MLST profiles: Download Image: Constant of the sent to keith jolley@zoo.ox.ac.uk Identifier adk abc2 aroc fumC gdh pdhC pgm Status Assigned ST Updates will be sent to keith jolley@zoo.ox.ac.uk 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 Corresponding isolate data has already been submitted (ids 43721-43722). Add message Add message					

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 (keith). GeLog out Change password					
Manage submissions					
Submission: BIG Sdb_20150619135509_21808_97411 Profiles You are submitting the following MLST profiles: Download C3 Identifier adk abc2 arce 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 Updates will be sent to keith.jolley@zoo.ox.ac.uk. ☑ E-mail submission updates	Action Finalize submission!			
Supporting files Please upload any supporting files required for curation. Ensure that these the appropriate submission item. Individual filesize is limited to 32 MB. Browse	are named unambiguously or add an explanatory note	so that they can be linked to			
Timestamp User Me 2015-06-19 13:00:33+00 Keith Jolley Corresponding isolate data has alre	essage eady been submitted (ids 43721-43722). .:i				
	Add message				

14.3.4 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'.

14.3.5 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 (keith). DeLog out Change password						
Manage submissions						
Submission: BIGSdb_20150619135509_21808_97411 Profiles	— E-mail	Action				
You are submitting the following MLST profiles: Download cst Identifier adk abcZ aroE fumC gdh pdhC pgm Status Assigned ST	Updates will be sent to keith.jolley@zoo.ox.ac.uk.	Finalize submission!				
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 a the appropriate submission item. Individual filesize is limited to 32 MB.	are named unambiguously or add an explanatory note	so that they can be linked to				
Browse No files selected. Upload files						
Messages						
Timestamp User Me 2015-06-19 13:00:33+00 Keith Jolley Corresponding isolate data has alre	ssage ady been submitted (ids 43721-43722).					
	i i i i i i i i i i i i i i i i i i i					
	Add message					

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 (keith). [#Log out Change password
Manage submissions
Submit new data
Data submitted here will go in to a queue for handling by a curator or by an automated script. You will be able to track the status of any submission.
Submission type:
alleles MLST profiles
Pending submissions
You have submitted the following submissions that are pending curation:
Submission id Submitted Updated Type Details BIGSdb_20150619135509_21808_97411 2015-06-19 2015-06-19 2 MLST profiles
Return to index page

14.4 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.

14.4.1 Start

Click the 'isolates' link under submission type on the submission management page.

PubMLST / Bre	ery: Search Browse Profile/ST List eakdown: Isolate fields Scheme/alleles Publications iks: Contents Home Options Profiles/sequences definitions Database submissions
Logged in: Keith Jolley (keit	th). DeLog out Change password
Manage subm	issions
Submit new data	
Data submitted here wil	I 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 	
Return to index page	

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 locu	is 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

14.4.2 Paste in isolate data

Fill in the template. Some fields are required and cannot be left blank. Check the 'Description of database fields' link on the database contents page to see a description of the fields and allowed values where these have been defined. Where allowed values have been set, the template will have dropdown boxes (although these require newer versions of Excel to work).

Some databases may have hundreds of loci defined, and most will not have a column in the template. You can add new columns for any loci that have been defined and for which you would like to include allelic information for. These locus names must be the primary locus identifier. A list of loci can be found in the 'allowed_loci' tab of the Excel submission template.

Copy and paste the entire contents of the submission worksheet. Click submit.

