BIGSdb Documentation

Release 1.18.0

Keith Jolley

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Contents

1 Concepts and terms **3**
- 1.1 BIGSdb . . . 3
- 1.2 Loci . . . 3
- 1.3 Alleles . . . 3
- 1.4 Schemes . . . 4
- 1.5 Profiles . . . 4
- 1.6 Classification groups . . . 4
- 1.7 Sequence tags . . . 4
- 1.8 Sets . . . 5

2 BIGSdb dependencies **7**
- 2.1 Required packages . . . 7
  - 2.1.1 Linux packages . . . 7
  - 2.1.2 Perl modules . . . 7
  - 2.1.3 Optional packages . . . 8

3 Installation and configuration of BIGSdb **9**
- 3.1 Software installation . . . 9
- 3.2 Configuring PostgreSQL . . . 10
  - 3.2.1 pg_hba.conf . . . 10
  - 3.2.2 pg_ident.conf . . . 11
- 3.3 Setting global connection parameters . . . 11
- 3.4 Site-specific configuration . . . 11
- 3.5 Setting up the offline job manager . . . 12
- 3.6 Setting up the submission system . . . 13
- 3.7 Setting up a site-wide user database . . . 13
- 3.8 Periodically delete temporary files . . . 15
- 3.9 Prevent preference database getting too large . . . 15
- 3.10 Purging old jobs from the jobs database . . . 16
- 3.11 Log file rotation . . . 16
- 3.12 Upgrading BIGSdb . . . 16
- 3.13 Running the BIGSdb RESTful interface . . . 17
  - 3.13.1 Proxying the API to use a standard web port . . . 19

4 Database setup **21**
- 4.1 Creating databases . . . 21
- 4.2 Database-specific configuration . . . 22

4.3 XML configuration attributes used in config.xml . . . 23
4.3.1 Isolate database XML attributes . . . 23
4.3.1.1 Special values . . . 29
4.3.2 Sequence definition database XML attributes . . . 29
4.4 Over-riding global defaults set in bigsdb.conf . . . 32
4.5 Over-riding values set in config.xml . . . 33
4.6 User authentication . . . 33
4.6.1 Apache authentication . . . 33
4.6.2 Built-in authentication . . . 33
4.7 Setting up the admin user . . . 34
4.8 Updating PubMed citations . . . 34
4.9 Configuring access to remote contigs . . . 34
4.9.1 Setting up authentication . . . 35
4.9.2 Processing remote contigs . . . 36

5 Administrator's guide **39**
5.1 Types of user . . . 39
5.2 User groups . . . 39
5.3 Curator permissions . . . 40
5.4 Locus and scheme permissions (sequence definition database) . . . 42
5.5 Controlling access . . . 44
5.5.1 Restricting particular configurations to specific user accounts . . . 44
5.6 Setting user passwords . . . 44
5.7 Setting the first user password . . . 45
5.8 Enabling plugins . . . 46
5.9 Temporarily disabling database updates . . . 46
5.9.1 Global . . . 47
5.9.2 Database-specific . . . 47
5.10 Host mapping . . . 47
5.11 Improving performance . . . 47
5.11.1 Use mod_perl . . . 47
5.11.2 Cache scheme definitions within an isolate database . . . 48
5.11.3 Use a ramdisk for the secure temporary directory . . . 49
5.12 Dataset partitioning . . . 49
5.12.1 Sets . . . 49
5.12.2 Configuration of sets . . . 50
5.12.3 Set metadata . . . 51
5.12.4 Set views . . . 53
5.12.5 Using only defined sets . . . 53
5.13 Setting a site-wide users database . . . 53
5.14 Adding new loci . . . 54
5.14.1 Sequence definition databases . . . 54
5.14.1.1 Single locus . . . 54
5.14.1.2 Batch adding . . . 57
5.14.2 Isolate databases . . . 58
5.14.2.1 Single locus . . . 58
5.14.2.2 Batch adding . . . 64
5.15 Defining locus extended attributes . . . 66
5.16 Defining schemes . . . 69
5.16.1 Sequence definition databases . . . 69
5.16.2 Isolate databases . . . 73
5.17 Organizing schemes into hierarchical groups . . . 76
5.18 Setting up client databases . . . 80
5.18.1 Look up isolates with given allele . . . 82

5.18.2 Look up isolates with a given scheme primary key . . . 84
5.18.3 Look up specific isolate database fields linked to a given allele . . . 85
5.19 Rule-based sequence queries . . . 86
5.19.1 Example rule code . . . 86
5.19.1.1 Rule files . . . 88
5.19.1.2 Linking to the rule query . . . 88
5.19.1.3 Adding descriptive text . . . 88
5.20 Workflow for setting up a MLST scheme . . . 88
5.21 Automated assignment of scheme profiles . . . 89
5.22 Scheme profile clustering - setting up classification schemes . . . 90
5.22.1 Defining classification scheme in sequence definition database . . . 90
5.22.2 Defining classification scheme in isolate database . . . 92
5.22.3 Clustering . . . 93
5.23 Defining new loci based on annotated reference genome . . . 95
5.24 Genome filtering . . . 98
5.24.1 Filtering by *in silico* PCR . . . 98
5.24.2 Filtering by *in silico* hybridization . . . 101
5.25 Setting locus genome positions . . . 102
5.26 Defining composite fields . . . 107
5.27 Extended provenance attributes (lookup tables) . . . 110
5.28 Sequence bin attributes . . . 113
5.29 Checking external database configuration settings . . . 115
5.30 Exporting table configurations . . . 116
5.31 Authorizing third-party client software to access authenticated resources . . . 119

6 Curator's guide **121**
6.1 Adding new sender details . . . 121
6.2 Adding new allele sequence definitions . . . 122
6.2.1 Single allele . . . 122
6.2.2 Batch adding multiple alleles . . . 125
6.2.2.1 Upload using a spreadsheet . . . 125
6.2.2.2 Upload using a FASTA file . . . 128
6.3 Updating and deleting allele sequence definitions . . . 131
6.4 Retiring allele identifiers . . . 133
6.5 Updating locus descriptions . . . 135
6.6 Adding new scheme profile definitions . . . 138
6.7 Updating and deleting scheme profile definitions . . . 142
6.8 Retiring scheme profile definitions . . . 144
6.9 Adding isolate records . . . 145
6.10 Updating and deleting single isolate records . . . 149
6.11 Batch updating multiple isolate records . . . 153
6.12 Deleting multiple isolate records . . . 156
6.13 Retiring isolate identifiers . . . 157
6.14 Setting alternative names for isolates (aliases) . . . 158
6.15 Linking isolate records to publications . . . 160
6.16 Uploading sequence contigs linked to isolate records . . . 162
6.16.1 Select isolate from drop-down list . . . 162
6.16.2 Select from isolate query . . . 164
6.16.3 Upload options . . . 166
6.17 Linking remote contigs to isolate records . . . 167
6.18 Automated web-based sequence tagging . . . 170
6.19 Projects . . . 173
6.19.1 Creating the project . . . 173
6.19.2 Explicitly adding isolates to a project . . . 174

6.20 Isolate record versioning . . . 178

7 Curating submitted data **181**
7.1 Alleles . . . 182
7.1.1 Individual allele curation . . . 183
7.1.2 Batch allele curation . . . 185
7.1.3 Rejecting sequences . . . 188
7.1.4 Requesting additonal information . . . 188
7.1.5 Closing the submission . . . 188
7.2 Profiles . . . 189
7.2.1 Individual profile curation . . . 190
7.2.2 Batch profile curation . . . 193
7.2.3 Rejecting profiles . . . 195
7.2.4 Requesting additonal information . . . 196
7.2.5 Closing the submission . . . 196
7.3 Isolates . . . 196
7.3.1 Requesting additonal information . . . 199
7.3.2 Closing the submission . . . 199

8 Offline curation tools **201**
8.1 Automated offline sequence tagging . . . 201
8.2 Defining exemplar alleles . . . 204
8.3 Automated offline allele definition . . . 205
8.4 Cleanly interrupting offline curation . . . 207
8.5 Uploading contigs from the command line . . . 207

9 Definition downloads **209**
9.1 Allele sequence definitions . . . 209
9.1.1 Scheme tree . . . 210
9.1.2 Alphabetical list . . . 212
9.1.3 All loci by scheme . . . 213
9.1.4 Download locus table . . . 213
9.2 Scheme profile definitions . . . 214

10 Data records **217**
10.1 Isolate records . . . 217
10.1.1 Projects . . . 219
10.1.2 Provenance metadata . . . 219
10.1.3 Publications . . . 220
10.1.4 Sequence bin summary . . . 221
10.1.5 Scheme and locus data . . . 221
10.2 Allele definition records . . . 222
10.3 Sequence tag records . . . 223
10.4 Profile records . . . 223
10.5 Sequence bin records . . . 224

11 Querying data **225**
11.1 Querying sequences to determine allele identity . . . 225
11.1.1 Querying whole genome data . . . 227
11.2 Querying multiple sequences to identify allele identities . . . 228
11.3 Searching for specific allele definitions . . . 230
11.3.1 General (all loci) sequence attribute search . . . 230
11.3.2 Locus-specific sequence attribute search . . . 234
11.4 Browsing scheme profile definitions . . . 237
11.5 Querying scheme profile definitions . . . 238

11.6 Identfying allelic profile definitions . . . 242
11.7 Batch profile queries . . . 246
11.8 Investigating allele differences . . . 248
11.8.1 Sequence similarity . . . 248
11.8.2 Sequence comparison . . . 249
11.9 Browsing isolate data . . . 251
11.10 Querying isolate data . . . 253
11.10.1 Query by allele designation/scheme field . . . 256
11.10.2 Query by allele designation count . . . 257
11.10.3 Query by allele designation status . . . 259
11.10.4 Query by sequence tag count . . . 260
11.10.5 Query by tagged sequence status . . . 261
11.10.6 Query by list of attributes . . . 263
11.10.7 Query filters . . . 264
11.11 Querying by allelic profile . . . 265
11.12 Retrieving isolates by linked publication . . . 268
11.13 User-configurable options . . . 271
11.13.1 General options . . . 272
11.13.2 Main results table . . . 273
11.13.3 Isolate record display . . . 274
11.13.4 Provenance field display . . . 276
11.13.5 Query filters . . . 277
11.13.6 Modifying locus and scheme display options . . . 279

12 User projects **283**
12.1 Adding isolates to a user project following a query . . . 284
12.2 Adding or removing isolates belonging to a user project by editing a list . . . 285
12.3 Accessing project isolates . . . 286
12.4 Allowing other users to share your project . . . 287
12.5 Deleting a user project . . . 288

13 Private records **291**
13.1 Uploading private records . . . 291
13.2 Modifying private records . . . 293
13.3 Sharing access to private records . . . 294

14 Data analysis plugins **295**
14.1 Locus explorer . . . 295
14.1.1 Polymorphic site analysis . . . 296
14.1.2 Codon usage . . . 299
14.1.3 Aligned translations . . . 300
14.2 Field breakdown . . . 301
14.3 Two field breakdown . . . 305
14.4 Scheme and allele breakdown . . . 308
14.5 Sequence bin breakdown . . . 315
14.6 Genome comparator . . . 317
14.6.1 Analysis using defined loci . . . 318
14.6.2 Analysis using annotated reference genome . . . 321
14.6.3 Include in identifiers fieldset . . . 322
14.6.4 Reference genome fieldset . . . 322
14.6.5 Parameters/options fieldset . . . 323
14.6.6 Distance matrix calculation fieldset . . . 323
14.6.7 Alignments fieldset . . . 324
14.6.8 Core genome analysis fieldset . . . 325

14.6.9 Filter fieldset . . . 325
14.6.10 Understanding the output . . . 325
14.6.10.1 Distance matrix . . . 325
14.6.10.2 Unique strains . . . 326
14.7 BLAST . . . 326
14.7.1 Include in results table fieldset . . . 329
14.7.2 Parameters fieldset . . . 330
14.7.3 No matches . . . 330
14.7.4 Filter fieldset . . . 330
14.8 BURST . . . 331
14.9 Codon usage . . . 334
14.10 Unique combinations . . . 337
14.11 Polymorphisms . . . 339
14.12 Presence/absence . . . 341
14.12.1 Options . . . 344
14.13 Tag status . . . 344

15 Data export plugins **349**
15.1 Isolate record export . . . 349
15.1.1 Advanced options . . . 351
15.1.2 Molecular weight calculation . . . 351
15.2 Sequence export . . . 352
15.2.1 Aligning sequences . . . 354
15.3 Contig export . . . 355
15.3.1 Filtering by tagged status of contigs . . . 357

16 Submitting data using the submission system **359**
16.1 Registering a user account . . . 360
16.2 Allele submission . . . 360
16.2.1 Start . . . 360
16.2.2 Select the submission locus . . . 361
16.2.3 Enter details of sequencing method . . . 362
16.2.4 Paste in sequence(s) . . . 363
16.2.5 Add message to curator . . . 365
16.2.6 Add supporting files . . . 367
16.2.7 Finalize submission . . . 370
16.3 Profile submission . . . 371
16.3.1 Start . . . 371
16.3.2 Paste in profile(s) . . . 373
16.3.3 Add message to curator . . . 374
16.3.4 Add supporting files . . . 375
16.3.5 Finalize submission . . . 376
16.4 Isolate submission . . . 377
16.4.1 Start . . . 377
16.4.2 Paste in isolate data . . . 378
16.4.3 Add message to curator . . . 380
16.4.4 Add supporting files . . . 381
16.4.5 Finalize submission . . . 383
16.5 Genome submission . . . 385
16.6 Removing submissions from your notification list . . . 385

17 RESTful Application Programming Interface (API) **387**
17.1 Passing additional/optional parameters . . . 387
17.2 Paging using request headers . . . 387

17.3 Resources . . . 388
17.3.1 GET / or /db - List site resources . . . 389
17.3.2 GET /db/{database} - List database resources . . . 390
17.3.3 GET /db/{database}/classification_schemes - List classification schemes . . . 390
17.3.4 GET /db/{database}/classification_schemes/{classification_scheme_id} - Retrieve classification scheme information and groups . . . 390
17.3.5 GET /db/{database}/classification_schemes/{classification_scheme_id}/groups/{group_id} - List isolates belonging to a classification scheme group . . . 391
17.3.6 GET /db/{database}/loci - List loci . . . 391
17.3.7 GET /db/{database}/loci/{locus} - Retrieve locus record . . . 392
17.3.8 GET /db/{database}/loci/{locus}/alleles - Retrieve list of alleles defined for a locus . . . 393
17.3.9 GET /db/{database}/loci/{locus}/alleles_fasta - Download alleles in FASTA format . . . 394
17.3.10 GET /db/{database}/loci/{locus}/alleles/{allele_id} - Retrieve full allele information . . . 394
17.3.11 POST /db/{database}/loci/{locus}/sequence - Query sequence to identify allele . . . 394
17.3.12 POST /db/{database}/sequence - Query sequence to identify allele without specifying locus 395
17.3.13 GET /db/{database}/schemes - List schemes . . . 395
17.3.14 GET /db/{database}/schemes/{scheme_id} - Retrieve scheme information . . . 396
17.3.15 GET /db/{database}/schemes/{scheme_id}/fields/{field} - Retrieve information about scheme field . . . 396
17.3.16 GET /db/{database}/schemes/{scheme_id}/profiles - List allelic profiles defined for scheme 396
17.3.17 GET /db/{database}/schemes/{scheme_id}/profiles_csv - Download allelic profiles in CSV (tab-delimited) format . . . 397
17.3.18 GET /db/{database}/schemes/{scheme_id}/profiles/{profile_id} - Retrieve allelic profile record . . . 397
17.3.19 GET /db/{database}/isolates - Retrieve list of isolate records . . . 398
17.3.20 GET /db/{database}/isolates/{isolate_id} - Retrieve isolate record . . . 399
17.3.21 GET /db/{database}/isolates/{isolate_id}/allele_designations - Retrieve list of allele designation records . . . 400
17.3.22 GET /db/{database}/isolates/{isolate_id}/allele_designations/{locus} - Retrieve full allele designation record . . . 400
17.3.23 GET /db/{database}/isolates/{isolate_id}/allele_ids - Retrieve allele identifiers . . . 401
17.3.24 GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_designations - Retrieve scheme allele designation records . . . 402
17.3.25 GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_ids - Retrieve list of scheme allele identifiers . . . 402
17.3.26 GET /db/{database}/isolates/{isolate_id}/contigs - Retrieve list of contigs . . . 402
17.3.27 GET /db/{database}/isolates/{isolate_id}/contigs_fasta - Download contigs in FASTA format 403
17.3.28 POST /db/{database}/isolates/search - Search isolate database . . . 403
17.3.29 GET /db/{database}/contigs/{contig_id} - Retrieve contig record . . . 404
17.3.30 GET /db/{database}/fields - Retrieve list of isolate provenance field descriptions . . . 405
17.3.31 GET /db/{database}/fields/{field} - Retrieve values set for a provenance field . . . 405
17.3.32 GET /db/{database}/users/{user_id} - Retrieve user information . . . 406
17.3.33 GET /db/{database}/projects - Retrieve list of projects . . . 406
17.3.34 GET /db/{database}/projects/{project_id} - Retrieve project information . . . 407
17.3.35 GET /db/{database}/projects/{project_id}/isolates - Retrieve list of isolates belonging to a project . . . 407
17.3.36 GET /db/{database}/submissions - retrieve list of submissions . . . 407
17.3.37 POST /db/{database}/submissions - create new submission . . . 408
17.3.38 GET /db/{database}/submissions/{submission_id} - Retrieve submission record . . . 409
17.3.39 DELETE /db/{database}/submissions/{submission_id} - Delete submission record . . . 410
17.3.40 GET /db/{database}/submissions/{submission_id}/messages - Retrieve submission correspondence . . . 411
17.3.41 POST /db/{database}/submissions/{submission_id}/messages - Add submission correspondence . . . 411

17.3.42 GET /db/{database}/submissions/{submission_id}/files - Retrieve list of supporting files uploaded for submission . . . 411
17.3.43 POST /db/{database}/submissions/{submission_id}/files - Upload submission supporting file 412
17.3.44 GET /db/{database}/submissions/{submission_id}/files/{filename} - Download submission supporting file . . . 412
17.3.45 DELETE /db/{database}/submissions/{submission_id}/files/{filename} - Delete submission supporting file . . . 412
17.4 Authentication . . . 412
17.4.1 Developer sign up to get a consumer key . . . 413
17.4.2 Getting a request token . . . 413
17.4.3 Getting user authorization . . . 414
17.4.4 Getting an access token . . . 415
17.4.5 Getting a session token . . . 416
17.4.6 Accessing protected resources . . . 416

18 Frequently asked questions (FAQs) 419
18.1 General . . . 419
18.2 Installation . . . 420
18.3 Administration . . . 420

19 Appendix 423
19.1 Query operators . . . 423
19.2 Sequence tag flags . . . 424
19.3 Allele sequence flags . . . 425

20 Database schema 427

Gene-by-gene population annotation and analysis

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

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

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

CHAPTER 1

Concepts and terms

1.1 BIGSdb

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

1.2 Loci

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

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

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

1.3 Alleles

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

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

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

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

1.4 Schemes

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

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

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

1.5 Profiles

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

1.6 Classification groups

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

1.7 Sequence tags

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

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

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

1.8 Sets

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

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

CHAPTER 2

BIGSdb dependencies

2.1 Required packages

BIGSdb requires a number of software components to be installed:

2.1.1 Linux packages

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

2.1.2 Perl modules

These are included with most Linux distributions.

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

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

2.1.3 Optional packages

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

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

CHAPTER 3

Installation and configuration of BIGSdb

3.1 Software installation

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

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

- *Software requirements*
- Download from SourceForge.net or GitHub.

1. Unpack the distribution package in a temporary directory:

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

2. Copy the bigsdb.pl and bigscurate.pl scripts to a subdirectory of your web server's cgi-bin directory. Make sure these are readable and executable by the web server daemon.
3. 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.
4. Copy the javascript directory to the root directory of your website, i.e. accessible from http://your_website/javascript/.
5. Copy the css directory to root directory of your website, i.e. accessible from http://your_website/css/.
6. Copy the fonts directory to the root directory of your website, 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/

3.2.1 pg_hba.conf

```
# Database administrative login by UNIX sockets
local   all         postgres                            ident map=mymap

# TYPE  DATABASE    USER        CIDR-ADDRESS          METHOD

# "local" is for Unix domain socket connections only
local   all         all                                 ident map=mymap
# IPv4 local connections:
```

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

3.2.2 pg_ident.conf

```
# MAPNAME      SYSTEM-USERNAME    PG-USERNAME

  mymap        postgres           postgres
  mymap        webmaster          postgres
  mymap        www-data           apache
  mymap        bigsdb             bigsdb
  mymap        bigsdb             apache
```

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

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

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

See Tuning Your PostgreSQL Server for more details.

Restart PostgreSQL after any changes, e.g.

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

3.3 Setting global connection parameters

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

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

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

3.4 Site-specific configuration

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

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

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

3.5 Setting up the offline job manager

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

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

```
sudo useradd -s /bin/sh bigsdb
```

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

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

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

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

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

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

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

4. Copy the job_logging.conf file to the /etc/bigsdb directory.

5. Set the script to run frequently (preferably every minute) from CRON. Note that CRON does not like '.' in executable filenames, so either rename the script to 'bigsjobs' or create a symlink and call that from CRON, e.g.:

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

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

   Add the following to /etc/crontab::

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

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

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

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

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

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

3.6 Setting up the submission system

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

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

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

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

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

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

3.7 Setting up a site-wide user database

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

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

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

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

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

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

```
05  *  *  *  *  bigsdb   /usr/local/bin/sync_user_dbase_users.pl --user_database␣
↪pubmlst_bigsdb_users
```

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

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

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

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

```
site_user_dbs=PubMLST|pubmlst_bigsdb_users
```

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

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

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

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

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

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

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

   e.g.

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

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

3.8 Periodically delete temporary files

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

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

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

#Remove .jnlp files from web tree older than 1 day
find /var/www/tmp/ -name '*.jnlp' -type f -mmin +1440 -exec rm -f {} \; 2>/dev/null

#Remove other tmp files from web tree older than 1 week
find /var/www/tmp/ -type f -mmin +10080 -exec rm -f {} \; 2>/dev/null
```

3.9 Prevent preference database getting too large

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

```
#Prevent prefs database getting too large
00   18 *  *  0  postgres    psql -c "DELETE FROM guid WHERE last_accessed < NOW() -␣
↪INTERVAL '6 months'" bigsdb_prefs
```

3.10 Purging old jobs from the jobs database

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

```
#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()-interval '7 days') OR (status LIKE 'rejected%' AND submit_time <␣
↪now()-interval '7 days')" bigsdb_jobs > /dev/null 2>&1
```

3.11 Log file rotation

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

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

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

3.12 Upgrading BIGSdb

Major version changes, e.g. 1.7 -> 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 -> 1.8, requires upgrading to 1.7 first.

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

3.13 Running the BIGSdb RESTful interface

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

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

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

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

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

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

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

```
psql bigsdb_rest
```

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

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

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

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

Finally, add the database resources to the group:

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

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

```
./bigsrest.pl
```

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

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

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

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

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

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

```
description "Start BIGSdb REST interface"
version "1.0"
author "Keith Jolley"

start on runlevel [12345]

## tell upstart we're creating a daemon
expect fork

script

exec su -s /bin/sh -c 'exec "$0" "$@"' bigsdb -- /usr/local/bin/plackup -a /var/rest/
↪bigsrest.pl -s Starman -E deployment

end script
```

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

```
sudo service bigsdb-rest start
```

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

```
[Unit]
Description=BIGSdb REST interface
After=network.target

[Service]
```

```
User=bigsdb
ExecStart=/usr/bin/plackup -a /var/rest/bigsrest.pl -s Starman -E deployment
Restart=always

[Install]
WantedBy=multi-user.target
```

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

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

It can also be manually started by calling:

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

3.13.1 Proxying the API to use a standard web port

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

```
<VirtualHost *>
  ServerName rest.pubmlst.org
  DocumentRoot /var/rest
  ServerAdmin keith.jolley@zoo.ox.ac.uk
   <Directory /var/rest>
    AllowOverride None
    Require all granted
  </Directory>

  ProxyPass / http://rest.pubmlst.org:5000/
  ProxyPassReverse / http://rest.pubmlst.org:5000/

  <Proxy *>
      Order allow,deny
      Allow from all
  </Proxy>

  ErrorLog  /var/log/apache2/rest.pubmlst.org-error.log
  CustomLog /var/log/apache2/rest.pubmlst.org-access.log common

</VirtualHost>
```

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

CHAPTER 4

Database setup

There are two types of BIGSdb database:

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

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

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

4.1 Creating databases

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

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

```
sudo su postgres
```

then

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

Create an isolate database the same way:

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

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

```
psql bigsdb_test_isolates
```

and alter the isolate table:

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

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

4.2 Database-specific configuration

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

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

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

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

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

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

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

4.3 XML configuration attributes used in config.xml

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

4.3.1 Isolate database XML attributes

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

```
<db>
```

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

```
<system>
```

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

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

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

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

  - Display locus aliases and use them in dropdown lists by default: must be either 'yes' or 'no', default 'no'. This option can be overridden by a user preference.

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

- script_path_includes
  - Partial path of the bigsdb.pl script used to access the database. See *user authentication*.
- seqbin_size_threshold
  - Sets the size values in Mbp to enable for the *seqbin filter*.
  - Example: seqbin_size_threshold="0.5,1,2,4".
- seq_export_limit
  - Overrides the sequence export limit (records x loci) in the Sequence Export plugin. Default: '1000000'.
- sets
  - Use *sets*: either 'yes' or 'no', default 'no'.
- set_id
  - Force the use of a specific set when accessing database via this XML configuration: Value is the name of the set.
- start_id
  - Defines the minimum record id to be used when uploading new isolate records. This can be useful when it is anticipated that two databases may be merged and it would be easier to do so if the id numbers in the two databases were different. Default: '1'.
- submissions
  - Enable automated submission system: either 'yes' or 'no', default 'no' (version 1.11+).
  - The curate_script and query_script paths should also be set, either in the bigsdb.conf file (for site-wide configuration) or within the system attribute of config.xml.
- submissions_deleted_days
  - Overrides the default number of days before closed submissions are deleted from the system. Default: '90'.
- tblastx_tagging
  - Sets whether tagging can be performed using TBLASTX: either 'yes' or 'no', default 'no'.
- total_pending_submissions
  - Overrides the total limit on pending submissions that a user can submit via the web submission system. Default: '20'.
- user
  - Username for access to isolates database, default 'apache'.
- user_job_quota
  - Integer with number of offline jobs that can be queued or currently running for this database by any specific user - this parameter is only effective if users have to log in.
- user_projects
  - Sets whether authenticated users can create their own projects in order to group isolates: either 'yes' or 'no', default 'no'.
- view
  - Database view containing isolate data, default 'isolates'.
- views

  - Comma-separated list of views of the isolate table defined in the database. This is used to set a view for a set.

- webroot
  - URL of web root, which can be relative or absolute. This is used to provide a hyperlinked item in the dropdown menu. Default '/'.

```
<field>
```

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

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

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

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

4.3.1.1 Special values

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

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

```
<sample>
```

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

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

4.3.2 Sequence definition database XML attributes

Required attributes are in **bold**.

```
<db>
```

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

```
<system>
```

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

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

  - Name of database on system.
- **dbtype**
  - Type of database: either 'isolates' or 'sequences'.
- **description**
  - Description of database used throughout interface.
- align_limit
  - Overrides the sequence export record alignment limit in the Sequence Export plugin. Default: '200'.
- allele_comments
  - Enable comments on allele sequences: either 'yes' or 'no', default 'no'.
  - This is not enabled by default to discourage the practice of adding isolate information to allele definitions (this sort of information belongs in an isolate database).
- allele_flags
  - Enable flags to be set for alleles: either 'yes' or 'no', default 'no'.
- curate_config
  - The database configuration that should be used for curation if different from the current configuration. This is used when the submission system is being used so that curation links in the 'Manage submissions' pages for curators load the correct database configuration.
- curate_path_includes
  - Partial path of the bigscurate.pl script used to curate the database. See *user authentication*.
- curate_script
  - Relative web path to curation script. Default 'bigscurate.pl' (version 1.11+).
  - This is only needed if automated submissions are enabled. If bigscurate.pl is in a different directory from bigsdb.pl, you need to include the whole web path, e.g. /cgi-bin/private/bigsdb/bigscurate.pl.
- curator_home
  - URL of curator's index page, which can be relative or absolute. This will be used to add a link in the dropdown menu.
- curators_only
  - Set to 'yes' to prevent ordinary authenticated users having access to database configuration. This is only effective if read_access is set to 'authenticated_users'. This may be useful if you have different configurations for curation and querying with some data hidden in the configuration used by standard users. Default 'no'.
- daily_pending_submissions
  - Overrides the daily limit on pending submissions that a user can submit via the web submission system. Default: '15'.
- daily_rest_submissions_limit
  - Overrides the limit on number of submissions that can be made to the database via the RESTful interface. This is useful to prevent flooding of the submission system by aberrant scripts. Default: '100'.
- diploid
  - Allow IUPAC 2-nuclotide ambiguity codes in allele definitions for use with diploid typing schemes: either 'yes' or 'no', default 'no'.

- disable_seq_downloads
  - Prevent users or curators from downloading all alleles for a locus (admins always can). 'yes' or 'no', default 'no'.
- exemplars
  - Use exemplar sequences in the BLAST caches used for the sequence query pages. This is useful on larger databases as it speeds up the query significantly. *Exemplar alleles MUST* be defined otherwise sequence queries will fail. 'yes' or 'no', default 'no'.
- isolate_database
  - The config name of the isolate database. This is used to provide a link to isolate submissions. You also need to set isolate_submissions="yes".
- isolate_submissions
  - Set to yes to provide a link to isolate submissions. The isolate_database attribute also needs to be set. Default: 'no'.
- job_priority
  - Integer with default job priority for offline jobs (default:5).
- job_quota
  - Integer with number of offline jobs that can be queued or currently running for this database.
- profile_submissions
  - Enable profile submissions (automated submission system): either 'yes' or 'no', default 'no' (version 1.11+).
  - To enable, you will also need to set submissions="yes". By default, profile submissions are disabled since generally new profiles should be accompanied by representative isolate data, and the profile can be extracted from that.
- public_login
  - Optionally allow users to log in to a public database - this is useful as any jobs will be associated with the user and their preferences will also be linked to the account. Set to 'no' to disable. Default 'yes'.
- query_script
  - Relative web path to bigsdb script. Default 'bigsdb.pl' (version 1.11+).
  - This is only needed if automated submissions are enabled. If bigsdb.pl is in a different directory from bigscurate.pl, you need to include the whole web path, e.g. /cgi-bin/bigsdb/bigsdb.pl.
- read_access
  - Describes who can view data: either 'public' for everybody, or 'authenticated_users' for anybody who has been able to log in. Default 'public'.
- related_databases
  - Semi-colon separated list of links to related BIGSdb databases on the system. This should be in the form of database configuration name followed by a '|' and the description, e.g. 'pubmlst_neisseria_isolates|Isolates'. This is used to populate the dropdown menu.
- script_path_includes
  - Partial path of the bigsdb.pl script used to access the database. See *user authentication*.
- seq_export_limit

  - Overrides the sequence export limit (records x loci) in the Sequence Export plugin. Default: '1000000'.

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

4.4 Over-riding global defaults set in bigsdb.conf

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

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

- ref_db
  - The name of the references database.

4.5 Over-riding values set in config.xml

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

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

4.6 User authentication

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

4.6.1 Apache authentication

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

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

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

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

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

4.6.2 Built-in authentication

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

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

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

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

4.7 Setting up the admin user

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

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

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

4.8 Updating PubMed citations

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

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

```
pubmlst_bigsdb_neisseria_isolates          refs
pubmlst_bigsdb_neisseria_seqdef            profile_refs,sequence_refs,locus_refs
```

The script can be called as follows:

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

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

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

4.9 Configuring access to remote contigs

It is possible for isolate records to have contigs in an external BIGSdb database. These must be accessible via the *RESTful API*. The advantage of this is that it enables multiple isolate databases to use the same genome assemblies

without having to duplicate the storage of those assemblies. If access to the external database requires authenticated access, OAuth settings can be set to enable contig retrieval.

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

```
remote_contigs = "yes"
```

4.9.1 Setting up authentication

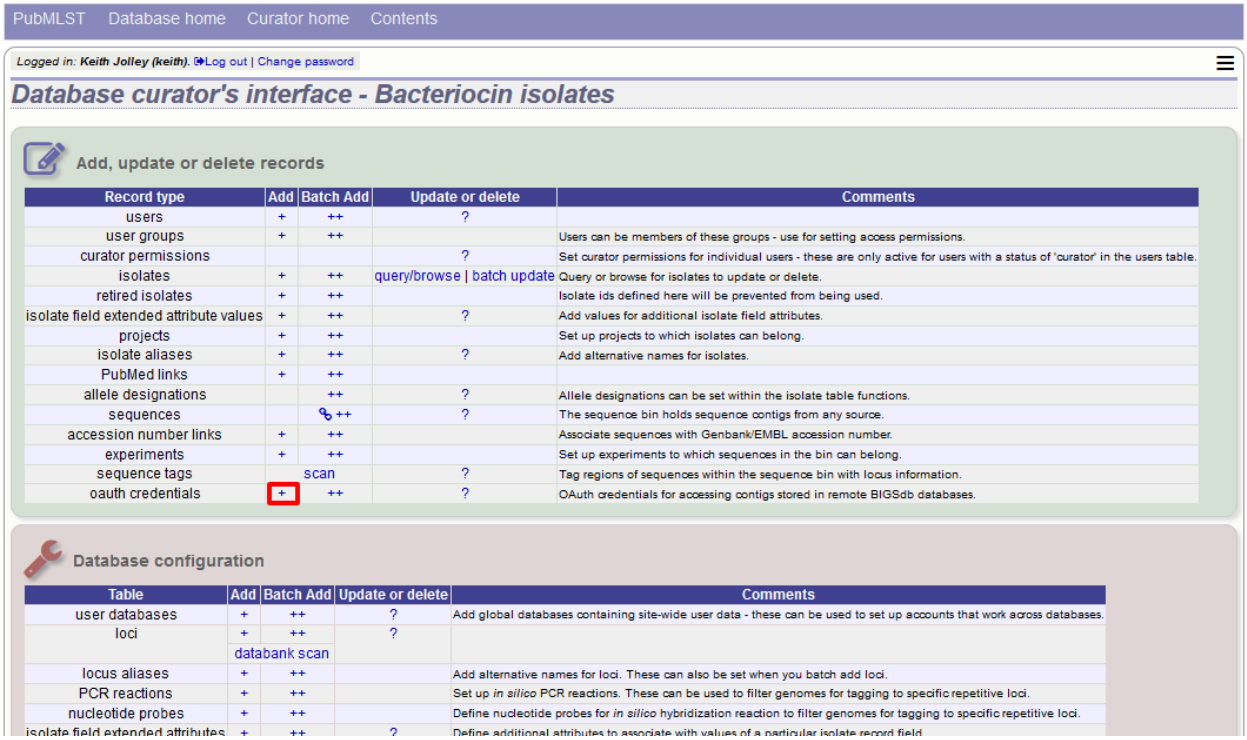
A client key for the BIGSdb remote contig manager needs to be generated. This can be done using the *create_client_credentials.pl* script, e.g.

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

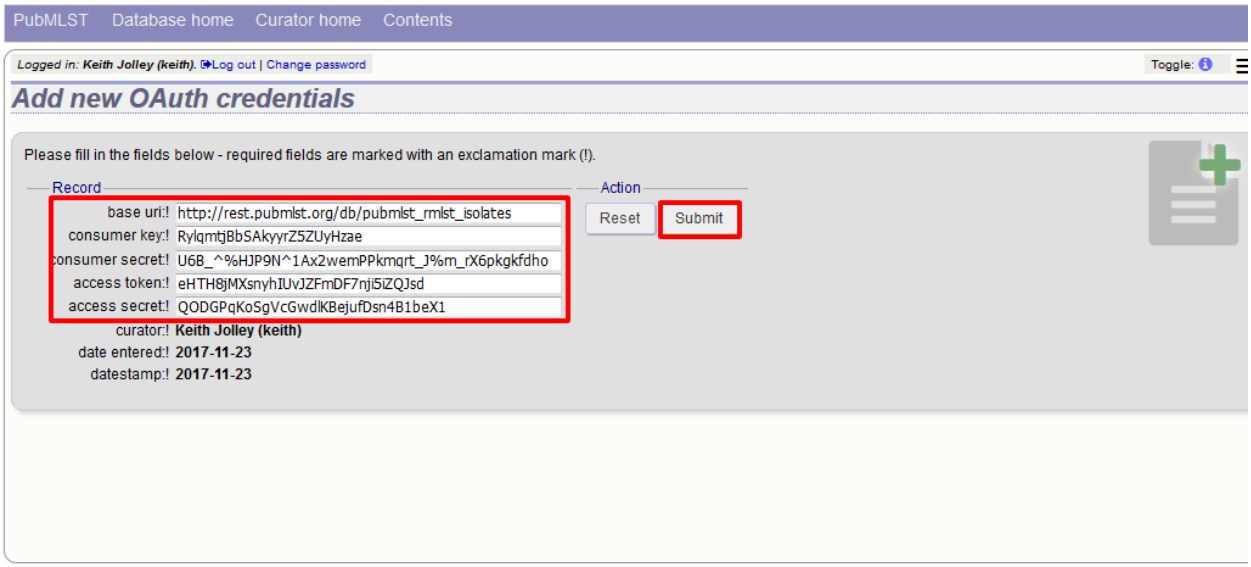
This will generate a client id (key) and a client secret and add them to the authentication database.

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

From the curators' page, click the oauth credentials add link.



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



4.9.2 Processing remote contigs

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

```
remote_contigs.pl --help
NAME
    process_remote_contigs.pl
    Download, check length and create checksum contigs stored as URIs

SYNOPSIS
    process_remote_contigs.pl --database NAME [options]

OPTIONS

--database NAME
    Database configuration name.

--exclude_isolates LIST
    Comma-separated list of isolate ids to ignore.

--exclude_projects LIST
    Comma-separated list of projects whose isolates will be excluded.

--help
    This help page.

--isolates LIST
    Comma-separated list of isolate ids to scan (ignored if -p used).

--isolate_list_file FILE
    File containing list of isolate ids (ignored if -i or -p used).
```

```
--min ID
    Minimum isolate id.

--max ID
    Maximum isolate id.

--projects LIST
    Comma-separated list of project isolates to scan.

--quiet
    Only display errors.
```

CHAPTER 5

Administrator's guide

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

5.1 Types of user

There are four types of user in BIGSdb:

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

5.2 User groups

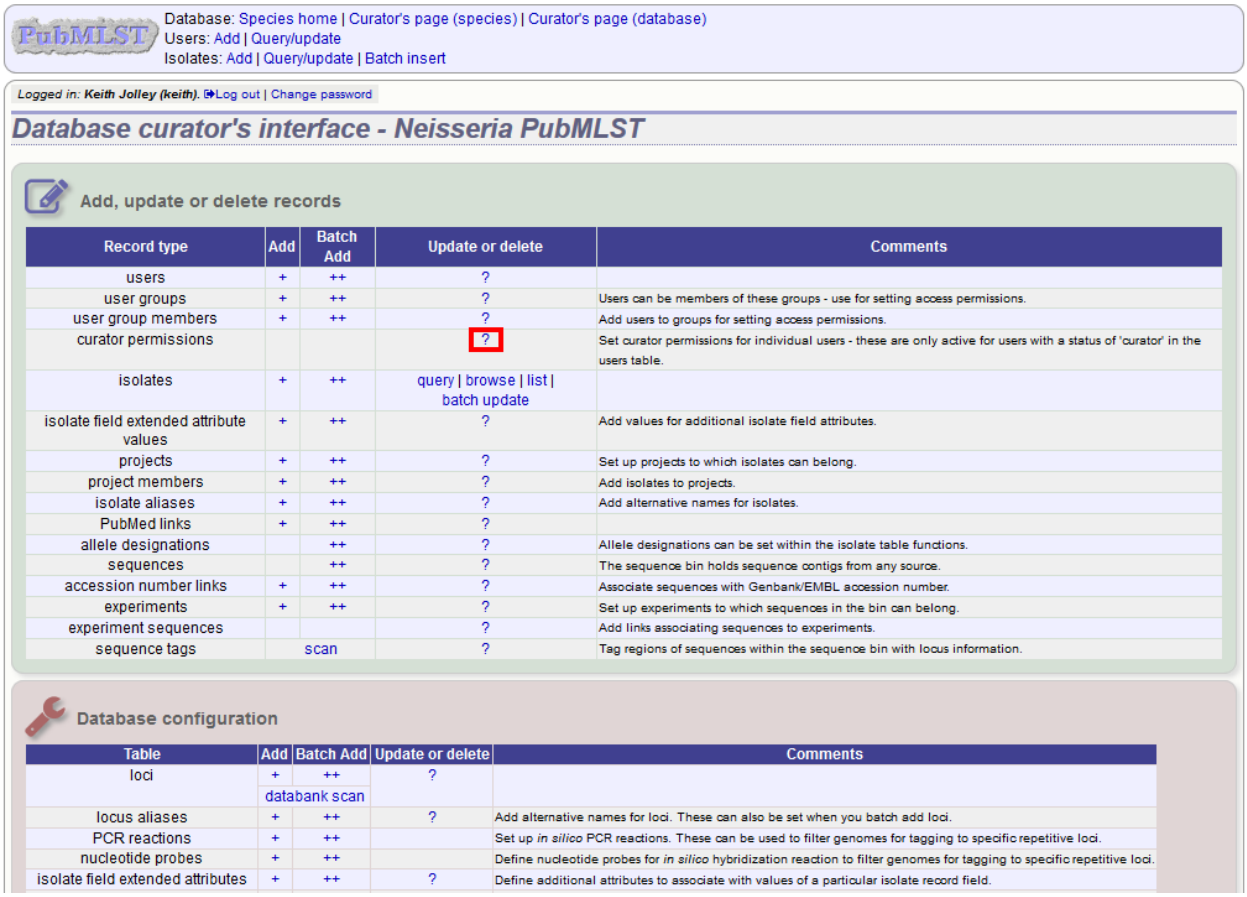
User groups allow submitter accounts to be grouped such that the submitter can edit isolates where the sender is either themselves or any member of a user group to which they belong.

5.3 Curator permissions

Individual permissions can be set for each curator:

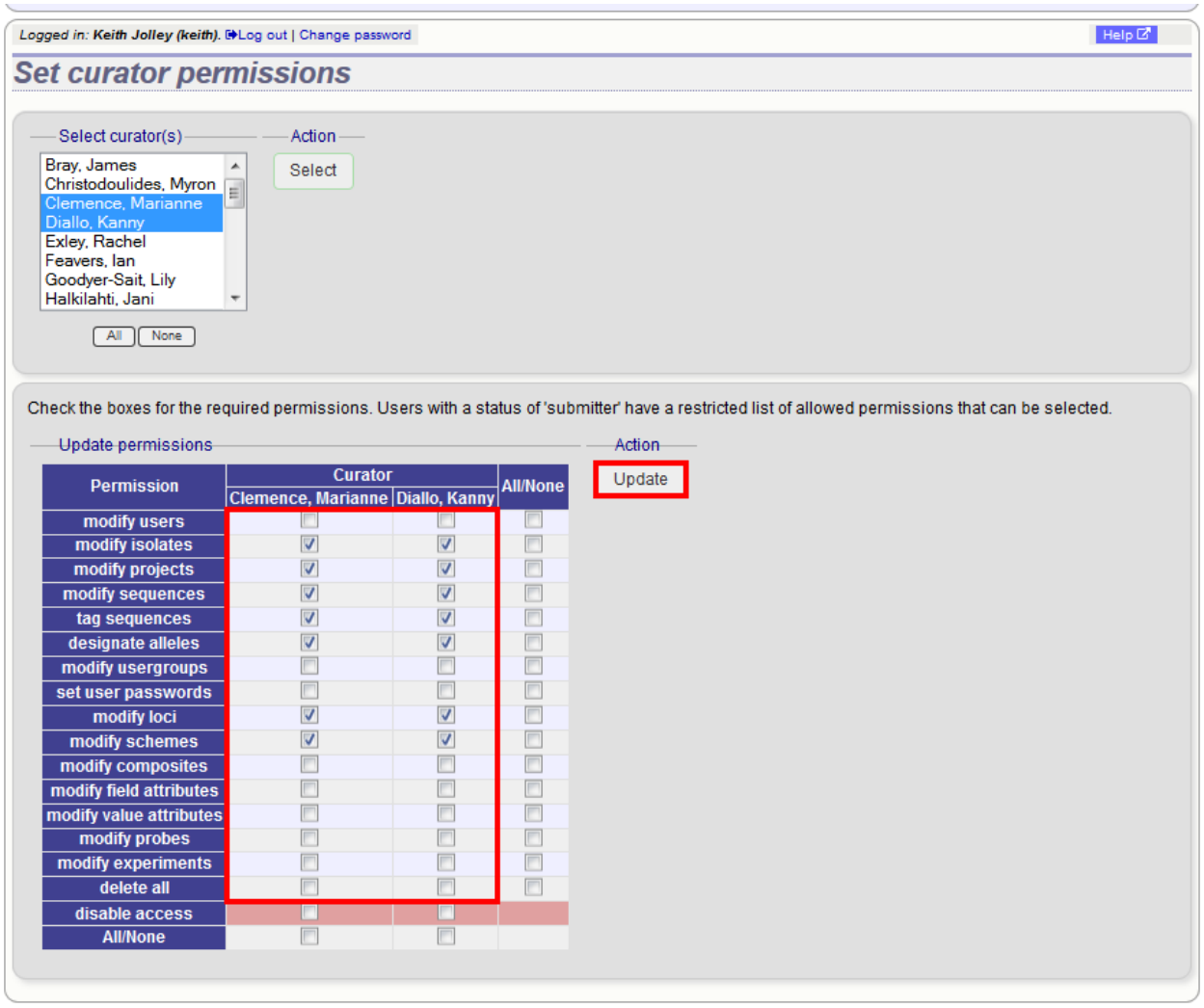
- disable_access - if set to true, this user is completely barred from access.
- modify_users - allowed to add or modify user records. They can change the status of users, but can not revoke admin privileges from an account. They can also not raise the status of a user to admin level.
- modify_usergroups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

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



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'.

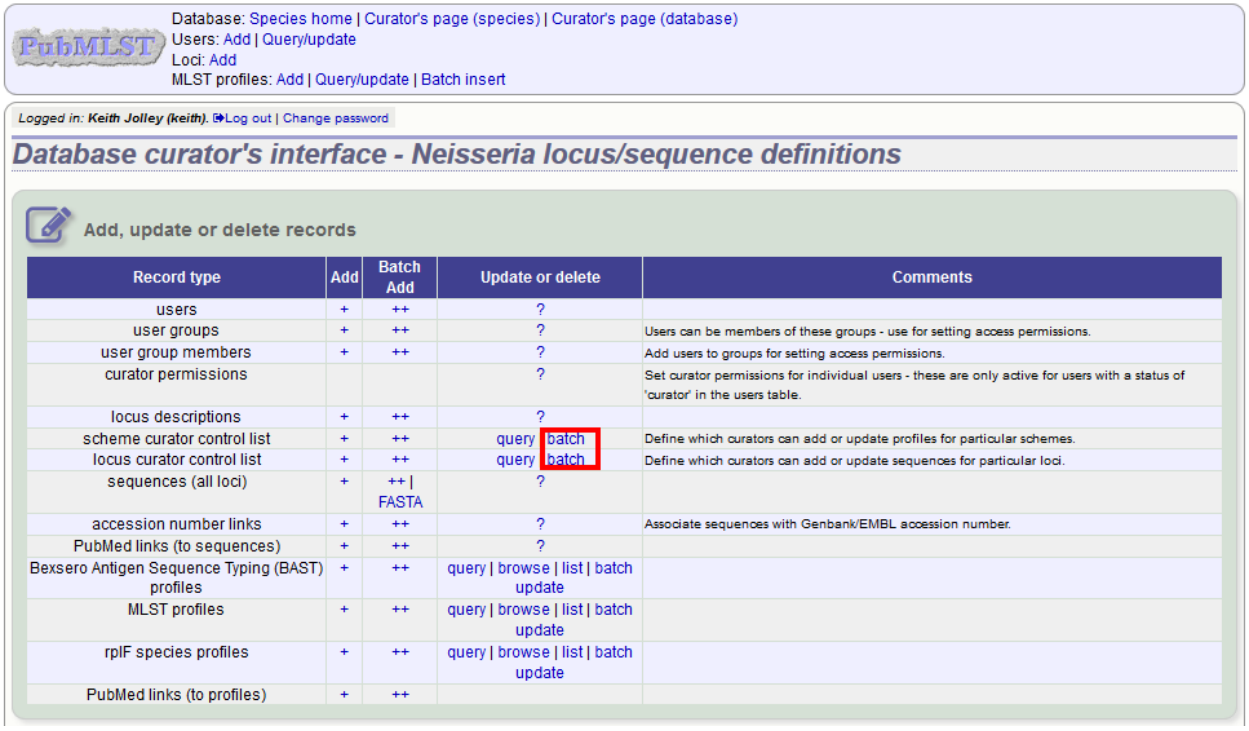


The 'disable access' option provides a quick way to disable access to a curator. This will not be selected by the 'All/None' buttons.

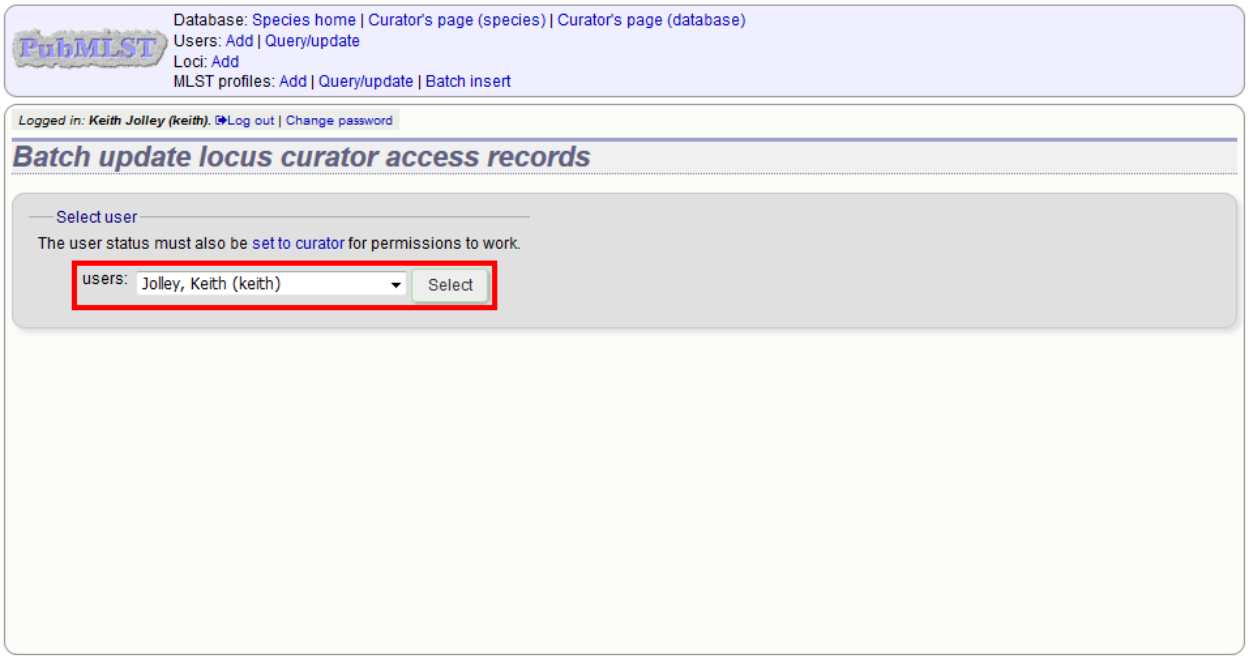
5.4 Locus and scheme permissions (sequence definition database)

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

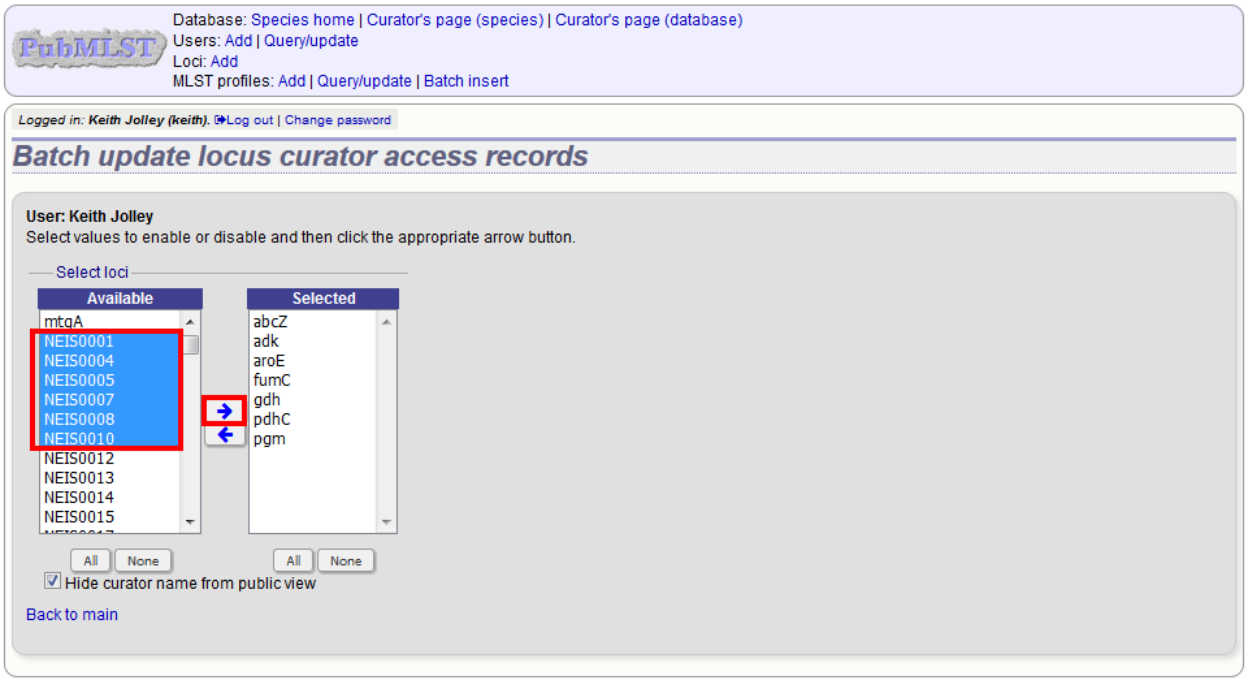
The easiest way to modify these lists is to use the batch update link next to 'locus curator control list' and 'scheme curator control list':



Select the curator from the list:



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:

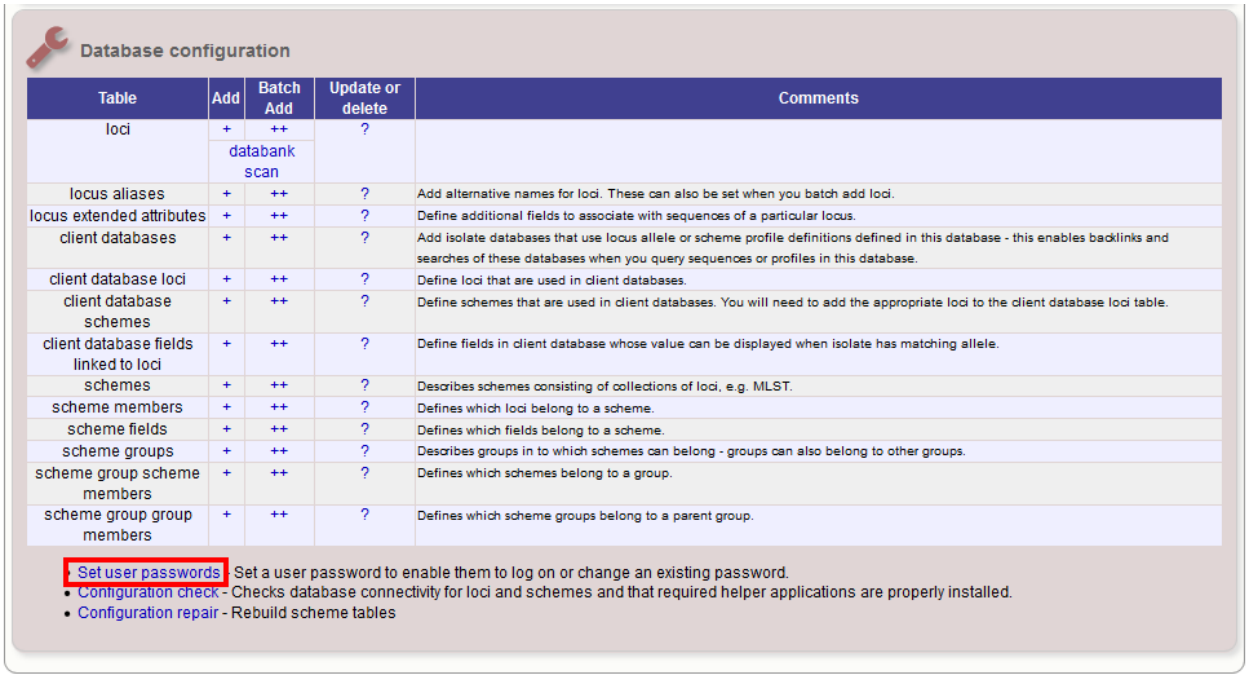
```
default_access="allow"
```

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.

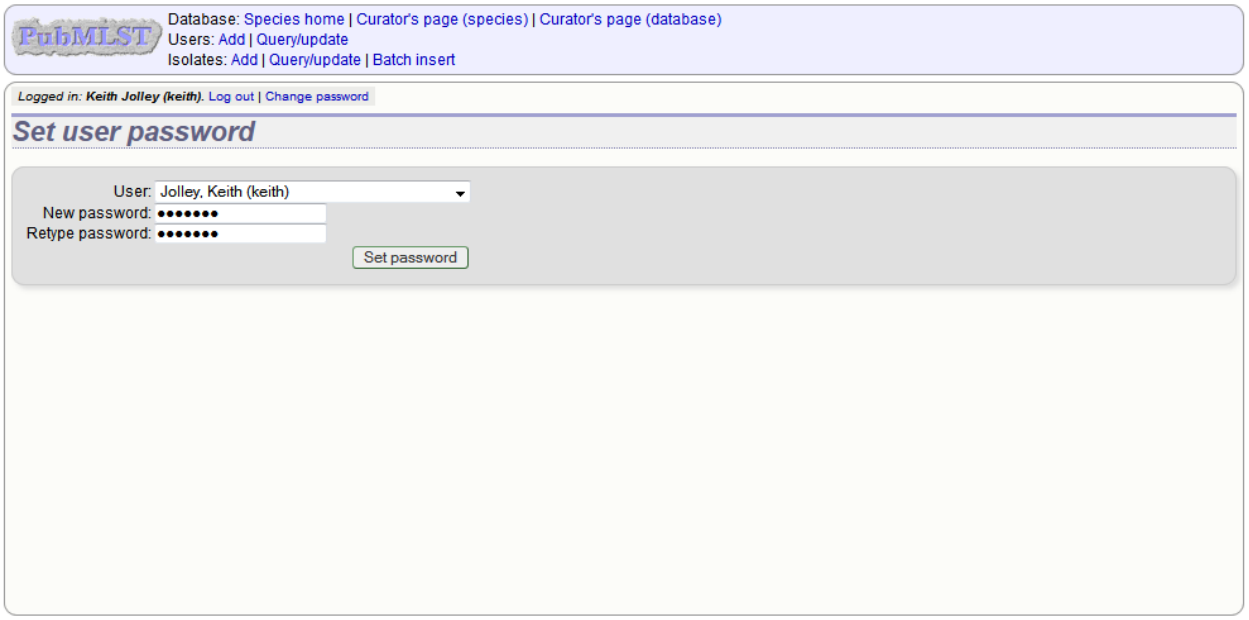
5.6 Setting user passwords

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.



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



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

5.7 Setting the first user password

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

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

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

5.8 Enabling plugins

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

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

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

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

```
BURST="yes"
```

to the system tag of the database XML file. If the system_flag value is not defined then the plugin is always enabled if it is installed on the system.

5.9 Temporarily disabling database updates

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

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

5.9.1 Global

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

```
disable_updates=yes
```

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

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

5.9.2 Database-specific

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

```
<system
  db="bigsdb_neisseria"
  dbtype="isolates"
  ...
  disable_updates="yes"
  disable_update_message="The server is currently undergoing maintenance."
```

5.10 Host mapping

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

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

```
#Existing_host      Mapped_host
 server1            server2
 localhost          server2
```

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

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

5.11 Improving performance

5.11.1 Use mod_perl

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

5.11.2 Cache scheme definitions within an isolate database

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

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

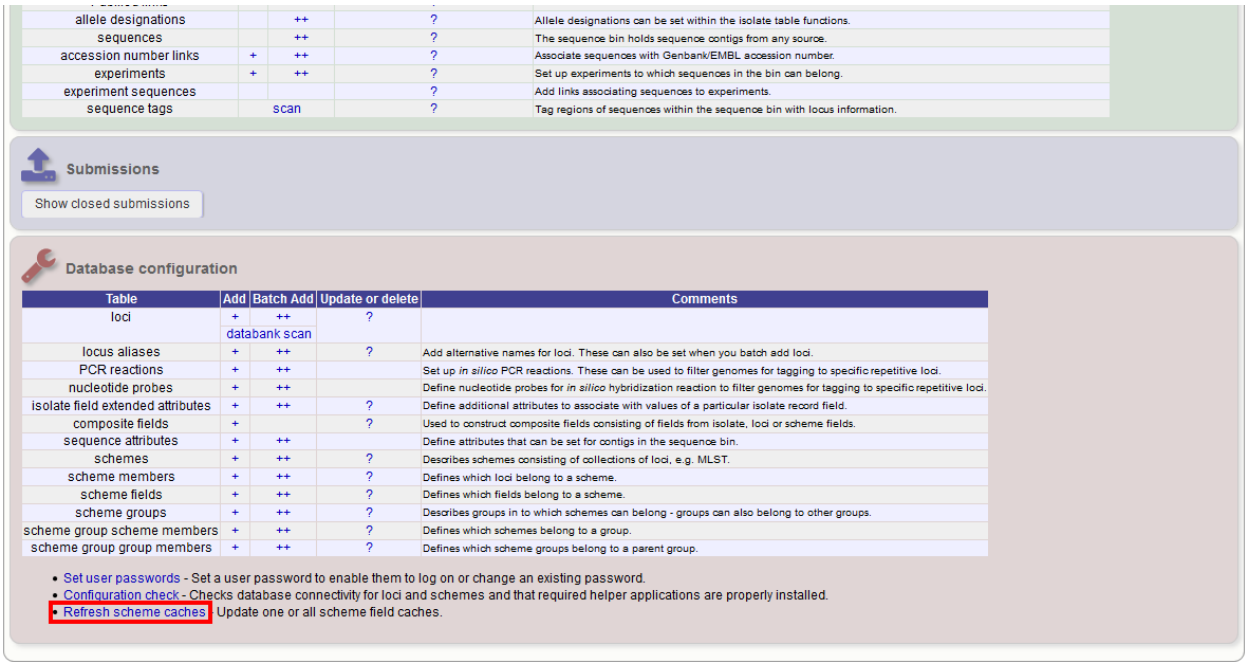
```
update_scheme_caches.pl --database pubmlst_bigsdb_neisseria_isolates
```

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

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

```
update_scheme_caches.pl --help

NAME
    update_scheme_caches.pl - Update scheme field caches

SYNOPSIS
    update_scheme_caches.pl --database NAME [options]

OPTIONS

--database NAME
    Database configuration name.

--help
    This help page.

--method METHOD
    Update method - the following values are allowed:
    full: Completely recreate caches
    incremental: Only add values for records not in cache.
    daily: Only add values for records not in cache updated today.
    daily_replace: Refresh values only for records updated today.

--quiet
    Don't output progress messages.

--schemes SCHEMES
    Comma-separated list of scheme ids to use.
    If left empty, all schemes will be updated.
```

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



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

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

5.11.3 Use a ramdisk for the secure temporary directory

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

5.12 Dataset partitioning

5.12.1 Sets

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

See also:

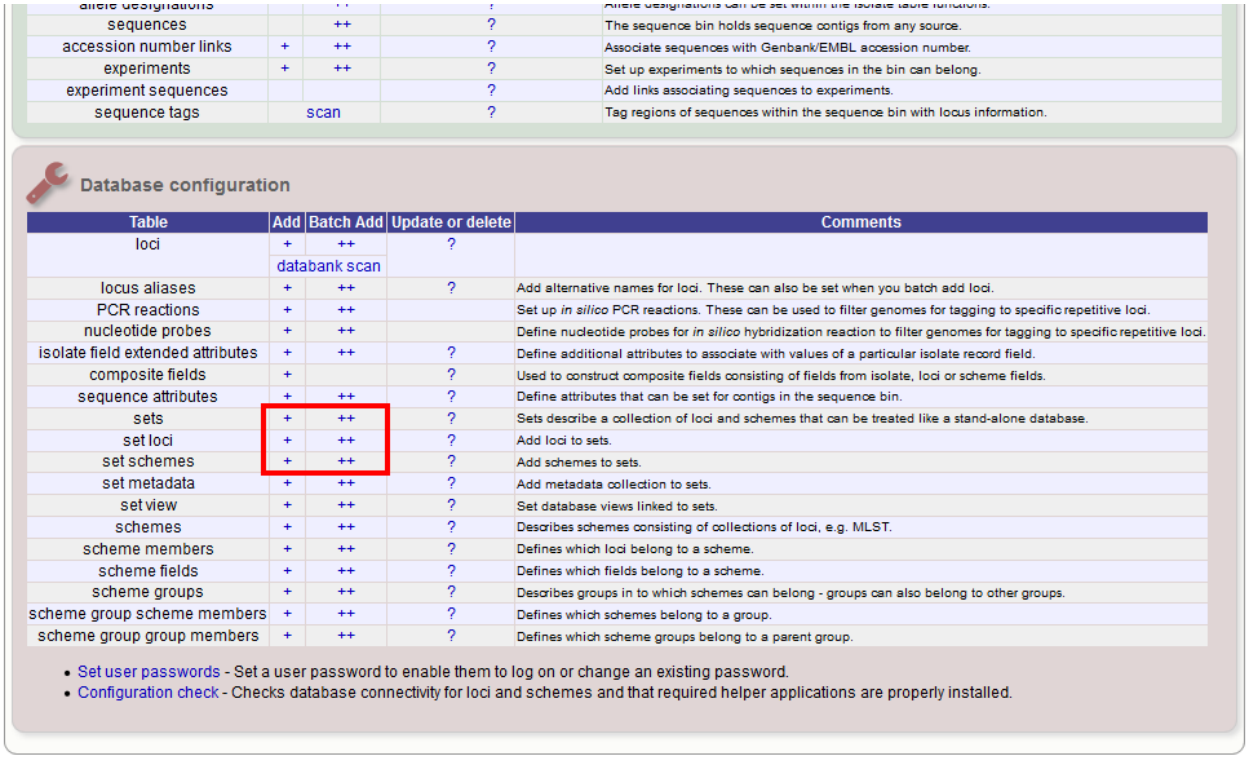
Sets (concept)

5.12.2 Configuration of sets

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

```
sets="yes"
```

With this attribute, the curation interface now has options to add sets, and then add loci or schemes to these sets.



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.

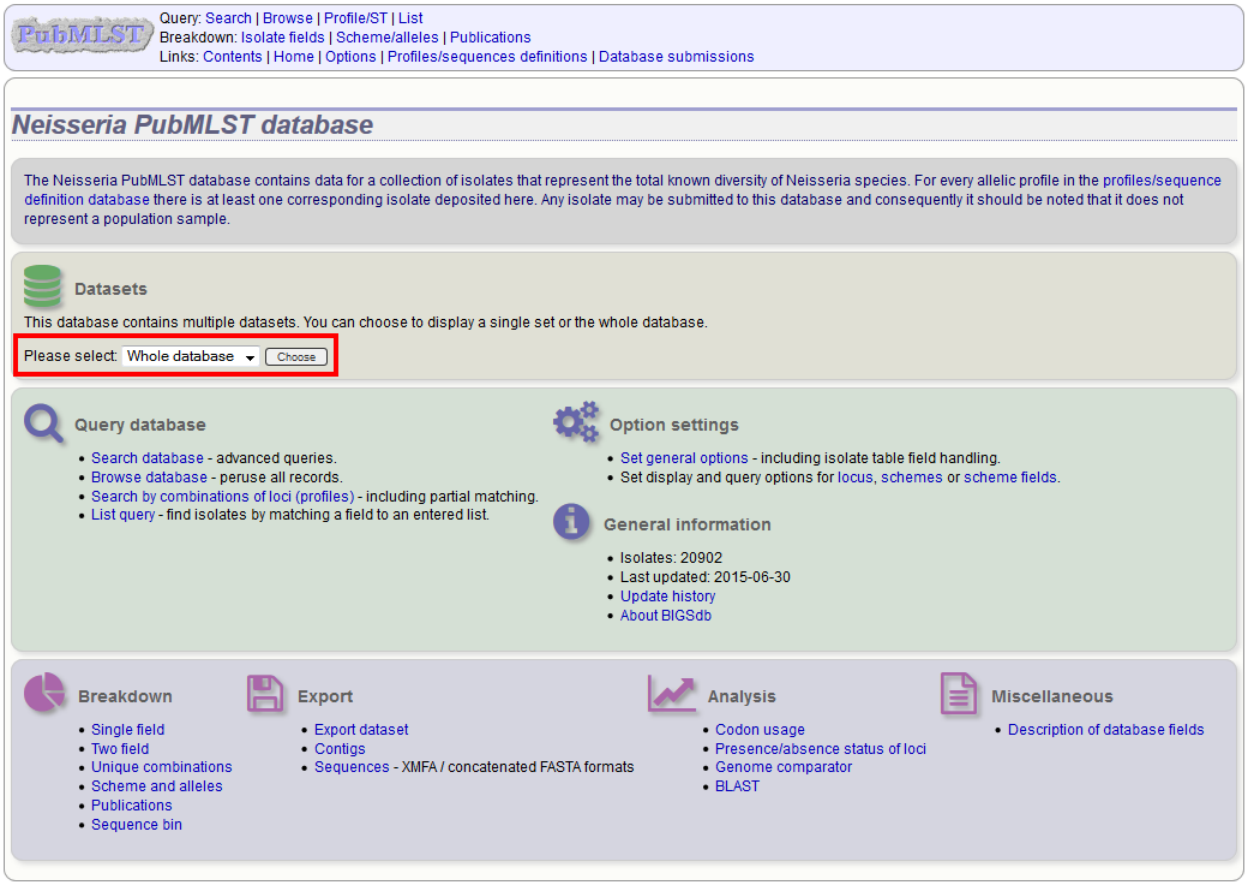
Database configuration

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.
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.
set view	+	++	?	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.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

- Set user passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

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

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



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

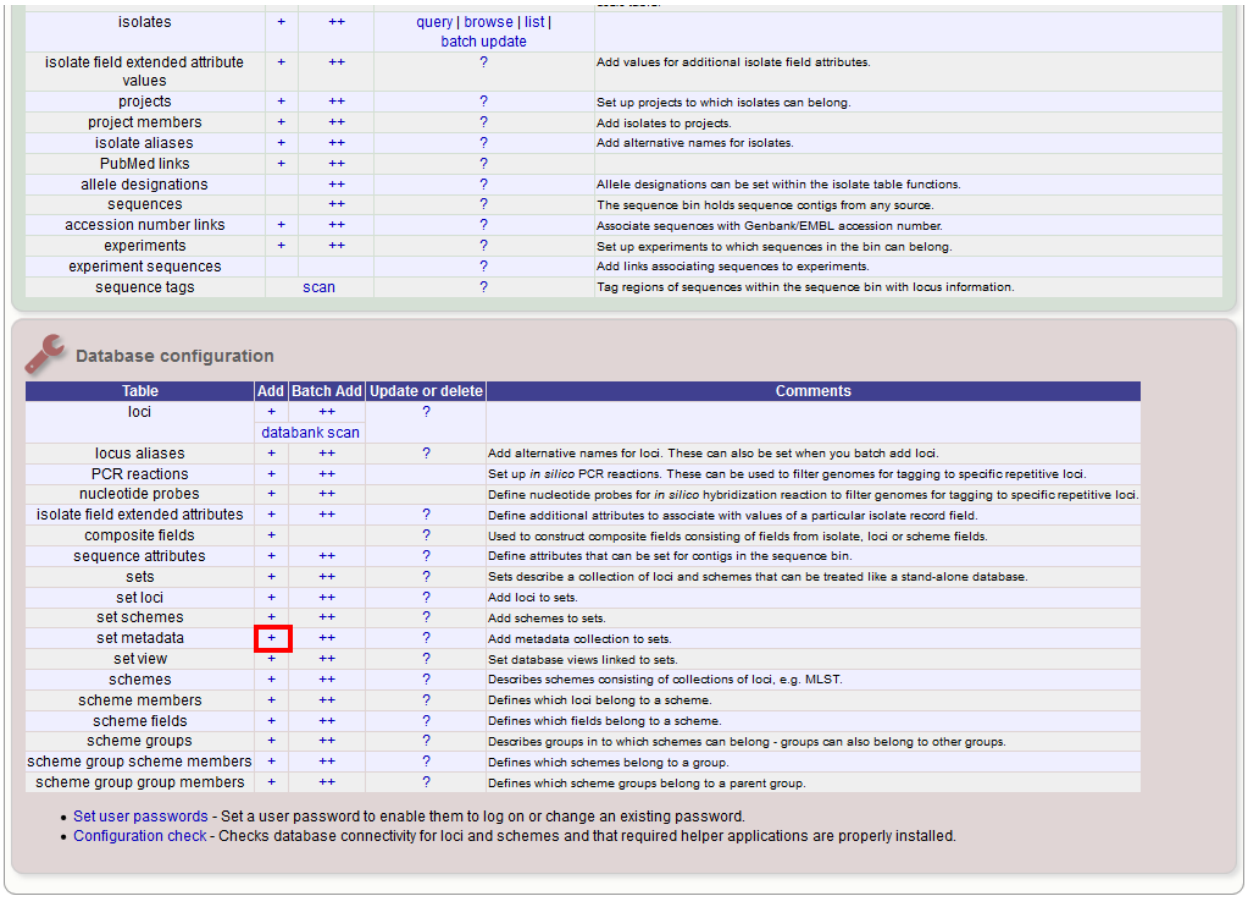
Additional metadata fields can be set within the XML configuration file. They are specified as belonging to a metaset by prefixing the field name with 'meta_NAME:' where NAME is the name of the metaset, e.g.

```
<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	+	++	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 configuration

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.
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.
set view	+	++	?	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.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

- Set user passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

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

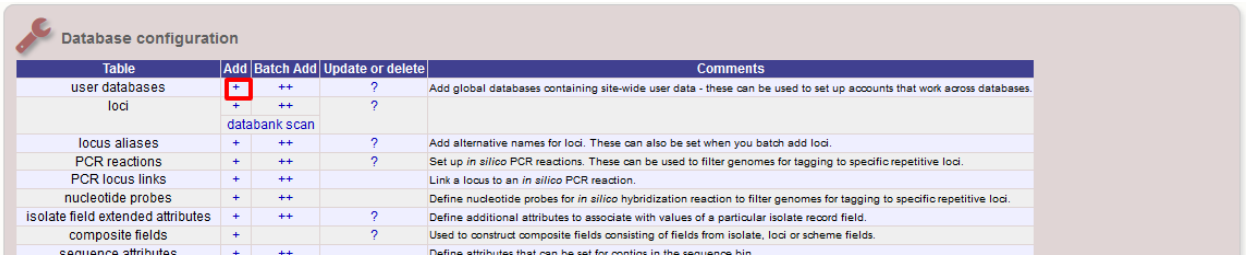
The only_sets attribute can be set to 'yes' to disable the option for 'Whole database' so that only sets can be viewed, e.g.

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

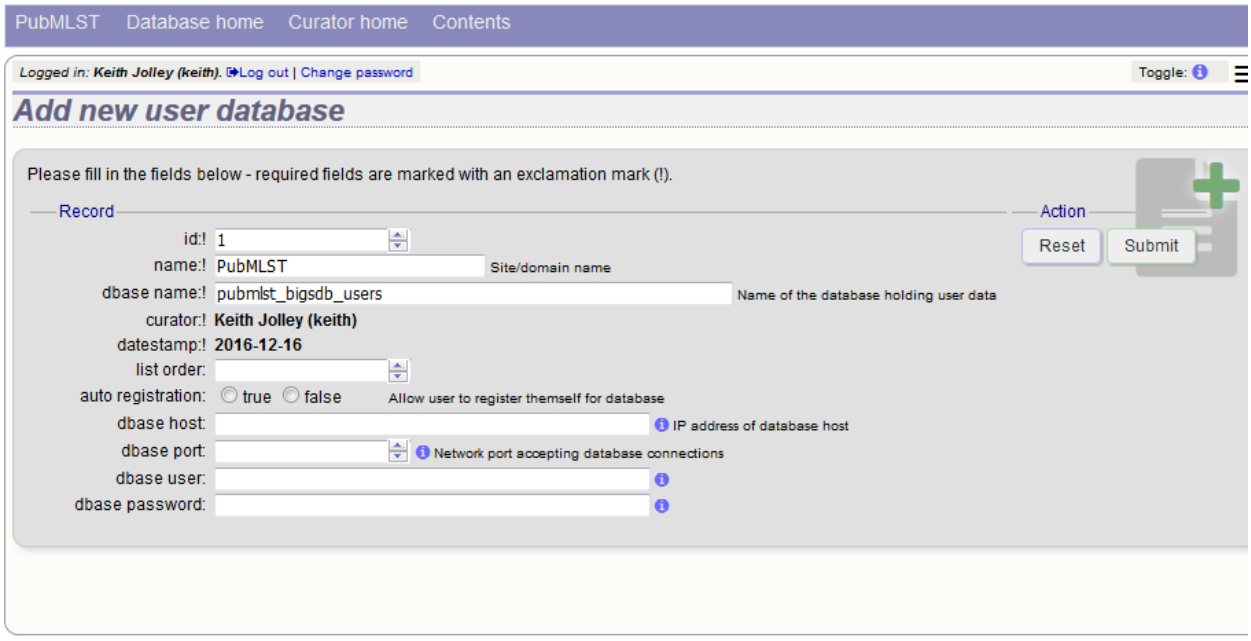
5.13 Setting a site-wide users database

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

Once a *site-wide user database has been set up*, this can be defined within each client database as follows. From the curators' contents page, click the add (+) user databases link:



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



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

5.14 Adding new loci

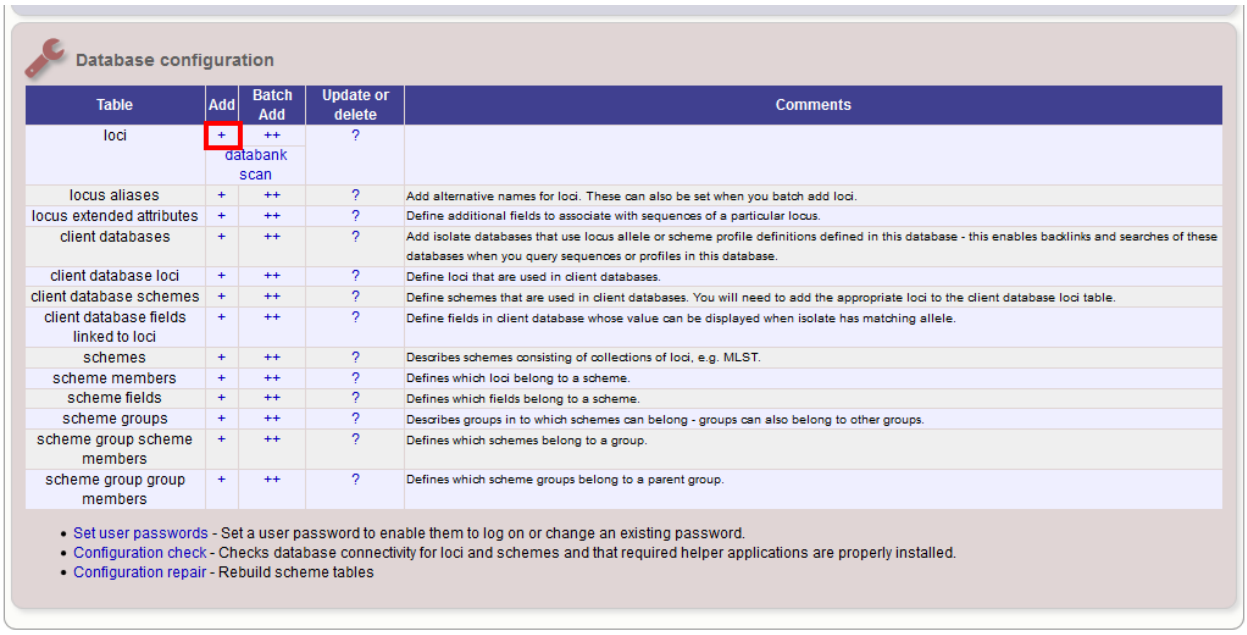
See also:

Loci (concept)

5.14.1 Sequence definition databases

5.14.1.1 Single locus

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



Database configuration

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.
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 passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.
- Configuration repair - Rebuild scheme tables

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

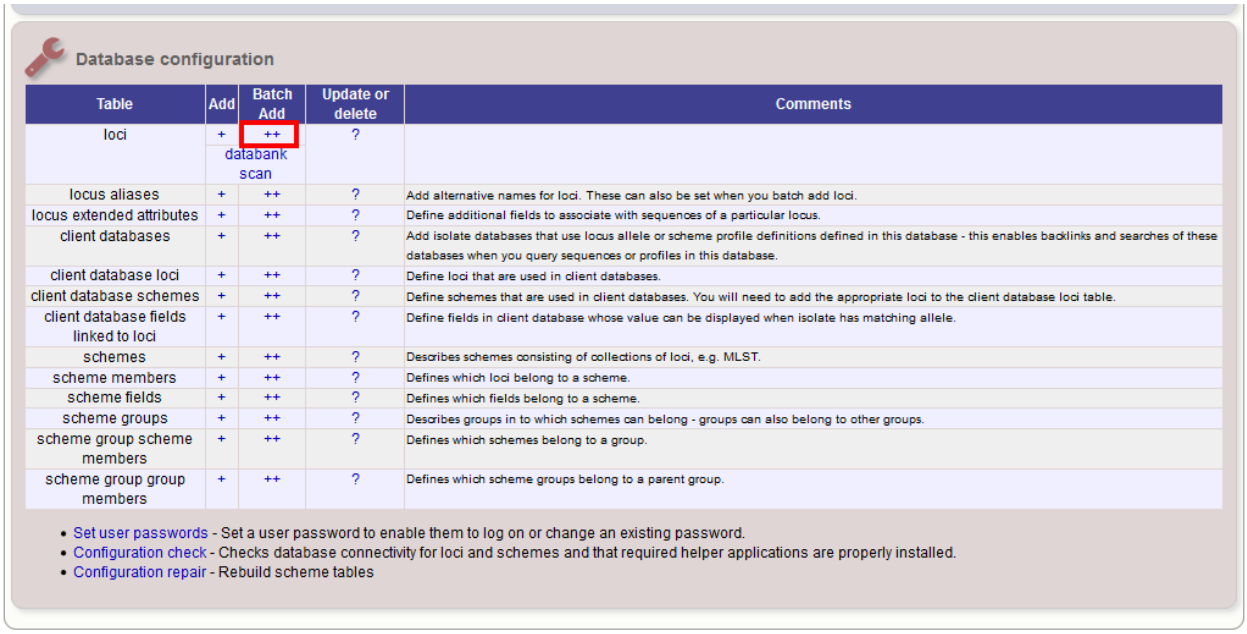
- id - The name of the locus.
  - Allowed: any value starting with a letter, number or underscore.
- data_type - Describes whether the locus is defined by nucleotide or peptide sequence.
  - Allowed: DNA/peptide.
- allele_id_format - The format for allele identifiers.
  - Allowed: integer/text.
- length_varies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

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

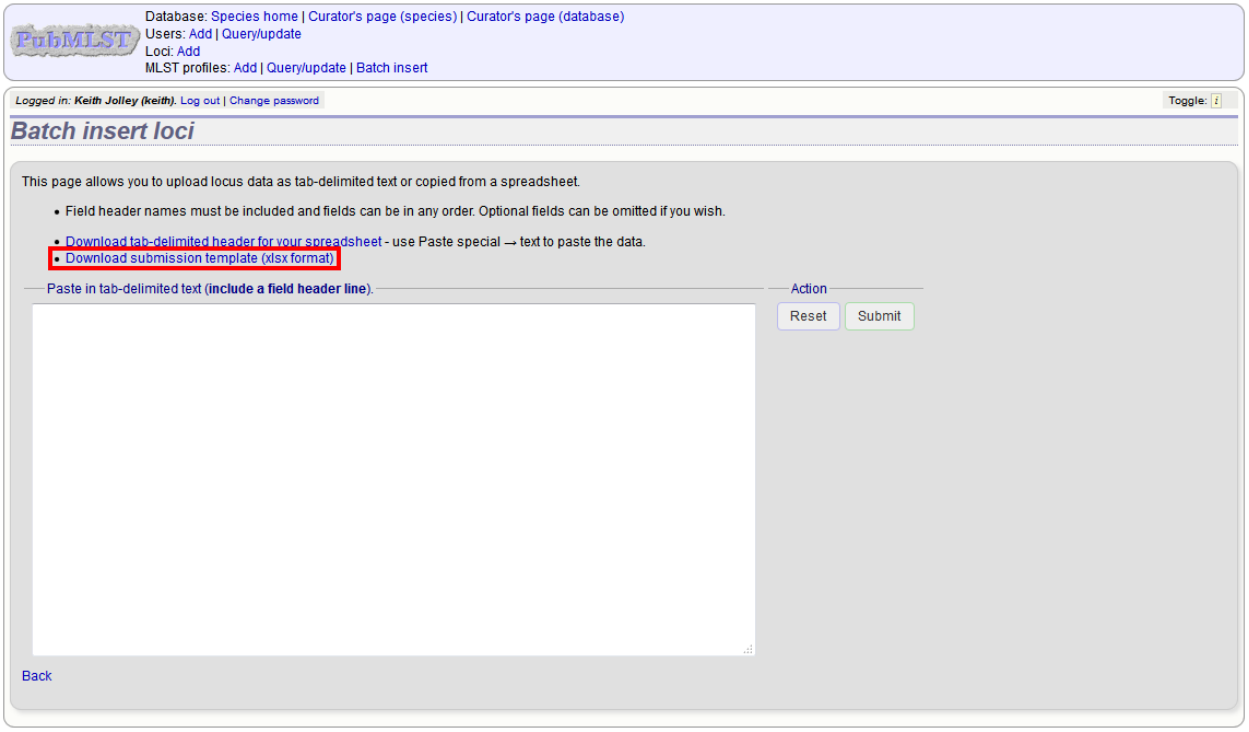
- links - Hyperlinks pointing to additional resources to display in the locus description (optional).
  - Enter each link on a separate line in the format with the URL first, followed by a | then the description (URL|description).

5.14.1.2 Batch adding

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



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



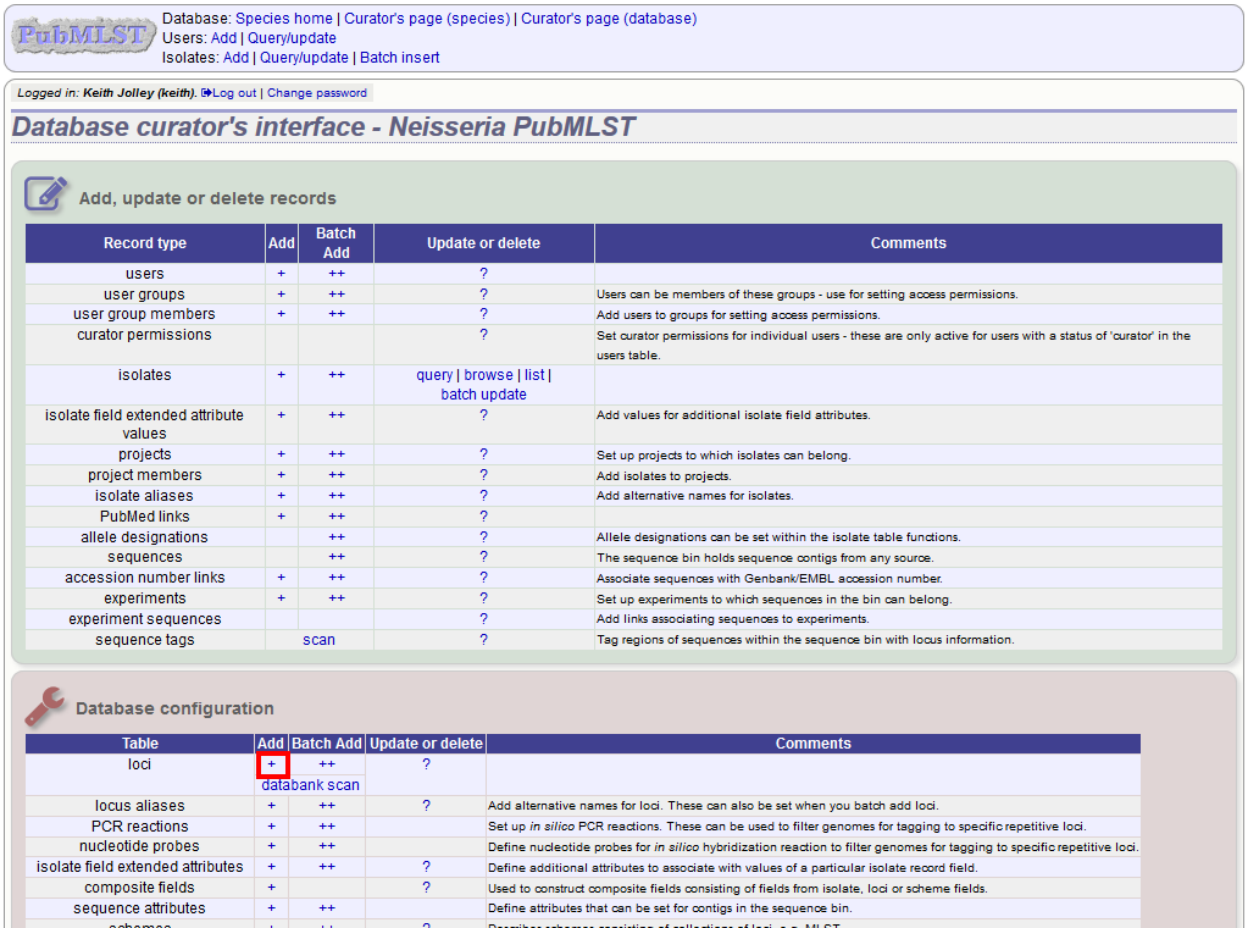
Fill in the spreadsheet using the fields described for *adding single loci*.

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

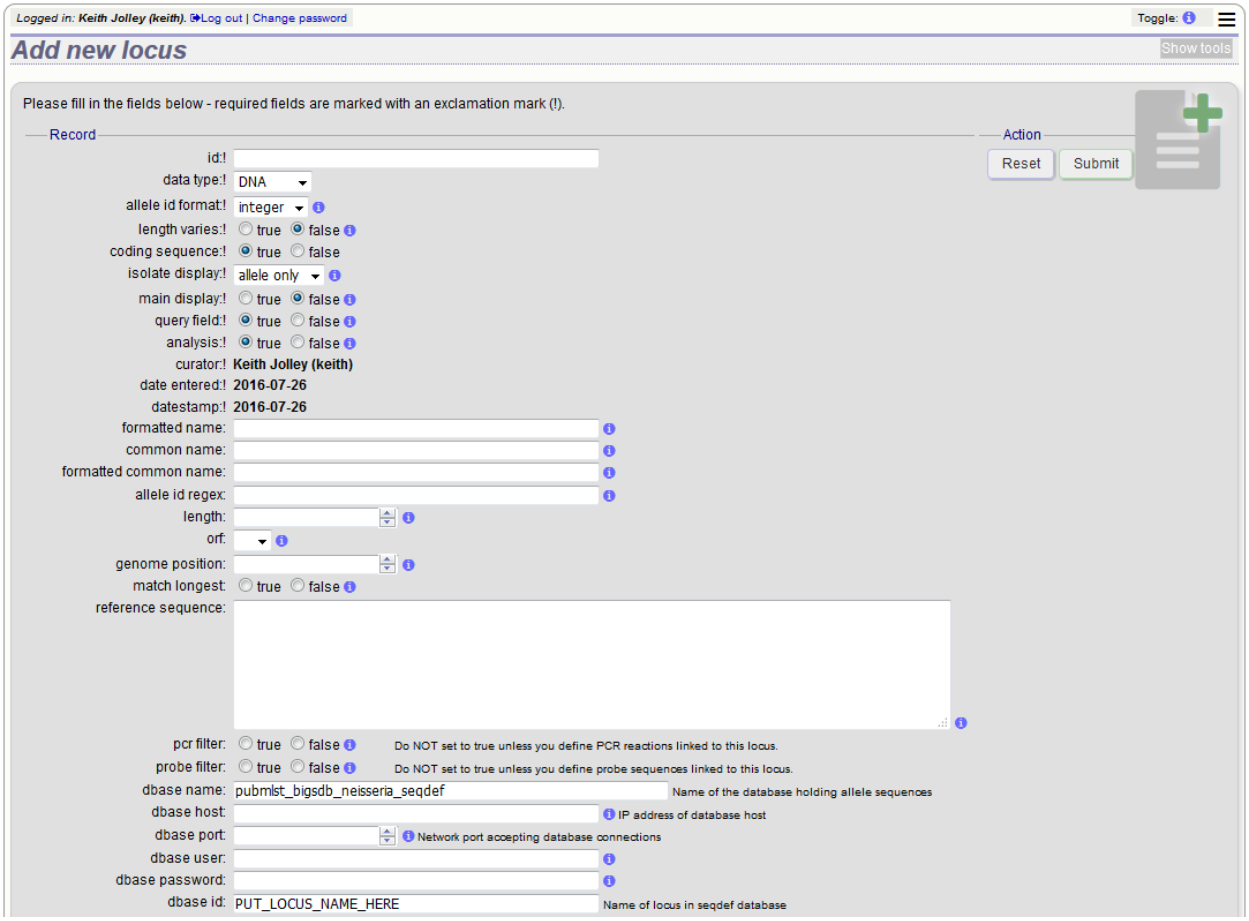
5.14.2 Isolate databases

5.14.2.1 Single locus

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



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.
- isolate_display - Sets how alleles for this locus are displayed in a detailed isolate record - this can be overridden by user preference.
  - Allowed: allele only/sequence/hide.
- main_display - Sets whether or not alleles for this locus are displayed in a main results table by default - this can be overridden by user preference.
  - Allowed: true/false.

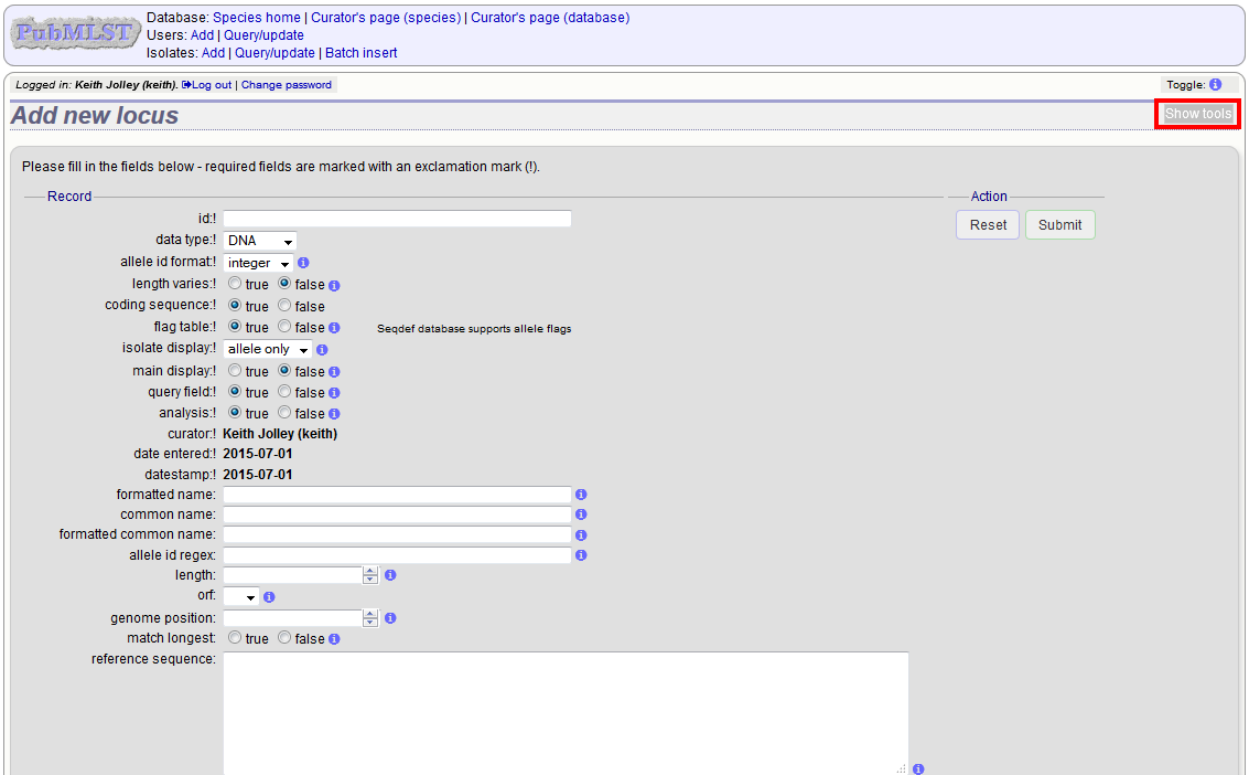
- query_field - Sets whether or not alleles for this locus can be used in queries by default - this can be overridden by user preference.
  - Allowed: true/false.
- analysis - Sets whether or not alleles for this locus can be used in analysis functions by default - this can be overridden by user preference.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

  - Allowed: true/false.

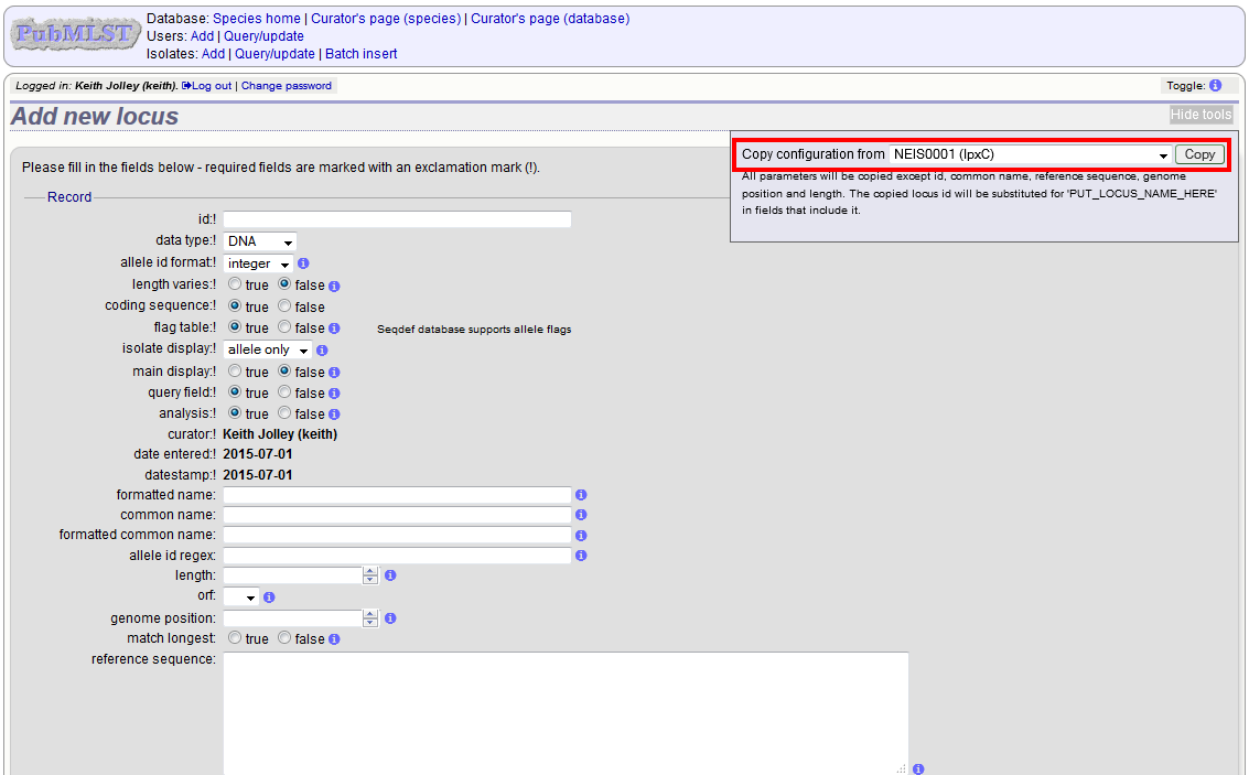
- reference_sequence - Sequence used by the automated sequence comparison algorithms to identify sequences matching this locus. **This is only used if a sequence definition database has not been set up for this locus.**
- pcr_filter - Set to true if this locus is further defined by genome filtering using in silico PCR.
  - Allowed: true/false.
- probe_filter - Set to true if this locus is further defined by genome filtering using in silico hybdridization.
  - Allowed: true/false.
- dbase_name - Name of database (system name).
  - Allowed: any text.
- dbase_host - Resolved name of IP address of database host - leave blank if running on the same machine as the isolate database.
  - Allowed: network address, e.g. 129.67.26.52 or zoo-oban.zoo.ox.ac.uk
- dbase_port - Network port on which the sequence definition database server is listening - leave blank unless using a non-standard port (5432).
  - Allowed: integer.
- dbase_user - Name of user with permission to access the sequence definition database - depending on the database configuration you may be able to leave this blank.
  - Allowed: any text (no spaces).
- dbase_password - Password of database user - again depending on the database configuration you may be able to leave this blank.
  - Allowed: any text (no spaces).
- dbase_id - Name of locus in seqdef database. This is usually the same as the id field.
  - Allowed: any text (no spaces).
- description_url - The URL used to hyperlink to locus information in the isolate information page. This can either be a relative (e.g. /cgi-bin/...) or an absolute (containing http://) URL.
  - Allowed: any valid URL.
- url - The URL used to hyperlink to information about the allele. This can either be a relative or absolute URL. If [?] (including the square brackets) is included then this will be substituted for the allele value in the resultant URL. To link to the appropiate 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:

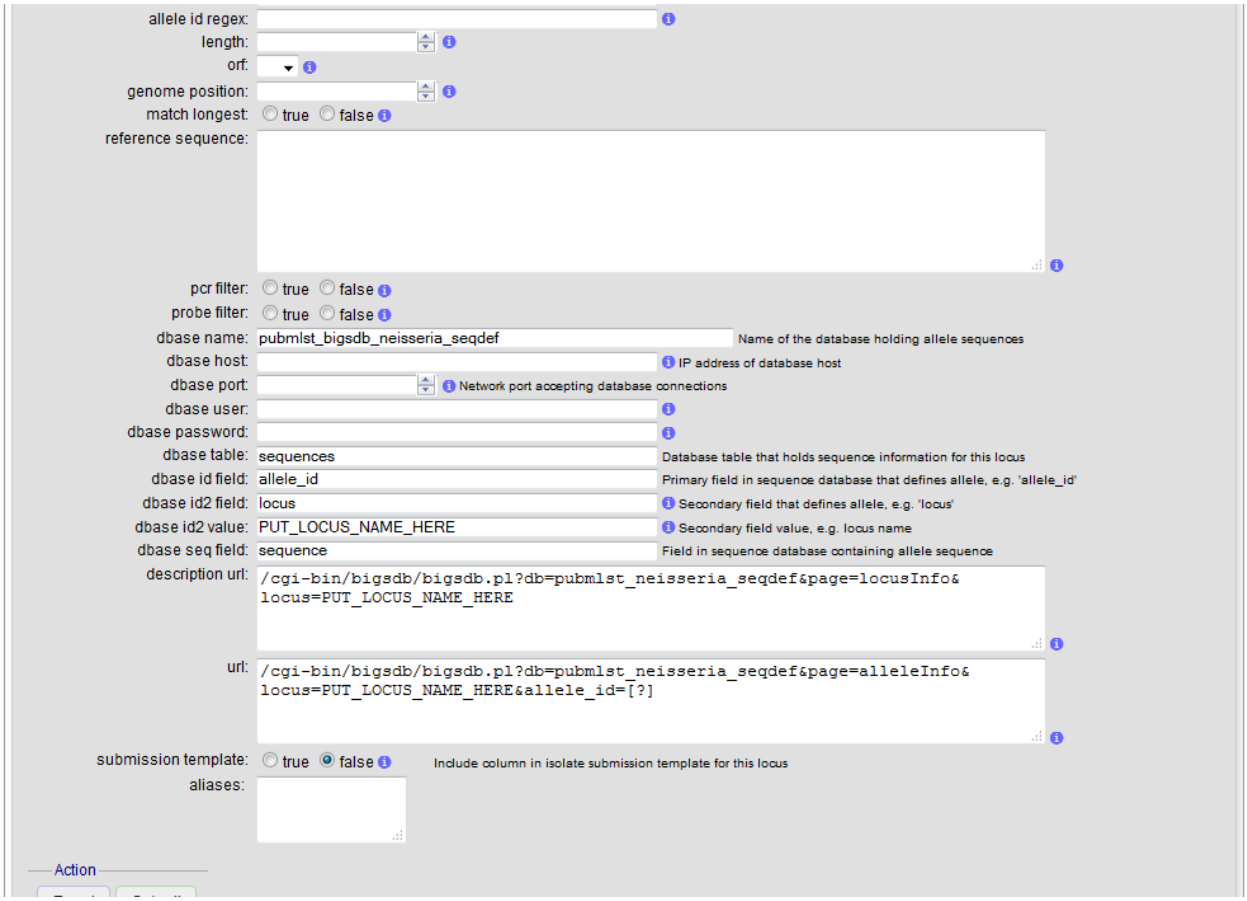


This displays a drop-down box containing existing loci. Select the locus that you wish to use as a template, and click 'Copy'.



The configuration will be copied over to the web form, with the exception of name fields. Some fields will require

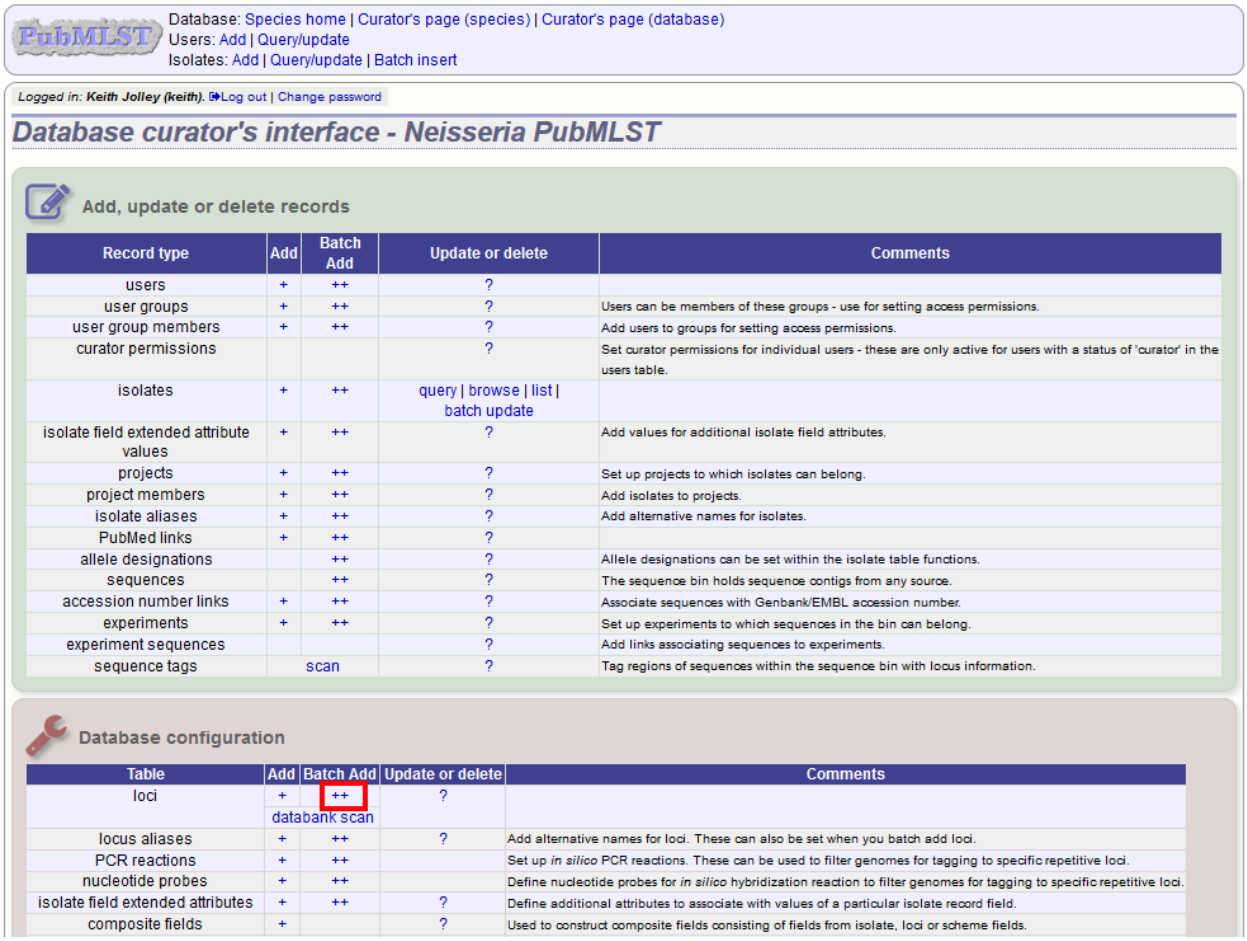
you to change the value 'PUT_LOCUS_NAME_HERE' with the value you enter in the id field. These are usually the dbase_id2_value, description_url and url fields:



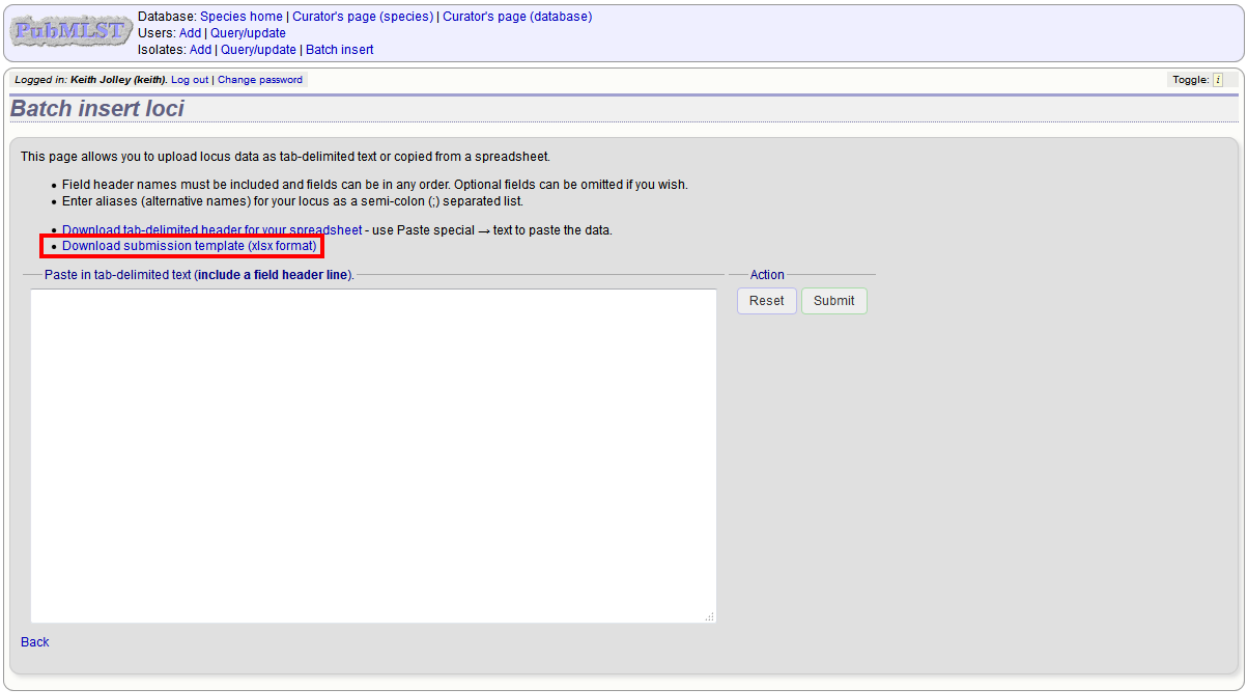
Complete the form and click 'Submit'.