PubMLST Breakdown: Isolate fields Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions								
Logged in: Keith Jalley (keith). @Log out Change password								
Manage submissions	Nanage submissions							
Submit new isolates								
Paste in your isolates for addition to the databa	ase using the template avai	lable below.						
Enter aliases (alternative names) for you Enter references for your isolates as a You can also upload additional allele fil	ur isolates as a semi-color semi-colon (;) separated lis	n (;) separated list. It of PubMed ids.	create a new colu	umn with the lo	ocus name.			
 Download tab-delimited header for you Download submission template (xlsx for 		Special 😋 Text' to p	aste the data.					
Please paste in tab-delimited text (include	a field header line)				— — Action —			
isolate aliases references disease source epidemiology serotype sero subtype amoxicillin sulphonamide	ET_no penicilli	MLEE C	age_mth s lesignation illin_range	ex	Submit			
chloramphenicol chloramphenico rifampicin rifampicin_ran pending assembly commen	l_range cefotaxim ge ciproflox ts abcZ a	ne cefota	axime_range loxacin_ran	ige Idh				
pdhC pgm FetA VR PorA V UK322 UK	R1 PorA_VR2 2015	~~~~~~~	····· ·	~~~				
meningitis and septicaemia B		Veisseria meni	ingitidis					
2 3 4 UK325 UK	3 8 4 2015	6	F1-5 5	2				
septicaemia CSF B	Neisseria meningi	itis						
2 3 4	3 8 4	6	F1-5 5	i-1 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.