5.14.2.2 Batch adding

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



Click the link to download an Excel template:

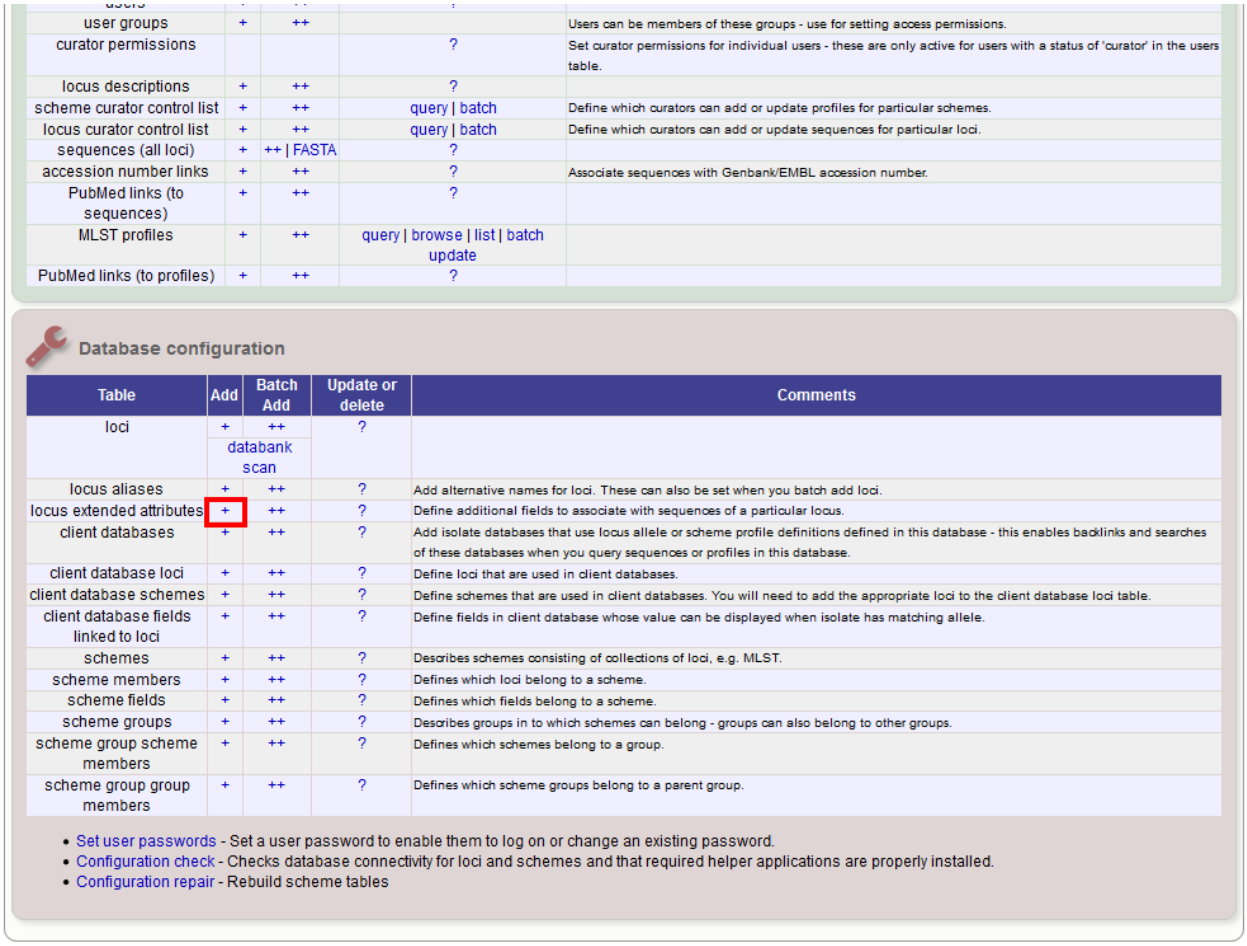


Fill in the spreadsheet fields using the *table above as a guide*, then paste the completed table into the web form and press 'Submit query'.

5.15 Defining locus extended attributes

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

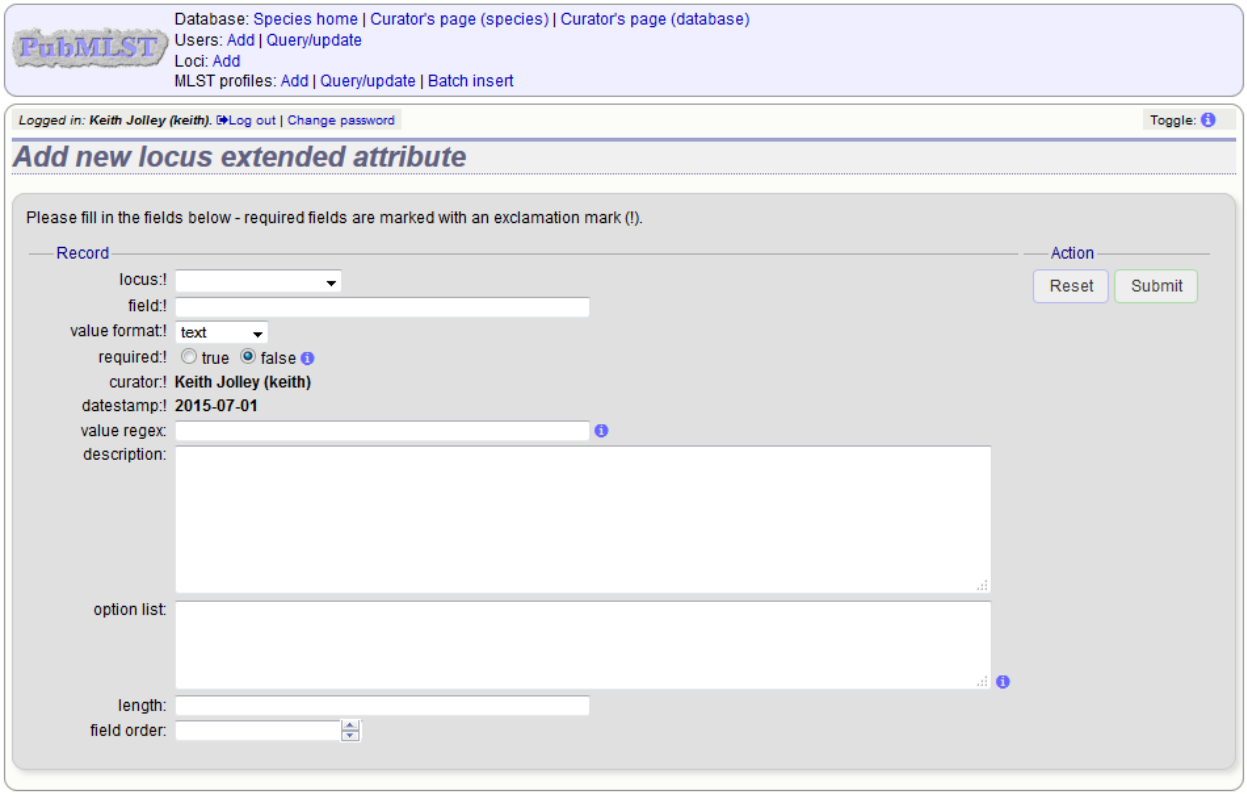
To add extended attributes for a locus, click add (+) locus extended attributes in the sequence definition database curator's interface contents page.



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 users table.
locus descriptions	+	++	?	
scheme curator control list	+	++	query | batch	Define which curators can add or update profiles for particular schemes.
locus curator control list	+	++	query | batch	Define which curators can add or update sequences for particular loci.
sequences (all loci)	+	++ | FASTA	?	
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
PubMed links (to sequences)	+	++	?	
MLST profiles	+	++	query | browse | list | batch update	
PubMed links (to profiles)	+	++	?	

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.
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.

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



- 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 (|) separated list of allowed values (optional).
- length - Maximum length of value (optional).
  - Allowed: any integer.
- field_order - Integer that sets the position of the field within scheme values in any results (optional).
  - Allowed: any integer.

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

5.16 Defining schemes

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

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

To set up a new scheme, you need to:

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

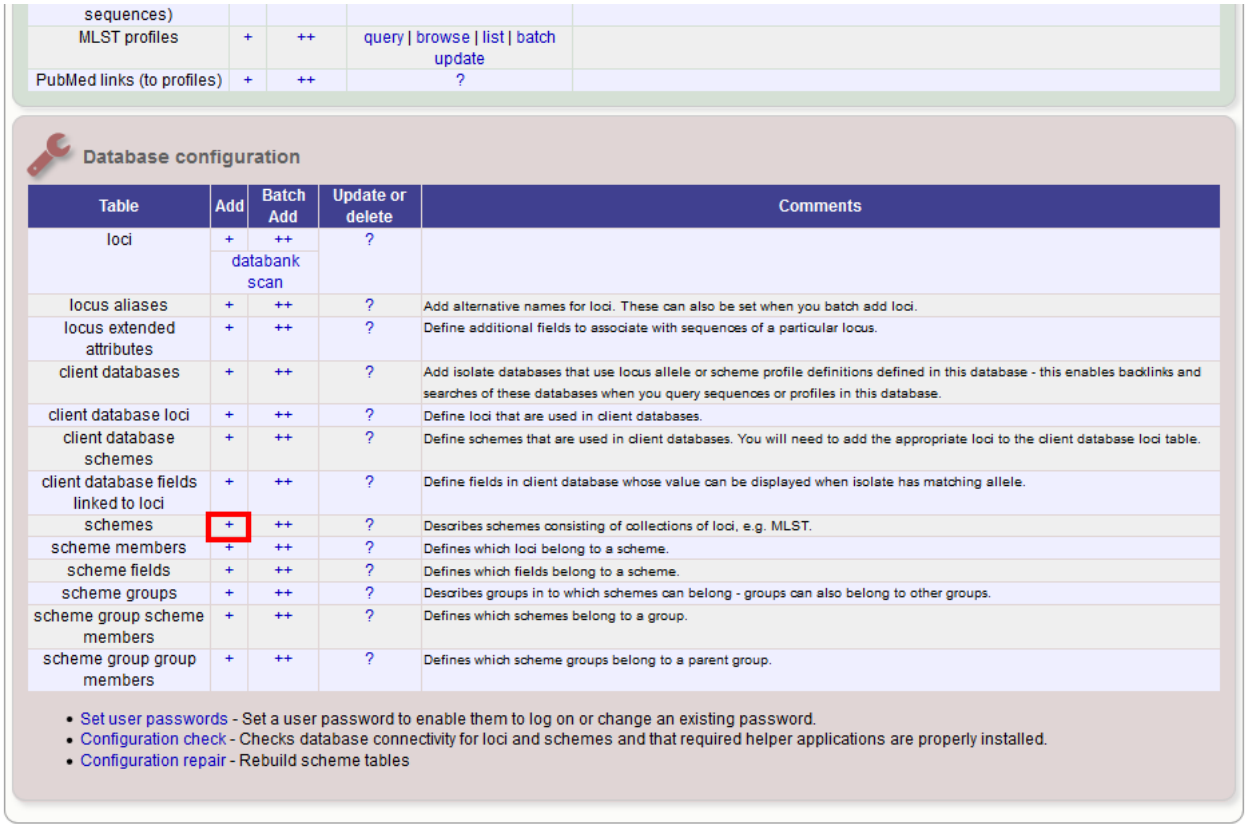
See also:

Schemes (concept)

5.16.1 Sequence definition databases

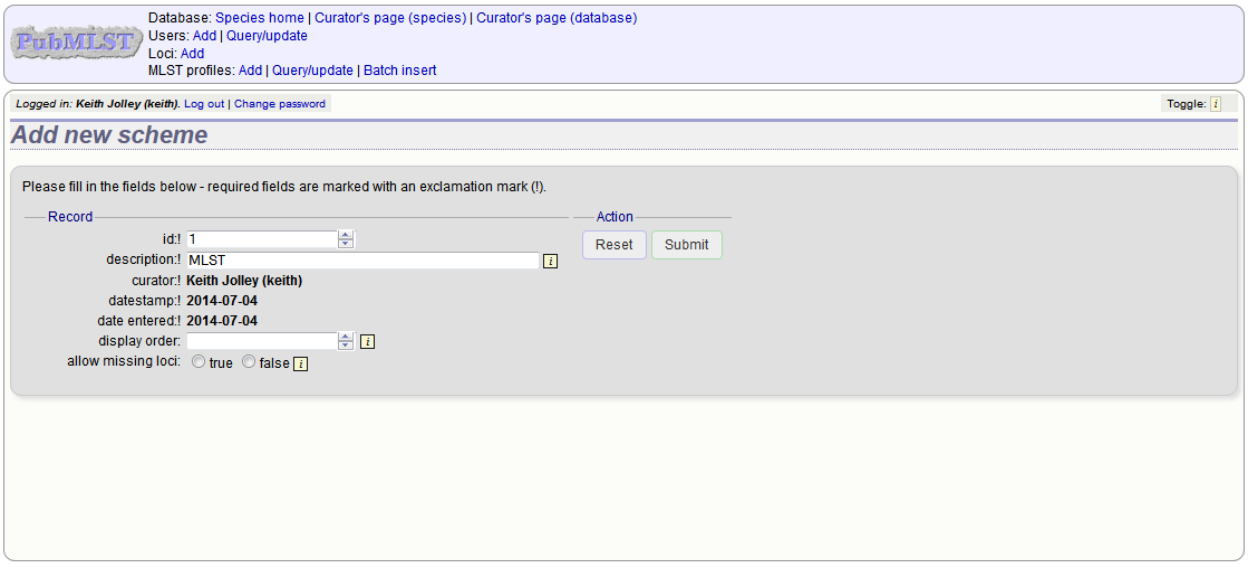
As with all configuration, tables can be populated using the batch interface (++) or one at a time (+). Details for the latter are described below:

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

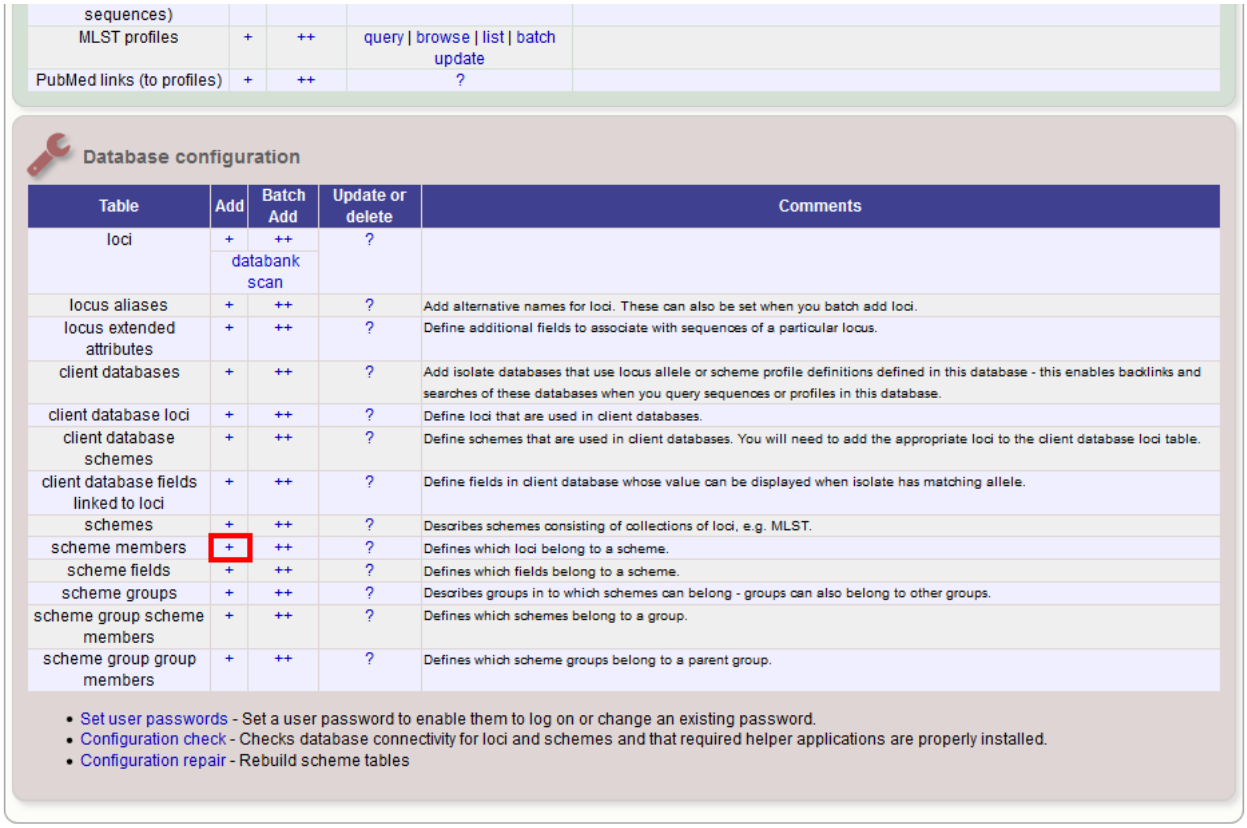


Fill in the scheme description in the web form. The next available scheme id number will be filled in already.

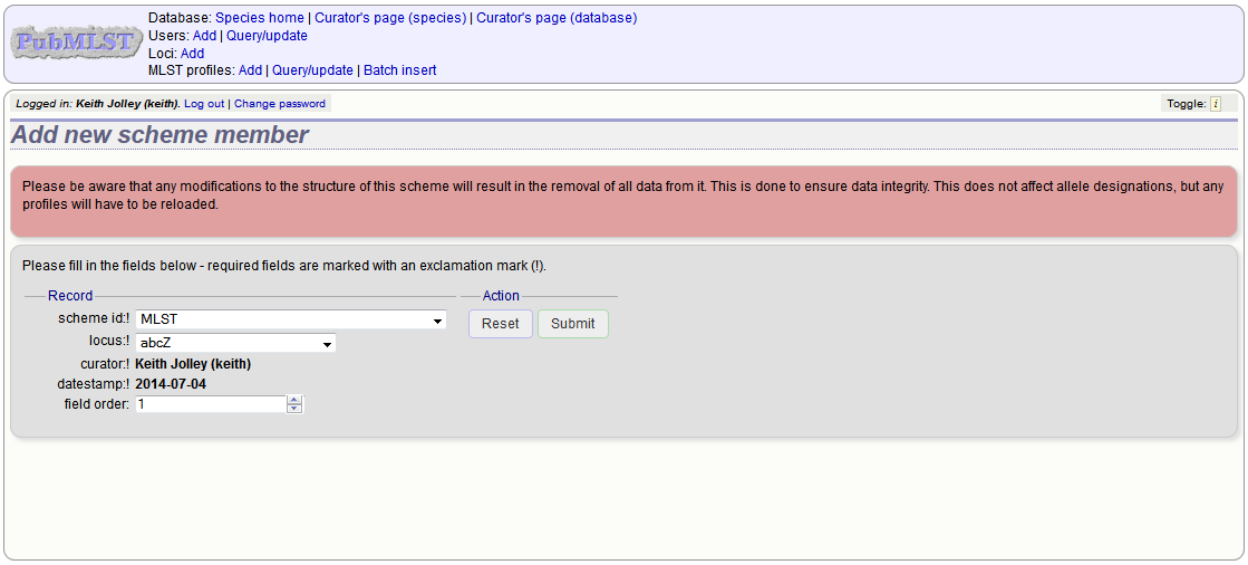
The display_order field accepts an integer that can be used to order the display of schemes in the interface - this can be left blank if you wish.



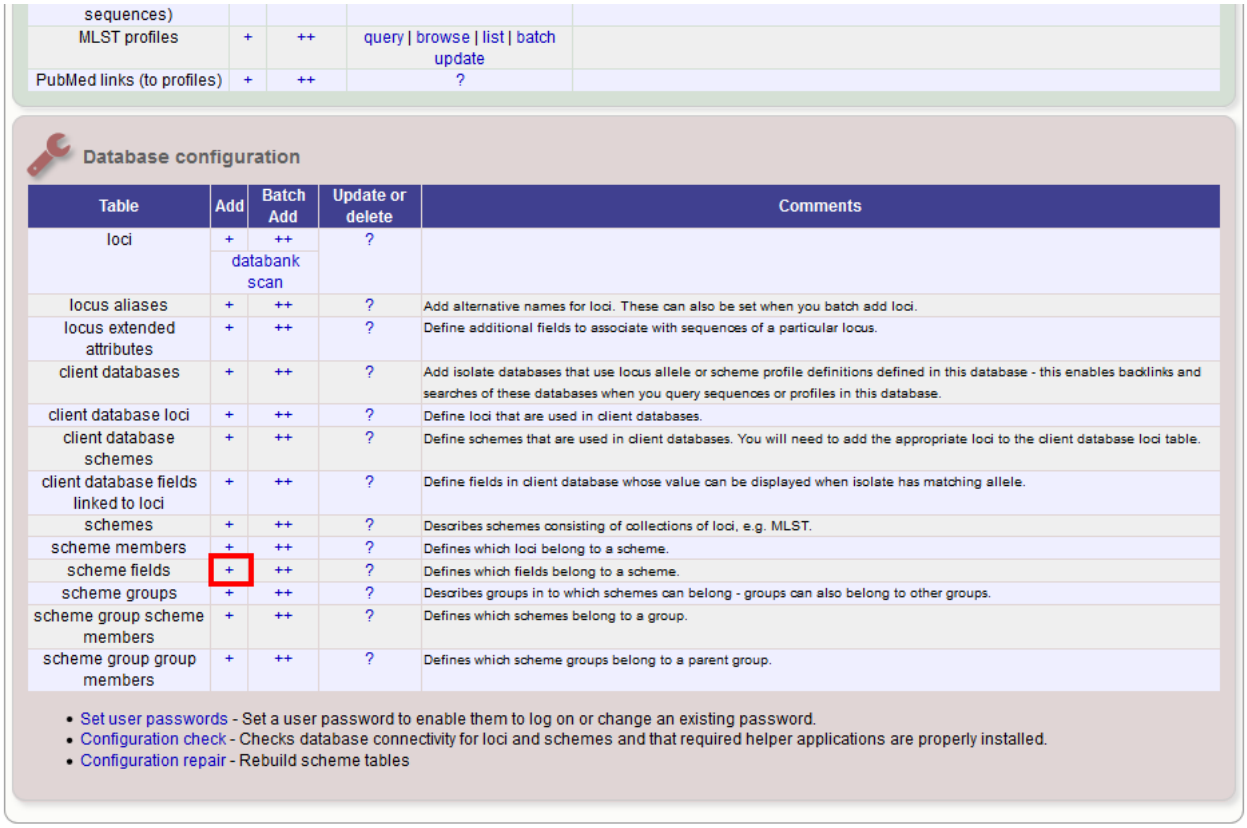
To add loci to the scheme, click the add (+) scheme members link on the curator's interface contents page.



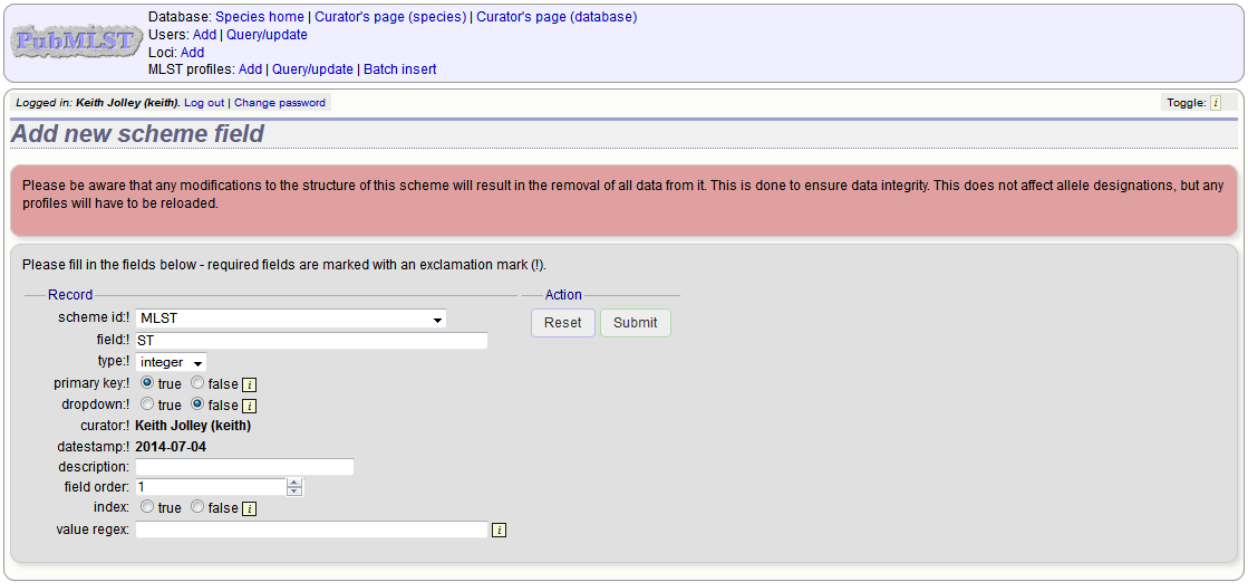
Select the scheme name and a locus that you wish to add to the scheme from the appropriate drop-down boxes. *Loci need to have already been defined*. The field_order field allows you to set the display order of the locus within a profile - if these are left blank that alphabetical ordering is used.



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



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



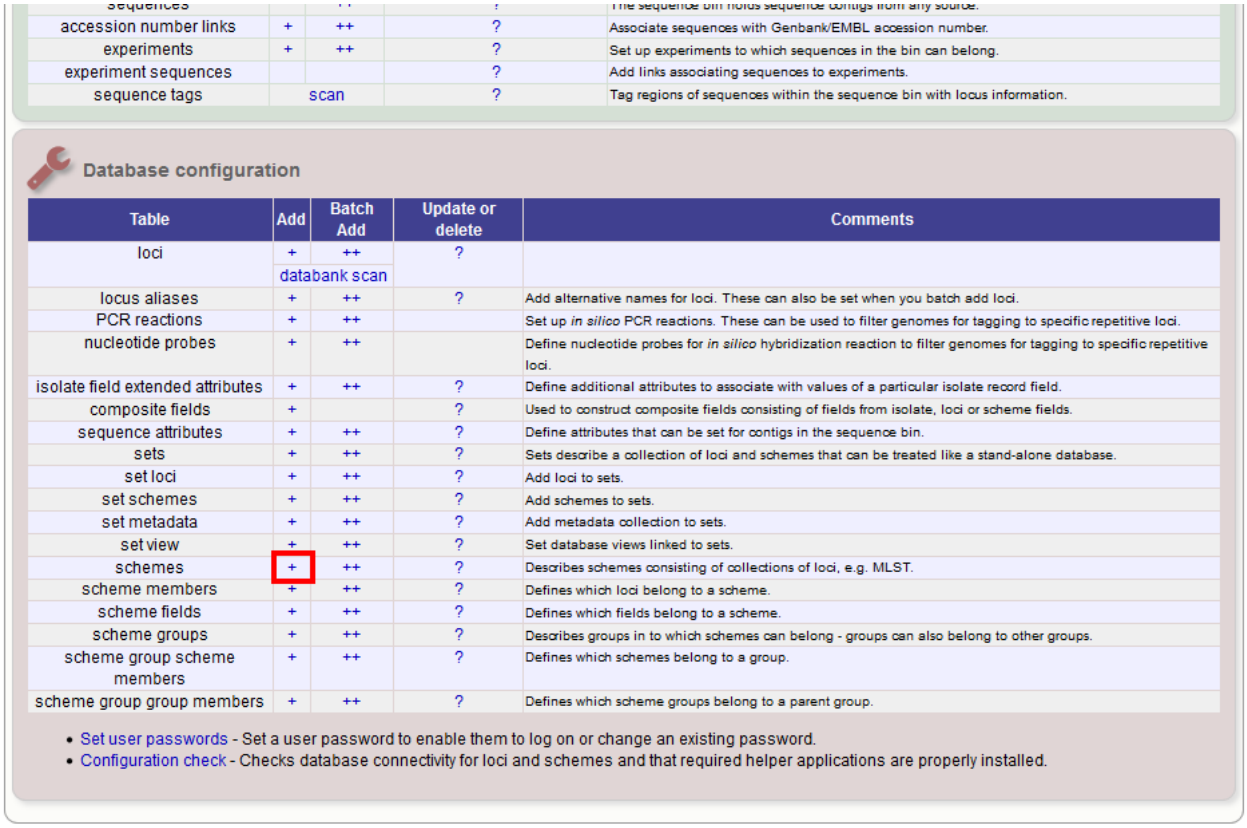
- scheme_id - Dropdown box of scheme names.
  - Allowed: selection from list.
- field - Field name.
  - Allowed: any value.

- type - Format for values.
  - Allowed: text/integer/date.
- primary_key - Set to true if field is the primary key. There can only be one primary key for a scheme.
  - Allowed: true/false.
- dropdown - Set to true if a dropdown box is displayed in the query interface, by default, for values of this field to be quickly selected. This option can be overridden by user preferences.
  - Allowed: true/false.
- description - This field isn't currently used.
- field_order - Integer that sets the position of the field within scheme values in any results.
  - Allowed: any integer.
- value_regex - Regular expression to enforce field values.
  - ^: the beginning of the string
  - $:the end of the string
  - d: digit
  - D: non-digit
  - s: white space character
  - S: non white space character
  - w: alpha-numeric plus '_'
  - .: any character
  - *: 0 or more of previous character
  - +: 1 or more of previous character

5.16.2 Isolate databases

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

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



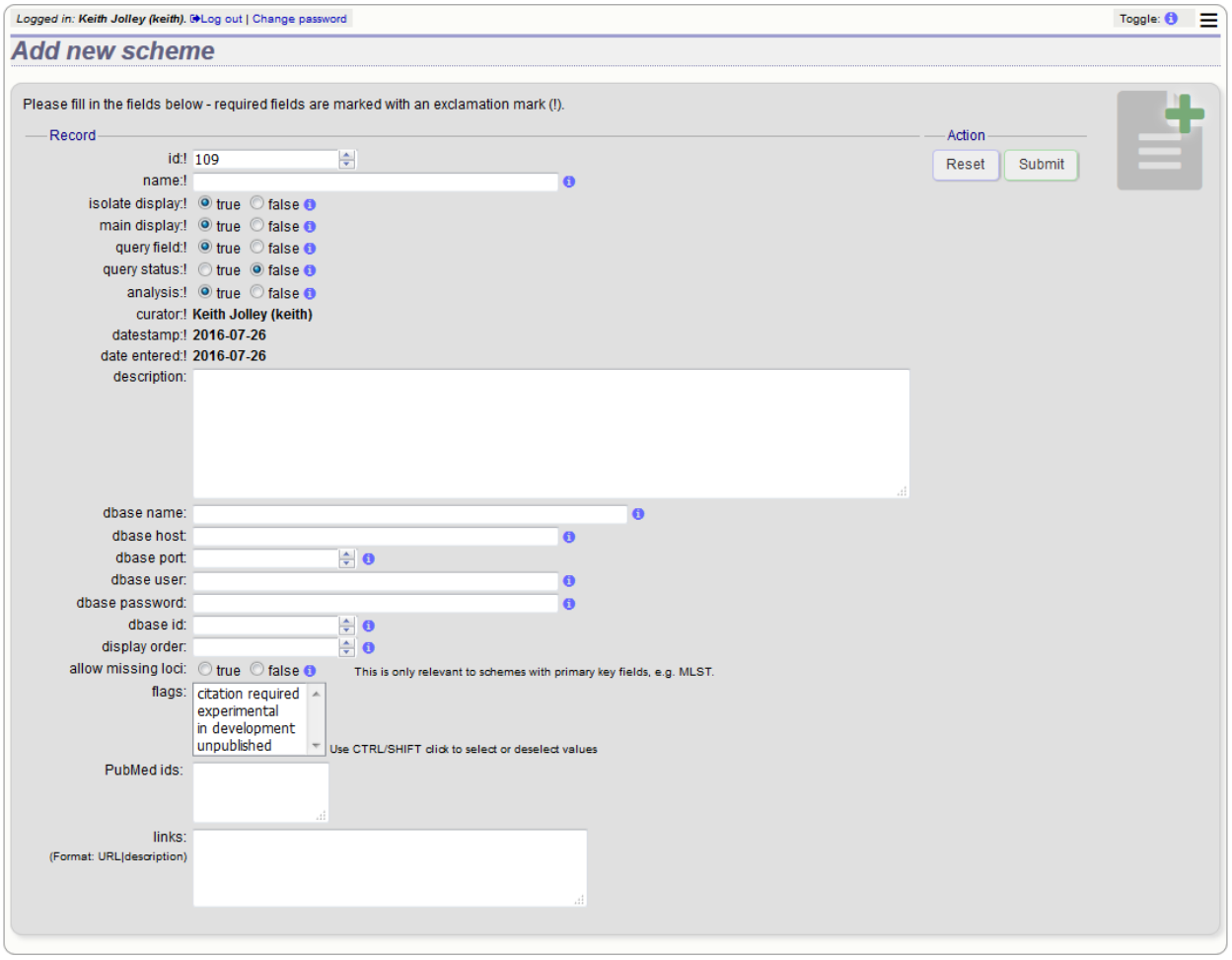
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.

Database configuration

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.
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.
set view	+	++	?	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.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

- Set user passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

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



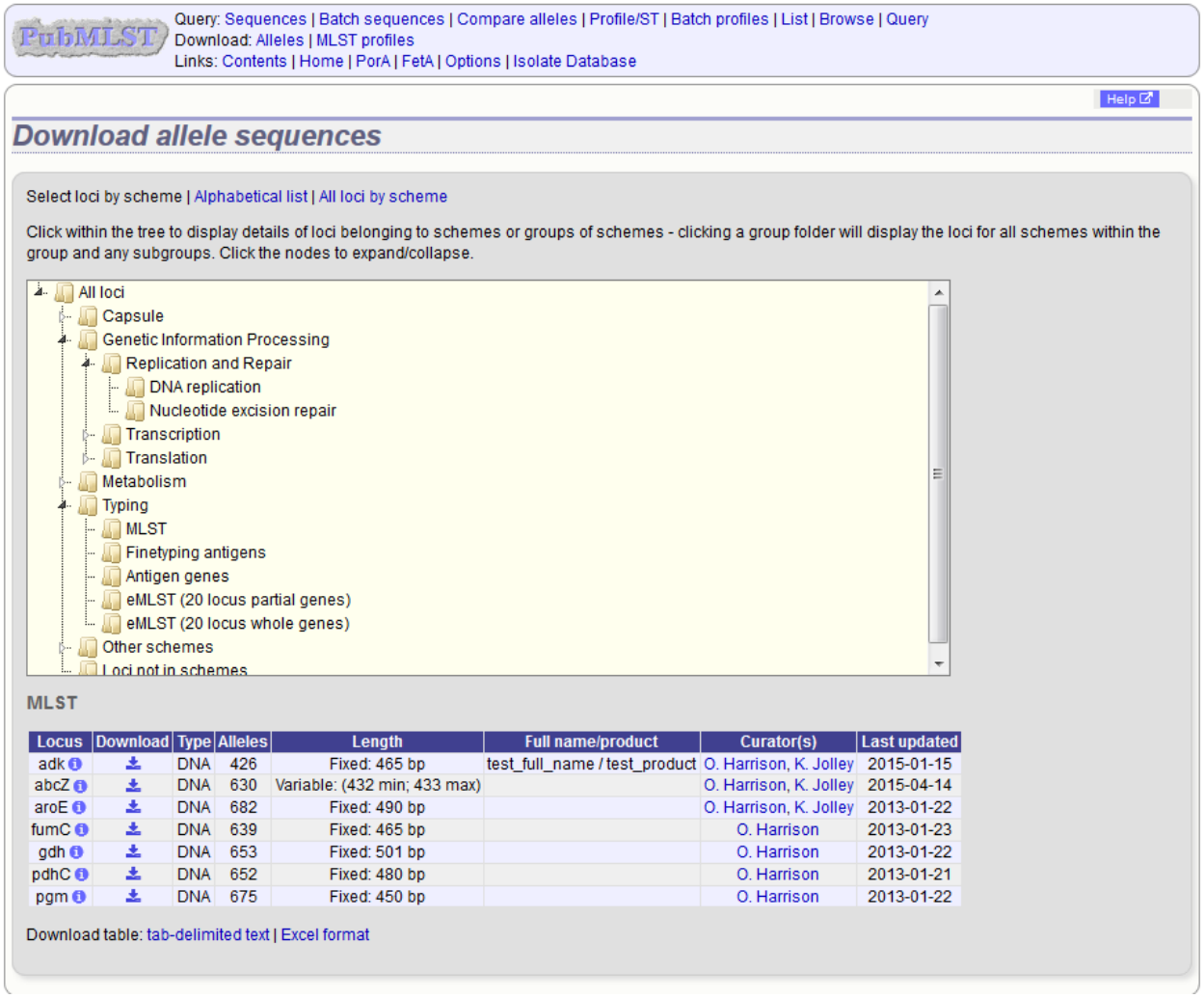
- id - Index number of scheme - the next available number will be entered automatically.
  - Allowed: any positive integer.
- description - Short description - this is used in tables so make sure it's not too long.
  - Allowed: any text.
- isolate_display - Sets whether or not fields for this scheme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

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

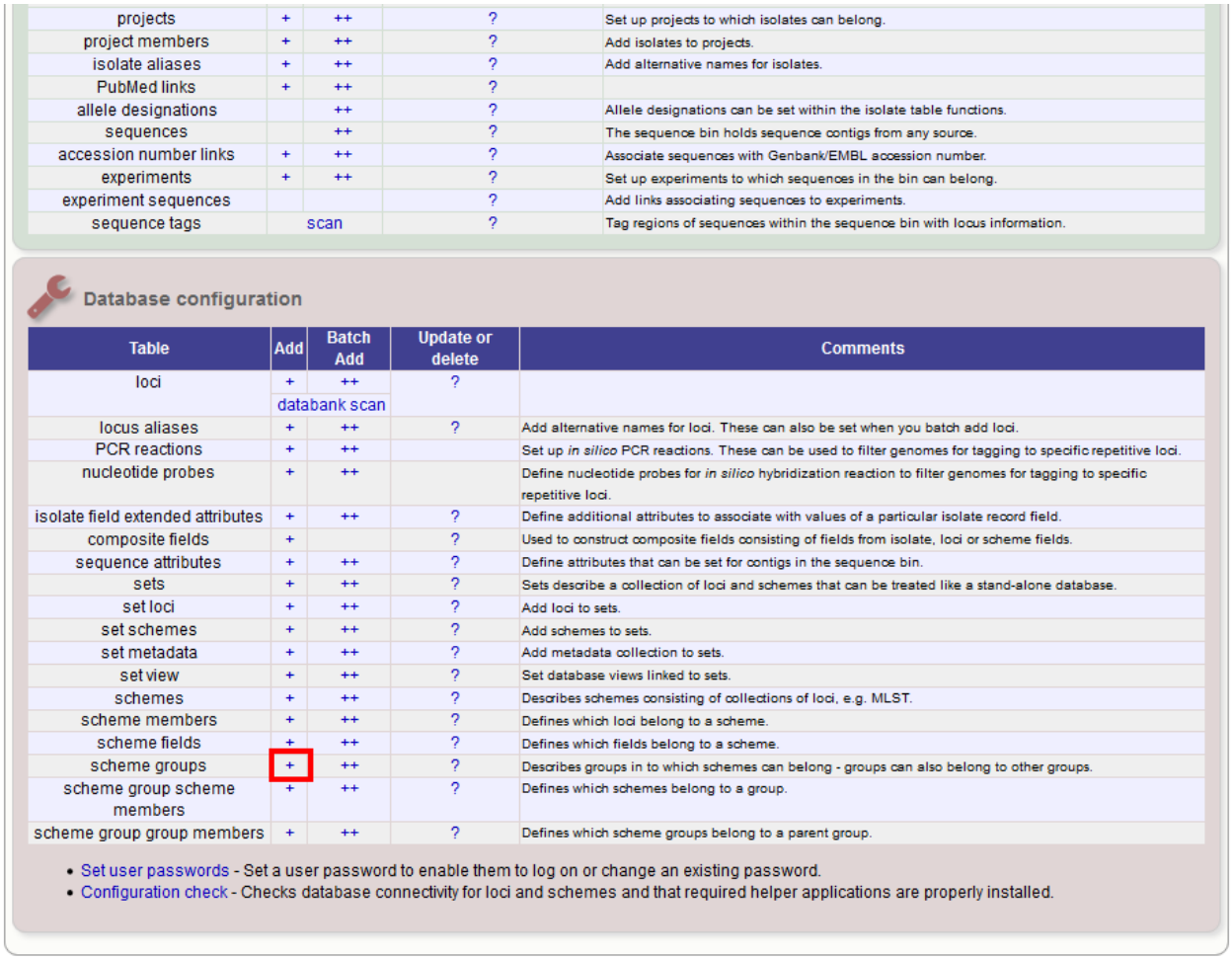
5.17 Organizing schemes into hierarchical groups

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

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



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 configuration

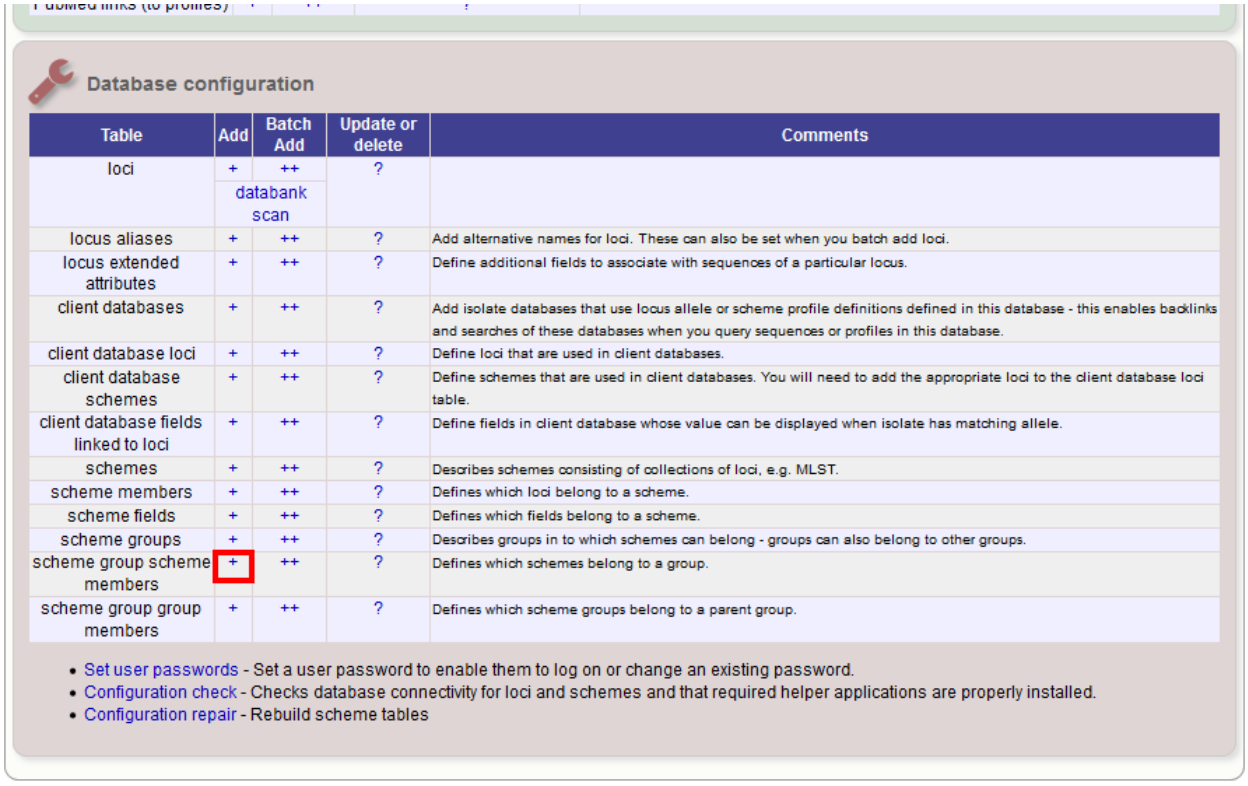
Table	Add	Batch Add	Update or delete	Comments
loci	+	++	?	
	databank scan			
locus aliases	+	++	?	Add alternative names for loci. These can also be set when you batch add loci.
PCR reactions	+	++		Set up *in silico* PCR reactions. These can be used to filter genomes for tagging to specific repetitive loci.
nucleotide probes	+	++		Define nucleotide probes for *in silico* hybridization reaction to filter genomes for tagging to specific repetitive loci.
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.
set view	+	++	?	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.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

- Set user passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

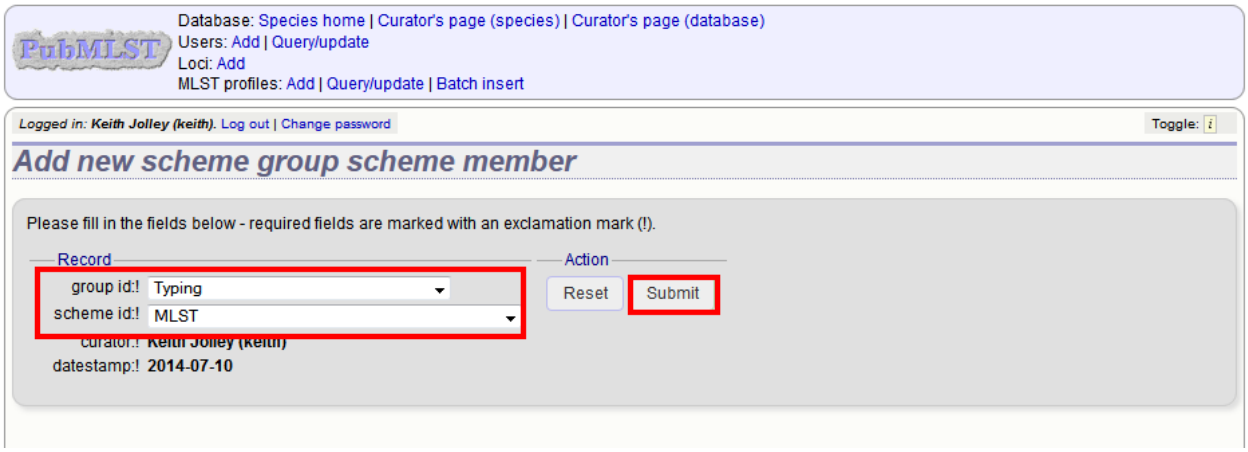
Enter a short name for the group - this will appear within drop-down list boxes and the hierarchical tree, so it needs to be fairly short.

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.



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



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

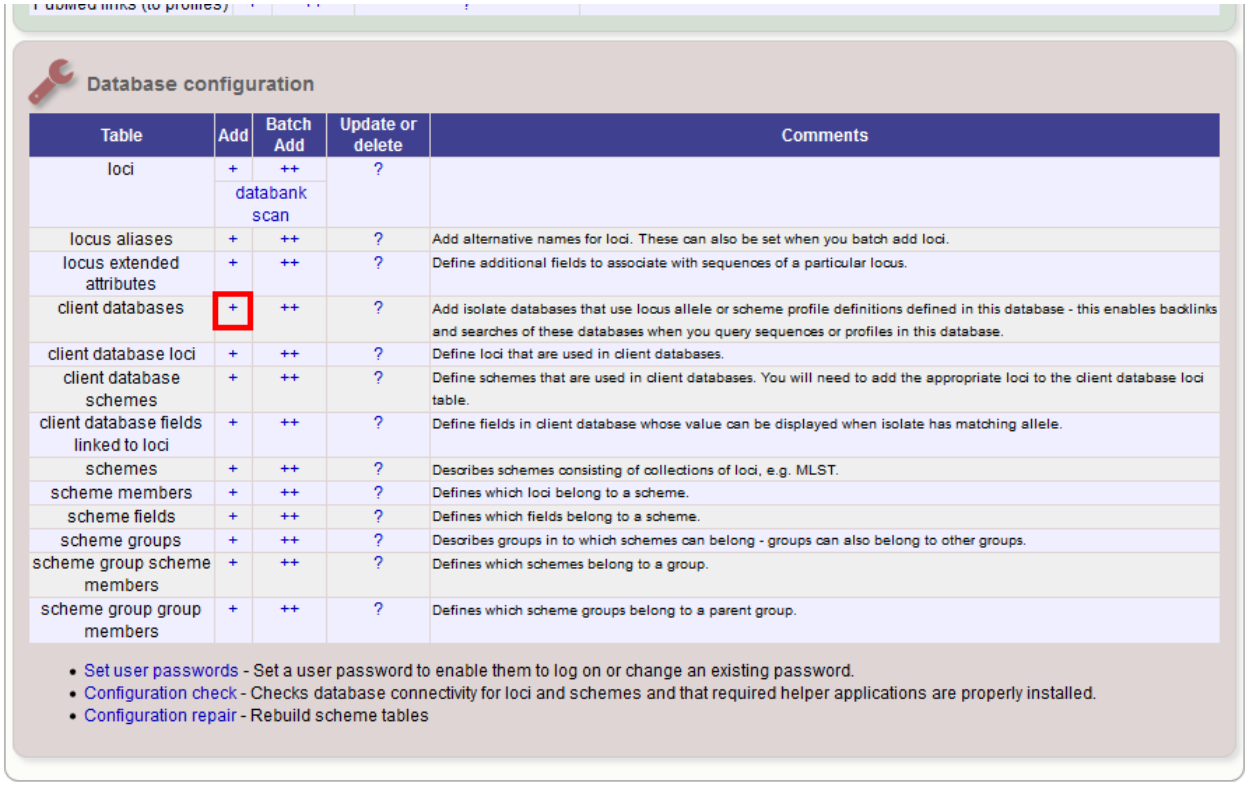
5.18 Setting up client databases

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

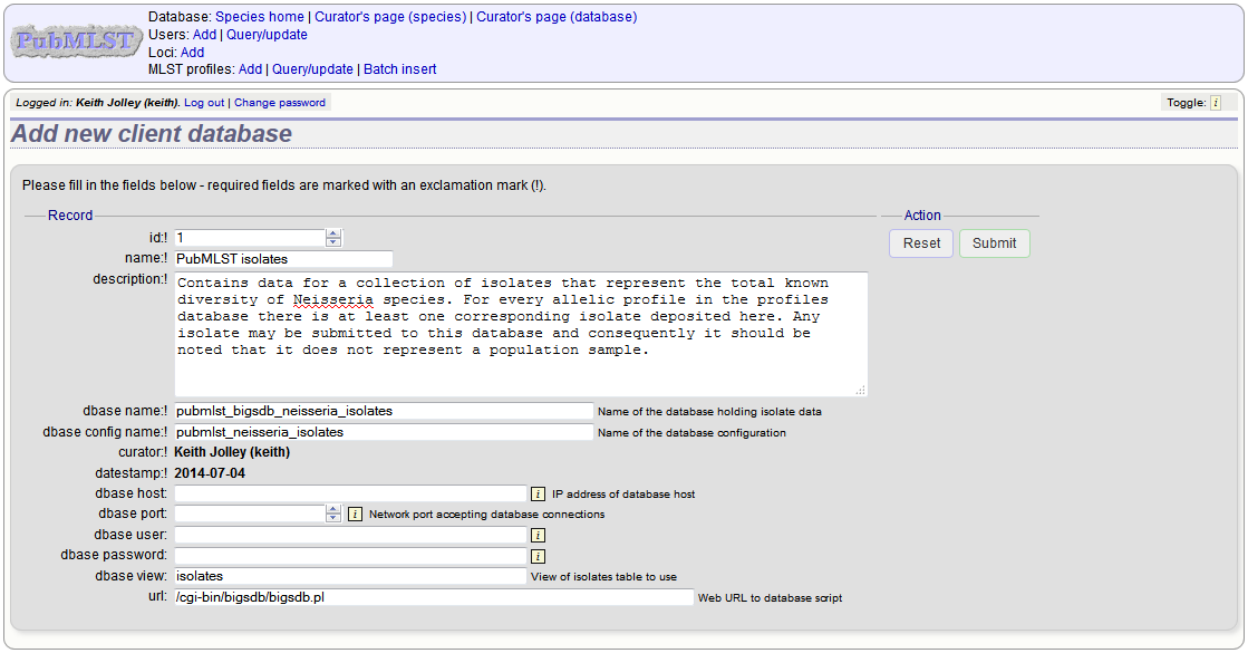
- Determine the number of isolates that a given allele is found in and link to these.
- Determine the number of isolates that a given scheme field, e.g. a sequence type, is found in and link to these.
- Retrieve specific attributes of isolates that have a given allele, e.g. species that have a particular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

Multiple client databases can be queried simultaneously.

To register a client isolate database for a sequence definition database, click the add (+) client database link on the curator's interface contents page.



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

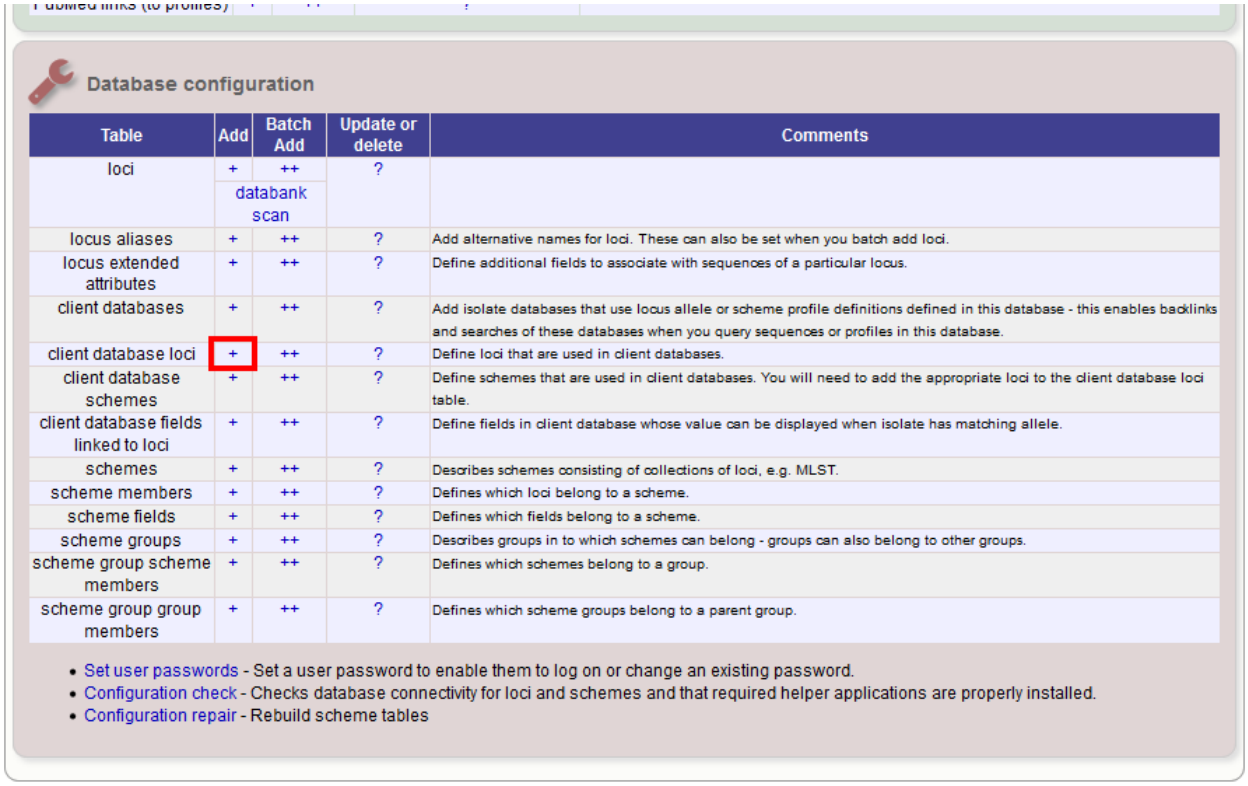


- id - Index number of client database. The next available number is entered automatically but can be overridden.
  - Allowed: any positive integer.
- name - Short description of database. This is used within the interface result tables so it is better to make it as short as possible.

  - 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.

5.18.1 Look up isolates with given allele

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



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

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

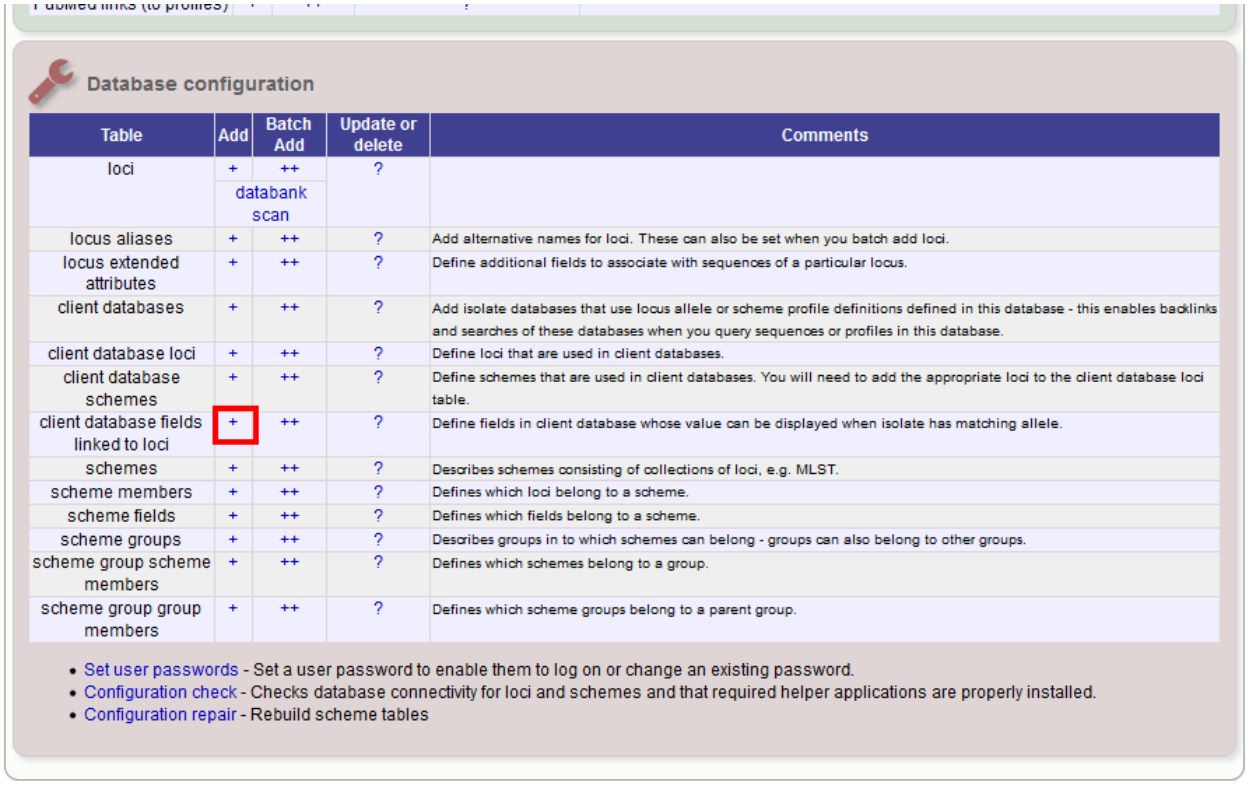
5.18.2 Look up isolates with a given scheme primary key

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

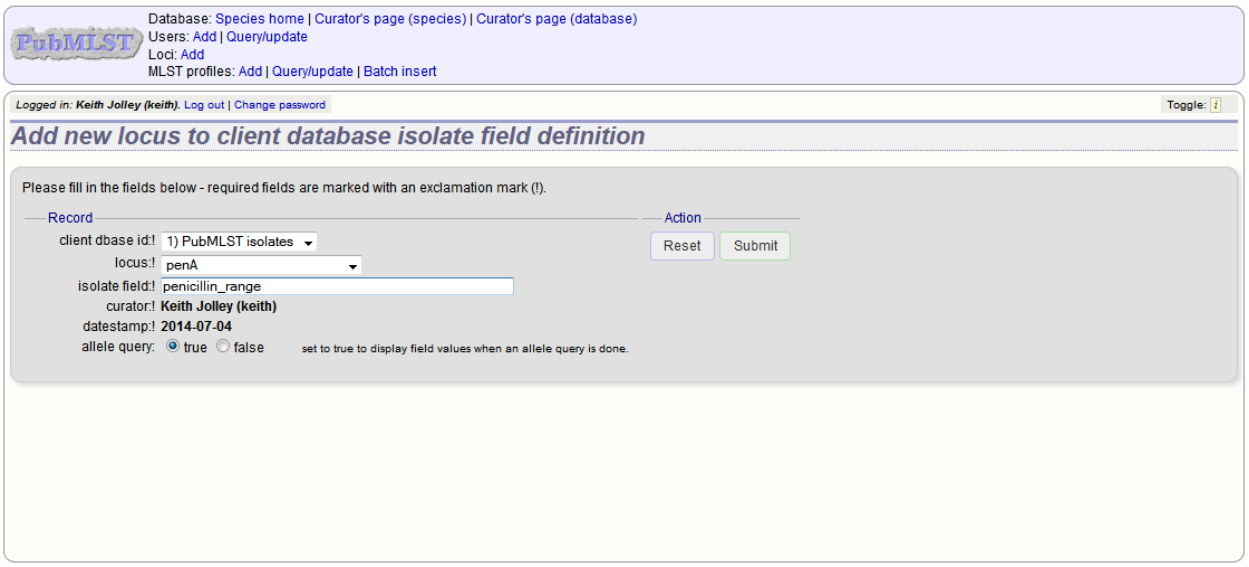
Now when information on a given scheme profile (e.g. MLST sequence type) is shown following a query, the software will list the number of isolates with that profile and link to a search on the database to retrieve these.

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

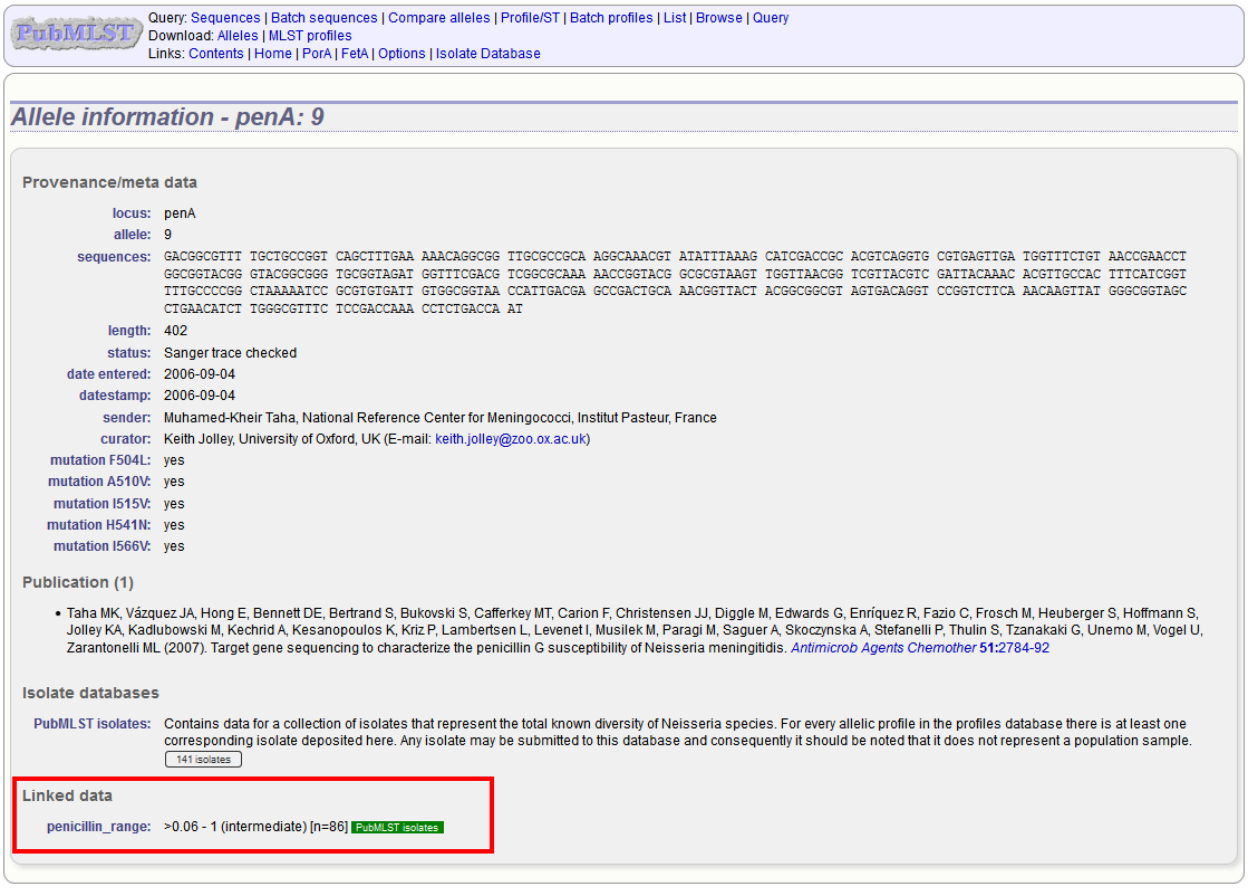
To link an allele to an isolate field, click the add (+) 'client database fields linked to loci' link on the curator's interface contents page.



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



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.



5.19 Rule-based sequence queries

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

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

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

5.19.1 Example rule code

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

The code for this rule is as follows:

```
#Clinical identification rule

#Update job viewer status
update_status({stage=>'Scanning MLST loci'});

#Scan genome against all scheme 1 (MLST) loci
scan_scheme(1);
```

```
#Update job viewer status
update_status({percent_complete=>30, stage=>'Scanning PorA and FetA VRs'});

#Scan genome against the PorA VR and FetA VR loci
scan_locus($_) foreach qw(PorA_VR1 PorA_VR2 FetA_VR);

Add text to main output
append_html("<h1>Strain type</h1>");

#Set variables for the scanned results.  These can be found in the
#$results->{'locus'} hashref
my %alleles;
$alleles{$_} = $results->{'locus'}->{$_} // 'ND' foreach qw(PorA_VR1 PorA_VR2);
$alleles{'FetA_VR'} = $results->{'locus'}->{'FetA_VR'} // 'F-ND';

#Scheme field values are automatically determined if a complete
#profile is available.  These are stored in the $results->{'scheme'} hashref
my $st = $results->{'scheme'}->{1}->{'ST'} // 'ND';
append_html("<ul><li>P1.$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("($cc)</li></ul>");
if ($st eq 'ND'){
  append_html("<p>ST not defined.  If individual MLST loci have been found "
  . "they will be displayed below:</p>");

  #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><ul>");
  if (defined $results->{'locus'}->{'penA'}){
    append_html("<li><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("</li>");
  }
```

```
  if (defined $results->{'locus'}->{'rpoB'}){
    append_html("<li><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("</li>");
  }
  append_html("</ul>");
}
```

5.19.1.1 Rule files

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

5.19.1.2 Linking to the rule query

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

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

To place a link to this within the database contents page an HTML file called job_query.html can be placed in a contents directory within the database configuration directory, e.g. in /etc/bigsdb/dbases/pubmlst_neisseria_seqdef/contents/job_query.html. This file should contain a list entry (i.e. surrounded with <li> and tags) that will appear in the 'Query database' section of the contents page.

5.19.1.3 Adding descriptive text

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

5.20 Workflow for setting up a MLST scheme

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

Seqdef database

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

Isolate database

1. Create the same loci with the following additional parameters (example locus 'atpD')

- dbase_name: seqdef_db
- dbase_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_id: 1 (or whatever the id of your seqdef scheme is)

3. Add scheme_field ST as before
4. Add loci as scheme_members

5.21 Automated assignment of scheme profiles

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

The script is run as follows:

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

A full list of options can be found by typing:

```
define_profiles.pl --help
NAME
    define_profiles.pl - Define scheme profiles found in isolate database

SYNOPSIS
    define_profiles.pl --database NAME --scheme SCHEME_ID [options]

OPTIONS

--cache
    Update scheme field cache in isolate database.

--database NAME
    Database configuration name.

--help
    This help page.

--exclude_isolates LIST
    Comma-separated list of isolate ids to ignore.

--exclude_projects LIST
    Comma-separated list of projects whose isolates will be excluded.

--ignore_multiple_hits
```

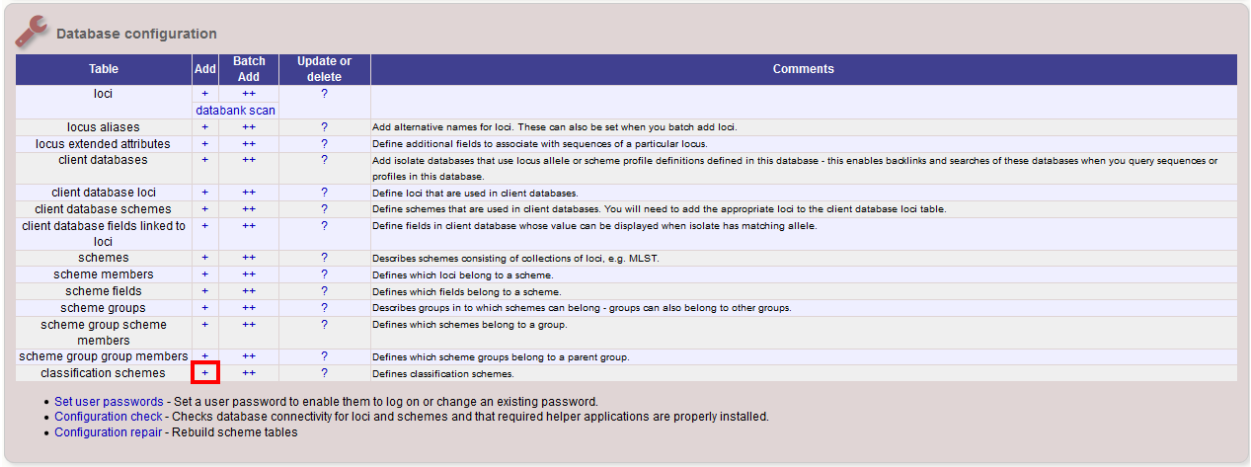
```
    Set allele designation to 'N' if there are multiple designations set for
    a locus. The default is to use the lowest allele value in the profile
    definition.

--isolates LIST
    Comma-separated list of isolate ids to scan (ignored if -p used).

--isolate_list_file FILE
    File containing list of isolate ids (ignored if -i or -p used).

--match_missing
    Treat missing loci as specific alleles rather than 'any'. This will
    allow profiles for every isolate that has <= threshold of missing alleles
    to be defined but may result in some isolates having >1 ST.

--max ID
    Maximum isolate id.

--min ID
    Minimum isolate id.

--min_size SIZE
    Minimum size of seqbin (bp) - limit search to isolates with at least this
    much sequence.

--missing NUMBER
    Set the number of loci that are allowed to be missing in the profile. If
    the remote scheme does not allow missing loci then this number will be set
    to 0.  Default=0.

--projects LIST
    Comma-separated list of project isolates to scan.

--scheme SCHEME_ID
    Scheme id number.
```

5.22 Scheme profile clustering - setting up classification schemes

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

5.22.1 Defining classification scheme in sequence definition database

Once a scheme has been defined, add a classification scheme by clicking the add classification schemes (+) link on the curator's interface contents page.



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

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

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

rather than

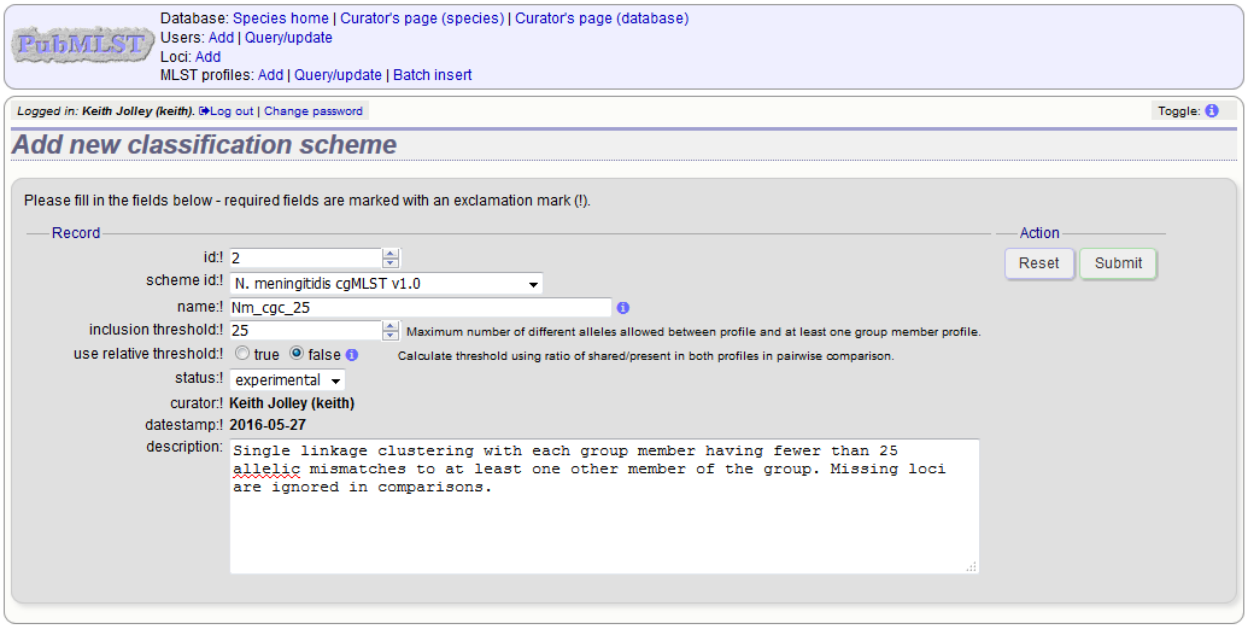
```
total loci - defined threshold
```

when an absolute threshold is used.

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

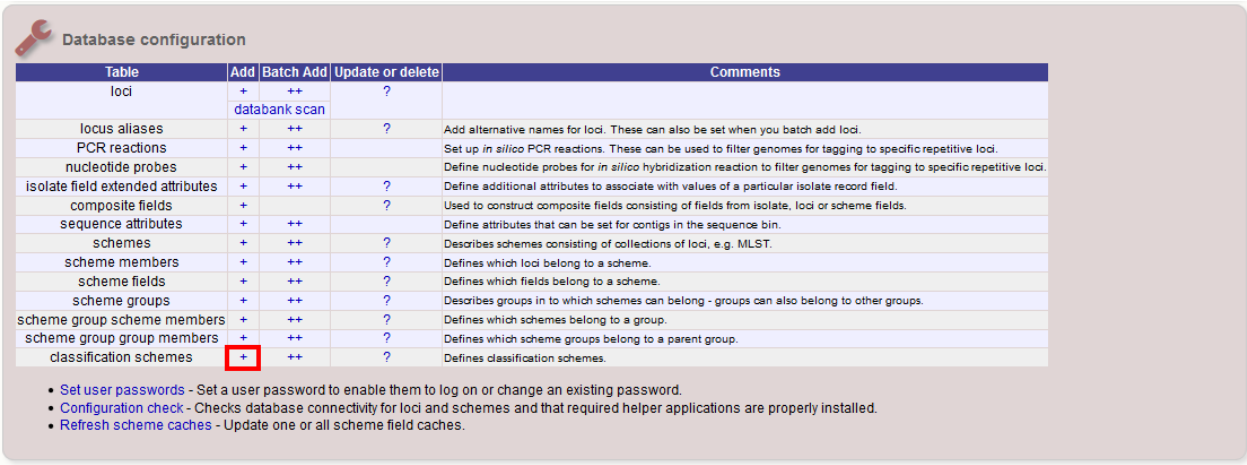
The status can be 'experimental' or 'stable'. The status of a scheme will be shown in the web interface to indicate that any groupings are subject to change and do not form part of the stable nomenclature.

Press 'Submit' to create the classification scheme.



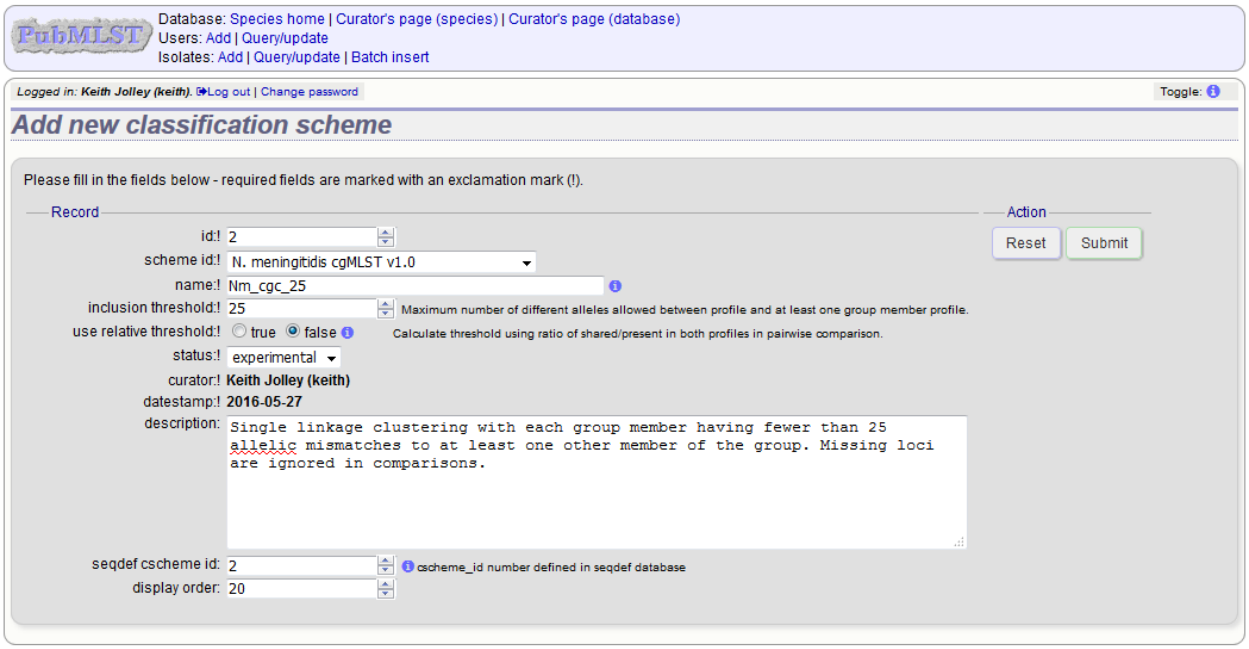
5.22.2 Defining classification scheme in isolate database

Duplicate the scheme definition from the sequence definition database. Click the add classification schemes (+) link on the curator's interface contents page.



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

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



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

5.22.3 Clustering

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

Currently only single-linkage clustering is supported.

The script is run as follows from the command line:

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

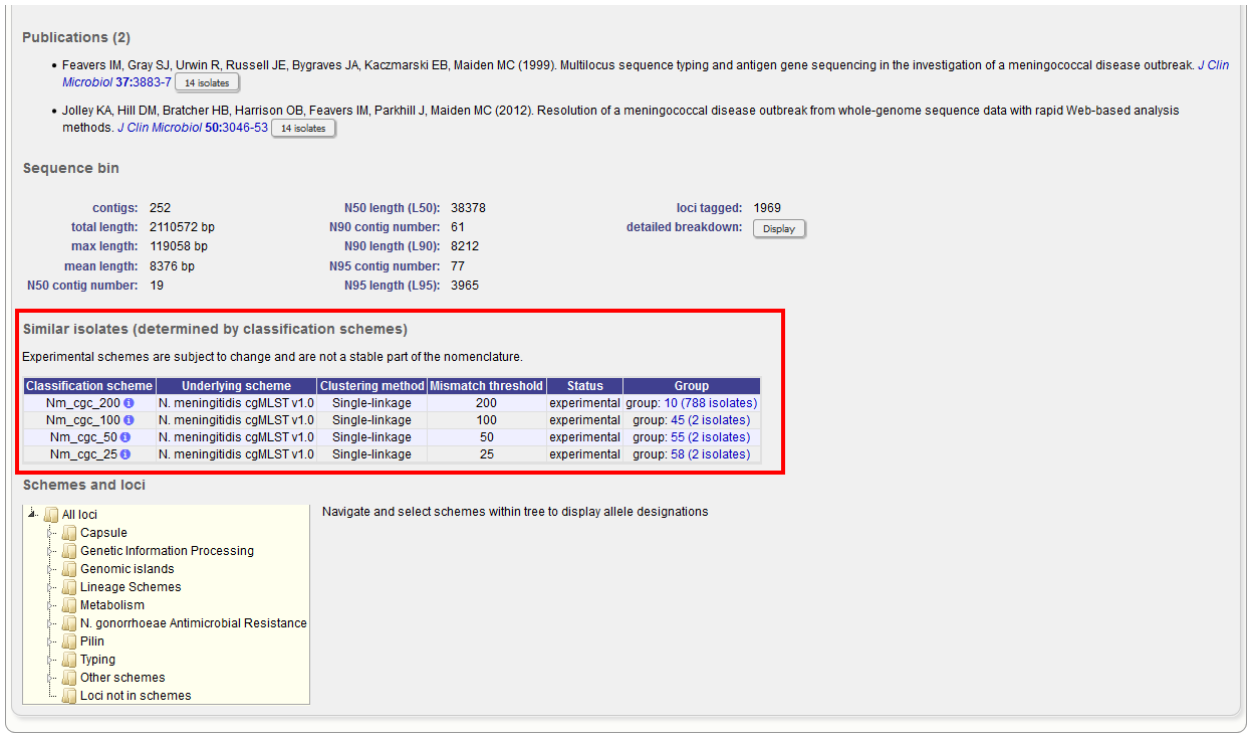
A full list of options can be found by typing:

```
cluster.pl --help
NAME
    cluster.pl - Cluster cgMLST profiles using classification groups.

SYNOPSIS
    cluster.pl --database NAME --cscheme_id SCHEME_ID [options]

OPTIONS

--cscheme CLASSIFICATION_SCHEME_ID
    Classification scheme id number.

--database NAME
    Database configuration name.

--help
    This help page.
```

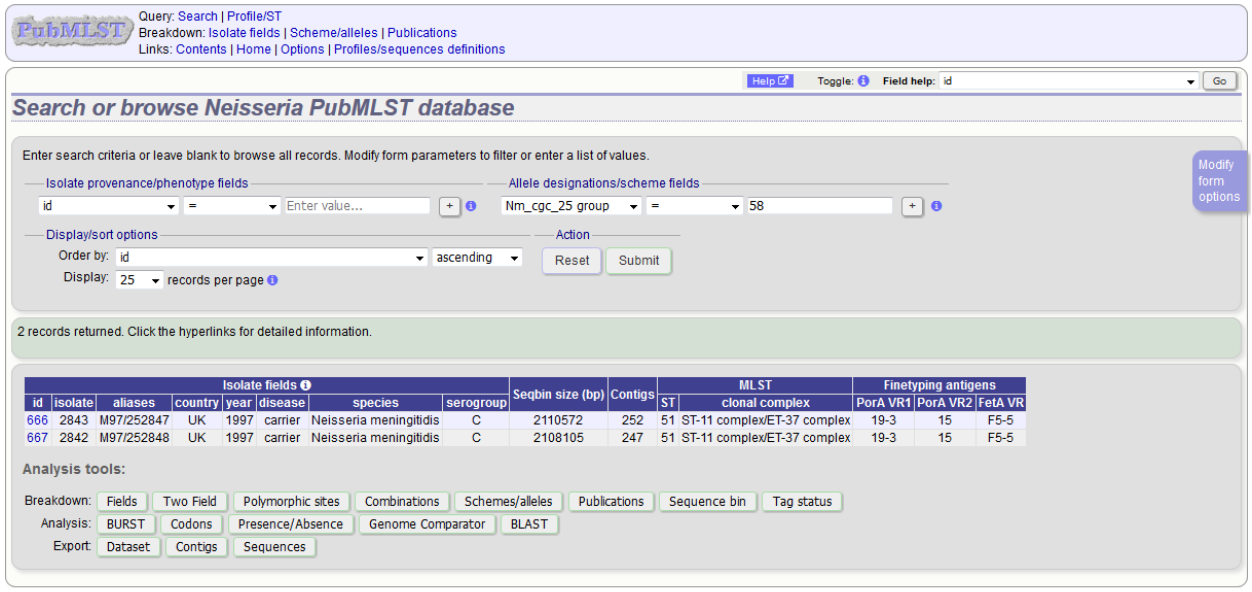
```
--reset
    Remove all groups and profiles currently defined for classification group.
```

Note: Note that for classification schemes to be accessible within the isolate database, *scheme cache tables* must be generated and kept up-to-date.

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



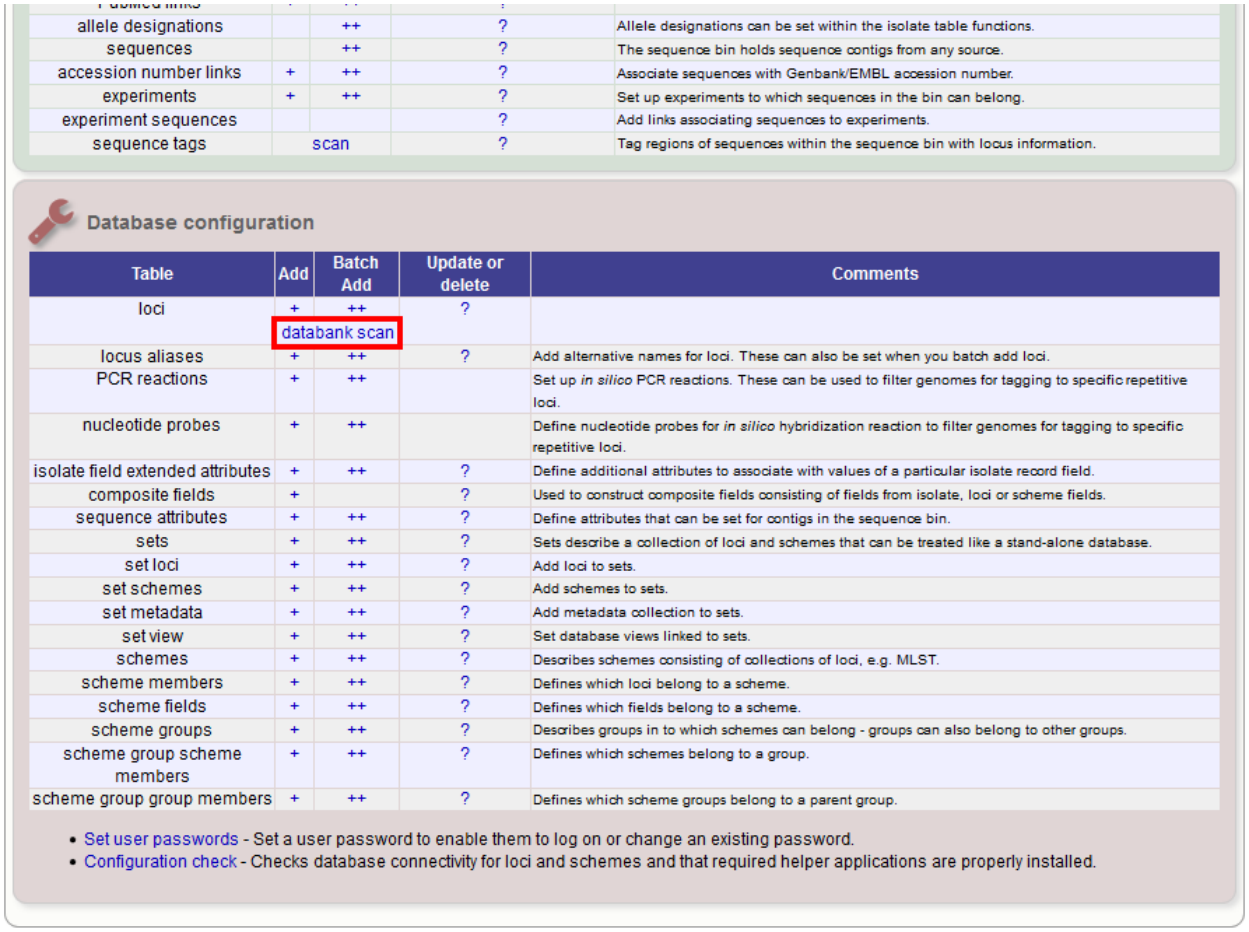
Clicking the hyperlinks will take you to a table containing matching isolates, from where standard analyses can be performed.



5.23 Defining new loci based on annotated reference genome

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

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



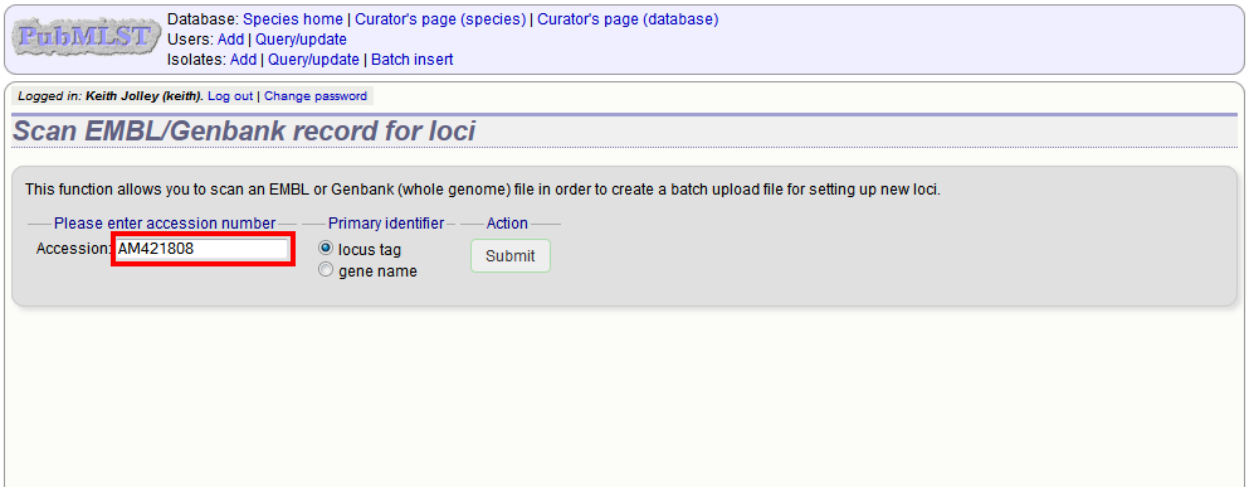
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences		++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences 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

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.
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.
set view	+	++	?	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.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

- Set user passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

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



PubMLST

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

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

Scan EMBL/Genbank record for loci

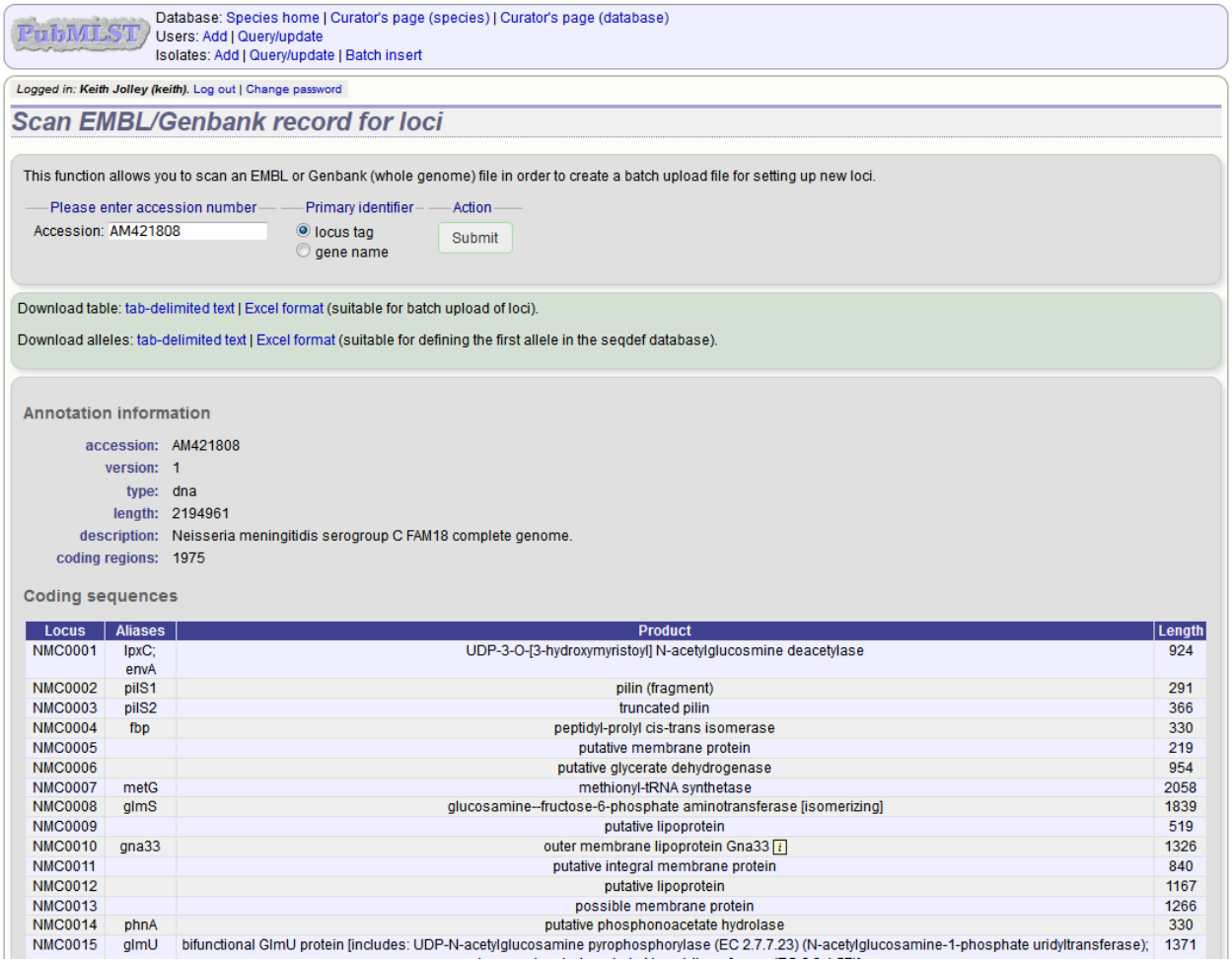
This function allows you to scan an EMBL or Genbank (whole genome) file in order to create a batch upload file for setting up new loci.

Please enter accession number — Accession: AM421808

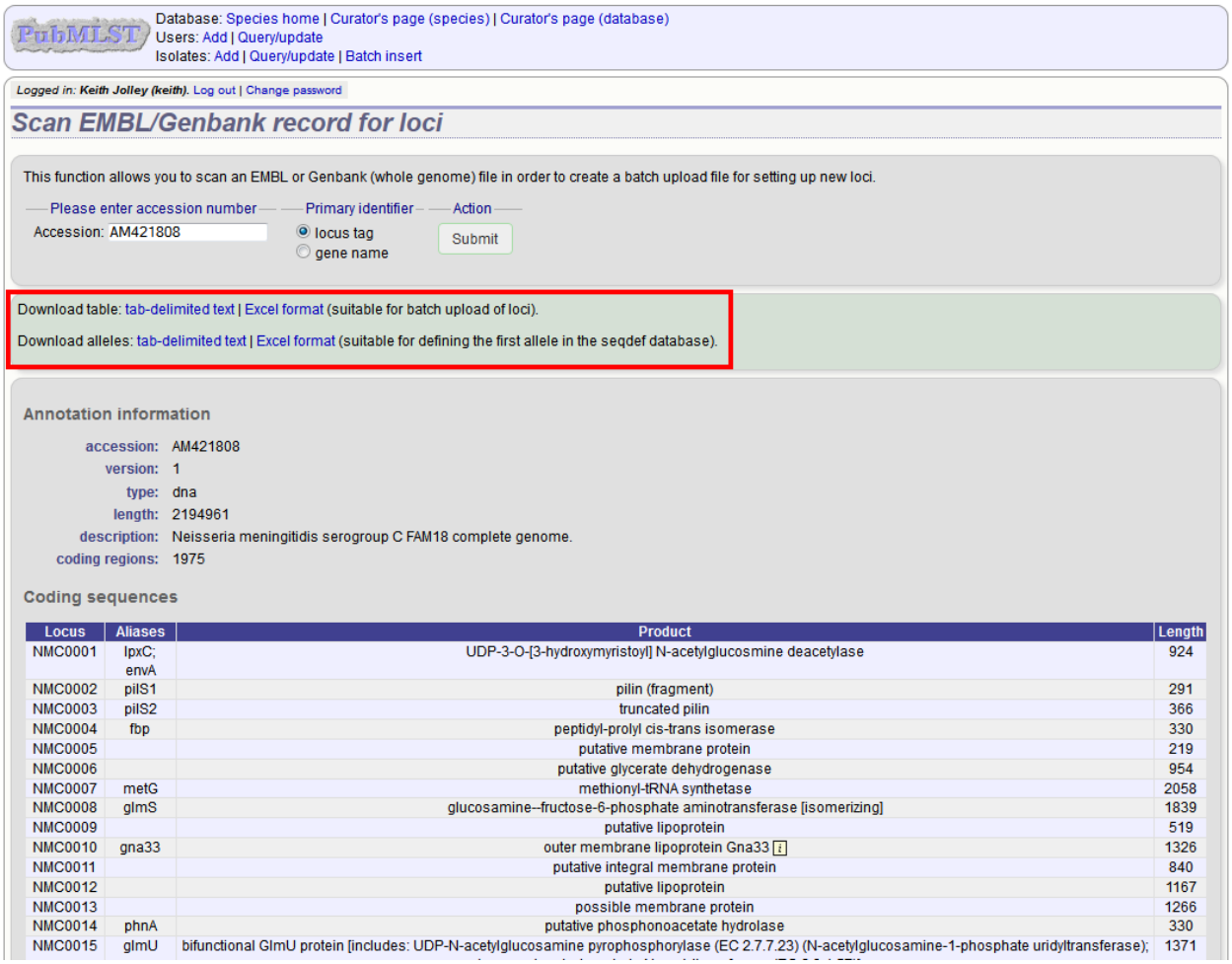
Primary identifier — locus tag / gene name

Action — Submit

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



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.



5.24 Genome filtering

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

5.24.1 Filtering by *in silico* PCR

Provided a locus can be predicted to be specifically amplifed by a PCR reaction, the genome can be filtered to only look at regions 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.

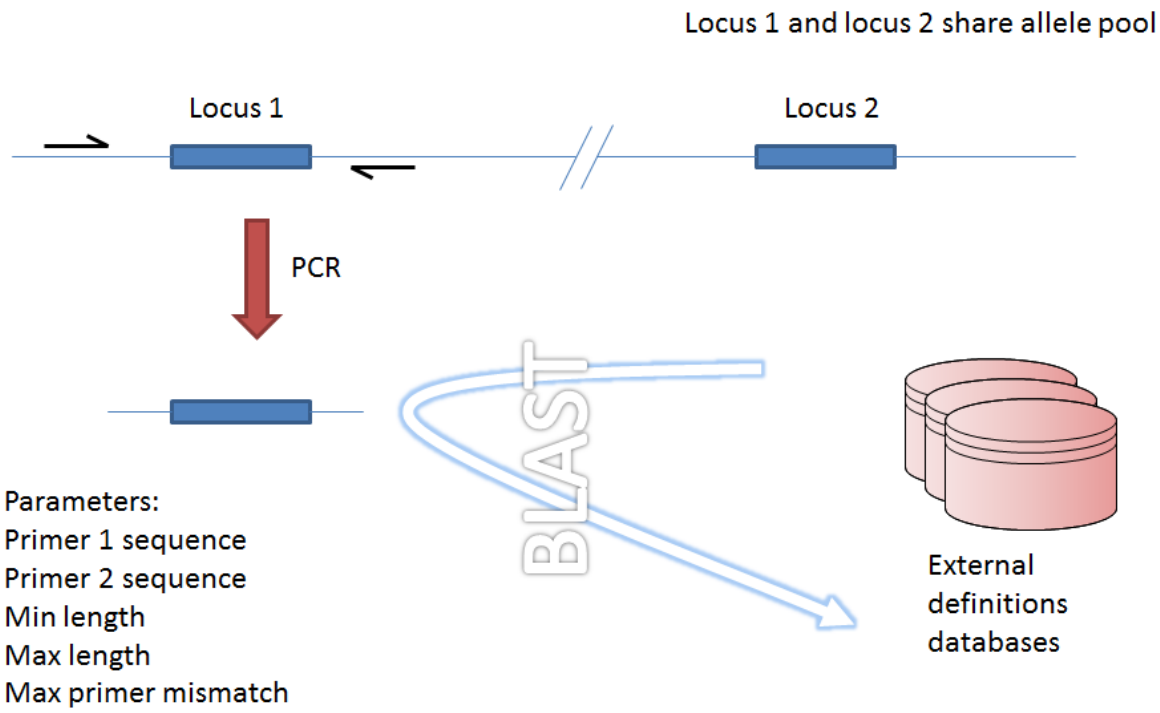


Fig. 5.1: Genome filtering by *in silico* PCR.

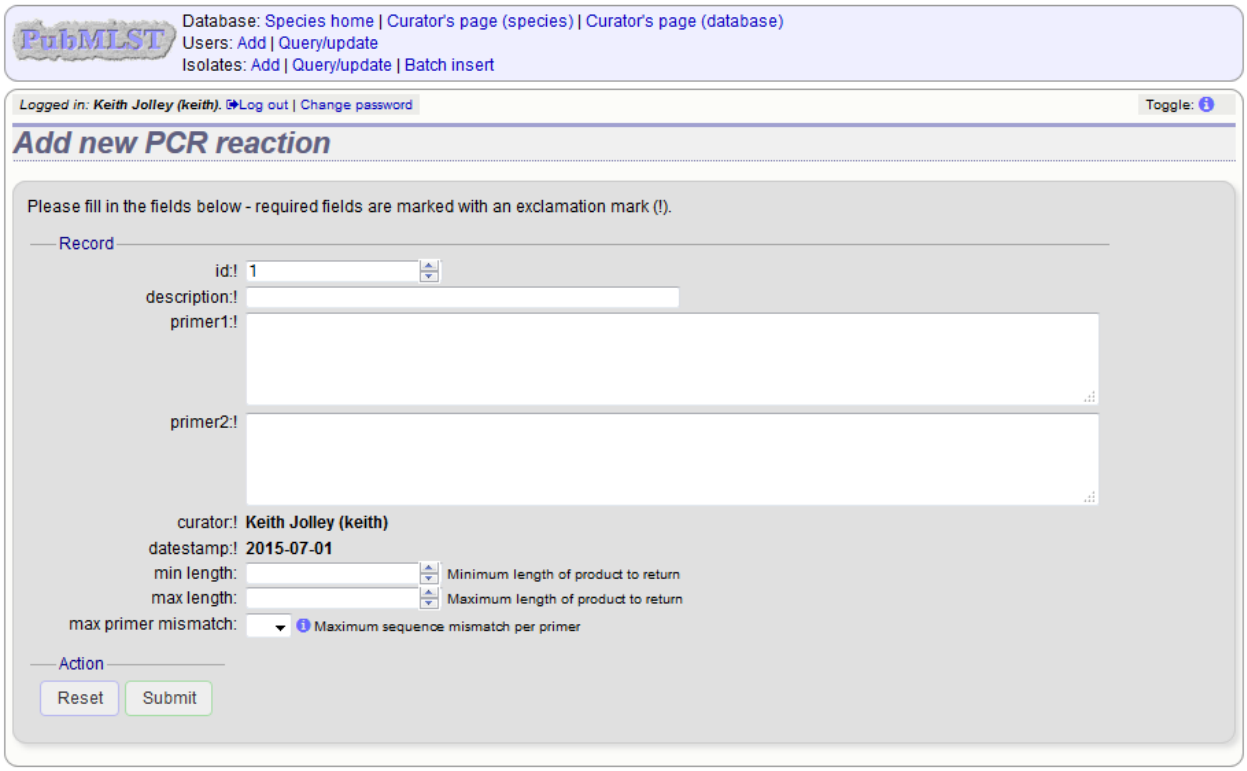
allele designations		++	?	Allele designations can be set within the isolate table functions.
sequences		++	?	The sequence bin holds sequence contigs from any source.
accession number links	+	++	?	Associate sequences with Genbank/EMBL accession number.
experiments	+	++	?	Set up experiments to which sequences 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

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.
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.
set view	+	++	?	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.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

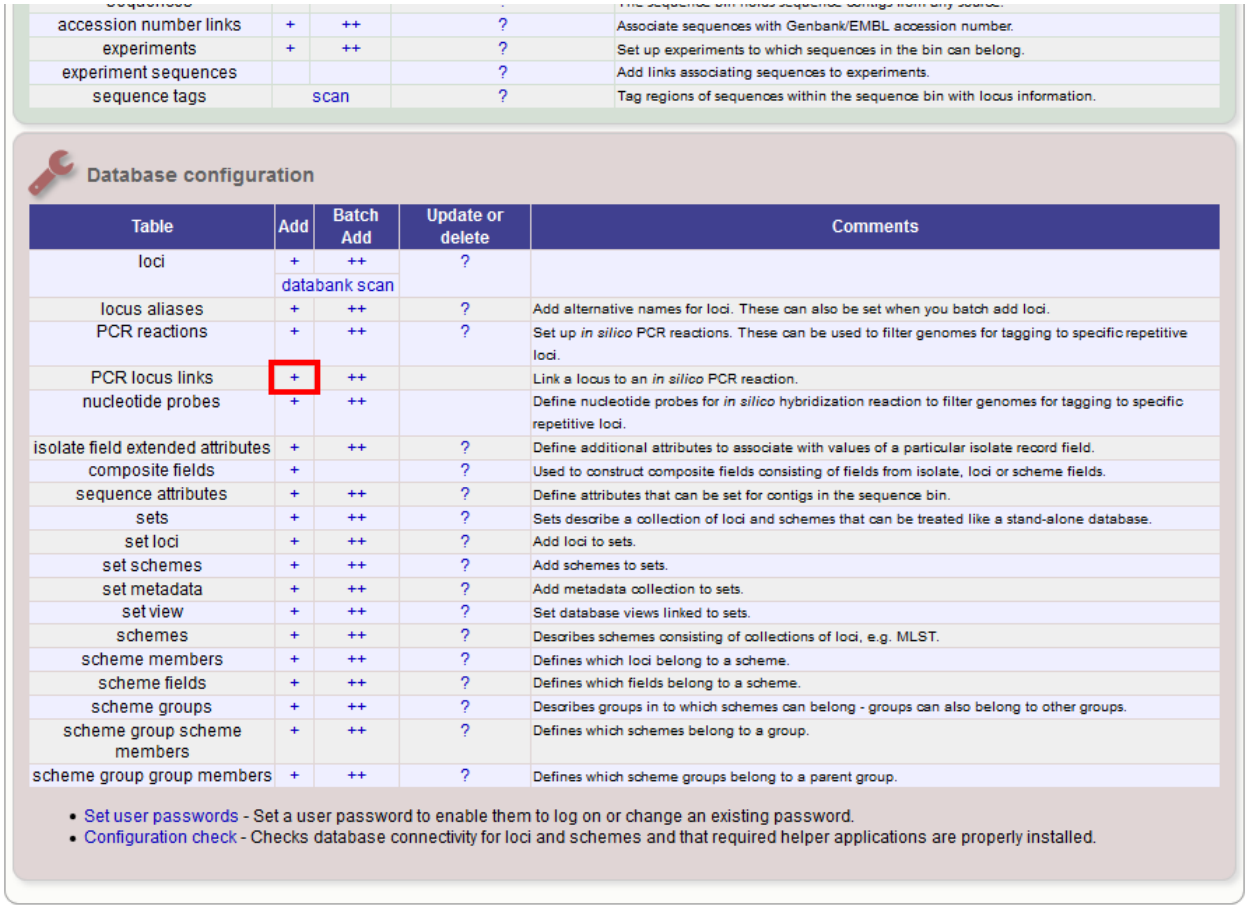
- Set user passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

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.



- 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.



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

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.
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.
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.
set view	+	++	?	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.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

- Set user passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci 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.

5.24.2 Filtering by *in silico* hybridization

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

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.