K3225 has problems - species: Neisseria meningitis' is not on the list of allowed values for this field. ubmit new isolates aste 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 aliases (untrative names) for your isolates as a semi-colon () separated list. • For preferences for your isolates as a semi-colon () separated list. • You can also upload additional allele fields along with the other isolate data - simply create a new column with the locus name. • Download tab-delimited header for your spreadsheet - use 'Paste Special O Text to paste the data. • Download tab-delimited text (include a field header line) Please paste in tab-delimited text (include a field header line) Action isolate aliases references Country region year age yr age mth sex disease source epidemiology species scrogroup MLEE_designation Submit serotype ser_or peictriaxone ceftriaxone_range chloramphenicol_chloramphenicol_range cefotaxime_range cefotaxime_range chloramphenicol_chloramphenicol_range ciprofloxacin_range gel yr yoth 2 3 4 6 F1-5 2 yoth	anade). 🕩 Log out	Change pass	word								
JK325 has problems - species: 'Neisseria meningilis' is not on the list of allowed values for this field. Submit new isolates Paste in your isolates for addition to the database using the template available below. • Enter aliases (alternative names) for your isolates as a semi-colon () separated list. • Enter aliases (alternative names) for your isolates as a semi-colon () separated list. • Enter aliases (alternative names) for your isolates as a semi-colon () separated list. • Enter aliases (alternative names) for your isolates as a semi-colon () separated list. • Enter aliases (alternative names) for your isolates as a semi-colon () separated list. • Enter aliases (alternative names) for your isolates as a semi-colon () separated list. • Download tab-delimited header for your spreadsheet - use 'Paste Special © Text' to paste the data. • Download tab-delimited text (include a field header line) Please paste in tab-delimited text (include a field header line) isolate a liases references country region year age_yr age_mth sex isolate aliases references country region year age_yr age_mth sex isolate aliases references certriaxone ceftriaxone ceftriaxone range chloramphenicol chloramphenicol_range ceftoraxime ciprofloxacin_range pandC pgm FetA_VR PorA_VR1 2015 <th>3</th> <th>e subm</th> <th>ission</th> <th>S</th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th> <th></th>	3	e subm	ission	S									
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 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 locus name. 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 isolate aliases references country region year age_yr age_mth sex disease source epidemiology species serogroup MLEE_designation serotype sero_subtype ET_no penicillin penicillin_range chloramphenicol chloramphenicol_range ceftotaxime ceftotaxime_range ciprofloxacin_ciprofloxacin_range pending_assembly comments abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2 UK322 UK 2015 2 3 4 3 8 4 6 F1-5 5 2 UK325 UK 2015	rror:												
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 locus 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 isolate aliases references country region year age_yr age_mth sex disease source epidemiology species serogroup MLEE_designation serotype sero_subtype ET_no penicillin penicillin_range amoxicillin sulphonamide ceftriaxone ceftriaxone_range chloramphenicol chloramphenicol_range cefotaxime cefotaxime_range rifampicin rifampicin_range ciprofloxacin_ciprofloxacin_range pending_assembly comments abc2 adk arocE func gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2 UK322 UK 2015 2 3 4 3 8 4 6 F1-5 5 2 UK325 UK 2015	K325 has	problems - s	pecies: 'Nei	sseria mer	ingitis' is no	ot on the list	t of allowed	values for t	his field.				
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 locus name. Download tab-delimited header for your spreadsheet - use 'Paste Special © Text to paste the data. Download tab-delimited header for your spreadsheet - use 'Paste Special © Text to paste the data. Download tab-delimited header for your spreadsheet - use 'Paste Special © Text to paste the data. Download tab-delimited text (include a field header line) Please paste in tab-delimited text (include a field header line) Action isolate aliases references country region year age_yr age_mth sex disease source epidemiology species serogroup MLEE_designation serotype sero subtype ET_no penicillin penicillin_range amoxicillin sulphonamide ceftriaxone ceftriaxone_range chloramphenicol chloramphenicol_range cliptofloxacin_range pending_asembly comments abc2 adk arooE ydn C y													
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 locus name. 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 isolate aliases references country region year age_yr age_mth sex disease source epidemiology species serogroup MLEE_designation serotype sero subtype ET_no penicillin penicillin, range amoxicillin sulphonamide ceftriaxone ceftriaxone_range chloramphenicol chloramphenicol_range ciprofloxacin_range ciprofloxacin_range pending_assembly comments abc2 adk arooE MLEE_datk Action Submit	ubmit no	ew isolates											
 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 locus 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 isolate aliases references country region year age_yr age_mth sex disease source epidemiology species serogroup MLEE_designation serotype sero_subtype ET_no penicillin penicillin_range chloramphenicol chloramphenicol_range ciprofloxacin ciprofloxacin range pending_assembly comments abcZ adk aros fum for your yona blood Neisseria meningitidis 				the databas	e using the	template a	vailable bel	0.00					
 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 locus 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 isolate aliases references country region year age_yr age_mth sex disease source epidemiology species serogroup MLEE_designation serotype sero_subtype ET_no penicillin penicillin_range chloramphenicol chloramphenicol_range ceftotaxime ceftotaxime_range ciprofloxacin_ciprofloxacin_range pending_assembly comments abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2 UK322 UK 2015 2 3 4 3 8 4 6 F1-5 5 2 UK325 UK 2015					-								
 You can also upload additional allele fields along with the other isolate data - simply create a new column with the locus name. Download tab-delimited header for your spreadsheet - use 'Paste Special Q Text to paste the data. Download submission template (xlsx format) Please paste in tab-delimited text (include a field header line) Action isolate aliases references country region year age_yr age_mth sex disease source epidemiology species serogroup MLEE_designation serotype sero_subtype ET_no penicillin penicillin_range amoxicillin sulphonamide ceftriaxone ceftriaxone_range chloramphenicol chloramphenicol_range ciprofloxacin ciprofloxacin_range pending_assembly comments abc2 adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2 UK322 UK 2015 UK 2015 													
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	chloram rifampi pending pdhC UK322 meningi	icin g_assembly pgm	/ FetA_VR	comment PorA_VR UK	3 1	PorA_VF		ria meni	ngitidis				
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	chloram rifampi pending pdhC UK322 meningi B UK325 septica	cin g_assembly pgm ltis and s 2 aemia	/ FetA_VR septicaen 3 CSF	comment PorA_VR UK nia 4 UK	s 1 blood 3 Neisser	PorA_VF 2015 8 2015 ia menir	Neisser 4 ngitis	6	F1-5				
	chloram rifampi pending pdhC UK322 meningi B UK325 septica	cin g_assembly pgm ltis and s 2 aemia	/ FetA_VR septicaen 3 CSF	comment PorA_VR UK nia 4 UK	s 1 blood 3 Neisser	PorA_VF 2015 8 2015 ia menir	Neisser 4 ngitis	6	F1-5				

Provided the checks pass, you will then be able to add additional information to your submission.

14.4.3 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Add message'.

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). 6+Log out Change password
Manage submissions
Submission: BIGSdb_20150622133440_1412_50186
Isolates
You are submitting the following isolates: Download est
isolate country year disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA VR PorA VR1 PorA VR2
UK322 UK 2015 meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2 UK325 UK 2015 septicaemia CSF Neisseria meningitidis B 2 3 4 3 18 4 6 F1-5 5-1 2
Updates will be sent to keith.jolley@zoo.ox.ac.uk.
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
Messages
I think UK325 has a new MLST profile requiring definition of a new ST
number. Thanks.
Add message

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 Scheme/alleles Publications Links: Contents Home Options Profiles/sequences definitions Database submissions	
Logged in: Keith Jolley (keith). @Log out Change password	
Manage submissions	
Submission: BIGSdb_20150622133440_1412_50186	
Isolates	
You are submitting the following isolates: Download	
isolate country year disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2	
UK322 UK 2015 meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2	
UK325 UK 2015 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	
- 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 appropriat	te
submission item. Individual filesize is limited to 32 MB.	
Browse No files selected. Upload files	
Messages	
Timestamp User Message	
2015-06-22 12:36:41+00 Keith Jolley I think UK325 has a new MLST profile requiring definition of a new ST number. Thanks.	
Add message	

14.4.4 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.

Man	LST	Break	: Search Browse down: Isolate fiel : Contents Home	ds Schen	ne/allele	s Publications s/sequences definitions	Database	subm	issior	ıs								
.ogged in: Ke	ith Joll	ey (keith). I	€Log out Change	password														
lanag	e sı	ıbmis	ssions															
Submissi	ion: E	GSdb	20150622133	440 141:	2 5018	6												
Isolate	s ——			-	_													
You are s	ubmitti	ng the fol	llowing isolates: I	Download	CST													
isolate o	countr	u voar	disease		source	species	COLOGICOUD	ahc7	adk	aroE f	umC	adb	ndhC	nam	FotA VD		1 PorA_VR2	
UK322	UK		neningitis and se			Neisseria meningitidis	B	2	3	4	3	8	4	6	F1-5	5	2	
UK325	UK	2015	septicaem	ia	CSF	Neisseria meningitidis	В	2	3	4	3	18	4	6	F1-5	5-1	2	
- E-mail					Action													
Updates v	will be	sent to ke	eith.jolley@zoo.ox	.ac.uk.	Finaliz	e submission!												
🗖 E-mai	il subn	nission u	pdates															
-Suppor	rting fil	es																
						ure that these are name	d unambig	uously	or ad	d an ex	plana	itory r	note s	o that	they can I	oe linked to	the appropriat	te
submissi	on iter	n. Individi	ual filesize is limit	ted to 32 M	В.													
Browse	N	o files sel	lected.	Ipload files	3													
Messa	aes —																	
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2015-06	-22 12	36:41+00	0 Keith Jolley I th	ink UK325	has a n	ew MLST profile requirin	g definition	of a n	ew ST	numbe	er. Th	anks						
I thin	k UK:	825 has	s a new MLST	profile	e requ	iring definition	of a ne	w ST	numl	ber.	Tha	inks	•					
										Add r	ness	age						
												-						

Select the file in the selection box, then click 'Upload files'.