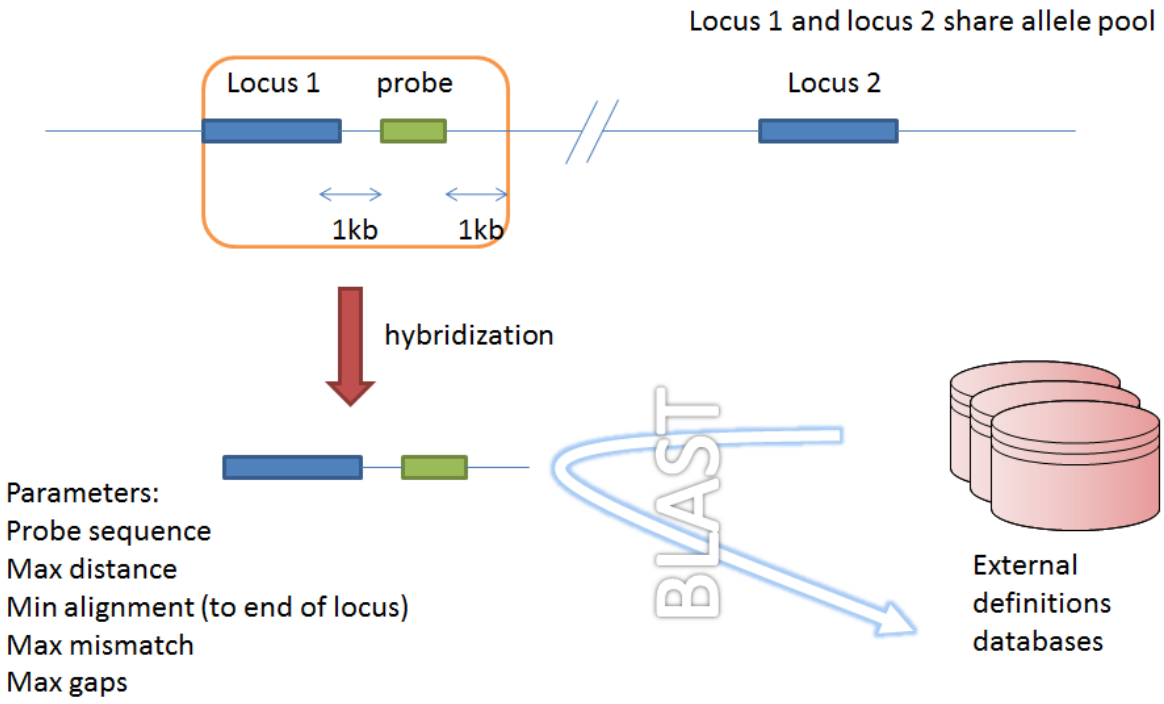


Fig. 5.2: Filtering by *in silico* hybridization

  - 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.

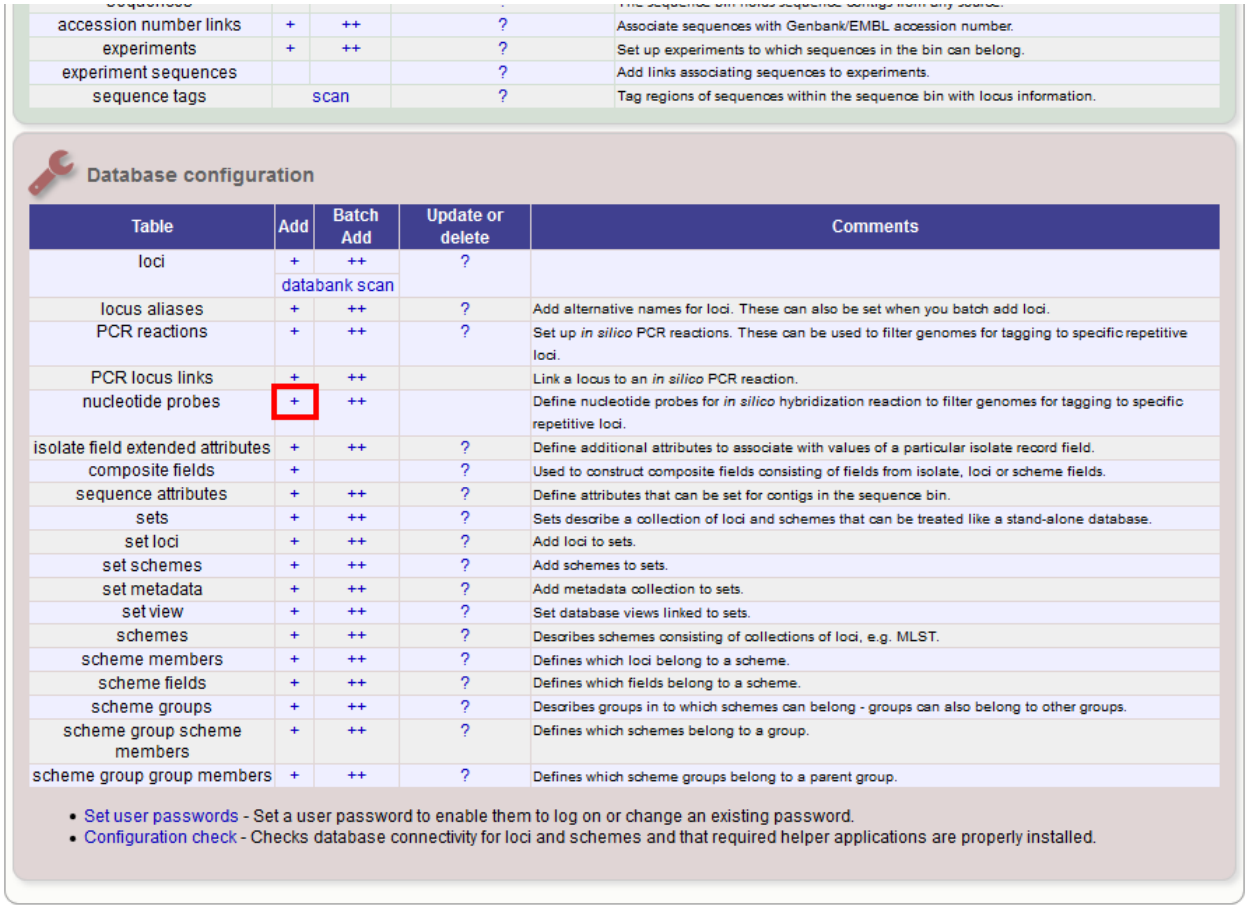
Finally edit the locus table and set the probe_filter field for the specified locus to 'true'.

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

5.25 Setting locus genome positions

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

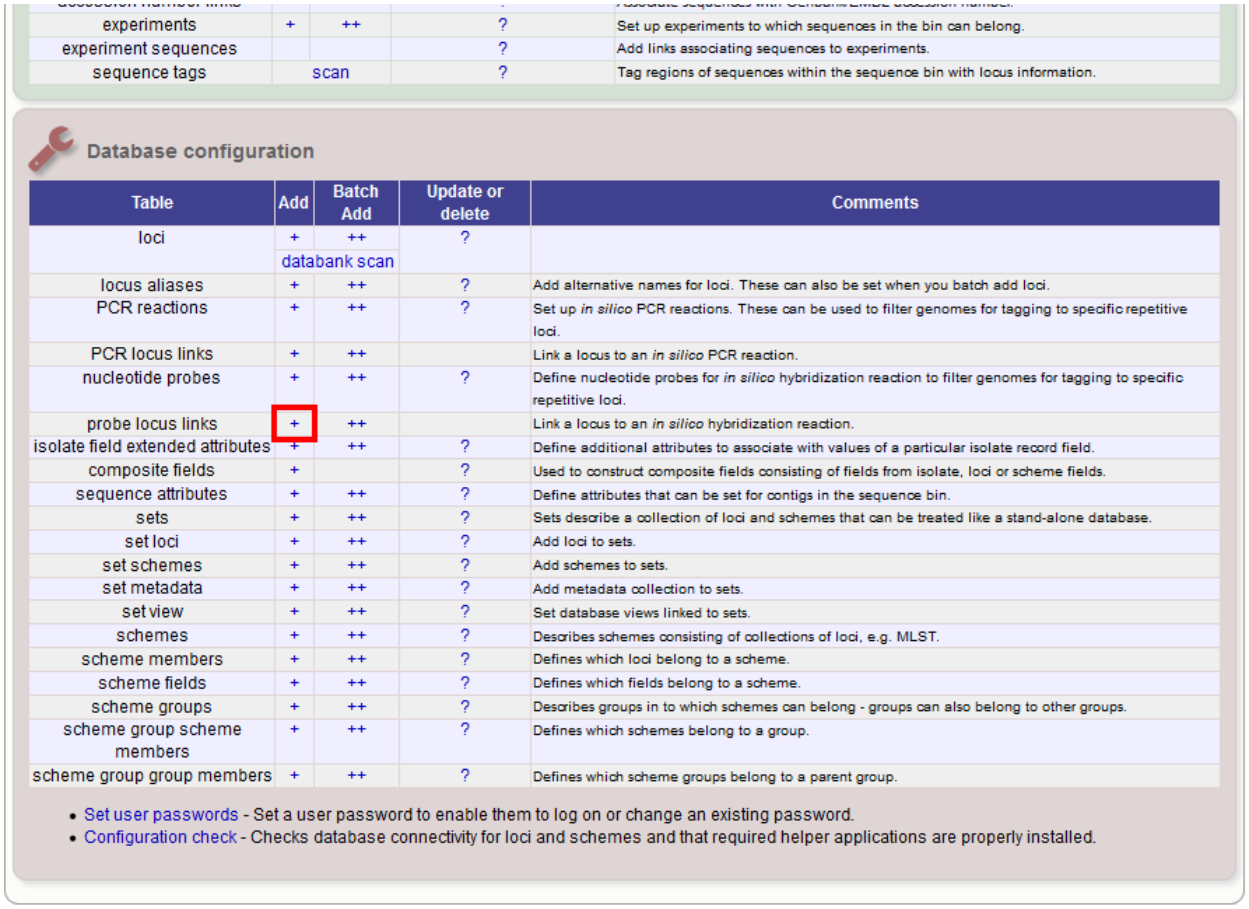
From the curator's main page, you need to do a query to find the isolate that you will base your numbering on. Click 'isolate query' to take you to a standard query form.



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.

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.
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.
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.
set view	+	++	?	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.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

- Set user passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

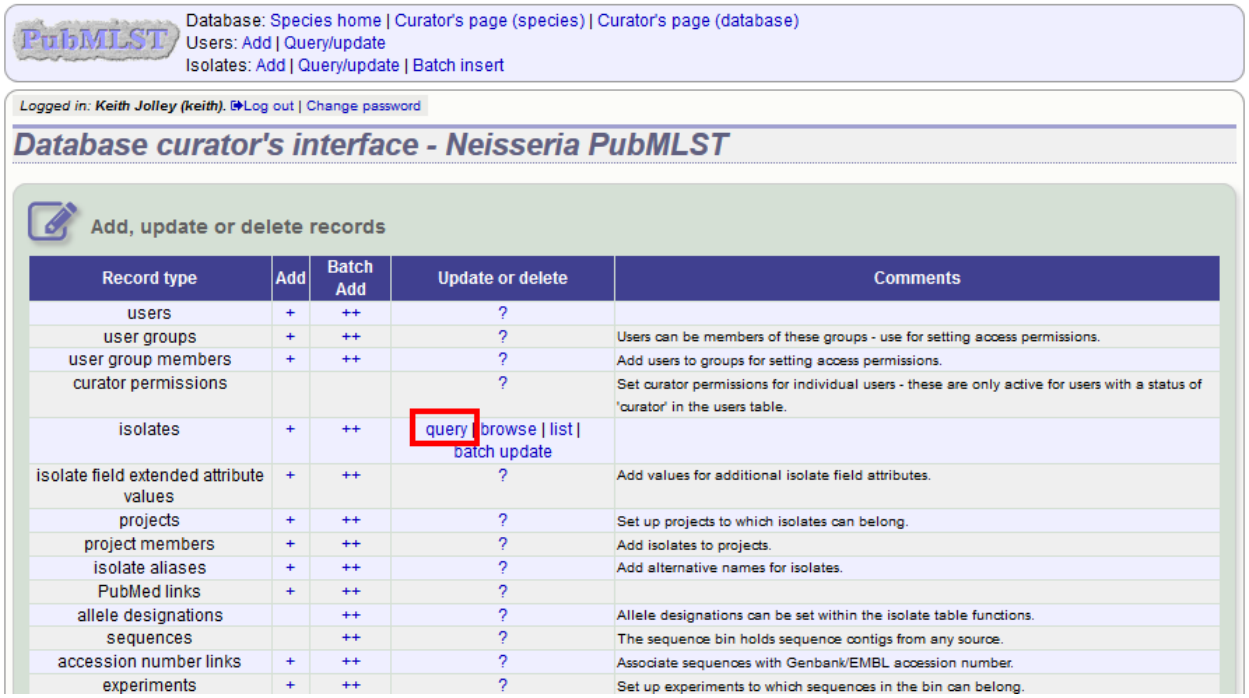


experiments	+	++	?	Set up experiments to which sequences in the bin can belong.
experiment sequences			?	Add links associating sequences to experiments.
sequence tags		scan	?	Tag regions of sequences within the sequence bin with locus information.

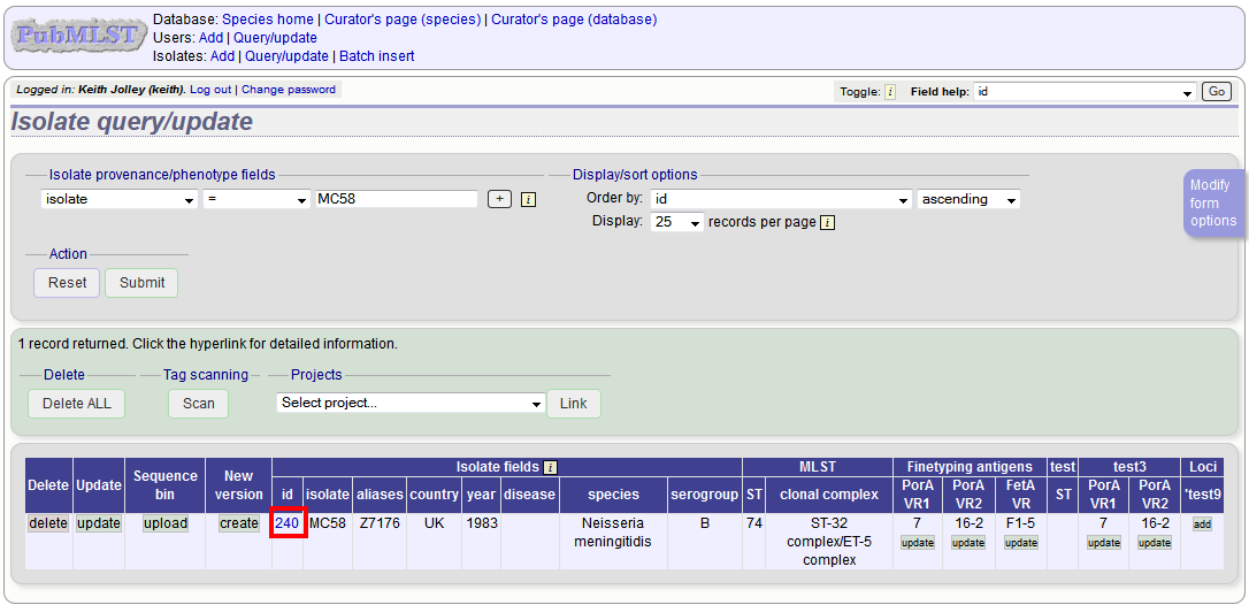
Database configuration

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.
PCR locus links	+	++		Link a locus to an *in silico* PCR reaction.
nucleotide probes	+	++	?	Define nucleotide probes for *in silico* hybridization reaction to filter genomes for tagging to specific repetitive loci.
probe locus links	+	++		Link a locus to an *in silico* hybridization reaction.
isolate field extended attributes	+	++	?	Define additional attributes to associate with values of a particular isolate record field.
composite fields	+		?	Used to construct composite fields consisting of fields from isolate, loci or scheme fields.
sequence attributes	+	++	?	Define attributes that can be set for contigs in the sequence bin.
sets	+	++	?	Sets describe a collection of loci and schemes that can be treated like a stand-alone database.
set loci	+	++	?	Add loci to sets.
set schemes	+	++	?	Add schemes to sets.
set metadata	+	++	?	Add metadata collection to sets.
set view	+	++	?	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.
scheme group group members	+	++	?	Defines which scheme groups belong to a parent group.

- Set user passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

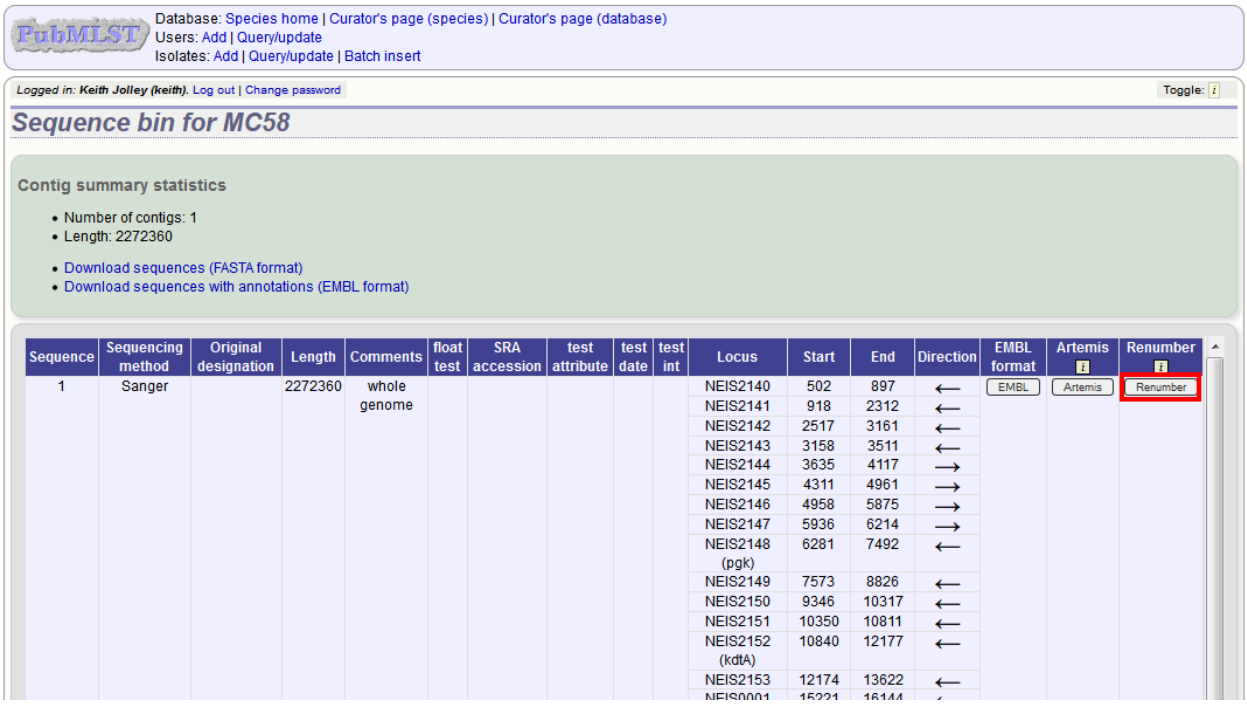


Perform your search and click the hyperlinked id number of the record.

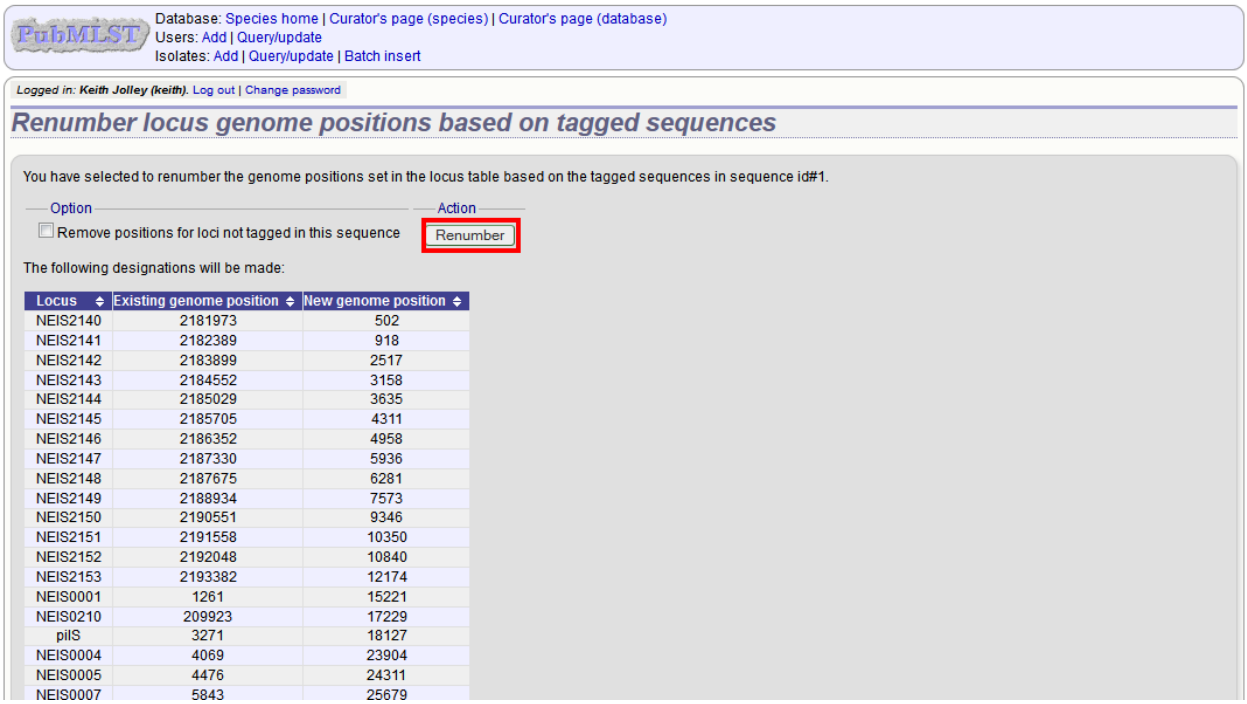


In the isolate record, click the sequence bin 'Display' button to bring up details of the isolate contigs.

Click the 'Renumber' button:



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



5.26 Defining composite fields

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

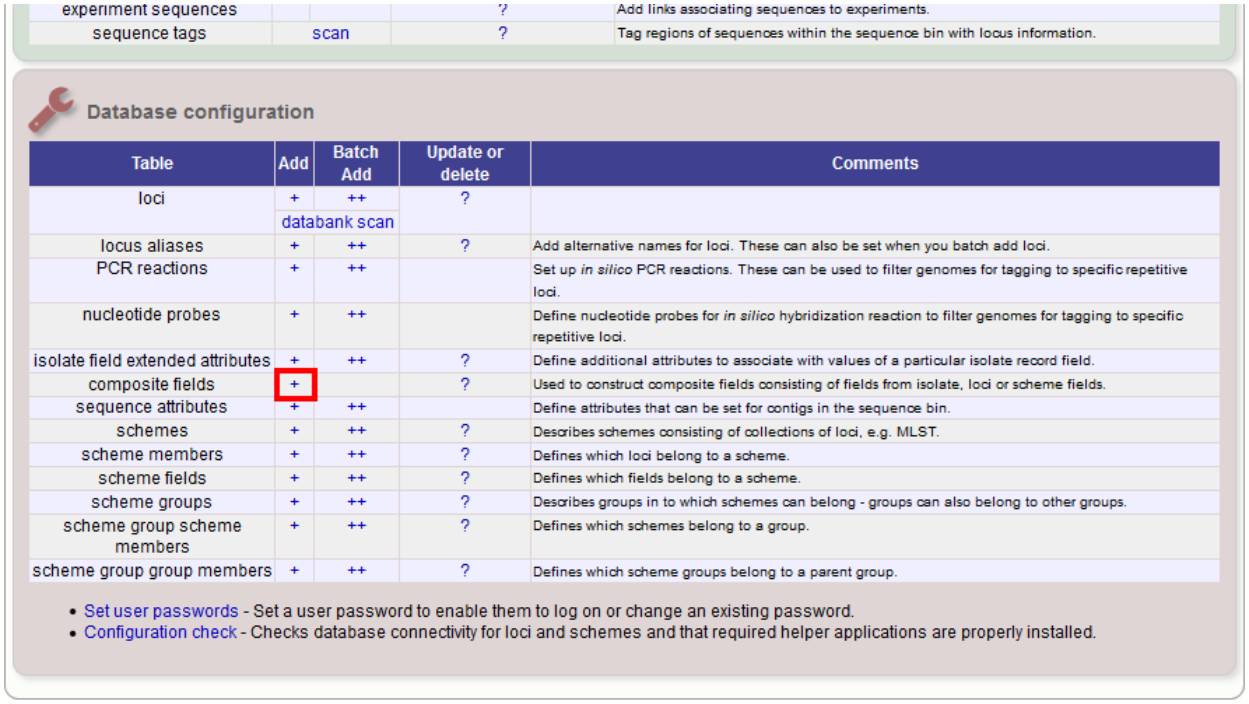
One example of a composite field is used in the Neisseria PubMLST database which has a strain designation composite field made up of serogroup, PorA VR1 and VR2, FetA VR, ST and clonal complex designations in the format:

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

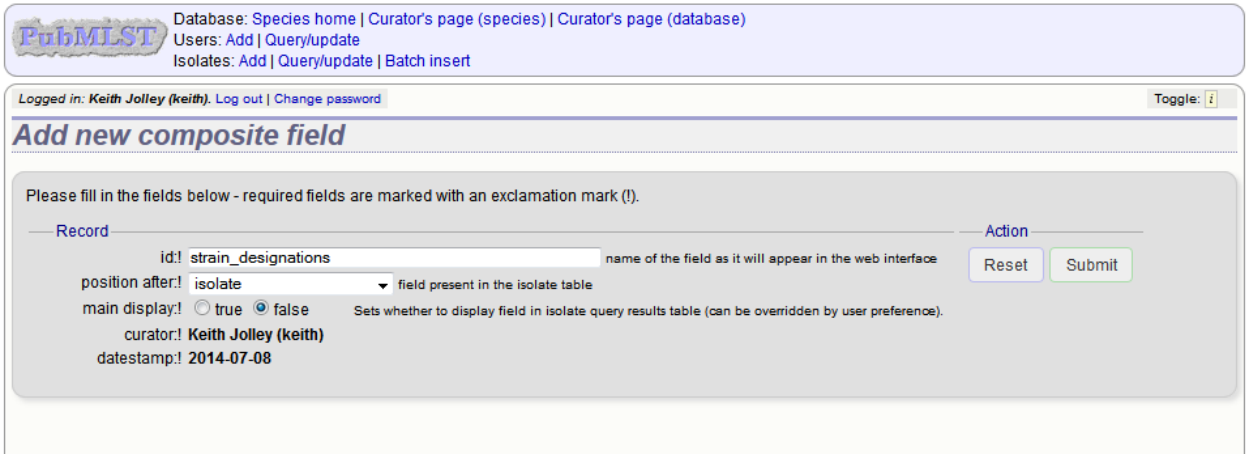
e.g. A: P1.5-2,10: F1-5: ST-4 (cc4)

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

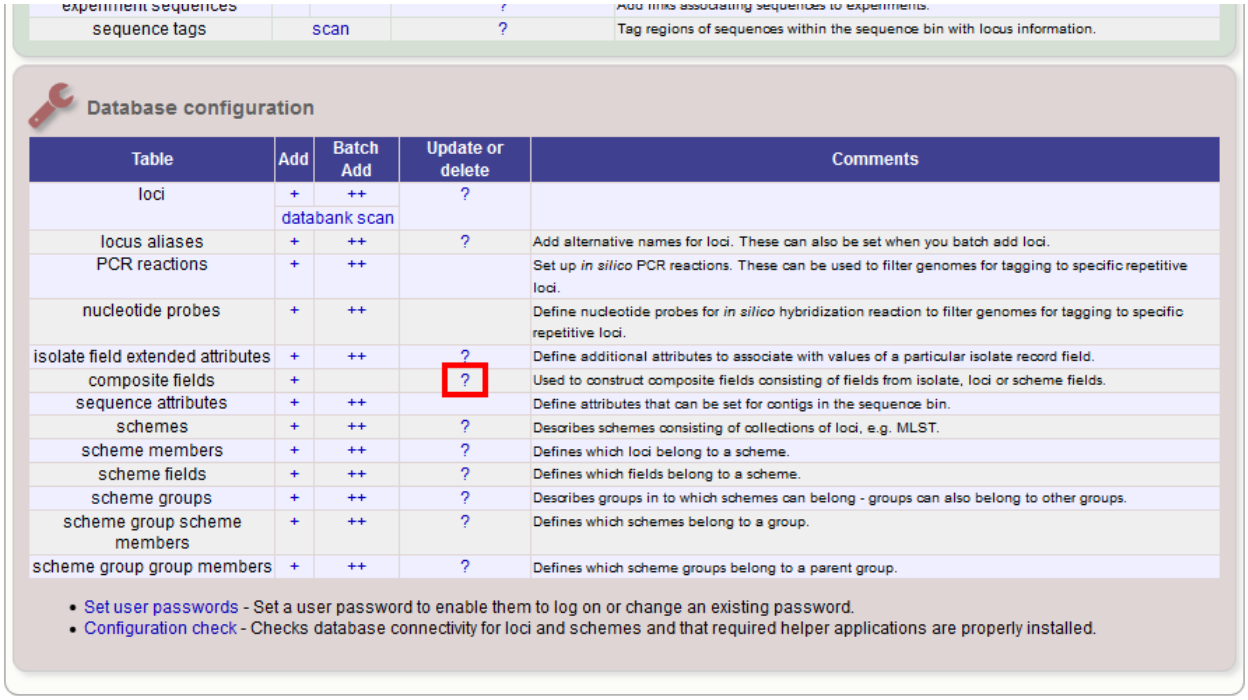
Composite fields can be added to the database by clicking the add (+) composite fields link on the curator's main page.



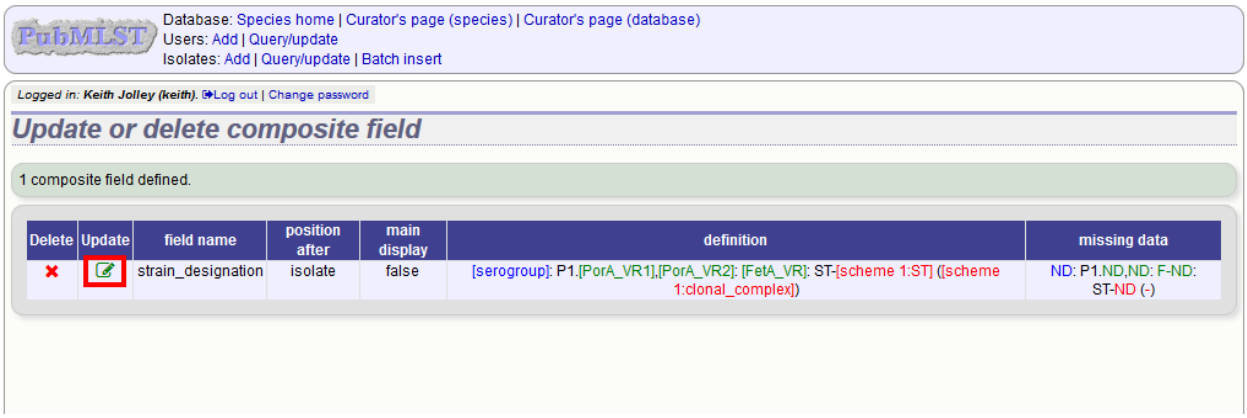
Initially you just enter a name for the composite field and after which field it should be positioned. You can also set whether or not it should be displayed by default in main results tables following a query - this is overrideable by user preferences.



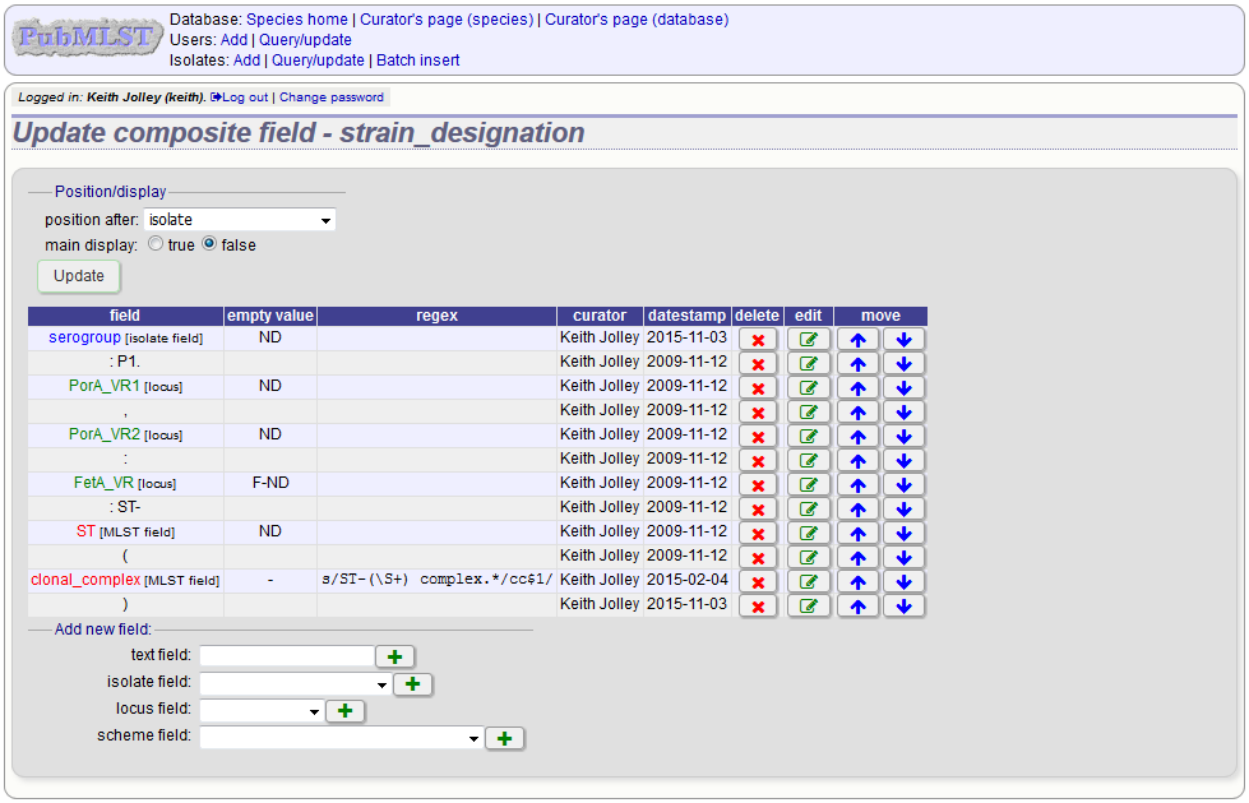
Once the field has been created it needs to be defined. This can be done from query composite field link on the main curator's page.



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



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.



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

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

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

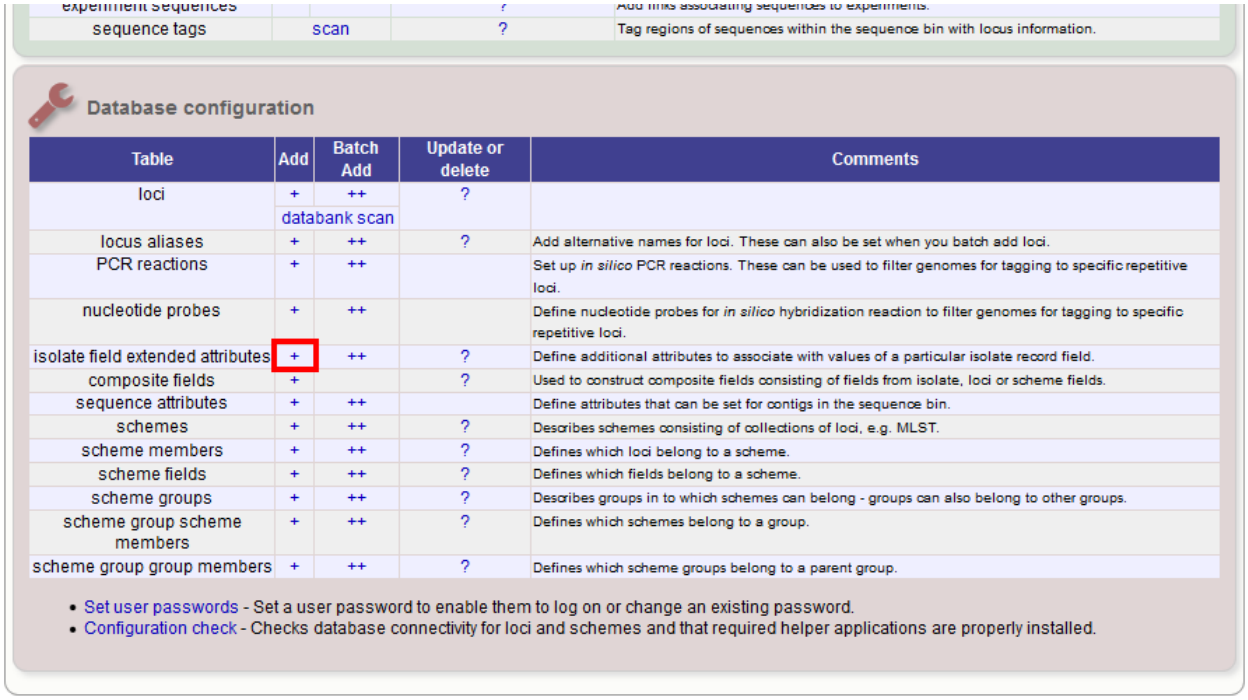
This will convert 'ST-4 complex/subgroup IV' to 'cc4'.

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

5.27 Extended provenance attributes (lookup tables)

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

To set up such an extended attribute, click the add (+) isolate field extended attributes link on the curator's main page.



experiment sequences		?	Add links associating sequences to experiments.
sequence tags	scan	?	Tag regions of sequences within the sequence bin with locus information.

Database configuration

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.
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.
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.

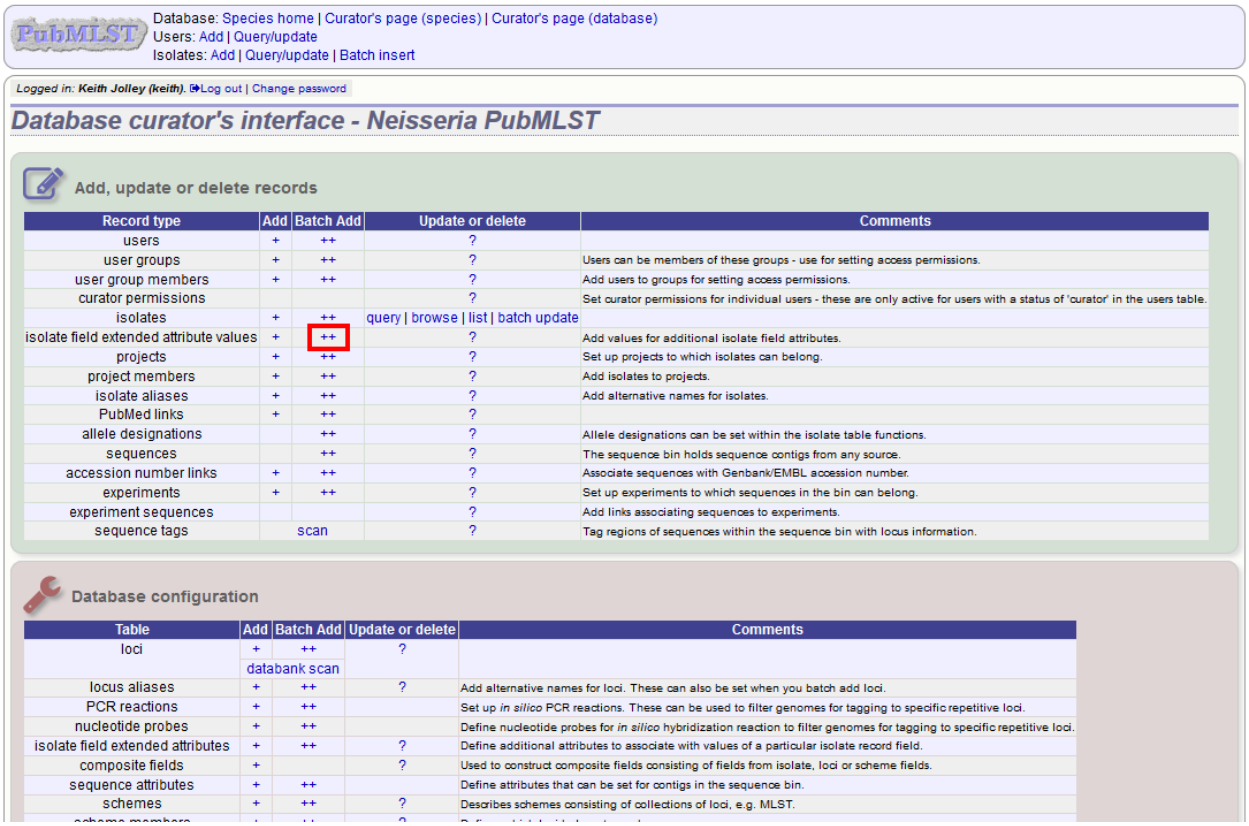
- Set user passwords - Set a user password to enable them to log on or change an existing password.
- Configuration check - Checks database connectivity for loci and schemes and that required helper applications are properly installed.

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

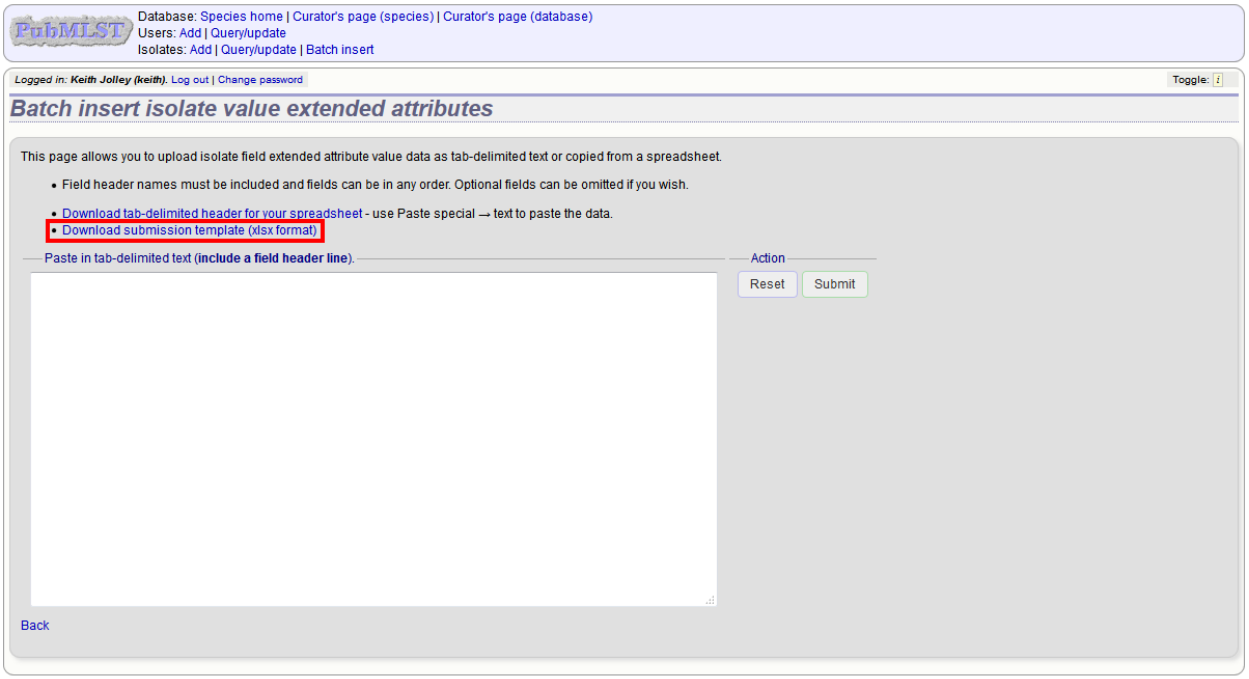
- isolate_field - Dropdown list of isolate fields.
  - Allowed: selection from list.
- attribute - Name of extended attribute, e.g. continent.
  - Allowed: any text (no spaces).
- value_format - Format for values.
  - Allowed: integer/float/text/date.
- value_regex - Regular expression to enforce allele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

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

The easiest way to populate the lookup table is to do a batch update copied from a spreadsheet. Click the batch add (++) isolate field extended attribute values link on the curator's main page (this link will only appear once an extended attribute has been defined).



Download the Excel template:



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

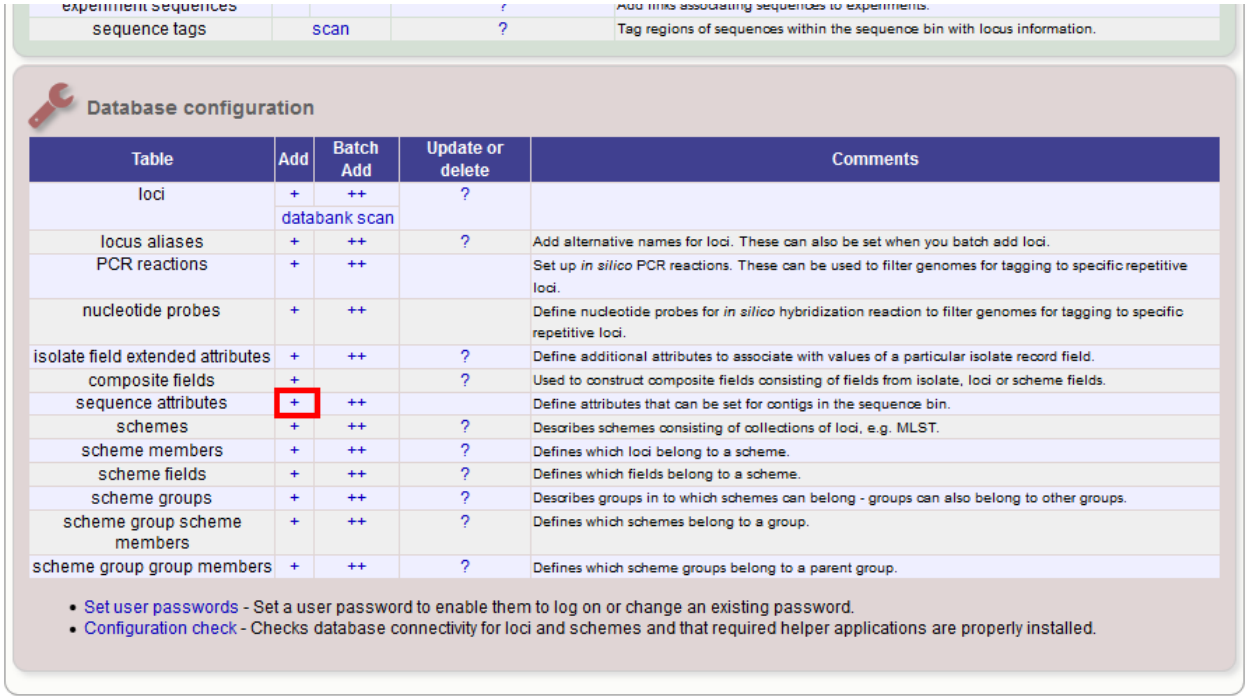
isolate_field	attribute	field_value	value
country	continent	Afghanistan	Asia
country	continent	Albania	Europe
country	continent	Algeria	Africa
country	continent	Andorra	Europe
country	continent	Angola	Africa

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

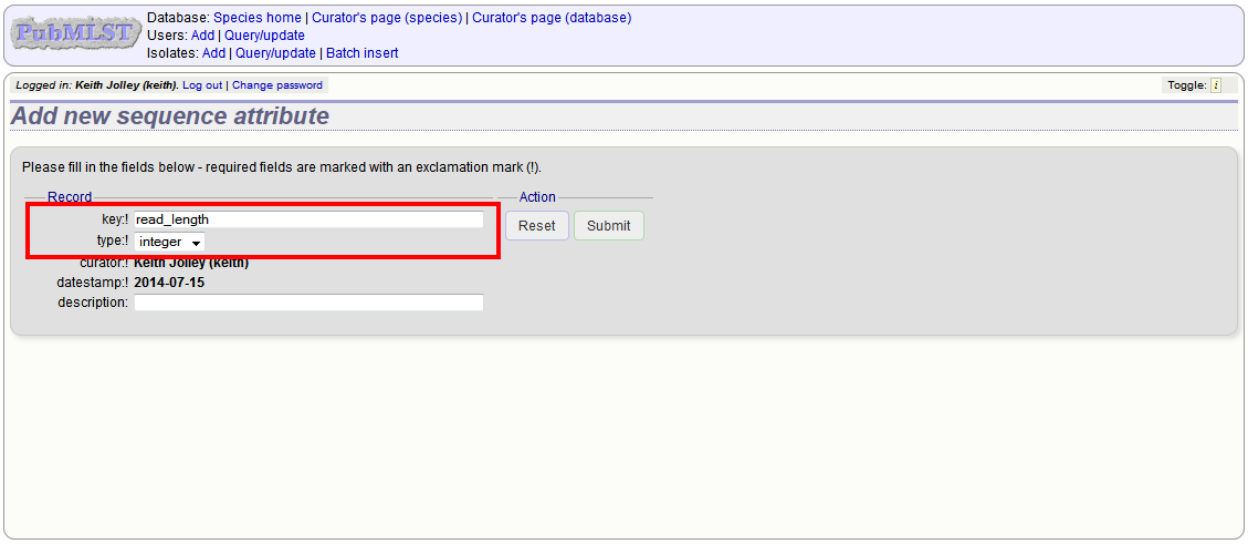
5.28 Sequence bin attributes

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

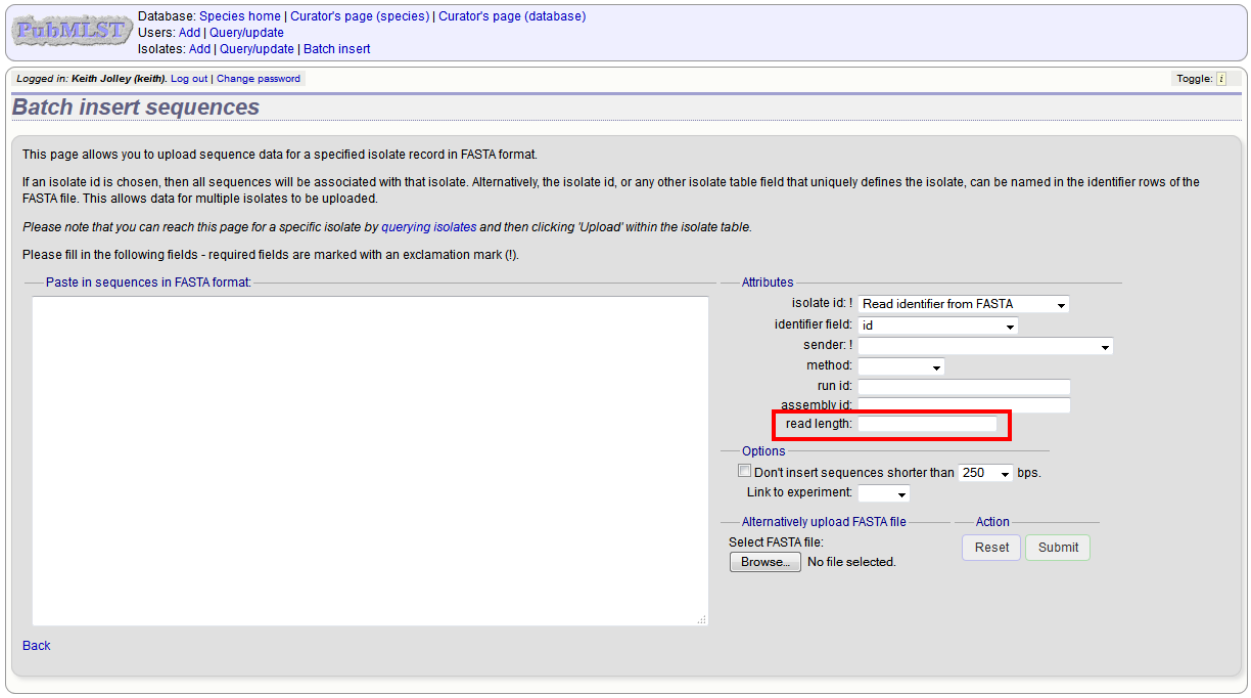
To set up new attributes, click the add (+) 'sequence attributes' link on the isolate database curator's index page.



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'.

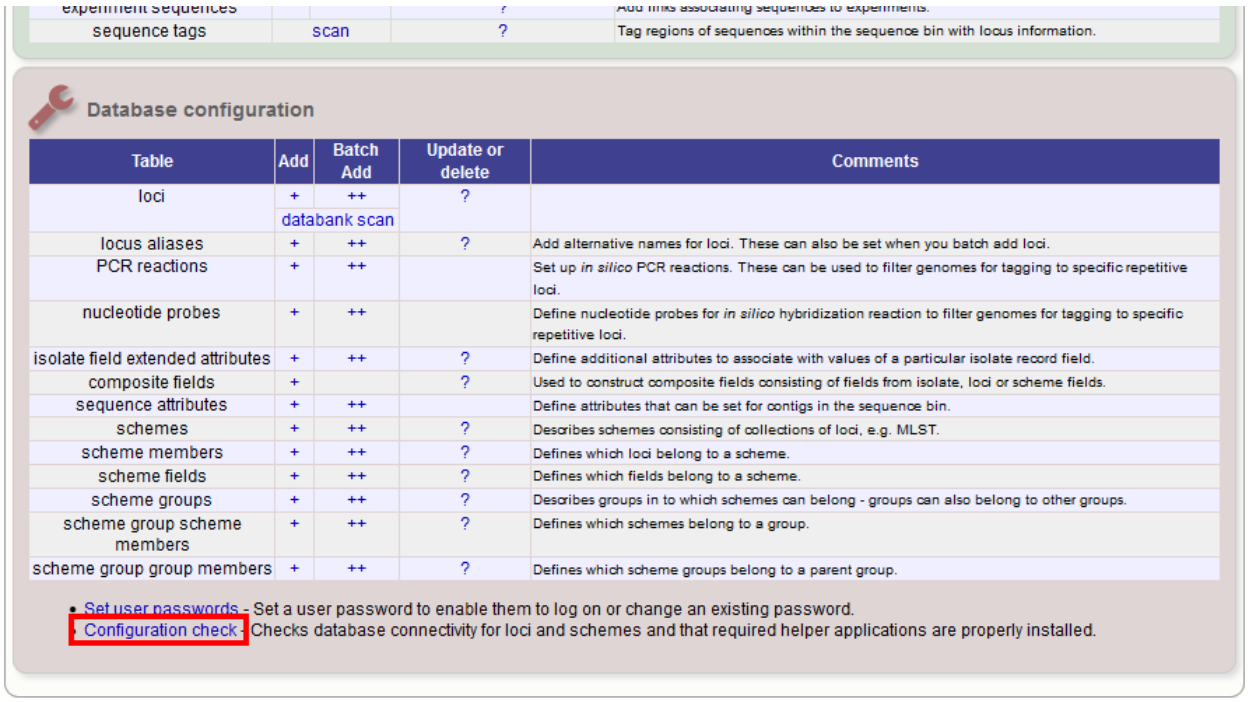


This new attribute will then be available when *uploading contig data*.

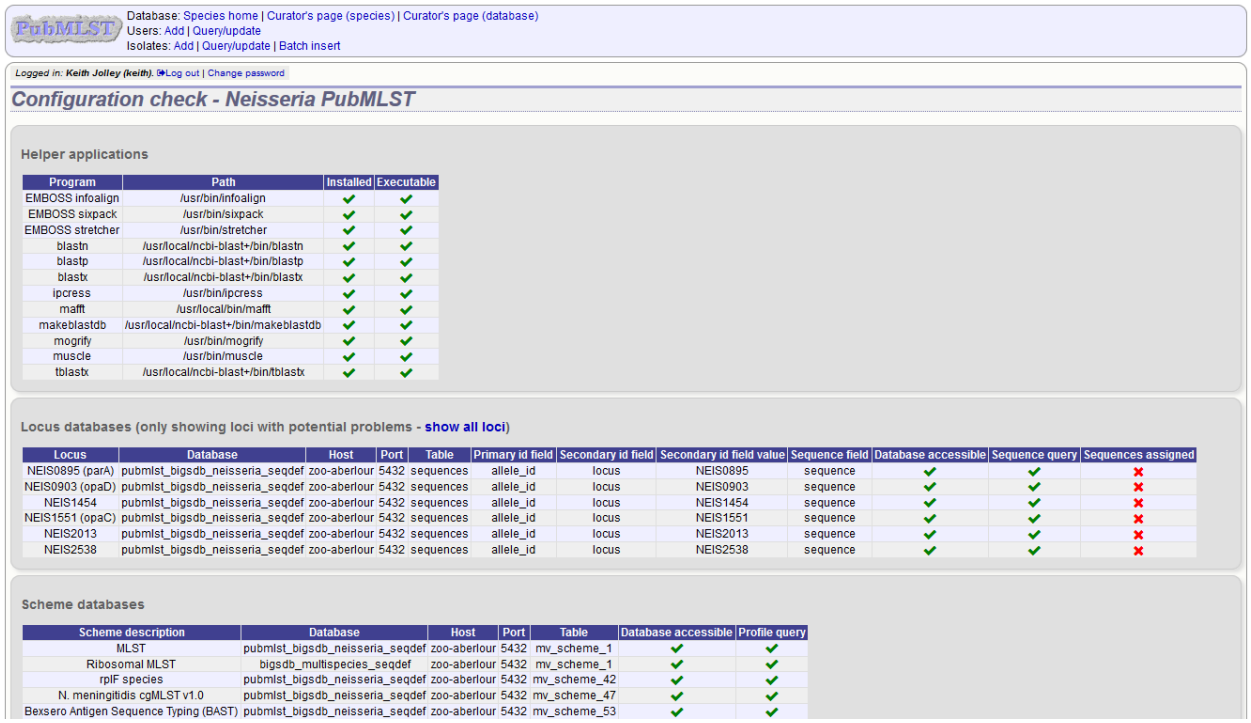


5.29 Checking external database configuration settings

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



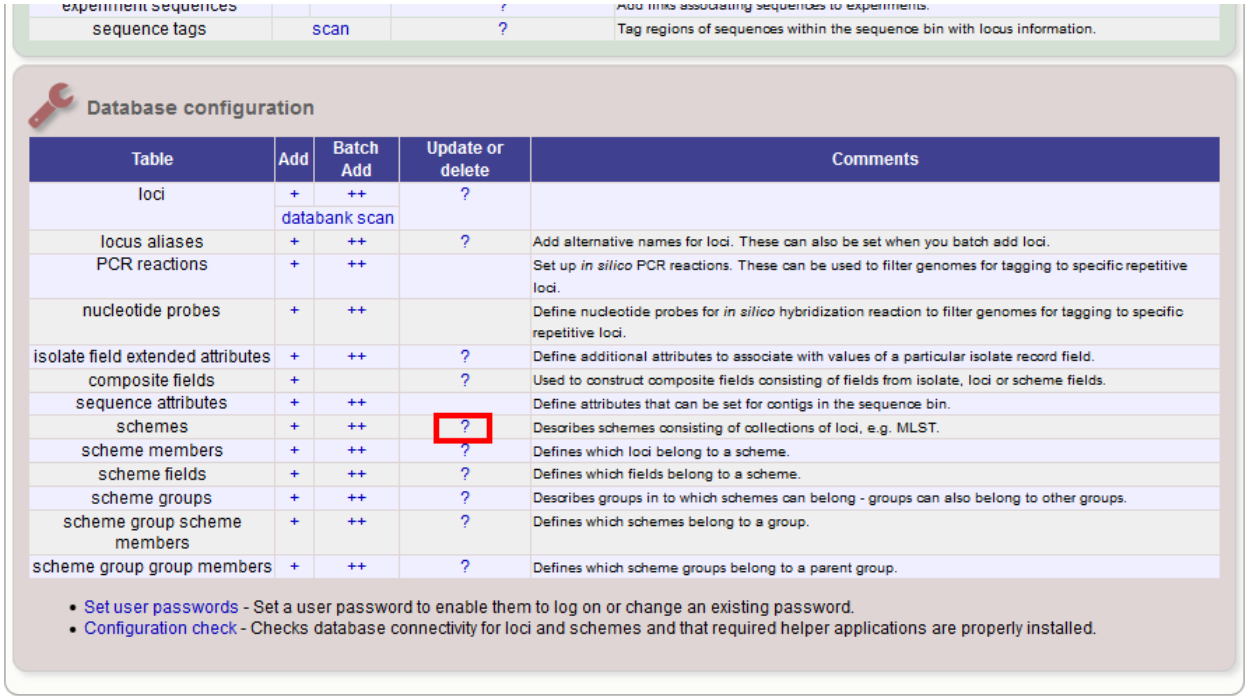
The software will check that required helper applications are installed and executable and, in isolate databases, test every locus and scheme external database to check for connectivity and that data can be retrieved. By default, only loci which have an issue will be displayed but you can click the 'show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



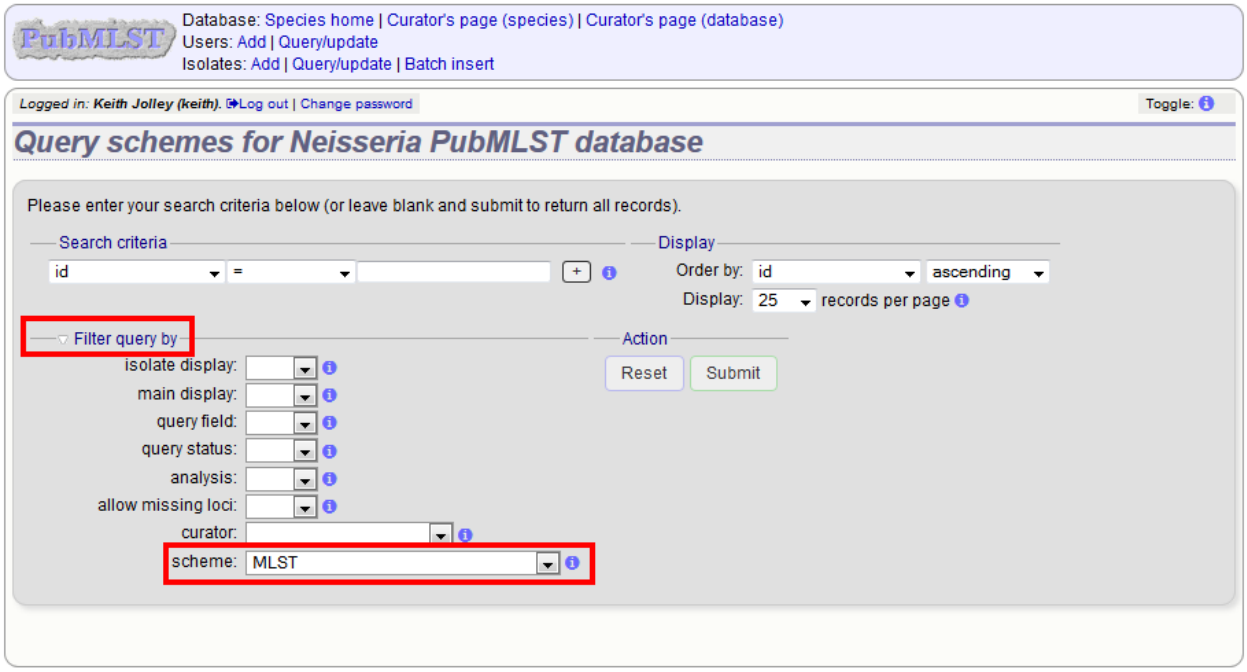
Any problems will be highlighted with a red X.

5.30 Exporting table configurations

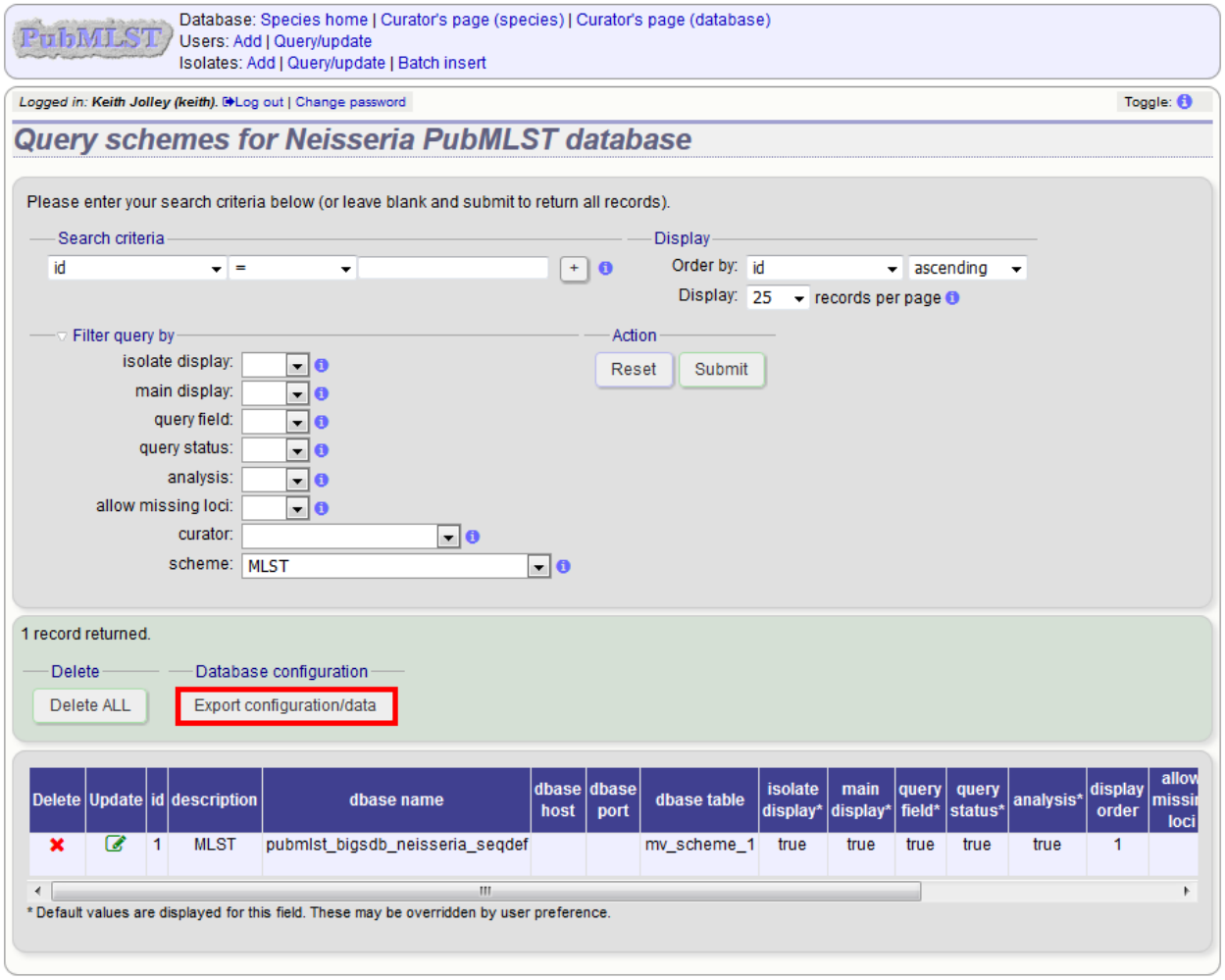
Sometimes it is useful to transfer configurations between different databases or to export a configuration for troubleshooting. Data from most of the tables can be exported in tab-delimited text format suitable for batch uploading. For example, to export scheme configuration data, click the '?' link (Update or delete) next to schemes in the curator's interface.



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



Click the button 'Export configuration/data'.



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

```
schemes
-------
id description dbase_name  dbase_host  dbase_port  dbase_user  dbase_password dbase_
↪table isolate_display   main_display   query_field query_status   analysis display_
↪order  allow_missing_loci   curator  datestamp   date_entered
1  MLST  pubmlst_bigsdb_neisseria_seqdef             mv_scheme_1 1  1  1  1  1  1
↪ 2  2012-03-22  2009-11-12

scheme_members
--------------
scheme_id   locus profile_name   field_order curator  datestamp
1  abcZ     1  2  2009-11-12
1  adk      2  2  2009-11-12
1  aroE     3  2  2009-11-12
1  fumC     4  2  2009-11-12
1  gdh      5  2  2009-11-12
1  pdhC     6  2  2009-11-12
1  pgm      7  2  2009-11-12

scheme_fields
-------------
```

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

5.31 Authorizing third-party client software to access authenticated resources

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

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

```
create_client_credentials.pl --help

NAME
    create_client_credentials.pl - Generate and populate
    authentication database with third party application (API client)
    credentials.

SYNOPSIS
    create_client_credentials.pl --application NAME [options]

OPTIONS
-a, --application NAME
    Name of application.

-d, --deny
    Set default permission to 'deny'.  Permissions for access to specific
    database configurations will have to be set.  If not included, the default
    permission will allow access to all resources by the client.

-h, --help
    This help page.

-i, --insert
    Add credentials to authentication database.  This will fail if a matching
    application version already exists (use --update in this case to overwrite
    existing credentials).

-u, --update
    Update exisitng credentials in the authentication database.

-v, --version VERSION
    Version of application (optional).
```

CHAPTER 6

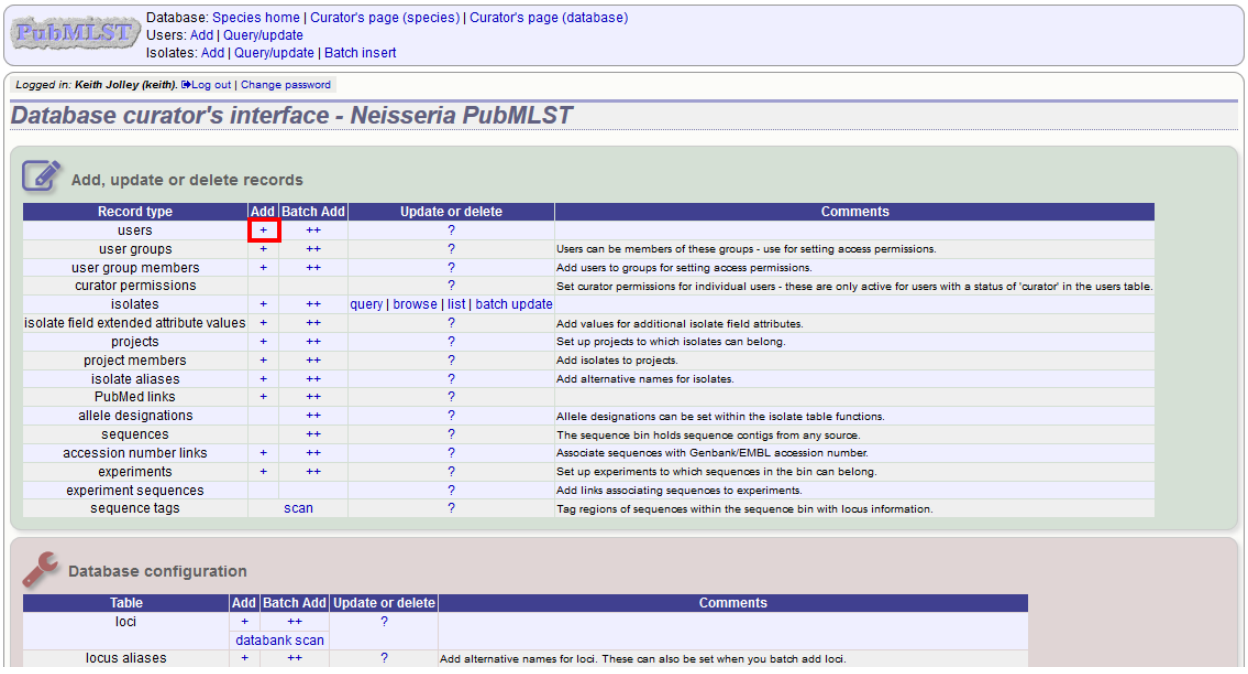
Curator's guide

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

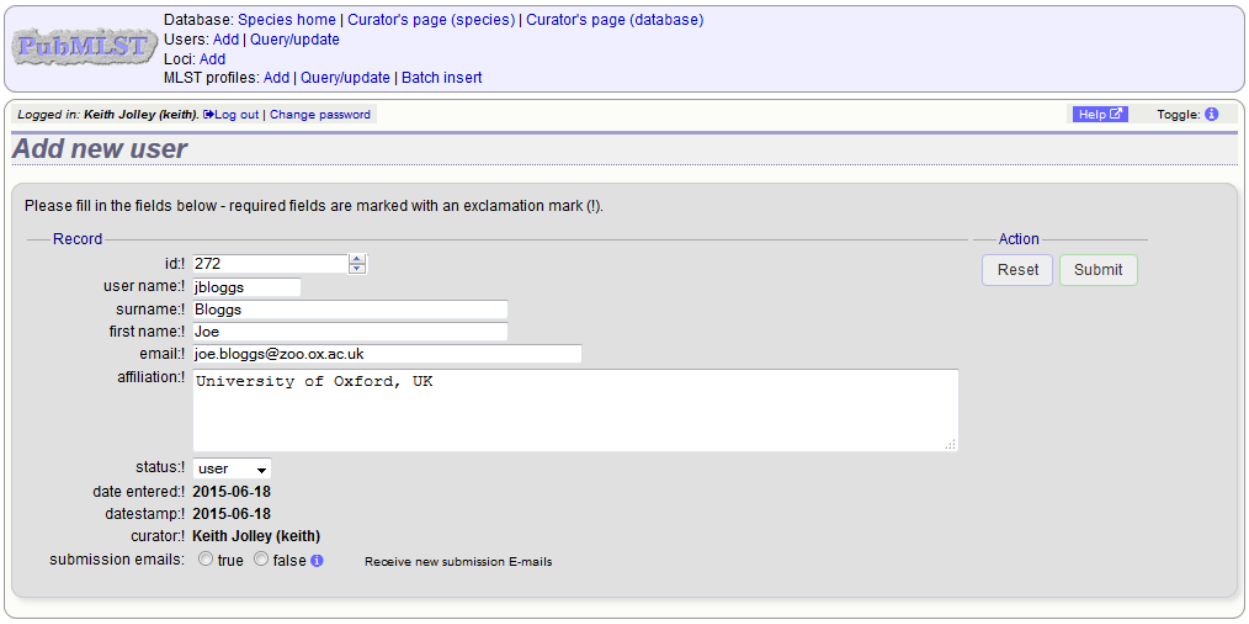
6.1 Adding new sender details

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.



Enter the user's details in to the form.



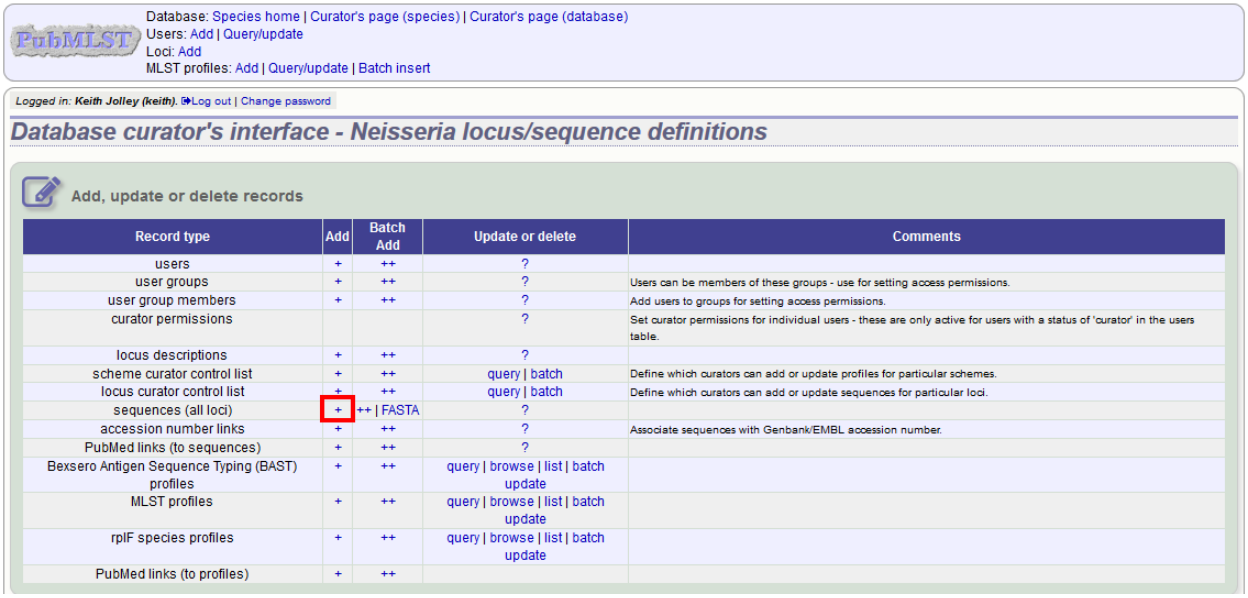
Normally the status should be set as 'user'. Only admins and curators with special permissions can create users with a status of curator or admin.

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.

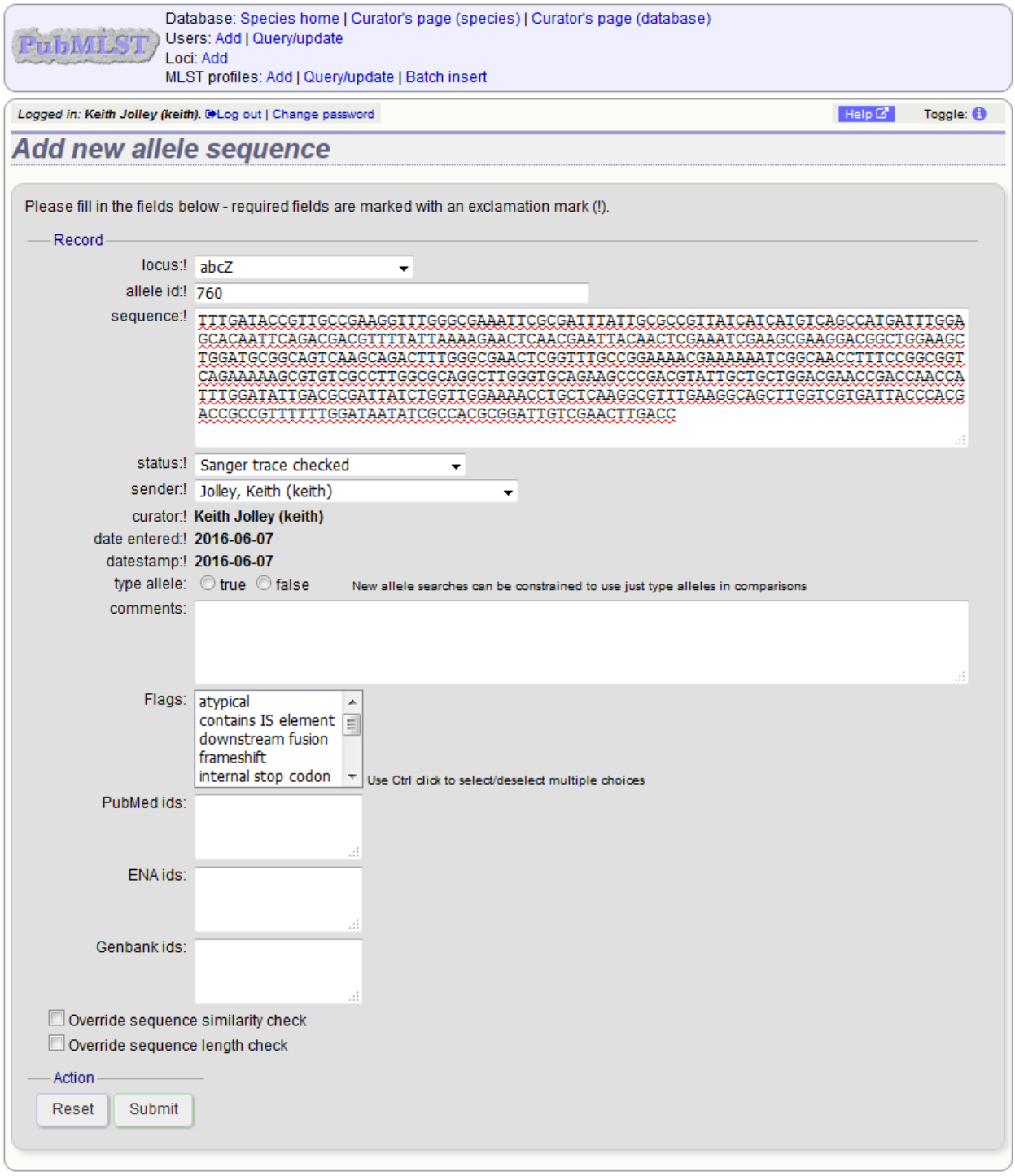


Select the locus from the dropdown list box. The next available allele id will be entered automatically (if the allele id format is set to integer). Paste the sequence in to form, set the status and select the sender name from the dropdown box. If the sender does not appear in the box, you will need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

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

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

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



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

See also:

allele sequence flags

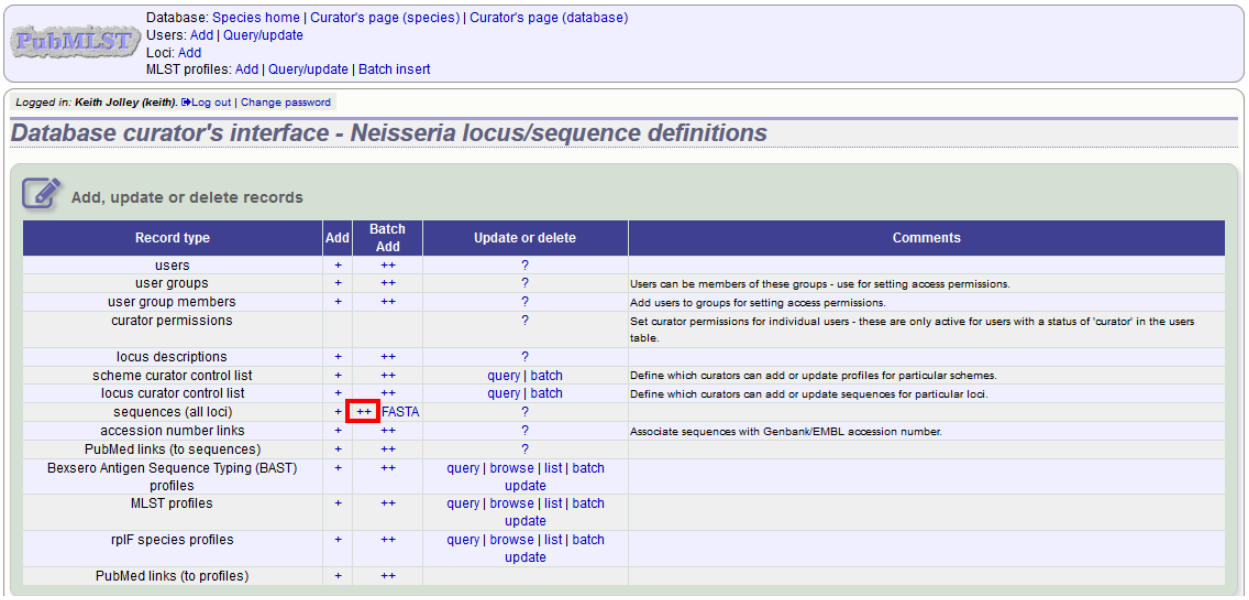
Sequences can also be associated with PubMed, ENA or Genbank id numbers by entering these as lists (one value per line) in the appropriate form box.

6.2.2 Batch adding multiple alleles

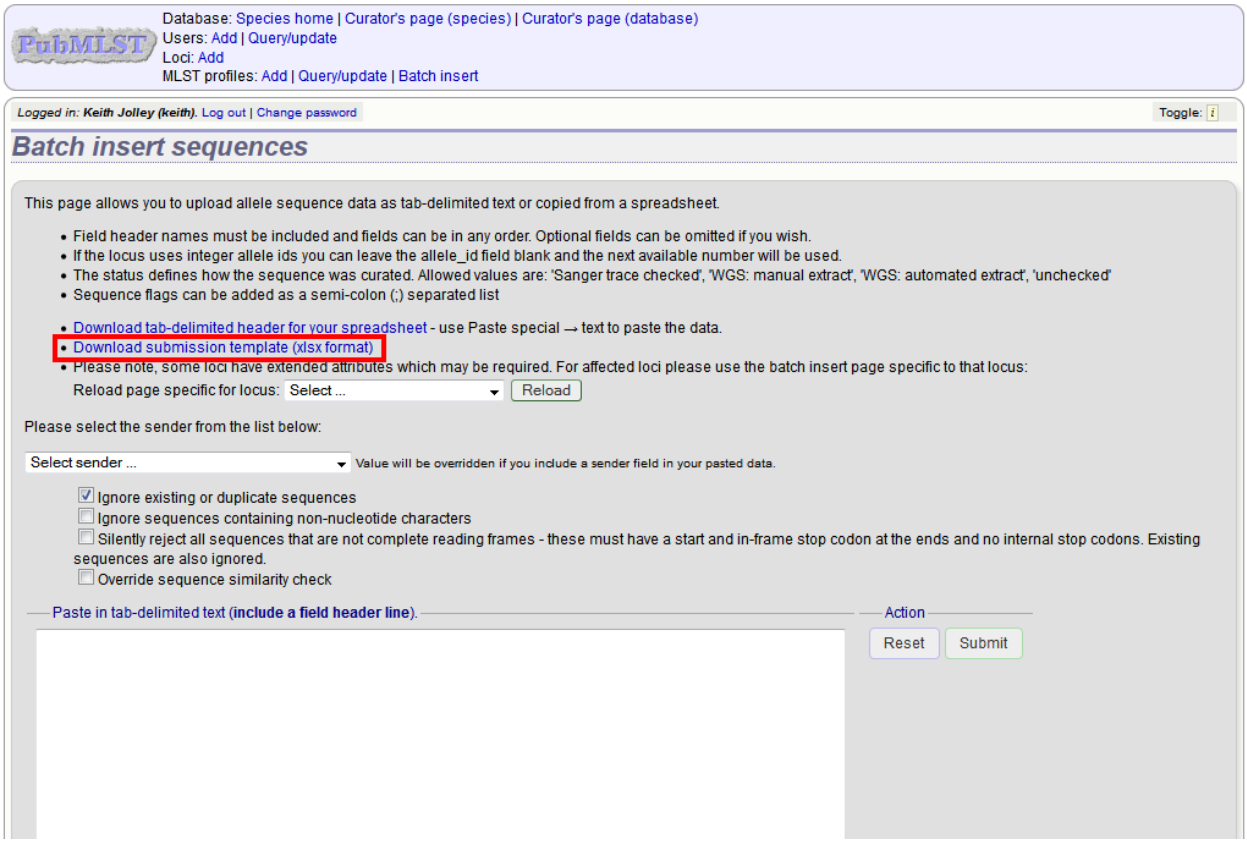
There are two methods of batch adding alleles. You can either upload a spreadsheet with all fields in tabular format, or you can upload a FASTA file provided all sequences are for the same locus and have the same status.

6.2.2.1 Upload using a spreadsheet

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



Download a template Excel file from the following page.



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

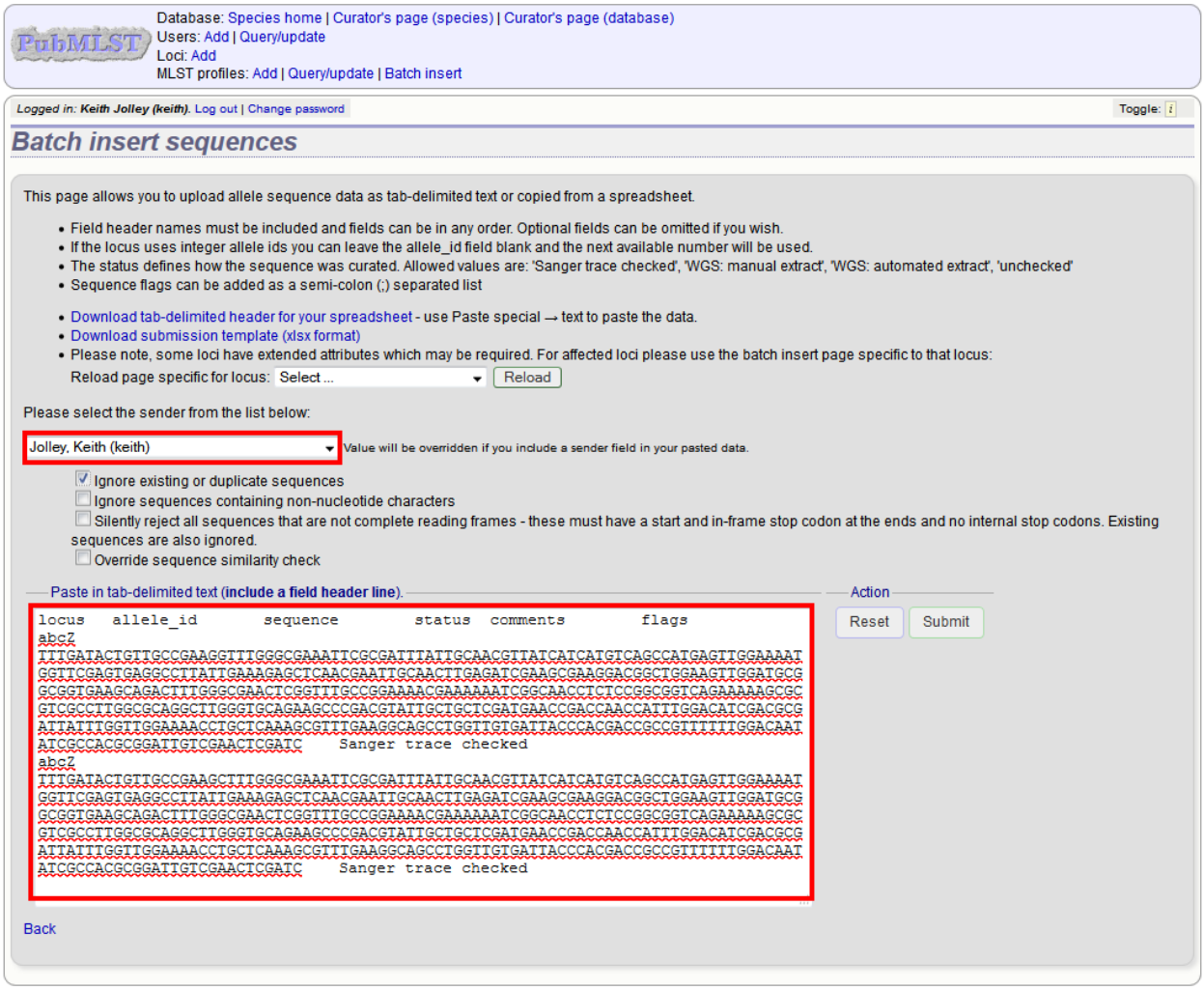
The status can be either: 'Sanger trace checked', 'WGS: manual extract (BIGSdb)', 'WGS: automated extract (BIGSdb)', 'WGS: visually checked', 'WGS: automatically checked' or 'unchecked'. See full explanations for these in the *single allele upload* section.

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

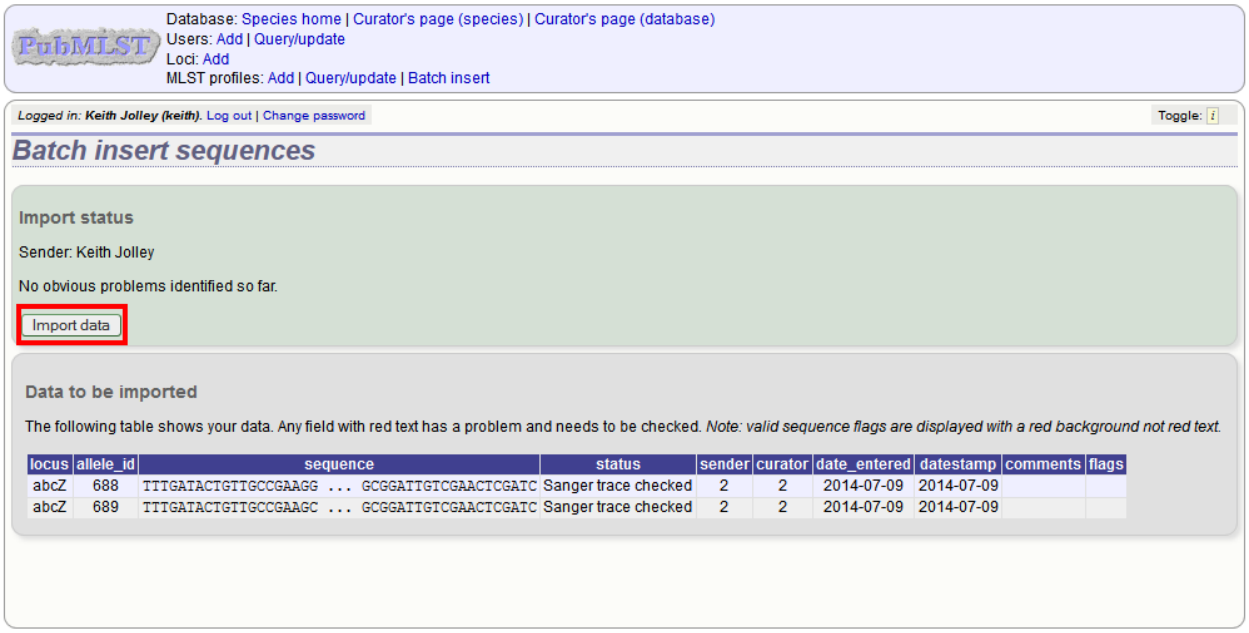
Paste the entire sheet in to the web form and select the sender from the dropdown box.

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

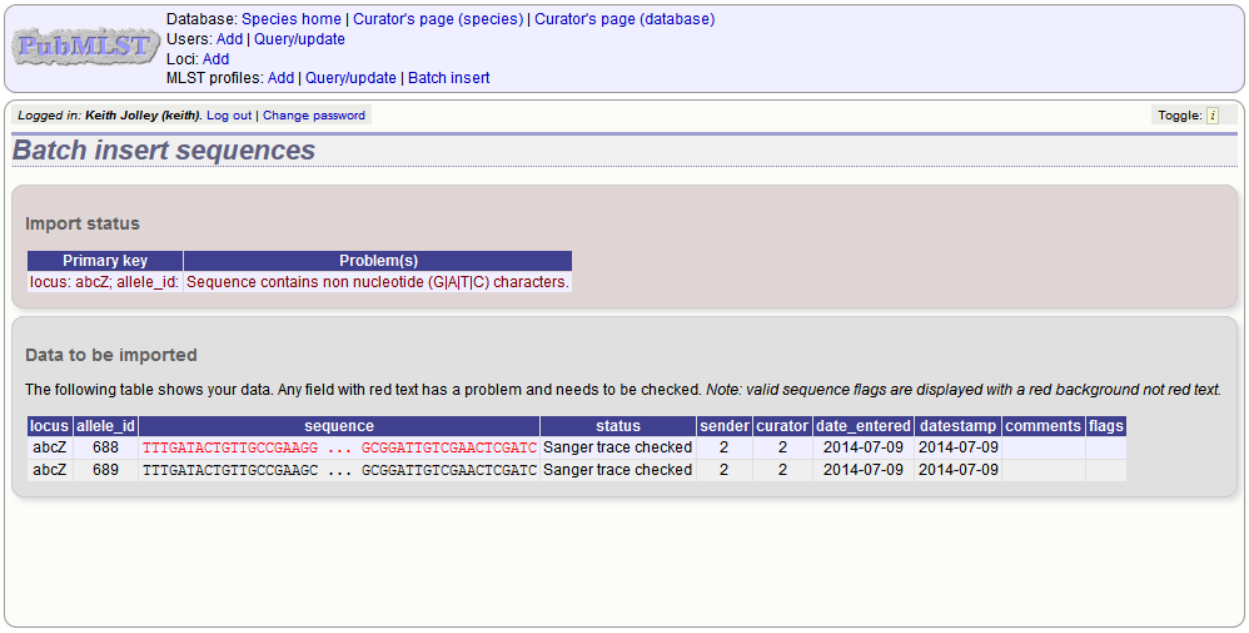
- Ignore existing or duplicate sequences.
- Ignore sequences containing non-nucleotide characters.
- Silently reject all sequences that are not complete reading frames - these must have a start and in-frame stop codon at the ends and no internal stop codons. Existing sequences are also ignored.
- Override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



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'.



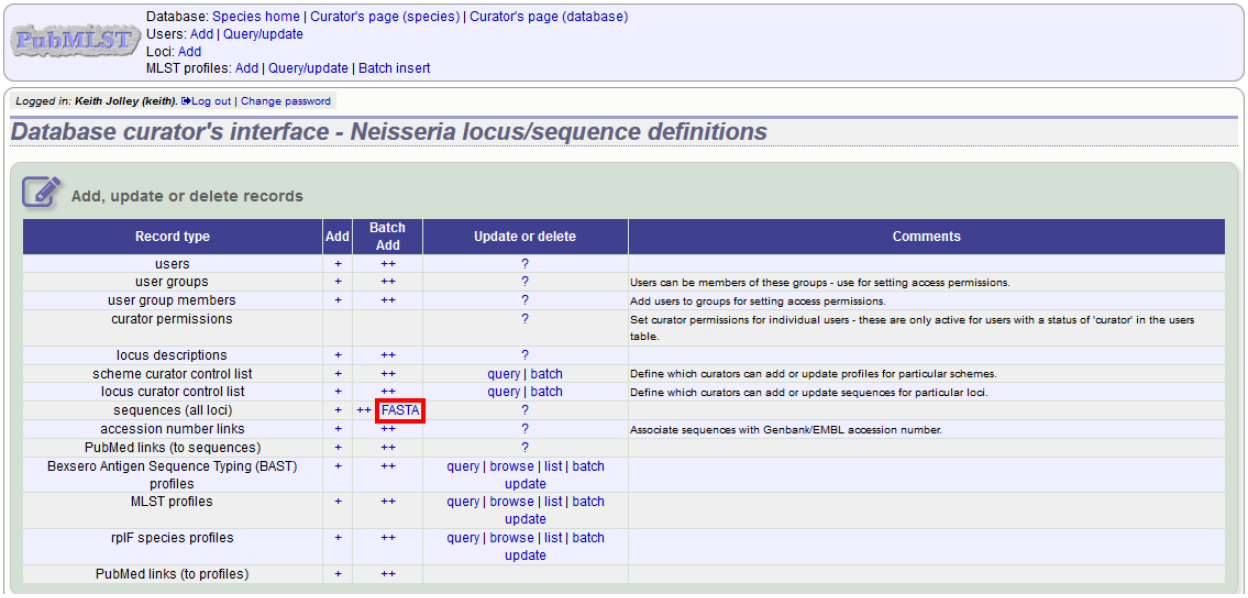
If there are any problems with the submission, these should be indicated at this stage, e.g.:



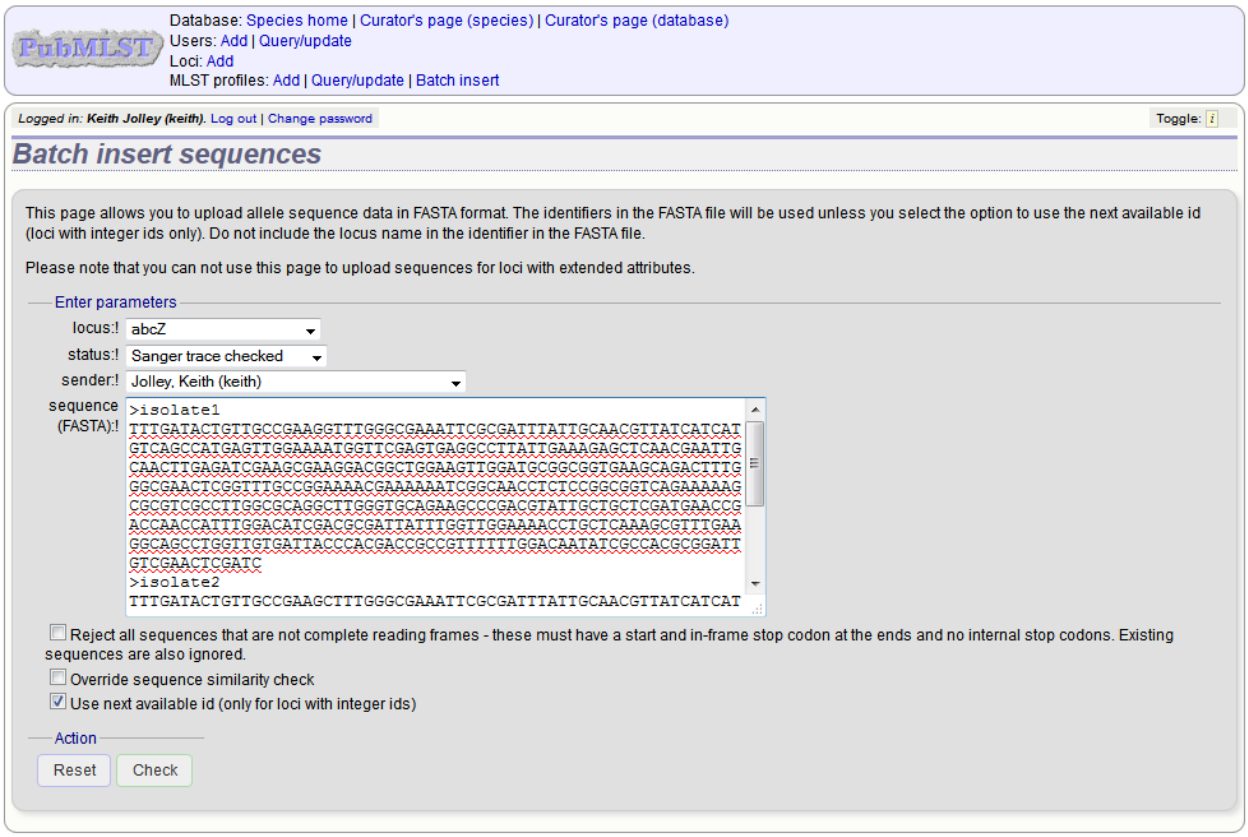
6.2.2.2 Upload using a FASTA file

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

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



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



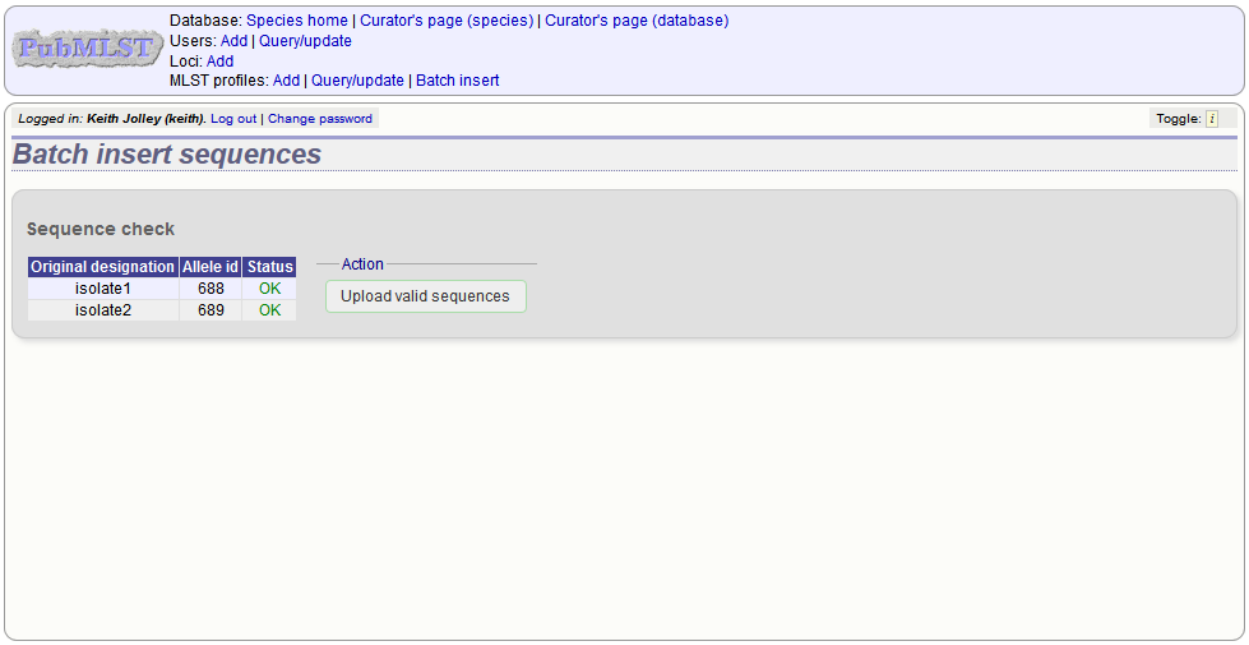
For loci with integer ids, the next available id number will be used by default (and the identifier in the FASTA file will be ignored). Alternatively, you can indicate the allele identifier within the FASTA file (do not include the locus name in this identifier).

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

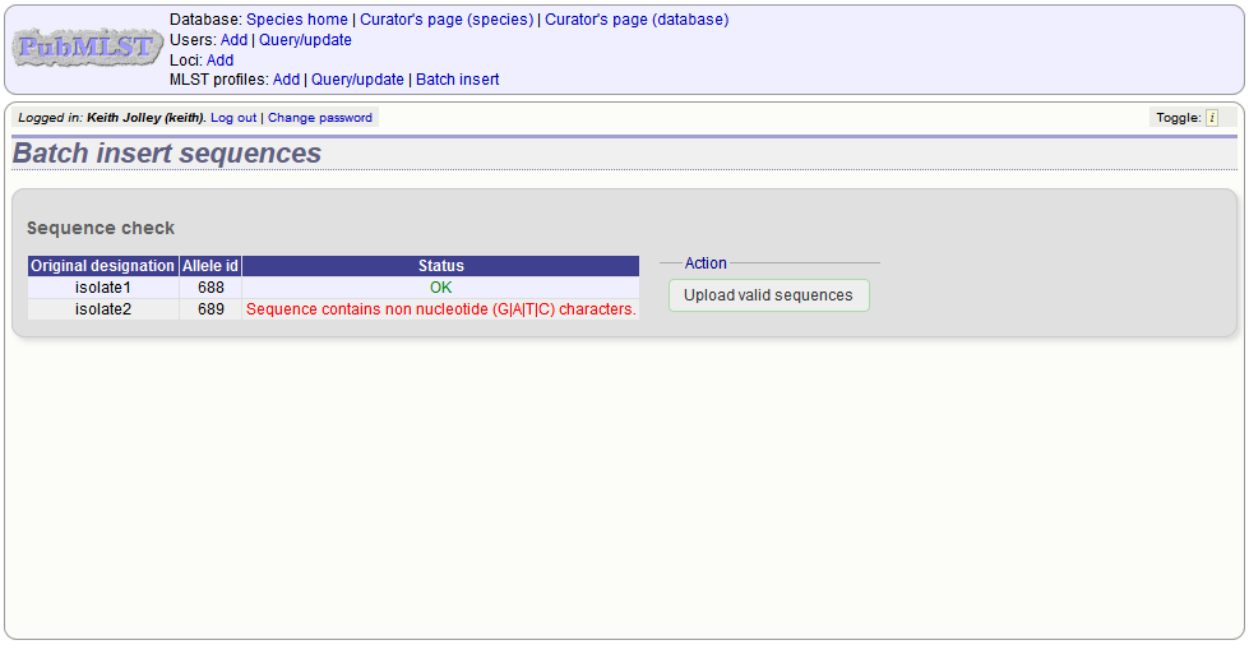
criteria.

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'.



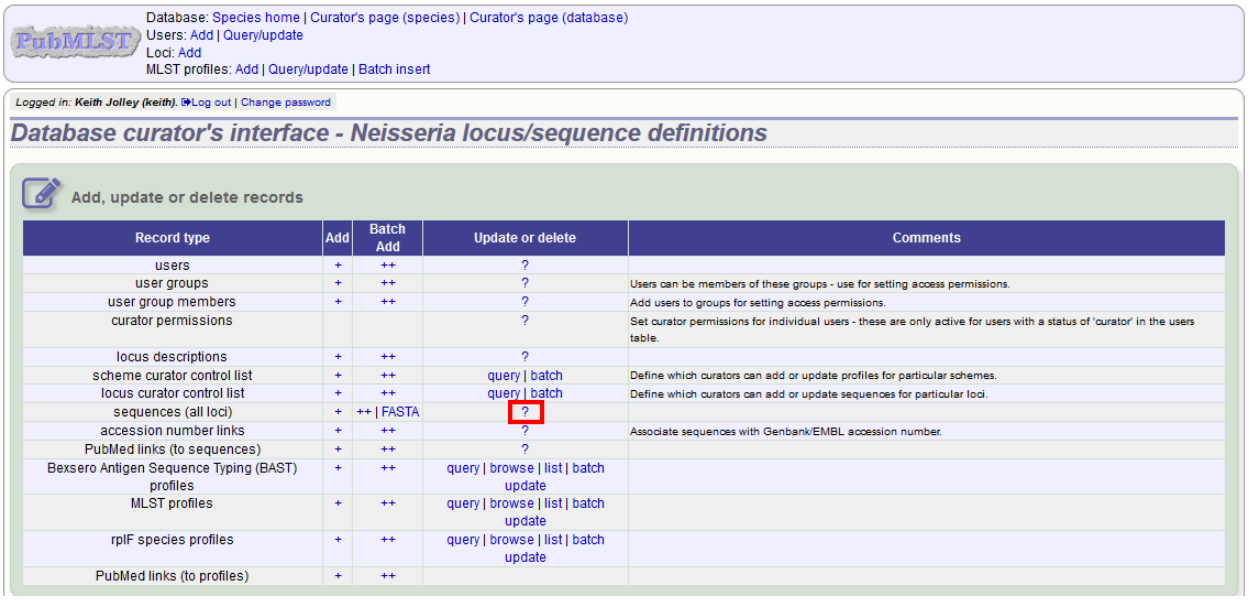
Any invalid sequences will be indicated in this confirmation page and these will not be uploaded (you can still upload the others), e.g.



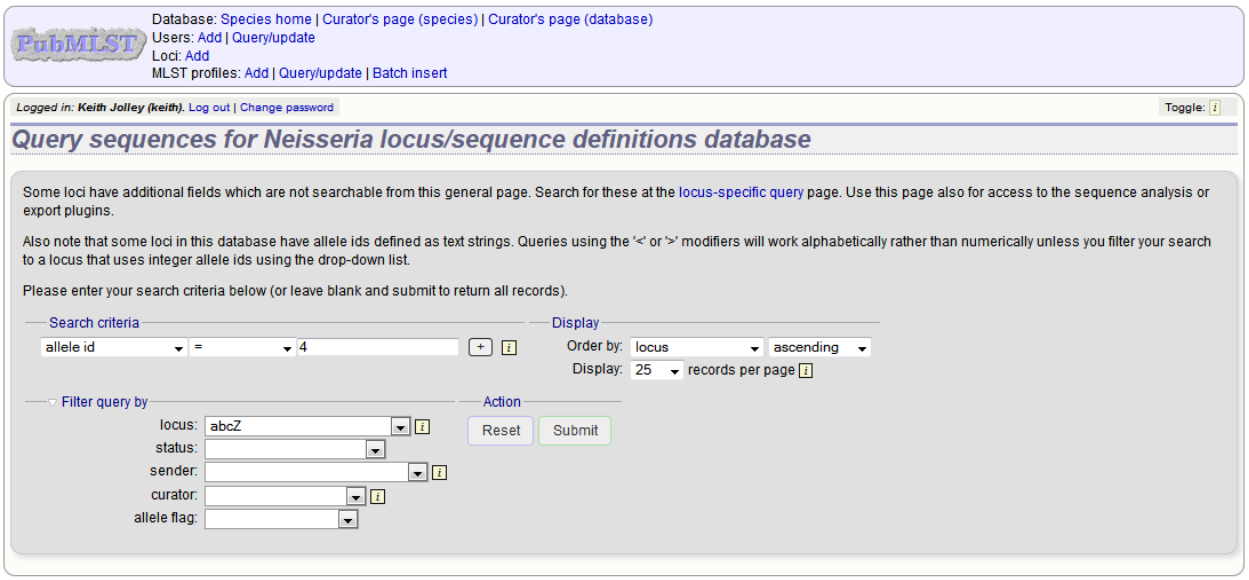
6.3 Updating and deleting allele sequence definitions

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.

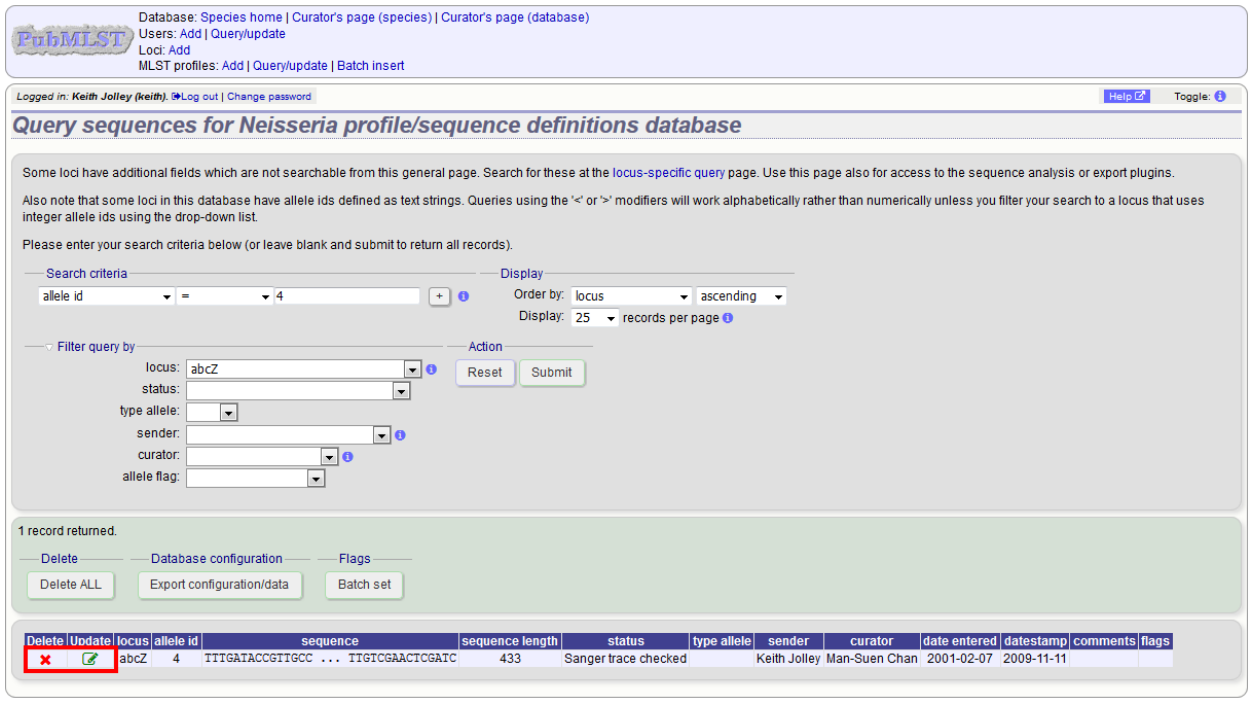
In order to update or delete an allele, first you must select it. Click the query (?) sequences (all loci) link - if only a few loci are defined with permission for the current user to curate then they will be listed individually and the specific locus query links can also be used.



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



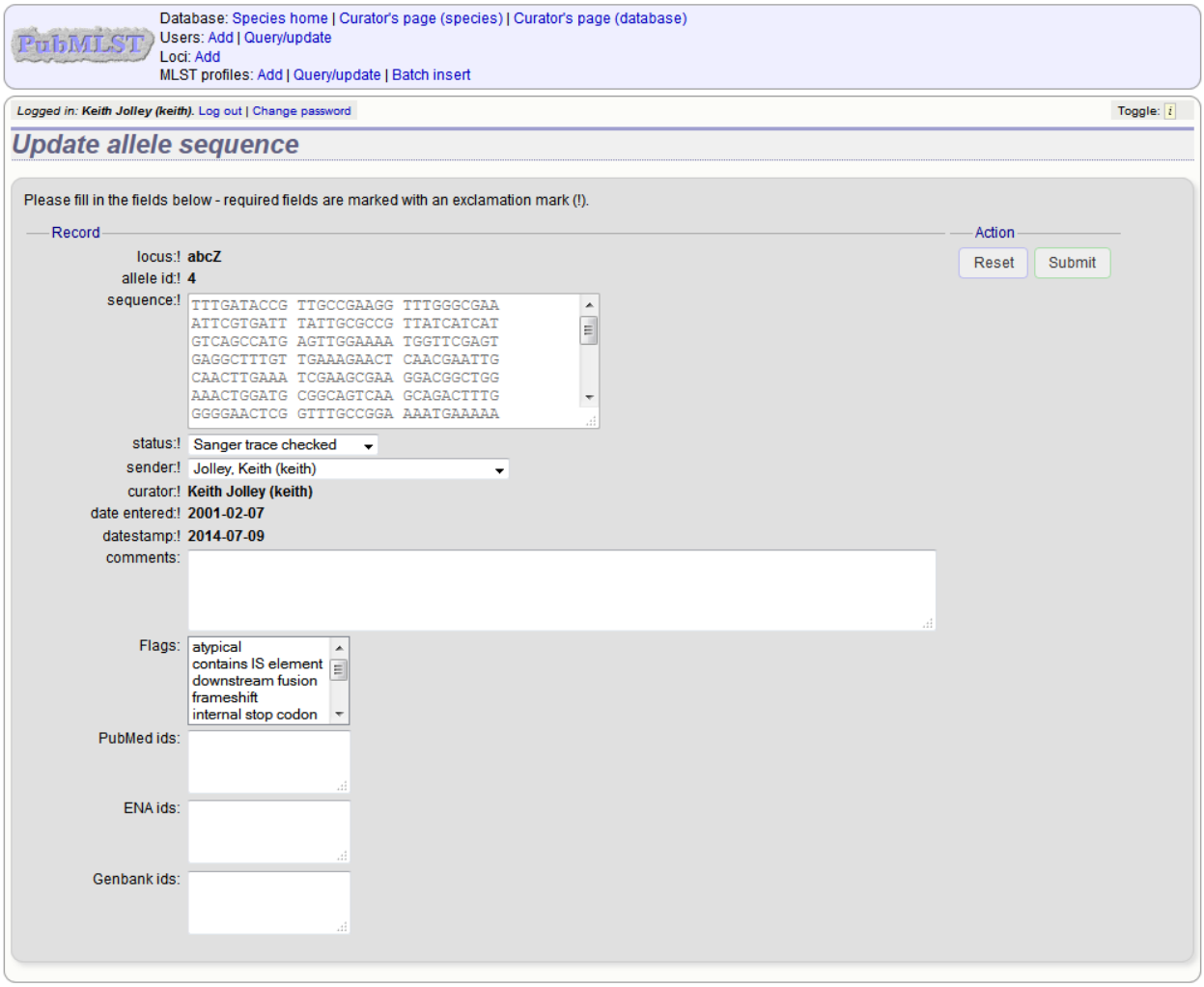
Click the appropriate link to either update the allele attributes or to delete it. If you have appropriate permissions, there may also be a link to 'Delete ALL'. This allows you to quickly delete all alleles returned from a search.



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

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.

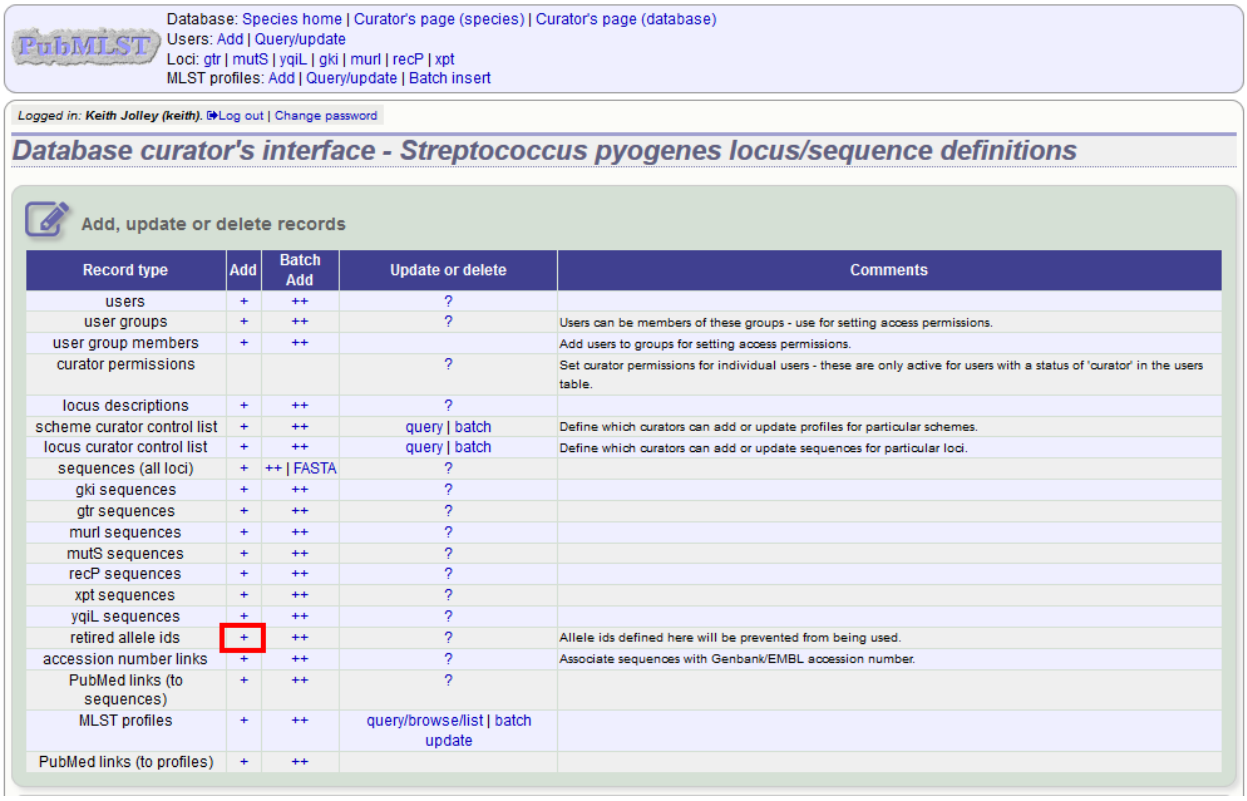
Note: Adding flags and comments to an allele record requires that this feature is enabled in the *database configuration*.



6.4 Retiring allele identifiers

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

You can retire an allele identifier by clicking the 'Add' retired allele ids link on the sequence database curators' page.



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

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

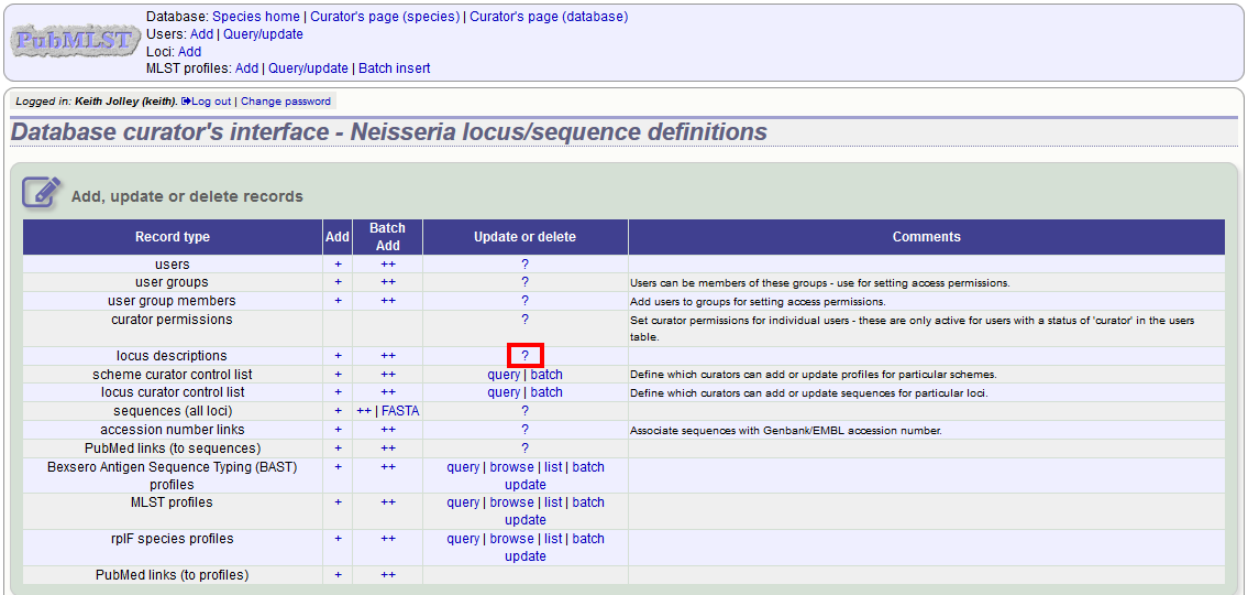
You can also retire an allele identifier when you *delete an allele*.

6.5 Updating locus descriptions

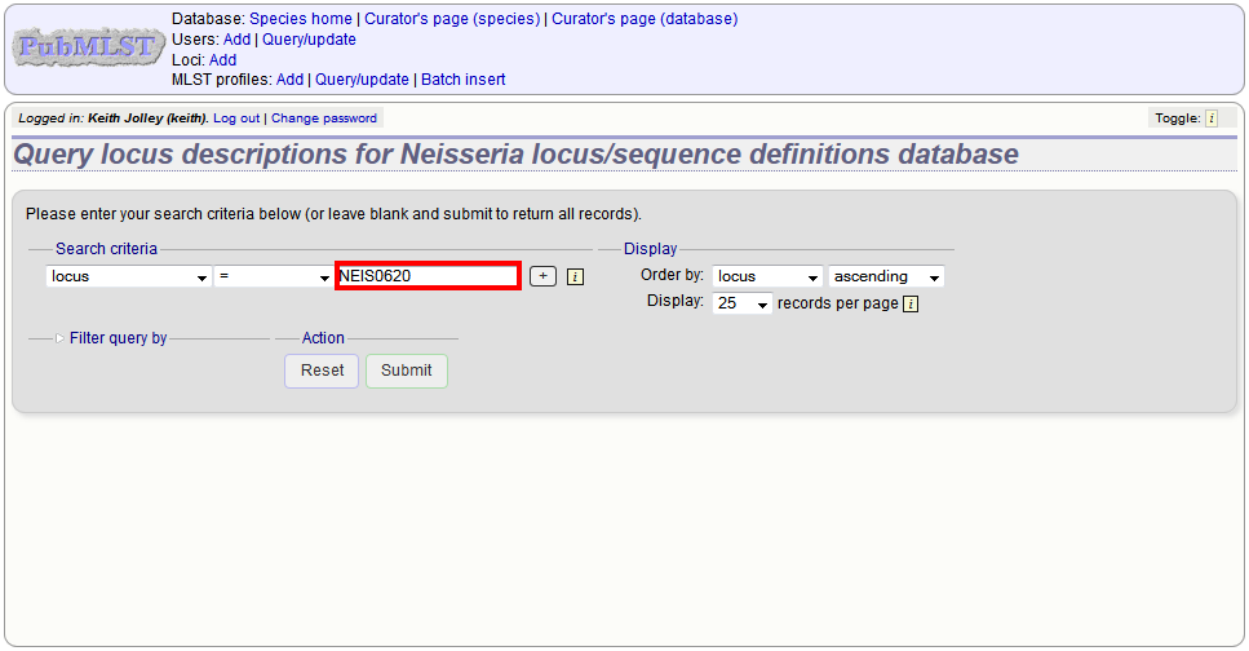
Loci in the sequence definitions database can have a description associated with them. This may contain information about the gene product, the biochemical reaction it catalyzes, or publications providing more detailed information etc. This description is accessible from various pages within the interface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

Note: In recent versions of BIGSdb, a blank description record is created when a new locus is defined. The following instructions assume that this is the case. It is possible for this record to be deleted or it may never have existed if the locus was created using an old version of BIGSdb. If the record does not exist, it can be added by clicking the Add (+) button next to 'locus descriptions'. Fill in the fields in the same way as described below.

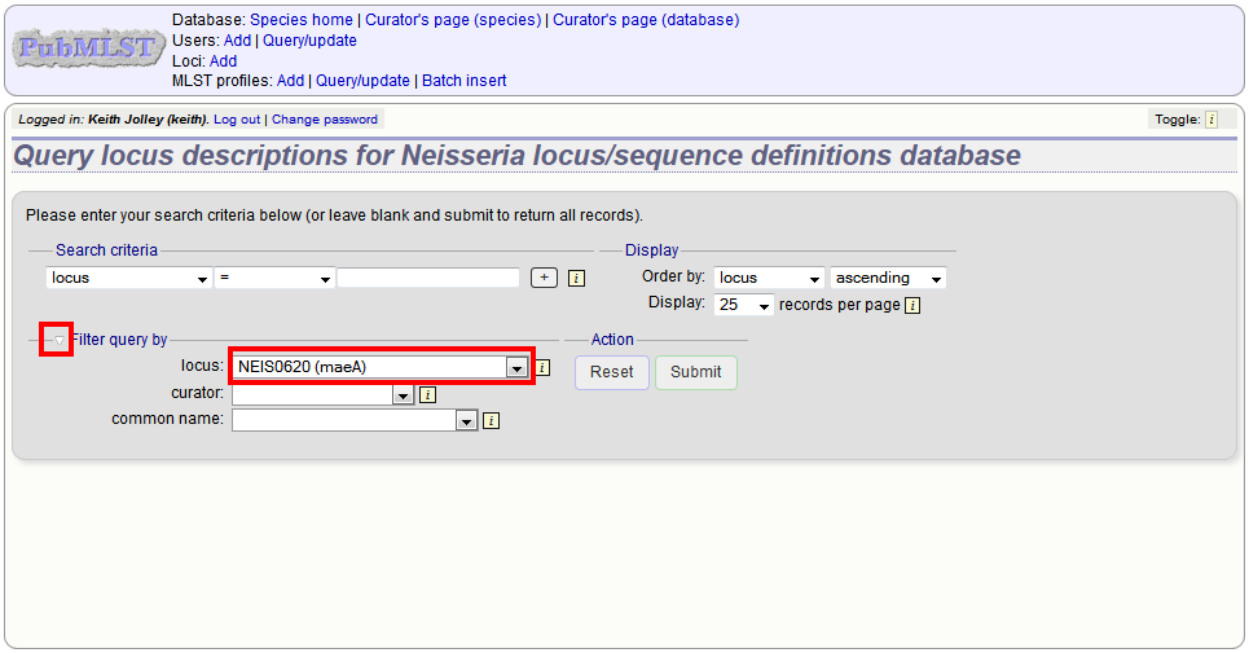
To edit a locus description, first you need to find it. Click the update/delete (?) button next to 'locus descriptions' on the sequence database curator's page (depending on the permissions set for your user account not all the links shown here may be displayed).



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

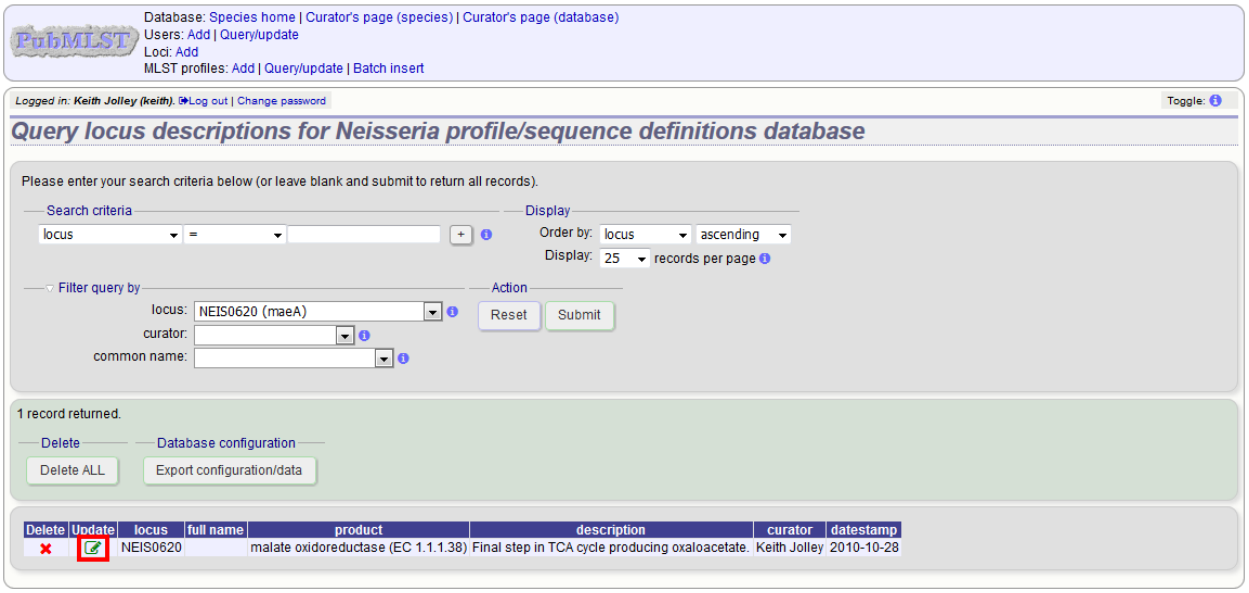


or expand the filter list and select it from the dropdown box:

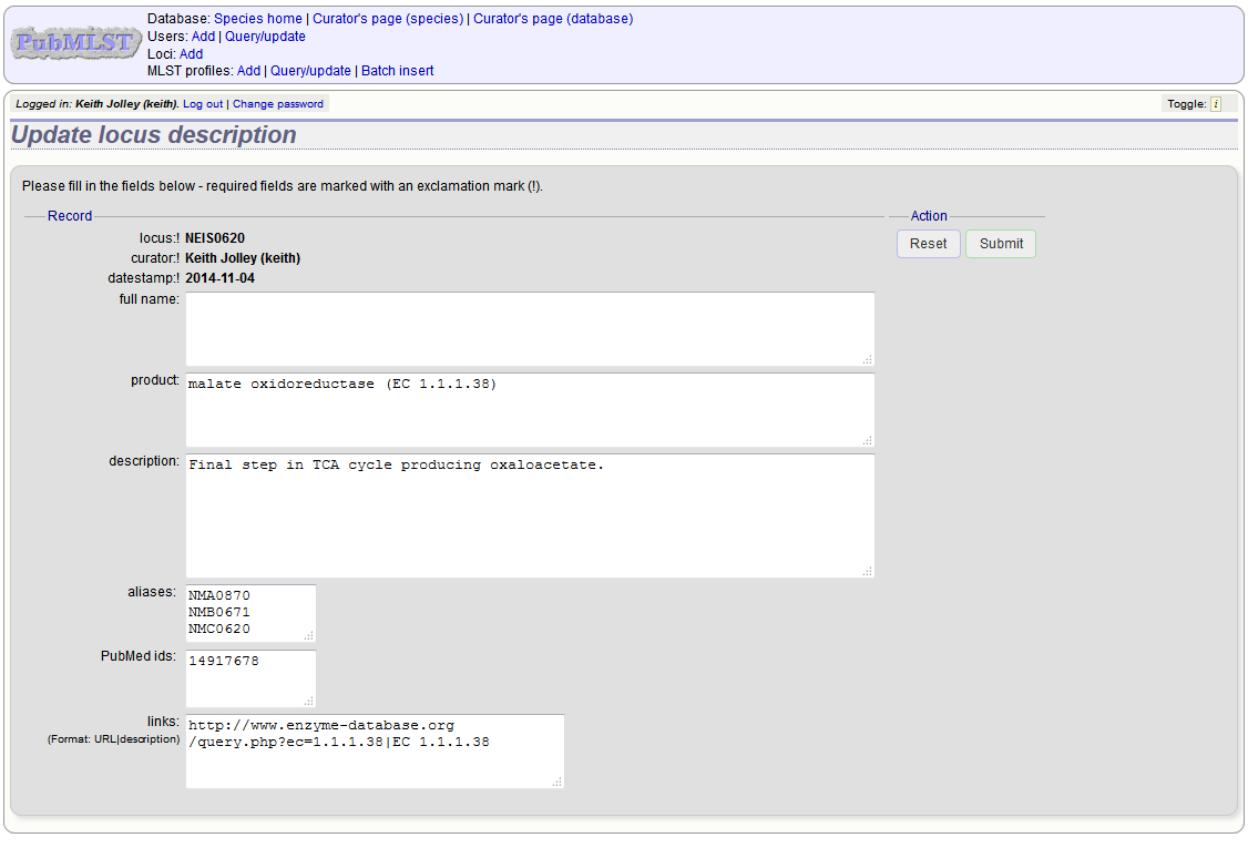


Click 'Submit'.

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



Fill in the form as needed:



- 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

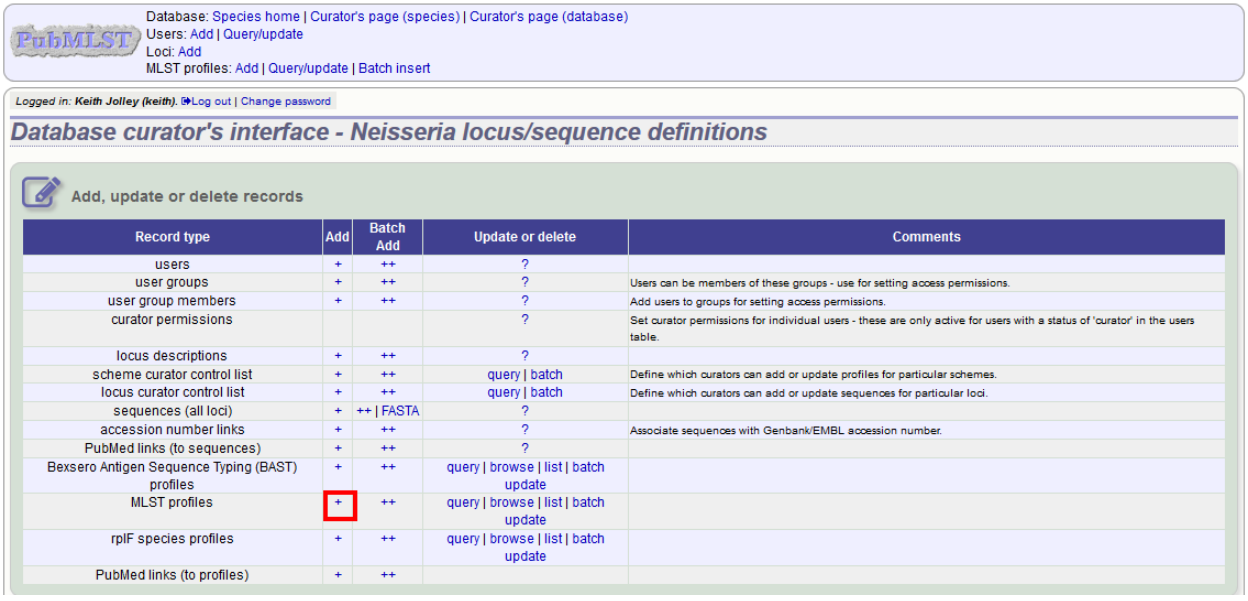
  Enter links to additional web-based resources. Enter the URL first followed by a pipe symbol (|) and then the description.

Click 'Submit' when finished.

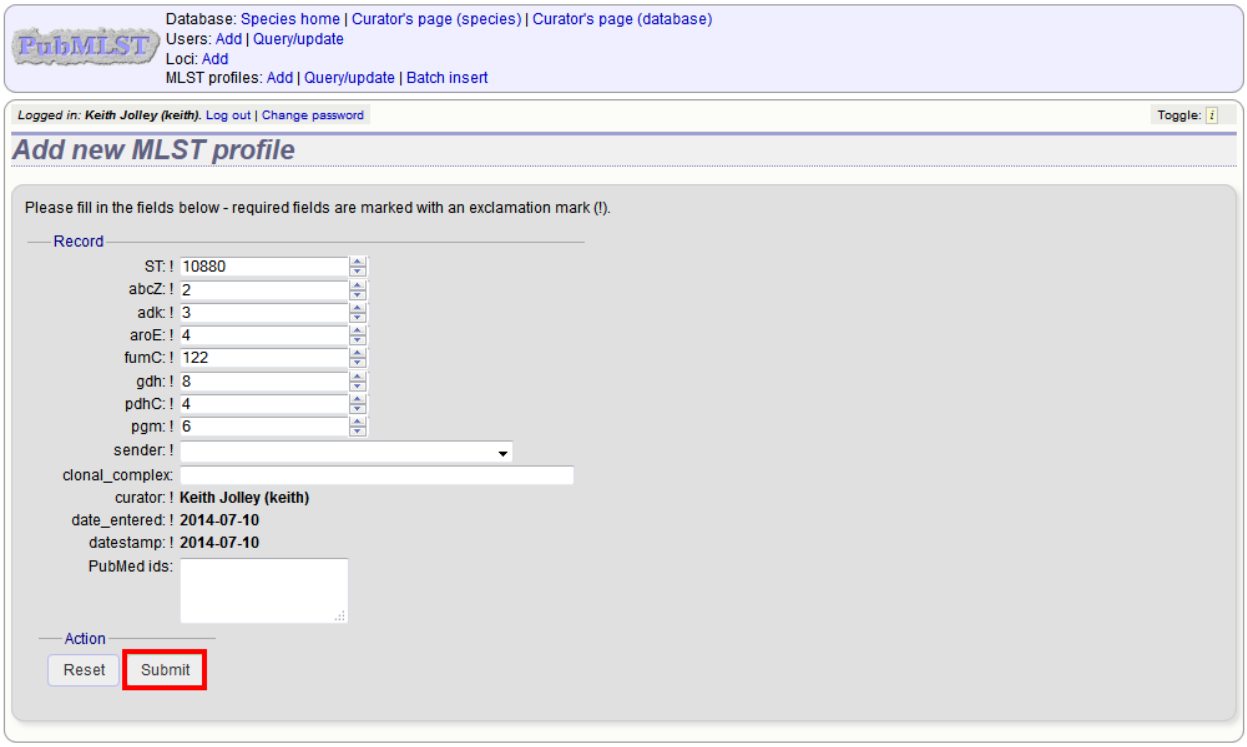
6.6 Adding new scheme profile definitions

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

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

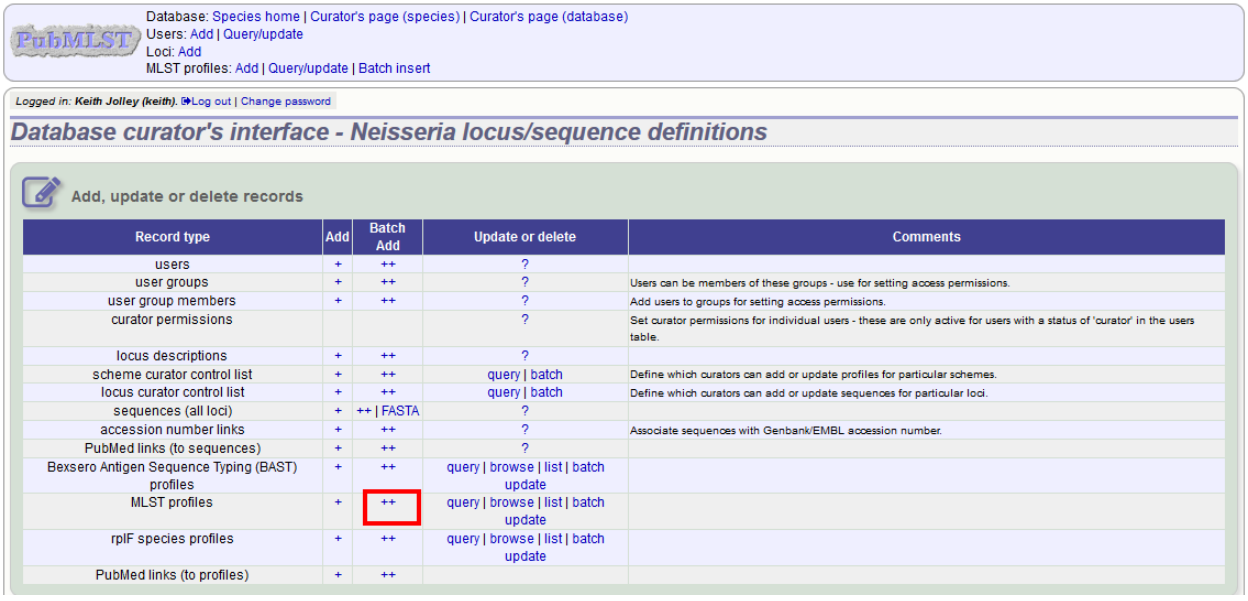


A form will be displayed with the next available primary key number already entered (provided integers are used for the primary key format). Enter the new profile, associated scheme fields, and the sender, then click 'Submit'. The new profile will be added provided the primary key or the profile has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



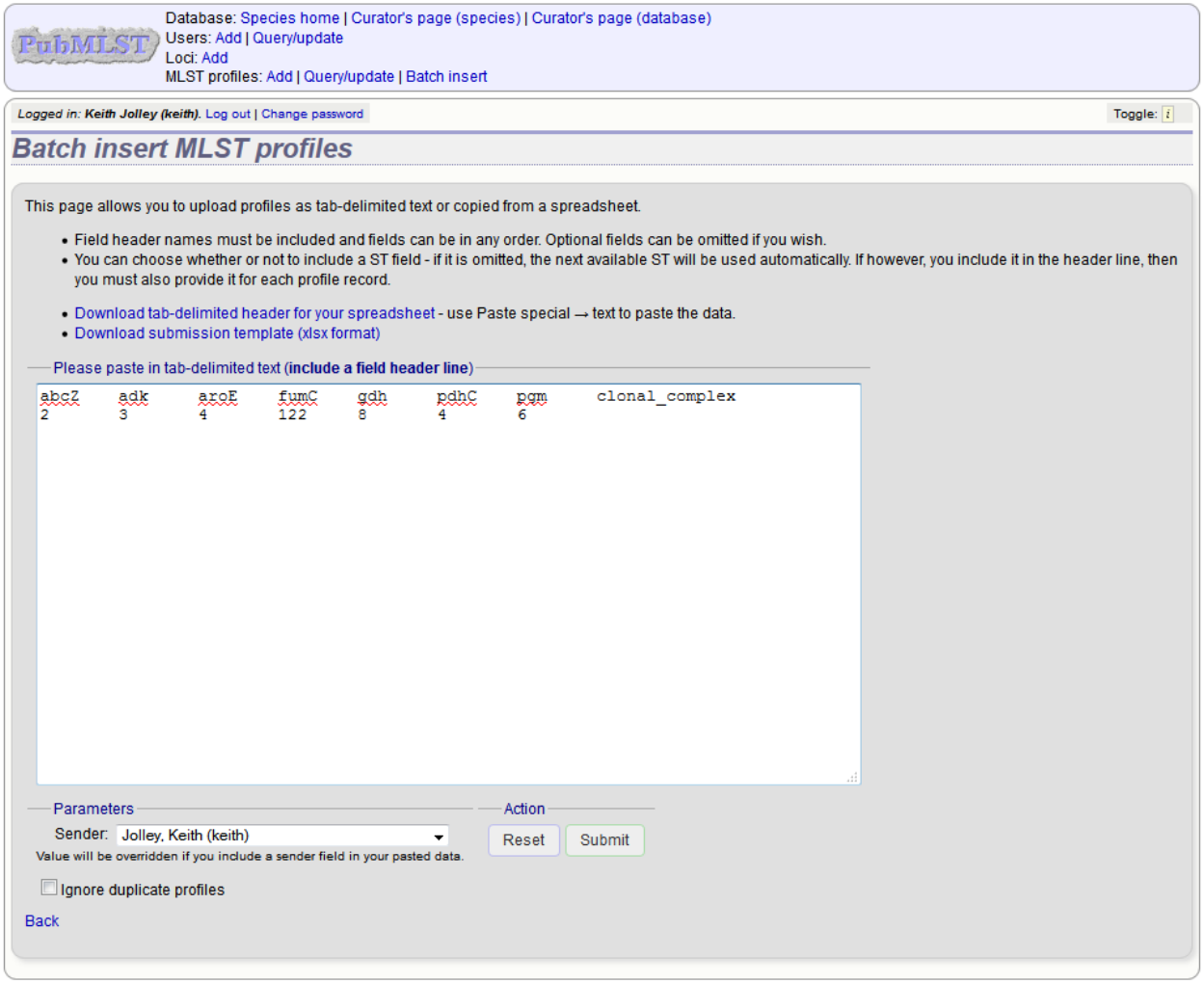
More usually, profiles are added in a batch mode. It is often easier to do this even for a single profile since it allows copying and pasting data from a spreadsheet.

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.

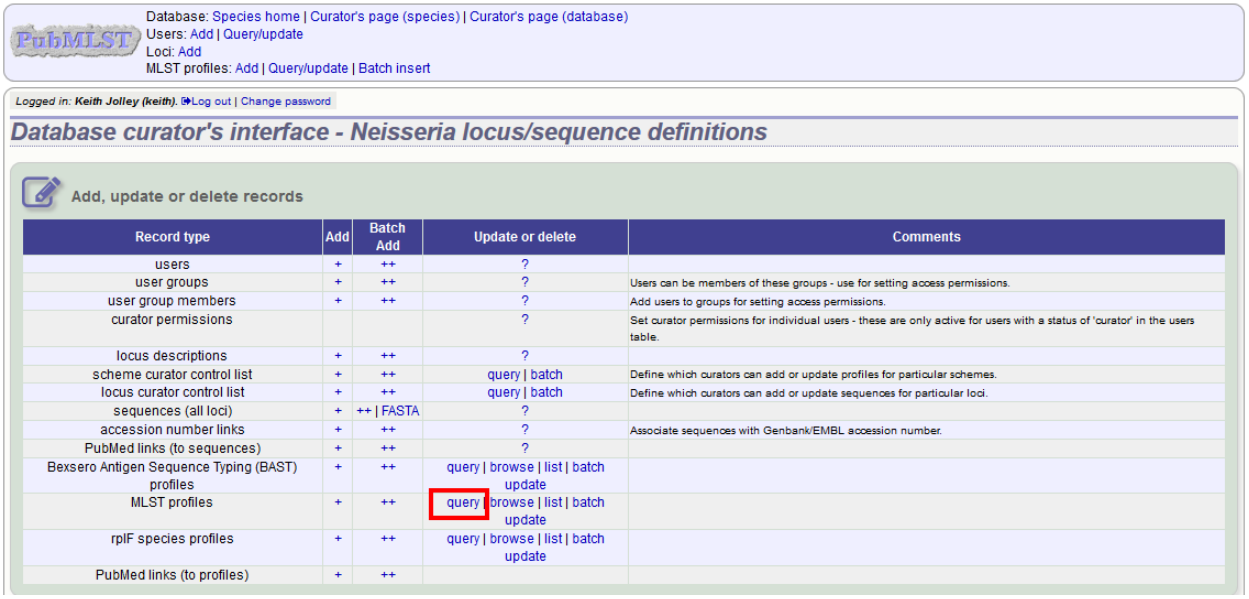
Fill in the spreadsheet using the copied template, then copy and paste the whole spreadsheet in to the large form on the upload page. If the primary key has an integer format, you can exclude this column and the next available number will be used automatically. If the column is included, however, a value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



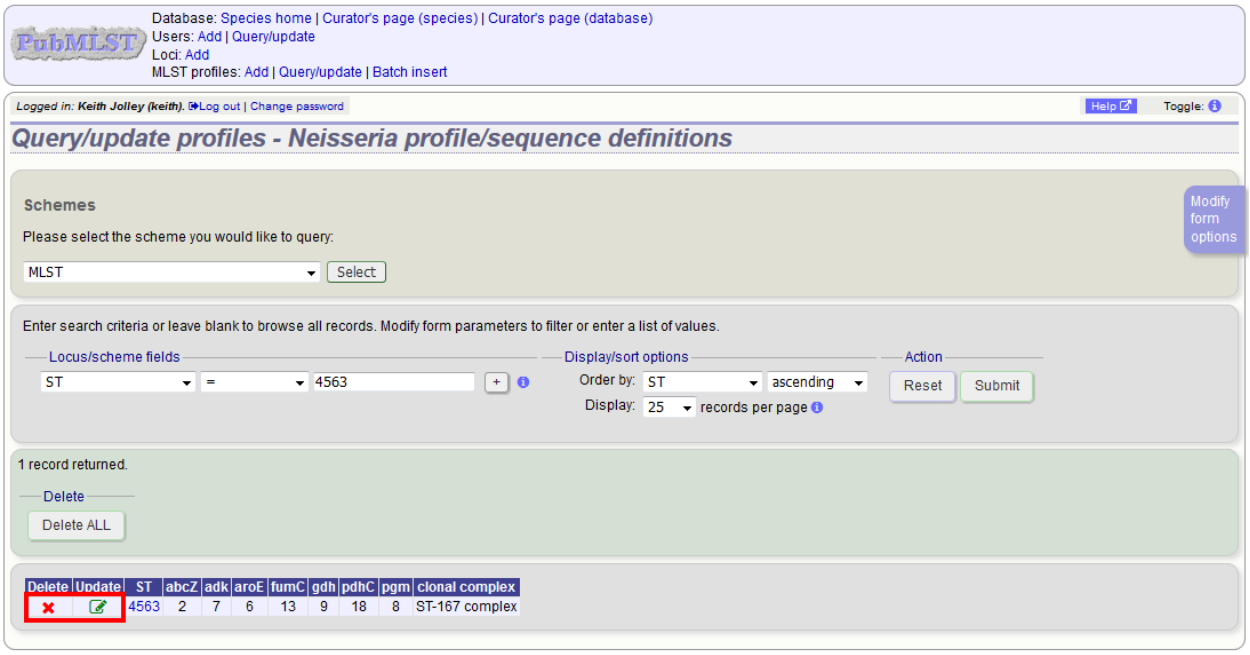
You will be given a final confirmation page stating what will be uploaded. If you wish to proceed with the submission, click 'Import data'.

6.7 Updating and deleting scheme profile definitions

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



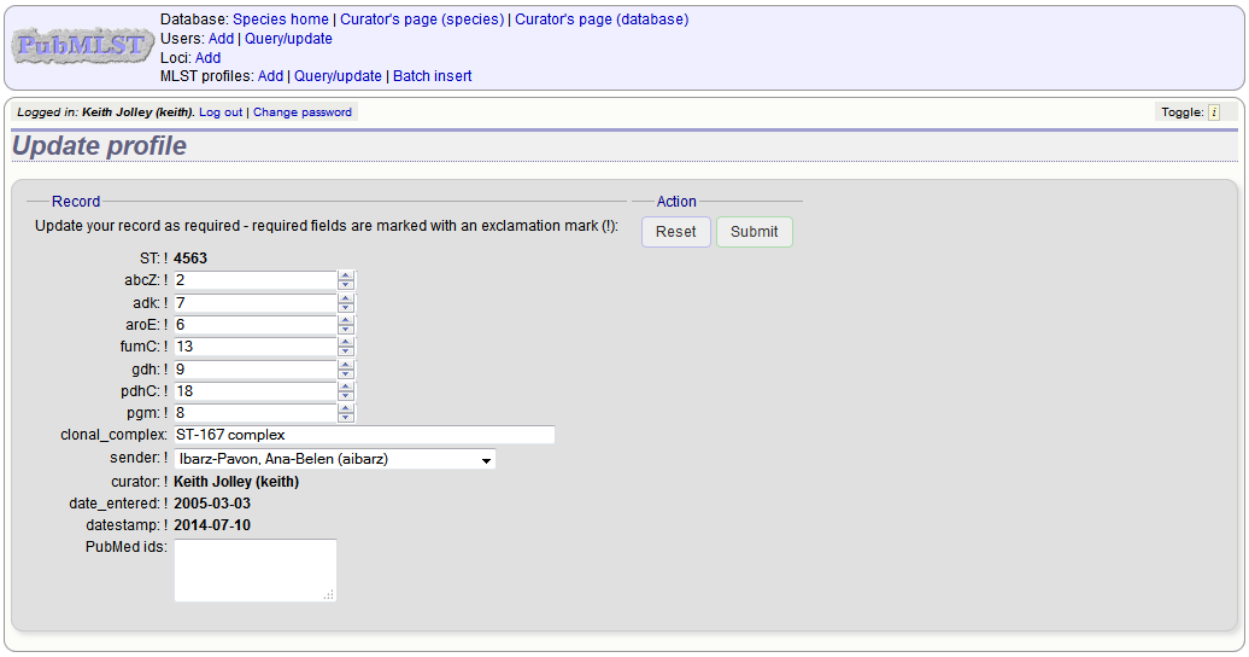
Search for your profile by entering search criteria (alternatively you can use the browse or list query functions).



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

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

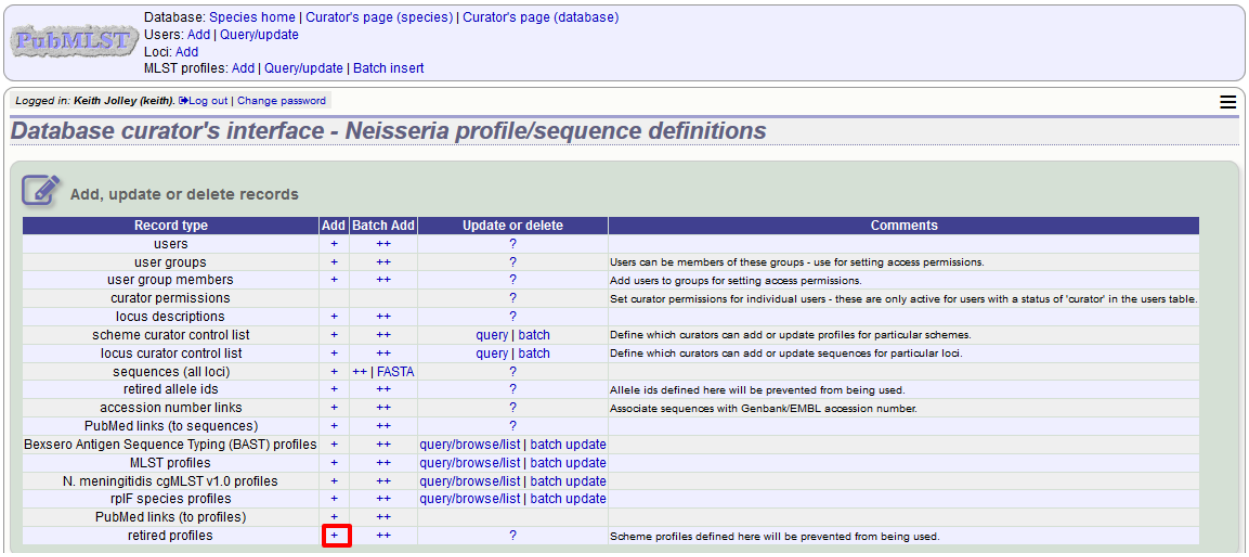
To modify the profile, click the 'Update' link next to the profile following the query. A form will be displayed - make any changes and then click 'Update'.



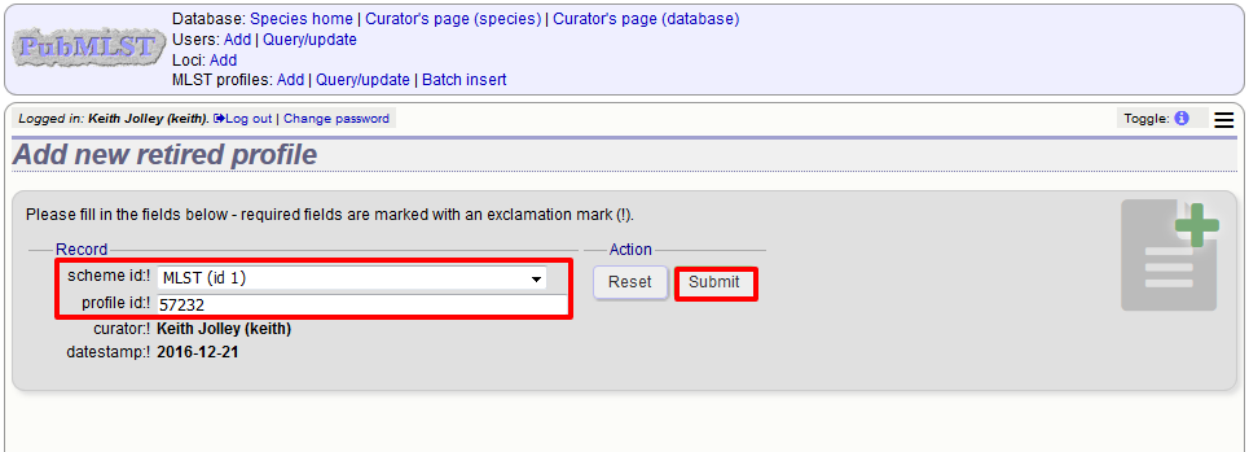
6.8 Retiring scheme profile definitions

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

You can retire a profile identifier by clicking the 'Add' retired profiles link on the sequence database curators' page.



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

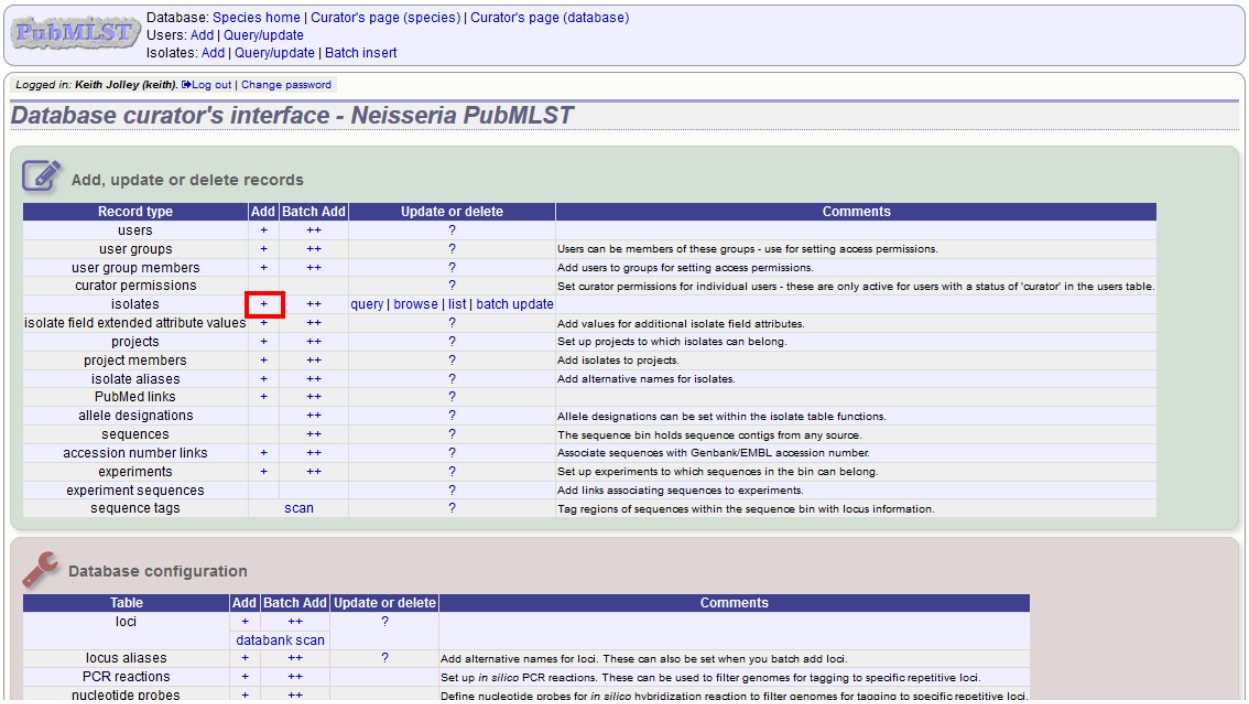


You cannot retire a profile identifier that already exists, so you must delete it before retiring it. Once an identifier is retired, you will not be able to create a new profile with that name.

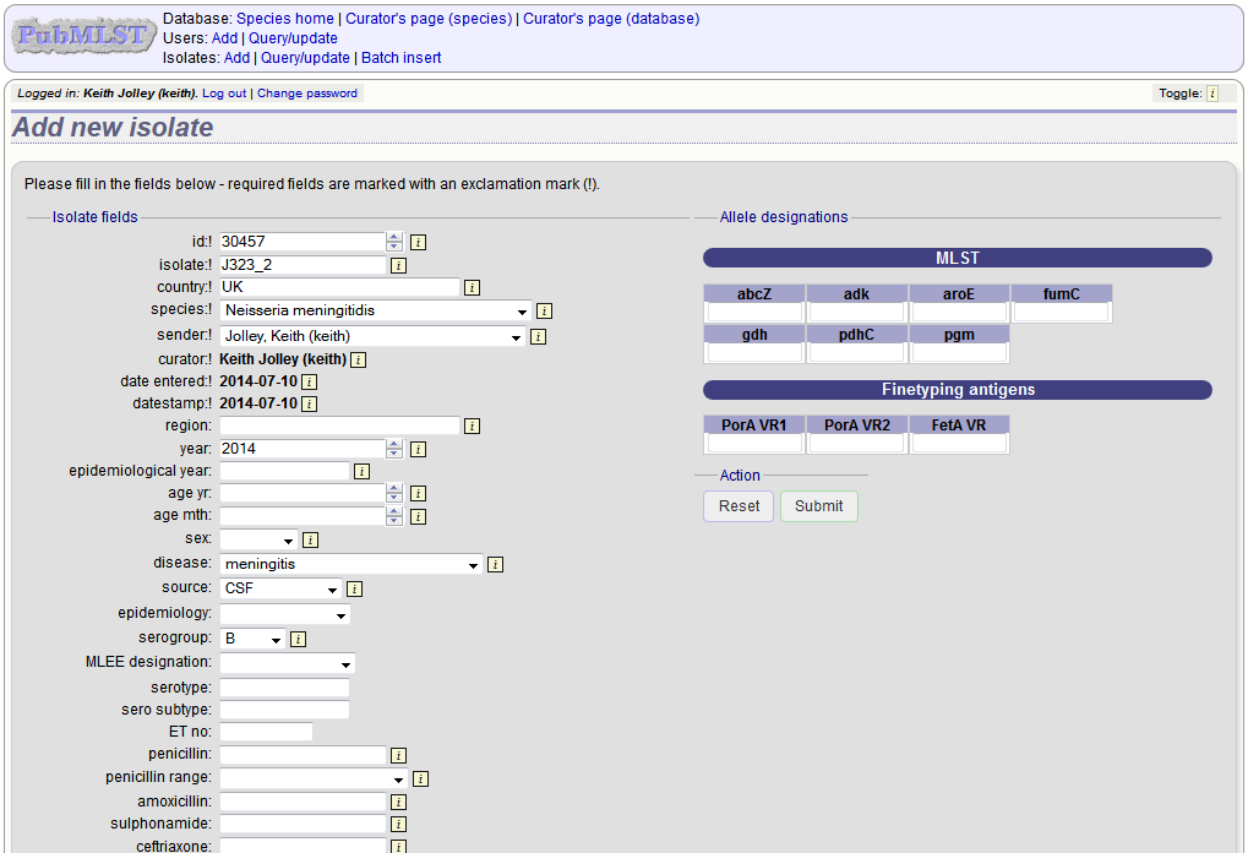
You can also retire a profile definition when you *delete a profile*.

6.9 Adding isolate records

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

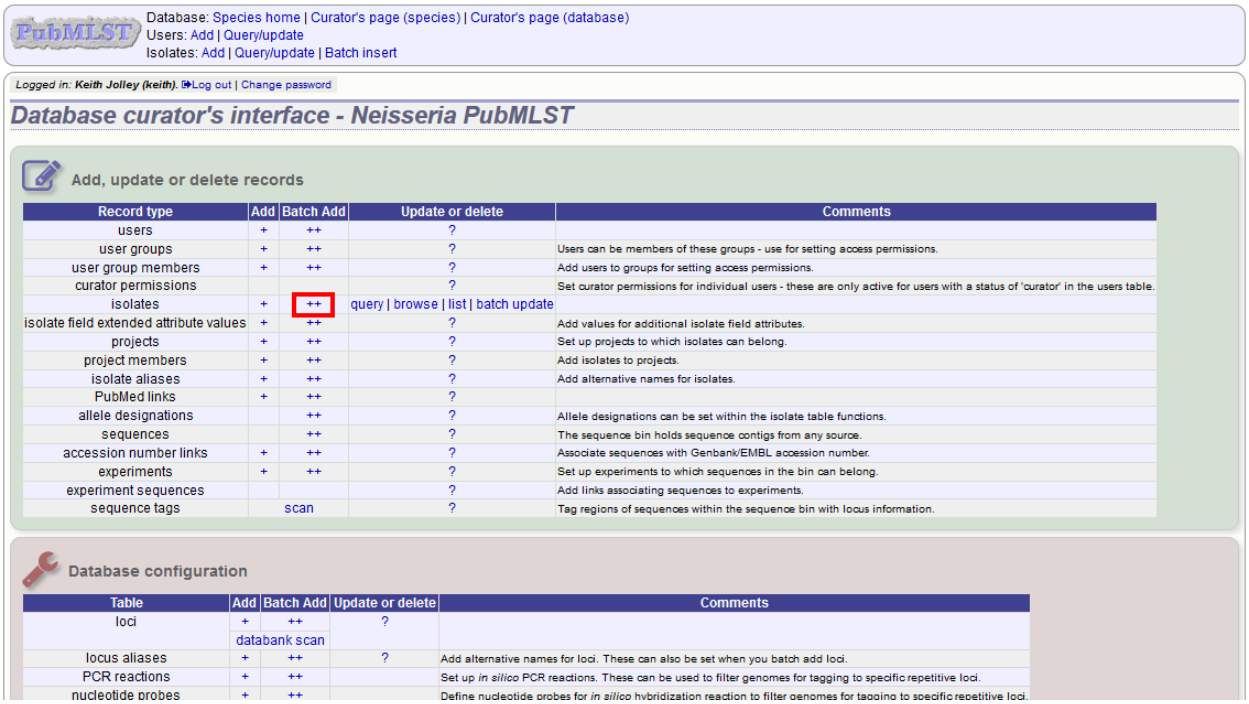


The next available id will be filled in automatically but you are free to change this. Fill in the individual fields. Required fields are listed first and are marked with an exclamation mark (!). Some fields may have drop-down list boxes of allowed values. You can also enter allele designations for any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

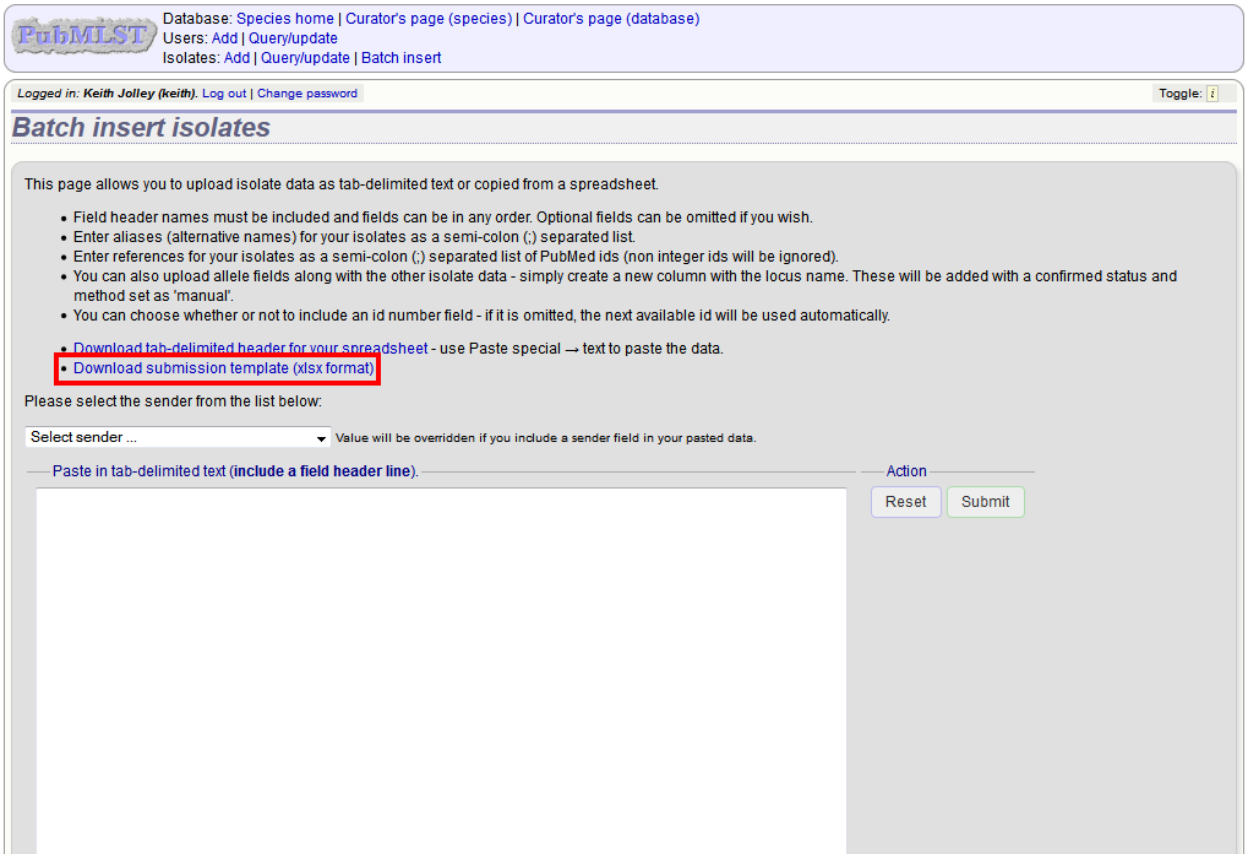


Press submit when finished. More usually, isolate records are added in batch mode, even when only a single record is added, since the submission can be prepared in a spreadsheet and copied and pasted.

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

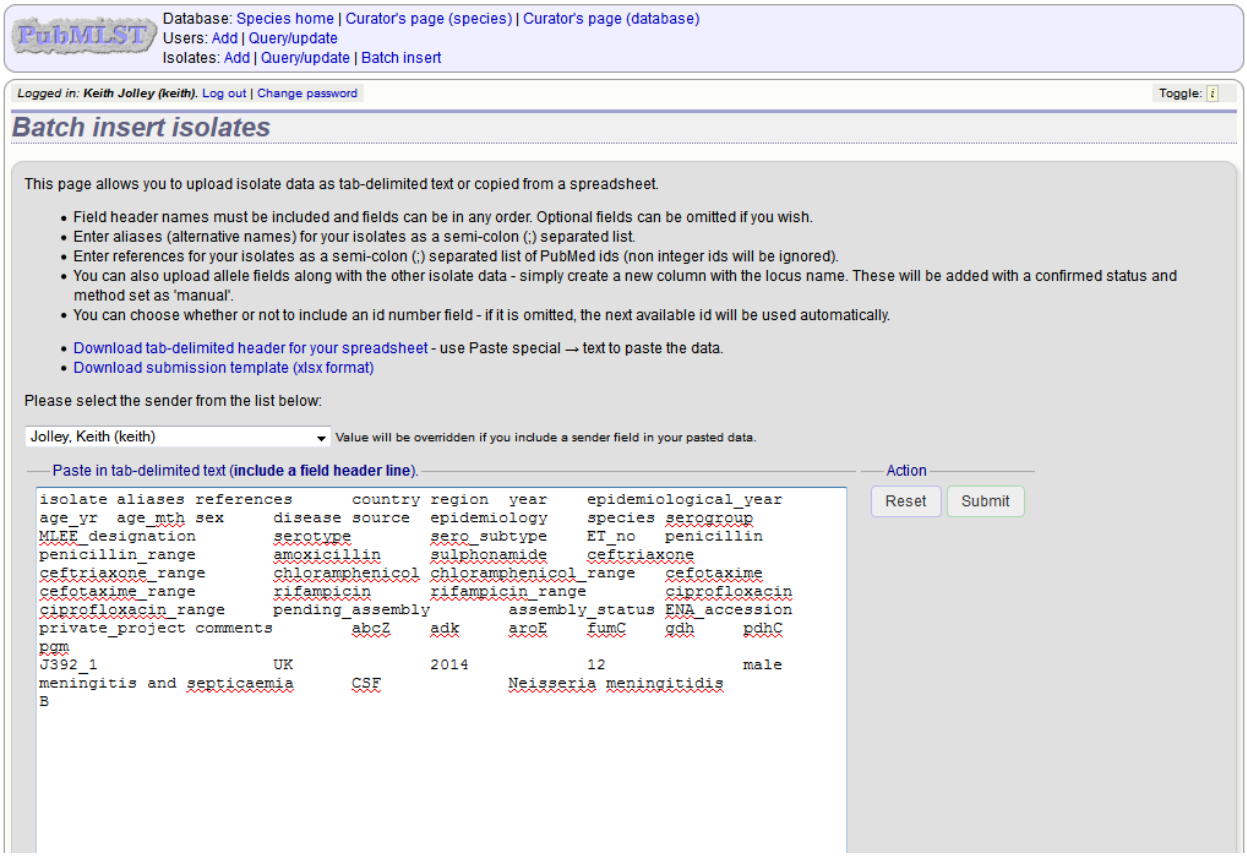


Download a submission template in Excel format from the link.

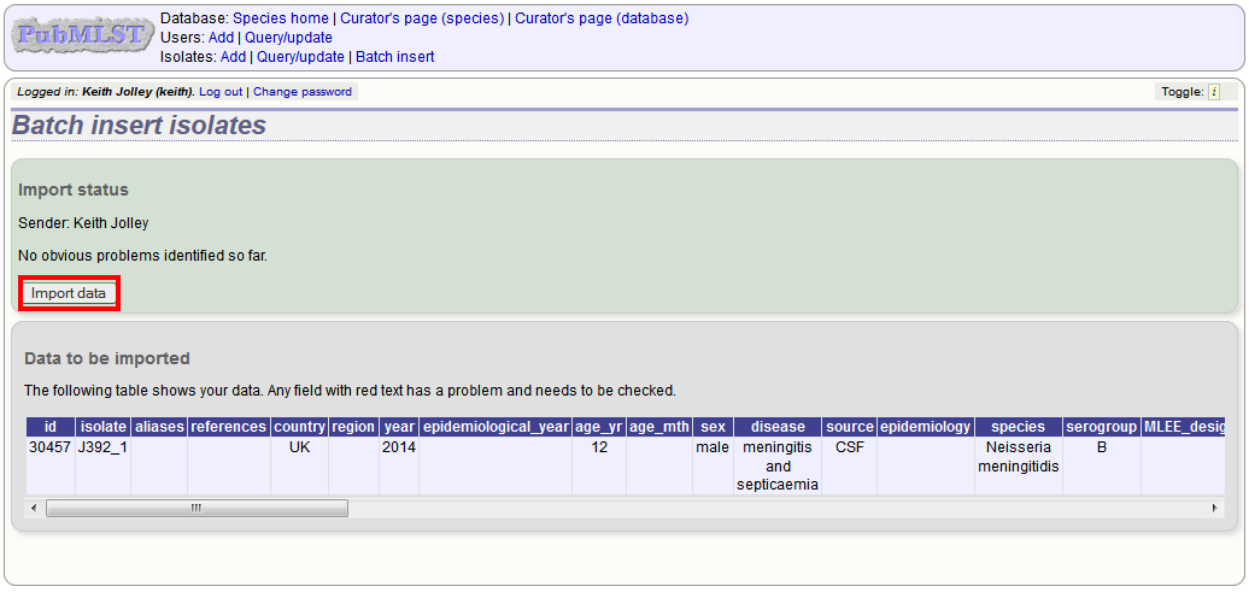


Prepare your data in the spreadsheet - the column headings must match the database fields. In databases with large numbers of loci, there won't be columns for each of these. You can, however, manually add locus columns.

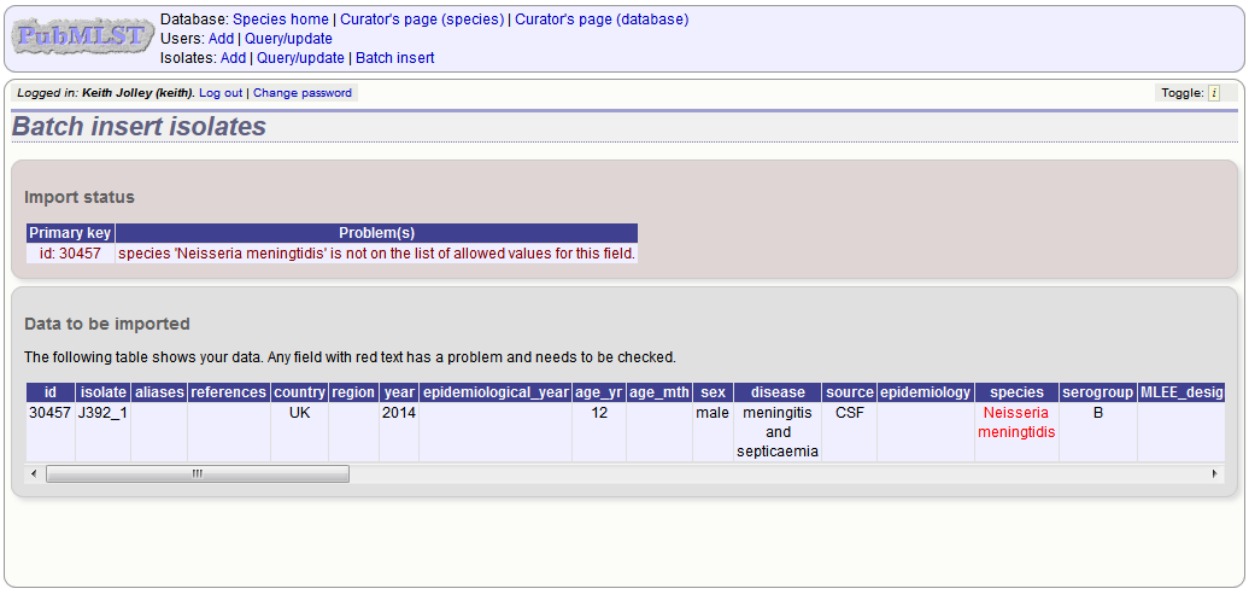
Pick a sender from the drop-down list box and paste the data from your spreadsheet in to the web form. The next available isolate id number will be used automatically (this can be overridden if you manually add an id column).



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

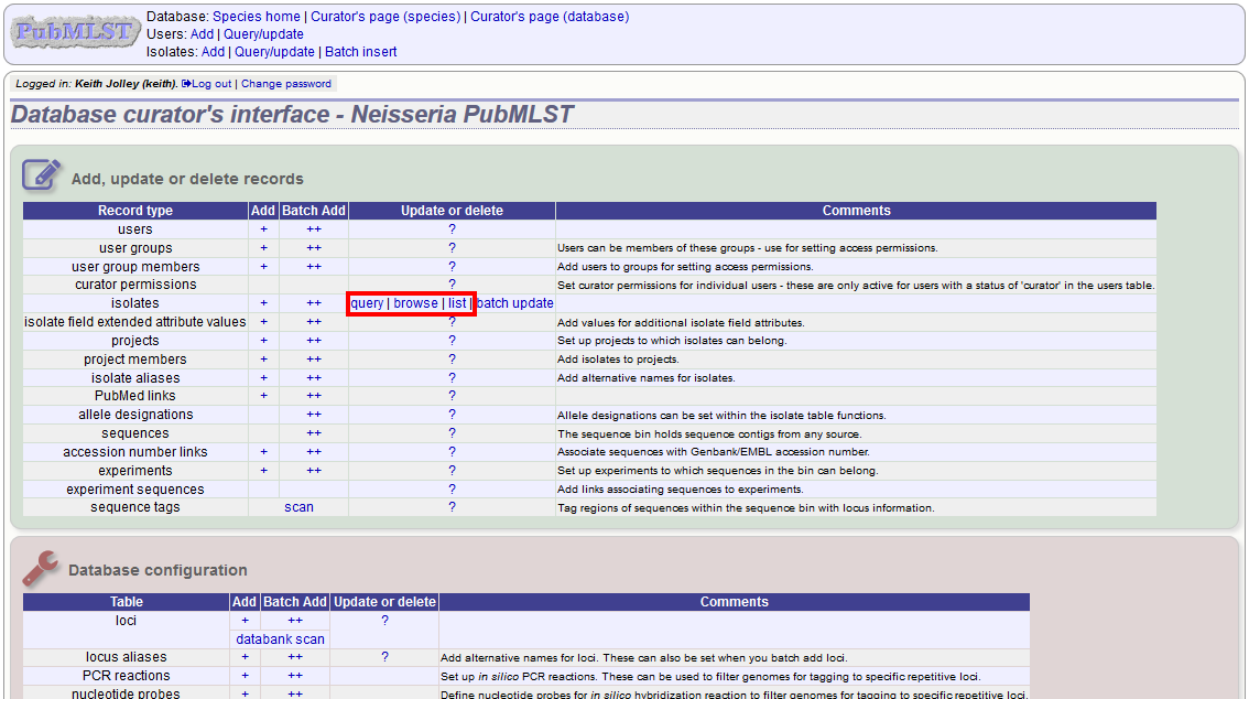


Any problems with the data will be listed and highlighted within the table. Fix the data and resubmit if this happens.

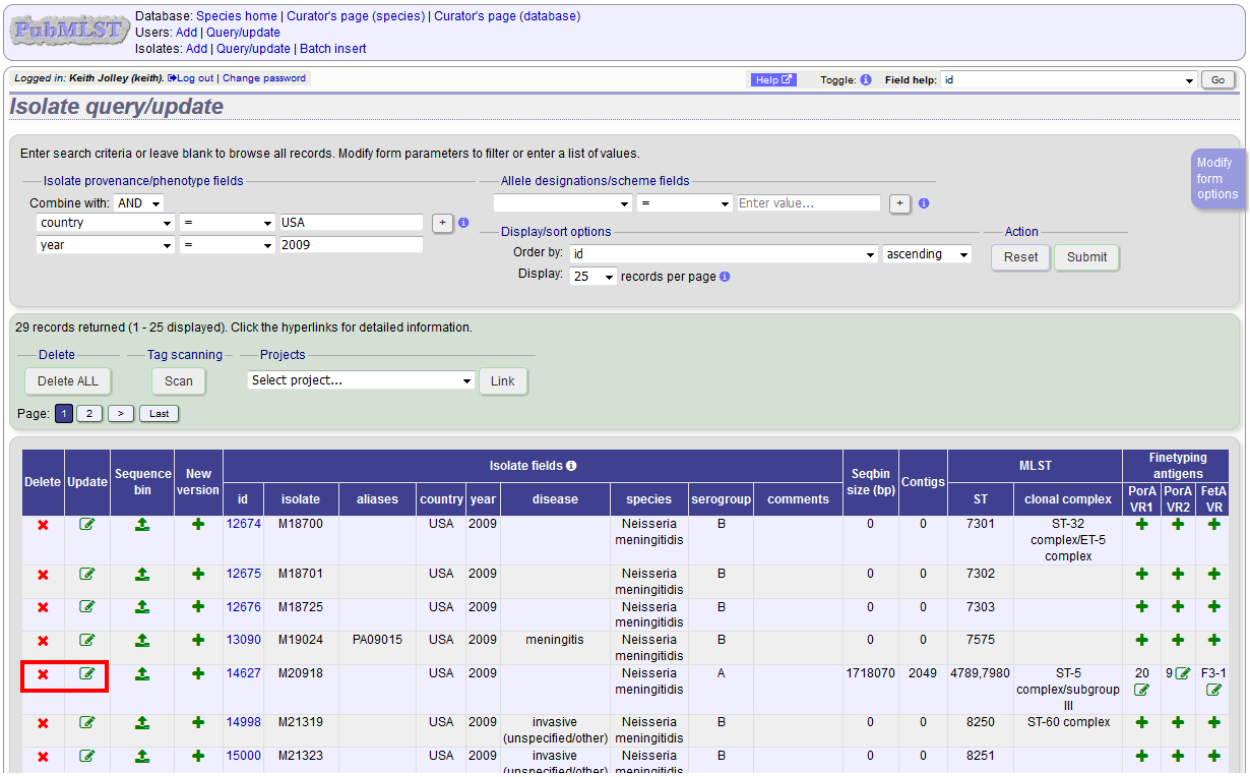


6.10 Updating and deleting single isolate records

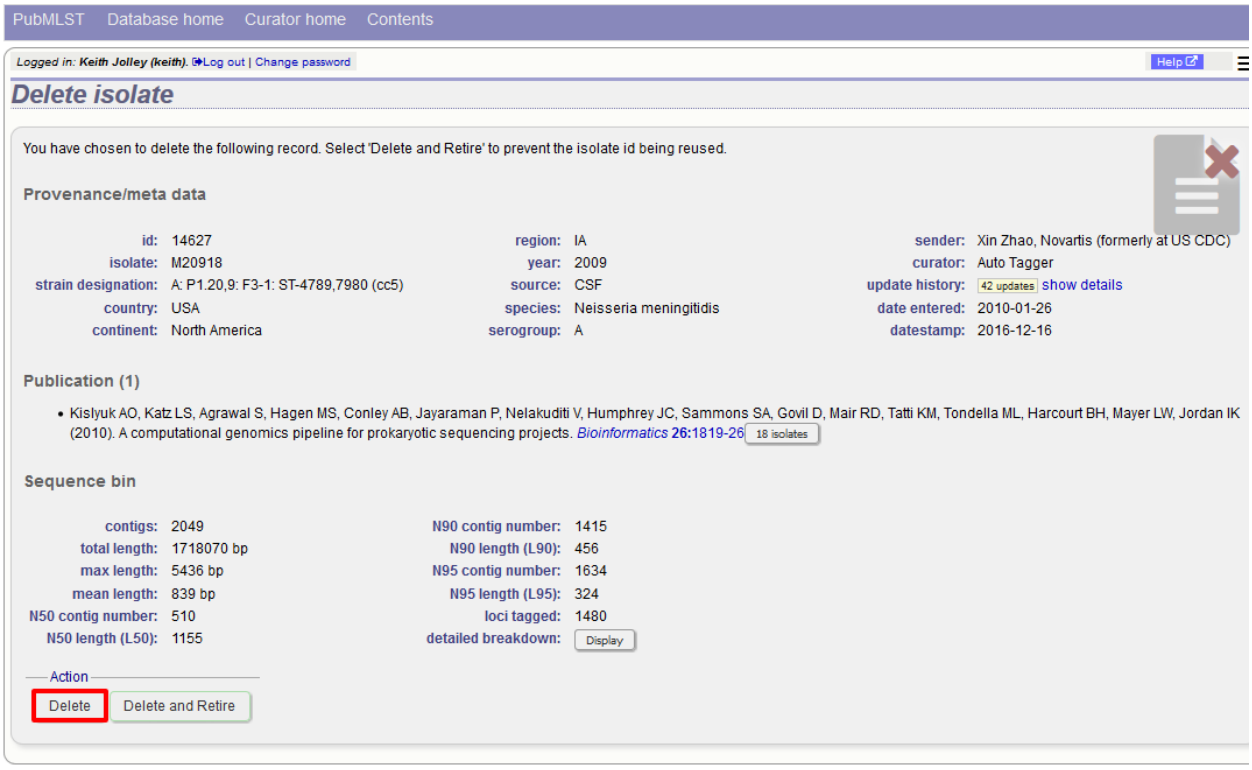
First you need to locate the isolate record. You can either browse or use a search or list query.



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.

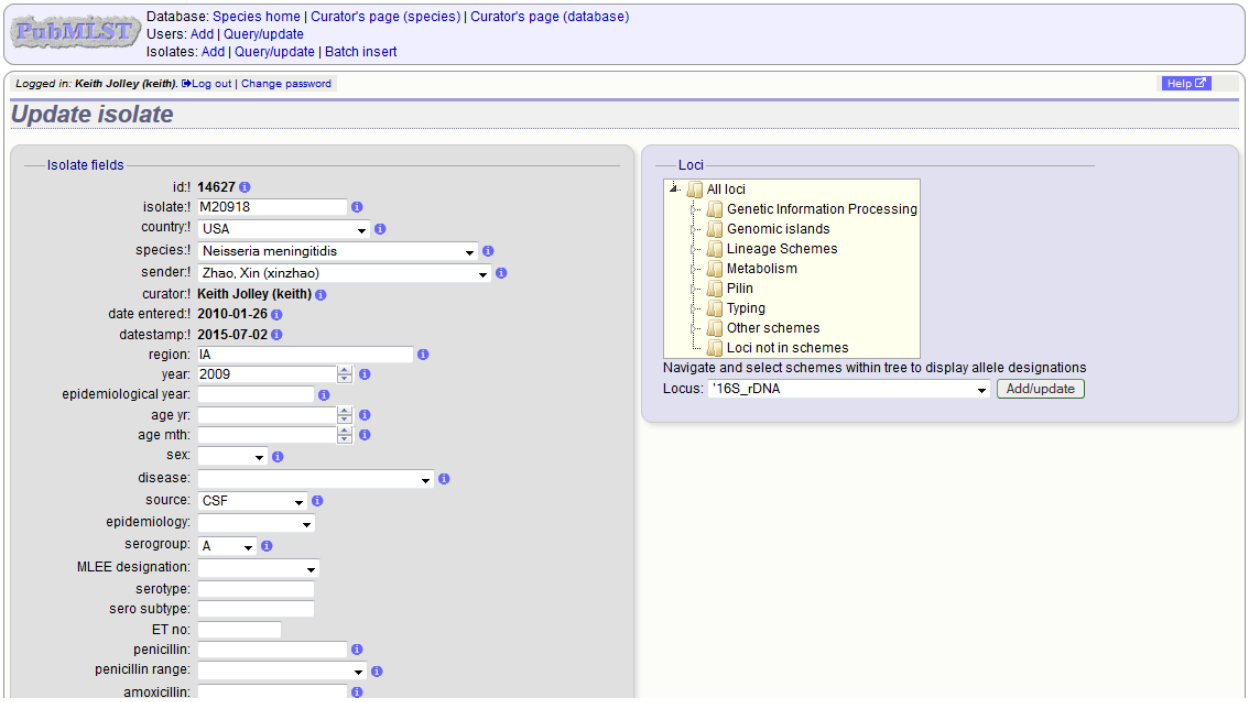


Clicking the 'Delete' link takes you to a page displaying the full isolate record.

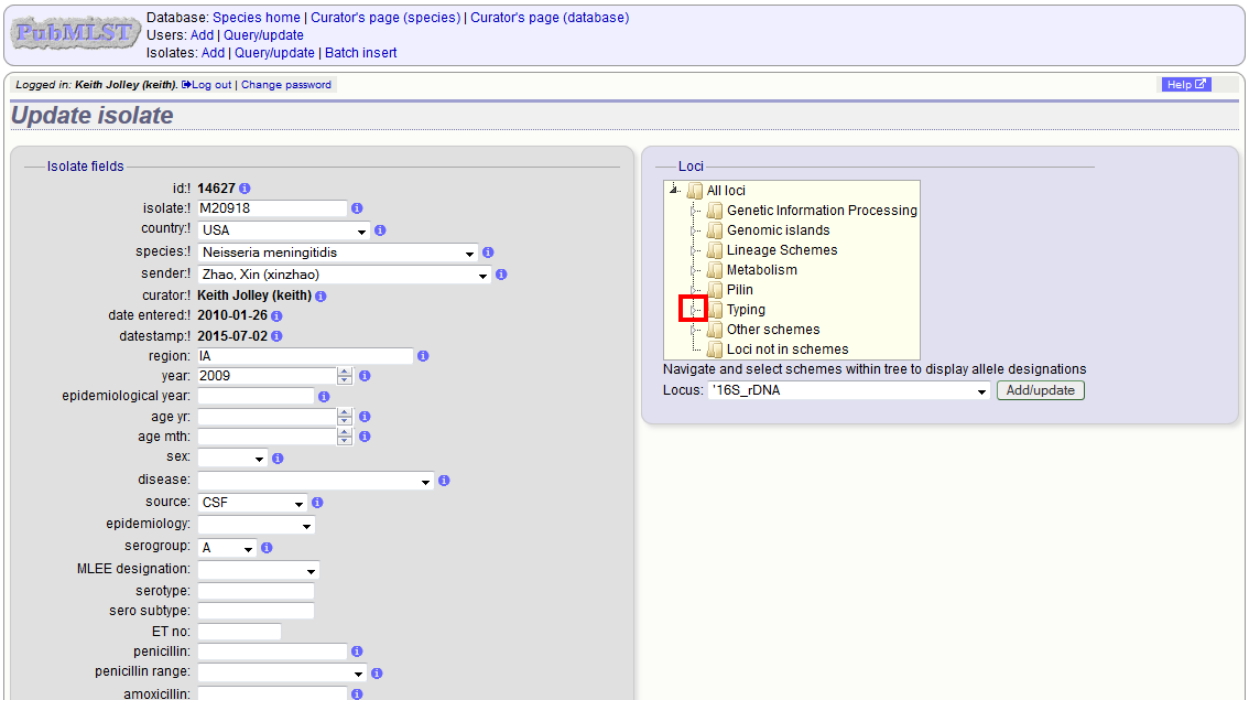


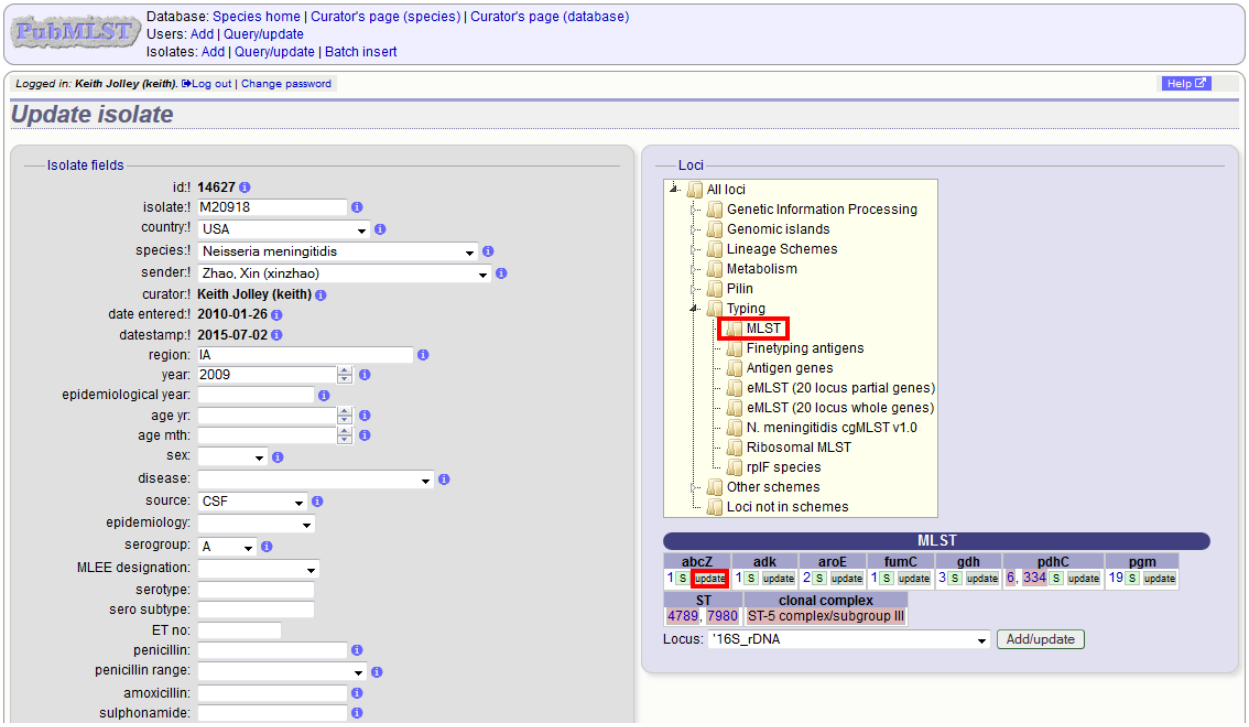
Pressing 'Delete' from this record page confirms the deletion.

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

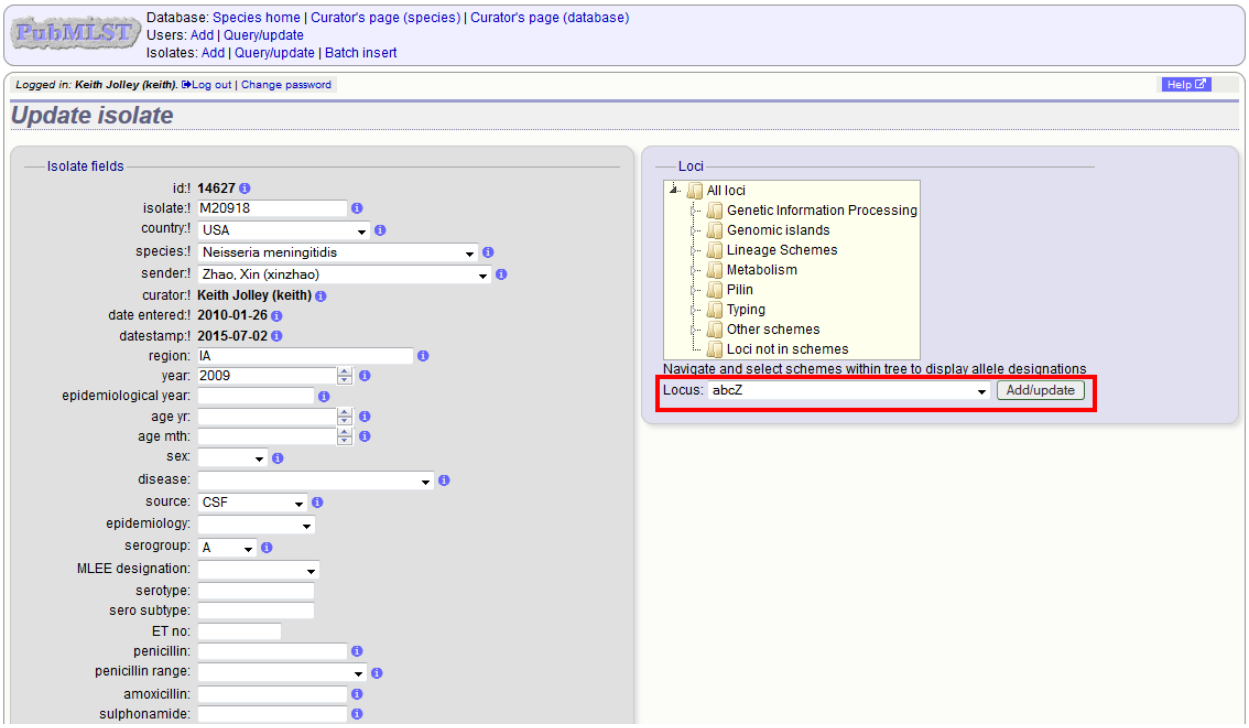


Allele designations can also be updated by clicking within the scheme tree and selecting the 'Add' or 'Update' link next to a displayed locus.

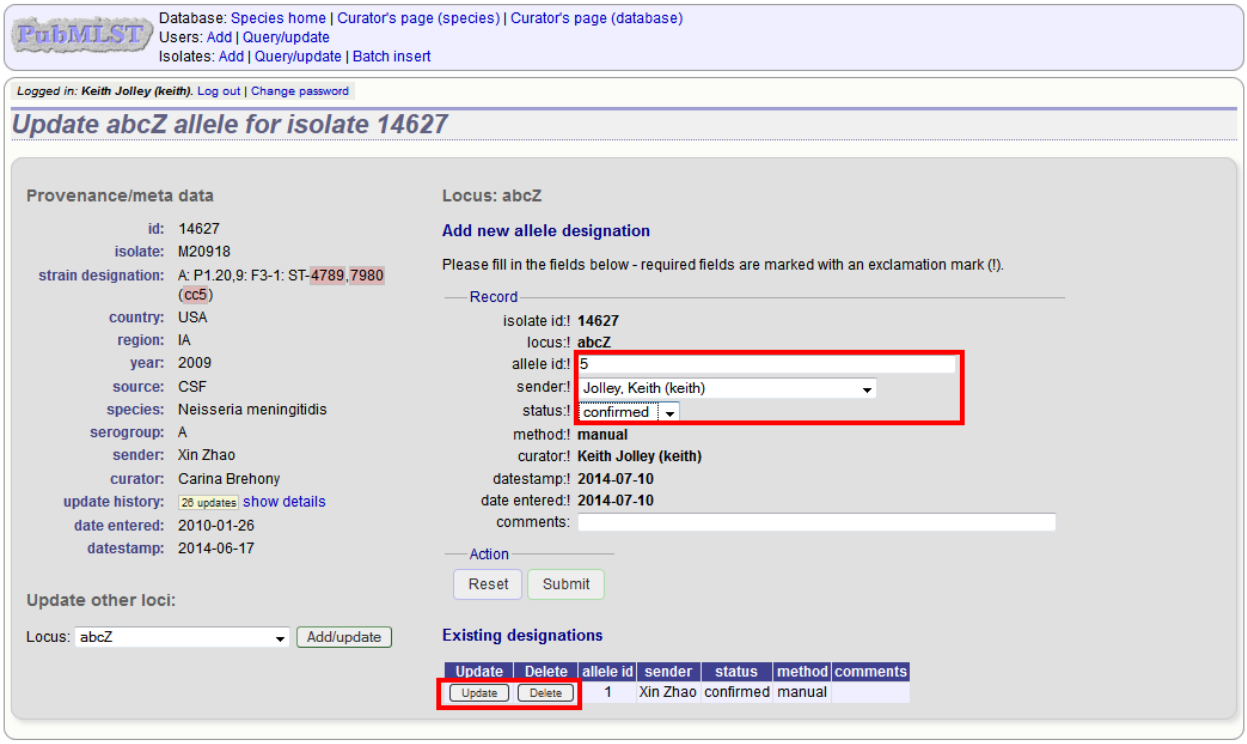




Schemes will only appear in the tree if data for at least one of the loci within the scheme has been added. You can additionally add or update allelic designations for a locus by choosing a locus in the drop-down list box and clicking 'Add/update'.

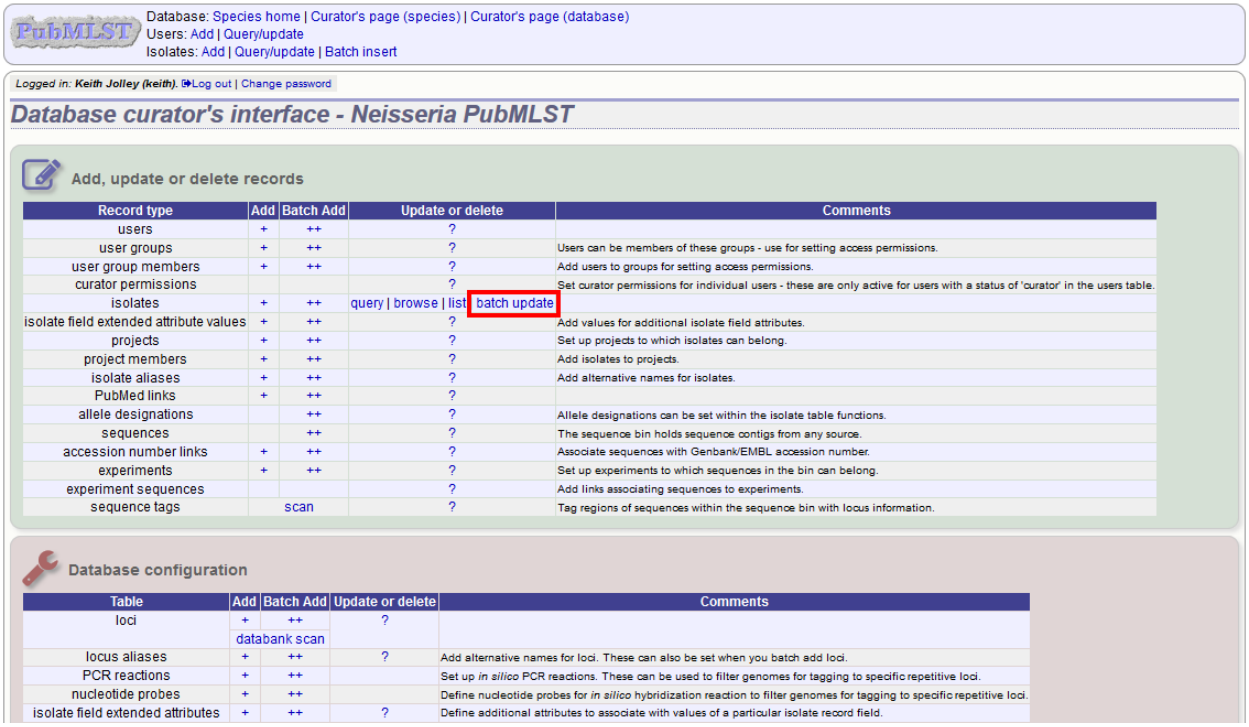


The allele designation update page allows you to modify an existing designation, or alternatively add additional designations. The sender, status (confirmed/provisional) and method (manual/automatic) needs to be set for each designation (all pending designations have a provisional status). The method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



6.11 Batch updating multiple isolate records

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



Prepare your update data in 3 columns in a spreadsheet:

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

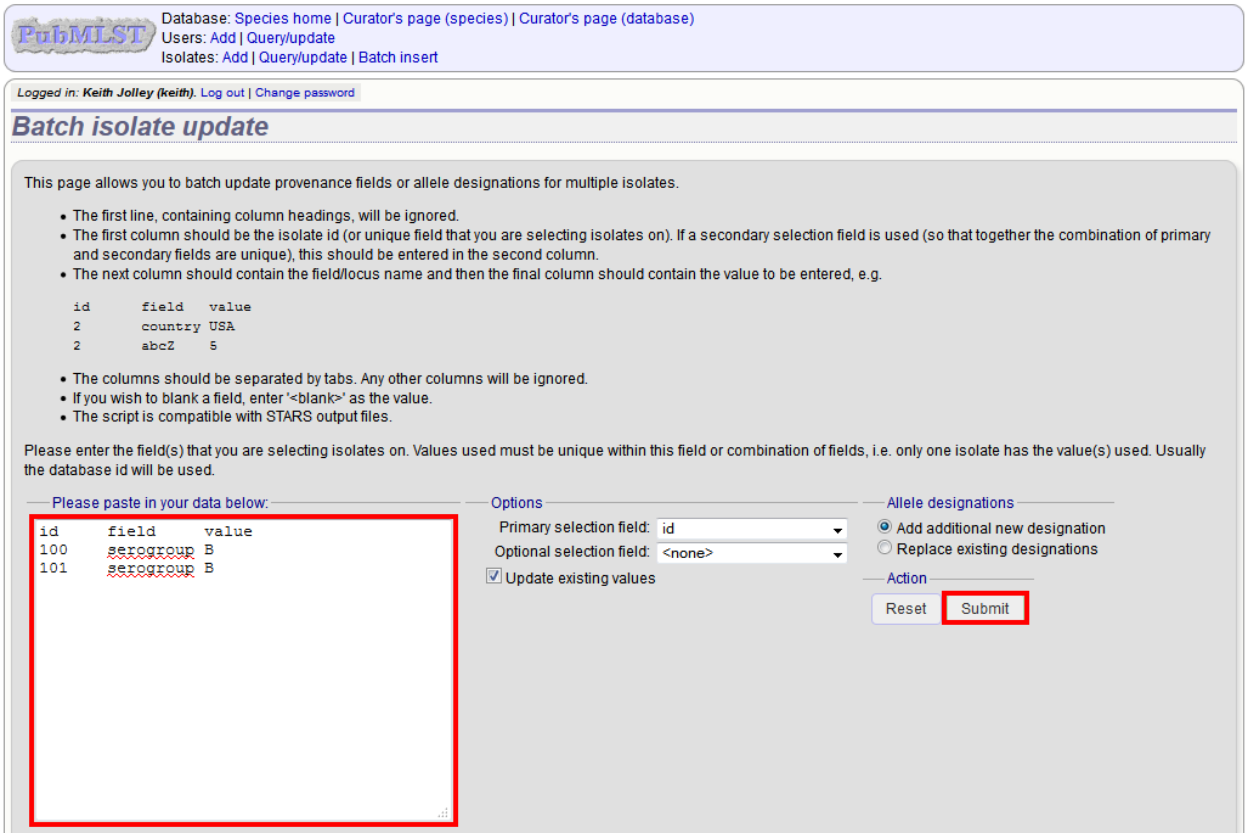
You should also include a header line at the top - this isn't used so can contain anything but it should be present.