Query: Search Browse Profile/S Breakdown: Isolate fields Schem Links: Contents Home Options	ne/alleles Publications	Database subm	issions					
Logged in: Keith Jolley (keith). DLog out Change password								
Manage submissions								
Submission: BIGSdb 20150622133440 1412	2 50186							
You are submitting the following isolates: Download	CST							
				fund a th	- 11-0	5-44-140	DA MD4	
isolate country year disease UK322 UK 2015 meningitis and septicaemia	source species blood Neisseria meningitidis	serogroup abcZ B 2	3 4	3 8	4 6	F1-5	5	2
UK325 UK 2015 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								
Supporting files								
Please upload any supporting files required for curat submission item. Individual filesize is limited to 32 M		ed unambiguously	or add an e	xplanatory	note so tha	t they can b	e linked to th	ne appropriate
	ID.							
Browse UK325_genome_contigs.fas Upload	lfiles							
Messages								
Timestamp User	Messa							
2015-06-22 12:36:41+00 Keith Jolley I think UK325		-			_			
I think UK325 has a new MLST profile	e requiring definition	of a new ST	number.	Thanks				
			Add	message				

The file will be uploaded and shown in a table.

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	
Manage submissions	
Submission: BIGSdb 20150622133440 1412 50186	
You are submitting the following isolates: Download 🕞	
isolate country year disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2 UK322 UK 2015 meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2	
UK325 UK 2015 septicaemia CSF Neisseria meningitidis B 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. Finalize submission!	
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 appropria submission item. Individual filesize is limited to 32 MB.	e
Browse No files selected. Upload files	
Filename Size Delete UK325_genome_contigs.fas 2 MB Image: Contigs.fas	
Delete selected files	
- Messages Timestamp User Message	
Timestamp User Message 2015-06-22 12:36:41+00 Keith Jolley I think UK325 has a new MLST profile requiring definition of a new ST number. Thanks.	
Add message	

Files can be removed from the submission by checking the appropriate 'Delete' box and clicking 'Delete selected files'.

14.4.5 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 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
Manage submissions
Submission: BIGSdb_20150622133440_1412_50186
Isolates
You are submitting the following isolates: Download est
isolate country year disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2
UK322 UK 2015 meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2
UK325 UK 2015 septicaemia CSF Neisseria meningitidis B 2 3 4 3 18 4 6 F1-5 5-1 2
E-mail Dpdates will be sent to keith.jolley@zoo.ox.ac.uk. Einalize submission
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
Messages
Timestamp User Message 2015-06-22 12:36:41+00 Keith Jolley I think UK325 has a new MLST profile requiring definition of a new ST number. Thanks.
Add message

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
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 idSubmittedUpdatedTypeDetailsBIGSdb_20150622133440_1412_501862015-06-222015-06-22isolates2
Return to index page

RESTful Application Programming Interface (API)

The REST API allows third-party applications to retrive data stored within BIGSdb databases. 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 file).

15.1 Passing optional parameters

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

15.2 Resources

- / or /db
- /db/{database}
- /db/{database}/loci
- /db/{database}/loci/{locus}
- /db/{database}/loci/{locus}/alleles
- /db/{database}/loci/{locus}/alleles_fasta
- /db/{database}/loci/{locus}/alleles/{allele_id}
- /db/{database}/schemes
- /db/{database}/schemes/{scheme_id}
- /db/{database}/schemes/{scheme_id}/fields/{field}
- /db/{database}/schemes/{scheme_id}/profiles
- /db/{database}/schemes/{scheme_id}/profiles_csv
- /db/{database}/schemes/{scheme_id}/profiles/{profile_id}
- /db/{database}/isolates
- /db/{database}/isolates/{isolate_id}
- /db/{database}/isolates/{isolate_id}/allele_designations

- /db/{database}/isolates/{isolate_id}/allele_designations/{locus}
- /db/{database}/isolates/{isolate_id}/allele_ids
- /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_designations
- /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_ids
- /db/{database}/isolates/{isolate_id}/contigs
- /db/{database}/isolates/{isolate_id}/contigs_fasta
- /db/{database}/contigs/{contig_id}
- /db/{database}/fields
- /db/{database}/users/{user_id}

15.2.1 / or /db

Lists database resources available using the API.