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

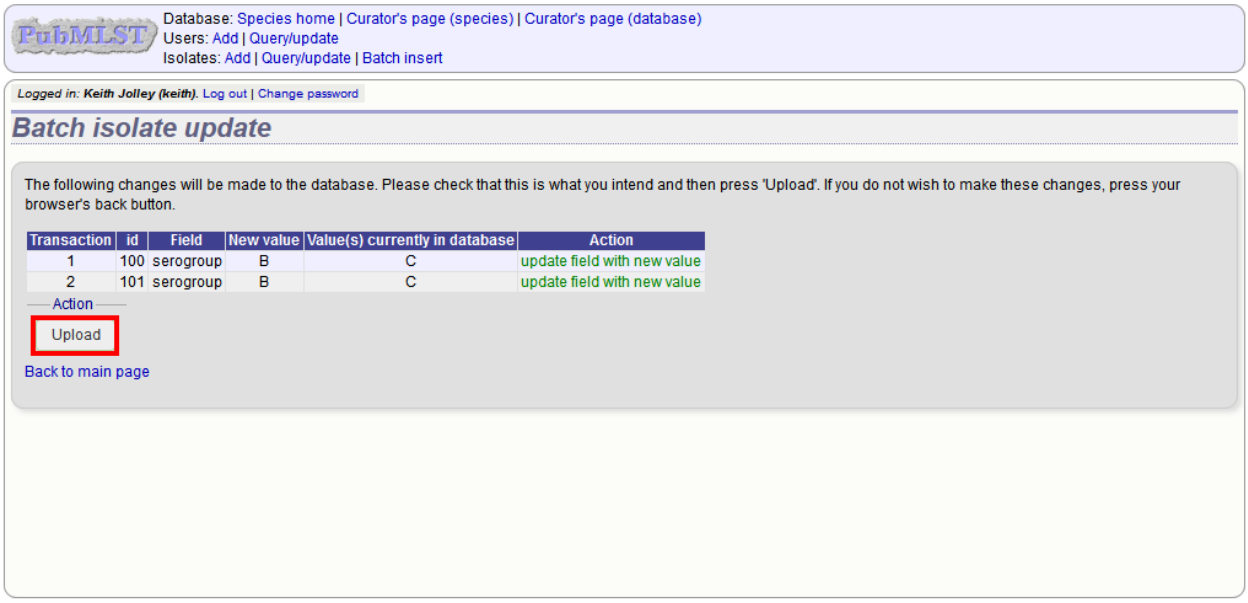
So, to update isolate id-100 and id-101 to serogroup B you would prepare the following:

```
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'.



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.



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.

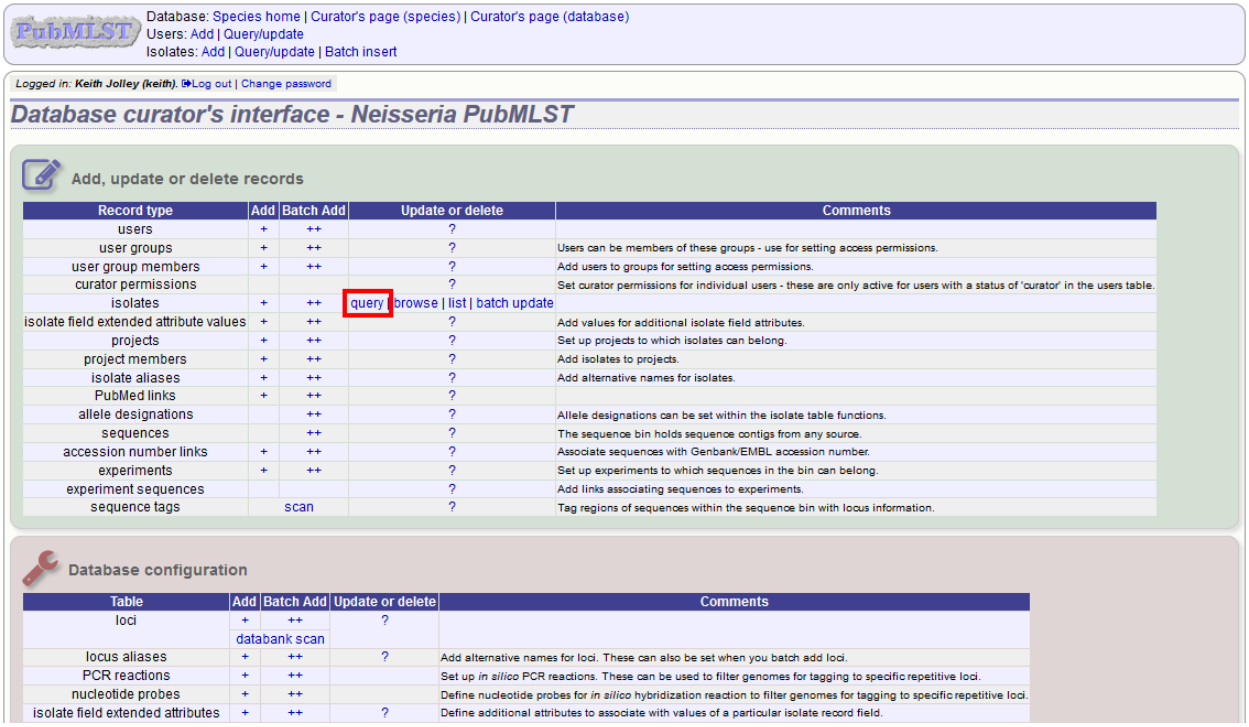
So, for example, to update the serogroups of isolates CN100 and CN103, both from the UK, select the appropriate primary and secondary fields and prepare the data as follows:

```
isolate     country     field       value
CN100       UK          serogroup   B
CN103       UK          serogroup   B
```

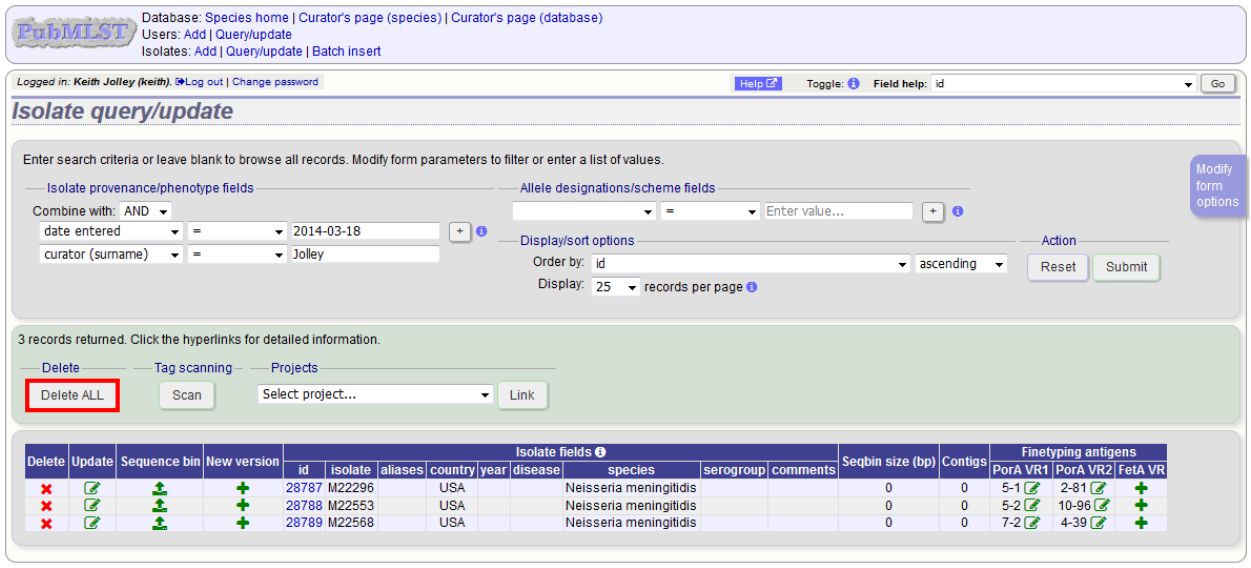
6.12 Deleting multiple isolate records

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

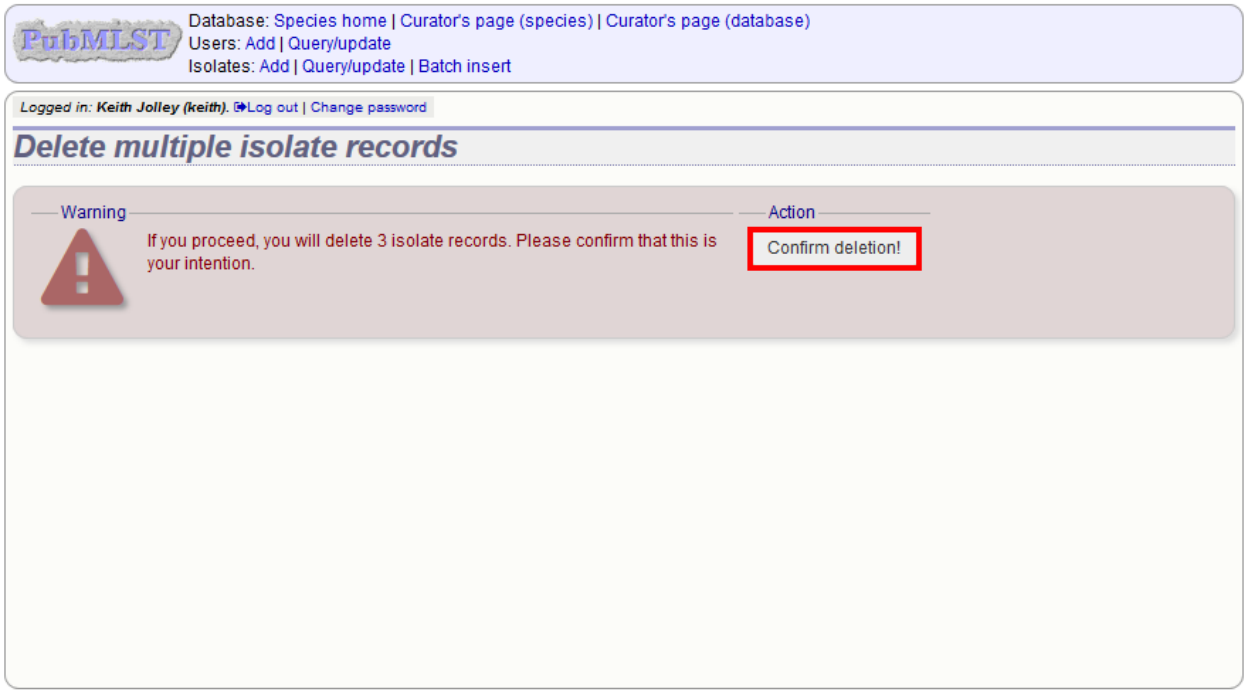
Before you can delete multiple records, you need to search for them. From the curator's main page, click the Query isolates link:



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



You will have a final chance to change your mind:

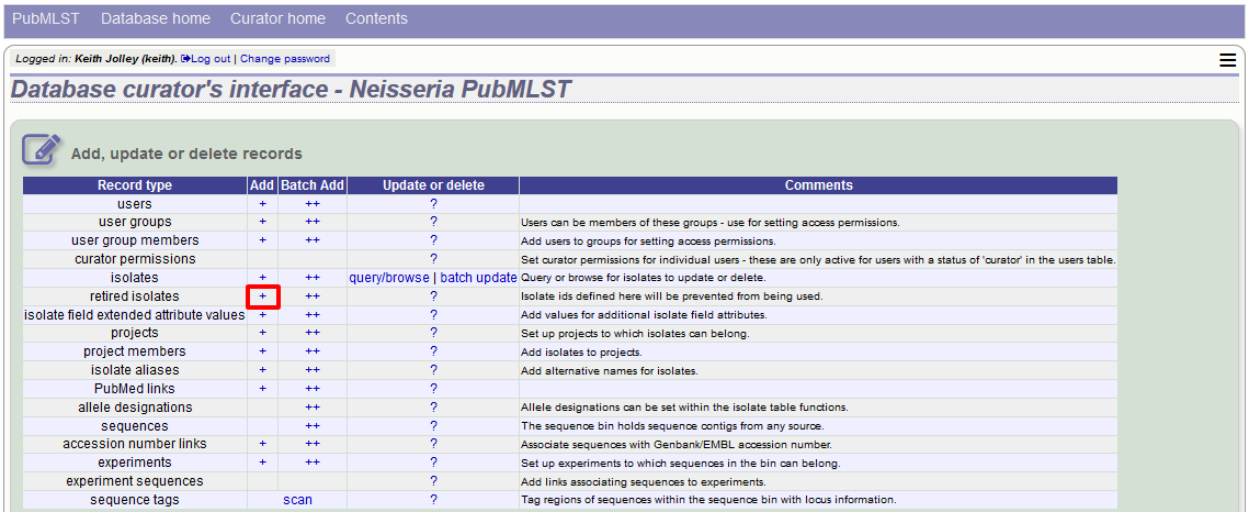


Click 'Confirm deletion!'.

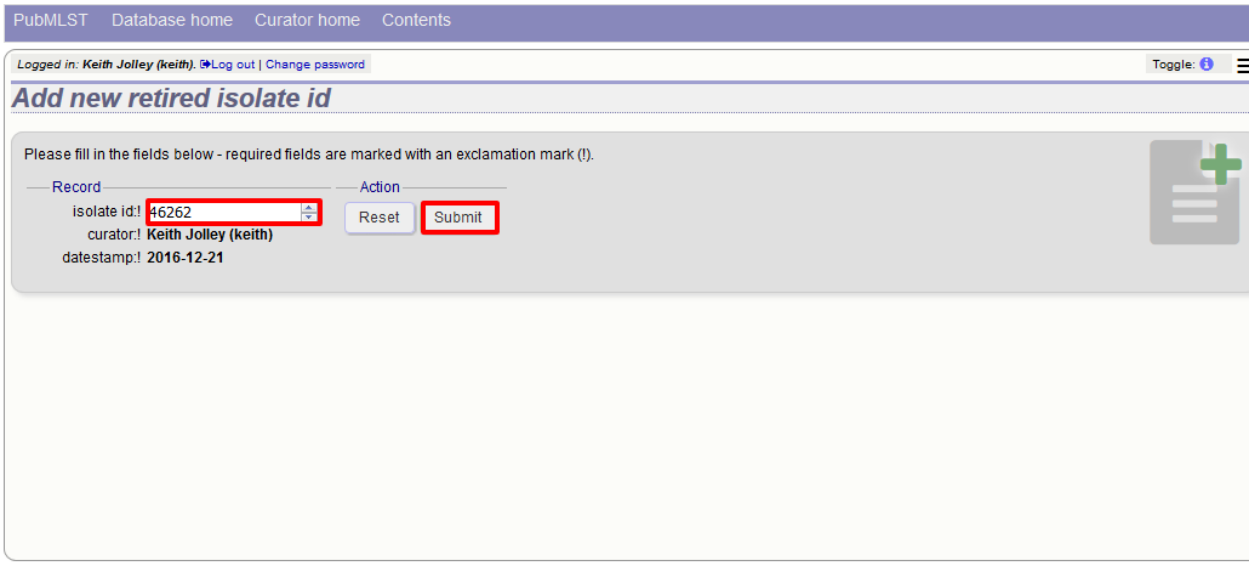
6.13 Retiring isolate identifiers

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

You can retire an isolate identifier by clicking the 'Add' retired isolates link on the isolates database curators' page.



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



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

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

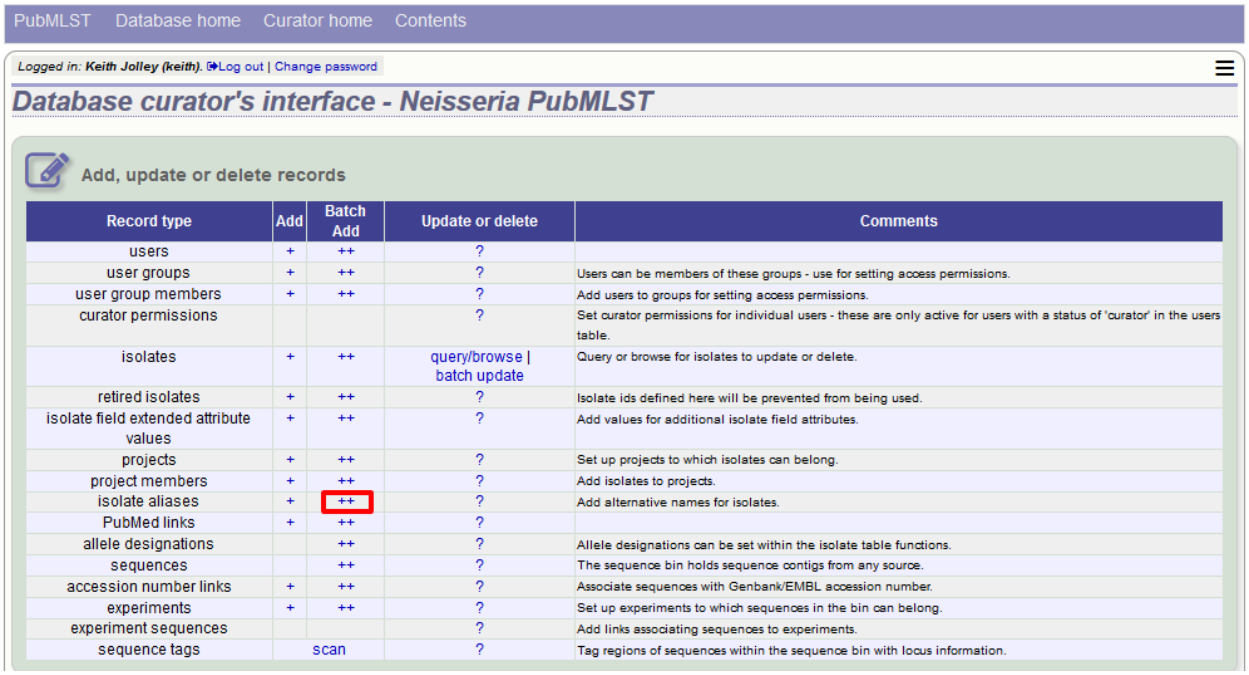
6.14 Setting alternative names for isolates (aliases)

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

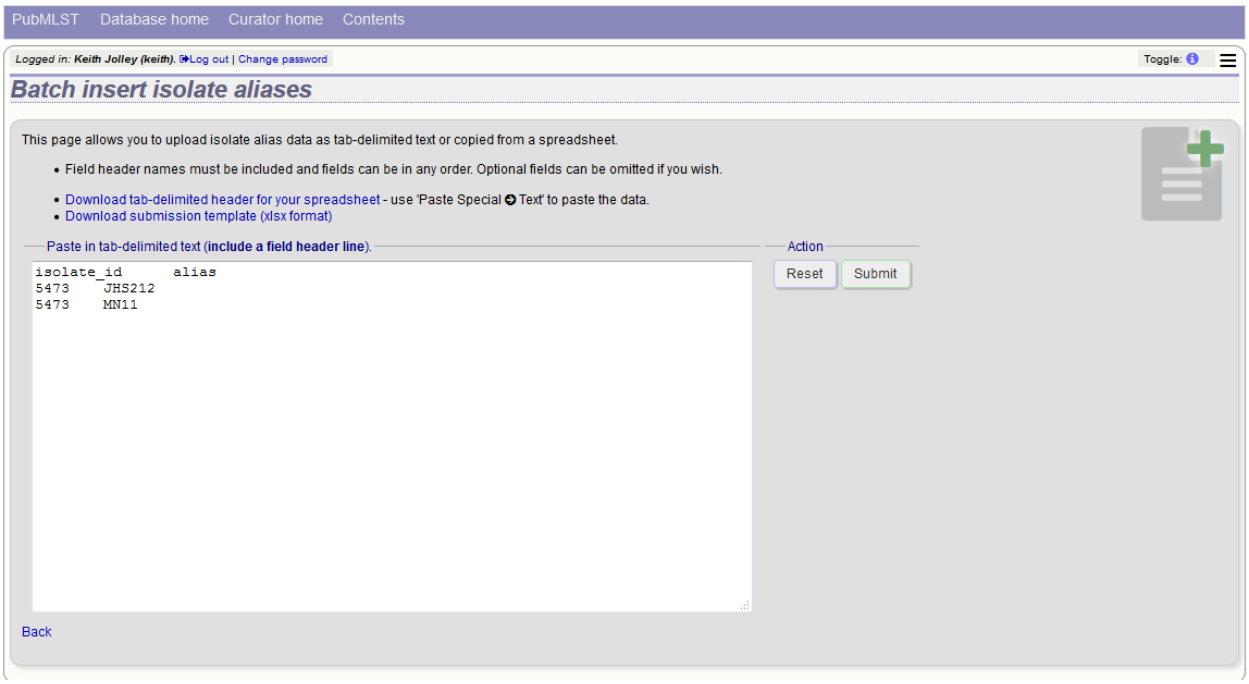
If *adding isolates* singly, add the aliases in to the aliases box (one alias per line):

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

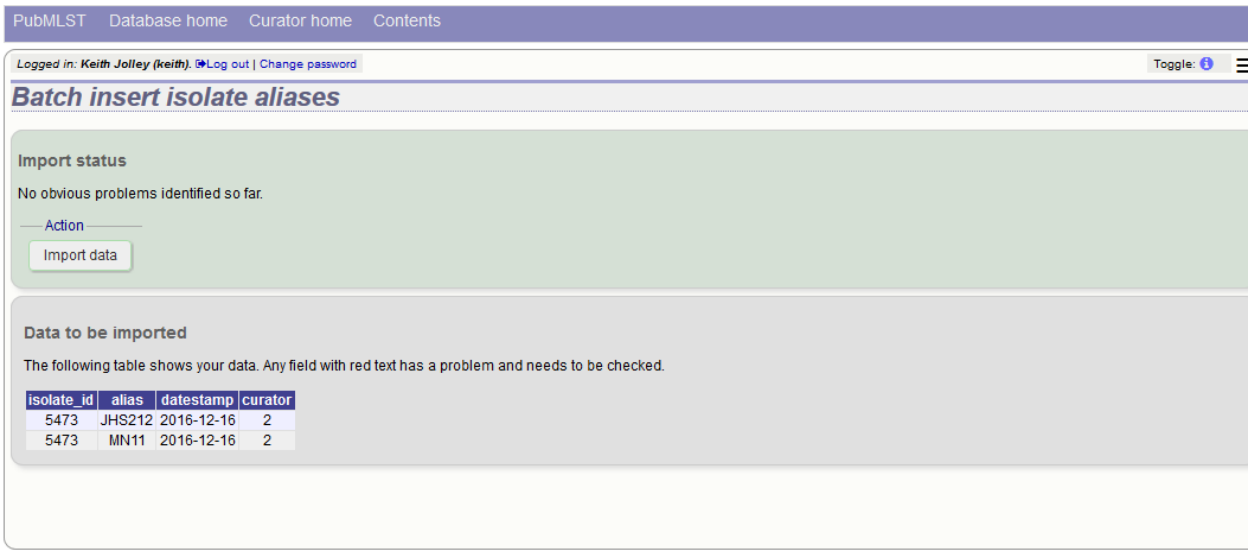
As stated above, aliases can also be batch added. To do this, click the batch add (++) link on the curator's index page.



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



A confirmation page will be displayed.

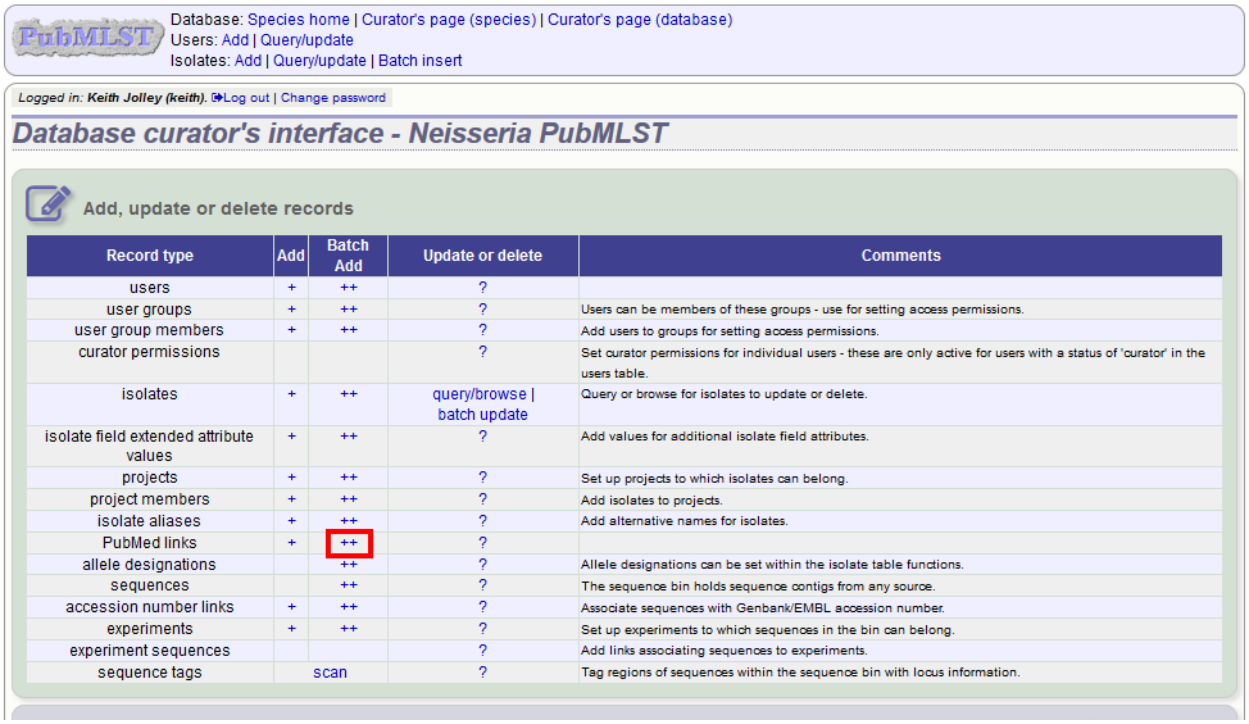


Click 'import data'.

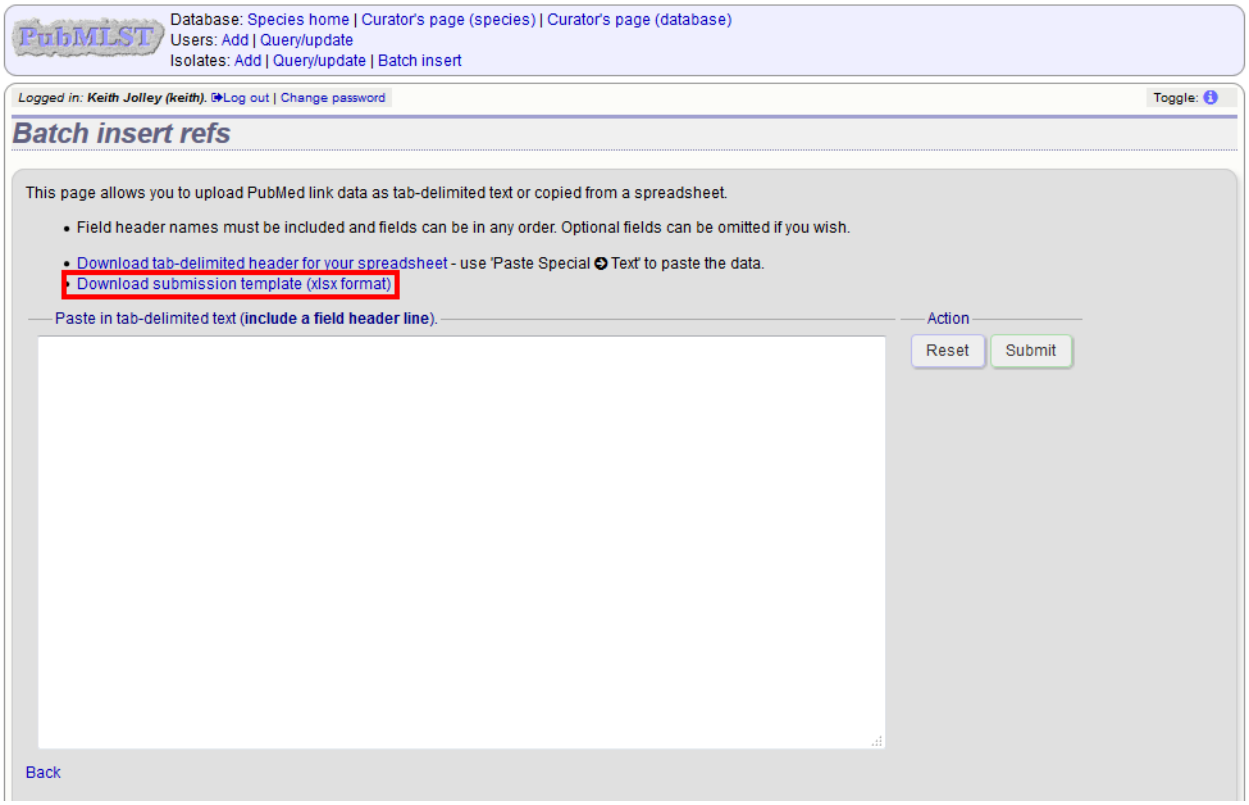
6.15 Linking isolate records to publications

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

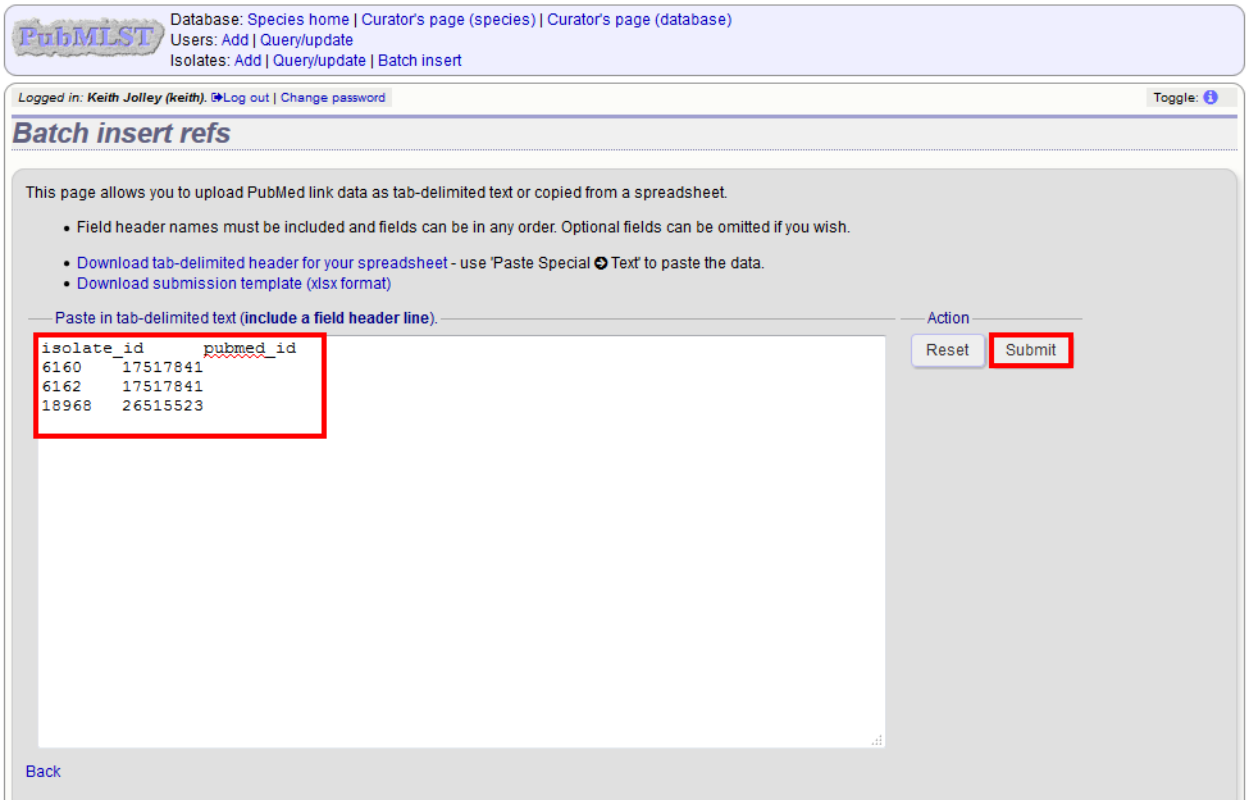
They can also be associated in batch after the upload of isolate records. Click the PubMed links batch add (++) link on the curator's main page.



Open the Excel template by clicking the link.



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



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

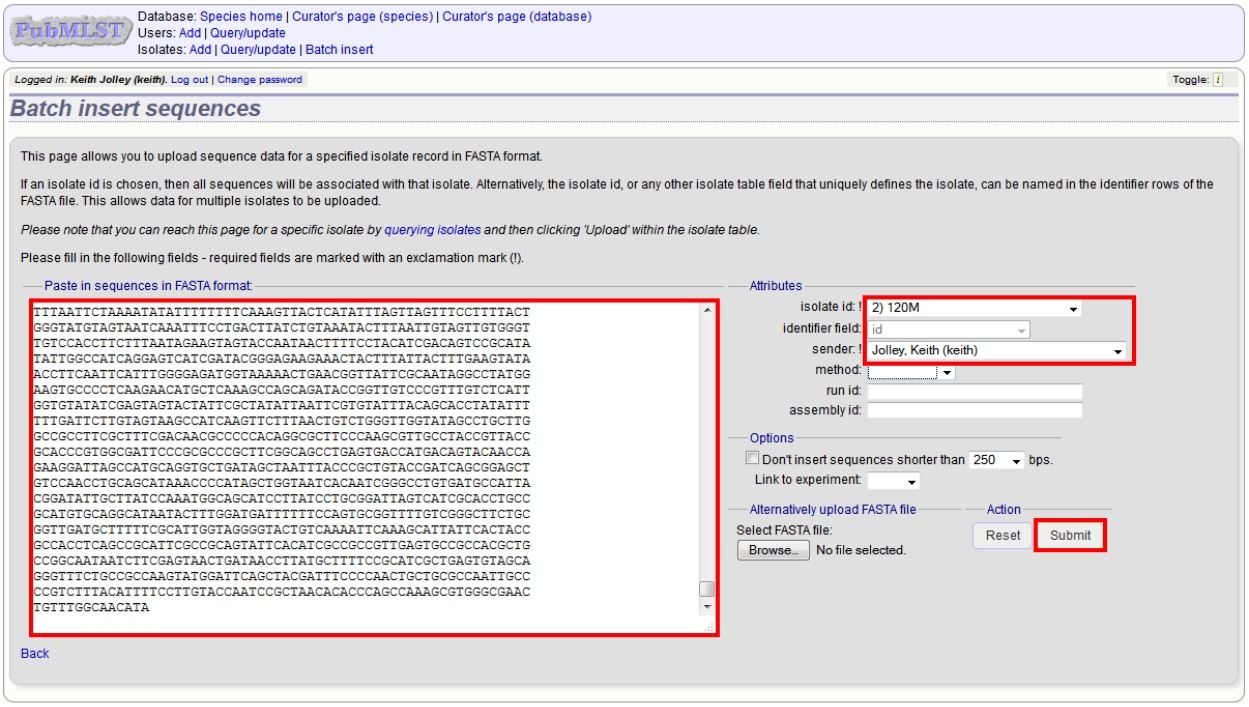
6.16 Uploading sequence contigs linked to isolate records

6.16.1 Select isolate from drop-down list

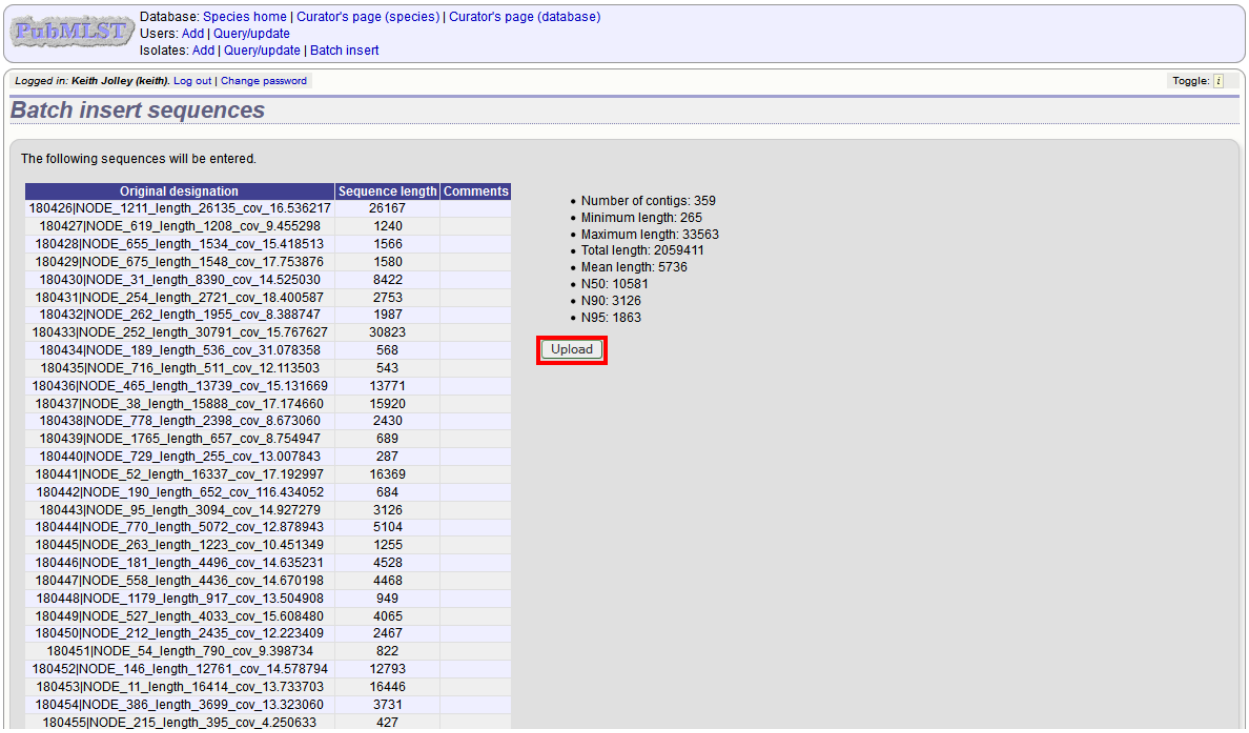
To upload sequence data, click the sequences batch add (++) link on the curator's main page.

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

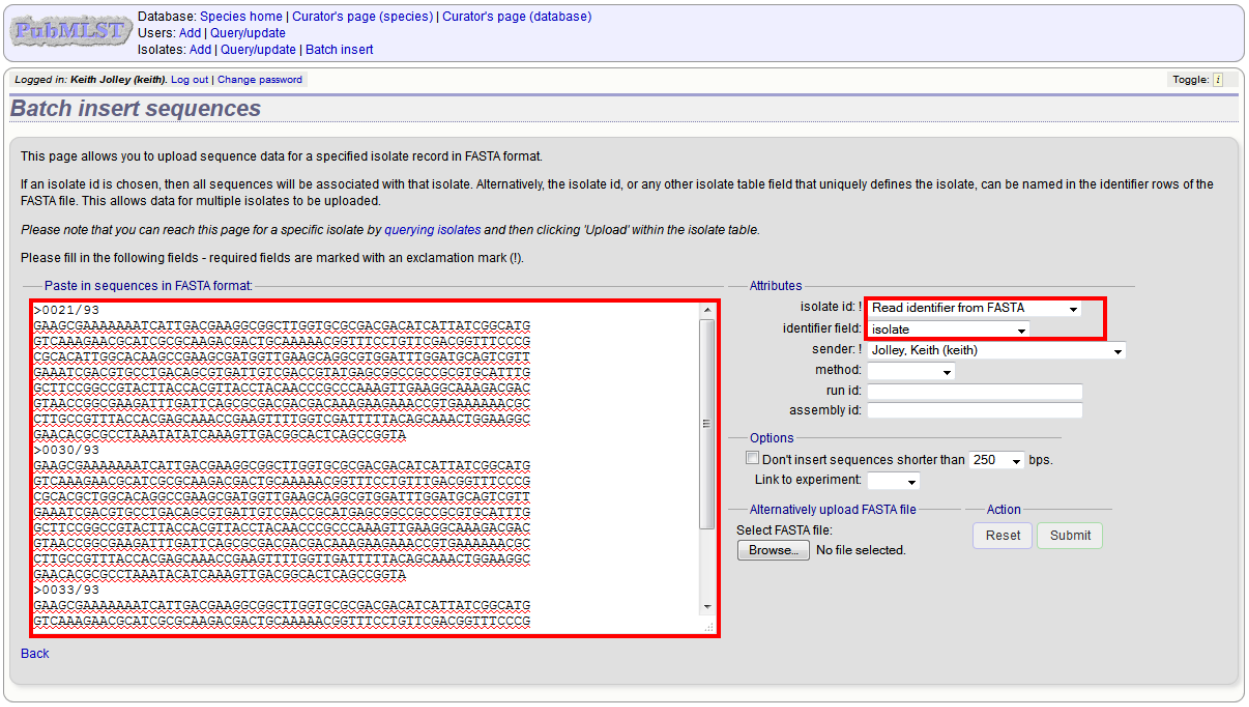
Paste sequence contigs in FASTA format in to the form.



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



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

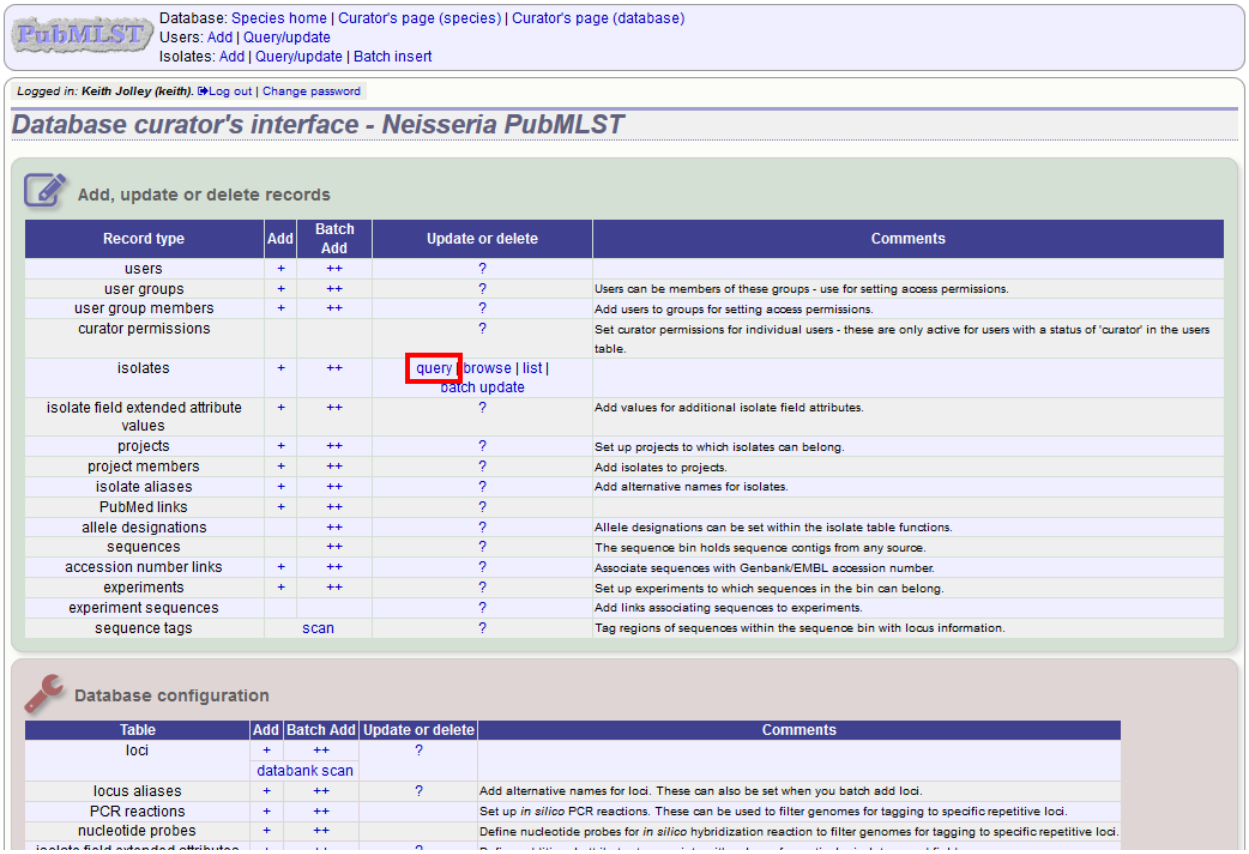


Provided the identifier used uniquely identifies the isolate you will get a confirmation screen. If the isolate name does not do this you'll probably have to use the database id number instead. Click 'Upload' to confirm.

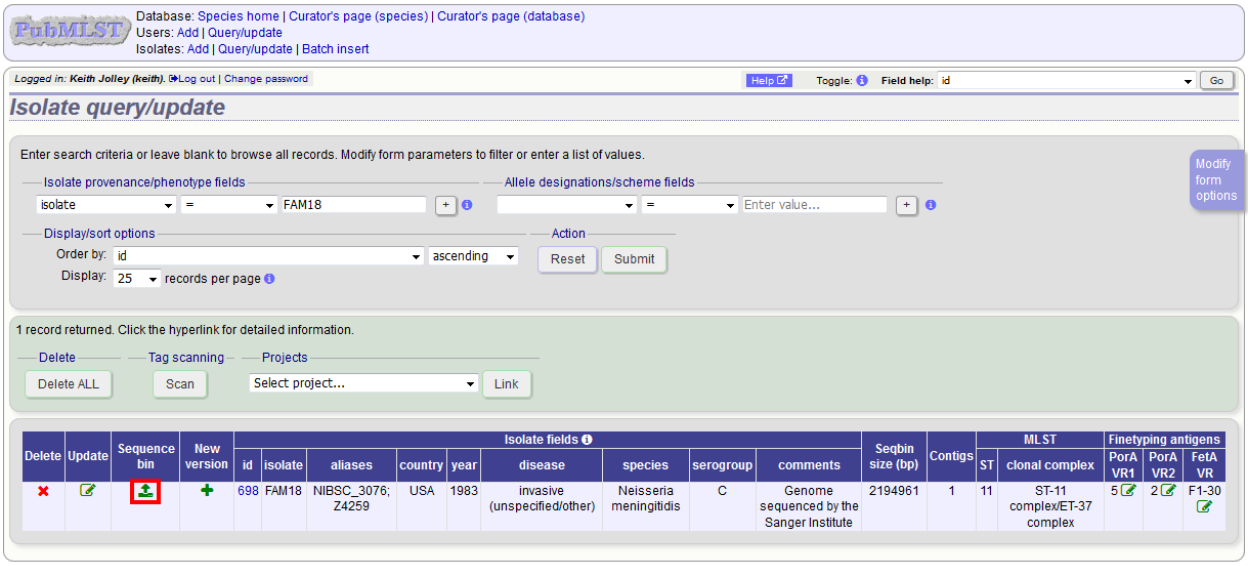
6.16.2 Select from isolate query

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.

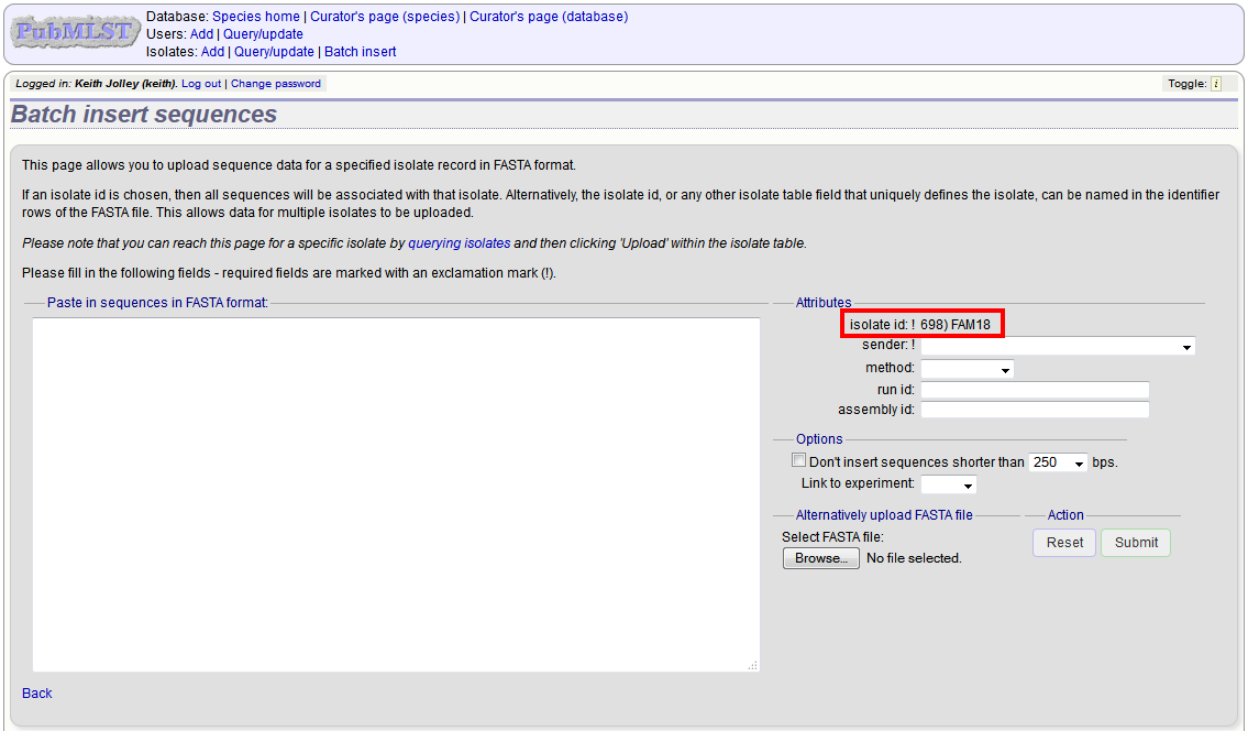
Click the isolate query link from the curator's main page.



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



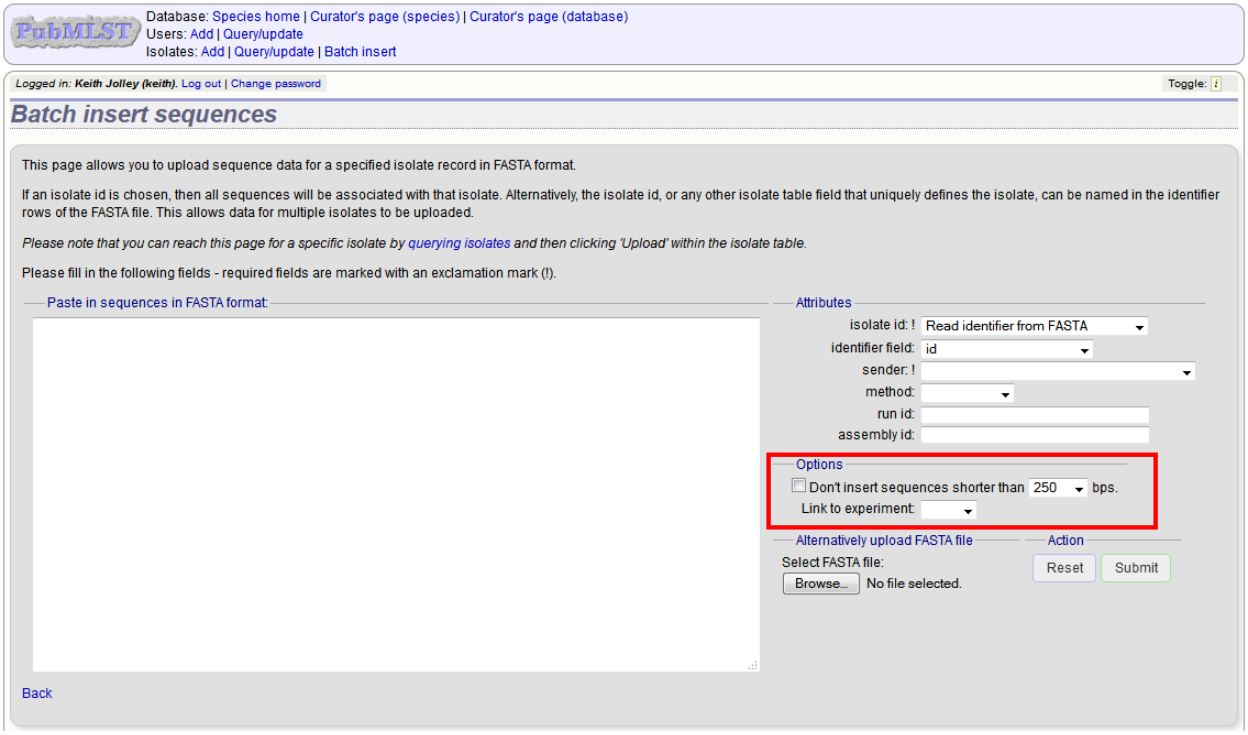
The same upload form as detailed above is shown. Instead of a dropdown list for isolate selection, however, the chosen isolate will be pre-selected.



6.16.3 Upload options

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

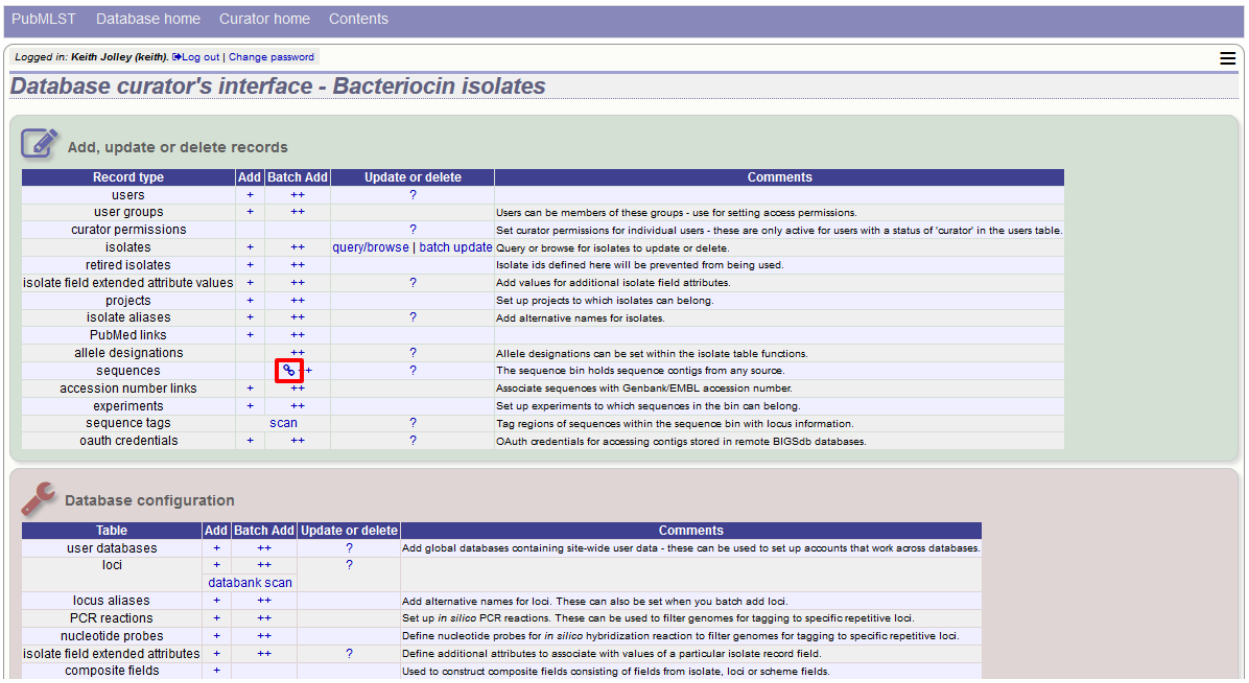
If your database has experiments defined (experiments are used for grouping sequences and can be used to filter the sequences used in *tag scanning*), you can also choose to upload your contigs as part of an experiment. To do this, select the experiment from the dropdown list box.



6.17 Linking remote contigs to isolate records

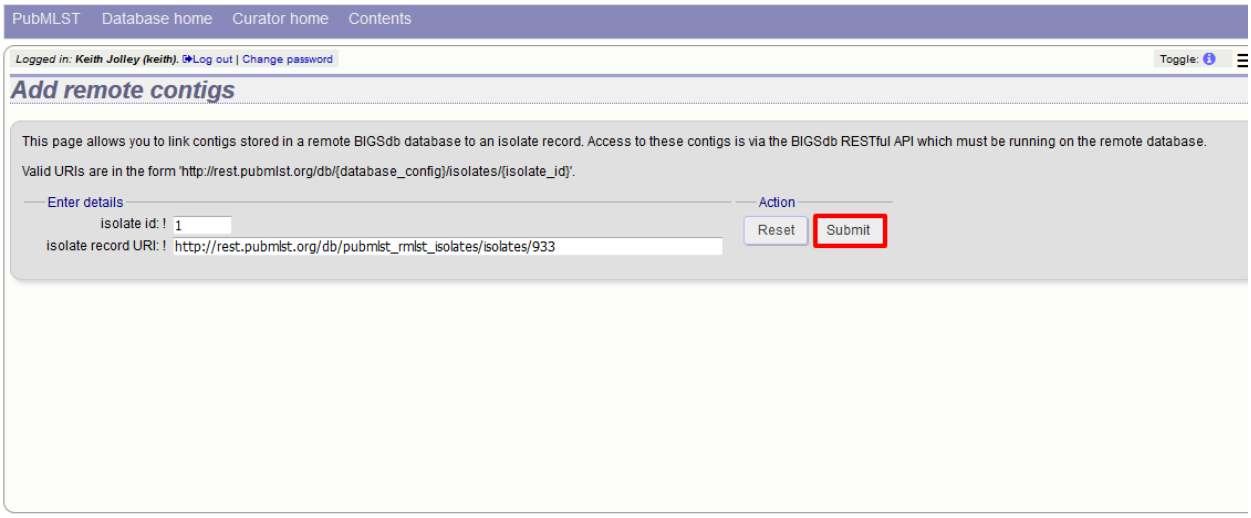
If *remote contigs have been enabled*, isolates can be linked to contigs stored in an external BIGSdb database, rather than directly uploaded. These well then be loaded when needed, for example during scanning or data export. This will be marginally slower than hosting contigs within the same database,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

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

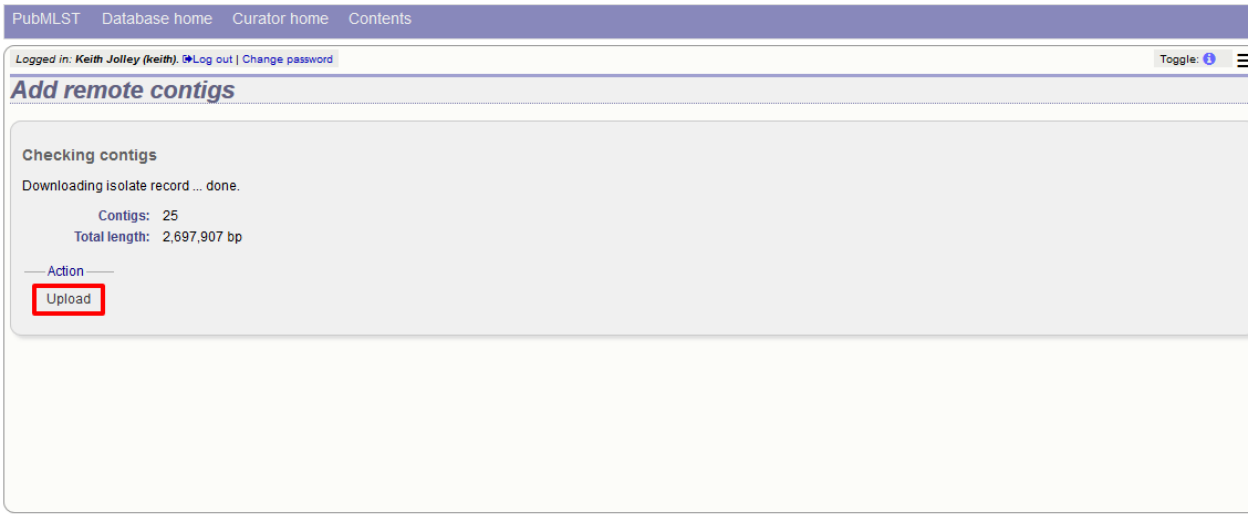


Either select the isolate id from the dropdown list, or enter it manually (list is disabled if there are >1000 records in the database). Enter the URI for the RESTful API of the parent isolate record, e.g. http://rest.pubmlst.org/db/pubmlst_rmlst_isolates/isolates/933. This URI can require authentication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

Press submit.

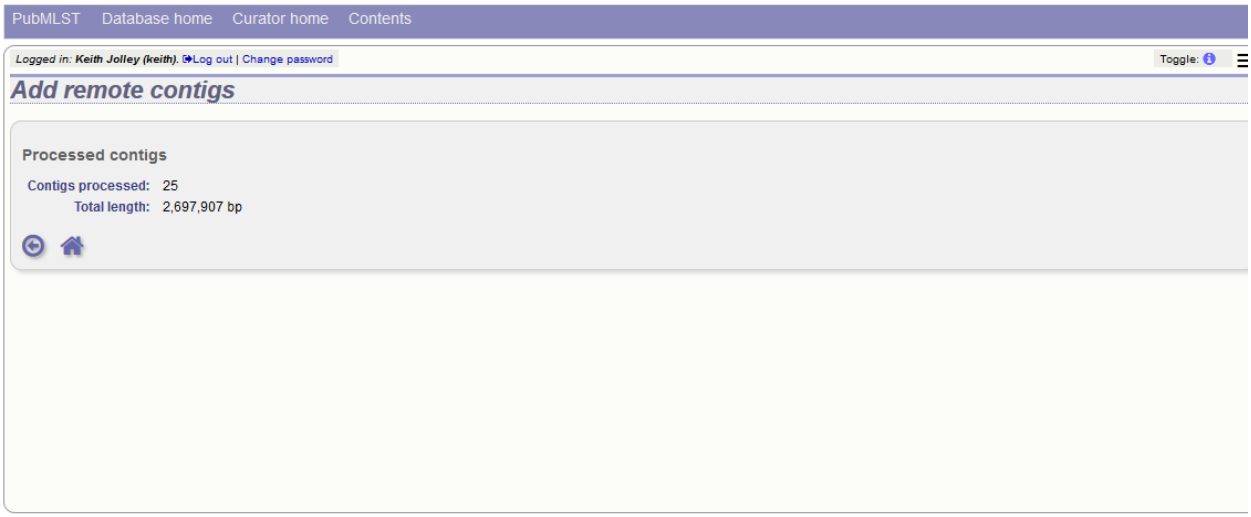


Summary information about the number of contigs and their total length will be downloaded from the remote isolate record. You will then be prompted to upload this information to the database, by clicking the 'Upload' button.



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

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

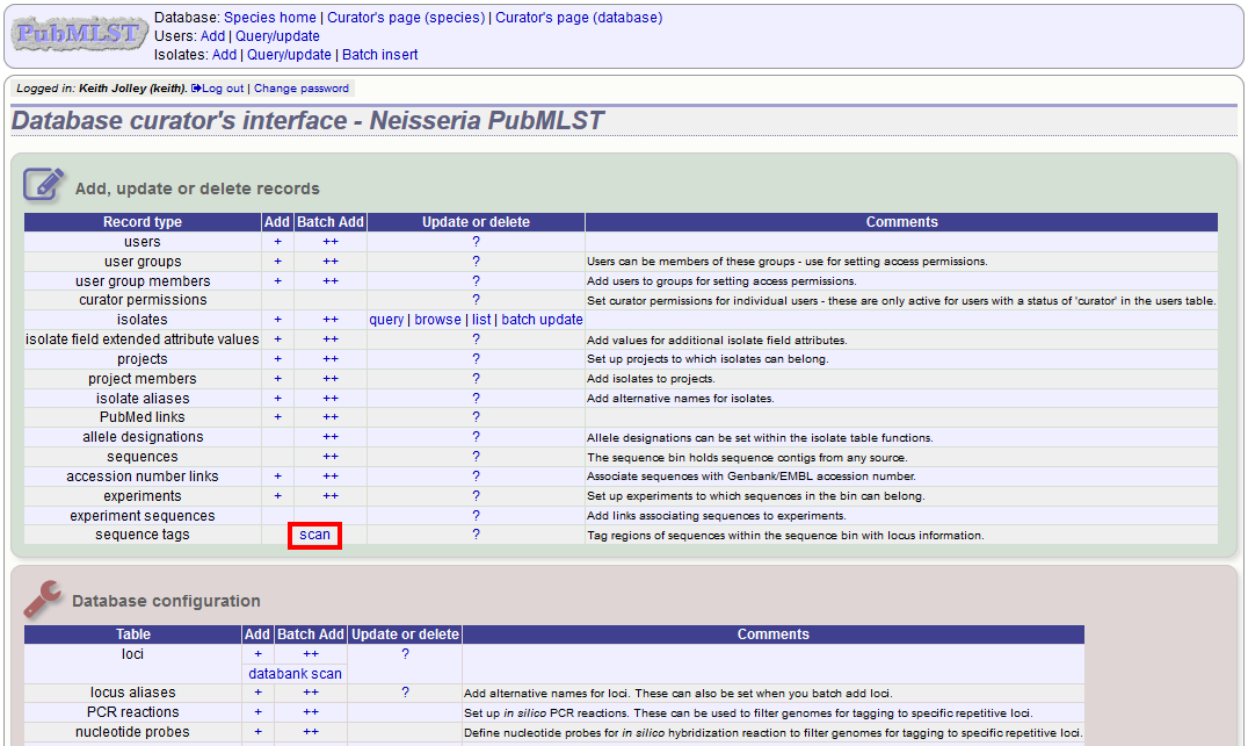


Alternatively, this step can be *performed offline automatically*.

6.18 Automated web-based sequence tagging

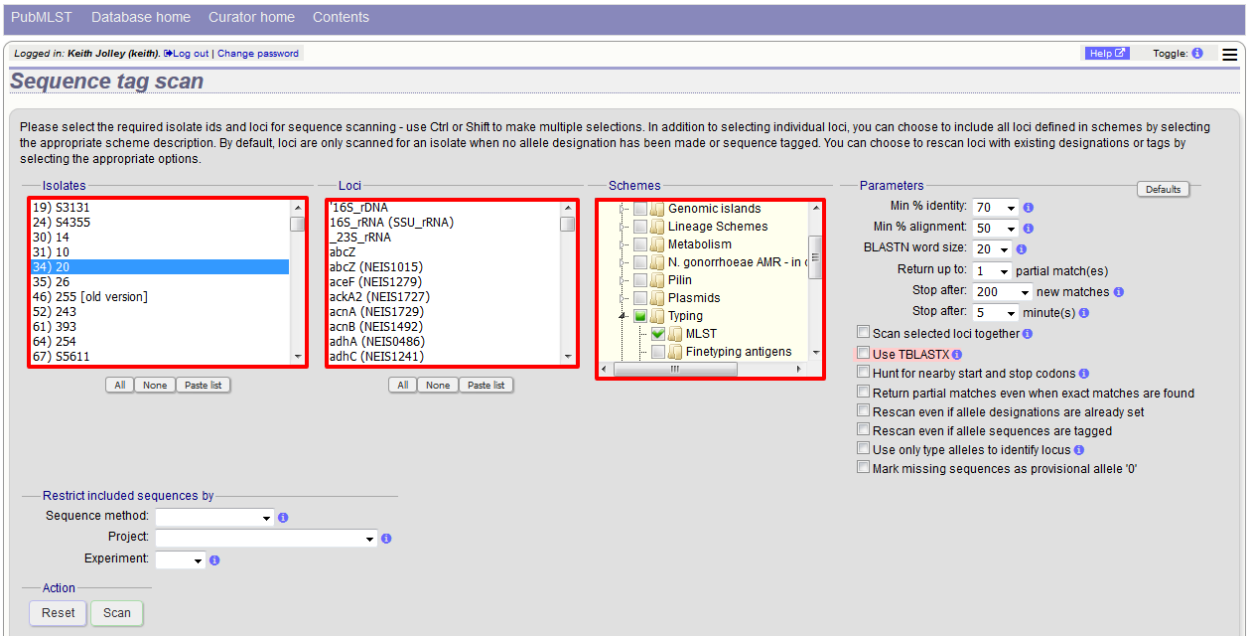
Sequence tagging, or tag-scanning, is the process of identifying alleles by scanning the sequence bin linked to an isolate record. Defined loci can either have a single reference sequence, that is defined in the locus table, or they can be linked to an external database that contains the sequences for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

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



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

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



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

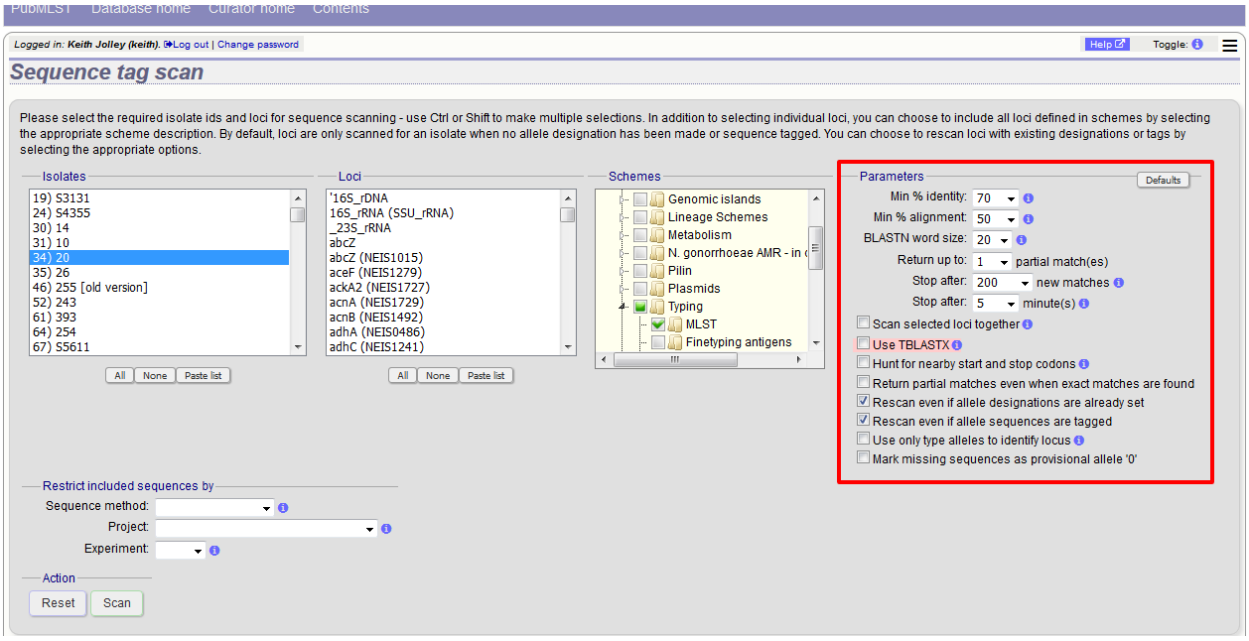
By default, for each isolate only loci that have not had either an allele designation made or a sequence region scanned will be scanned again. To rescan in these cases, select either or both the following:

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

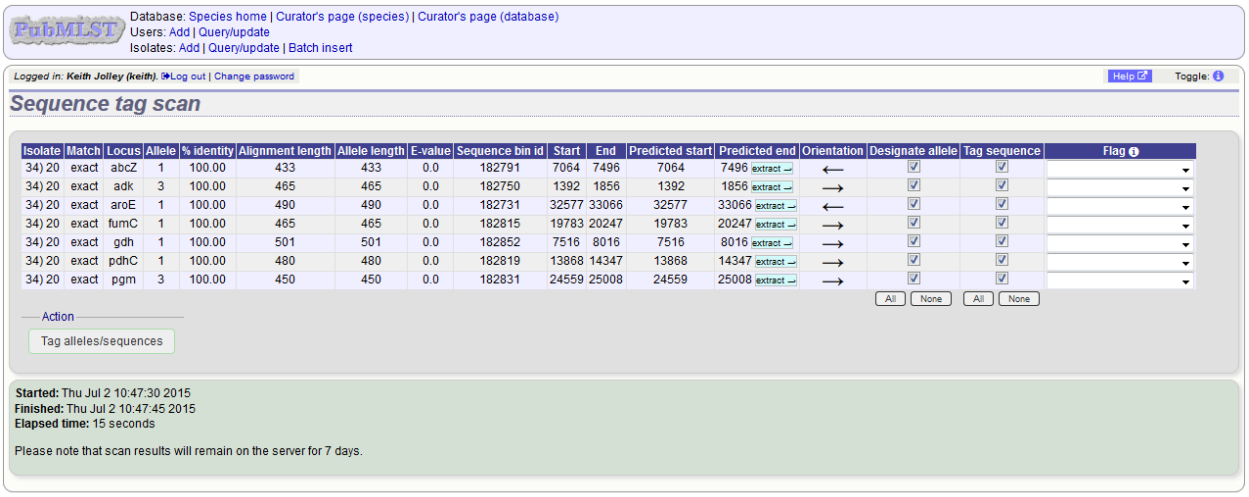
You can select to only use type alleles to identify the locus. This will constrain the search space so that allele definitions don't become more variable over time. If a partial match is found to a type allele then a full database lookup will be performed to identify any known alleles. An allele can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

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

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



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



Individual sequences can be extracted for inspection by clicking the ‘extract →’ 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

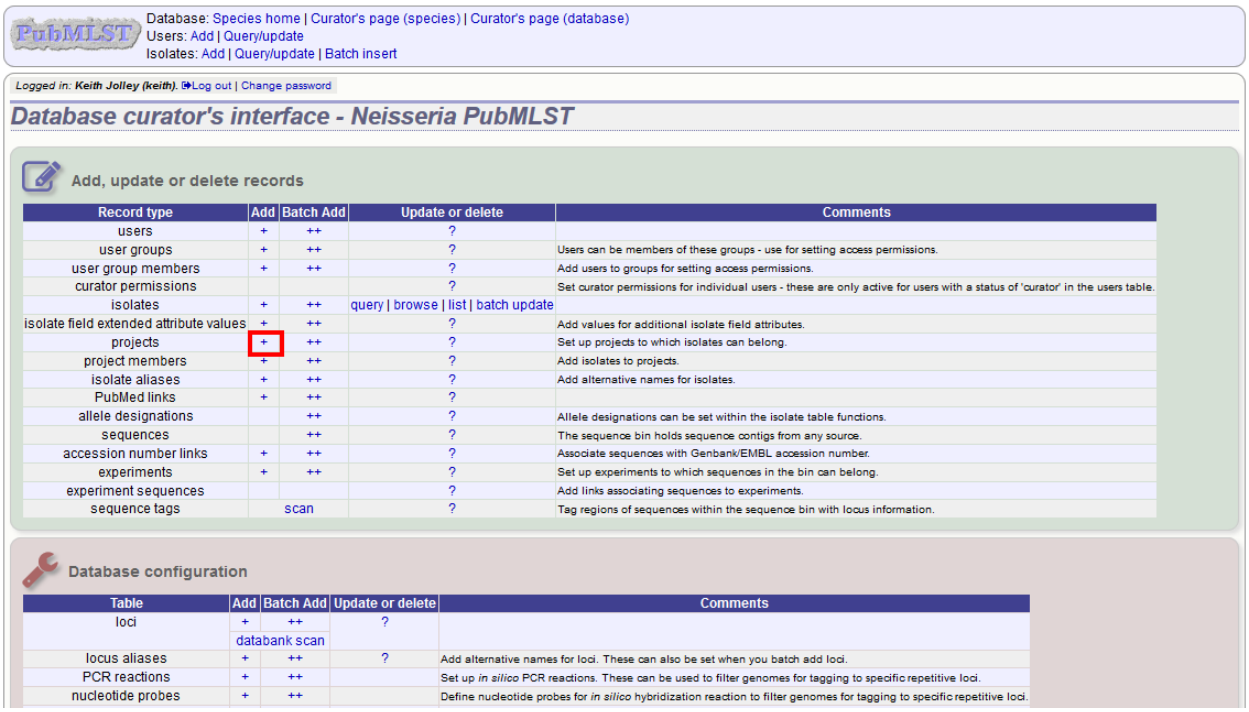
Automated offline sequence tagging

6.19 Projects

6.19.1 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.



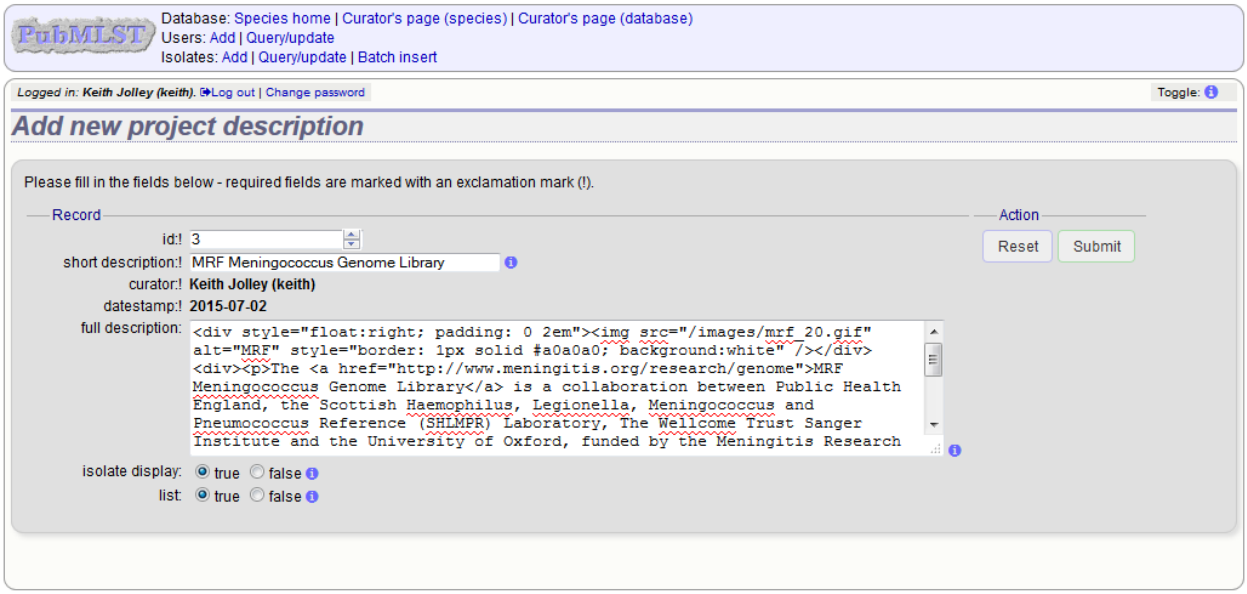
Enter a short description for the project. This is used in drop-down list boxes within the query interfaces, so make sure it is not too long.

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:

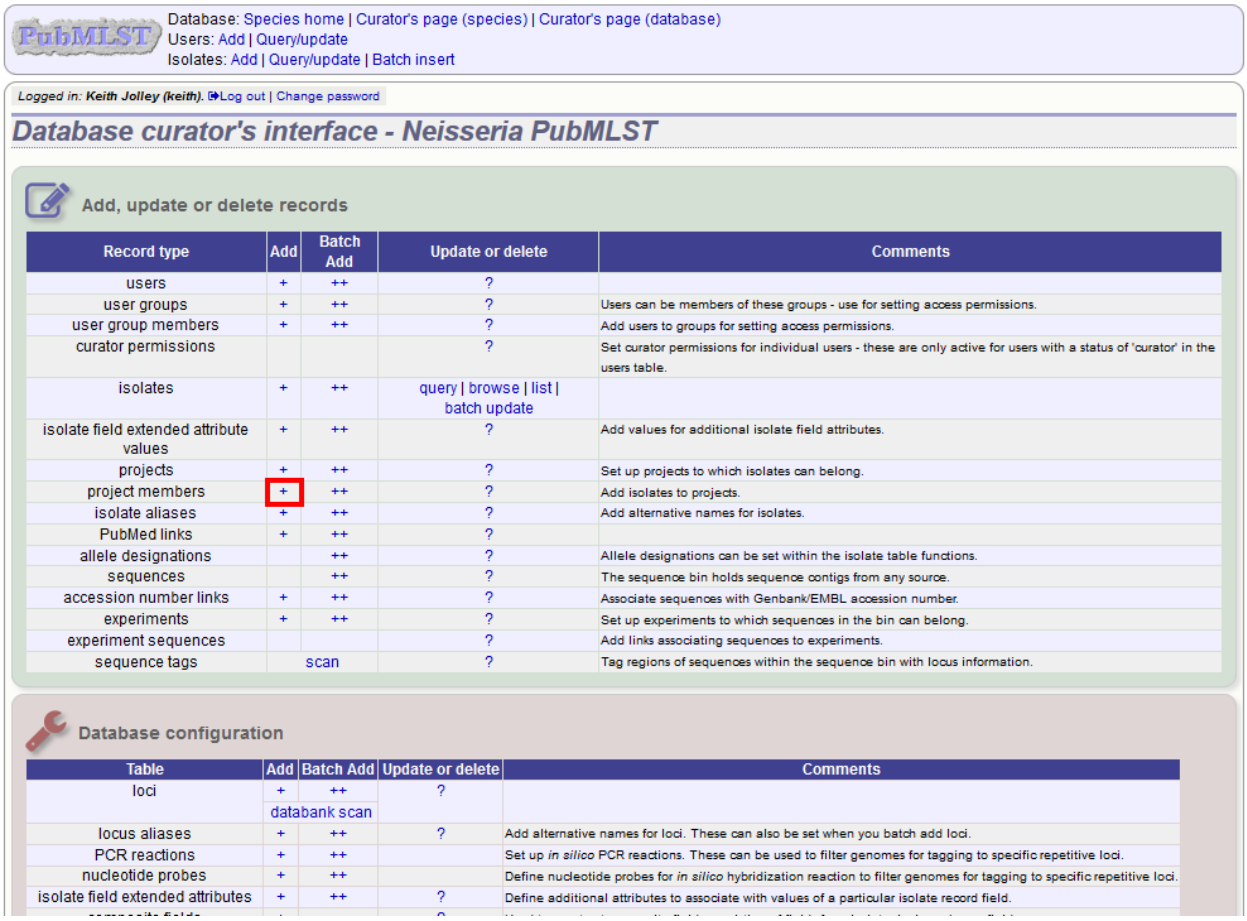
- isolate_display - Setting this is required for the project and its description to be listed at the top of an isolate record (default: false).
- list - Setting this is required for the project to be listed in a page of projects linked from the main contents page.

Click 'Submit'.

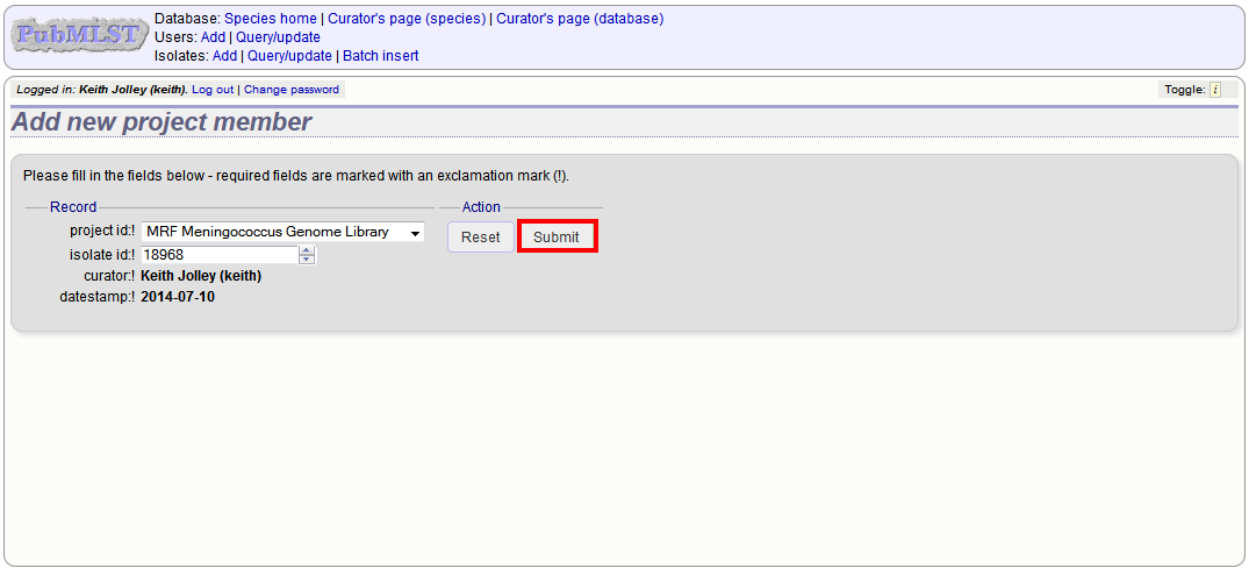


6.19.2 Explicitly adding isolates to a project

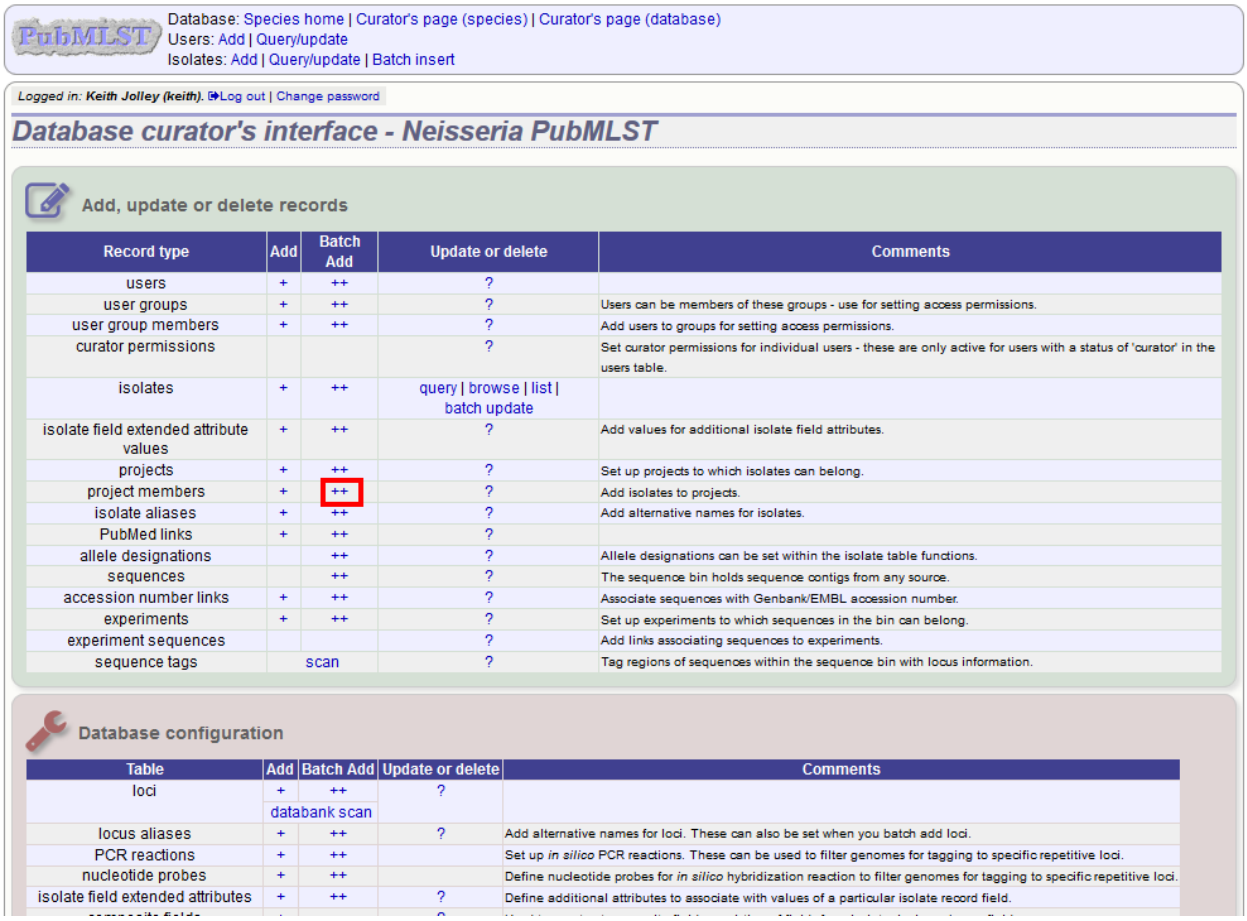
Explicitly adding isolates to the project can be done individually or in batch mode. To add individually, click the add (+) project member link on the curator's main page.



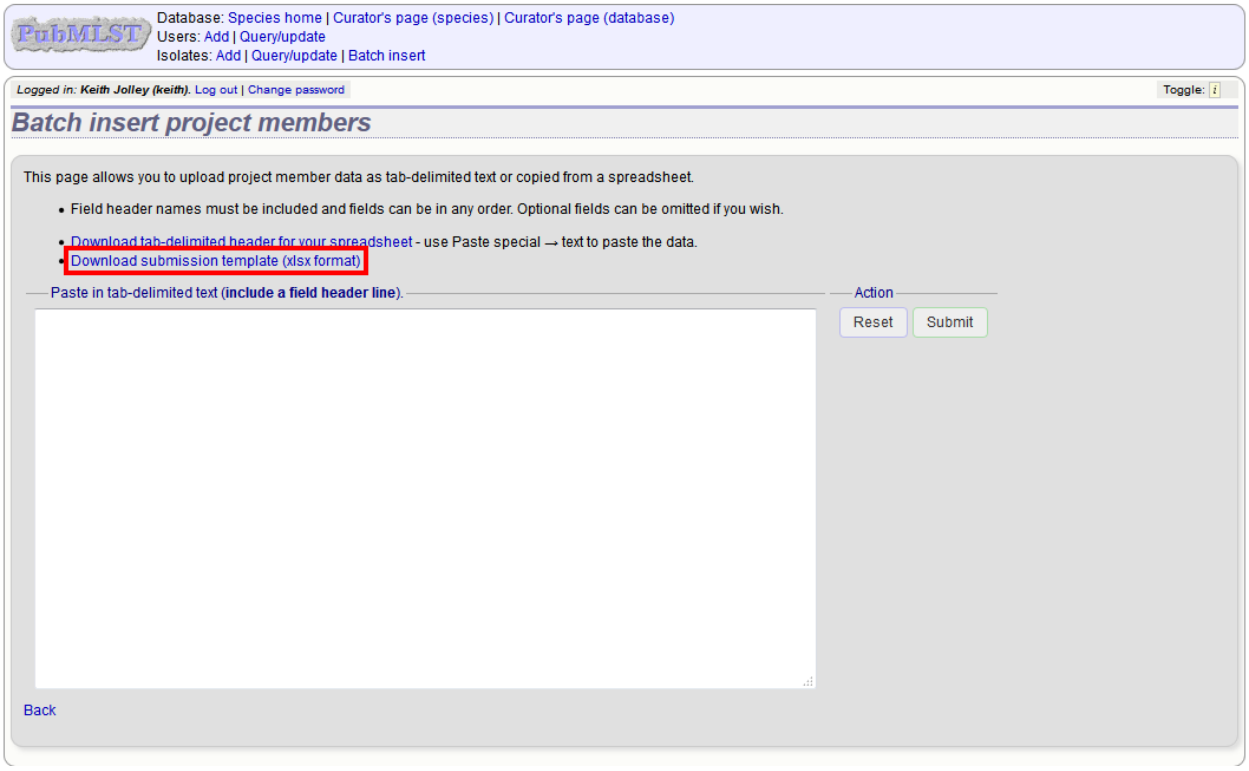
Select the project from the dropdown list box and enter the id of the isolate that you wish to add to the project. Click 'Submit'.



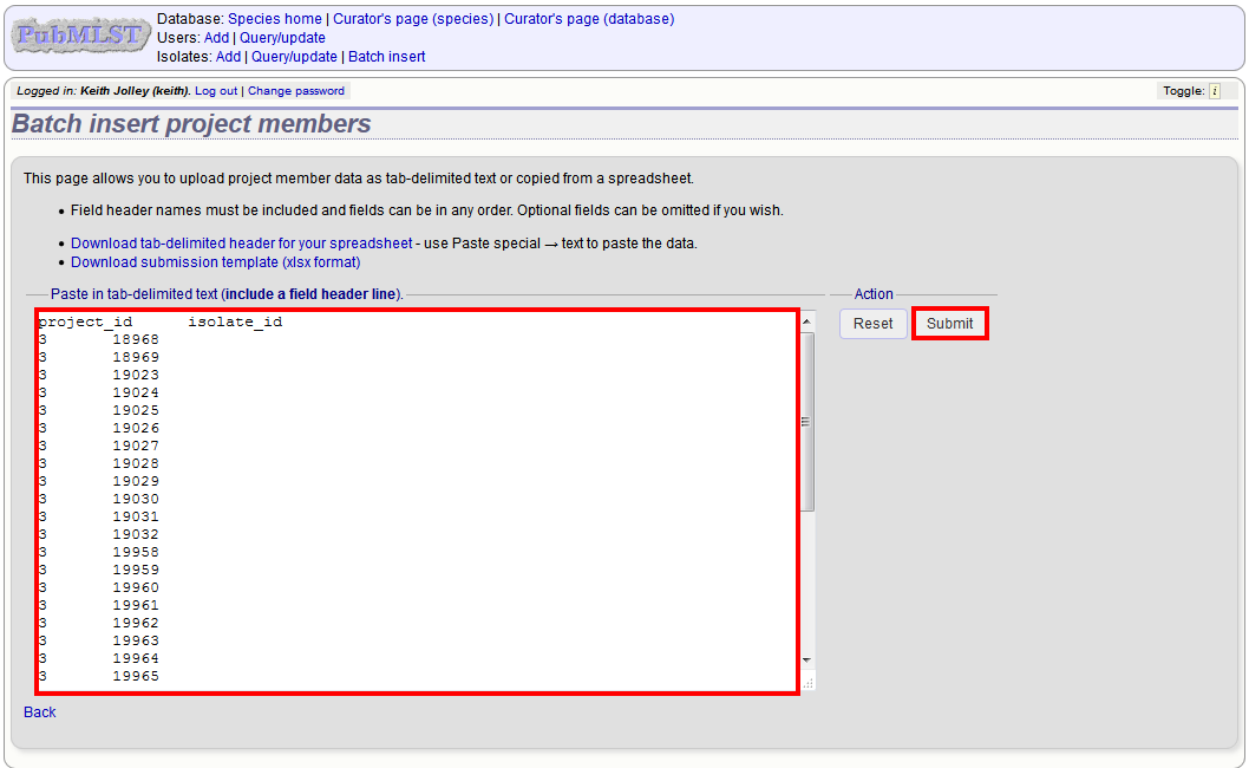
To add isolates in batch mode. Click the batch add (++) project members link on the curator's main page.



Download an Excel submission template:



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



6.20 Isolate record versioning

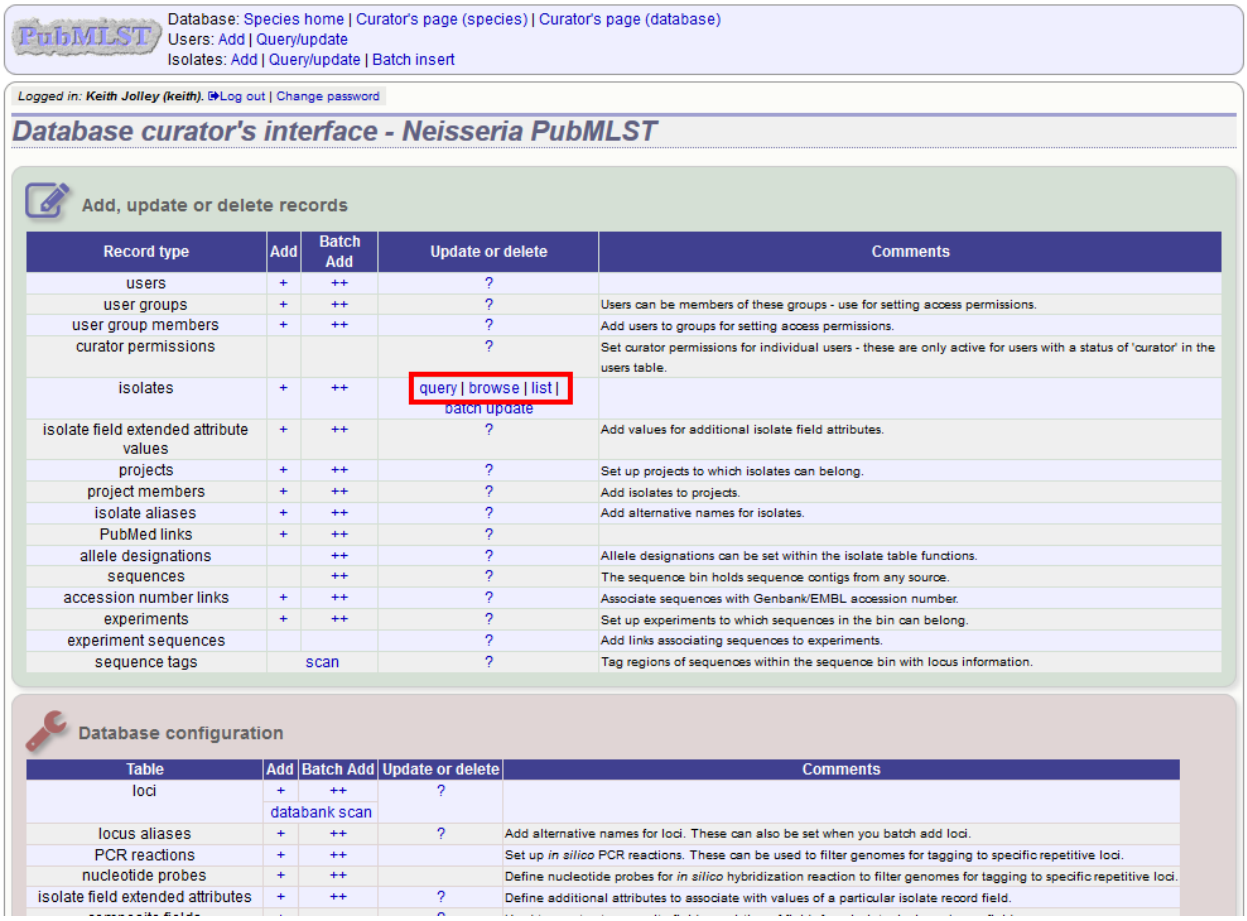
Versioning enables multiple versions of genomes to be uploaded to the database and be analysed separately. When a new version is created, a copy of the provenance metadata, and publication links are created in a new isolate record. The sequence bin and allele designations are not copied.

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.

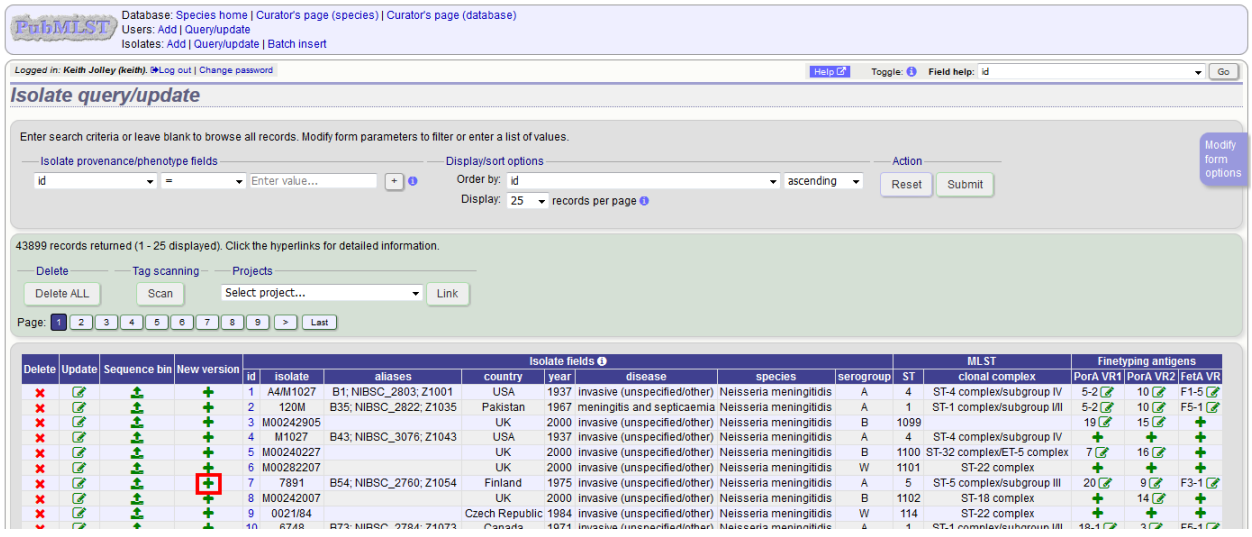
Links to different versions are displayed within an isolate record:

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

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

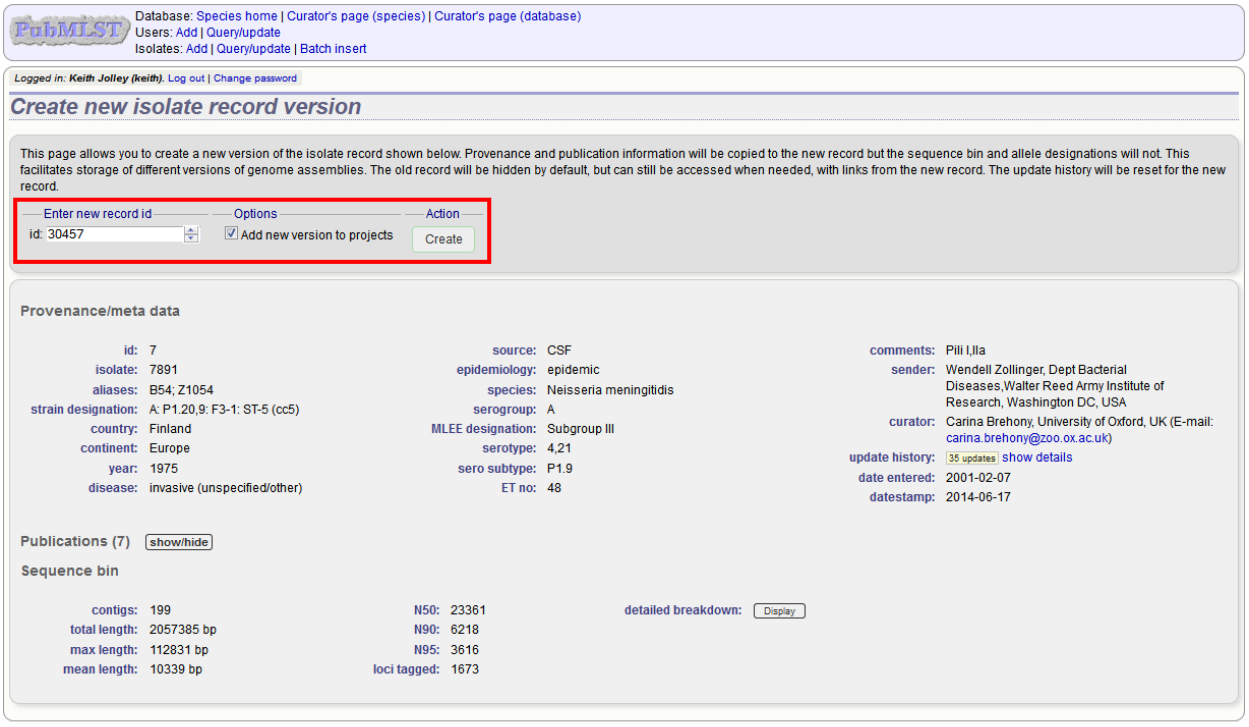


Click the 'create' new version link next to the isolate record:



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.

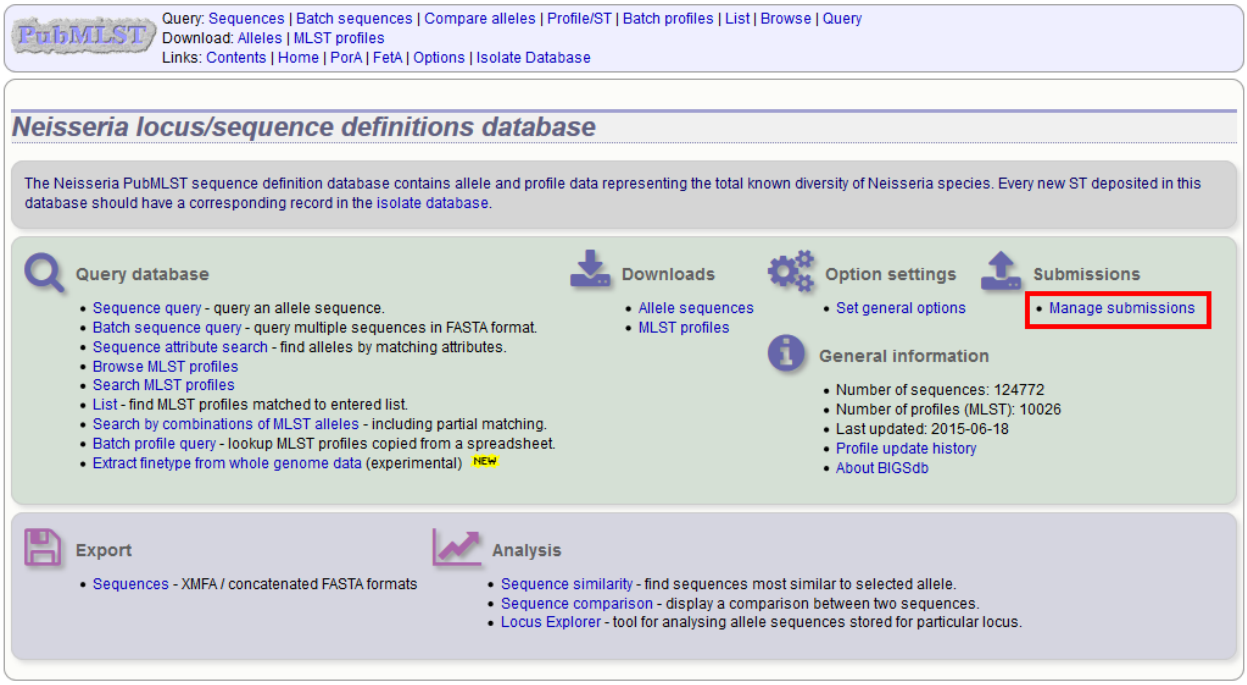
Click the 'Create' button.


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
Create new isolate record version
This page allows you to create a new version of the isolate record shown below. Provenance and publication information will be copied to the new record but the sequence bin and allele designations will not. This facilitates storage of different versions of genome assemblies. The old record will be hidden by default, but can still be accessed when needed, with links from the new record. The update history will be reset for the new record.
Enter new record id
id: 30457
Options
Add new version to projects
Action
Create
Provenance/meta data
id: 7
isolate: 7891
aliases: B54; Z1054
strain designation: A: P1.20,9: F3-1: ST-5 (cc5)
country: Finland
continent: Europe
year: 1975
disease: invasive (unspecified/other)
source: CSF
epidemiology: epidemic
species: Neisseria meningitidis
serogroup: A
MLEE designation: Subgroup III
serotype: 4,21
sero subtype: P1.9
ET no: 48
comments: Pili I,IIa
sender: Wendell Zollinger, Dept Bacterial Diseases,Walter Reed Army Institute of Research, Washington DC, USA
curator: Carina Brehony, University of Oxford, UK (E-mail: carina.brehony@zoo.ox.ac.uk)
update history: 35 updates show details
date entered: 2001-02-07
datestamp: 2014-06-17
Publications (7) show/hide
Sequence bin
contigs: 199
total length: 2057385 bp
max length: 112831 bp
mean length: 10339 bp
N50: 23361
N90: 6218
N95: 3616
loci tagged: 1673
detailed breakdown: Display

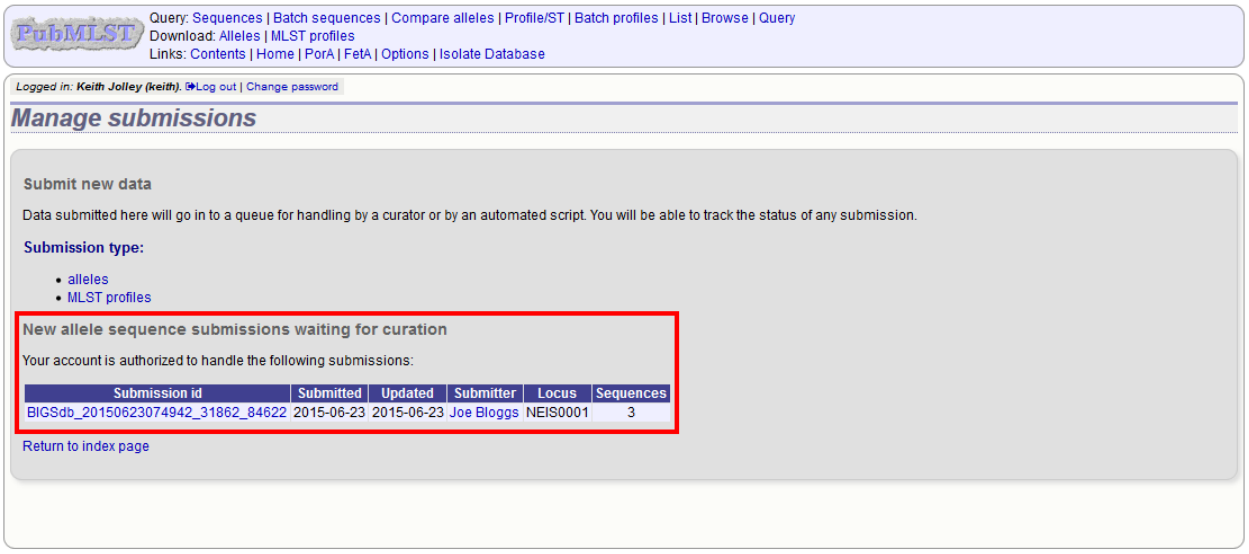
CHAPTER 7

Curating submitted data

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



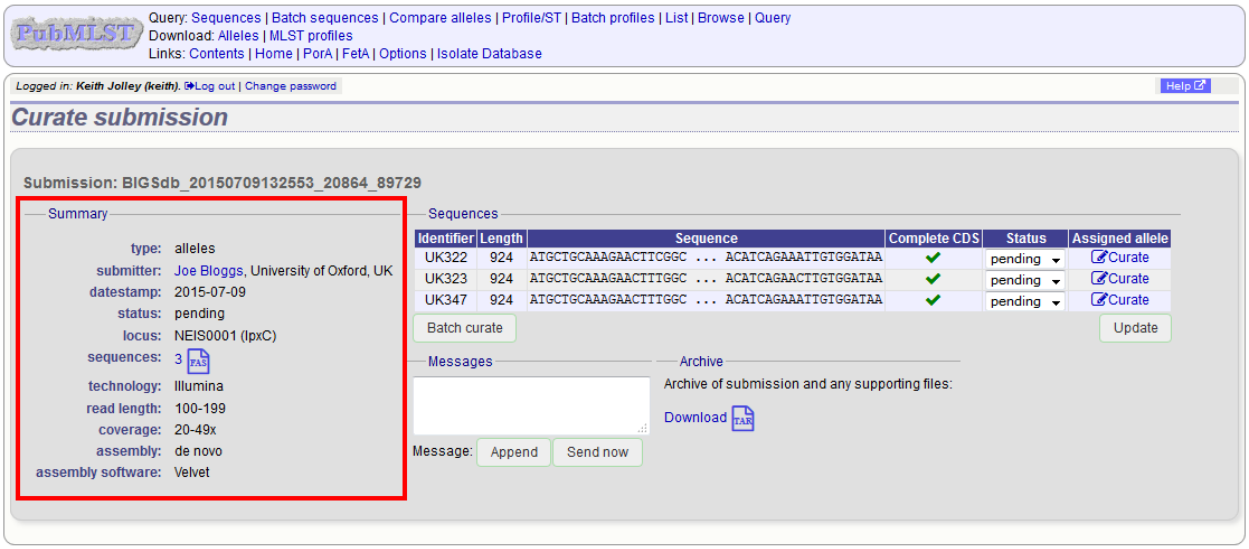
Any submissions for which you have sufficient privileges to curate will be shown.



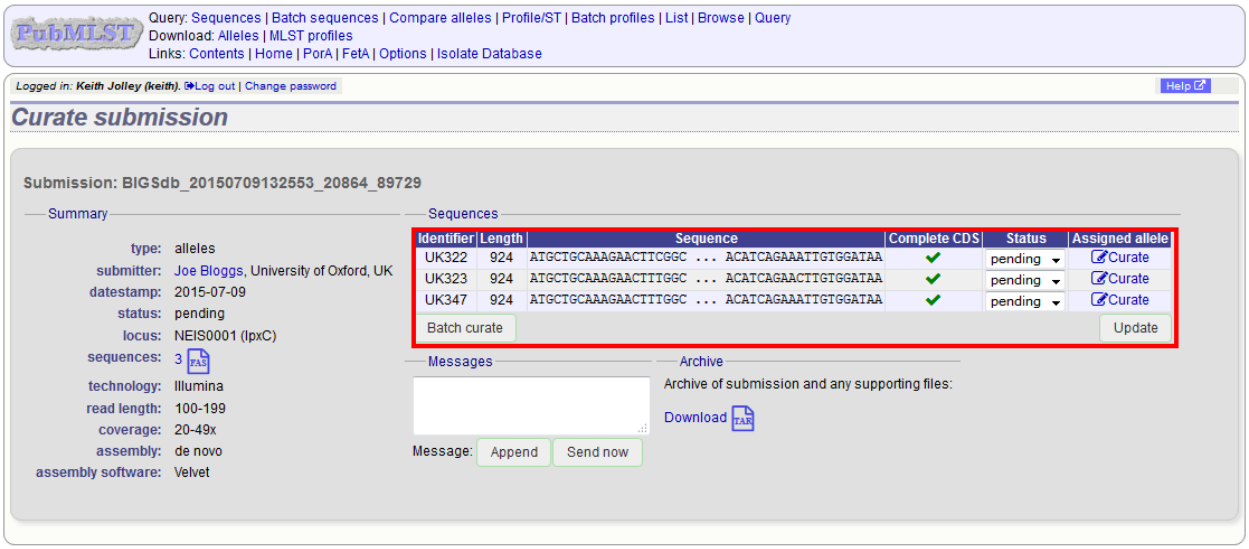
7.1 Alleles

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.

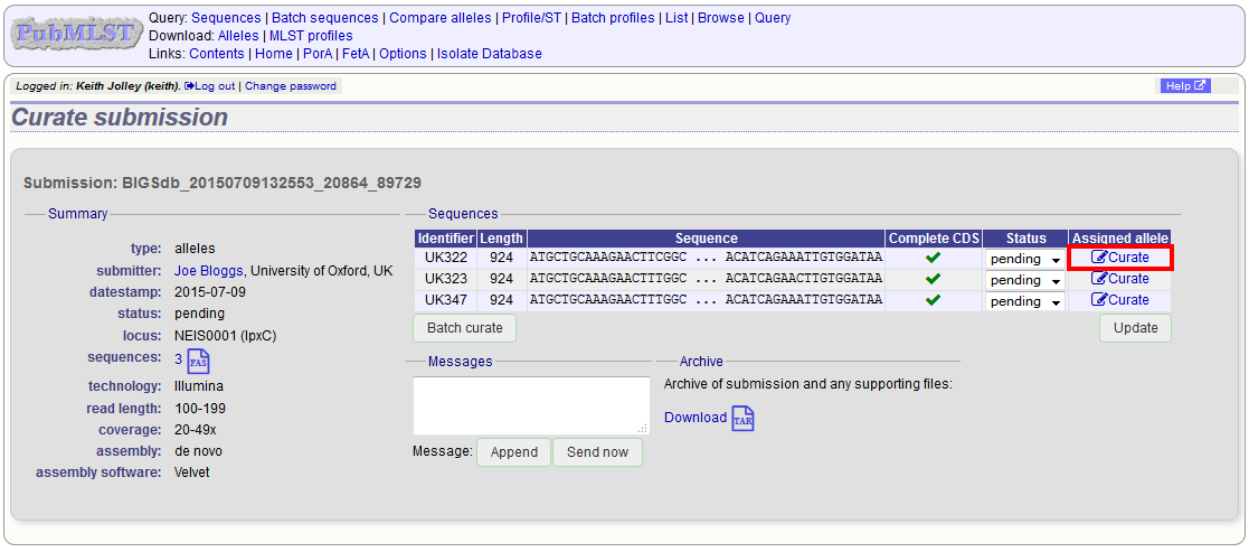


There will also be a table summarizing the sequences in the submission and their current submission status.

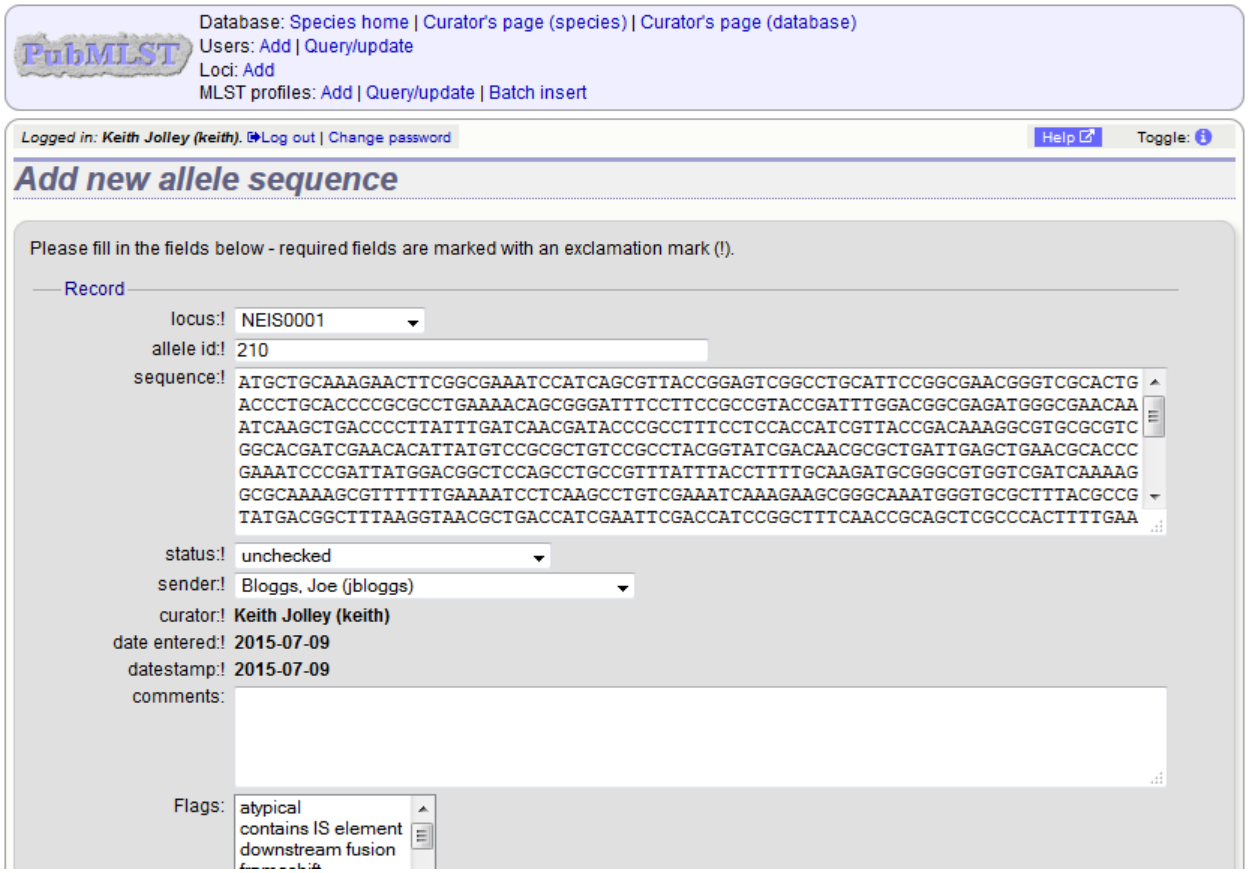


7.1.1 Individual allele curation

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.

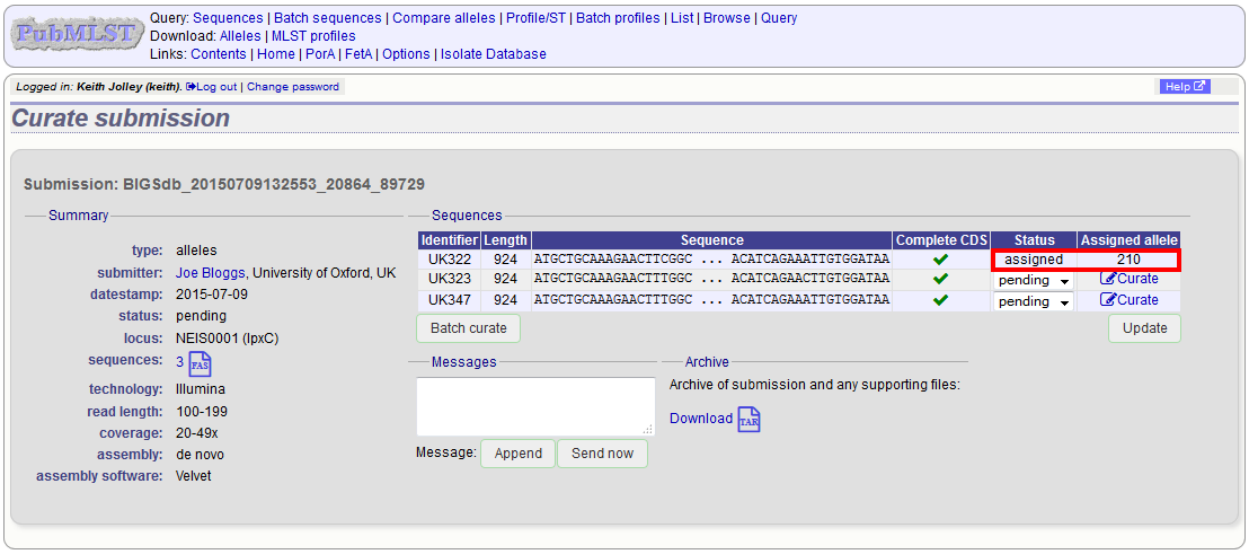


Clicking this link takes you to the curation interface *single sequence upload page*. The upload form will be filled with details from the submission. You may wish to manually change the status from the dropdown list of values.



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.

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.

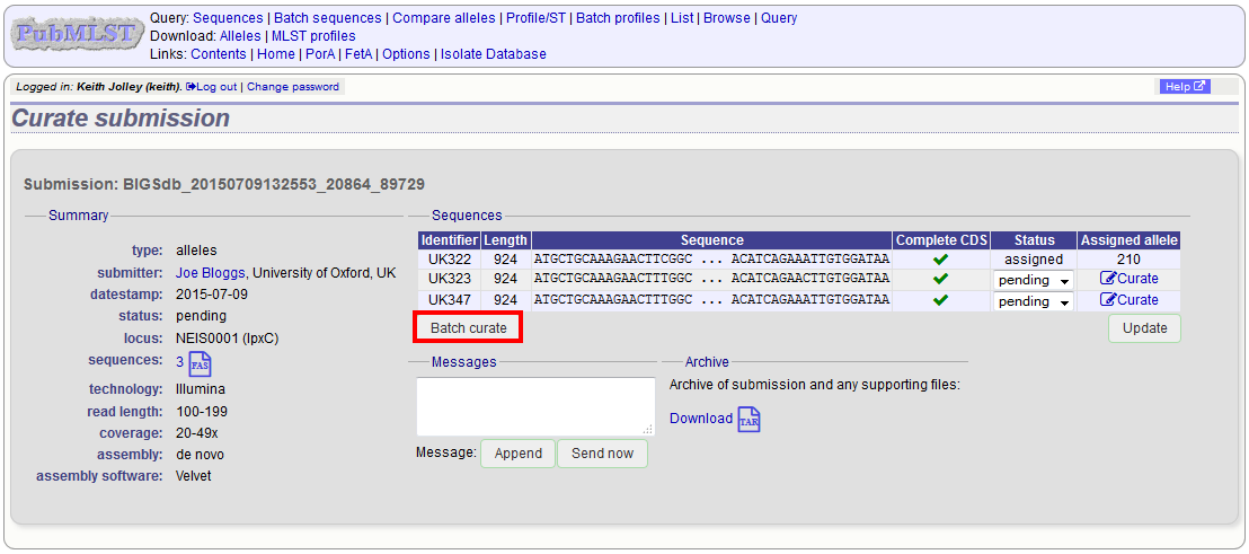


7.1.2 Batch allele curation

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

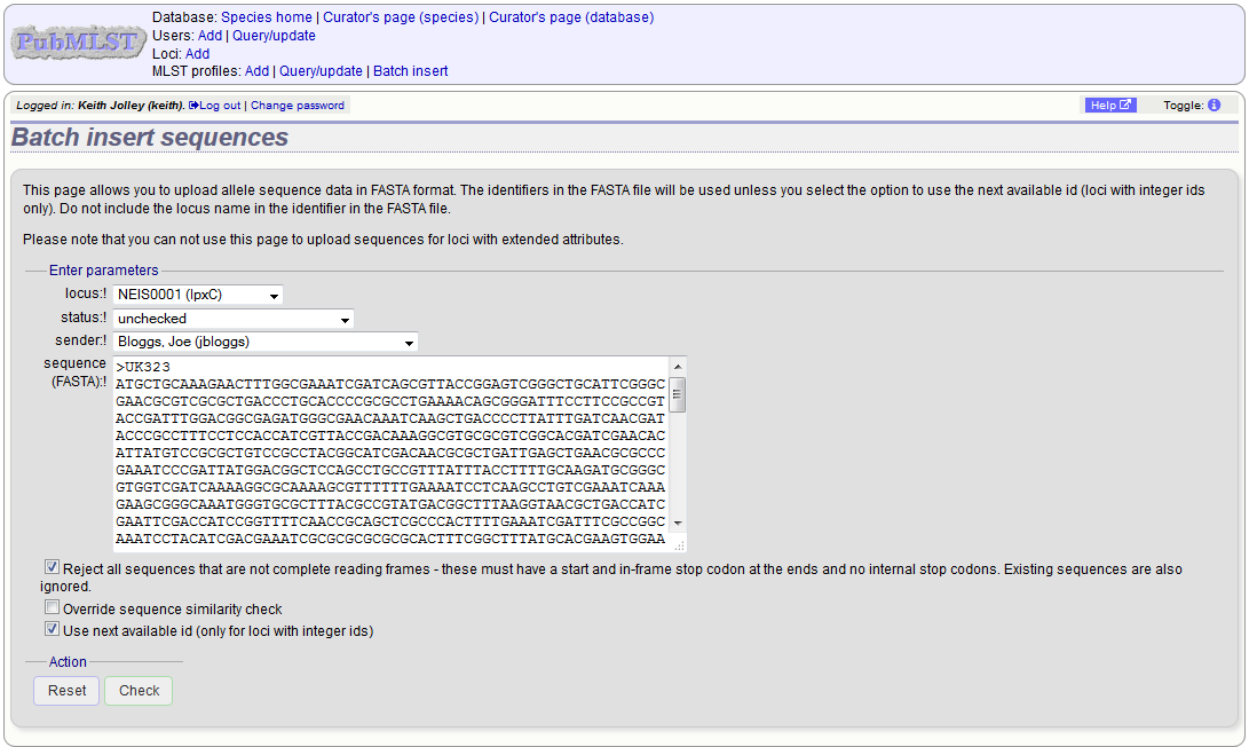
Note: Batch curation is only available for loci that do not have extended attributes defined. Entries for these loci

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

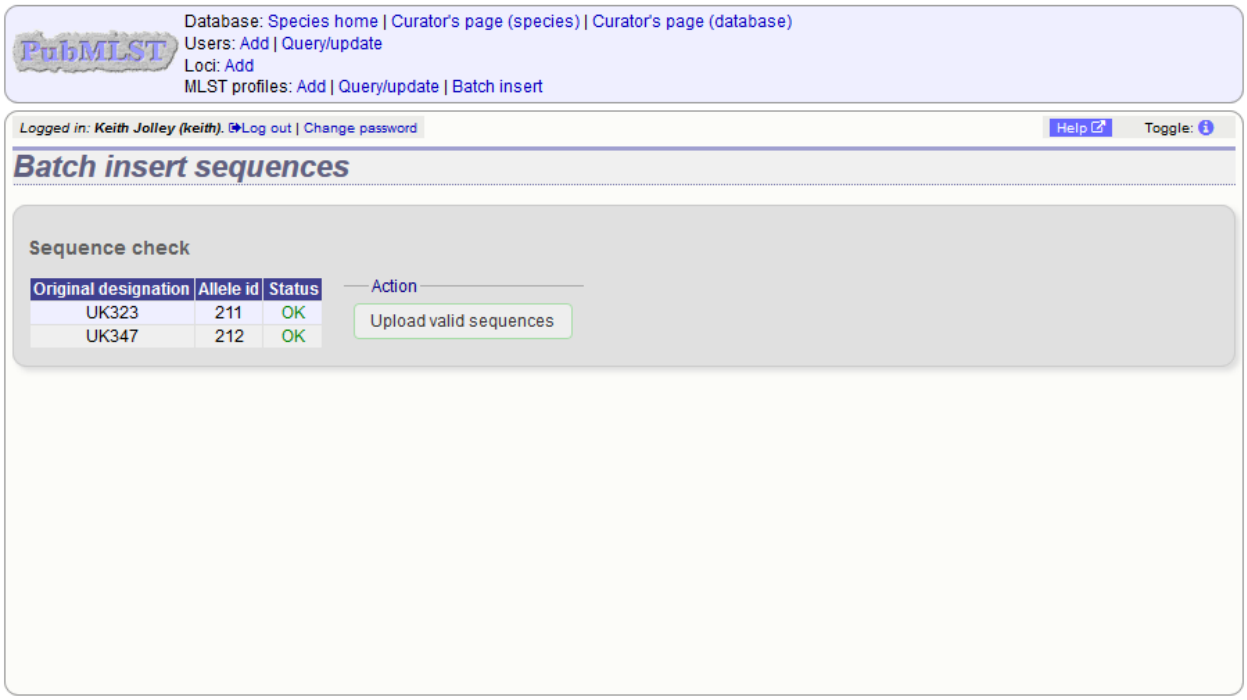


This takes you to the *batch FASTA upload page* in the curators' interface.

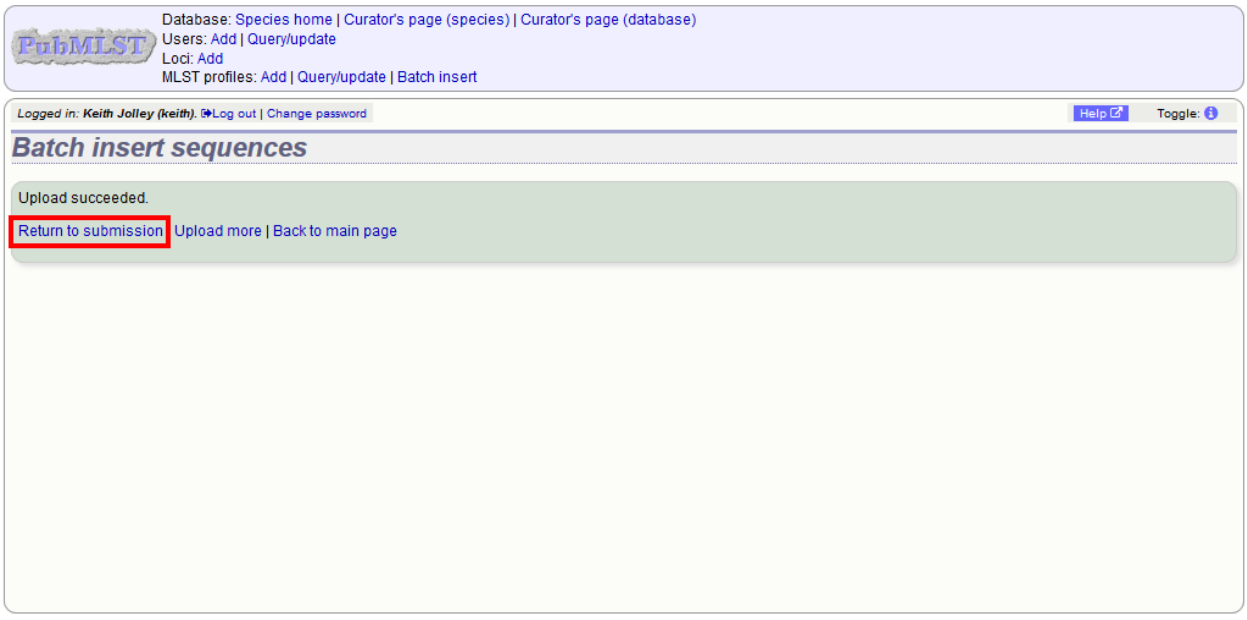
The upload form will be filled with details from the submission. You may wish to manually change the status from the dropdown list of values.



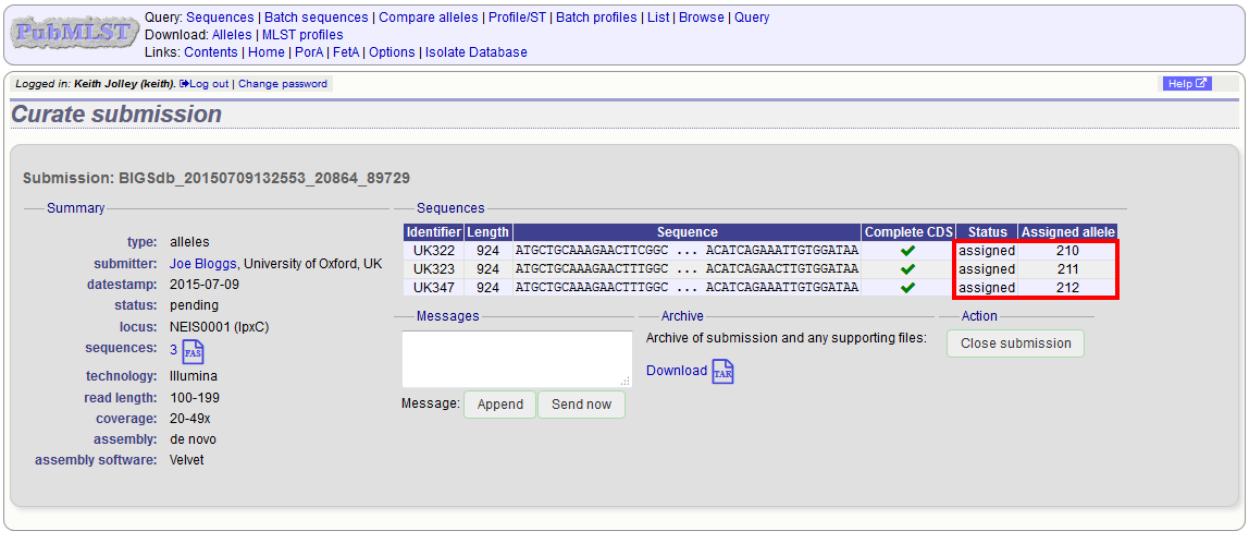
Click 'Check' on this form will perform some standard checks before allowing you to upload the sequences.



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

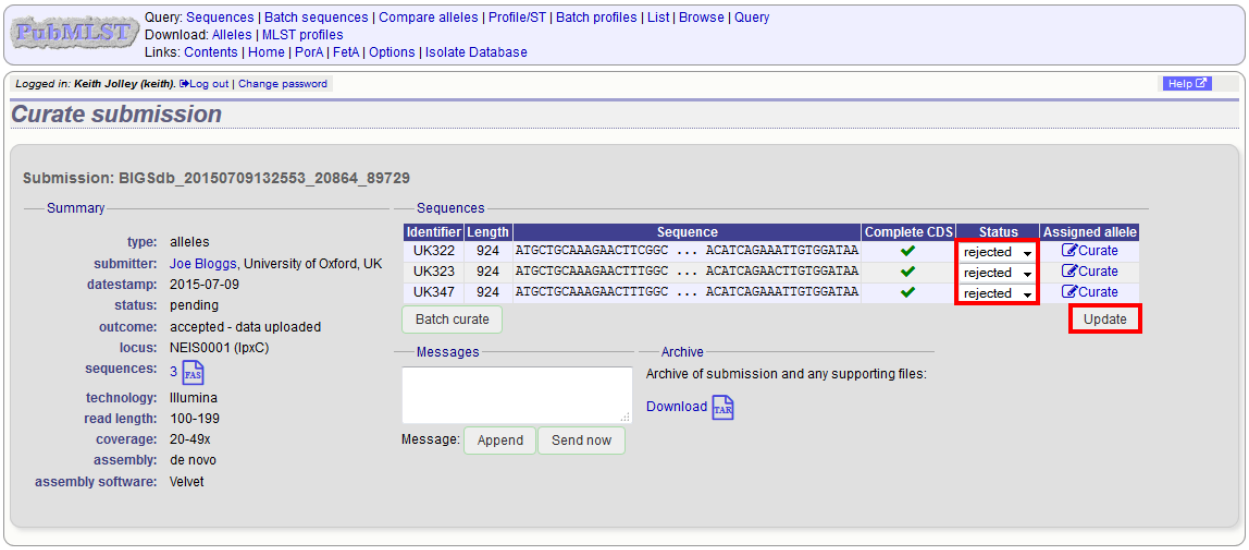


The status of the sequences should reflect their newly assigned status.



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.

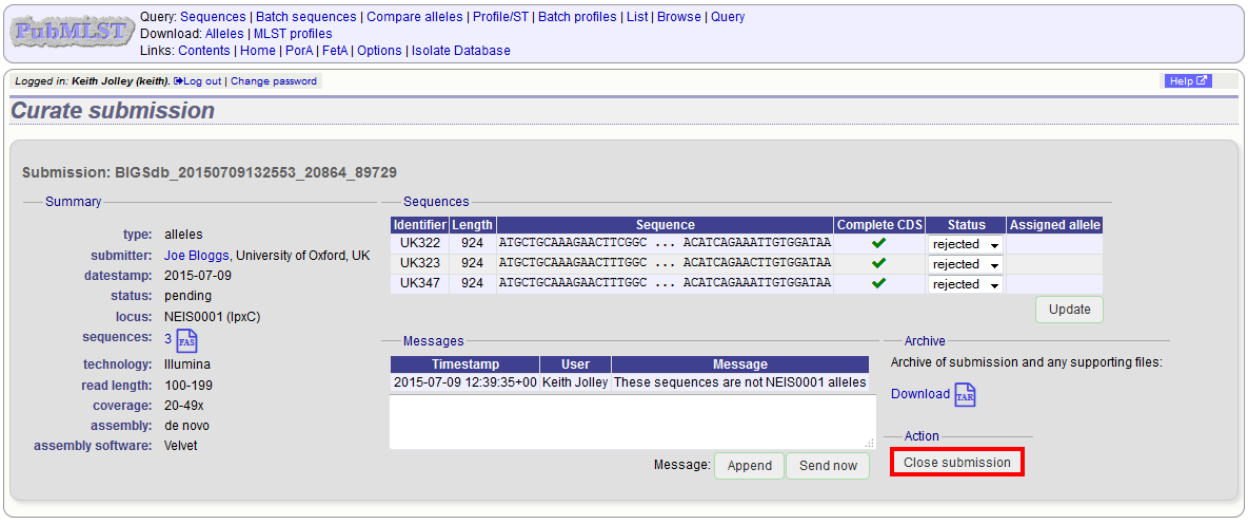


7.1.4 Requesting additonal information

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

7.1.5 Closing the submission

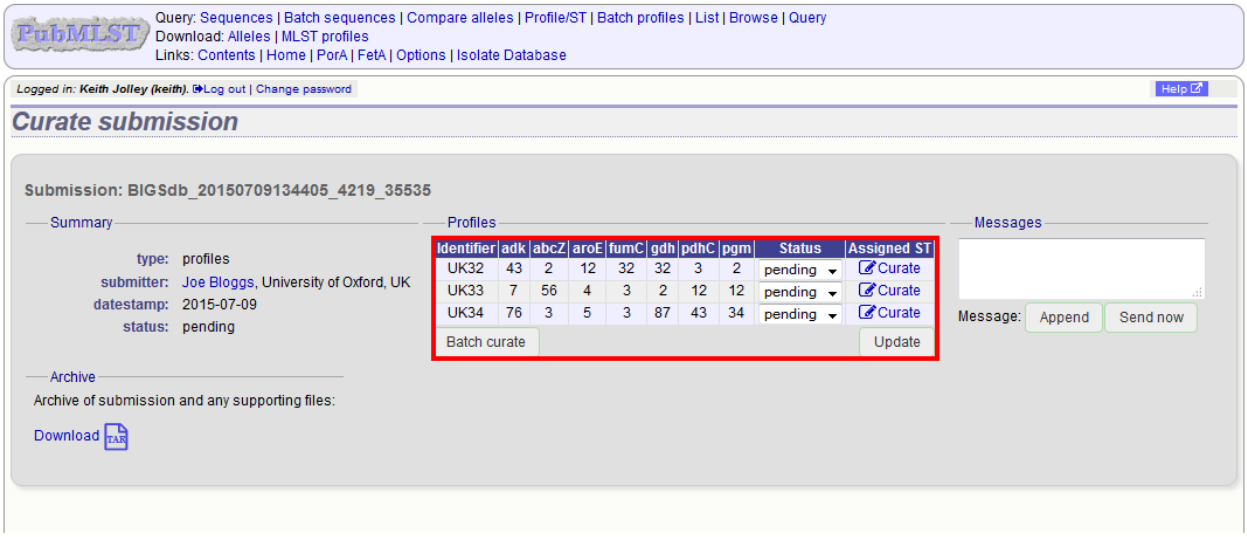
You can add a message to the submitter by entering it in the message box and clicking 'Append'. Once sequences have all been either assigned or rejected, the 'Close submission' button will be displayed. Click this to close the submission. The submitter will be notified of their submission status.



7.2 Profiles

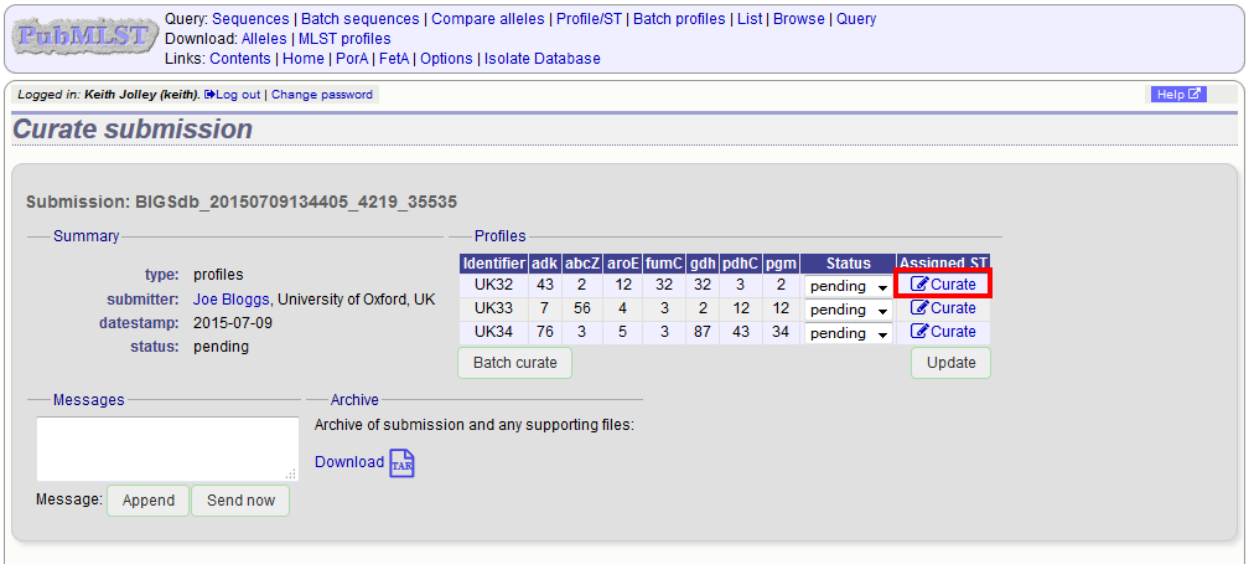
Click the appropriate submission on the 'Manage submissions' page.

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

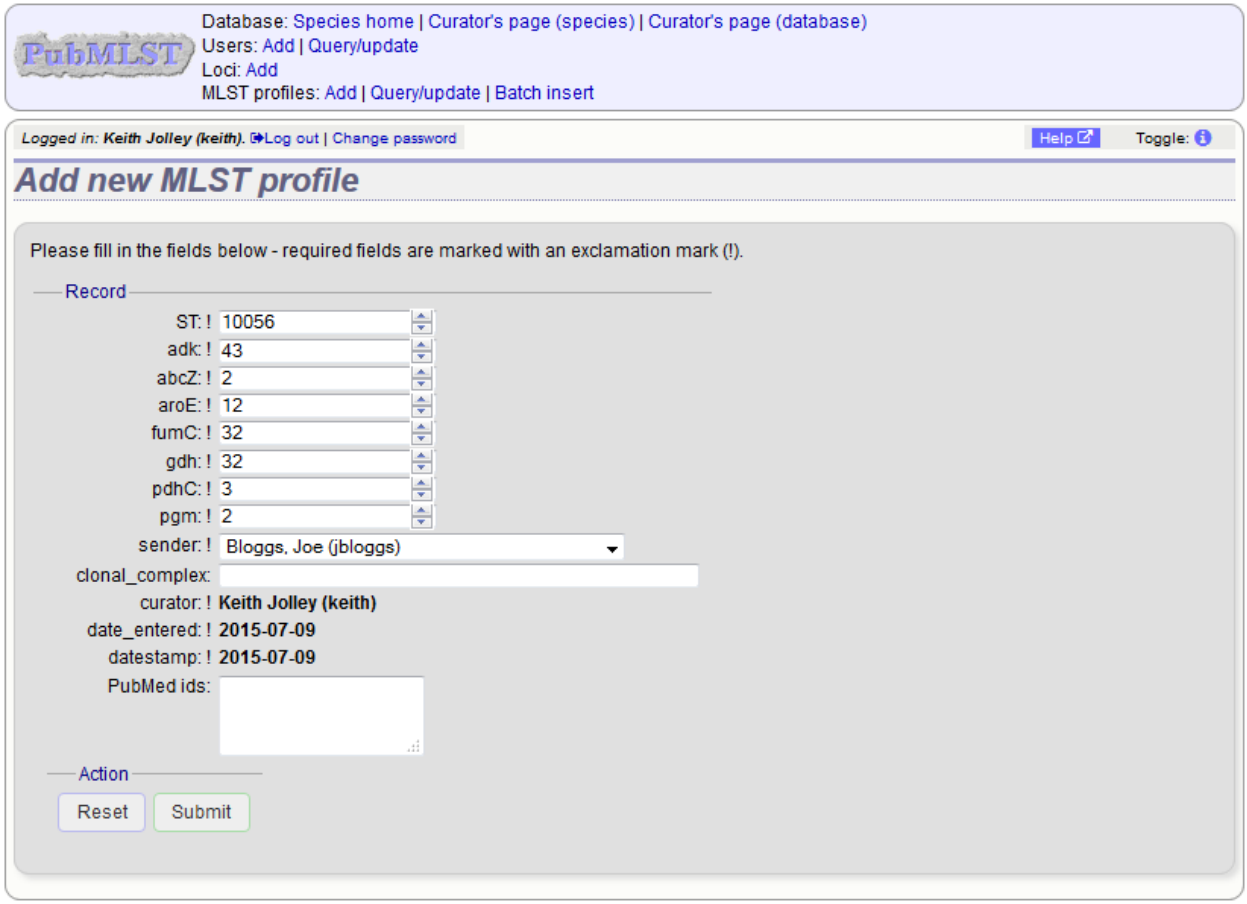


7.2.1 Individual profile curation

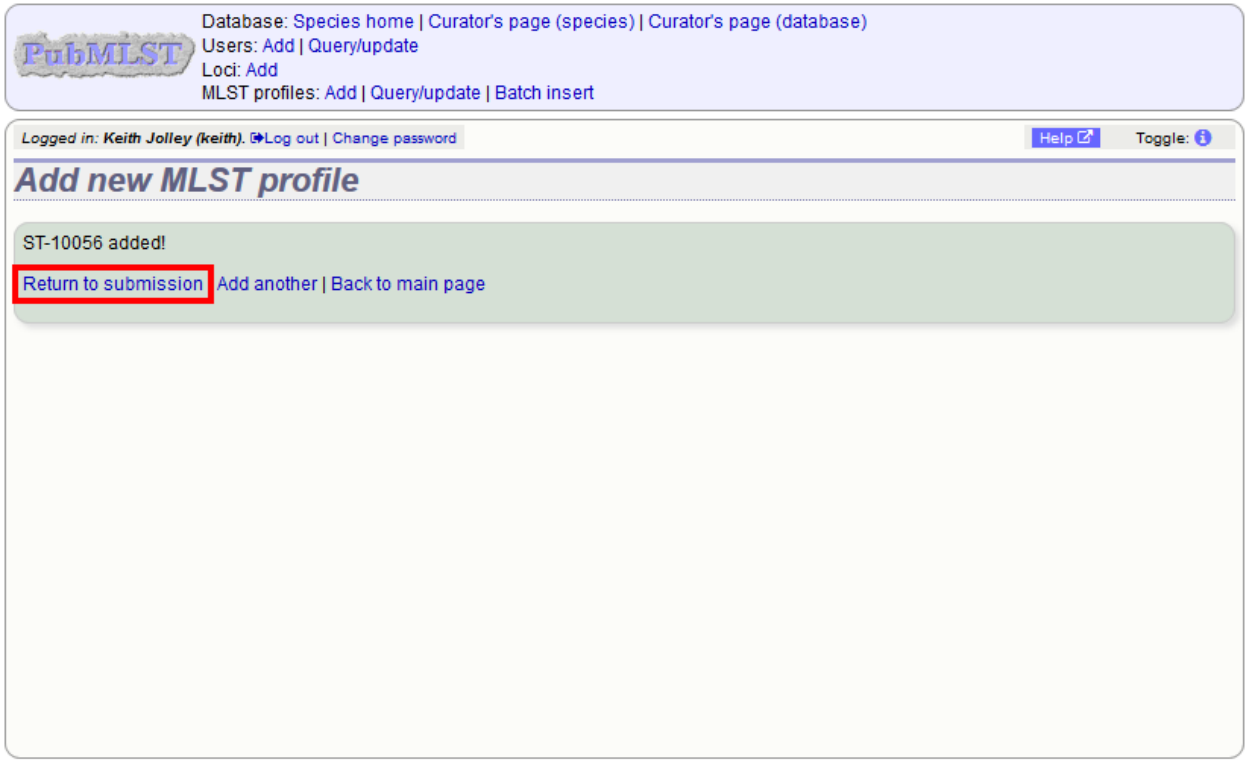
Individual profiles can be curated singly by clicking the 'Curate' links next to the profile in the table.



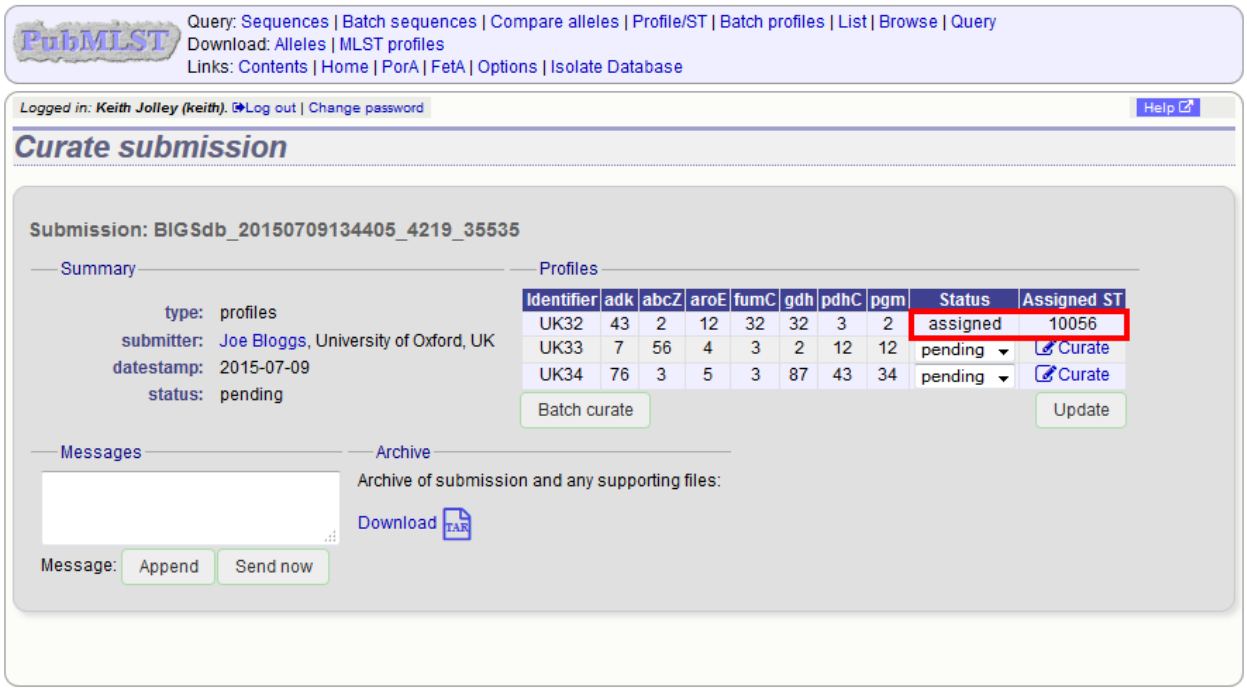
Clicking this link takes you to the curation interface *single profile upload page*. The upload form will be filled with details from the submission.



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.

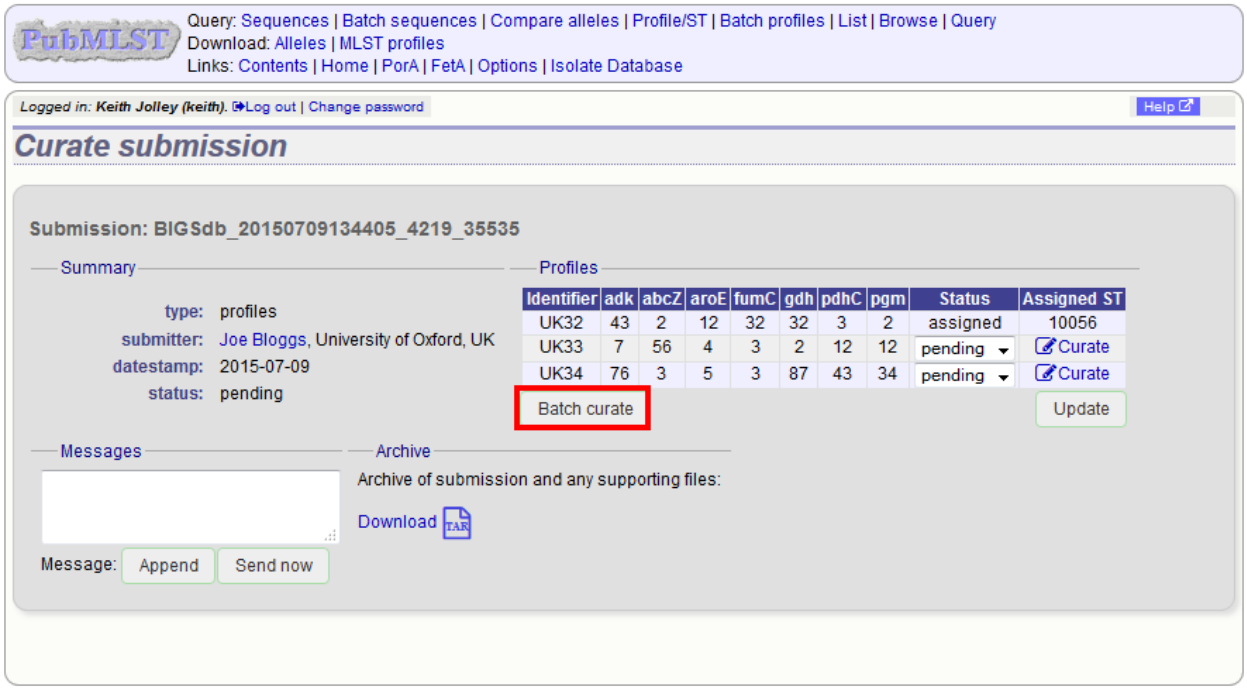


You will find that the status of the newly assigned profile has changed in the summary table. The assigned value and status are determined on display and should always reflect the live database values.



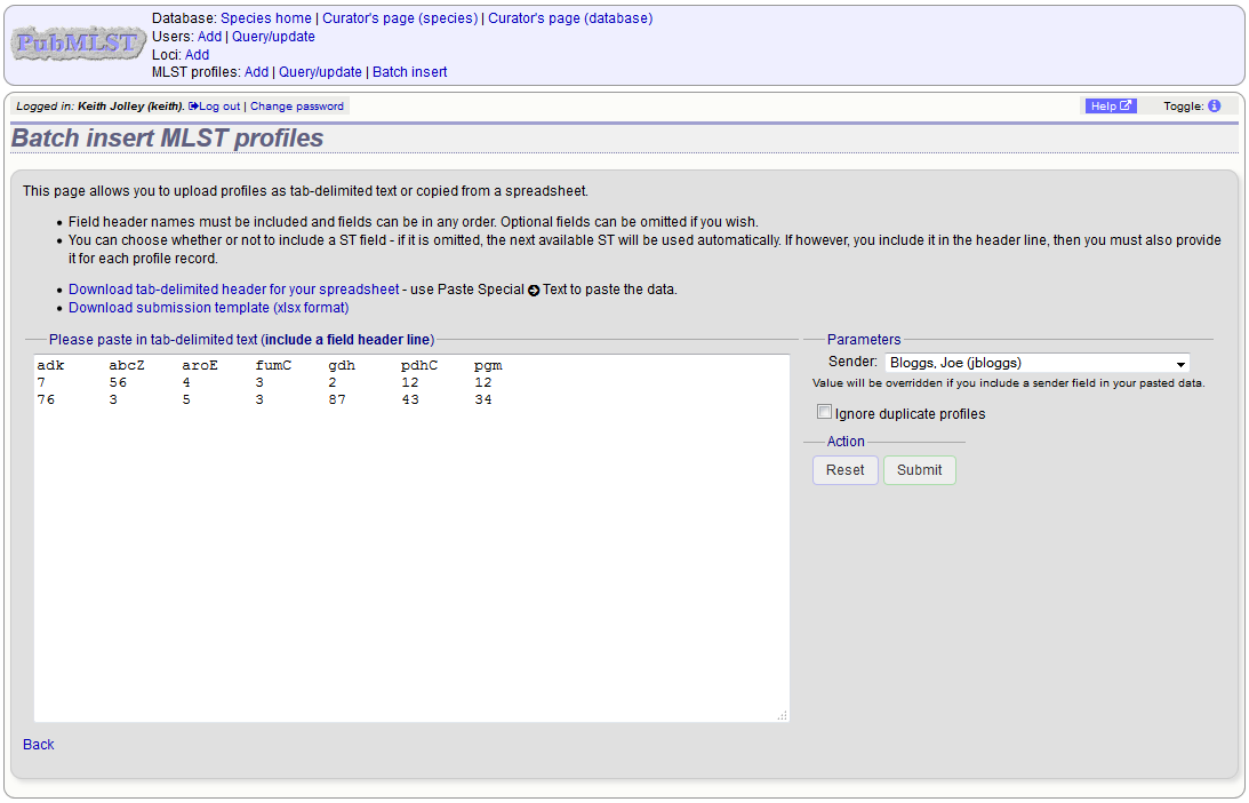
7.2.2 Batch profile curation

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



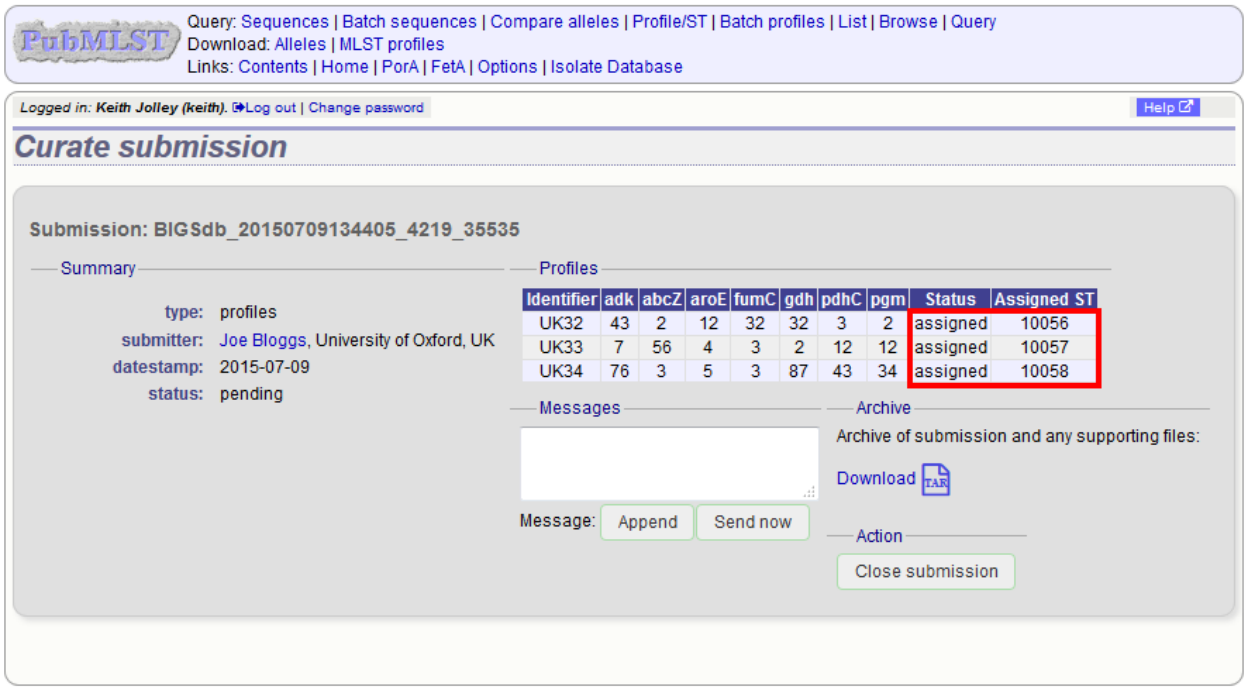
This takes you to the *batch profile upload page* in the curators' interface.

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



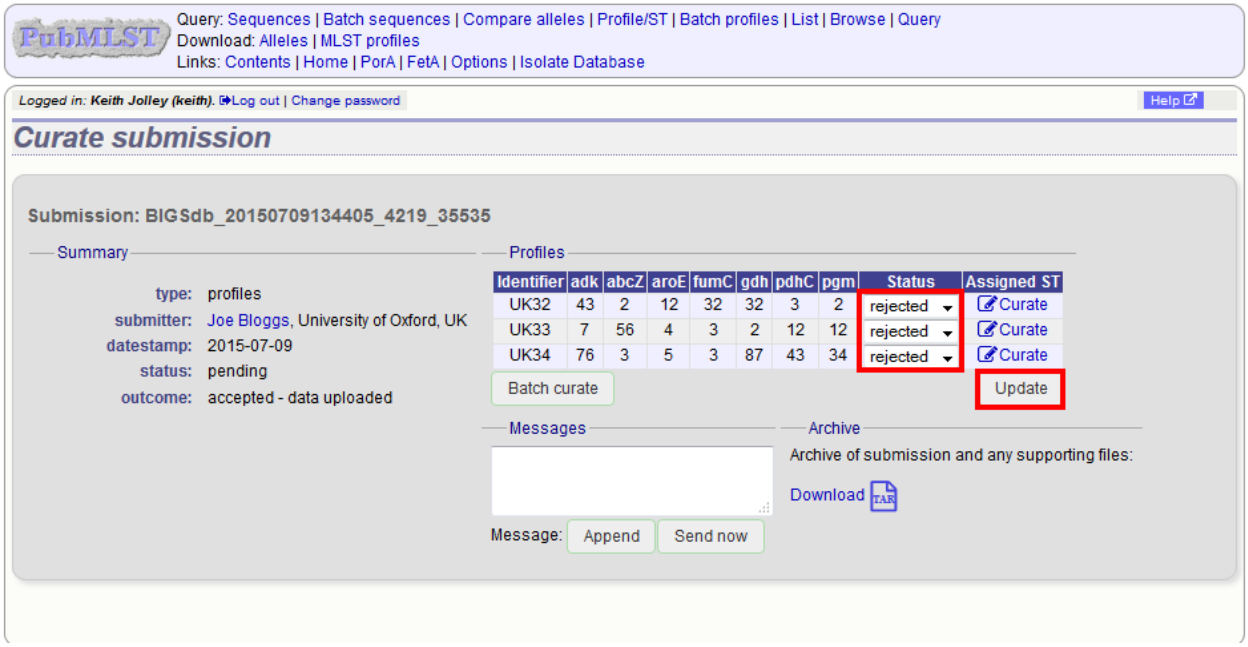
After upload, a link on the confirmation page leads back to the submission management page.

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



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.



7.2.4 Requesting additonal information

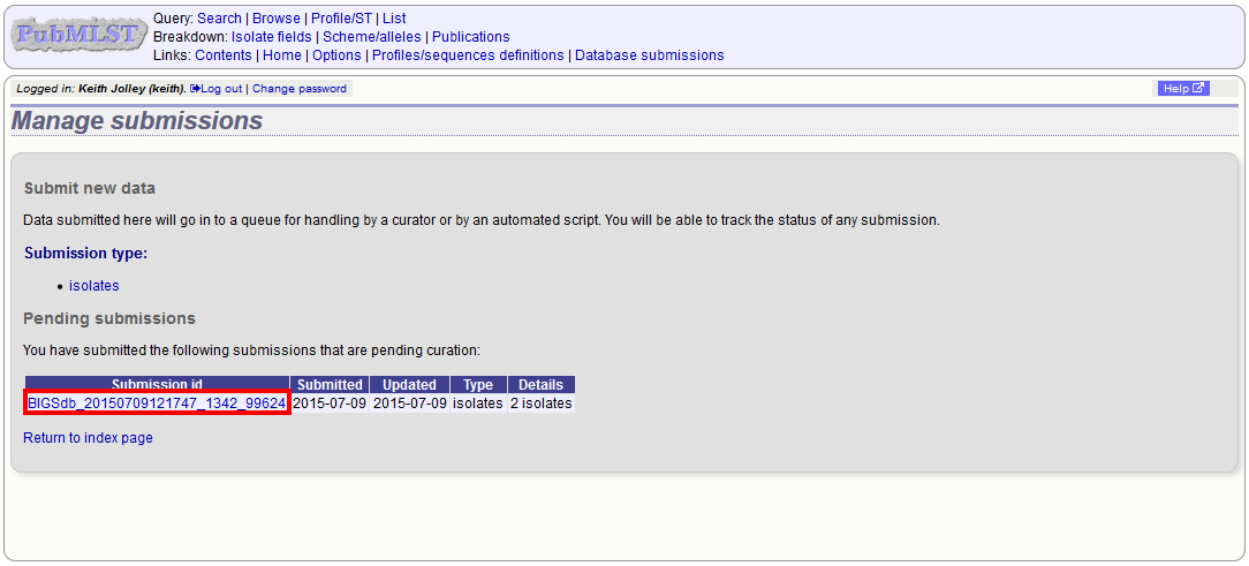
You can send a message to the submitter by entering it in the Messages box and clicking 'Send now'. This will append a message to the submission and send an update to the submitter so that they can respond.

7.2.5 Closing the submission

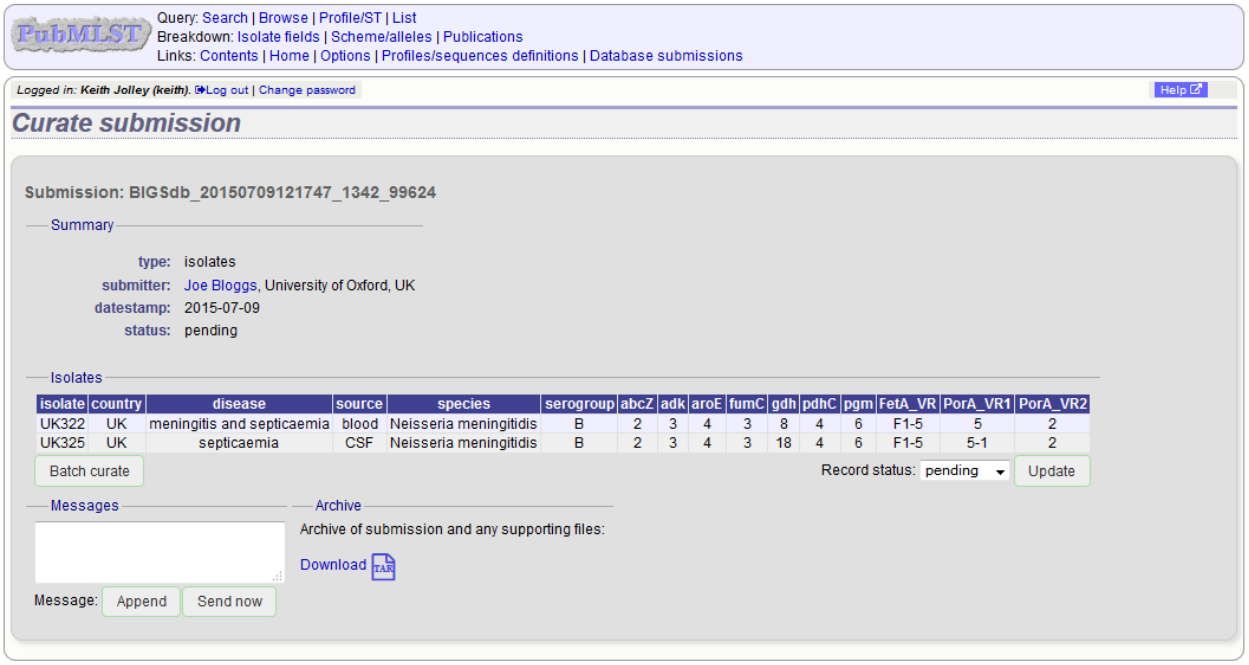
You can add a message to the submitter by entering it in the message box and clicking 'Append'. Once profiles have all been either assigned or rejected, the 'Close submission' button will be displayed. Click this to close the submission. The submitter will be notified of their submission status.

7.3 Isolates

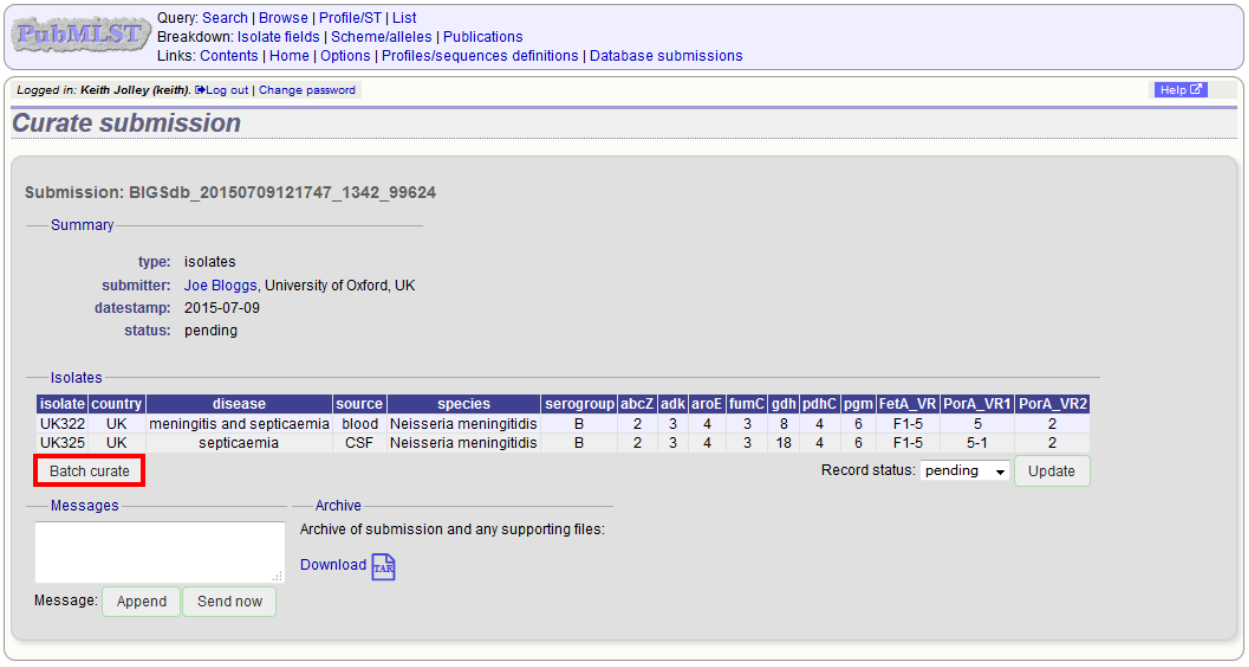
Clicking the appropriate submission on the 'Manage submissions' page.



You will see a table summarizing the submission.

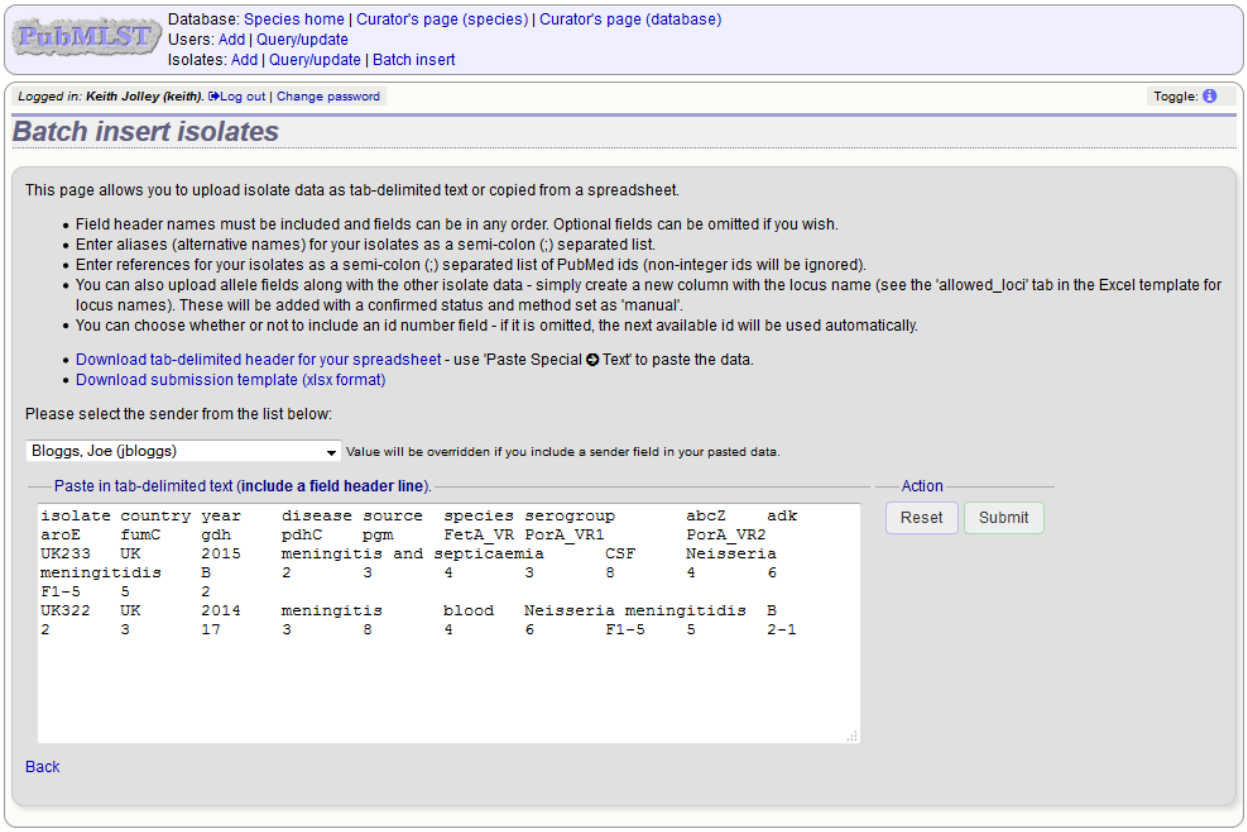


Click the 'Batch curate' button.



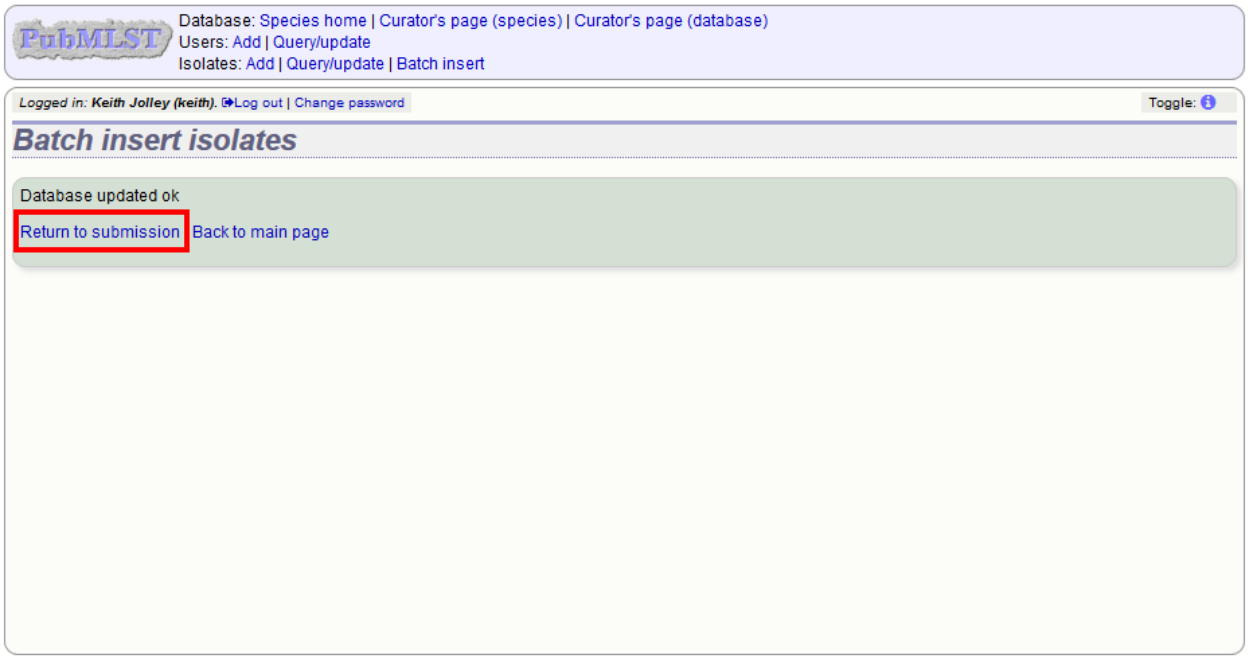
This will take you to the *batch isolate upload page* in the curators' interface.

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



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.



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

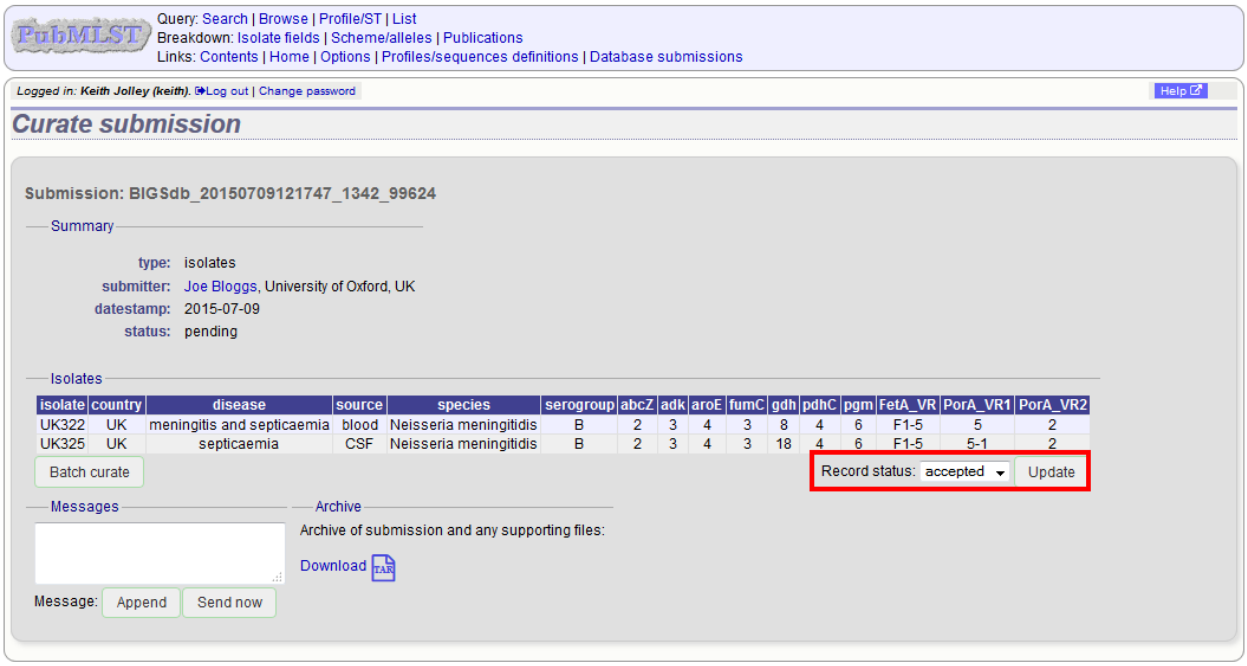
of representative isolate records. Where this is the case, the curator will need to extract the new profile from the submitted record. The tab-delimited isolate text file can be downloaded from the archive of supporting files linked to the submission and used directly for *batch adding new profiles*.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

7.3.1 Requesting additonal information

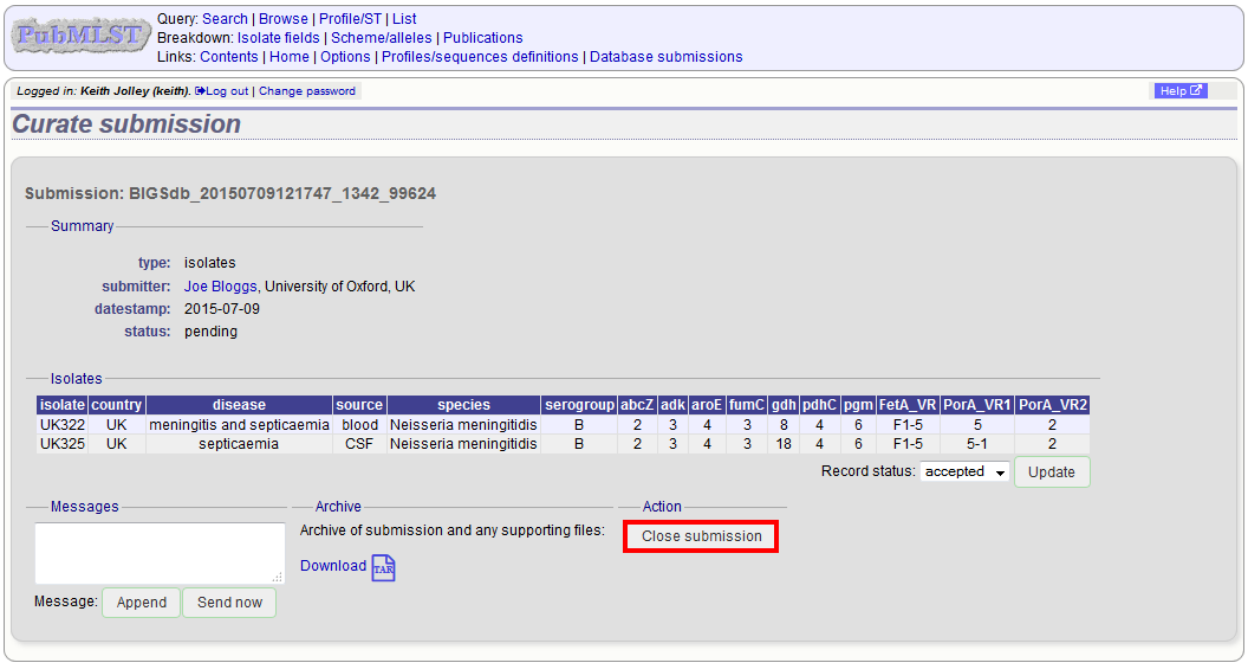
You can send a message to the submitter by entering it in the Messages box and clicking 'Send now'. This will append a message to the submission and send an update to the submitter so that they can respond.

7.3.2 Closing the submission

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



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


PubMLST
Query: Search | Browse | Profile/ST | List
Breakdown: Isolate fields | Scheme/alleles | Publications
Links: Contents | Home | Options | Profiles/sequences definitions | Database submissions
Logged in: Keith Jolley (keith). Log out | Change password
Help
Curate submission
Submission: BIGSdb_20150709121747_1342_99624
Summary
type: isolates
submitter: Joe Bloggs, University of Oxford, UK
datestamp: 2015-07-09
status: pending
Isolates
isolate country disease source species serogroup abcZ adk aroE fumC gdh pdhC pgm FetA_VR PorA_VR1 PorA_VR2
UK322 UK meningitis and septicaemia blood Neisseria meningitidis B 2 3 4 3 8 4 6 F1-5 5 2
UK325 UK septicaemia CSF Neisseria meningitidis B 2 3 4 3 18 4 6 F1-5 5-1 2
Record status: accepted
Update
Messages
Archive
Archive of submission and any supporting files:
Download
Action
Close submission
Message:
Append
Send now

CHAPTER 8

Offline curation tools

8.1 Automated offline sequence tagging

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

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

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

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

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

```
autotag.pl --database <database configuration>
```

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

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

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

A full list of options can be found by typing:

```
autotag.pl --help

NAME
    autotag.pl - BIGSdb automated allele tagger
```

```
SYNOPSIS
    autotag.pl --database NAME [options]

OPTIONS
-0, --missing
    Marks missing loci as provisional allele 0. Sets default word size to 15.

-d, --database NAME
    Database configuration name.

-e, --exemplar
    Only use alleles with the 'exemplar' flag set in BLAST searches to identify
    locus within genome. Specific allele is then identified using a database
    lookup. This may be quicker than using all alleles for the BLAST search,
    but will be at the expense of sensitivity. If no exemplar alleles are set
    for a locus then all alleles will be used. Sets default word size to 15.

-f --fast
    Perform single BLAST query against all selected loci together. This will
    take longer to return any results but the overall scan should finish
    quicker. This method will also use more memory - this can be used with
    --exemplar to mitigate against this.

-h, --help
    This help page.

-i, --isolates LIST
    Comma-separated list of isolate ids to scan (ignored if -p used).

--isolate_list_file FILE
    File containing list of isolate ids (ignored if -i or -p used).

-I, --exclude_isolates LIST
    Comma-separated list of isolate ids to ignore.

-l, --loci LIST
    Comma-separated list of loci to scan (ignored if -s used).

-L, --exclude_loci LIST
    Comma-separated list of loci to exclude

-m, --min_size SIZE
    Minimum size of seqbin (bp) - limit search to isolates with at least this
    much sequence.

-n, --new_only
    New (previously untagged) isolates only.  Combine with --new_max_alleles
    if required.

--new_max_alleles ALLELES
    Set the maximum number of alleles that can be designated or sequences
    tagged before an isolate is not considered new when using the --new_only
    option.

-o, --order
    Order so that isolates last tagged the longest time ago get scanned first
    (ignored if -r used).
```

```
--only_already_tagged
    Only check loci that already have a tag present (but no allele designation).
    This must be combined with the --already_tagged option or no loci will
    match. This option is used to perform a catch-up scan where a curator has
    previously tagged sequence regions prior to alleles being defined, without
    the need to scan all missing loci.

-p, --projects LIST
    Comma-separated list of project isolates to scan.

-P, --exclude_projects LIST
    Comma-separated list of projects whose isolates will be excluded.

-q, --quiet
    Only error messages displayed.

-r, --random
    Shuffle order of isolate ids to scan.

--reuse_blast
    Reuse the BLAST database for every isolate (when running --fast option).
    All loci will be scanned rather than just those missing from an isolate.
    Consequently, this may be slower if isolates have already been scanned,
    and for the first isolate scanned by a thread. On larger schemes, such as
    wgMLST, or when isolates have not been previously scanned, setting up the
    BLAST database can take a significant amount of time, so this may be
    quicker. This option is always selected if --new_only is used.

-R, --locus_regex REGEX
    Regex for locus names.

-s, --schemes LIST
    Comma-separated list of scheme loci to scan.

-t, --time MINS
    Stop after t minutes.

--threads THREADS
    Maximum number of threads to use.

-T, --already_tagged
    Scan even when sequence tagged (no designation).

-v, --view VIEW
    Isolate database view (overrides value set in config.xml).

-w, --word_size SIZE
    BLASTN word size.

-x, --min ID
    Minimum isolate id.

-y, --max ID
    Maximum isolate id.
```

8.2 Defining exemplar alleles

Exemplar alleles are a subset of the total number of alleles defined for a locus that encompass the known diversity within a specified identity threshold. They can be used to speed up *autotagging* as the BLAST queries are performed against exemplars to identify the locus region in the genome followed by a direct database lookup of the sequence found to identify the exact allele found. This is usually combined with the autotagger –fast option.

Once exemplars have been defined you may also wish to set the fast_scan="yes" option in the config.xml file. This enables their use for scanning within the web curators' interface.

There is a script called 'find_exemplars.pl' in the BIGSdb scripts/maintenance directory.

A full list of options can be found by typing:

```
find_exemplars.pl --help

NAME
    find_exemplars.pl - Identify and mark exemplar alleles for use
    by tagging functions

SYNOPSIS
    find_exemplars.pl --database NAME   [options]

OPTIONS

--database NAME
    Database configuration name.

--datatype DNA|peptide
    Only define exemplars for specified data type (DNA or peptide)

--exclude_loci LIST
    Comma-separated list of loci to exclude

--help
    This help page.

--loci LIST
    Comma-separated list of loci to scan (ignored if -s used).

--locus_regex REGEX
    Regex for locus names.

--schemes LIST
    Comma-separated list of scheme loci to scan.

--update
    Update exemplar flags in database.

--variation IDENTITY
    Value for percentage identity variation that exemplar alleles
    cover (smaller value will result in more exemplars). Default: 10.
```

8.3 Automated offline allele definition

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

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

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

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

```
scannew.pl --database <database configuration>
```

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

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

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

A full list of options can be found by typing:

```
scannew.pl --help

NAME
  scannew.pl - BIGSdb automated allele definer

SYNOPSIS
  scannew.pl --database NAME [options]

OPTIONS
-a, --assign
    Assign new alleles in definitions database.

--allow_frameshift
    Allow sequences to contain a frameshift so that the length is not a
    multiple of 3, or an internal stop codon. To be used with
    --coding_sequences option to allow automated curation of pseudogenes.
    New alleles assigned will be flagged either 'frameshift' or 'internal stop
    codon' if appropriate.  Essentially, combining these two options only
    checks that the sequence starts with a start codon and ends with a stop
    codon.

-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.

--type_alleles
    Only use alleles with the 'type_allele' flag set to identify locus.
    If a partial match is found then a full database lookup will be performed
    to identify any known alleles. Using this option will constrain the search
    space so that allele definitions don't become more variable over time. Note
    that you must have at least one allele defined as a type allele for a locus
    if you use this option otherwise you will not find any matches!

-T, --already_tagged
```

```
    Scan even when sequence tagged (no designation).

-v, --view VIEW
    Isolate database view (overrides value set in config.xml).

-w, --word_size SIZE
    BLASTN word size.

-x, --min ID
    Minimum isolate id.

-y, --max ID
    Maximum isolate id.
```

8.4 Cleanly interrupting offline curation

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

```
kill 23232
```

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

If these scripts are running using multiple threads, then you need to cleanly kill each of these. The simplest way to terminate all autotagger jobs is to type

```
pkill autotag
```

The parent process will wait for all forked processes to cleanly terminate and then exit itself.

Similarly, to terminate all allele autodefiner jobs, type

```
pkill scannew
```

8.5 Uploading contigs from the command line

There is a script called upload_contigs.pl in the BIGSdb scripts/maintenance directory. This can be used to upload contigs from a local FASTA file for a specified isolate record.

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

```
upload_contigs.pl --database <NAME> --isolate <ID> --file <FILE>
    --curator <ID> --sender <ID>
```

The script must be run by a user who has the appropriate database permissions and the local configuration settings should be modified to match the database user account to be used. The default setting uses the 'apache' user which is used by the BIGSdb web interface.

A full list of options can be found by typing:

```
upload_contigs.pl --help

NAME
    upload_contigs.pl - Upload contigs to BIGSdb isolate database

SYNOPSIS
    upload_contigs.pl --database NAME --isolate ID --file FILE
         --curator ID --sender ID [options]

OPTIONS
-a, --append
    Upload contigs even 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'.

--min_length LENGTH
    Exclude contigs with length less than value.

-s, --sender ID
    Sender id number.
```

CHAPTER 9

Definition downloads

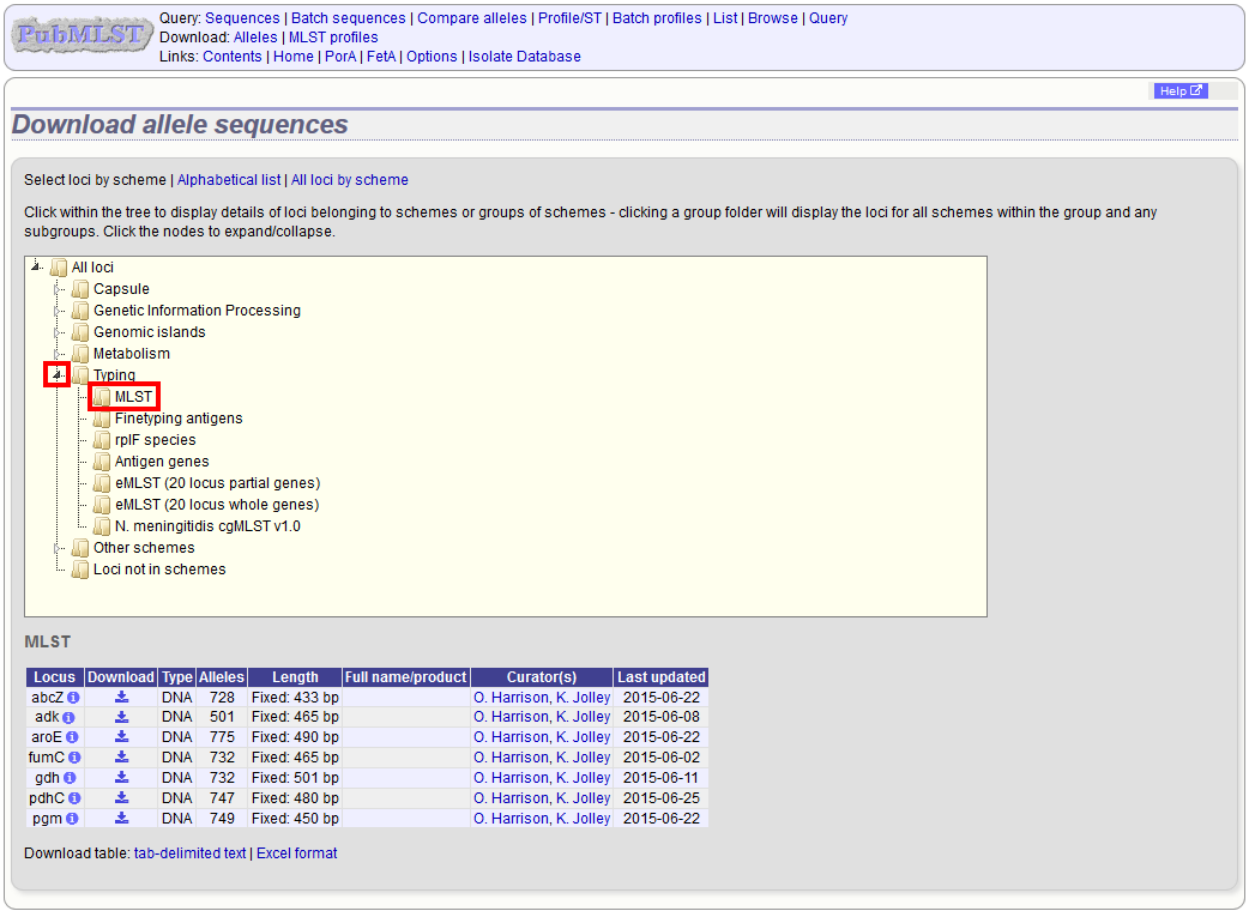
The sequence definition database defines alleles, i.e. links an allele identifier to a sequence. It also defines scheme, e.g. MLST, profiles.

9.1 Allele sequence definitions

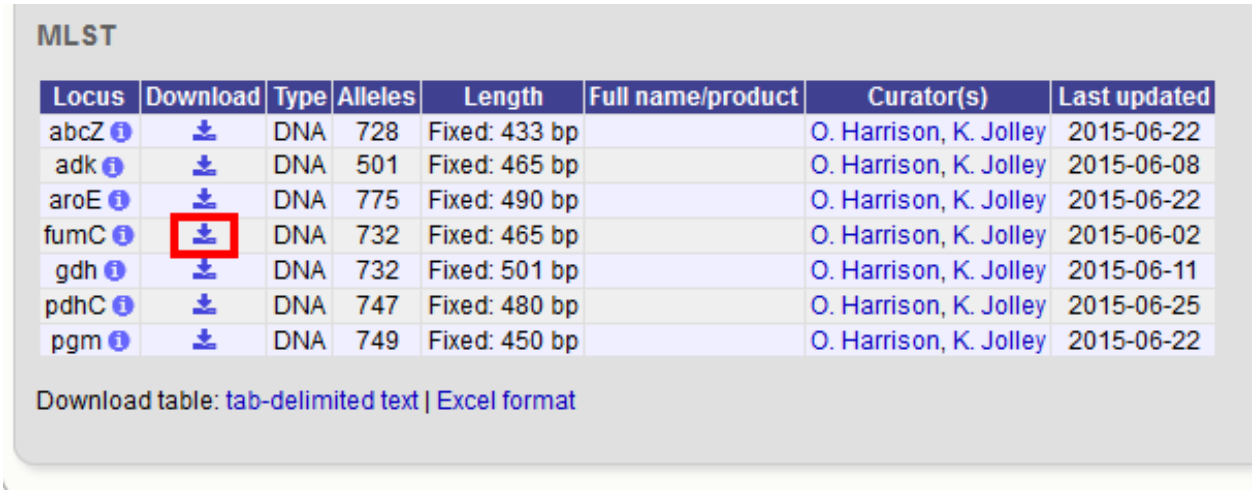
Click the 'Allele sequences' link in the 'Downloads' section. Depending on the database, you may see either a hierarchical scheme tree or a table of loci. You can choose to display links either by scheme using the scheme tree, as an alphabetical list or a page of all schemes, by selecting the approrpiate 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



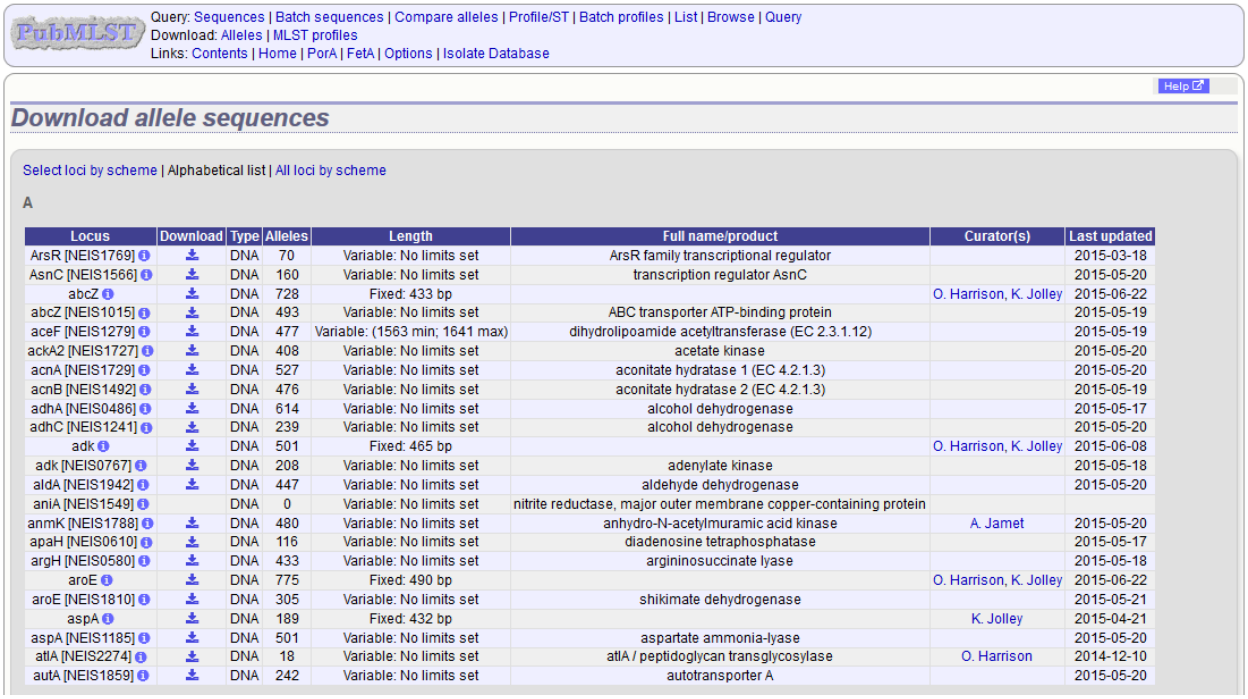
Alleles will be downloaded in FASTA format, e.g.

```
>fumC_1
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGGCAAGCGGCCCGCGCTGCGGT
TTGGGCGAAATCAAAATCCCCGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT
ACCATCGGTATGGCGGGCGCGTCGGGCAATTTCGAGCTGAACGTCTATATGCCCGTCATC
```

```
GCCTACAACCTCTTGCAATCCATCCGCCTGTTGGGCGACGCGTGCAACAGCTTCAACGAA
CACTGCGCCGTCGGCATTGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC
CTGATGCTCGTTACCGCGTTAAACCGCAAAATCGGTTACGAAAAC
>fumC_2
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGGCAAGCGGCCCGCGCTGCGGT
TTGGGCGAAATCAAAATCCCCGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT
ACCATCGGCATGGCGGGCGCGTCGGGCAATTTCGAGCTGAACGTCTATATGCCCGTTATC
GCCTACAACCTCTTGCAATCCATCCGCCTCTTGGGCGACGCGTGCAACAGCTTCAACGAA
CACTGCGCCATCGGCATCGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC
CTGATGCTCGTTACCGCGTTAAACCGCAAAATCGGTTACGAAAAC
>fumC_3
GAAGCCTTGGGCGGACGCGATGCCGCCGTTGCCGCTTCGGGCGCATTGAAAACGCTGGCG
GCAAGCCTGAATAAAATCGCCAACGACATCCGCTGGCTGGCAAGCGGCCCGCGCTGCGGT
TTGGGCGAAATCAAAATCCCCGAAAACGAGCCGGGTTCGTCCATCATGCCGGGCAAAGTC
AACCCGACCCAATGCGAAGCGATGACCATGGTGTGCTGCCAAGTGTTCGGCAACGACGTT
ACCATCGGCATGGCGGGCGCGTCGGGCAATTTCGAGCTGAACGTCTATATGCCCGTTATC
GCCTACAACCTCTTGCAATCCATCCGCCTGTTGGGCGACGCGTGCAACAGCTTCAACGAA
CACTGCGCCGTCGGCATCGAACCCGTACCGGAAAAAATCGACTATTTCCTGCACCATTCC
CTGATGCTGGTTACTGCGTTAAACCGTAAAATCGGCTACGAAAAC
```

9.1.2 Alphabetical list

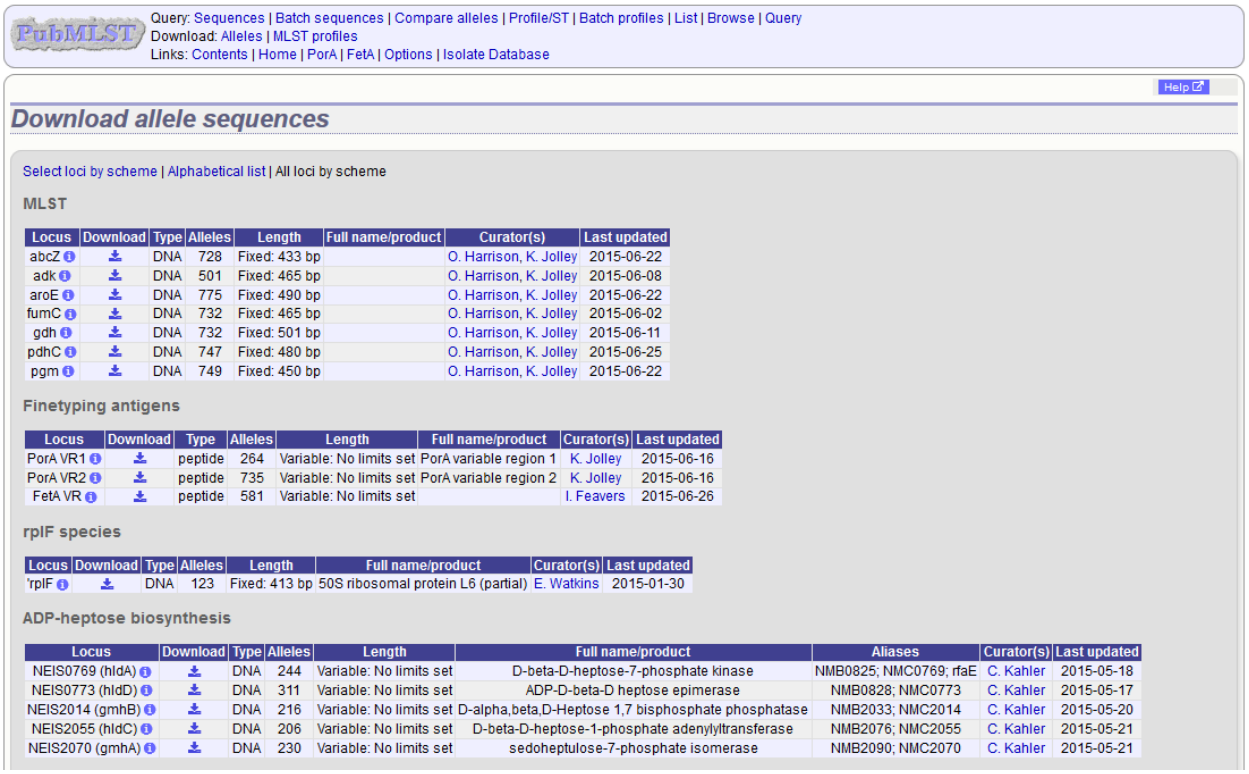
Loci can be displayed in an alphabetical list. Loci will be grouped in to tables by initial letter. If common names are set for loci, they will be listed by both primary and common names.



Click the download links for the required locus.

9.1.3 All loci by scheme

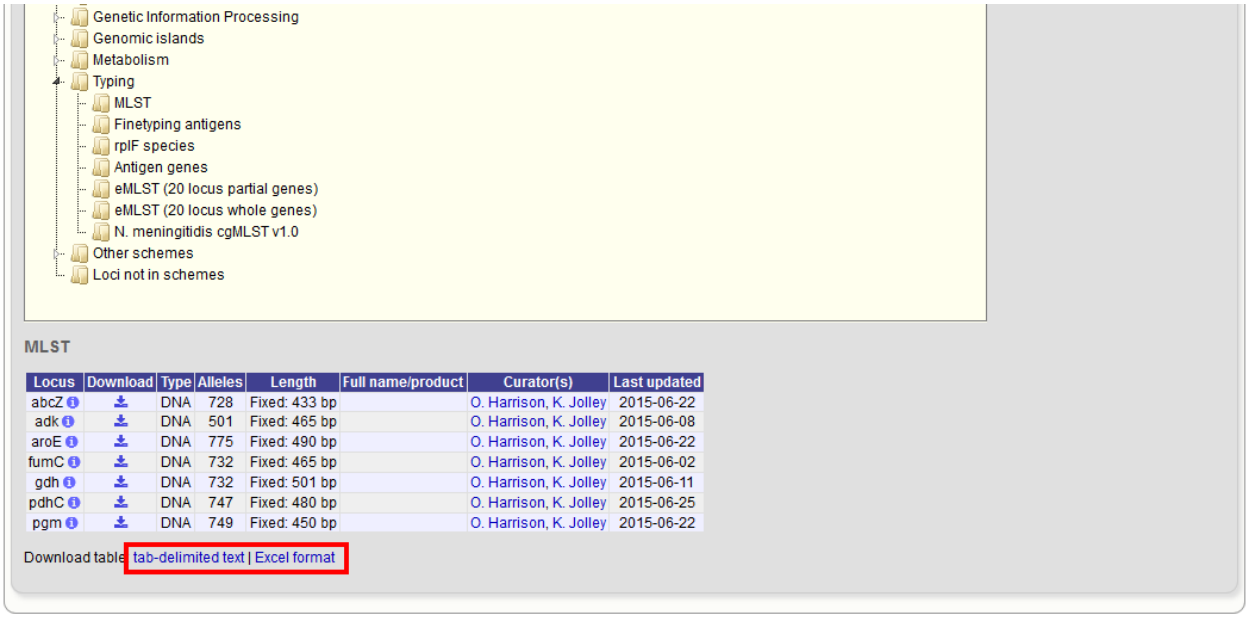
Loci can also be displayed by scheme with all schemes displayed.



Click the green download links for the required locus.

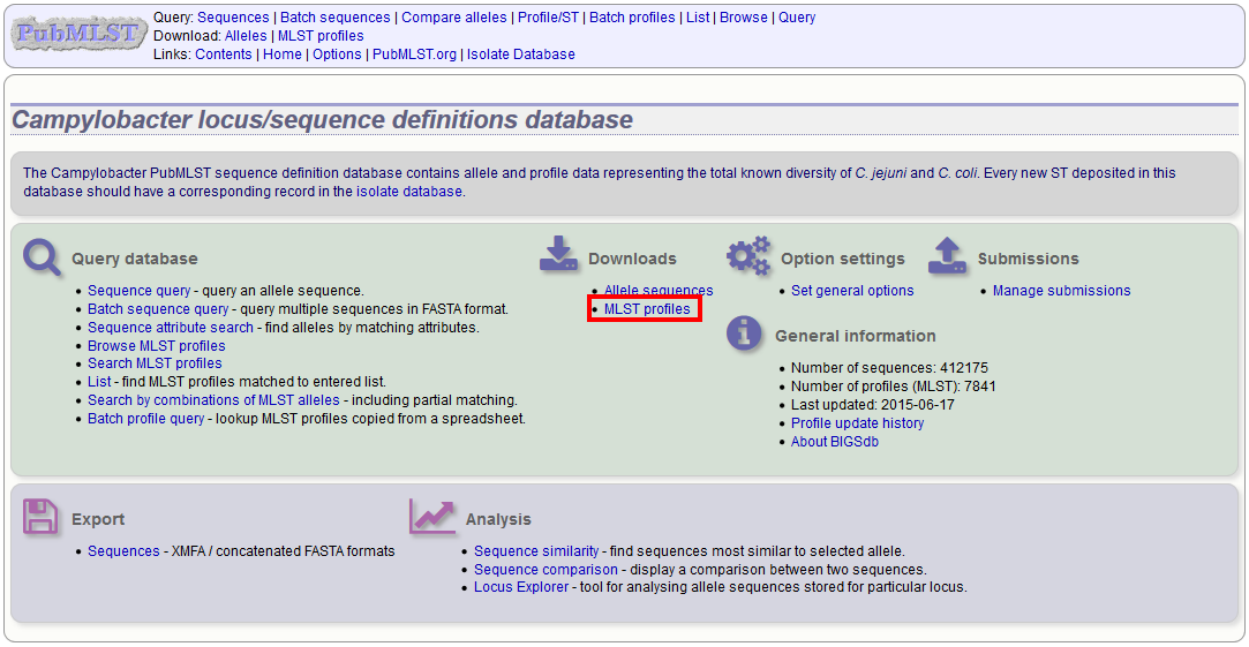
9.1.4 Download locus table

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

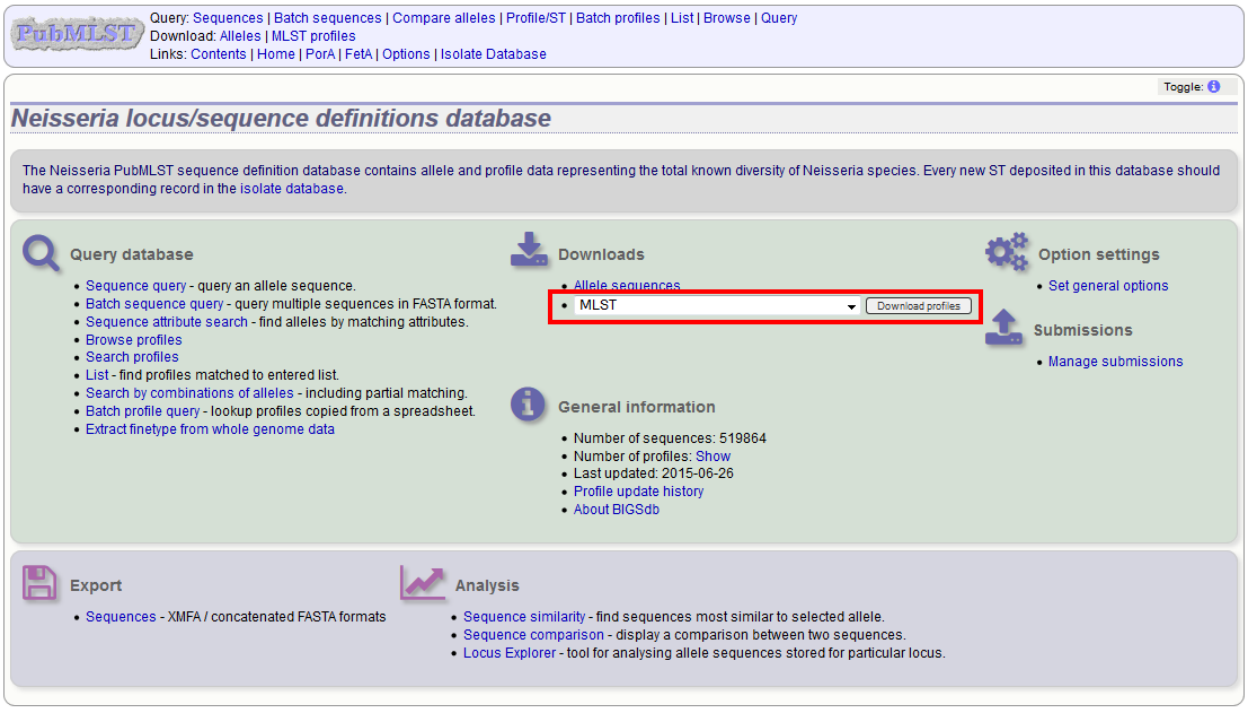


9.2 Scheme profile definitions

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



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



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