Supported methods: GET, POST

Required query 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

15.2.2 /db/{database}

Lists resources available for specified database configuration. These will vary depending on whether the resource is an isolate or a sequence definition database.

Supported methods: GET, POST

Required query parameter: {database} - Database configuration name [string]

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
- records [integer] count of available records

15.2.3 /db/{database}/loci

Lists loci defined within specified database configuration.

Supported methods: GET, POST

Required query parameter: {database} - Database configuration name [string]

Optional parameters:

- page [integer]
- page_size [integer] Set very large page size to return all results in one go.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci

Response: Object containing:

- 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

15.2.4 /db/{database}/loci/{locus}

Provides information about a locus, including links to allele sequences (in seqdef databases).

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {locus} Locus name [string]

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)

15.2.5 /db/{database}/loci/{locus}/alleles

Lists alleles defined for specific locus.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {locus} Locus name [string]

Optional parameters:

- page [integer]
- page_size [integer] Set very large page size to return all results in one go.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles

Response: Object containing:

- 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

15.2.6 /db/{database}/loci/{locus}/alleles_fasta

Provides all alleles defined for a locus in FASTA format.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {locus} Locus name [string]

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles_fasta

Response: FASTA format file of alleles sequences

15.2.7 /db/{database}/loci/{locus}/alleles/{allele_id}

Provides information about an allele including its sequence.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {locus} Locus name [string]
- {allele_id} Allele identifier [string]

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)

15.2.8 /db/{database}/schemes

Lists schemes defined within specified database configuration.

Supported methods: GET, POST

Required query parameter: {database} - Database configuration name [string]

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes

Response: List of scheme objects, each containing:

- scheme [string] URI to scheme information
- description [string]

15.2.9 /db/{database}/schemes/{scheme_id}

Provides information about a scheme, including links to allelic profiles (in seqdef databases, if appropriate).

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {scheme_id} Scheme id number [integer]

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
- profile_count [integer] number of defined profiles (only for schemes with primary keys defined only seqdef databases)
- profiles [array] URI to list of profile definitions (only seqdef databases)
- profiles_csv [string] URI to tab-delimited file of all scheme profiles

15.2.10 /db/{database}/schemes/{scheme_id}/fields/{field}

Provides information about scheme fields.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {scheme_id} Scheme id number [integer]
- {field} Field name [string]

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

15.2.11 /db/{database}/schemes/{scheme_id}/profiles

Lists allelic profiles defined for a specific scheme.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {scheme_id} Scheme id [integer]

Optional parameters:

- page [integer]
- page_size [integer] Set very large page size to return all results in one go.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles

Response: Object containing:

- 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

15.2.12 /db/{database}/schemes/{scheme_id}/profiles_csv

Provides all profiles defined for a scheme in CSV (tab-delimited) format.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {scheme_id} Scheme id [integer]

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles_csv

Response: Tab-delimited text file of allelic profiles

15.2.13 /db/{database}/schemes/{scheme_id}/profiles/{profile_id}

Provides information about a specific allelic profile defined for a scheme.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {scheme_id} Scheme id [integer]
- {profile_id} Profile id [string/integer]

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)

15.2.14 /db/{database}/isolates

Provides list of isolate records.

Supported methods: GET, POST

Required query parameter: {database} - Database configuration name [string]

Optional parameters:

• page [integer]

• page_size [integer] - Set very large page size to return all results in one go.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates

Response: Object containing:

- 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

15.2.15 /db/{database}/isolates/{isolate_id}

Provides information about an isolate.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {isolate_id} Isolate identifier [integer]

Optional parameters: None

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*. 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 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

15.2.16 /db/{database}/isolates/{isolate_id}/allele_designations

Provides a list of full allele designation records for the specified isolate.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {isolate_id} Isolate identifier [integer]

Optional parameters:

- page [integer]
- page_size [integer] Set very large page size to return all results in one go.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_designations

Response: Object containing:

- 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

15.2.17 /db/{database}/isolates/{isolate_id}/allele_designations/{locus}

Provides a full allele designation record.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {isolate_id} Isolate identifier [integer]
- {locus} Locus mame [string]

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)

15.2.18 /db/{database}/isolates/{isolate_id}/allele_ids

Returns array of allele identifiers for isolate.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {isolate_id} Isolate identifier [integer]

Optional parameters:

- page [integer]
- page_size [integer] Set very large page size to return all results in one go.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_ids

Response: Object containing:

- 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

15.2.19 /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_designations

Provides a list of full allele designation records for loci belonging to the specified scheme and isolate.

Supported methods: GET, POST

Required query parameters:

• {database} - Database configuration name [string]

- {isolate_id} Isolate identifier [integer]
- {scheme_id} Scheme identifier [integer]

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/schemes/1/allele_designations **Response:** Array containing *allele designation objects* for each locus in the specified scheme that has been designated.

15.2.20 /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_ids

Provides a list of allele identifiers for loci belonging to the specified scheme and isolate.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {isolate_id} Isolate identifier [integer]
- {scheme_id} Scheme identifier [integer]

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/schemes/1/allele_ids

Response: Array 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.

15.2.21 /db/{database}/isolates/{isolate_id}/contigs

Returns a list of contig records for the specified isolate.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {isolate_id} Isolate identifier [integer]

Optional parameters:

- page [integer]
- page_size [integer] Set very large page size to return all results in one go.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/contigs

Response: Object containing:

- 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

15.2.22 /db/{database}/isolates/{isolate_id}/contigs_fasta

Provides all contigs associated with an isolate record in FASTA format.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {isolate_id} Isolate identifier [integer]

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

15.2.23 /db/{database}/contigs/{contig_id}

Provides a record of a specified contig.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {contig_id} Contig identifier [integer]

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)

15.2.24 /db/{database}/fields

Provides a list of isolate provenance field descriptions.

Supported methods: GET, POST

Required query parameters:

• {database} - Database configuration name [string]

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 [string]

15.2.25 /db/{database}/users/{user_id}

Provides information about data senders and curators.

Supported methods: GET, POST

Required query parameters:

- {database} Database configuration name [string]
- {user_id} User id number [integer]

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

15.3 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.

15.3.1 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

15.3.2 Getting a request token

- Relative URL: /db/{database}/oauth/get_request_token
- Supported methods: GET, POST

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 ('POST')
- 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.

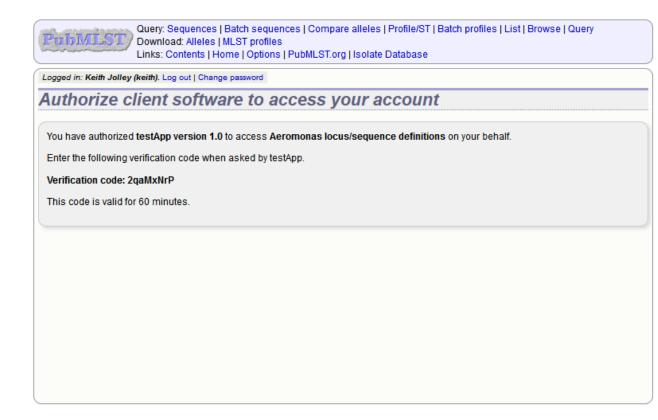
15.3.3 Getting user authorization

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=fKFm0WNhCfbEX8zQm6qhDA8K23FOWI

The user will be asked if they wish to grant access to the application on their behalf:

Duery: 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 — Action
testApp version 1.0 Aeromonas locus/sequence definitions Cancel Authorize
You will be able to revoke access for this application at any time.