```
ST    abcZ    adk    aroE    fumC    gdh    pdhC    pgm    clonal_complex
1     1       3      1       1       1      1       3      ST-1 complex/subgroup I/
↪II
2     1       3      4       7       1      1       3      ST-1 complex/subgroup I/
↪II
3     1       3      1       1       1      23      13     ST-1 complex/subgroup I/
↪II
4     1       3      3       1       4      2       3      ST-4 complex/subgroup IV
5     1       1      2       1       3      2       3      ST-5 complex/subgroup␣
↪III
6     1       1      2       1       3      2       11     ST-5 complex/subgroup␣
↪III
7     1       1      2       1       3      2       19     ST-5 complex/subgroup␣
↪III
8     2       3      7       2       8      5       2      ST-8 complex/Cluster A4
9     2       3      8       10      8      5       2      ST-8 complex/Cluster A4
10    2       3      4       2       8      15      2      ST-8 complex/Cluster A4
11    2       3      4       3       8      4       6      ST-11 complex/ET-37␣
↪complex
12    4       3      2       16      8      11      20
13    4       10     15      7       8      11      1      ST-269 complex
14    4       1      15      7       8      11      1      ST-269 complex
```

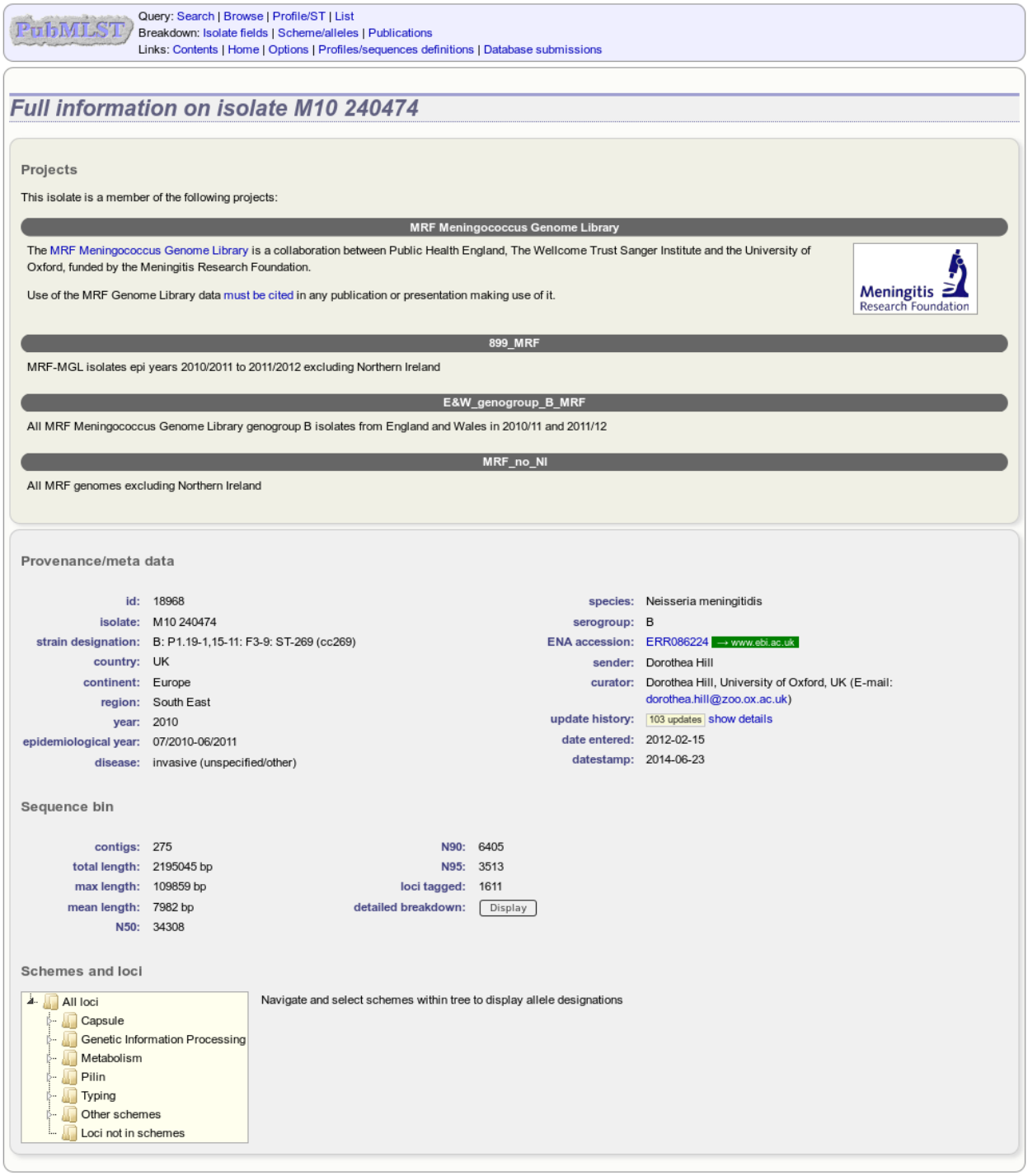
CHAPTER 10

Data records

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

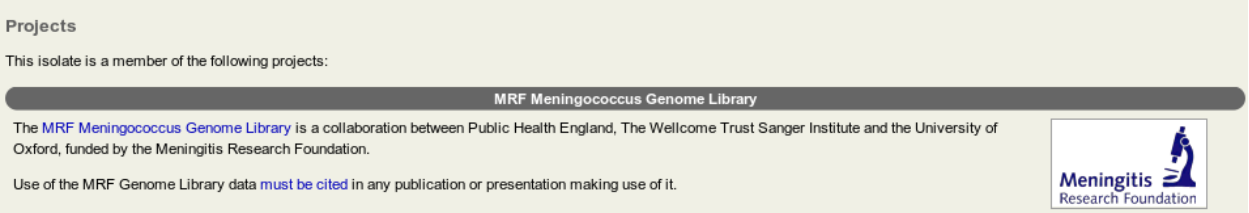
10.1 Isolate records

An Isolate record page displays everything known about an isolate.



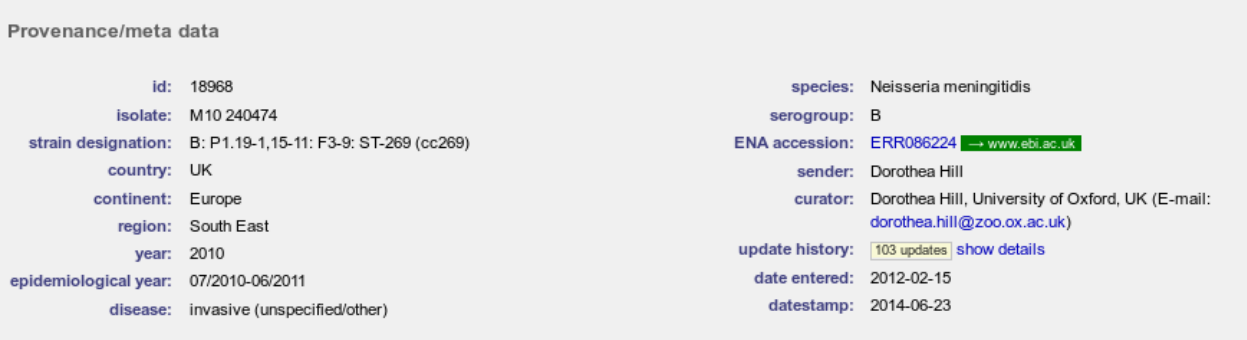
Each record will have some or all of the following sections:

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.

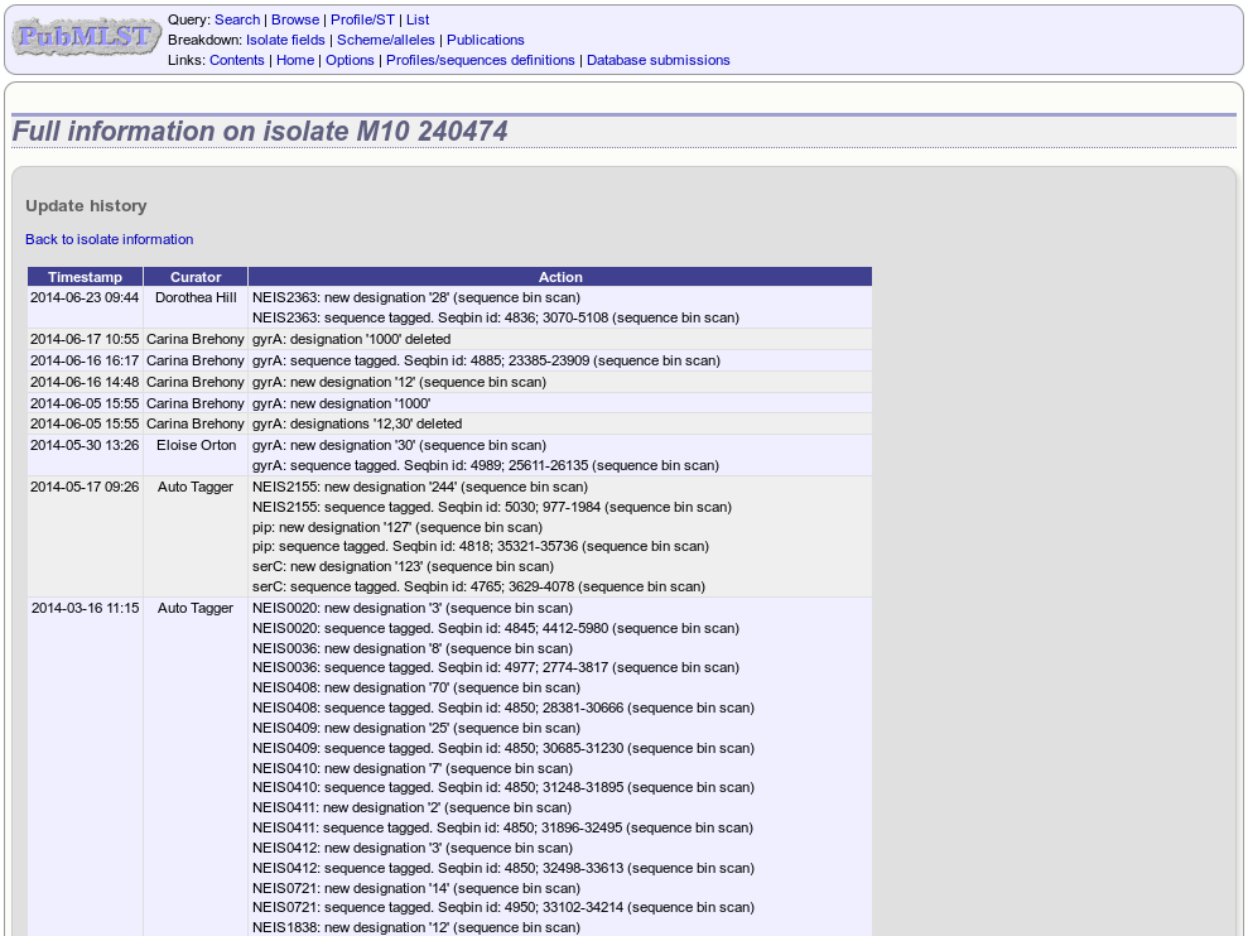
10.1.2 Provenance metadata



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.



PubMLST

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

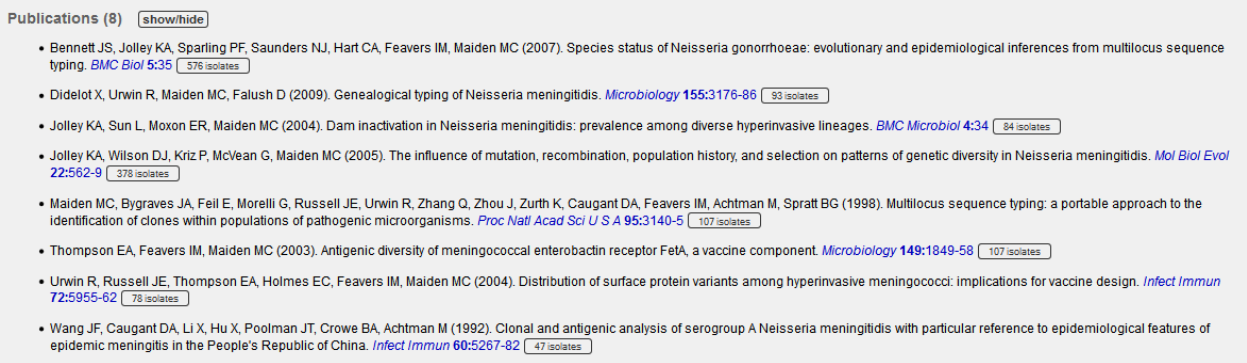
Full information on isolate M10 240474

Update history

Back to isolate information

Timestamp	Curator	Action
2014-06-23 09:44	Dorothea Hill	NEIS2363: new designation '28' (sequence bin scan) NEIS2363: sequence tagged. Seqbin id: 4836; 3070-5108 (sequence bin scan)
2014-06-17 10:55	Carina Brehony	gyrA: designation '1000' deleted
2014-06-16 16:17	Carina Brehony	gyrA: sequence tagged. Seqbin id: 4885; 23385-23909 (sequence bin scan)
2014-06-16 14:48	Carina Brehony	gyrA: new designation '12' (sequence bin scan)
2014-06-05 15:55	Carina Brehony	gyrA: new designation '1000'
2014-06-05 15:55	Carina Brehony	gyrA: designations '12,30' deleted
2014-05-30 13:26	Eloise Orton	gyrA: new designation '30' (sequence bin scan) gyrA: sequence tagged. Seqbin id: 4989; 25611-26135 (sequence bin scan)
2014-05-17 09:26	Auto Tagger	NEIS2155: new designation '244' (sequence bin scan) NEIS2155: sequence tagged. Seqbin id: 5030; 977-1984 (sequence bin scan) pip: new designation '127' (sequence bin scan) pip: sequence tagged. Seqbin id: 4818; 35321-35736 (sequence bin scan) serC: new designation '123' (sequence bin scan) serC: sequence tagged. Seqbin id: 4765; 3629-4078 (sequence bin scan)
2014-03-16 11:15	Auto Tagger	NEIS0020: new designation '3' (sequence bin scan) NEIS0020: sequence tagged. Seqbin id: 4845; 4412-5980 (sequence bin scan) NEIS0036: new designation '8' (sequence bin scan) NEIS0036: sequence tagged. Seqbin id: 4977; 2774-3817 (sequence bin scan) NEIS0408: new designation '70' (sequence bin scan) NEIS0408: sequence tagged. Seqbin id: 4850; 28381-30666 (sequence bin scan) NEIS0409: new designation '25' (sequence bin scan) NEIS0409: sequence tagged. Seqbin id: 4850; 30685-31230 (sequence bin scan) NEIS0410: new designation '7' (sequence bin scan) NEIS0410: sequence tagged. Seqbin id: 4850; 31248-31895 (sequence bin scan) NEIS0411: new designation '2' (sequence bin scan) NEIS0411: sequence tagged. Seqbin id: 4850; 31896-32495 (sequence bin scan) NEIS0412: new designation '3' (sequence bin scan) NEIS0412: sequence tagged. Seqbin id: 4850; 32498-33613 (sequence bin scan) NEIS0721: new designation '14' (sequence bin scan) NEIS0721: sequence tagged. Seqbin id: 4950; 33102-34214 (sequence bin scan) NEIS1838: new designation '12' (sequence bin scan)

10.1.3 Publications



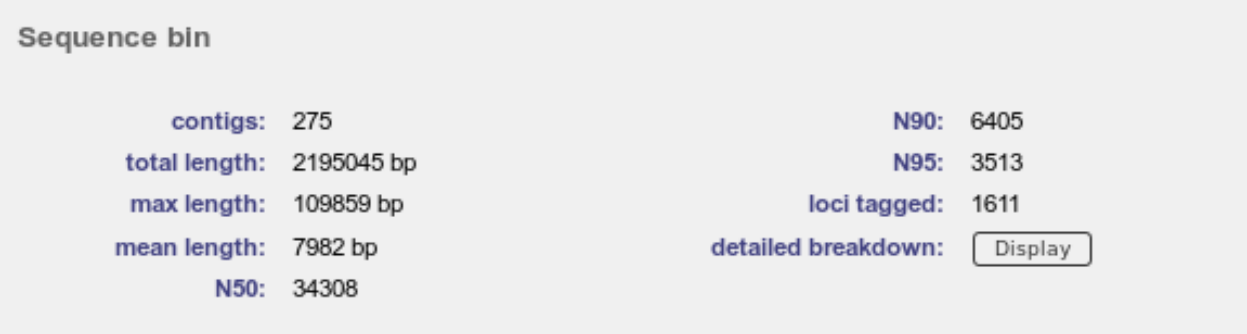
Publications (8) show/hide

- Bennett JS, Jolley KA, Sparling PF, Saunders NJ, Hart CA, Feavers IM, Maiden MC (2007). Species status of Neisseria gonorrhoeae: evolutionary and epidemiological inferences from multilocus sequence typing. *BMC Biol* **5**:35 576 isolates
- Didelot X, Urwin R, Maiden MC, Falush D (2009). Genealogical typing of Neisseria meningitidis. *Microbiology* **155**:3176-86 93 isolates
- Jolley KA, Sun L, Moxon ER, Maiden MC (2004). Dam inactivation in Neisseria meningitidis: prevalence among diverse hyperinvasive lineages. *BMC Microbiol* **4**:34 84 isolates
- Jolley KA, Wilson DJ, Kriz P, McVean G, Maiden MC (2005). The influence of mutation, recombination, population history, and selection on patterns of genetic diversity in Neisseria meningitidis. *Mol Biol Evol* **22**:562-9 378 isolates
- Maiden MC, Bygraves JA, Feil E, Morelli G, Russell JE, Urwin R, Zhang Q, Zhou J, Zurth K, Caugant DA, Feavers IM, Achtman M, Spratt BG (1998). Multilocus sequence typing: a portable approach to the identification of clones within populations of pathogenic microorganisms. *Proc Natl Acad Sci U S A* **95**:3140-5 107 isolates
- Thompson EA, Feavers IM, Maiden MC (2003). Antigenic diversity of meningococcal enterobactin receptor FetA, a vaccine component. *Microbiology* **149**:1849-58 107 isolates
- Urwin R, Russell JE, Thompson EA, Holmes EC, Feavers IM, Maiden MC (2004). Distribution of surface protein variants among hyperinvasive meningococci: implications for vaccine design. *Infect Immun* **72**:5955-62 78 isolates
- Wang JF, Caugant DA, Li X, Hu X, Poolman JT, Crowe BA, Achtman M (1992). Clonal and antigenic analysis of serogroup A Neisseria meningitidis with particular reference to epidemiological features of epidemic meningitis in the People's Republic of China. *Infect Immun* **60**:5267-82 47 isolates

This section includes full citation for papers linked to the isolate record. Each citation has a button that will return a dataset of all isolates linked to the paper.

If there are five or more references they will be hidden by default to avoid cluttering the page too much. Click the 'Show/hide' button to display them in this case.

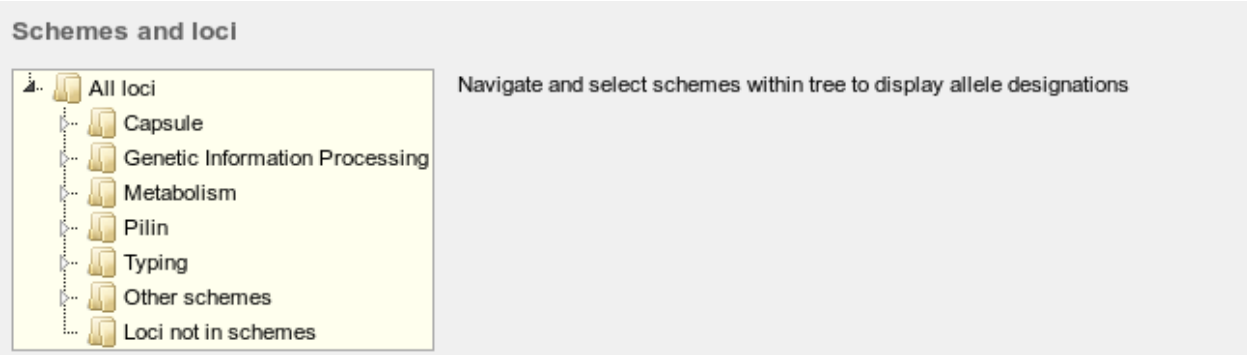
10.1.4 Sequence bin summary



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.



Clicking any terminal node will display data available for a scheme or group of schemes.

Click an allele number within the scheme profile, will display the appropriate *allele definition record*. Clicking the green 'S' link will display the appropriate *sequence tag record*.

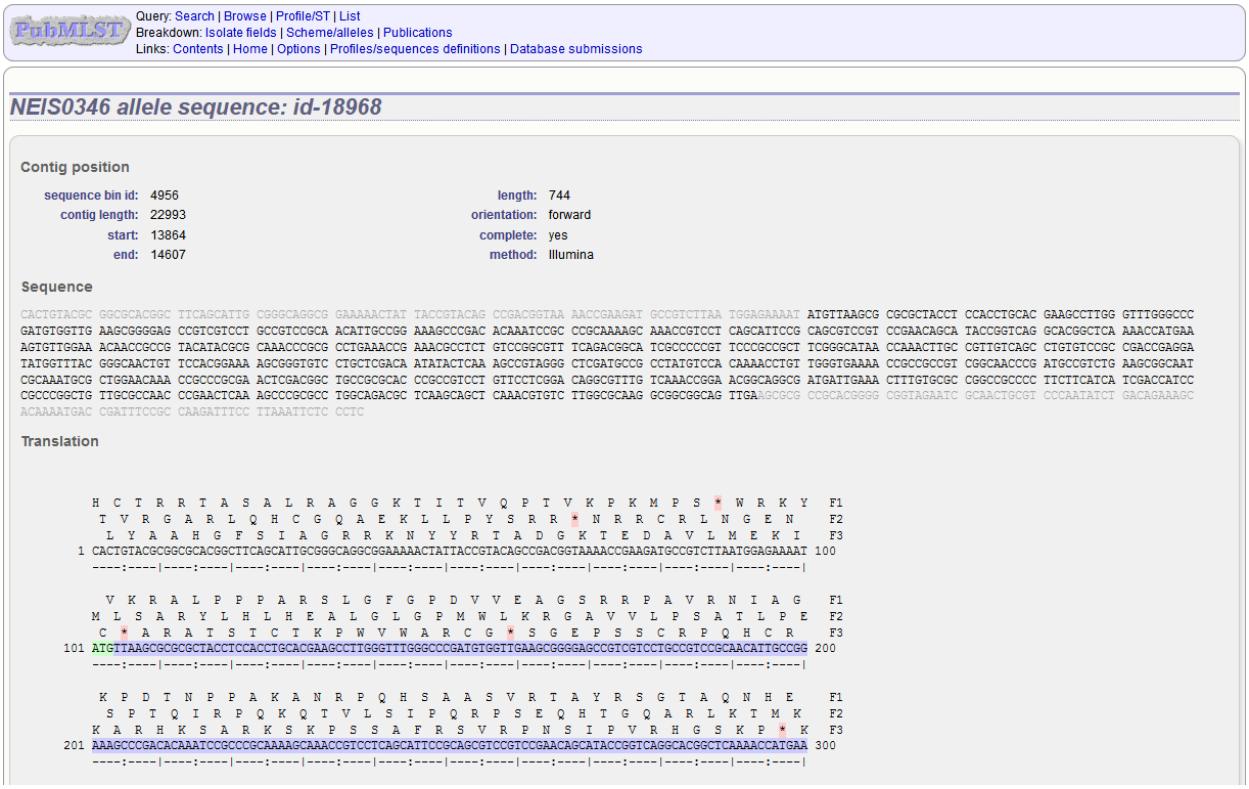
10.2 Allele definition records

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

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

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

10.3 Sequence tag records



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*.

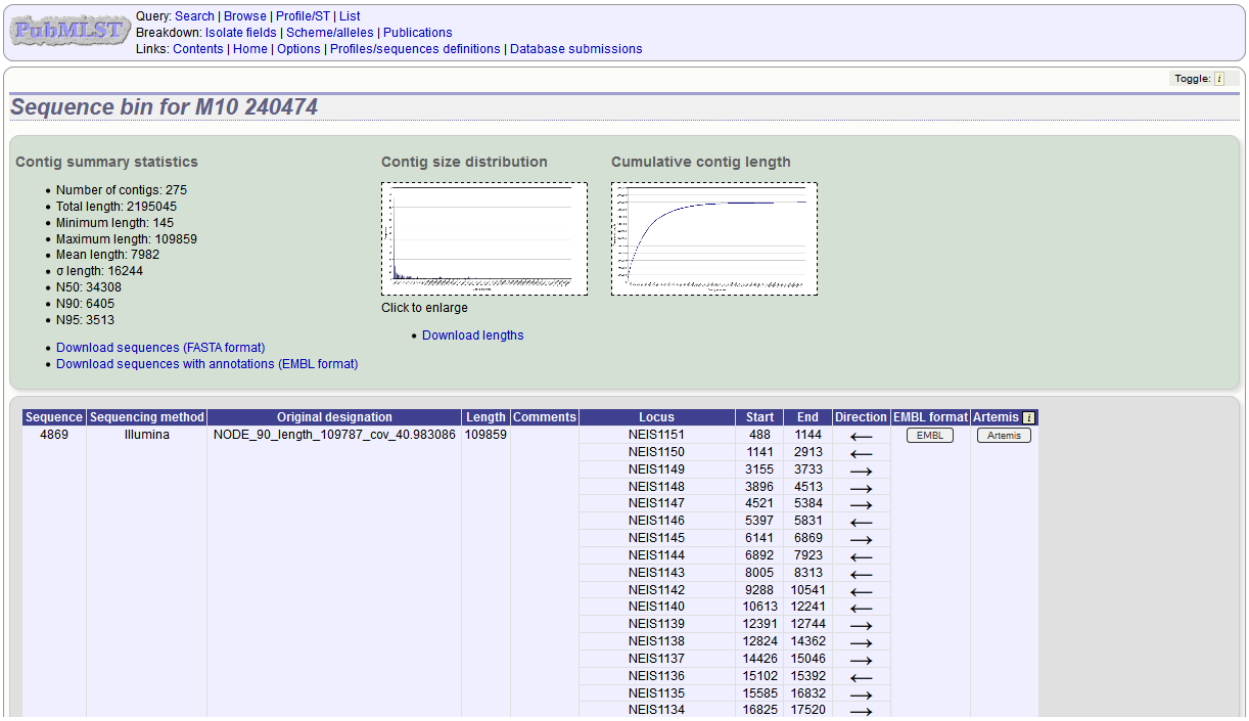
If the tag is for a DNA locus and it is marked as a coding sequence, the three-frame translation will also be displayed.

10.4 Profile records

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



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

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

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

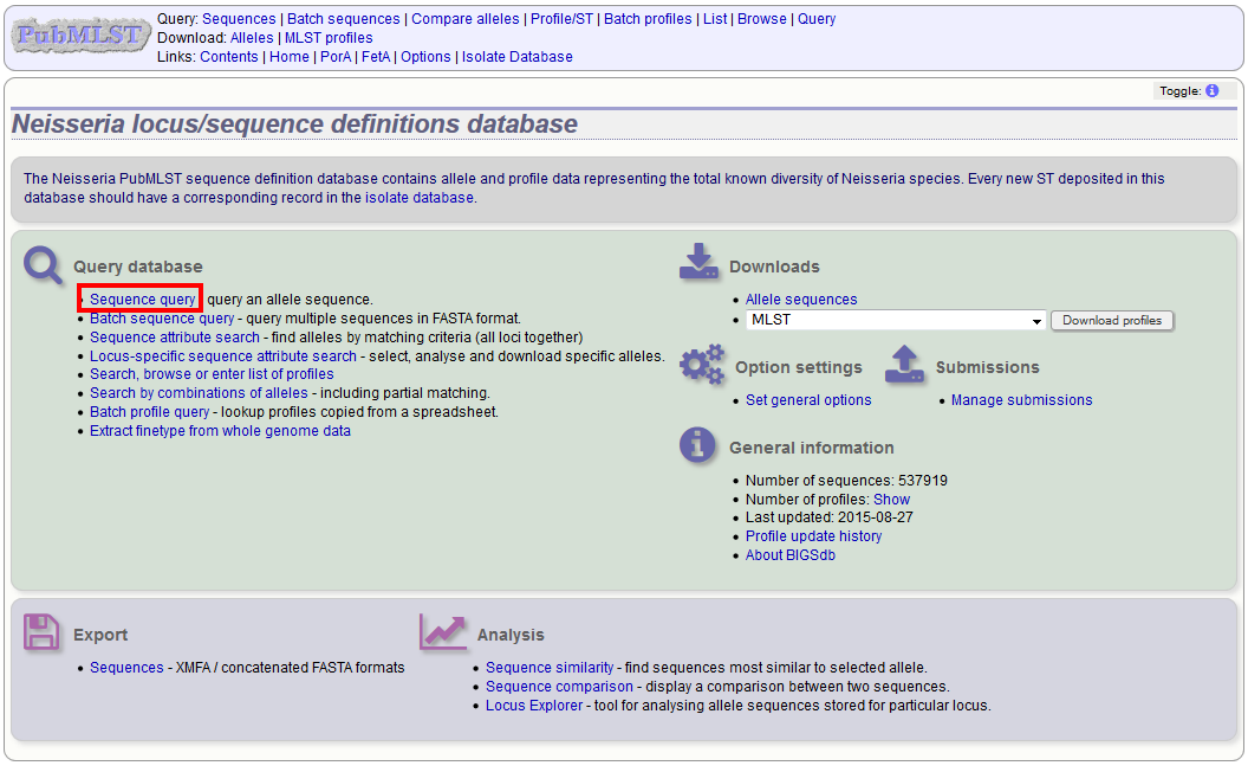
Finally there is a table that shows the loci that are tagged on each contig. Individual contigs can also be downloaded in EMBL format.

CHAPTER 11

Querying data

11.1 Querying sequences to determine allele identity

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

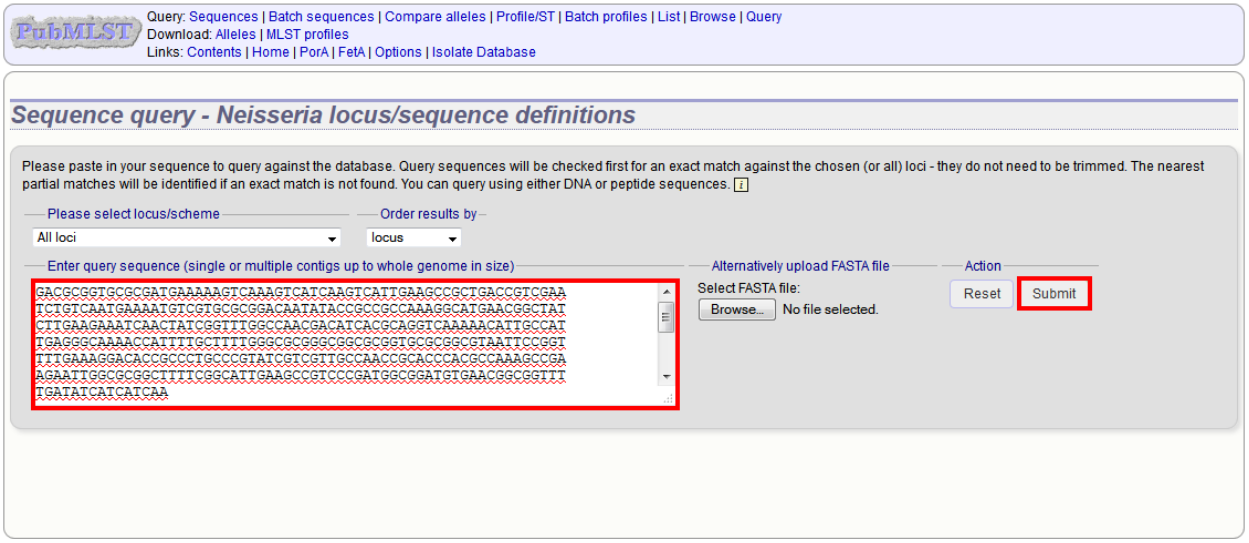


Paste your sequence in to the box - there is no need to trim. Normally, you can leave the locus setting on 'All loci' - the software should identify the correct locus based on your sequence. Sometimes, it may be quicker, however, to

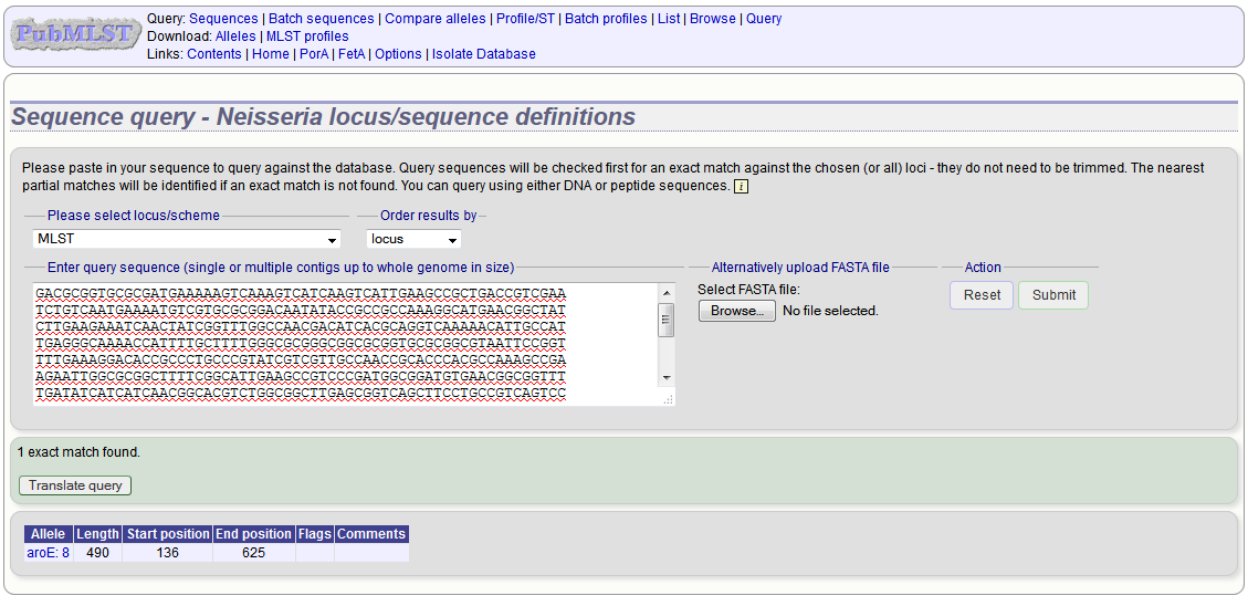
select the specific locus or scheme (e.g. MLST) that a locus belongs to.

Note: If the locus you are querying is a shorter version of another, e.g. an MLST fragment of a gene where the full length gene is also defined, you will need to select the specific locus or the scheme from the dropdown box. Leaving the selection on 'All loci' will return a match to the longer sequence in preference to the shorter one.

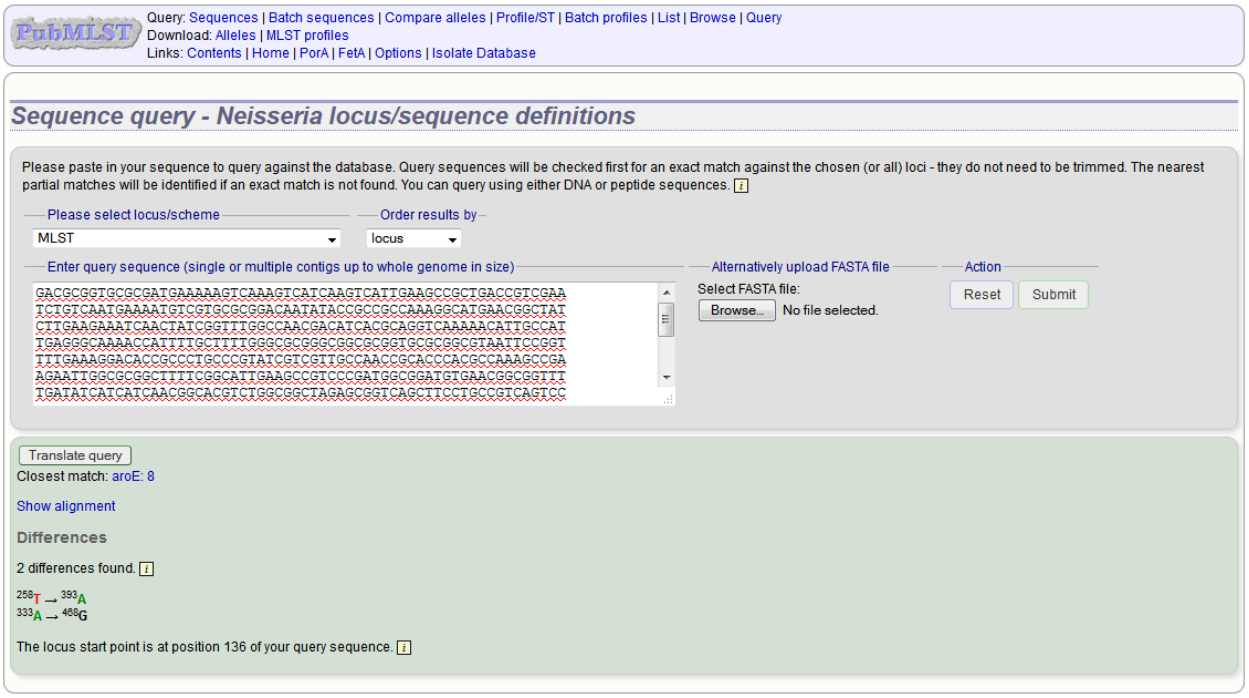
Click 'Submit'.



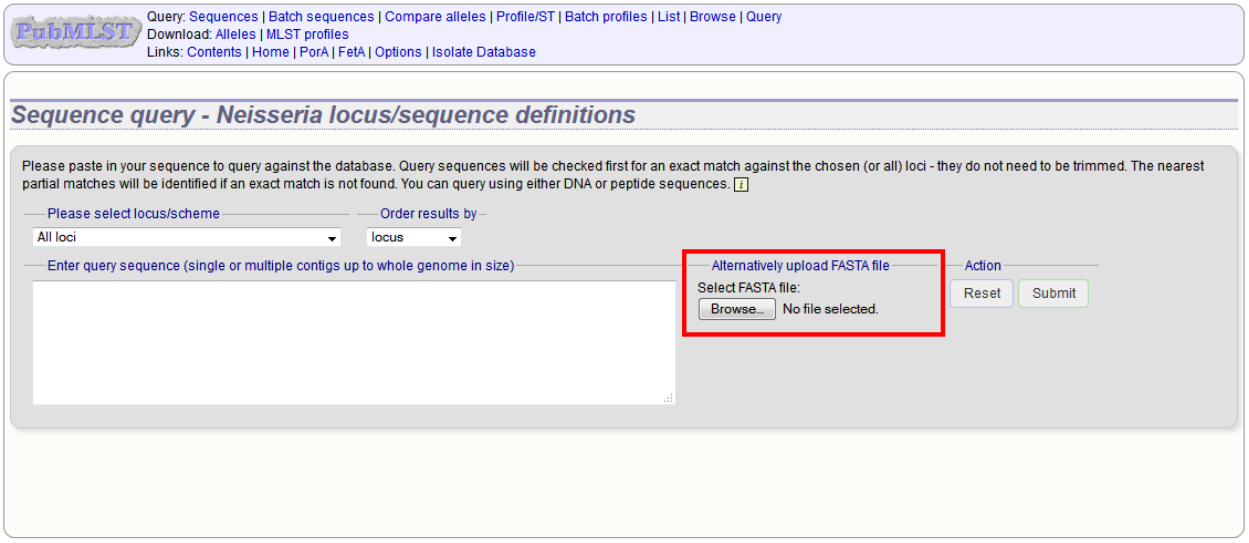
If an exact match is found, this will be indicated along with the start position of the locus within your sequence.



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.

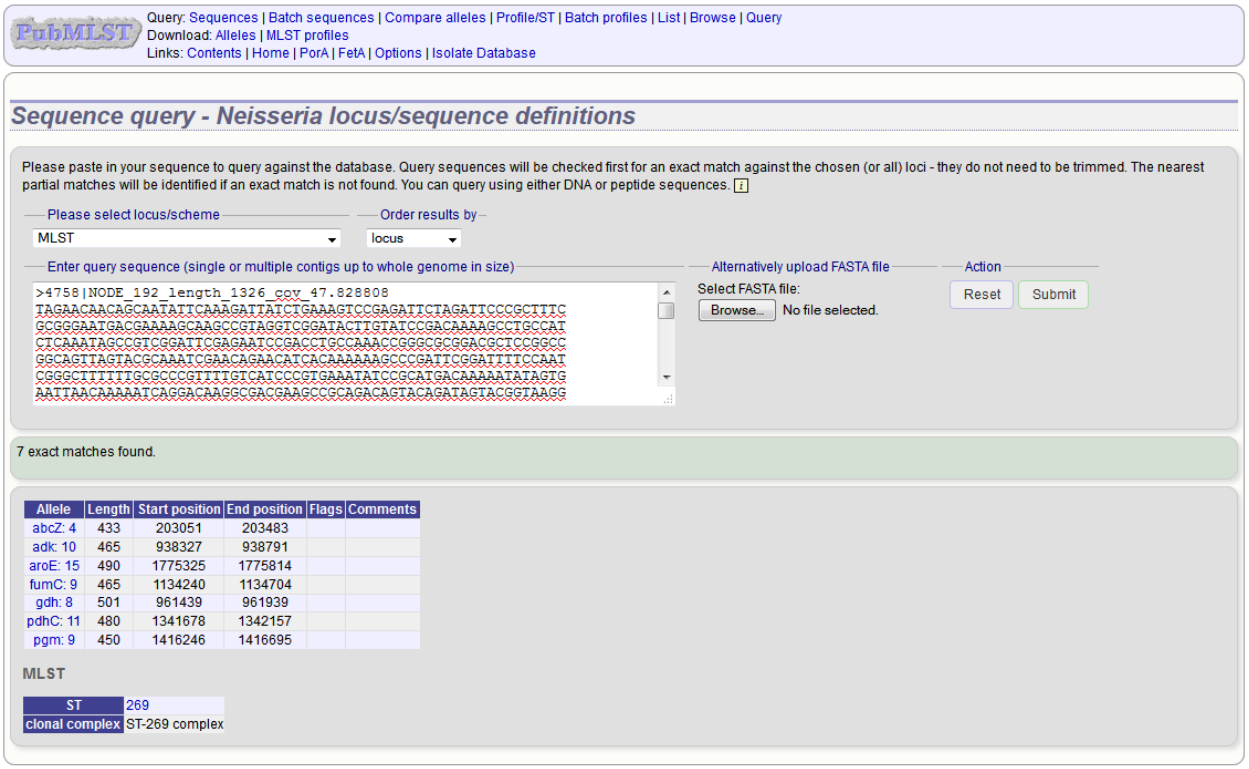


As an alternative to pasting a sequence in to the box, you can also choose to upload sequences in FASTA format by clicking the file browse button.



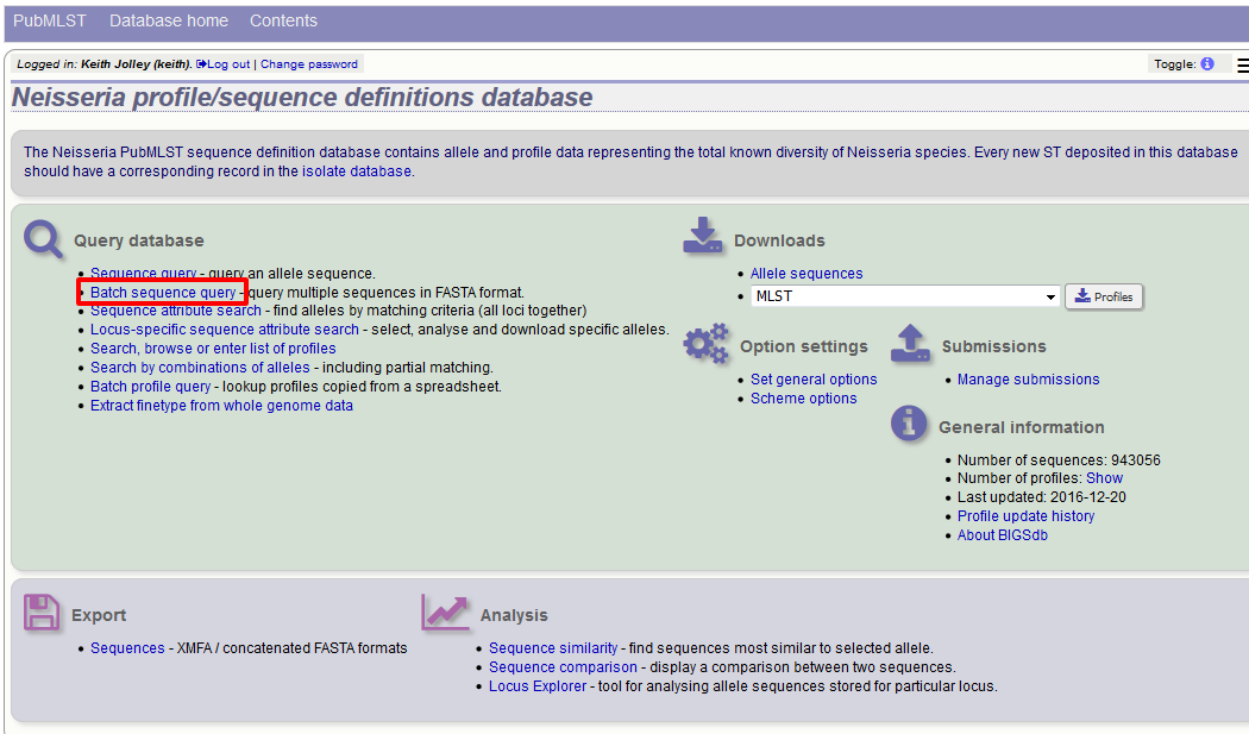
11.1.1 Querying whole genome data

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.

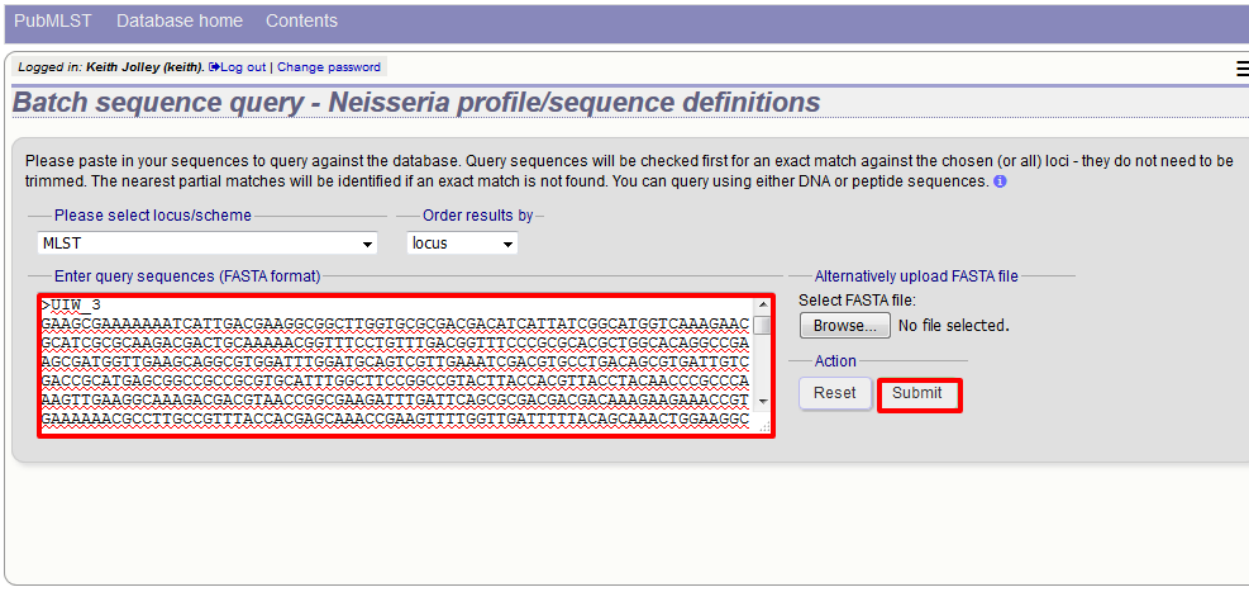


11.2 Querying multiple sequences to identify allele identities

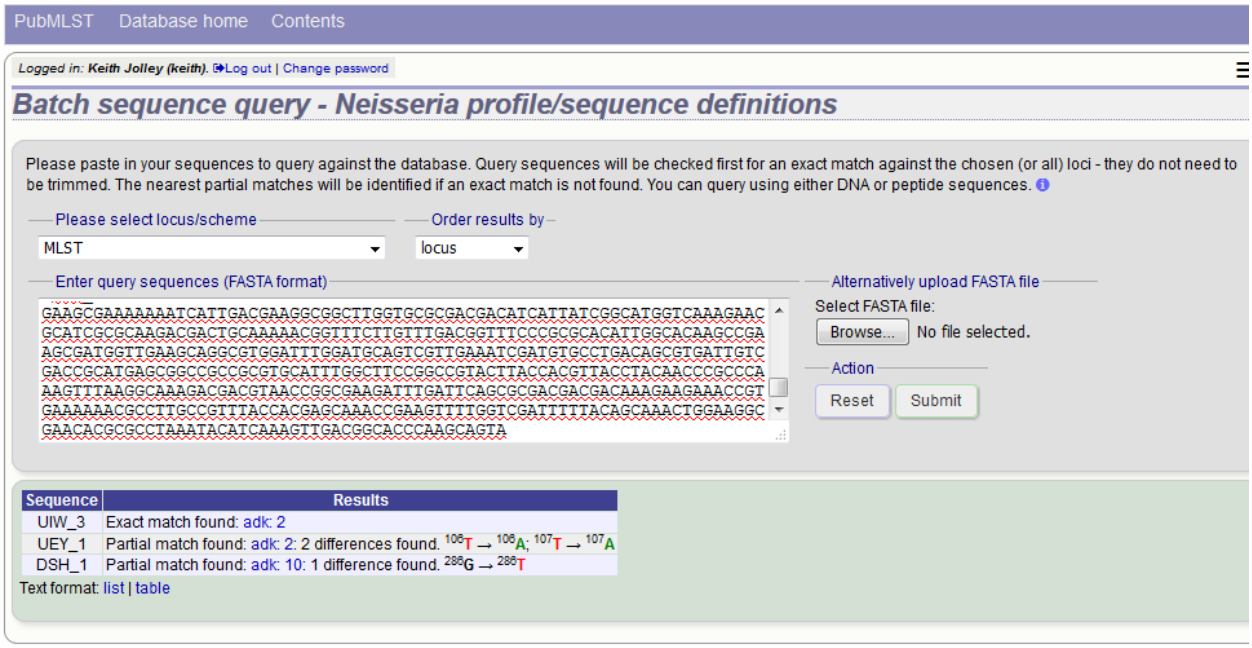
You can also query mutiple sequences together. These should be in FASTA format. Click 'Batch sequence query' from the contents page.



Paste your sequences (FASTA format) in to the box. Select a specific locus, scheme or 'All loci'.



The best match will be displayed for each sequence in your file. If this isn't an exact match, the differences will be listed.

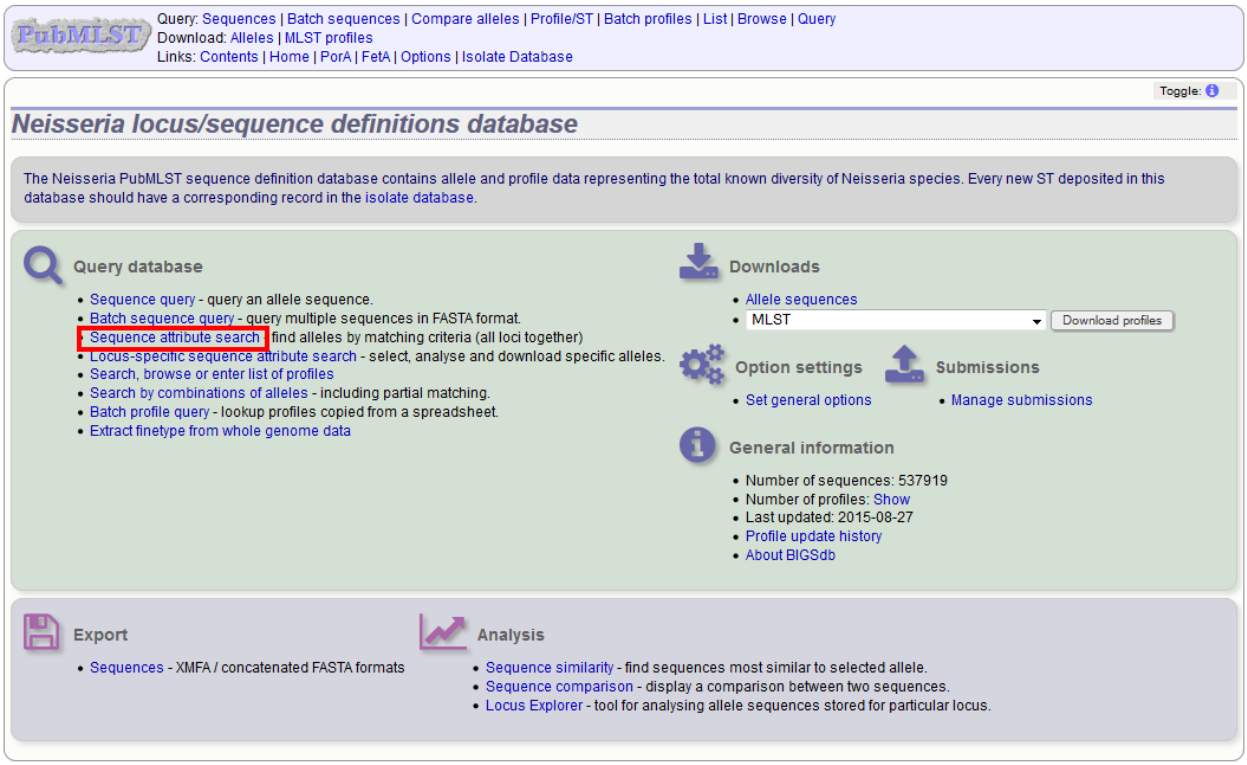


11.3 Searching for specific allele definitions

There are two query pages available that allow searching for specific allele definitions. The first allows querying of all loci together by criteria that are common to all. The second is a locus-specific attribute query that can search on any extended attributes that may be defined for a locus. This locus- specific query also allows you to paste in lists of alleles for download or analysis.

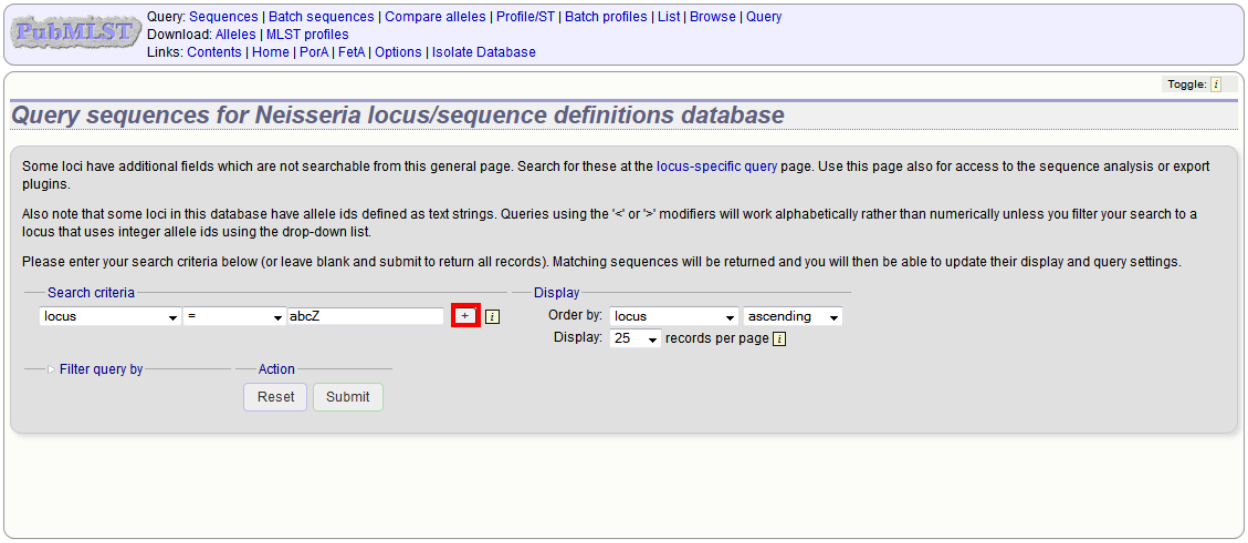
11.3.1 General (all loci) sequence attribute search

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

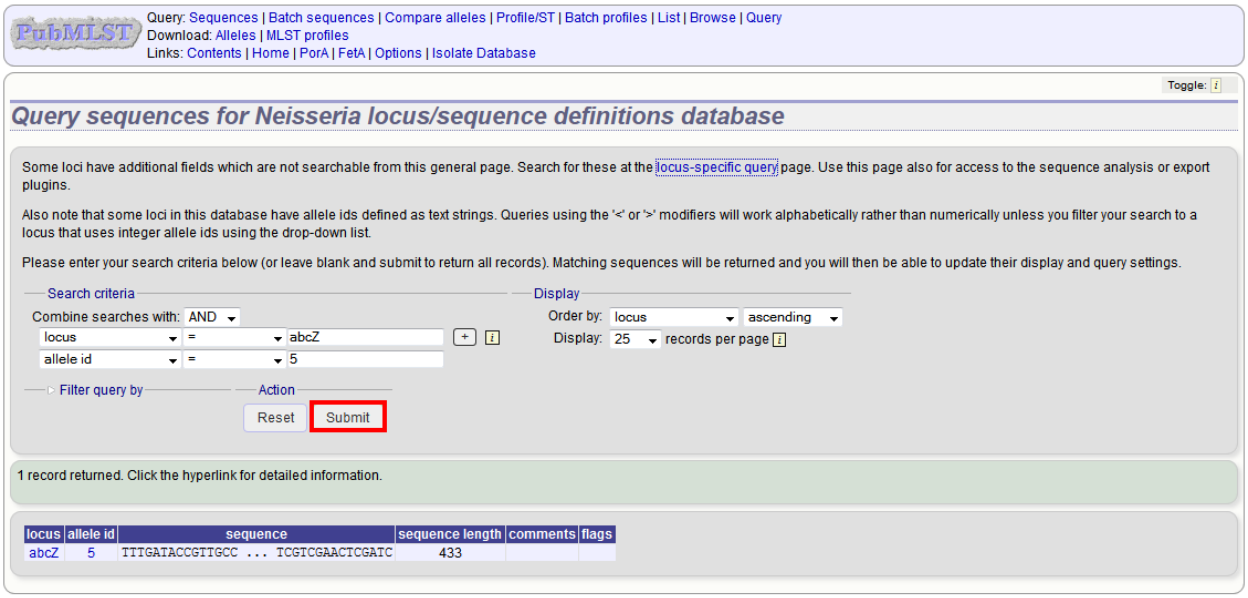


Enter your query using the dropdown search box - additional terms can be added by clicking the '+' button.

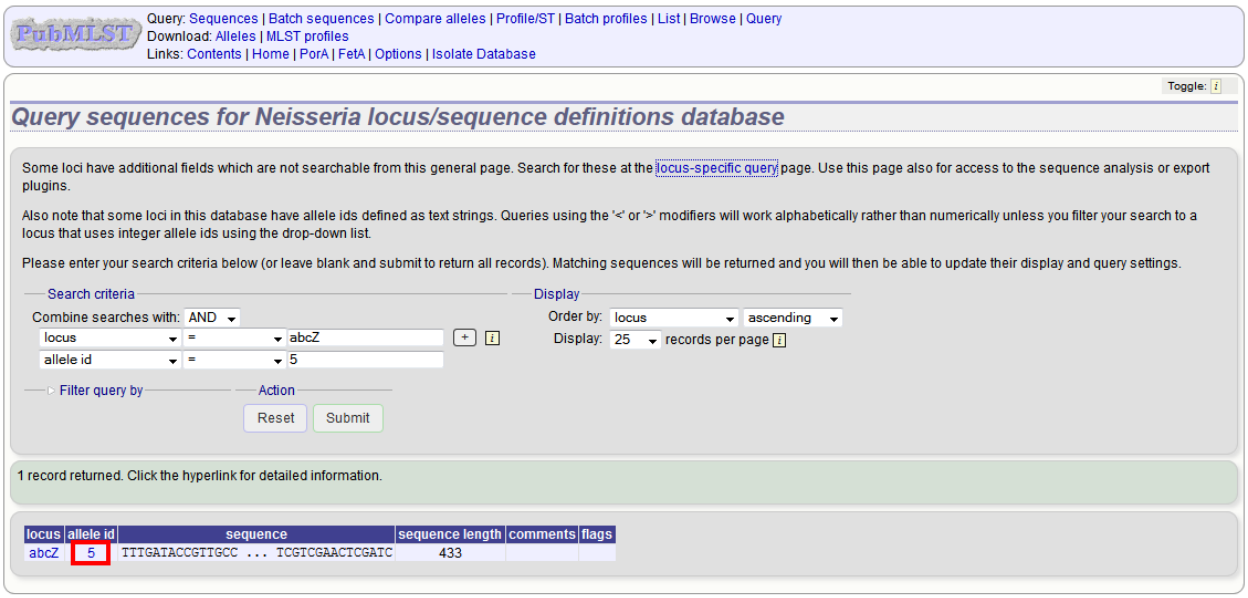
Designations can be queried using *standard operators*.



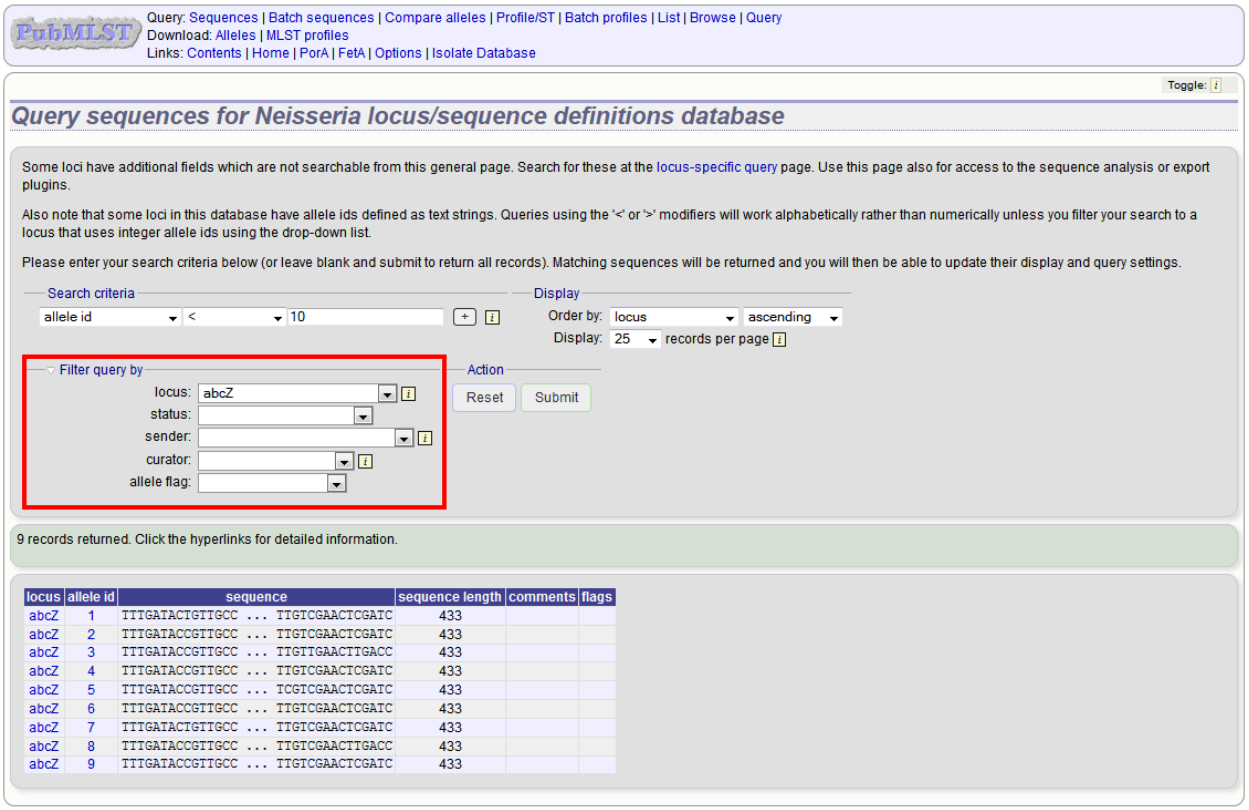
Click submit.



Click the hyperlinked results to display allele records.

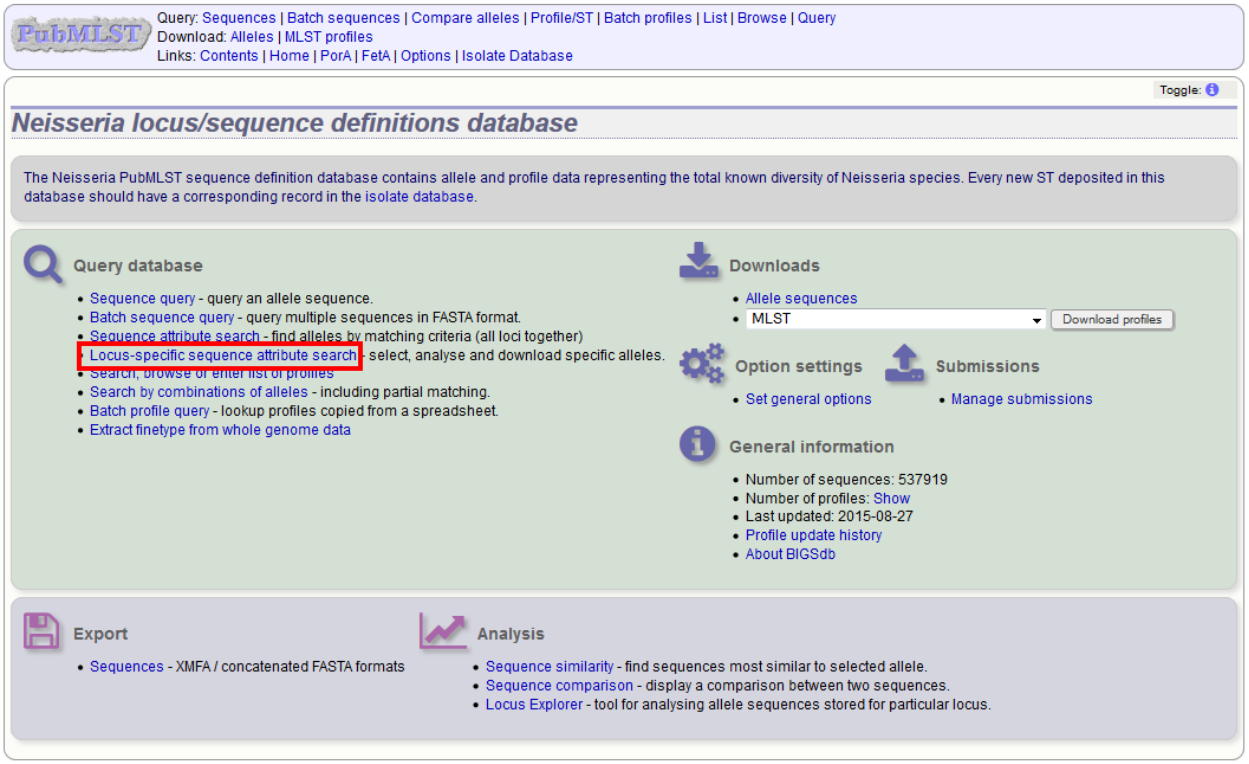


Various search criteria can also be selected by combining with filters. Click the filter heading to display these.

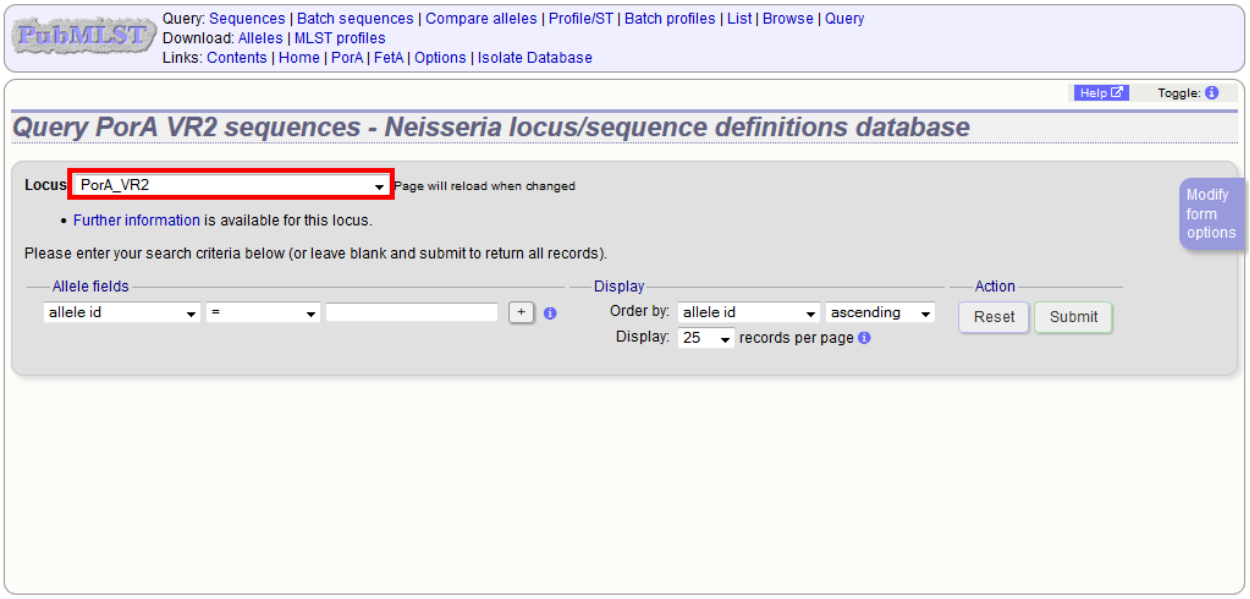


11.3.2 Locus-specific sequence attribute search

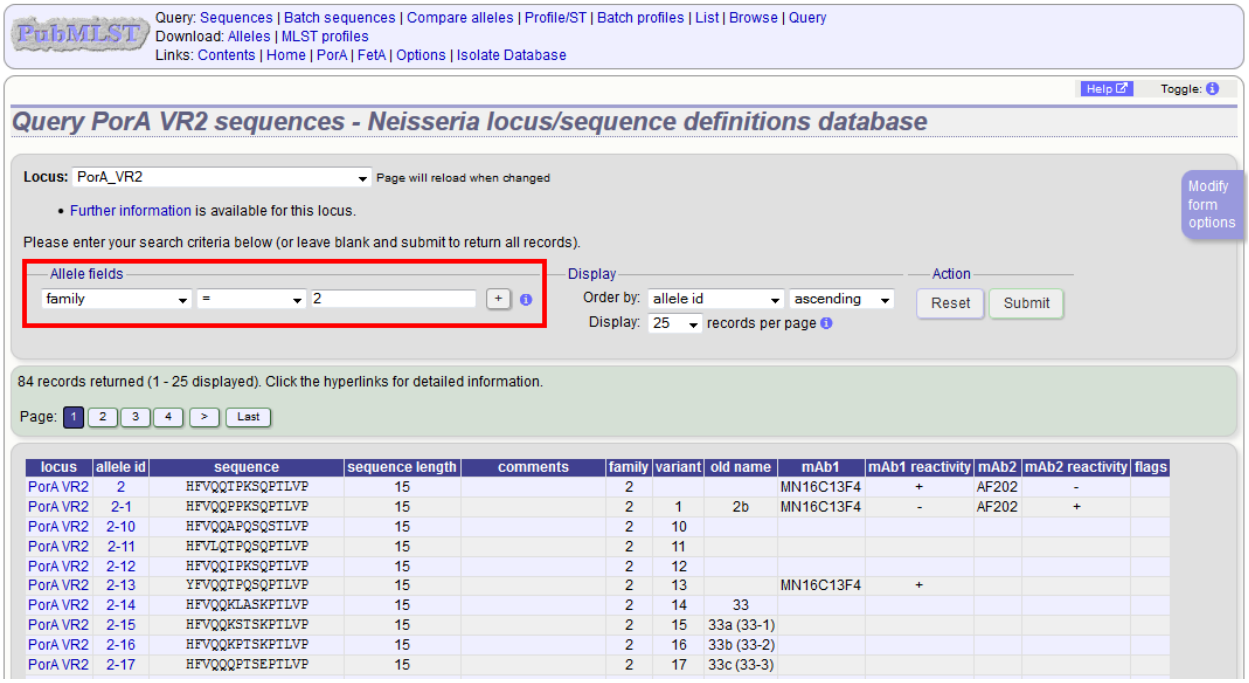
Some loci have *extended attribute fields*. To query these, click 'Locus-specific sequence attribute search' on a sequence definition database contents page.



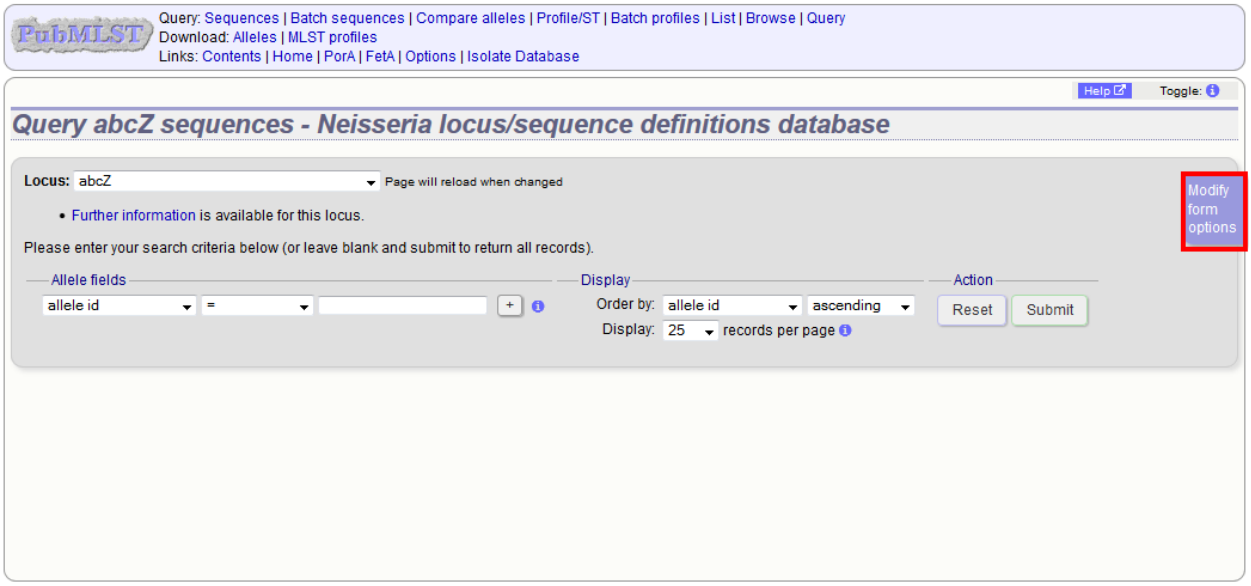
Pick the required locus from the dropdown box.



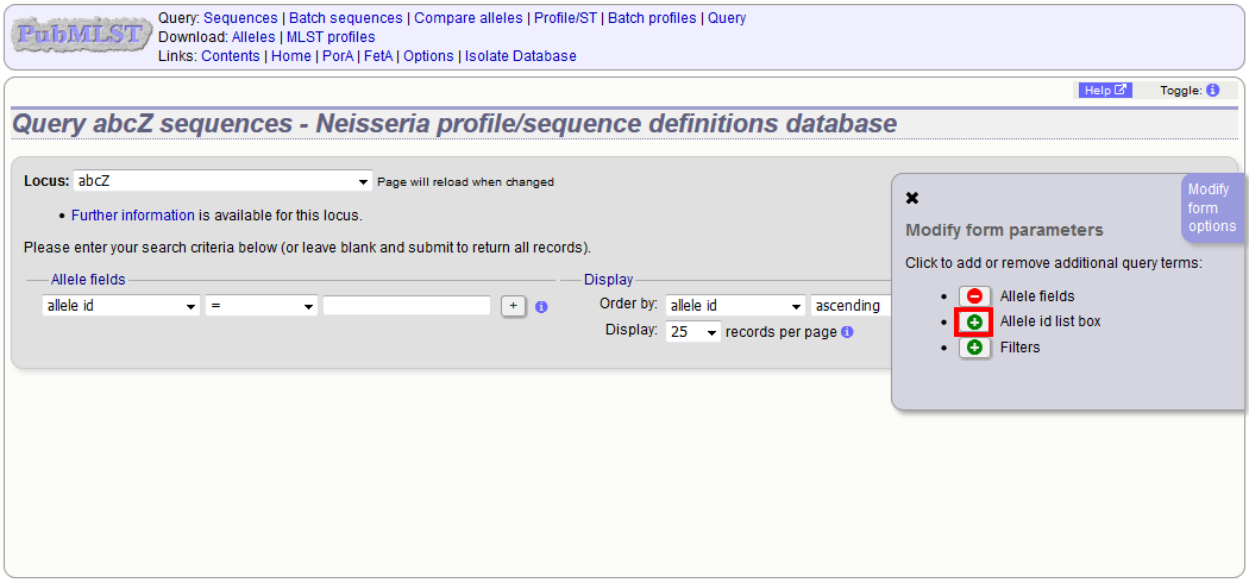
The fields specific for that locus will be added to the dropdown query boxes.



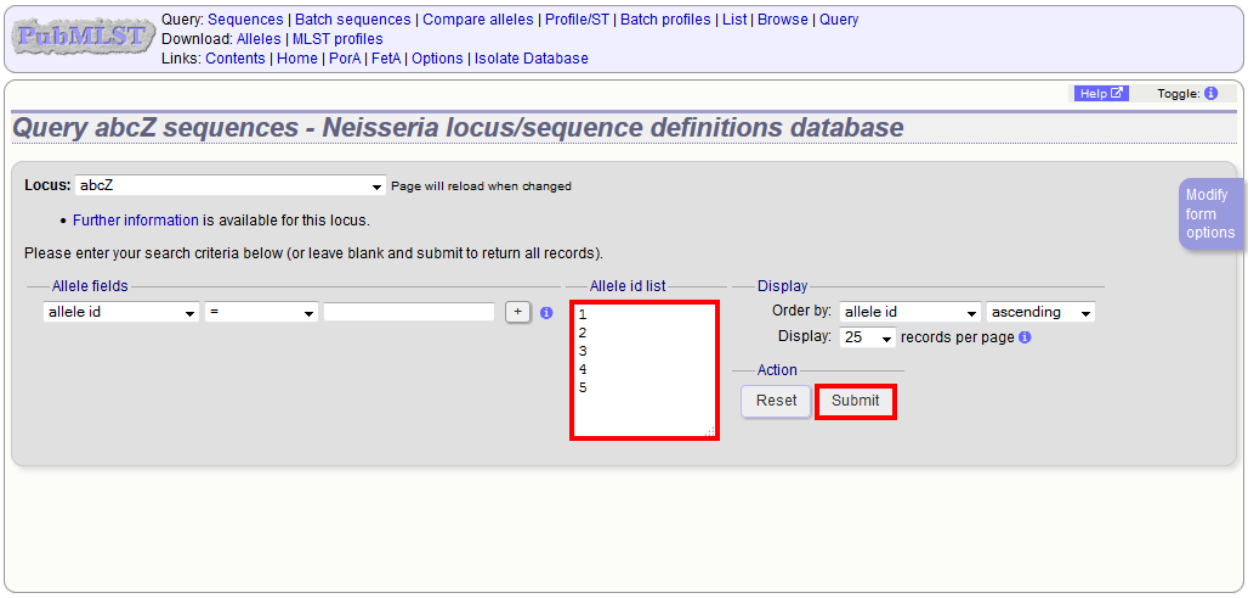
The query form can be modified by clicking the 'Modify form options' tab:



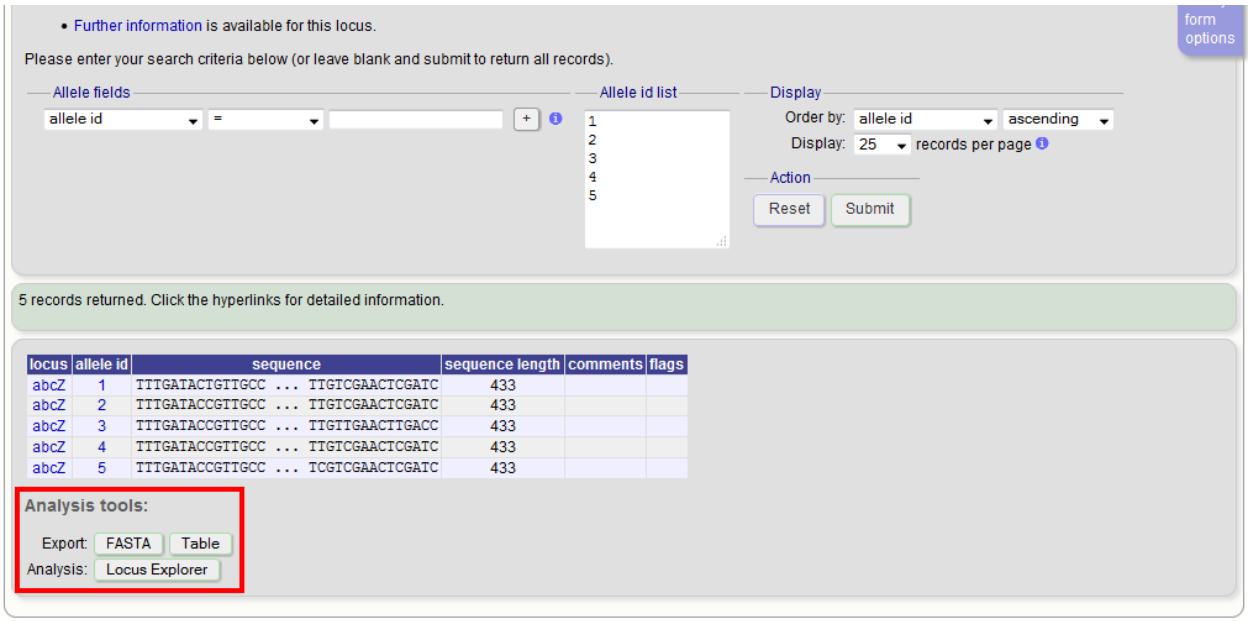
A list box can be added by clicking the 'Show' button for 'Allele id list box'.



Close the form modification tab and you can now enter a list of allele ids for retrieval.

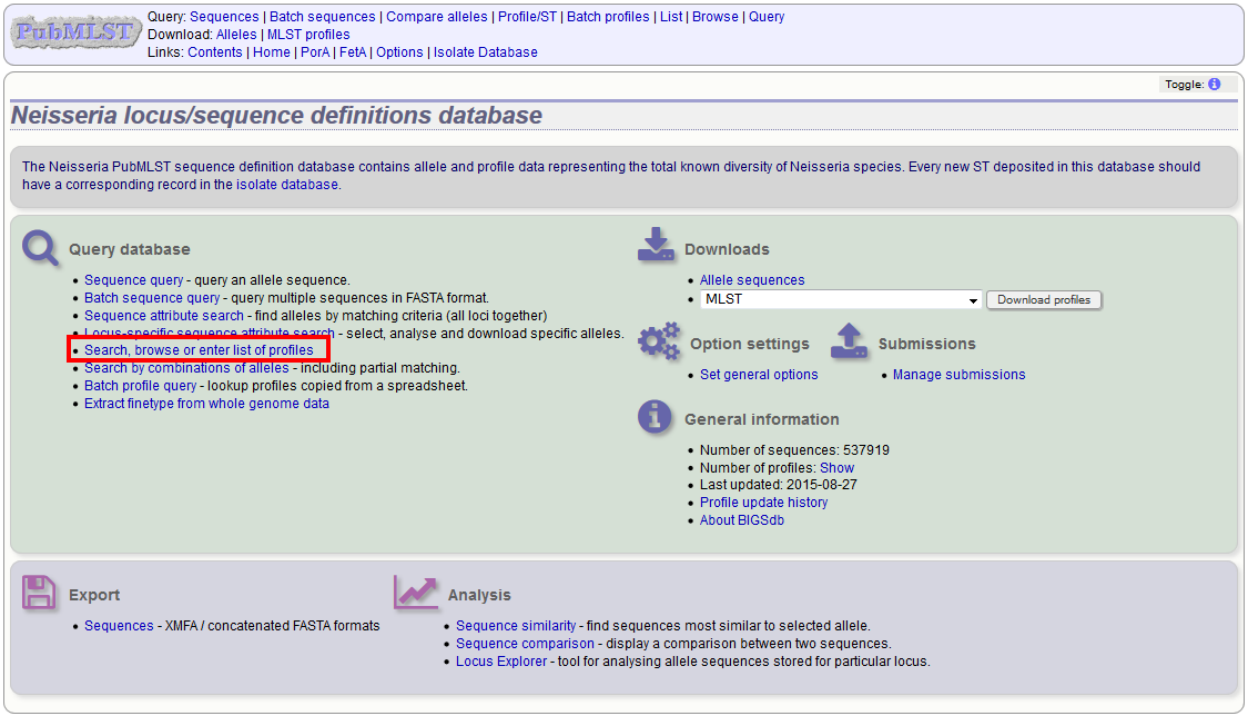


Various analysis and export options will be available for use on the retrieved sequences. These include FASTA output and *Locus Explorer* analysis.

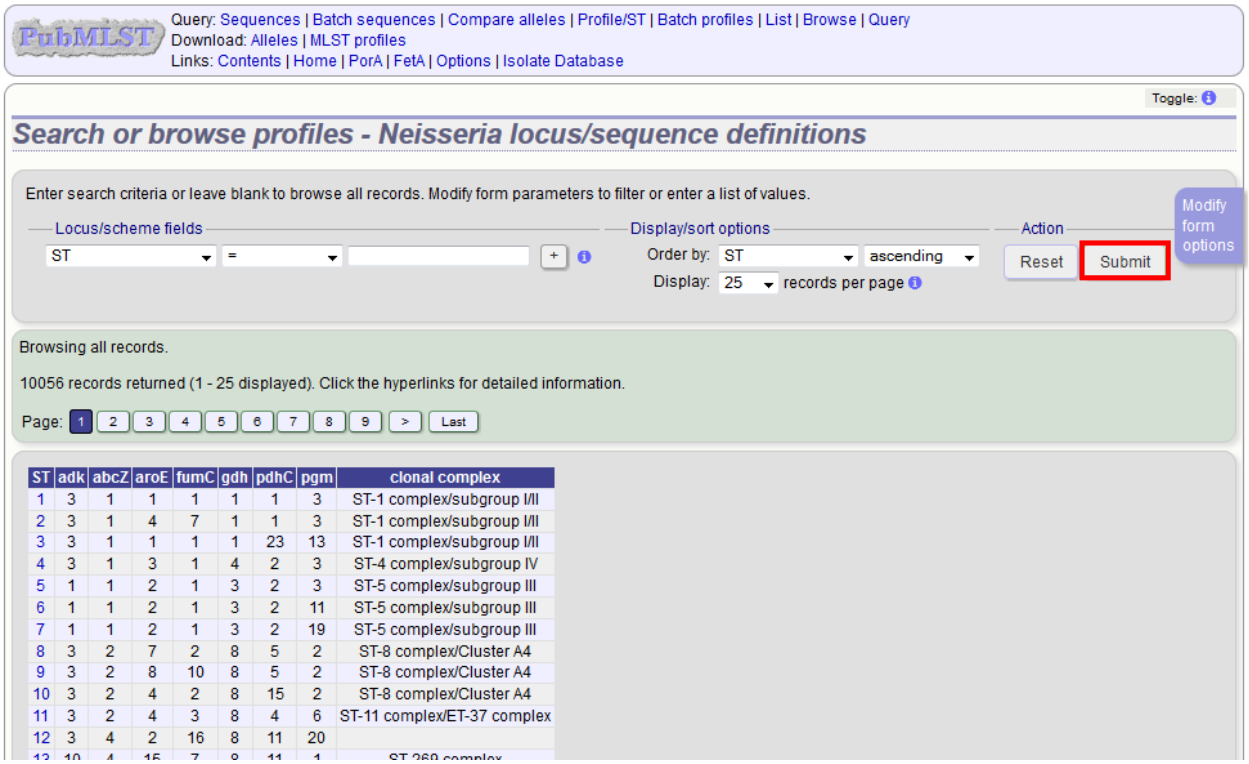


11.4 Browsing scheme profile definitions

If a sequence definition database has schemes defined that include a primary key field, i.e. collections of loci that together create profiles, e.g. for MLST, these can be browsed by clicking the link to 'Search, browse or enter list of profiles'.



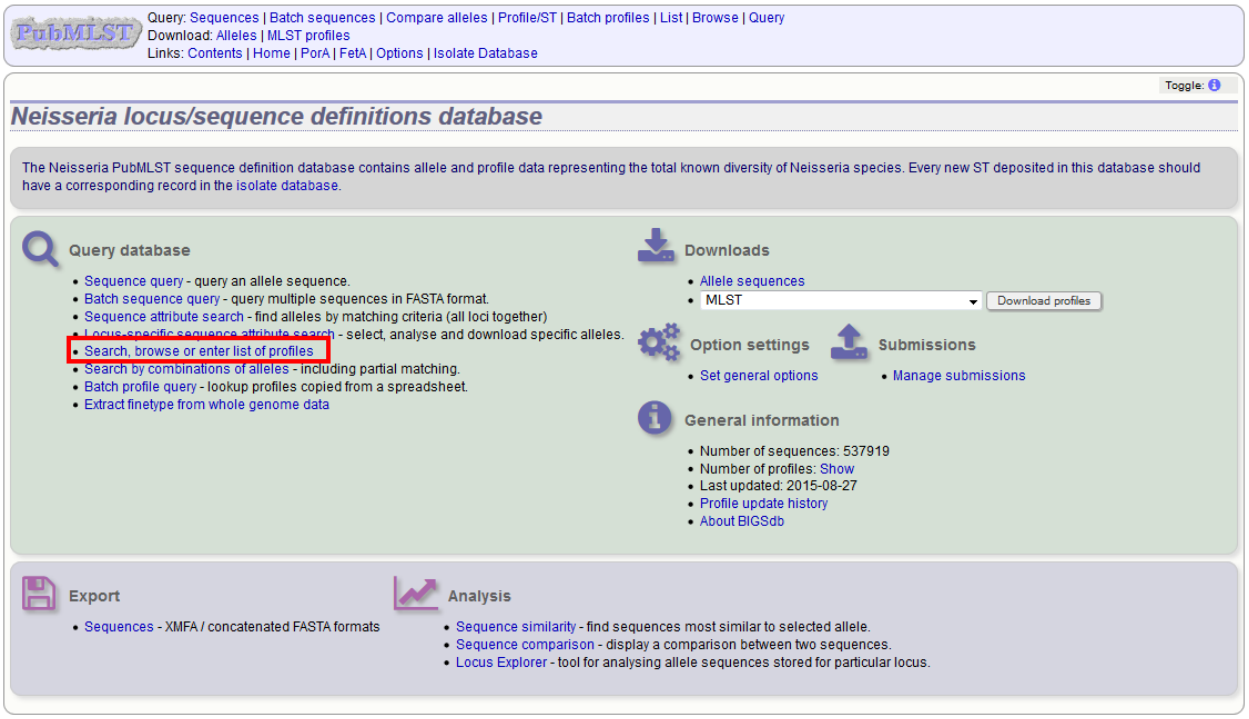
Leave query form fields blank (the display of these may vary depending on modification options set by the user). Choose the field to order the results by, the number of results per page to display, and click 'Submit'.



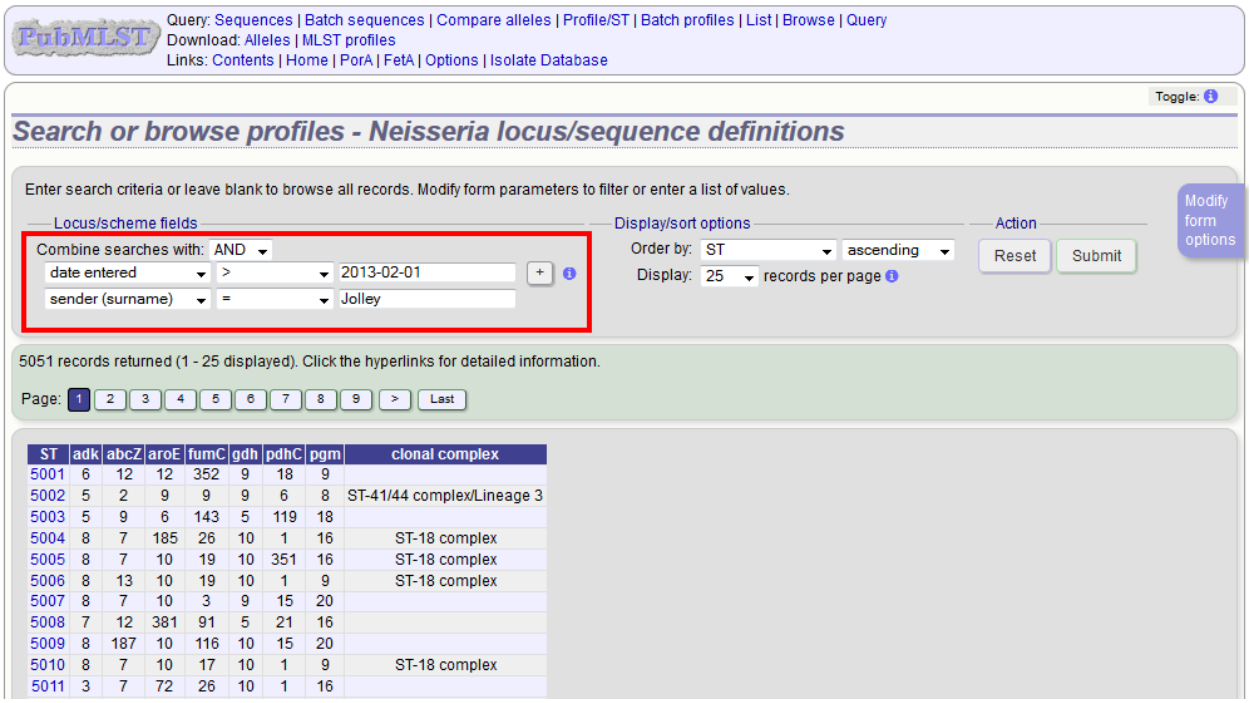
Clicking the hyperlink for any profile will display full information about the profile.

11.5 Querying scheme profile definitions

Click the link to 'Search, browse of enter list of profiles'.

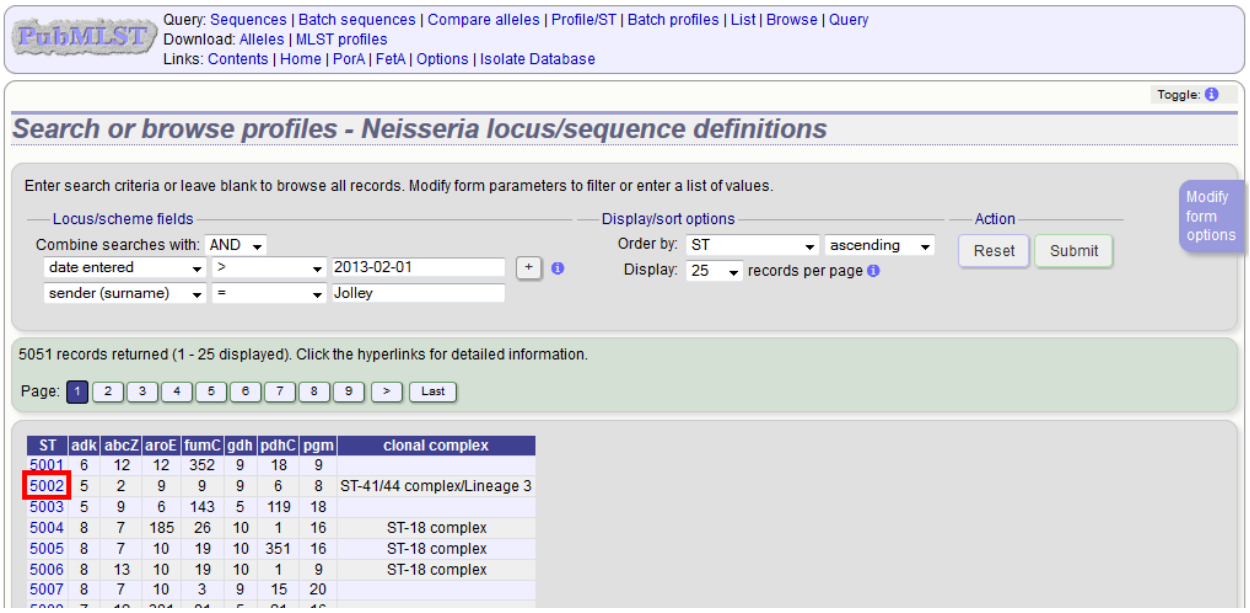


Enter the search criteria you wish to search on. You can add search criteria by clicking the '+' button in the 'Locus/scheme fields' section. These can be combined using 'AND' or 'OR'.

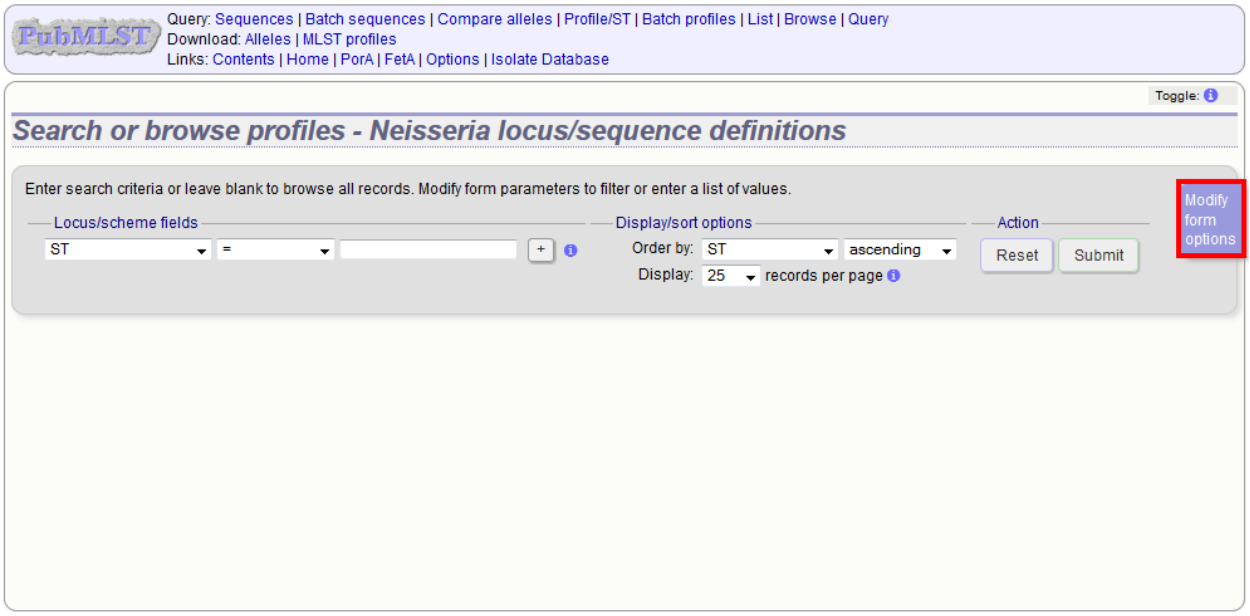


Each field can be queried using *standard operators*.

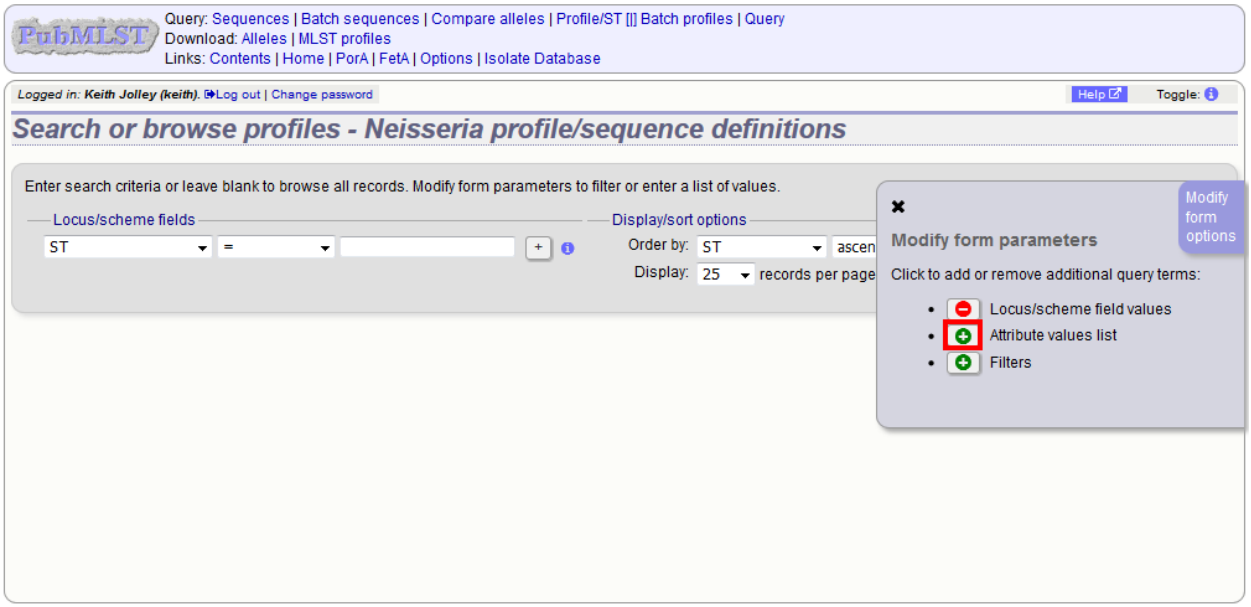
Clicking the hyperlink for any profile will display full information about the profile.



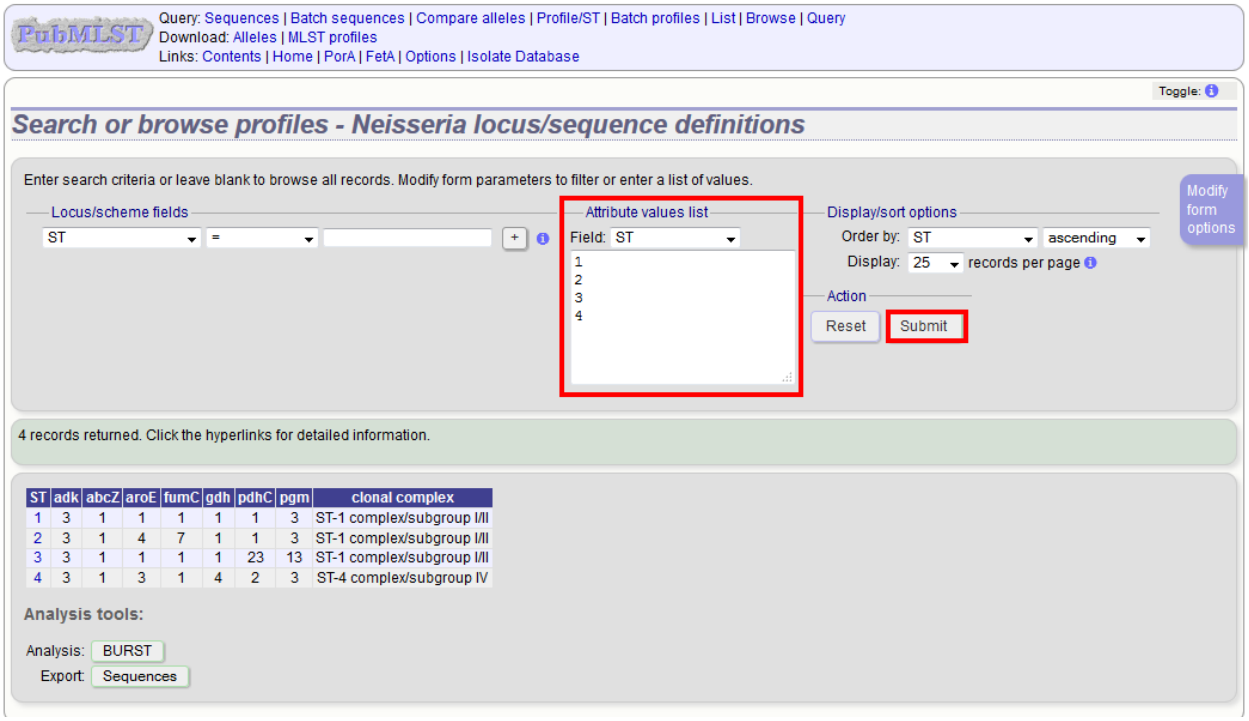
Other query options are available by clicking the 'Modify form options' tab.



For example, you can enter a list of attributes to query on by clicking the 'Show' button next to 'Attribute values list'.

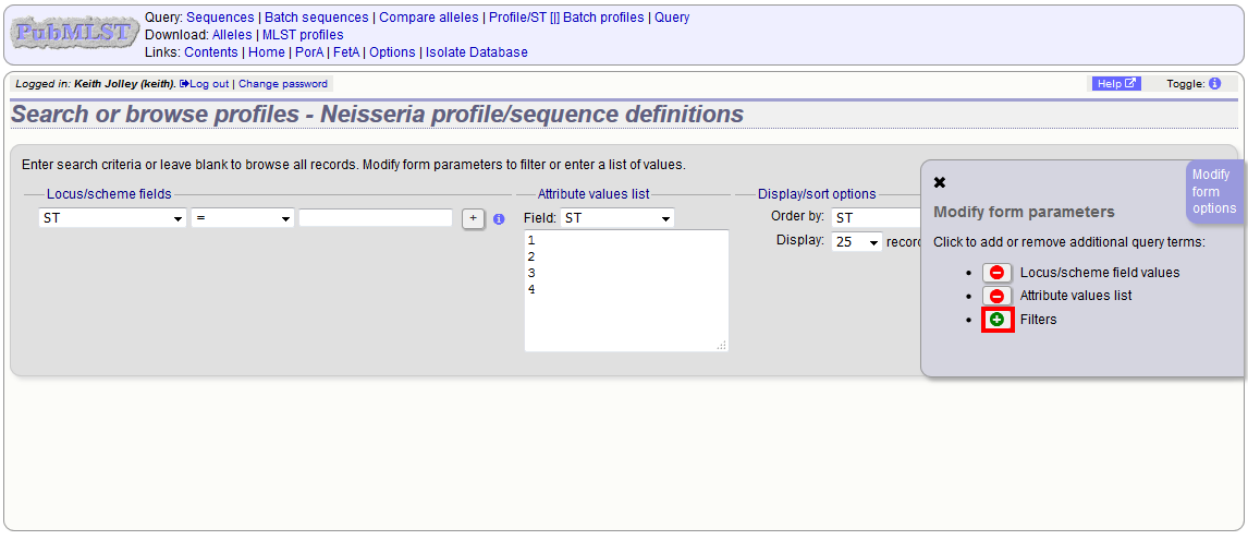


A list box will appear within the page. Hide the form modification tab by clicking the 'X' in the corner or the purple tab again. Now you can choose the attribute to search on along with a list of values.

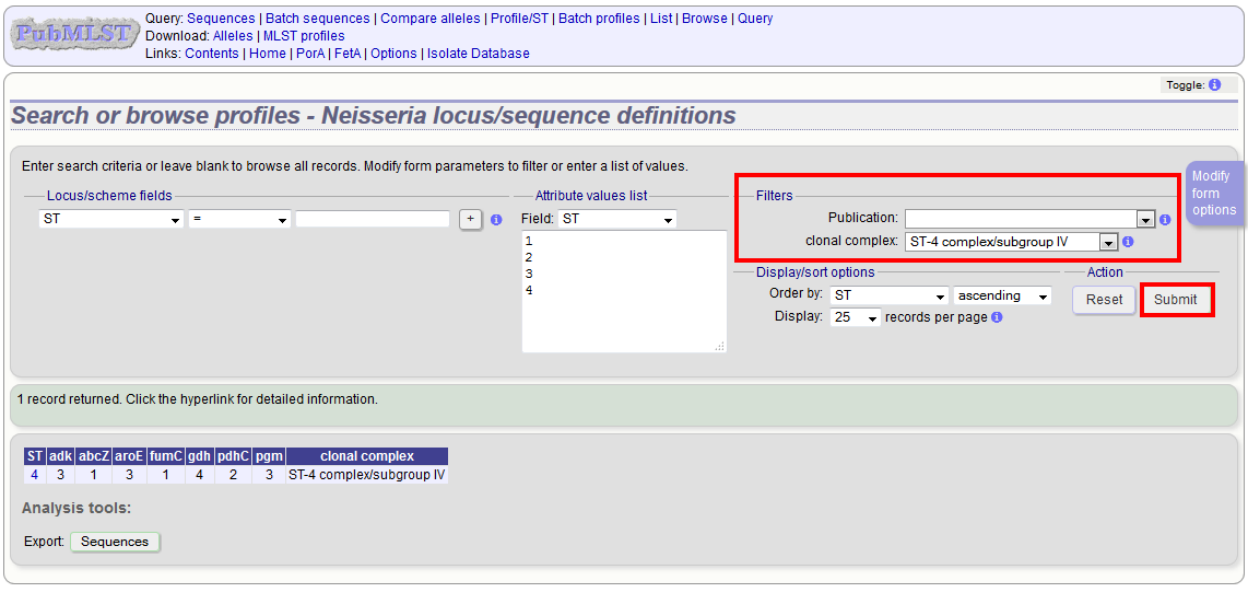


List values will be combined with any other attributes entered in the query form allowing complex queries can be constructed.

You can also add filters to the form by again clicking the 'Modify form options' tab and selecting 'Filters'.



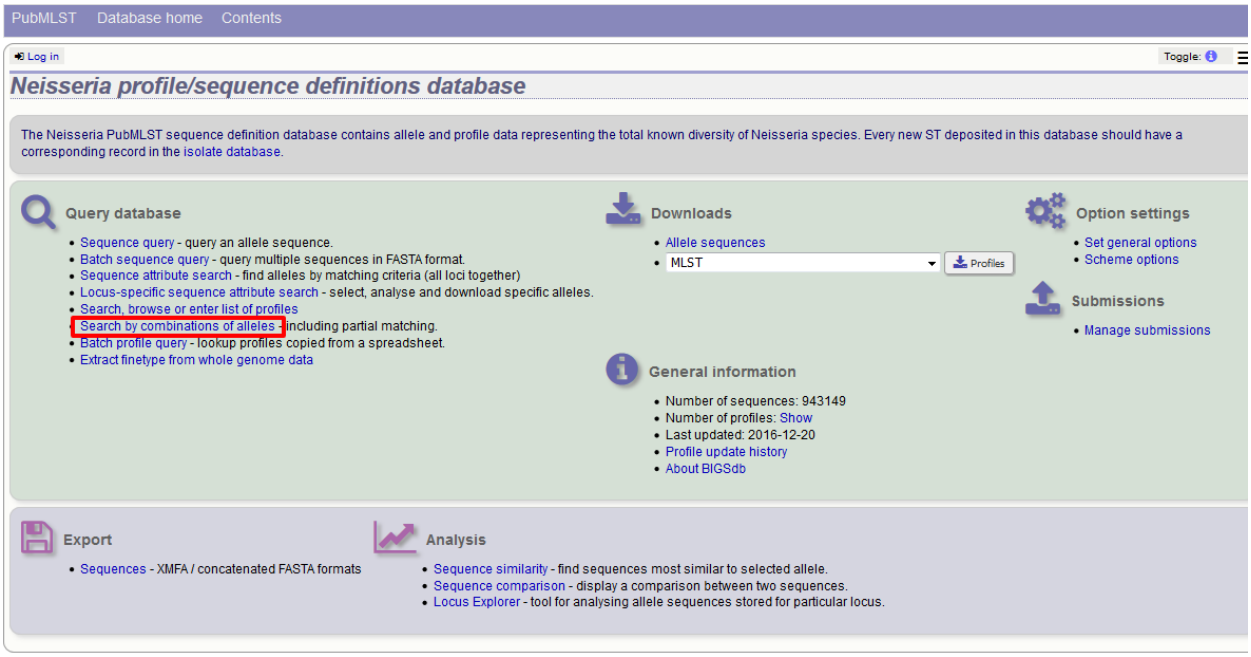
Available filters will vary depending on the database. These will be combined with other query criteria or lists of attributes.



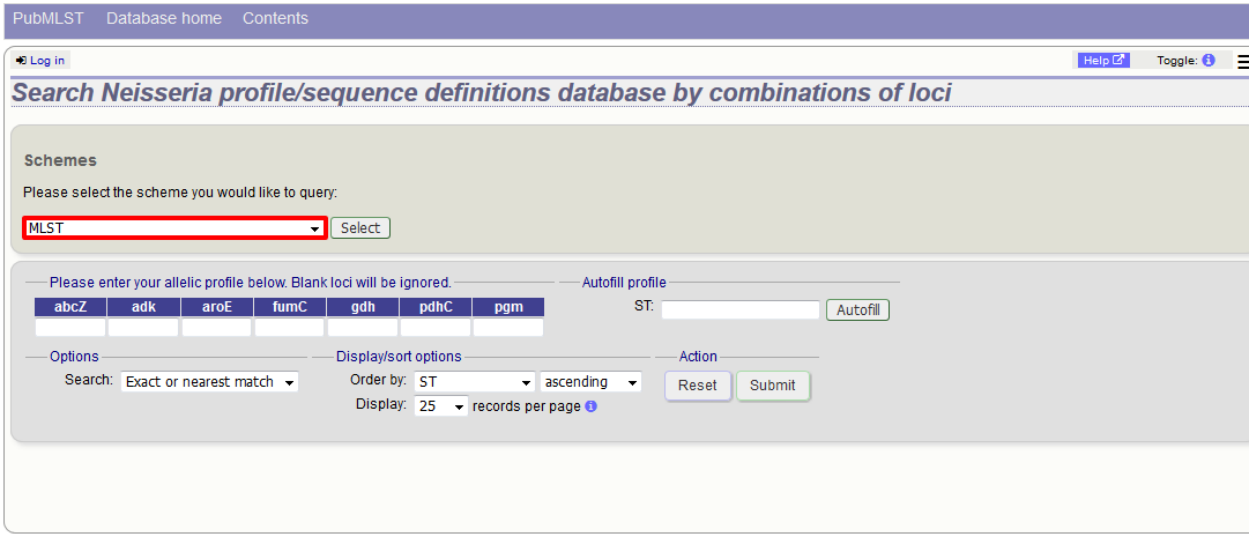
11.6 Identfying allelic profile definitions

For schemes such as MLST you can query allelic combinations to identify the sequence type (or more generically, the primary key of the profile).

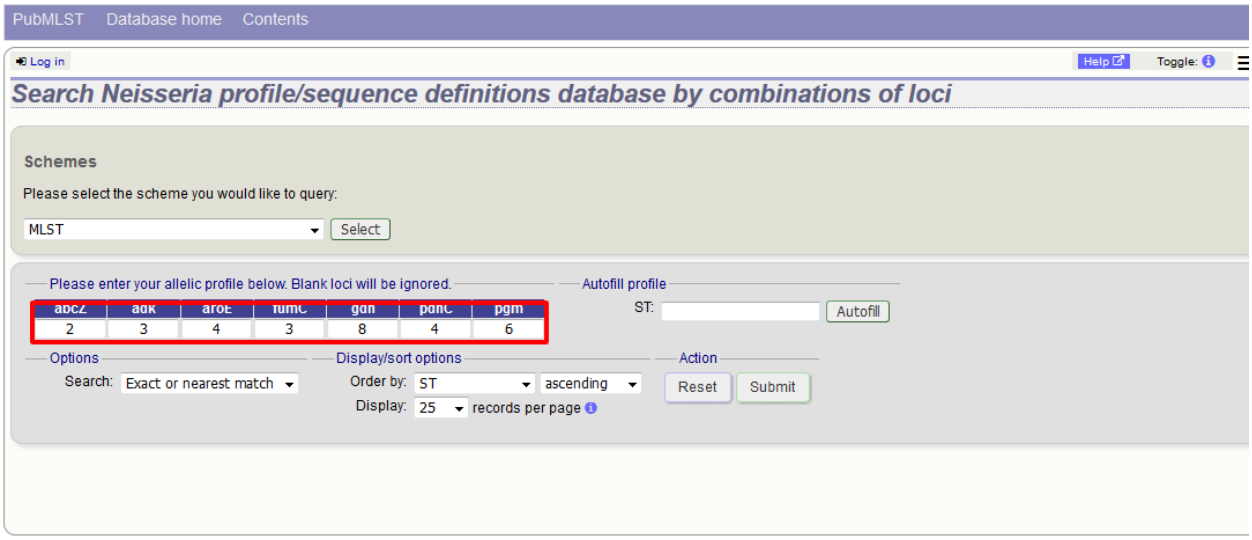
Click the 'Search by combinations of alleles' link from the sequence definition contents page.



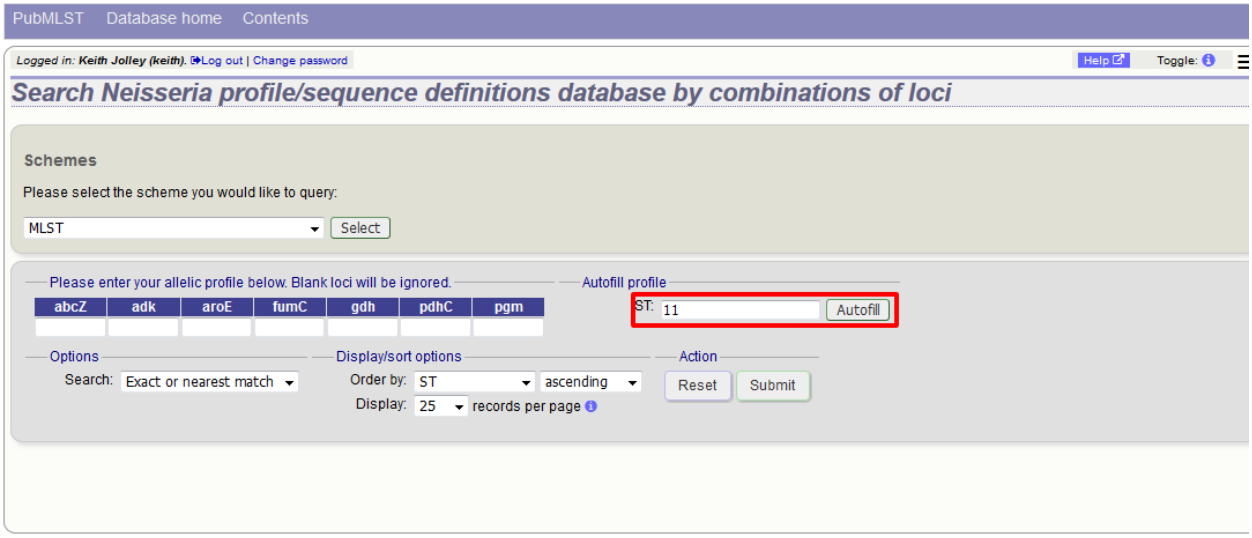
If multiple schemes are defined in the database you should select the scheme you wish to check.



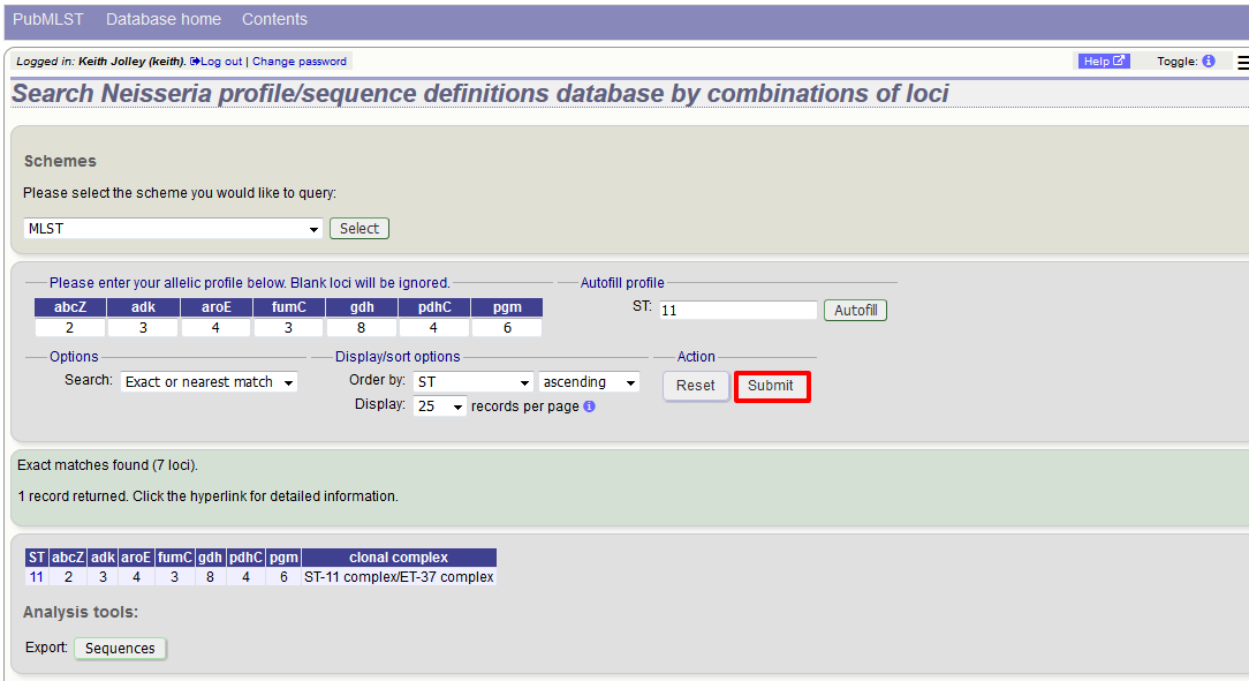
Enter a combination of allelic values (you can enter a partial profile if you wish).



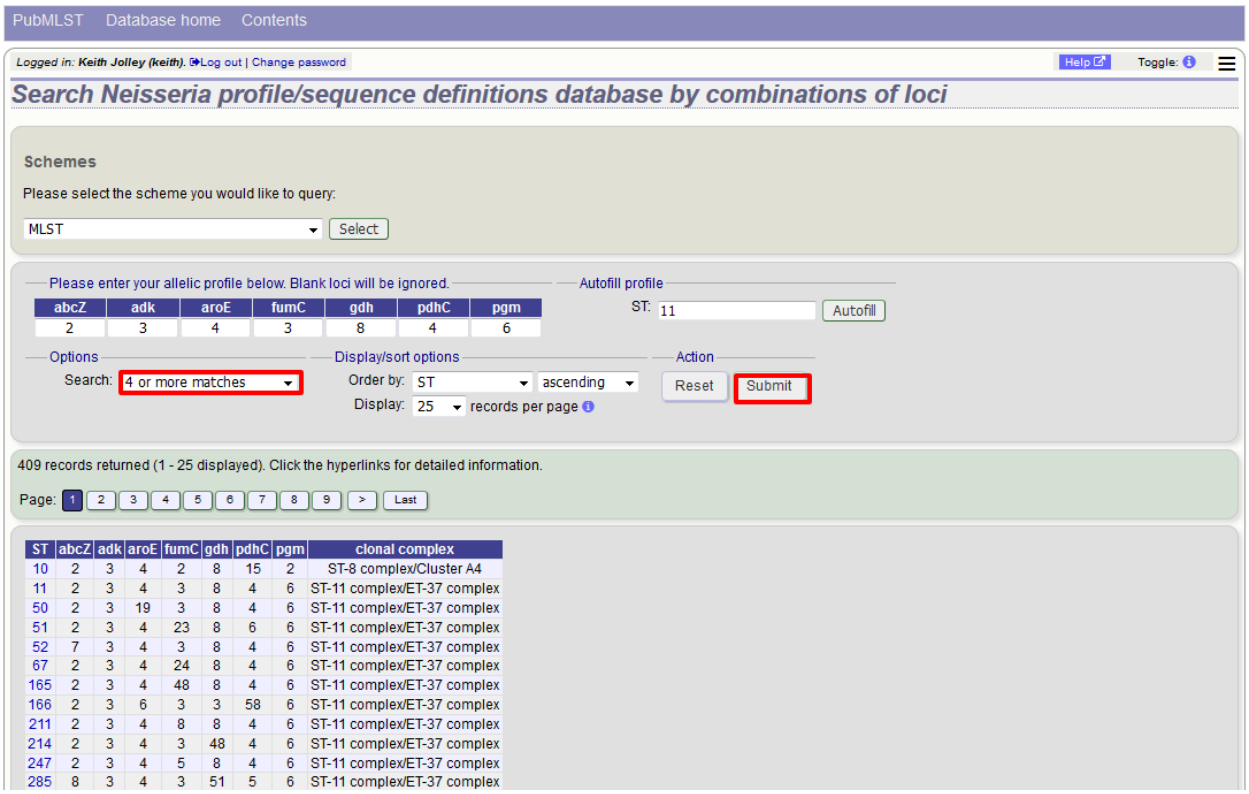
Alternatively, you can automatically populate a profile by entering a value for the scheme primary key field (e.g. ST) and clicking 'Autofill'.



To find the closest or exact match, leave the search box on 'Exact or nearest match' and click 'Submit'. The best match will be displayed.

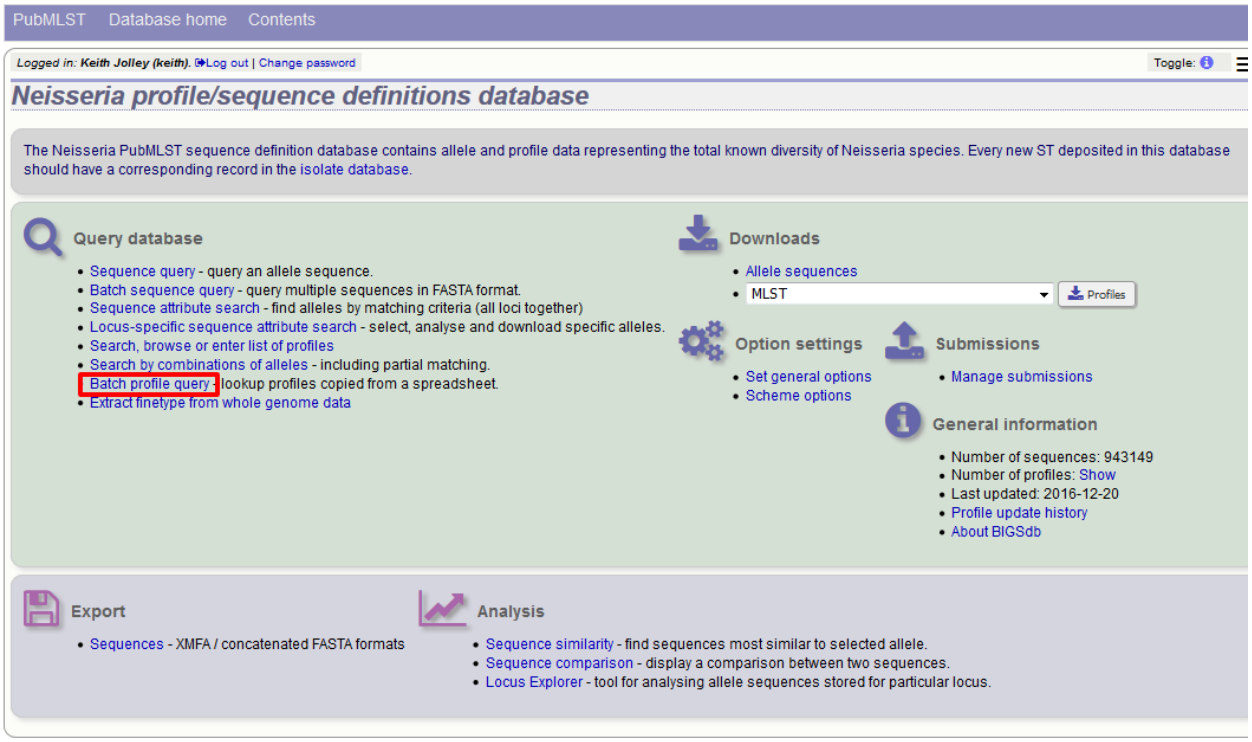


Alternatively, if you wish to find all profiles that match the query profile by at least a set number of loci, select the appropriate value in the search dropdown box, e.g. '4 or more matches' will show related profiles that share at least 4 alleles with the query.