If they authorize the access, they will be presented with a verifier code. This should be entered in to the client application which will use this together with the request token to request an access token.



The verifier code is valid for 60 minutes.

15.3.4 Getting an access token

- Relative URL: /db/{database}/oauth/get_access_token
- Supported methods: GET, POST

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 ('POST')
- 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

15.3.5 Getting a session token

- Relative URL: /db/{database}/oauth/get_session_token
- Supported methods: GET, POST

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 ('POST')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_token (access token)
- oauth_timestamp (UNIX timestamp seconds since Jan 1 1970) this must be within 600 seconds of the current time.
- oauth_nonce (random string)
- oauth_version ('1.0')

If the application has been registered and has been granted permission to access the specific resource, a JSON response will be returned containing the following parameters:

- oauth_token
 - This is the session token. It is usually a 32 character alphanumeric string.
 - e.g. H8CjIS8Ikq6hwCUqUfF1l4pTaCYl8Ljw
- oauth_token_secret
 - This is the secret associated with the session token. It is usually a 32 character alphanumeric string.
 - e.g. RfponbaNPO7tkZ2miHFISk0pMndePNfJ

15.3.6 Accessing protected resources

• Supported methods: GET, POST

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 ('POST')
- 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')

Frequently asked questions (FAQs)

16.1 General

1. What is the minimum specification of hardware required to run BIGSdb?

The software will run on very 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 a processor core each, 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* can be 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: 16 cores, 64GB RAM
- database server: 64 cores, 1TB RAM, 3TB RAID 10 local storage

16.2 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.

16.3 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.

Appendix

17.1 Query operators

Various query forms have operators for use with field values. Available operators are:

• =

- Exact match (case-insensitive).
- contains
 - Match to a partial string (case-insensitive), e.g. searching for clonal complex 'contains' st-11 would return all STs belonging to the ST-11 complex.
- · starts with
 - Match to values that start with the search term (case-insensitive).
- ends with
 - Match to values that end with the search term (case-sensitive).

• >

- Greater than the search term.

• <

- Less than the search term.
- NOT
 - Match to values that do not equal the search term (case-insensitive).
- NOT contain
 - Match to values that do not contain the search term (case-insensitive).

17.2 Sequence tag flags

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

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

- apparent misassembly
 - Sequence has a region of very high identity to existing allele in one region but looks completely different in another.
- atypical
 - Catch-all term for a sequence that is unusual compared to other alleles of locus.
- · contains IS element
 - Coding sequence is interrupted by insertion sequence.
- · downstream fusion
 - No stop codon present resulting in translation continuing.
- frameshift
 - Frameshift in sequence relative to other alleles, not resulting in internal stop codon.
- internal stop codon
 - Frameshift in sequence relative to other alleles, resulting in internal stop codon.
- no start codon
 - No apparent start codon in immediate vicinity of usual start.
- phase variable: off
 - Coding sequence has a homopolymeric run with a frameshift resulting in a stop codon preventing complete translation.
- truncated
 - Coding sequence is unusually short resulting in a truncated protein (not the same as running off the end of a contig).
- upstream fusion
 - No apparent start codon in immediate vicinity of usual start, likely due to a gene fusion (sequence is transcribed together with upstream coding sequence).

17.3 Allele sequence flags

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

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

- internal stop codon
 - Frameshift in sequence relative to other alleles, resulting in internal stop codon.
- no start codon
 - No apparent start codon in immediate vicinity of usual start.
- phase variable: off
 - Coding sequence has a homopolymeric run with a frameshift resulting in a stop codon preventing complete translation.
- truncated
 - Coding sequence is unusually short resulting in a truncated protein (not the same as running off the end of a contig).
- upstream fusion
 - No apparent start codon in immediate vicinity of usual start, likely due to a gene fusion (sequence is transcribed together with upstream coding sequence).

Database schema

- Sequence definition database
- Isolate database

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