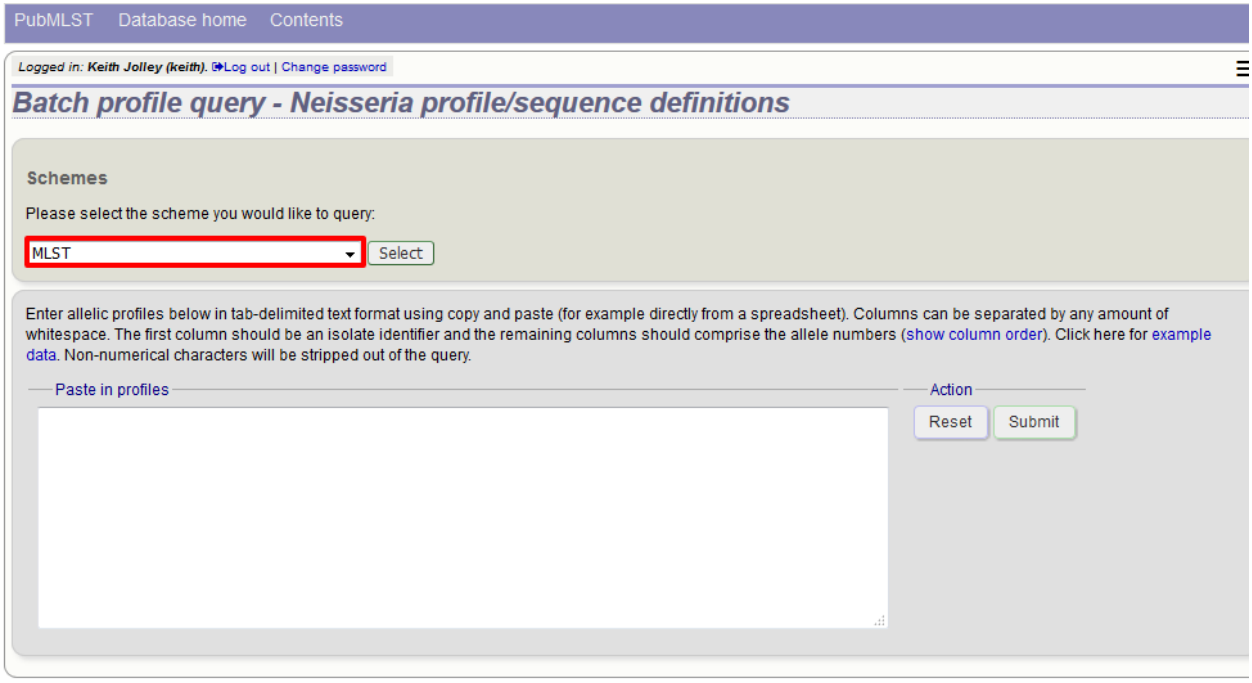


11.7 Batch profile queries

To lookup scheme definitions, e.g. the sequence type for multiple profiles, click 'Batch profile query' from the sequence definition contents page.

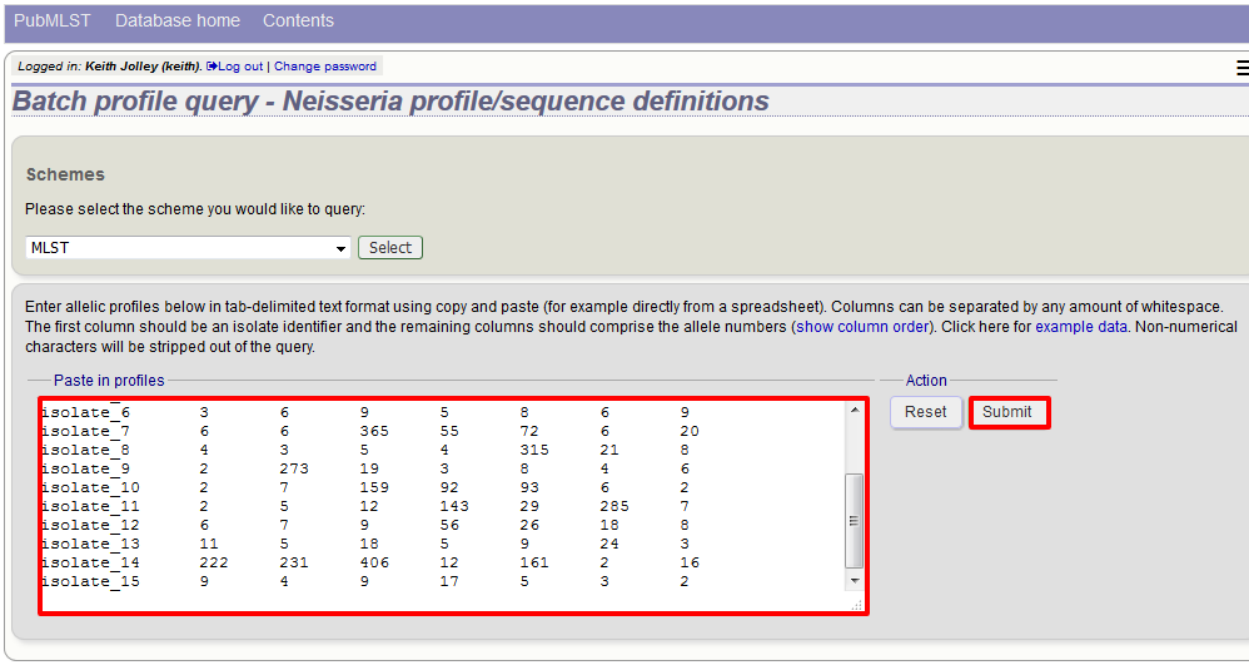


If multiple schemes are defined in the database you should select the scheme you wish to check.

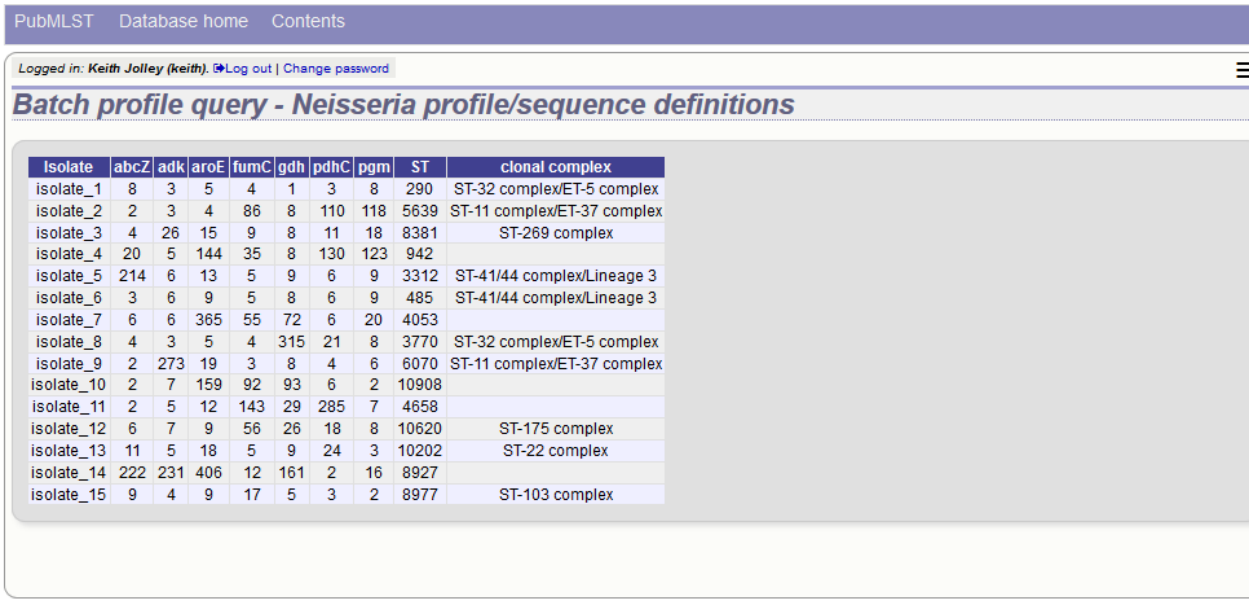


Copy and paste data from a spreadsheet. The first column is the record identifier, and the remaining columns are the alleles for each locus in the standard locus order defined for the scheme. There are links to the column order which can be used as a header line for your spreadsheet and to example data.

Click submit after pasting in the data.



A results table will be displayed.

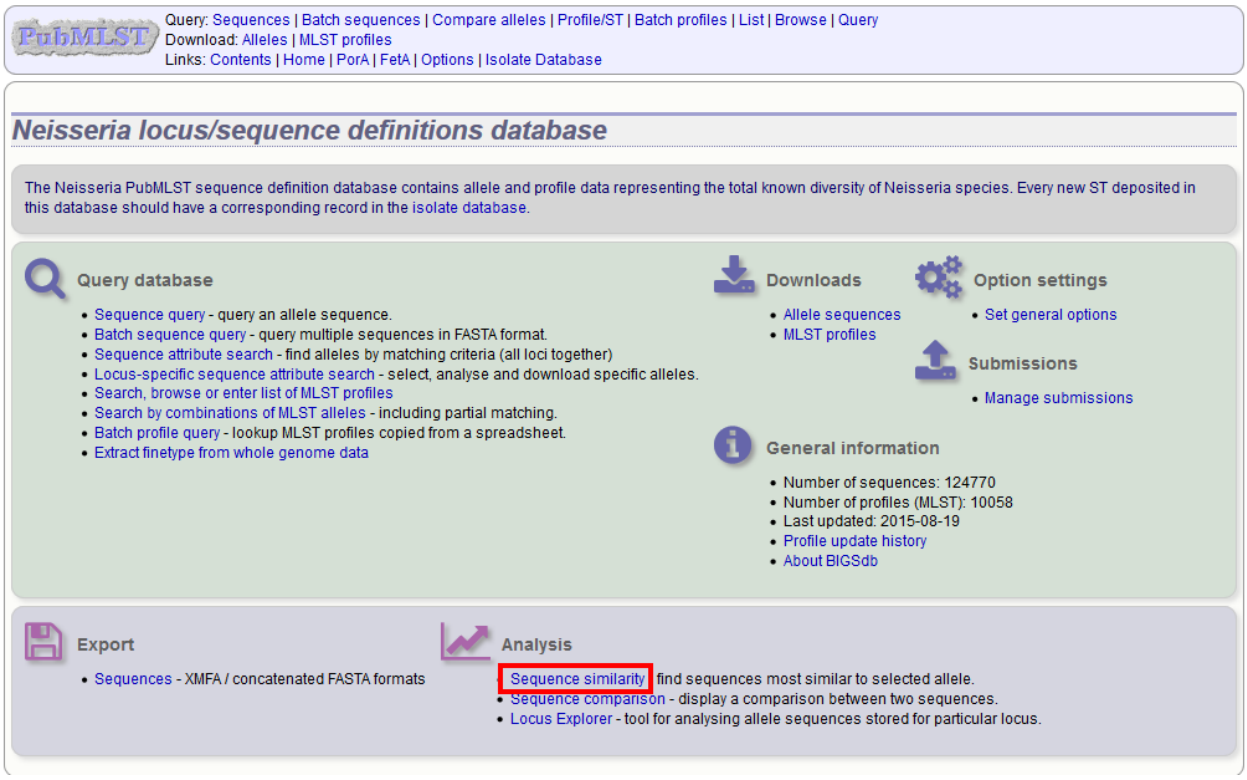


Isolate	abcZ	adk	aroE	fumC	gdh	pdhC	pgm	ST	clonal complex
isolate_1	8	3	5	4	1	3	8	290	ST-32 complex/ET-5 complex
isolate_2	2	3	4	86	8	110	118	5639	ST-11 complex/ET-37 complex
isolate_3	4	26	15	9	8	11	18	8381	ST-269 complex
isolate_4	20	5	144	35	8	130	123	942	
isolate_5	214	6	13	5	9	6	9	3312	ST-41/44 complex/Lineage 3
isolate_6	3	6	9	5	8	6	9	485	ST-41/44 complex/Lineage 3
isolate_7	6	6	365	55	72	6	20	4053	
isolate_8	4	3	5	4	315	21	8	3770	ST-32 complex/ET-5 complex
isolate_9	2	273	19	3	8	4	6	6070	ST-11 complex/ET-37 complex
isolate_10	2	7	159	92	93	6	2	10908	
isolate_11	2	5	12	143	29	285	7	4658	
isolate_12	6	7	9	56	26	18	8	10620	ST-175 complex
isolate_13	11	5	18	5	9	24	3	10202	ST-22 complex
isolate_14	222	231	406	12	161	2	16	8927	
isolate_15	9	4	9	17	5	3	2	8977	ST-103 complex

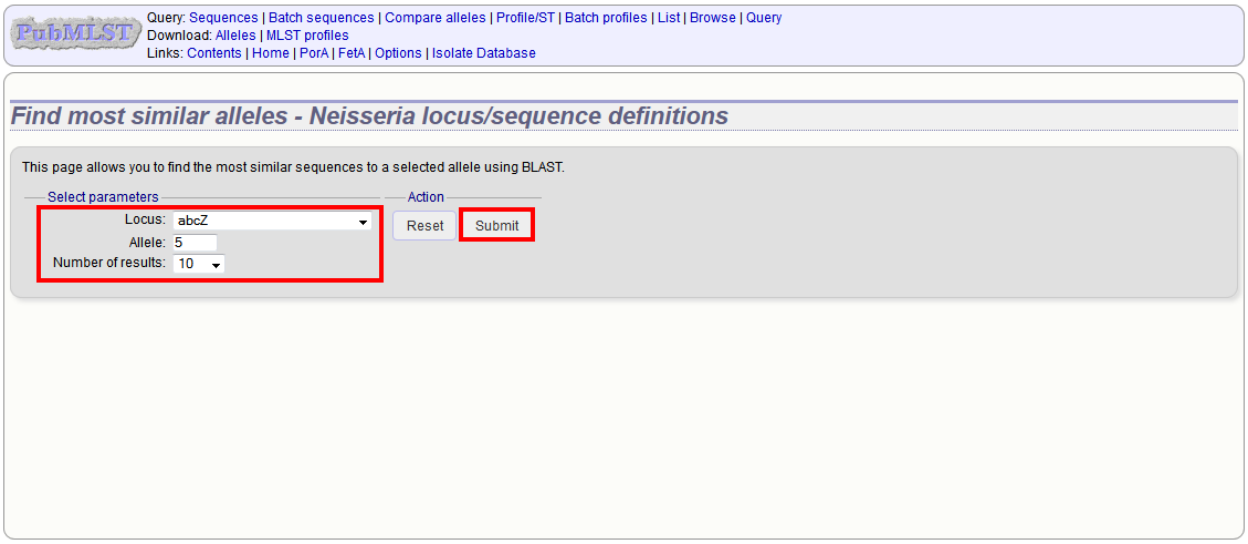
11.8 Investigating allele differences

11.8.1 Sequence similarity

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

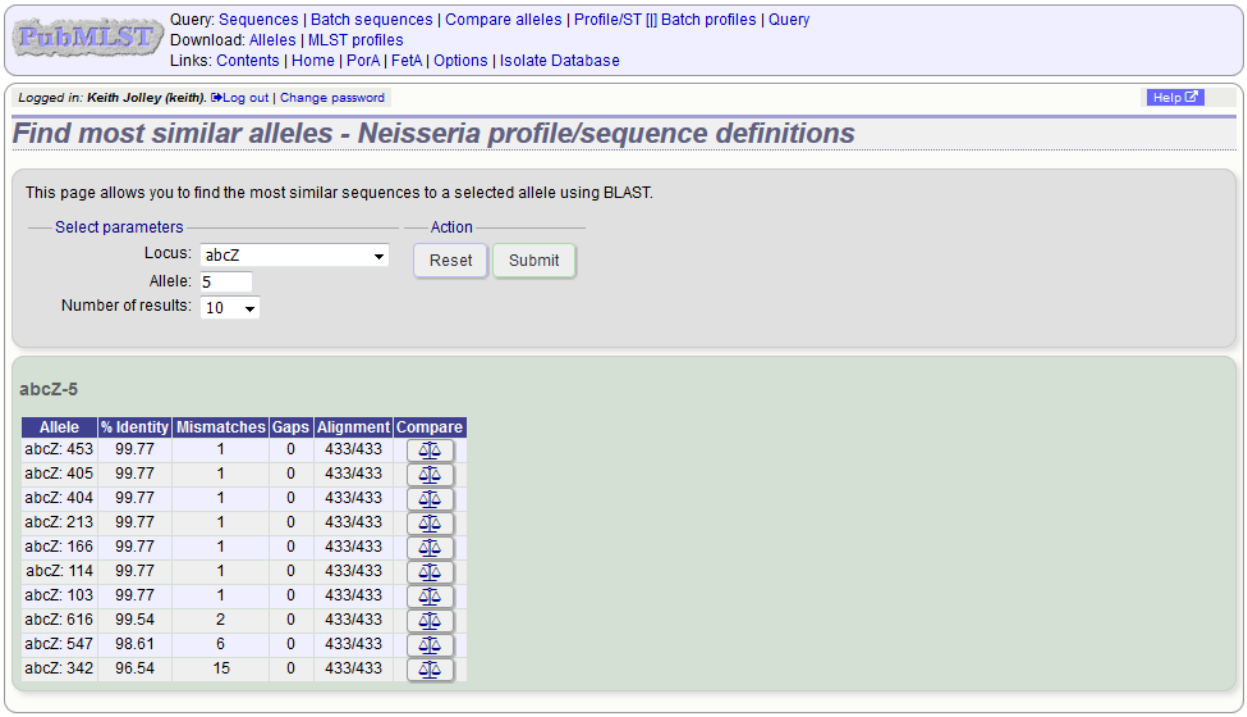


Enter the locus and allele identifer of the sequence to investigate and the number of nearest matches you'd like to see, then press submit.

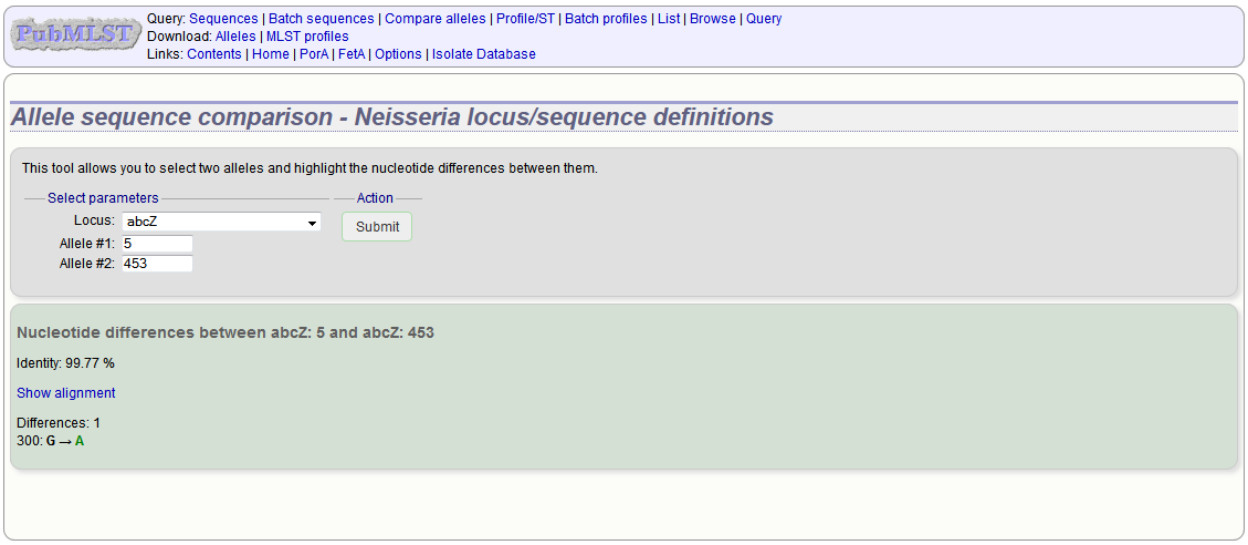


A list of nearest alleles will be displayed, along with the percentage identity and number of gaps between the se-

quences.

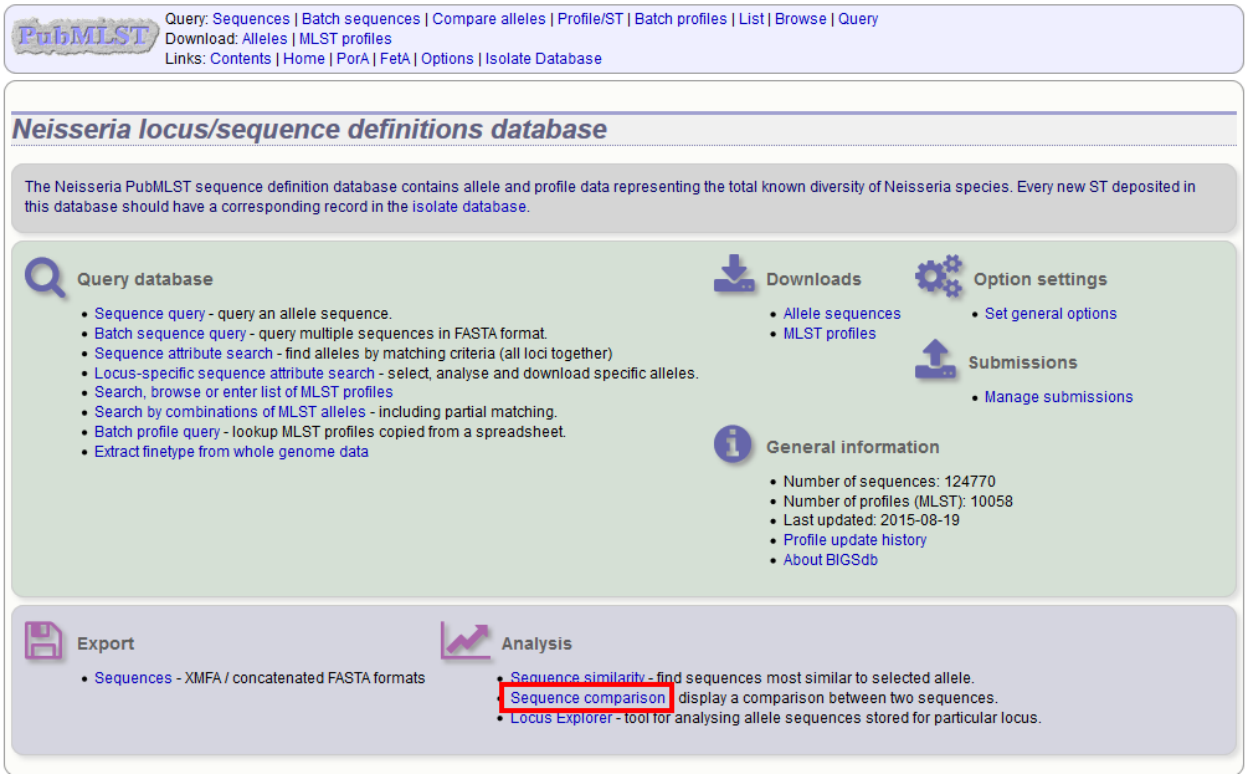


Click the appropriate 'Compare' button to display a list of nucleotide differences and/or a sequence alignment.

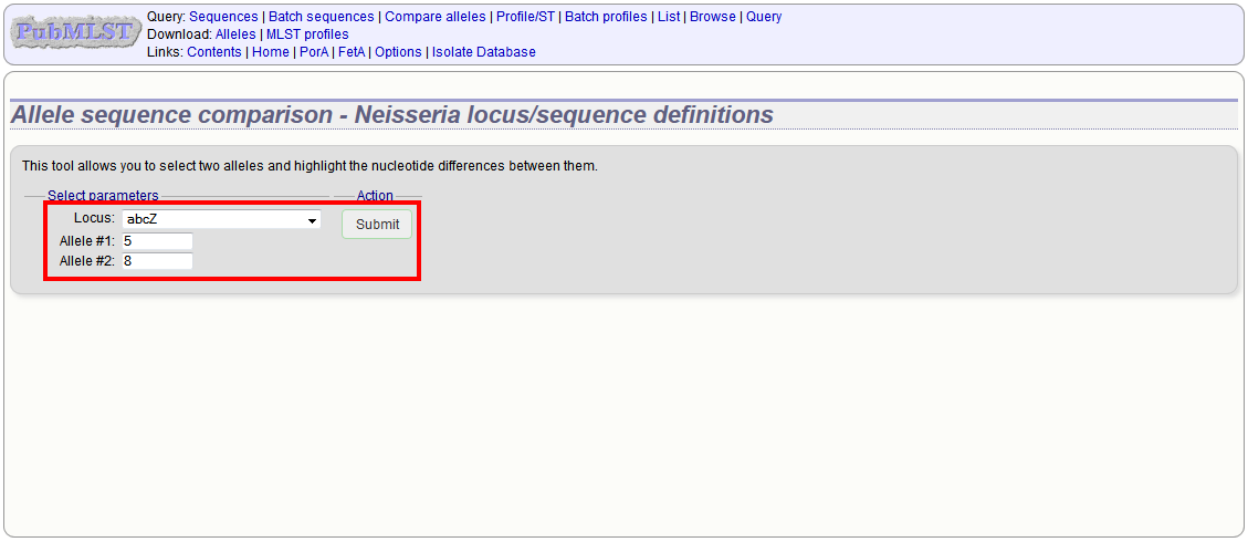


11.8.2 Sequence comparison

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



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



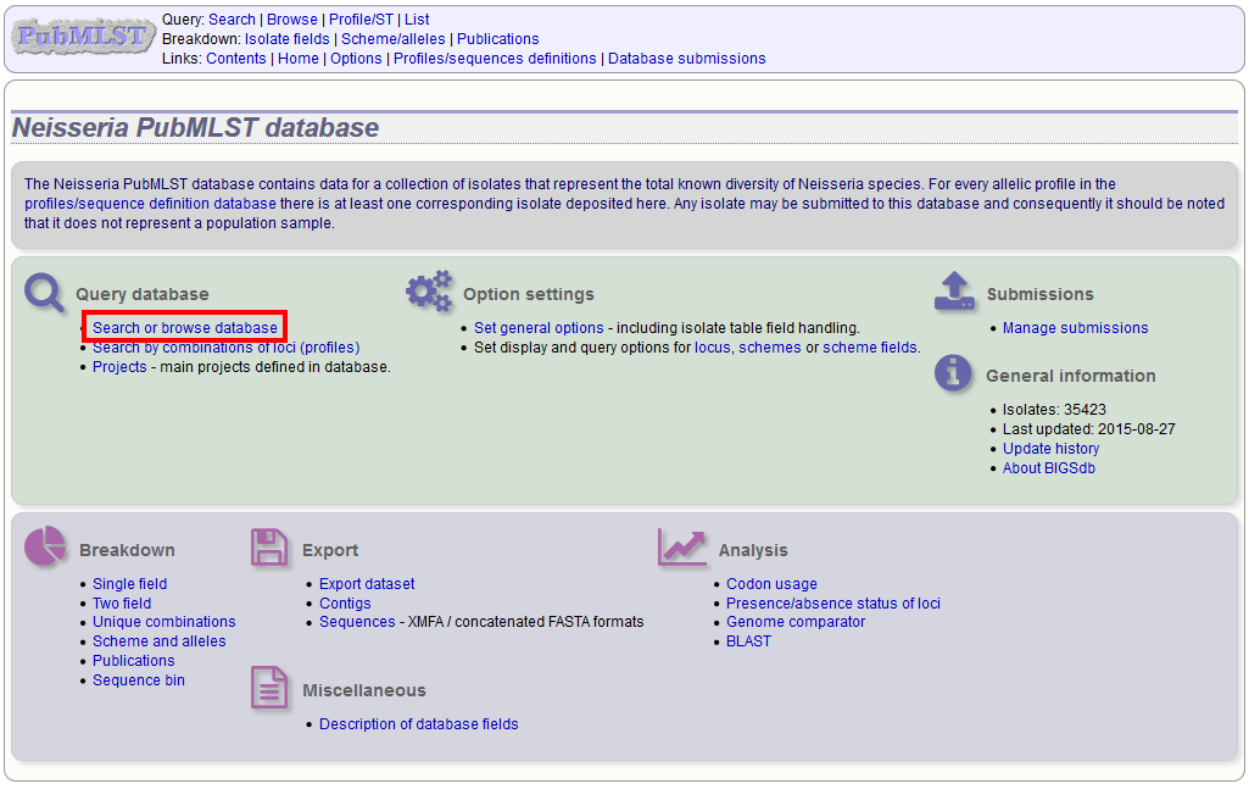
A list of nucleotide differences and/or an alignment will be displayed.

See also:

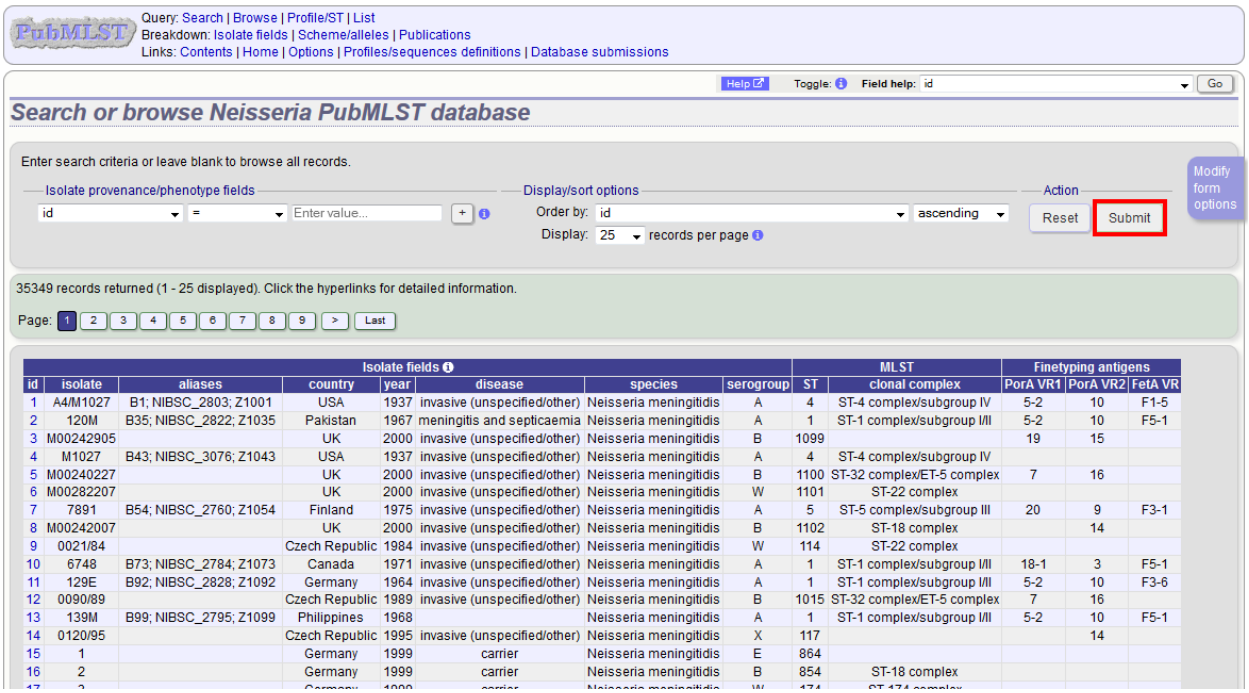
Locus explorer plugin.

11.9 Browsing isolate data

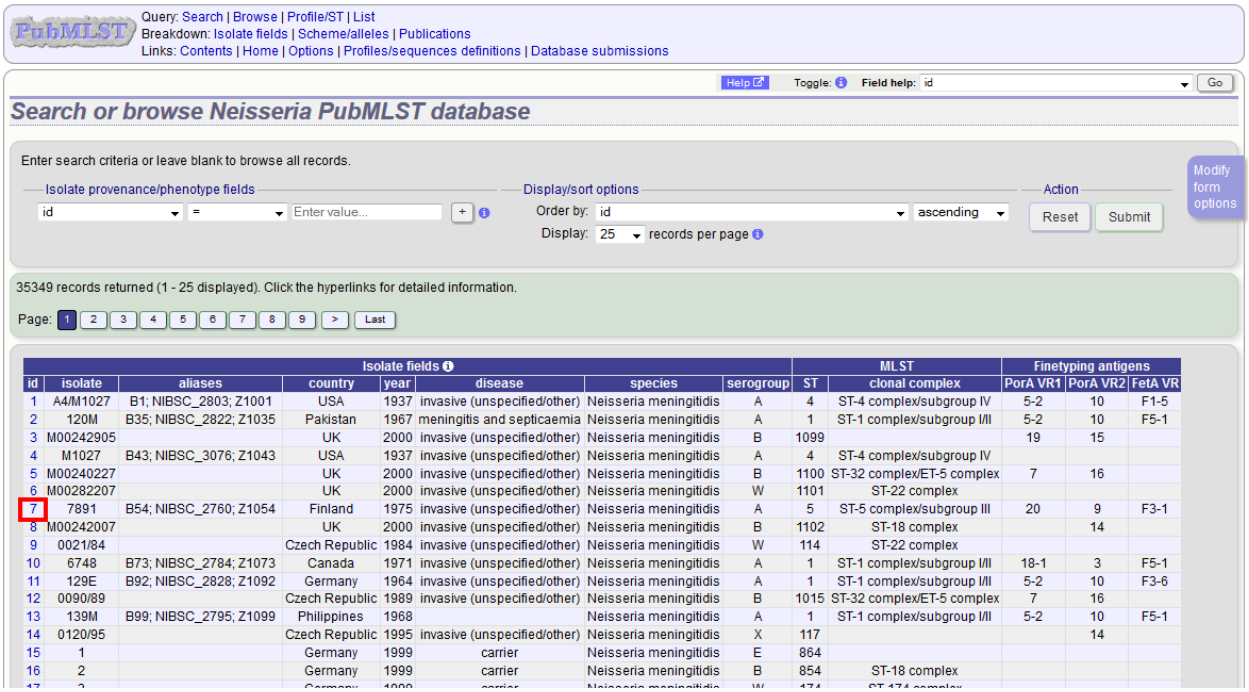
Isolate records can be browsed by clicking the link to 'Search or browse database'.



Leave query form fields blank (the display of these may vary depending on modification options set by the user). Choose the field to order the results by, the number of results per page to display, and click 'Submit'.



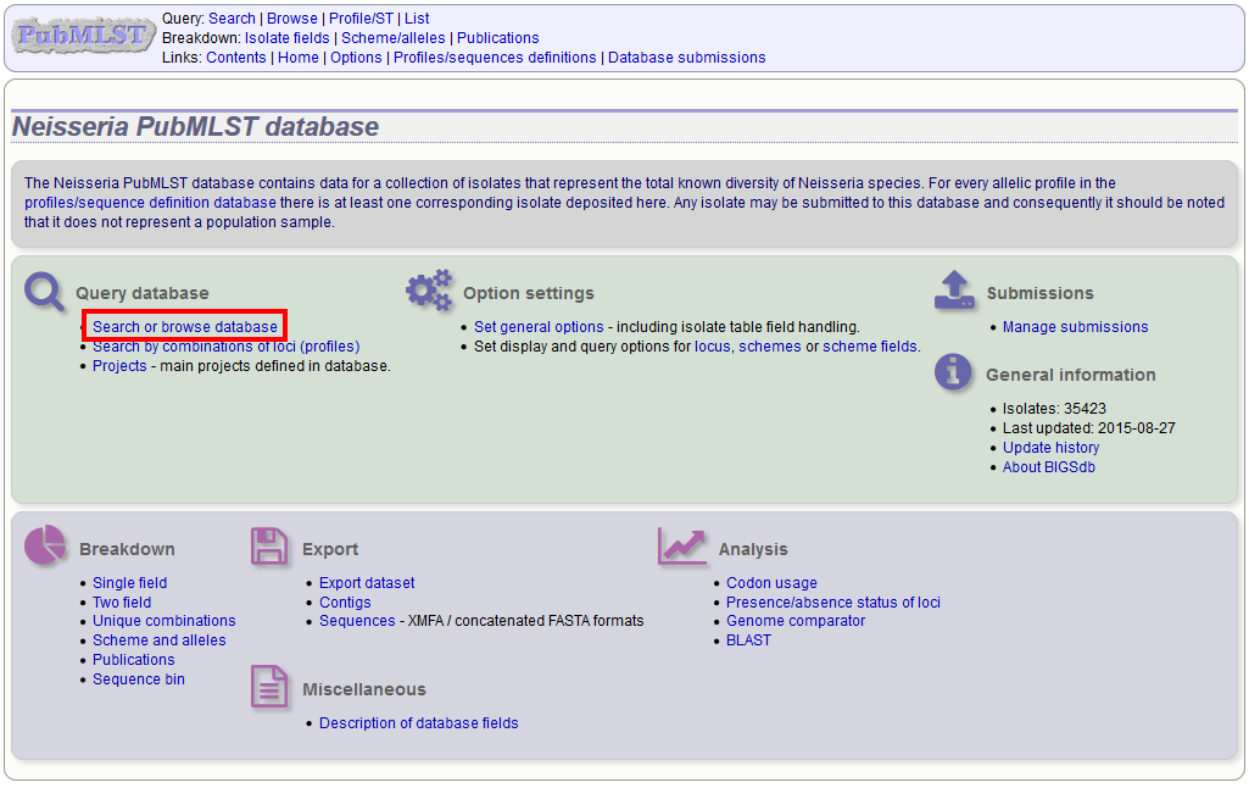
Clicking the hyperlink for any record will display full information about the profile.



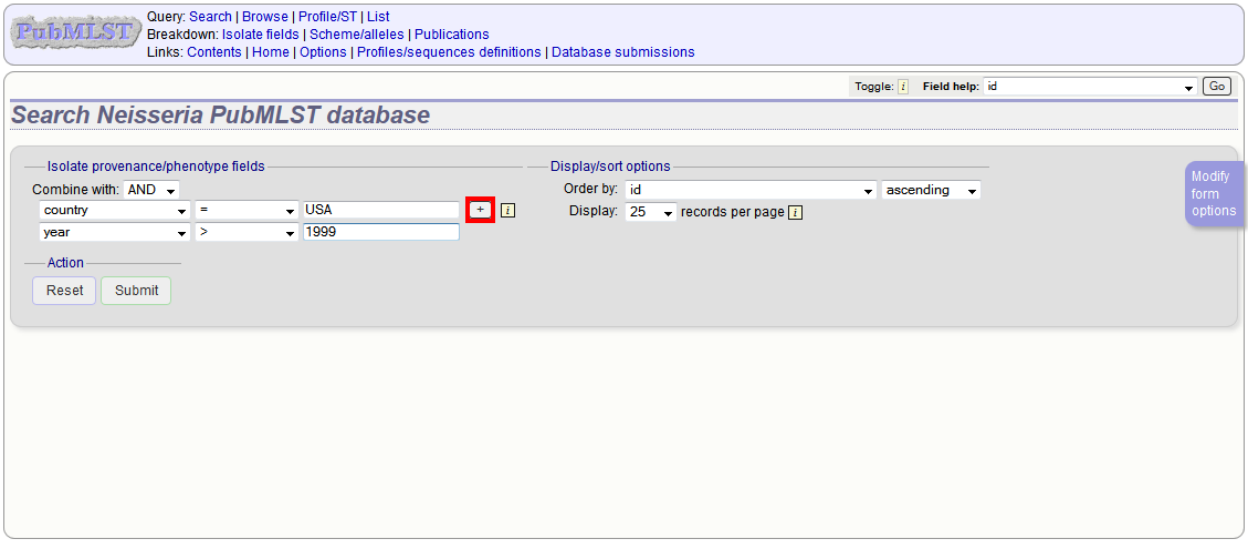
id	isolate	aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1	PorA VR2	FetA VR
1	A4/M1027	B1; NIBSC_2803; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; NIBSC_2822; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
3	M00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	B	1099		19	15	
4	M1027	B43; NIBSC_3076; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV			
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	B	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; NIBSC_2760; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	20	9	F3-1
8	M00242007		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	B	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; NIBSC_2784; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129E	B92; NIBSC_2828; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	B	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; NIBSC_2795; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	X	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	B	854	ST-18 complex			

11.10 Querying isolate data

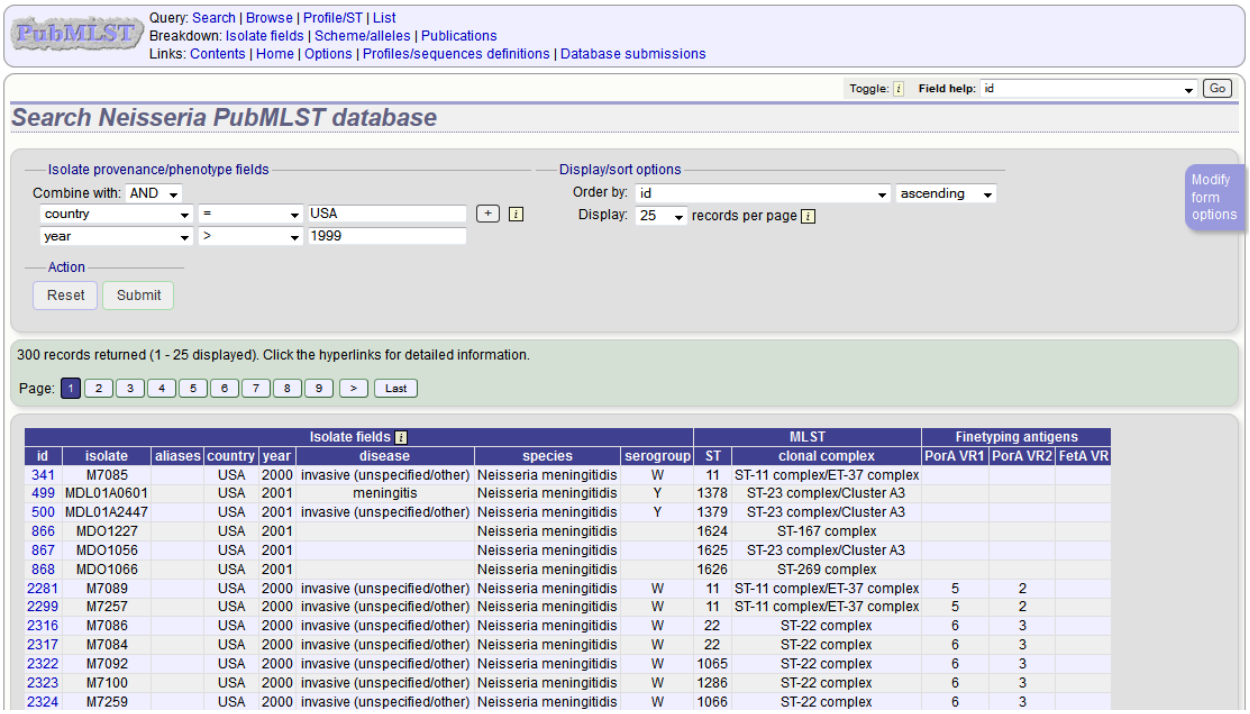
The 'Search or browse database' page of an isolate database allows you to also search by combinations of provenance criteria, scheme and locus data, and more.



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



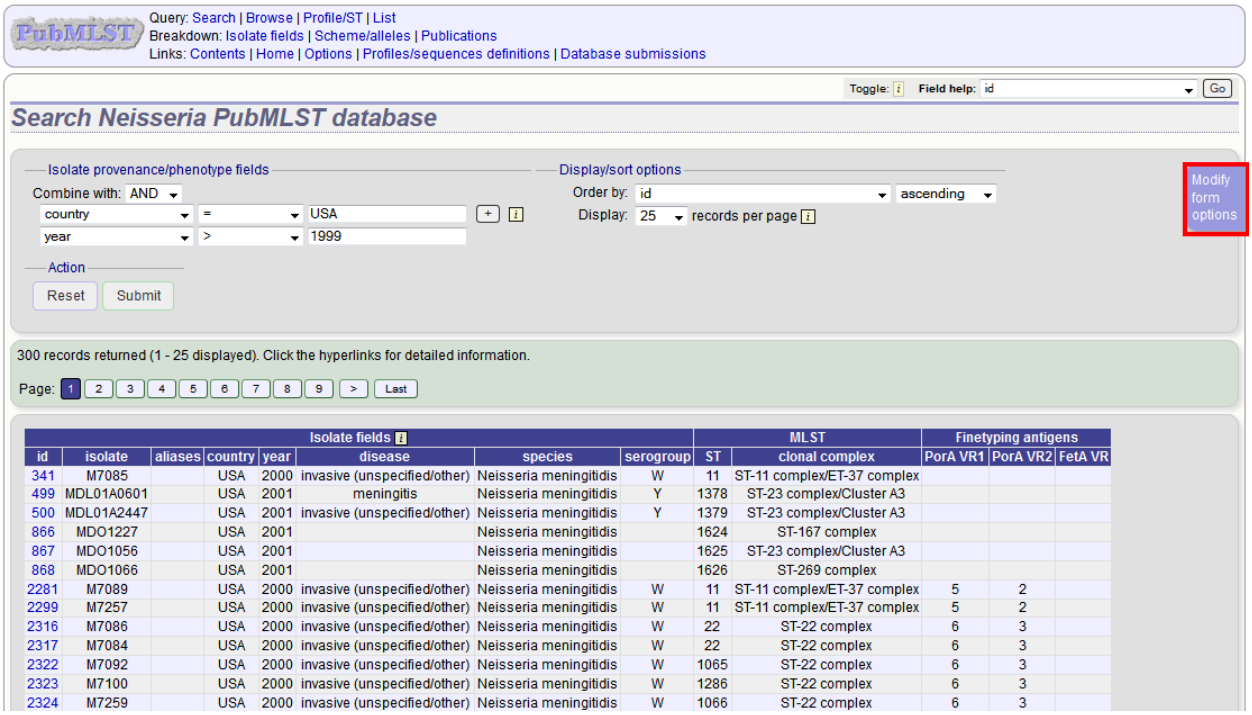
After the search has been submitted, the results will be displayed in a table.



Isolate fields								MLST		Finetyping antigens		
id	isolate	aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1	PorA VR2	FetA VR
341	M7085		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex			
499	MDL01A0601		USA	2001	meningitis	Neisseria meningitidis	Y	1378	ST-23 complex/Cluster A3			
500	MDL01A2447		USA	2001	invasive (unspecified/other)	Neisseria meningitidis	Y	1379	ST-23 complex/Cluster A3			
866	MDO1227		USA	2001		Neisseria meningitidis		1624	ST-167 complex			
867	MDO1056		USA	2001		Neisseria meningitidis		1625	ST-23 complex/Cluster A3			
868	MDO1066		USA	2001		Neisseria meningitidis		1626	ST-269 complex			
2281	M7089		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex	5	2	
2299	M7257		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex	5	2	
2316	M7086		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	22	ST-22 complex	6	3	
2317	M7084		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	22	ST-22 complex	6	3	
2322	M7092		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1065	ST-22 complex	6	3	
2323	M7100		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1286	ST-22 complex	6	3	
2324	M7259		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1066	ST-22 complex	6	3	

Each field can be queried using *standard operators*.

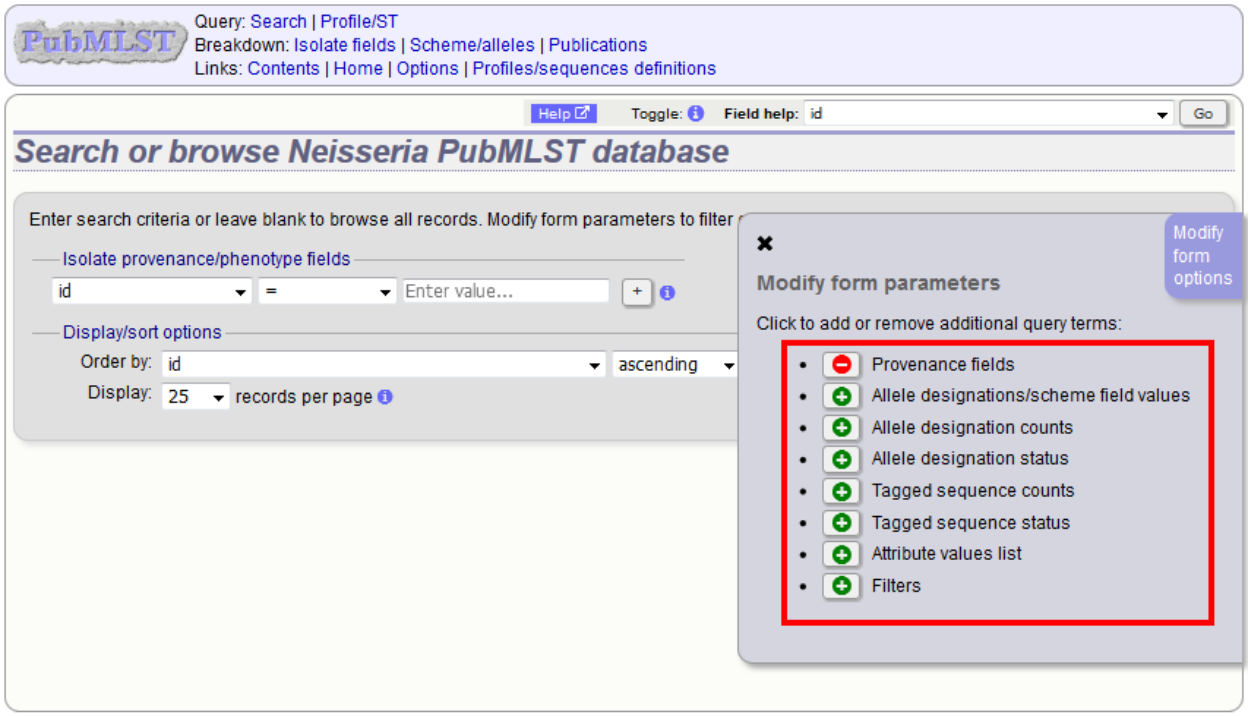
More search features are available by clicking the 'Modify form options' tab on the right-hand side of the screen.



Isolate fields								MLST		Finetyping antigens		
id	isolate	aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1	PorA VR2	FetA VR
341	M7085		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex			
499	MDL01A0601		USA	2001	meningitis	Neisseria meningitidis	Y	1378	ST-23 complex/Cluster A3			
500	MDL01A2447		USA	2001	invasive (unspecified/other)	Neisseria meningitidis	Y	1379	ST-23 complex/Cluster A3			
866	MDO1227		USA	2001		Neisseria meningitidis		1624	ST-167 complex			
867	MDO1056		USA	2001		Neisseria meningitidis		1625	ST-23 complex/Cluster A3			
868	MDO1066		USA	2001		Neisseria meningitidis		1626	ST-269 complex			
2281	M7089		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex	5	2	
2299	M7257		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	11	ST-11 complex/ET-37 complex	5	2	
2316	M7086		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	22	ST-22 complex	6	3	
2317	M7084		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	22	ST-22 complex	6	3	
2322	M7092		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1065	ST-22 complex	6	3	
2323	M7100		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1286	ST-22 complex	6	3	
2324	M7259		USA	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1066	ST-22 complex	6	3	

A tab will be displayed. Different options will be available here depending on the database. Queries will be combined from the values entered in all form sections. Possible options are:

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

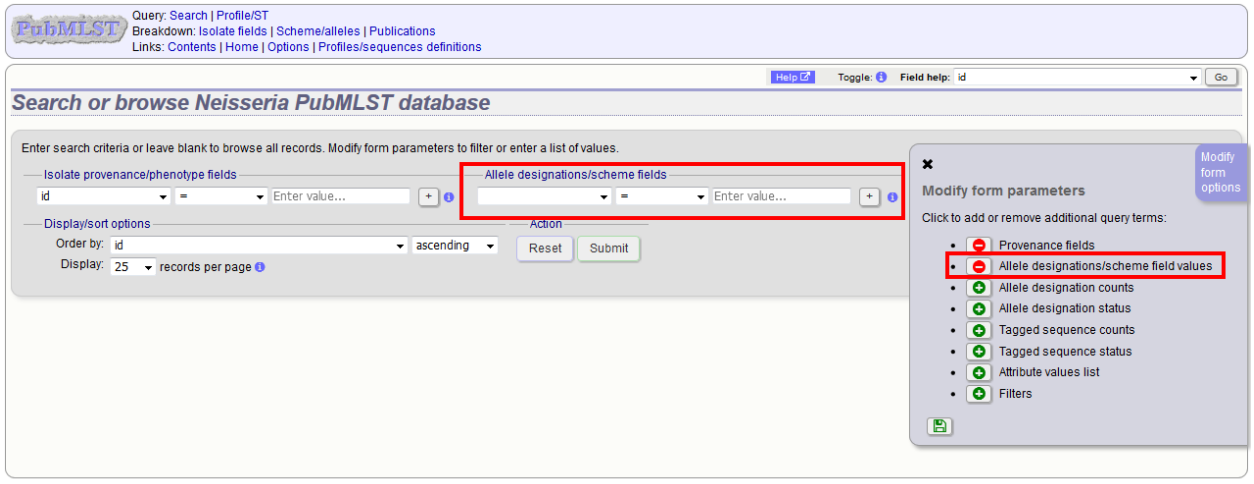


If the interface is modified, a button to save options becomes available within the tab. If this is clicked, the modified form will be displayed the next time you go to the query page.

11.10.1 Query by allele designation/scheme field

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

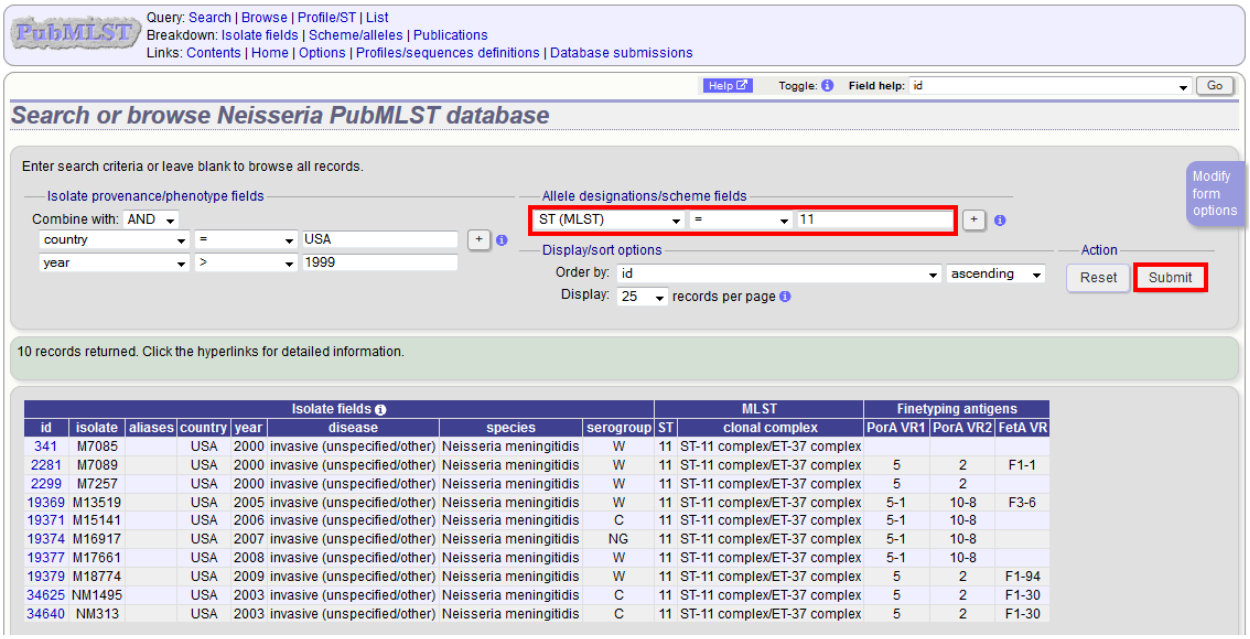
Make sure that the allele designation/scheme field values fieldset is displayed by selecting it in the 'Modify form options' tab.



Designations can be queried using *standard operators*.

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

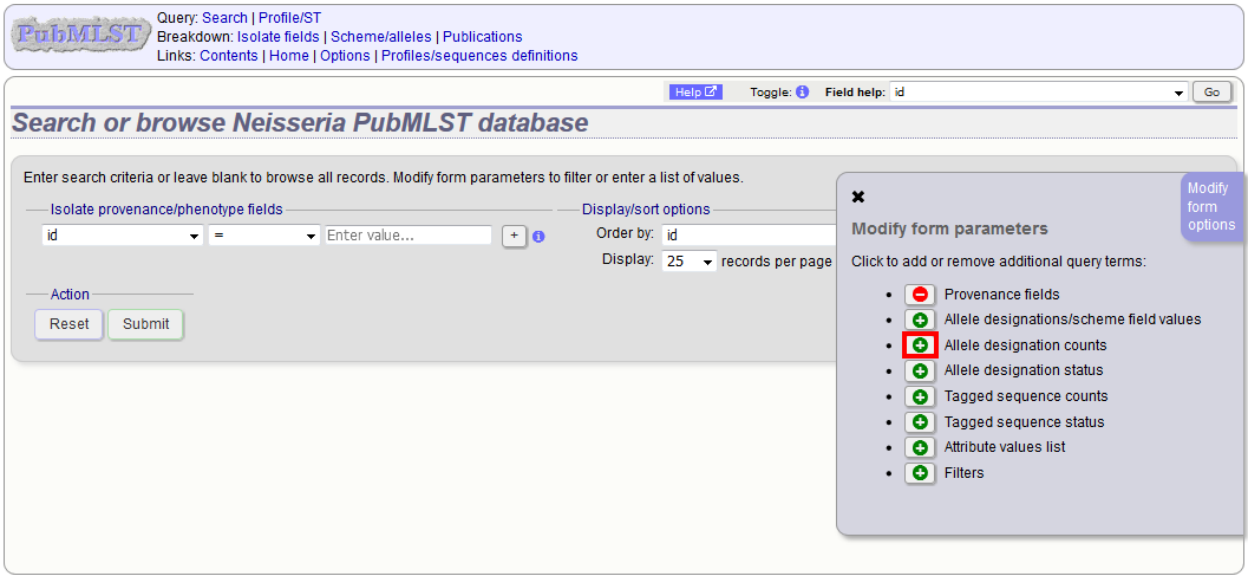
Add your search terms and click 'Submit'. Allele designation/scheme field queries will be combined with terms entered in other sections.



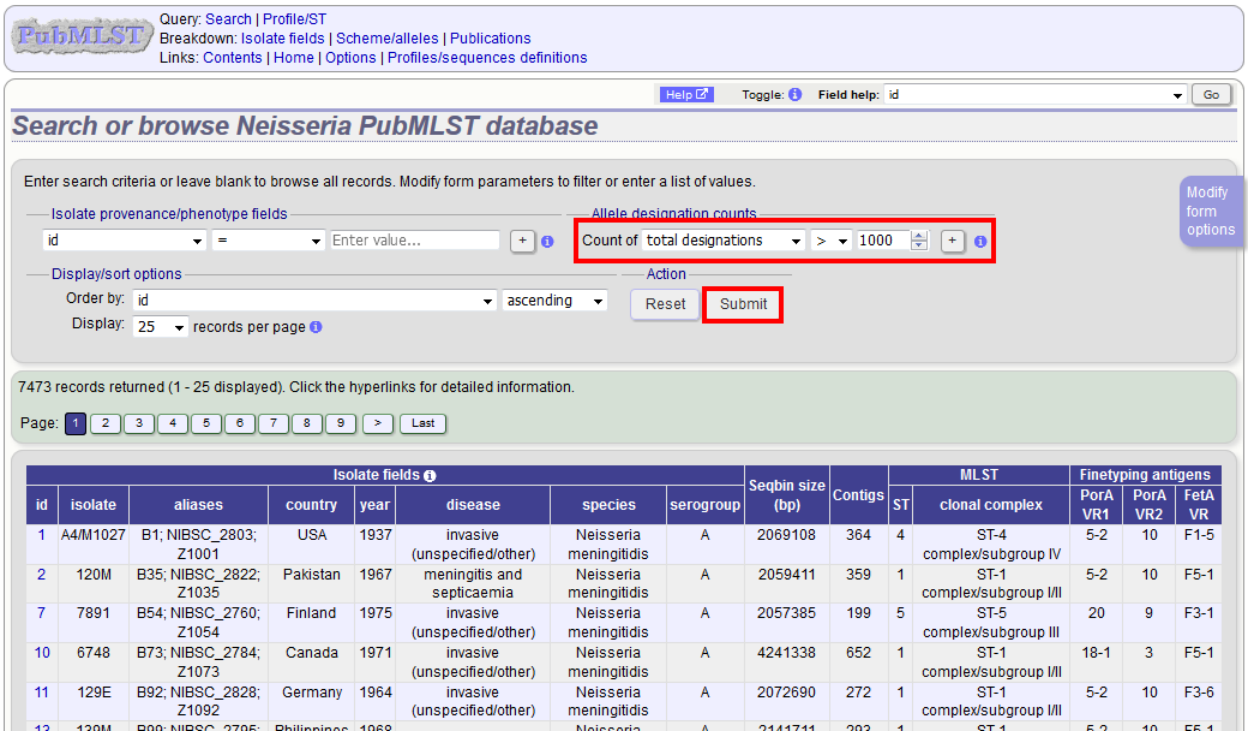
11.10.2 Query by allele designation count

Queries can be combined with counts of the total number of designations or for individual loci.

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

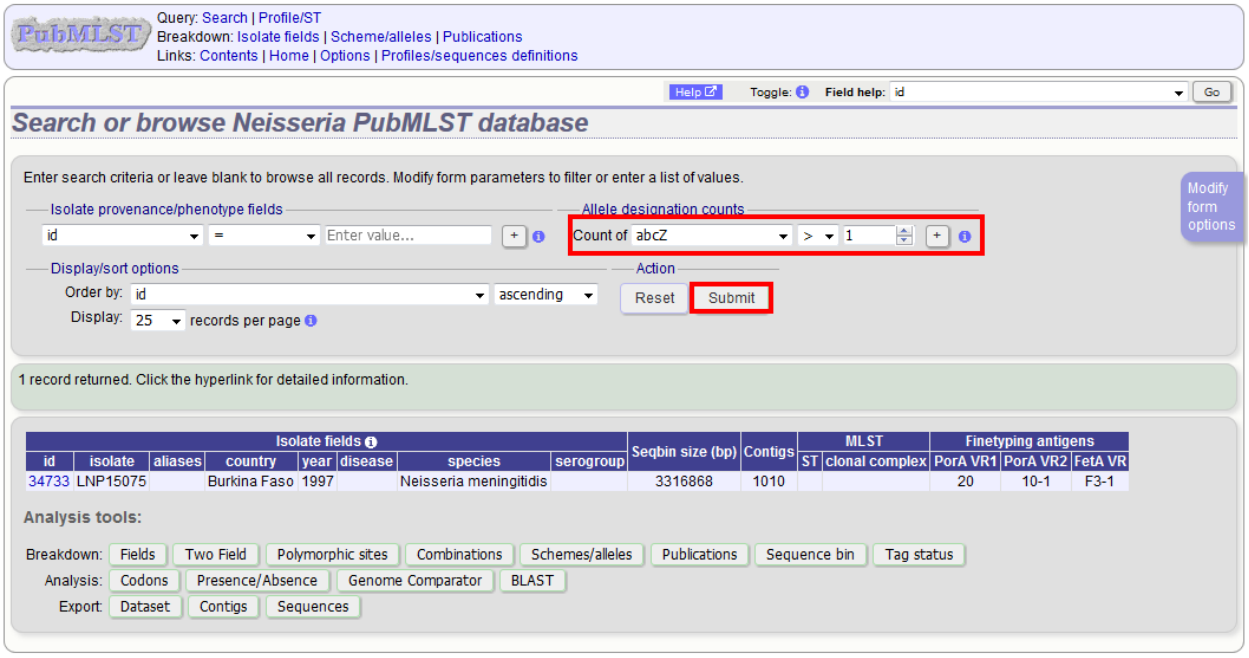


For example, to find all isolates that have designations at >1000 loci, select 'total designations > 1000', then click 'Submit'.



You can also search for isolates where any isolate has a particular number of designations. Use the term 'any locus' to do this.

Finally, you can search for isolates with a specific number of designations at a specific locus.



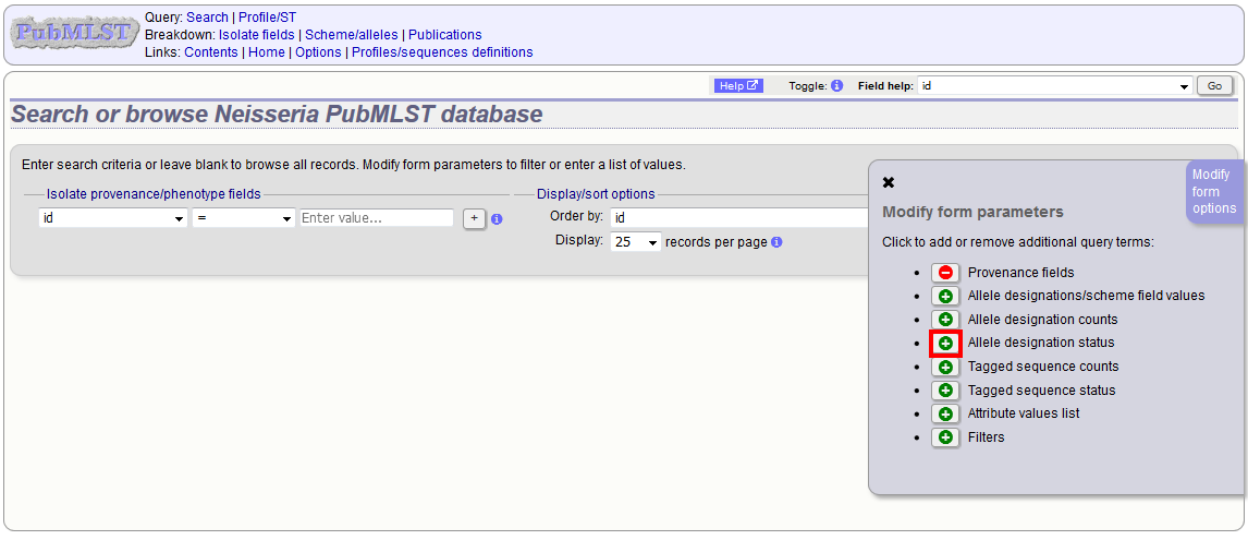
Additional search terms can be combined using the '+' button. Designation count queries will be combined with terms entered in other sections.

Note: Searches for 'all loci' with counts that include zero, e.g. 'count of any locus = 0' or with a '<' operator are not supported. This is because such searches have to identify every isolate for which one or more loci are missing. In databases with thousands of loci this can be a very expensive database query.

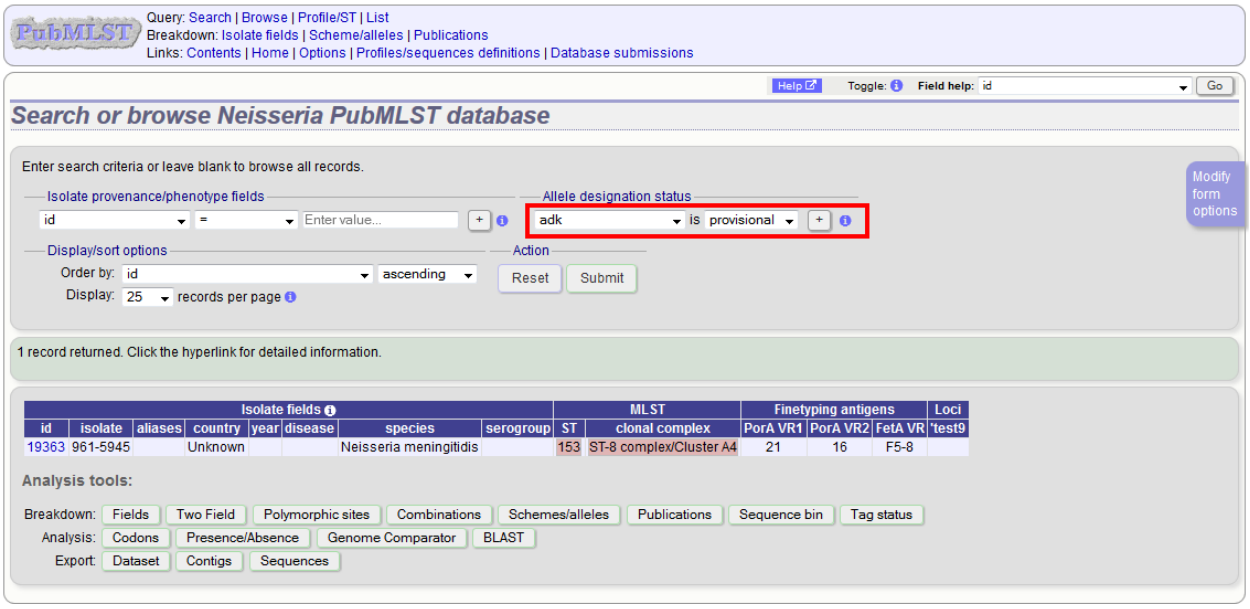
11.10.3 Query by allele designation status

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

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



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

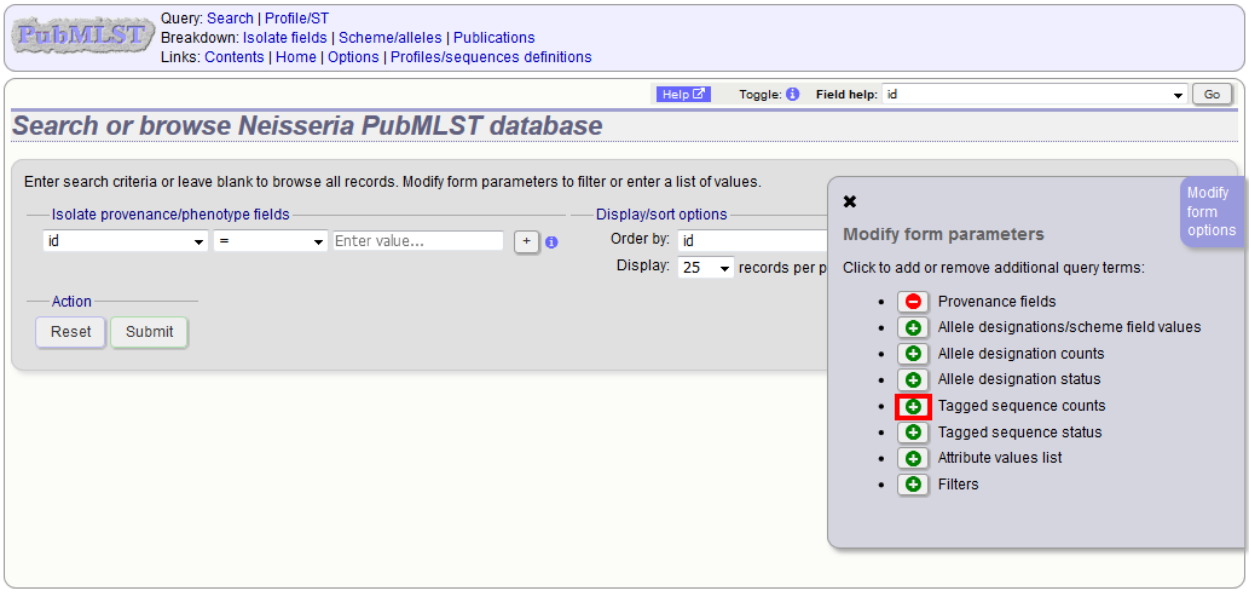


Provisional allele designations are marked within the results tables with a pink background. Any scheme field designations that depend on the allele in question, e.g. a MLST ST, will also be marked as provisional.

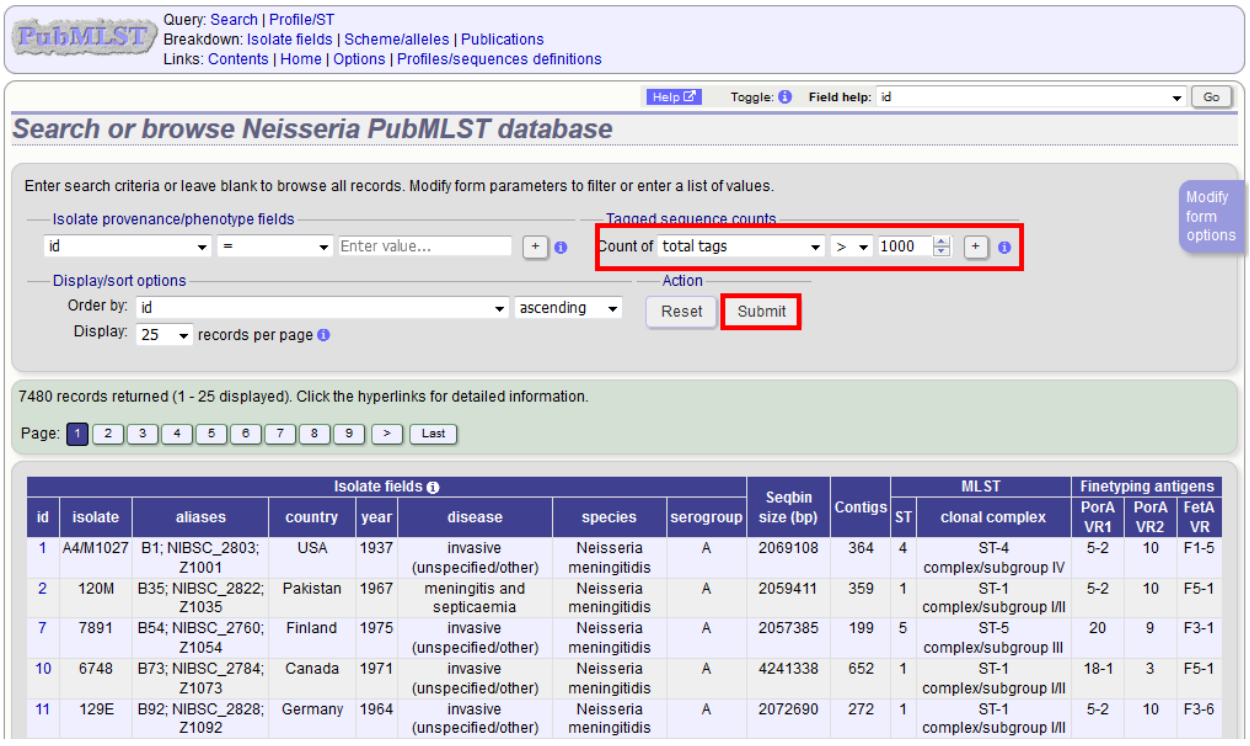
11.10.4 Query by sequence tag count

Queries can be combined with counts of the total number of tags or for individual loci.

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

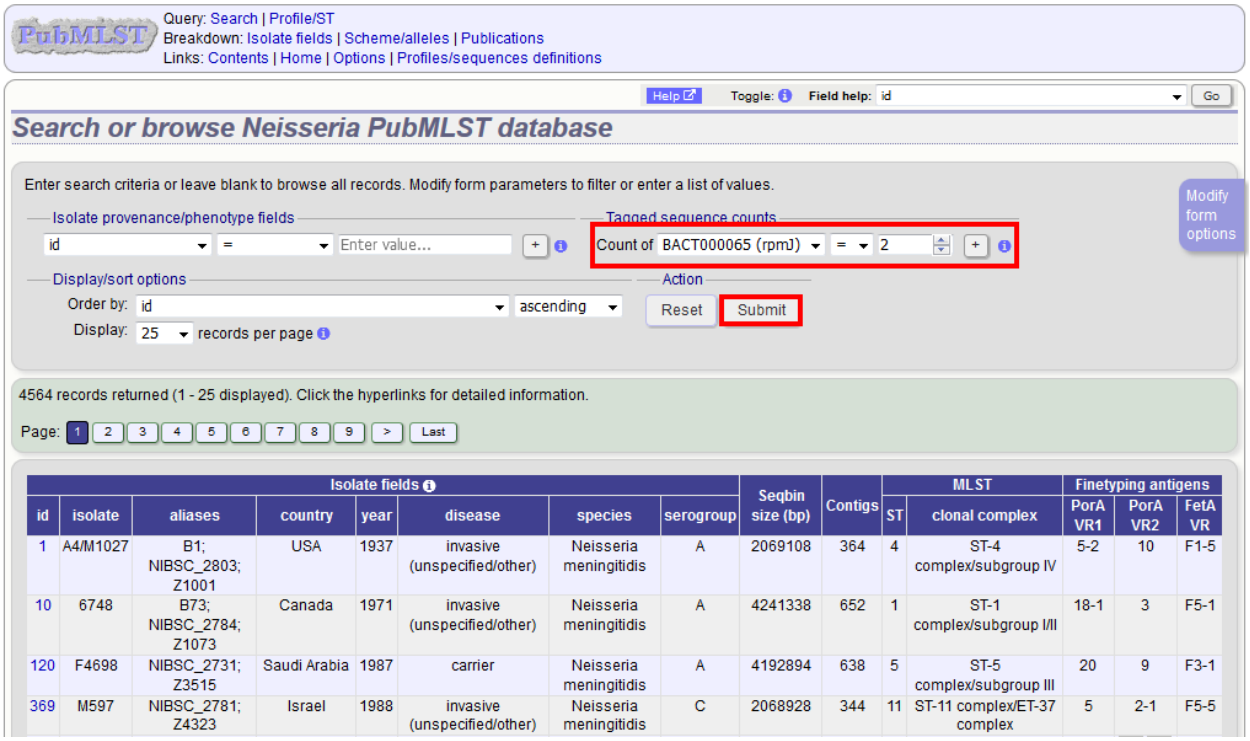


For example, to find all isolates that have sequence tags at >1000 loci, select 'total tags > 1000', then click 'Submit'.



You can also search for isolates where any isolate has a particular number of sequence tags. Use the term 'any locus' to do this.

Finally, you can search for isolates with a specific number of tags at a specific locus.



Isolate fields								Seqbin size (bp)	Contigs	MLST		Finetyping antigens		
id	isolate	aliases	country	year	disease	species	serogroup			ST	clonal complex	PorA VR1	PorA VR2	FetA VR
1	A4/M1027	B1; NIBSC_2803; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	2069108	364	4	ST-4 complex/subgroup IV	5-2	10	F1-5
10	6748	B73; NIBSC_2784; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	4241338	652	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
120	F4698	NIBSC_2731; Z3515	Saudi Arabia	1987	carrier	Neisseria meningitidis	A	4192894	638	5	ST-5 complex/subgroup III	20	9	F3-1
369	M597	NIBSC_2781; Z4323	Israel	1988	invasive (unspecified/other)	Neisseria meningitidis	C	2068928	344	11	ST-11 complex/ET-37 complex	5	2-1	F5-5

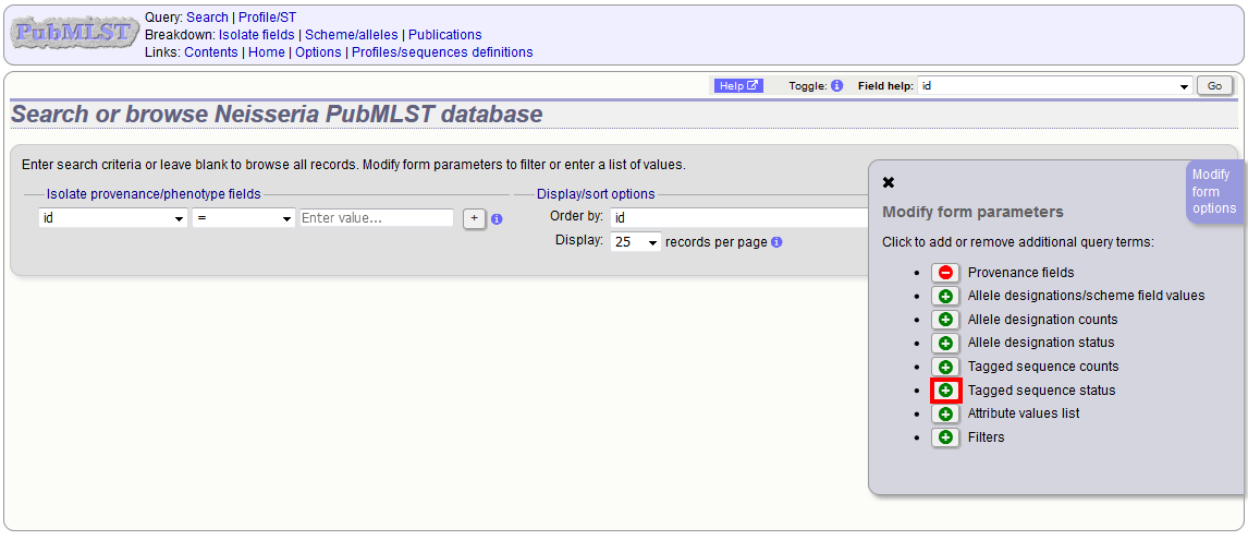
Additional search terms can be combined using the '+' button. Sequence tag count queries will be combined with terms entered in other sections.

Note: Searches for 'all loci' with counts that include zero, e.g. 'count of any locus = 0' or with a '<' operator are not supported. This is because such searches have to identify every isolate for which one or more loci are not tagged. In databases with thousands of loci this can be a very expensive database query.

11.10.5 Query by tagged sequence status

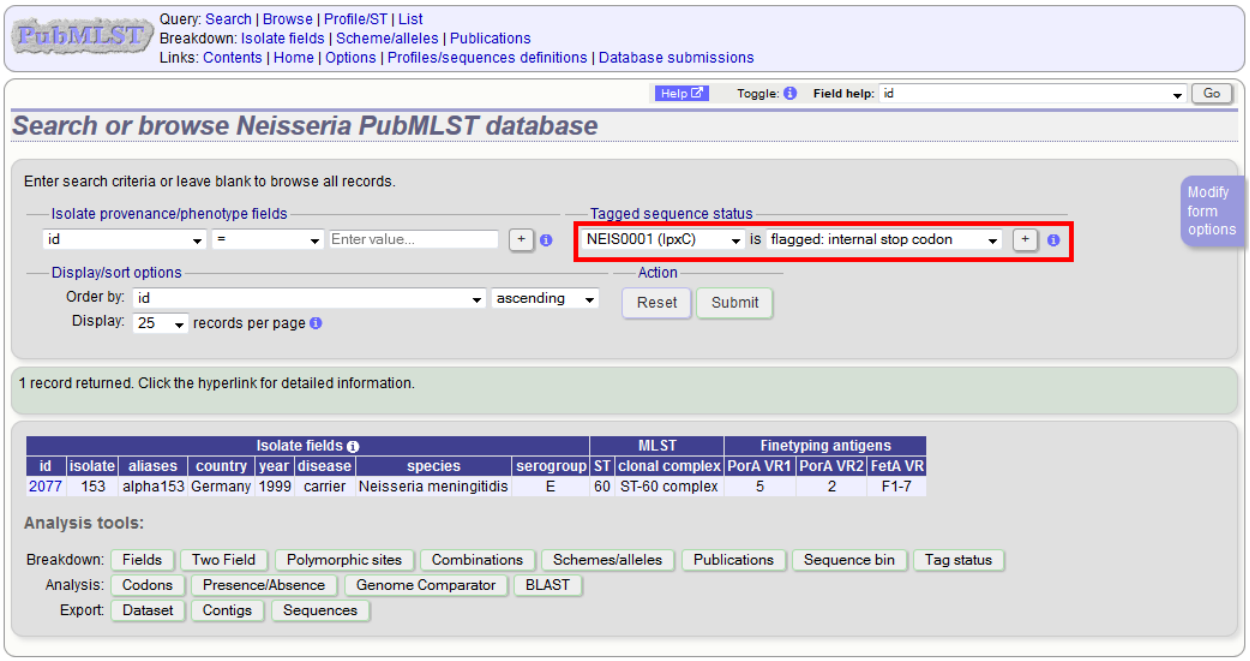
Sequence tags identify the region of a contig within an isolate's sequence bin entries that correspond to a particular locus. The presence or absence of these tags can be queried as can whether or not the sequence has an a flag associated with. These flags designate specific characteristics of the sequences.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

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



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.



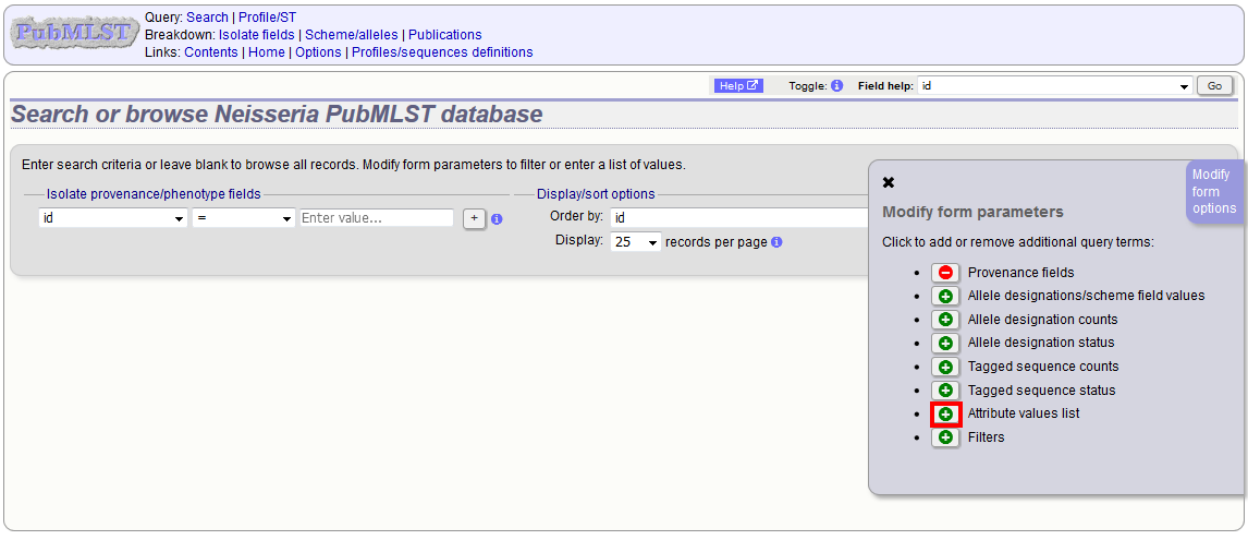
See also:

Sequence tag flags

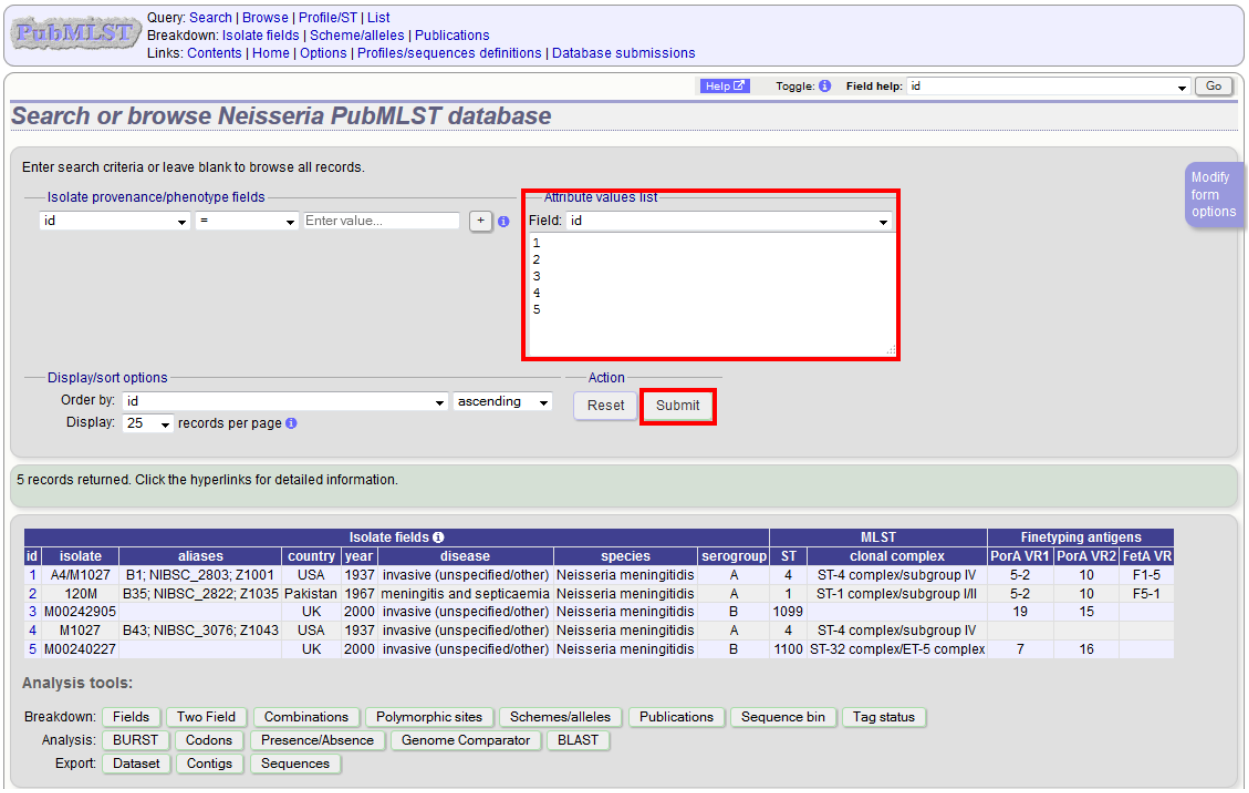
11.10.6 Query by list of attributes

The query form can be modified with a list box in to which a list of values for a chosen attribute can be entered - this could be a list of ids, isolate names, alleles or scheme fields. This list will be combined with any other criteria or filter used on the page.

If the list box is not shown, add it by selecting it in the 'Modify form options' tab.



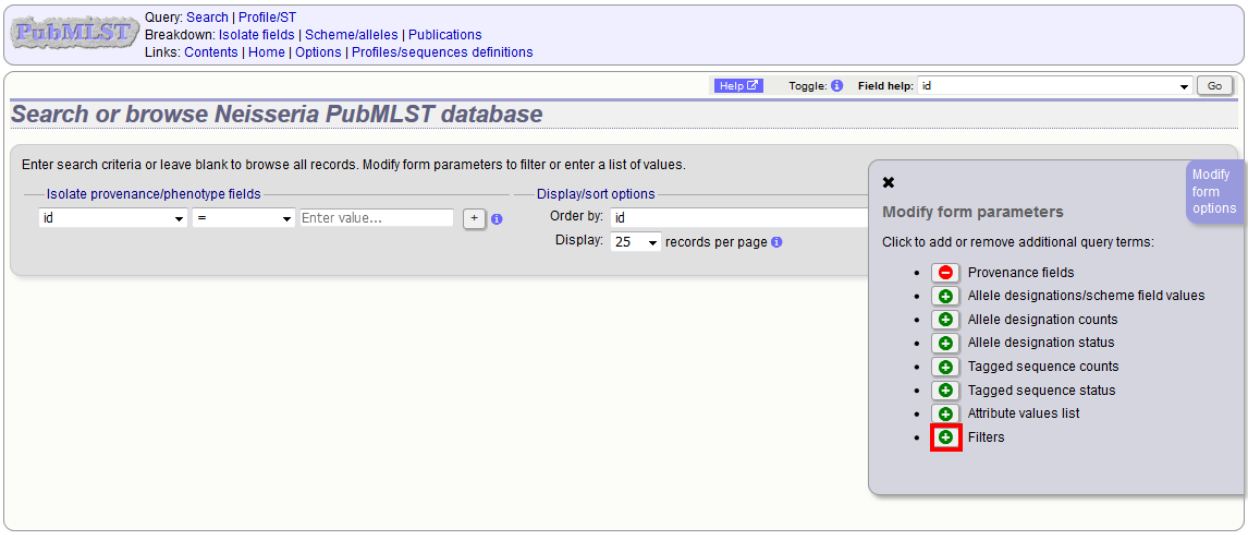
Select the attribute to query and enter a list of values.



11.10.7 Query filters

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

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



The filters displayed will depend on the database and what has been defined within it. Common filters are:

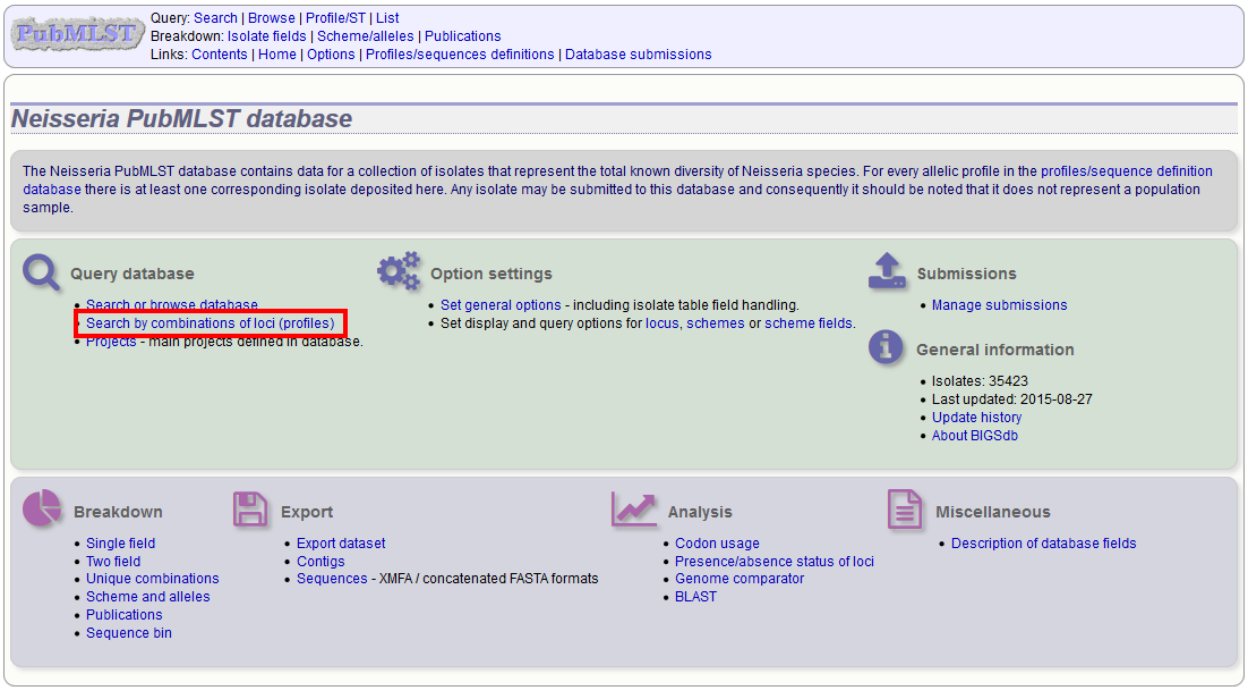
- Publication - Select one or more publication that has been linked to isolate records.

- Project - Select one or more project that isolates belong to.
- Profile completion - This is commonly displayed for MLST schemes. Available options are:
  - complete - All loci of the scheme have alleles designated.
  - incomplete - One or more loci have not yet been designated.
  - partial - The scheme is incomplete, but at least one locus has an allele designated.
  - started - At least one locus has an allele designated. The scheme mat be complete or partial.
  - not started - The scheme has no loci with alleles designated.
- Sequence bin - Specify whether any sequence data has been associated with a record. Specific threshold values may be selected if these have been *set up for the database*.
- Provenance fields - Dropdown list boxes of values for specific provenance fields may be present if set for the database. Users can choose to *add additional filters*.

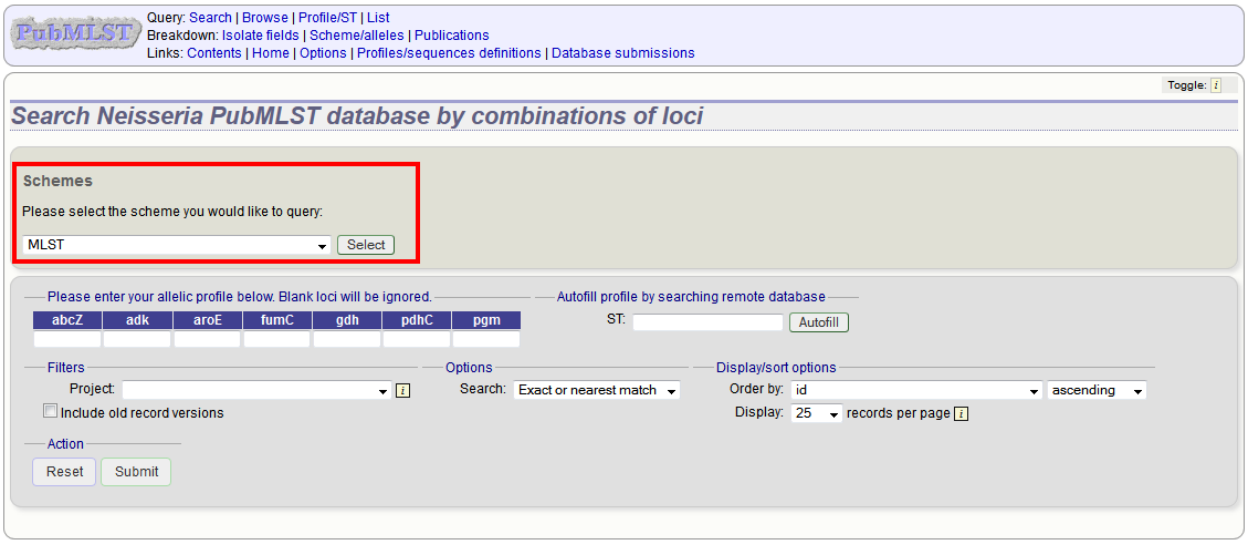
11.11 Querying by allelic profile

If a scheme, such as MLST, has been defined for an isolate database it is possible to query the database against complete or partial allelic profiles. Even if no scheme is defined, queries can be made against all loci.

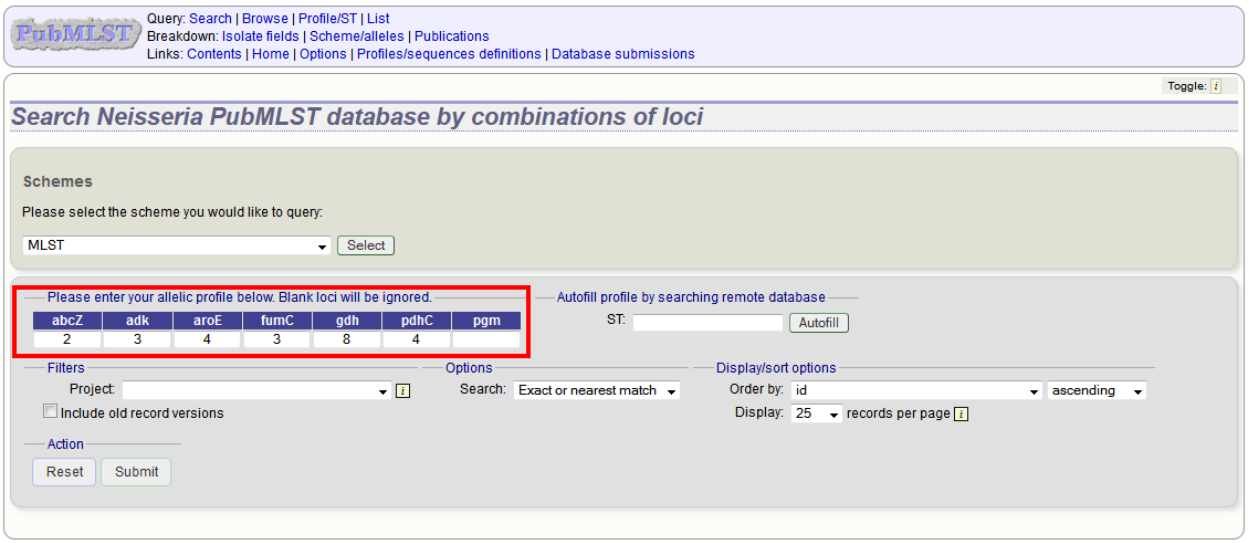
On the index page, click 'Search by combinations of loci (profiles)' for any defined scheme. Enter either a partial (any combination of loci) or complete profile.



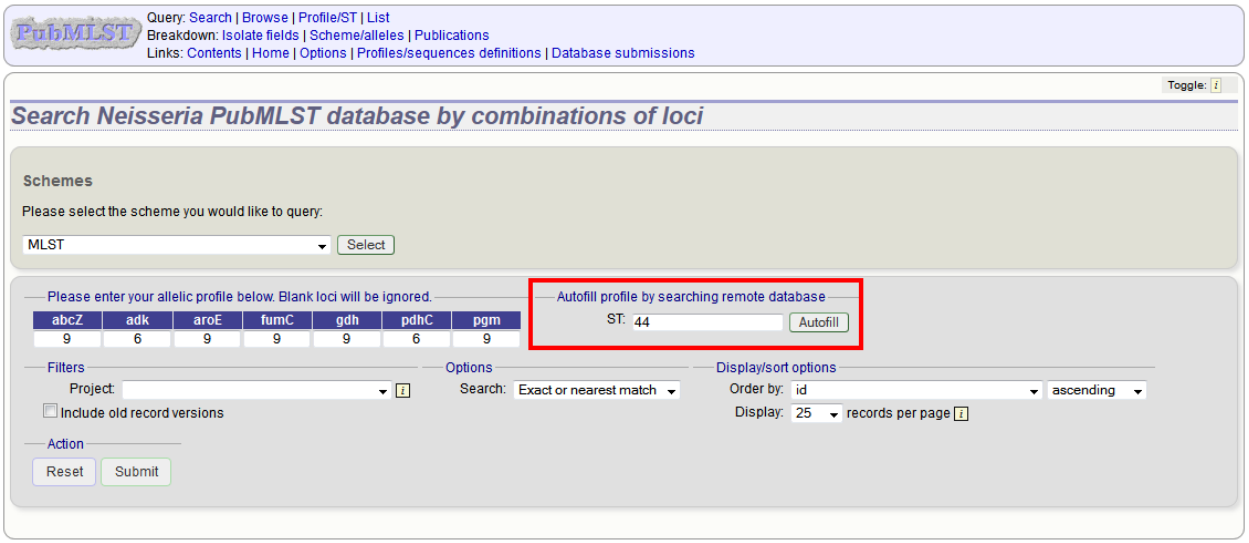
If multiple schemes are defined, you may have to select the scheme you wish to query in the 'Schemes' dropdown box and click 'Select'.



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



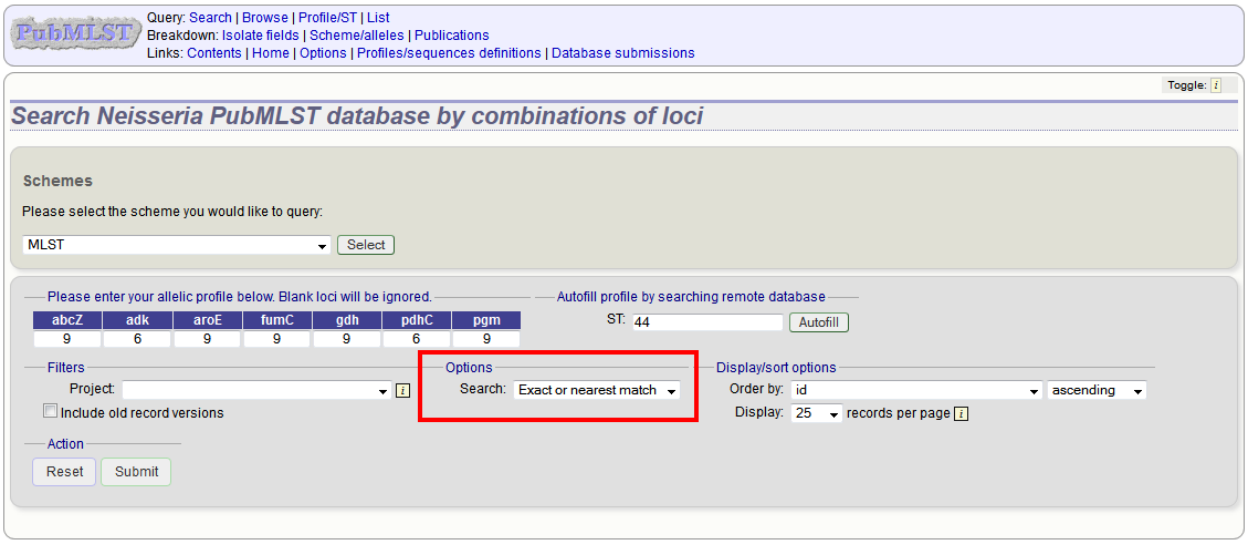
Alternatively, for scheme profiles, you can enter a primary key value (e.g. ST) and select 'Autofill' to automatically fill in the associated profile.



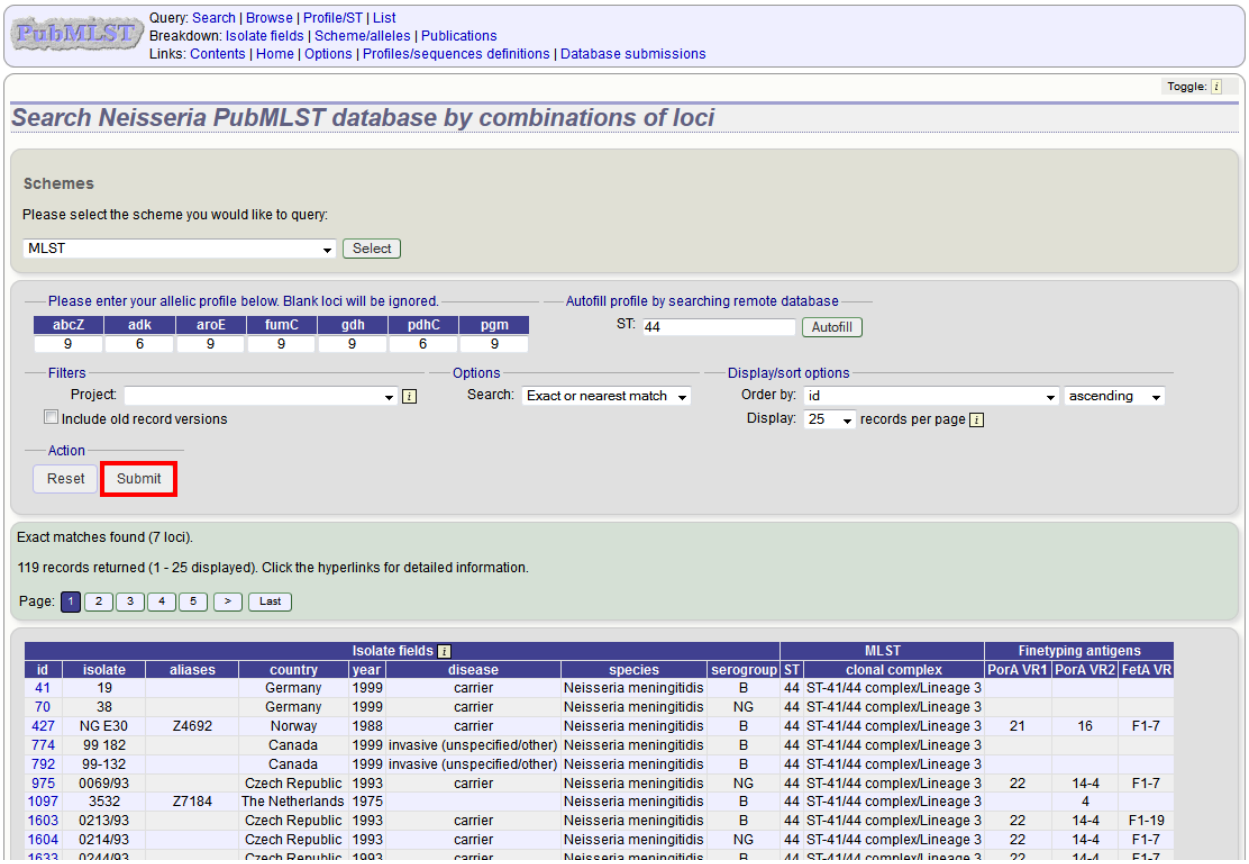
Select the number of loci that you'd like to match in the options dropdown box. Available options are:

- 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.

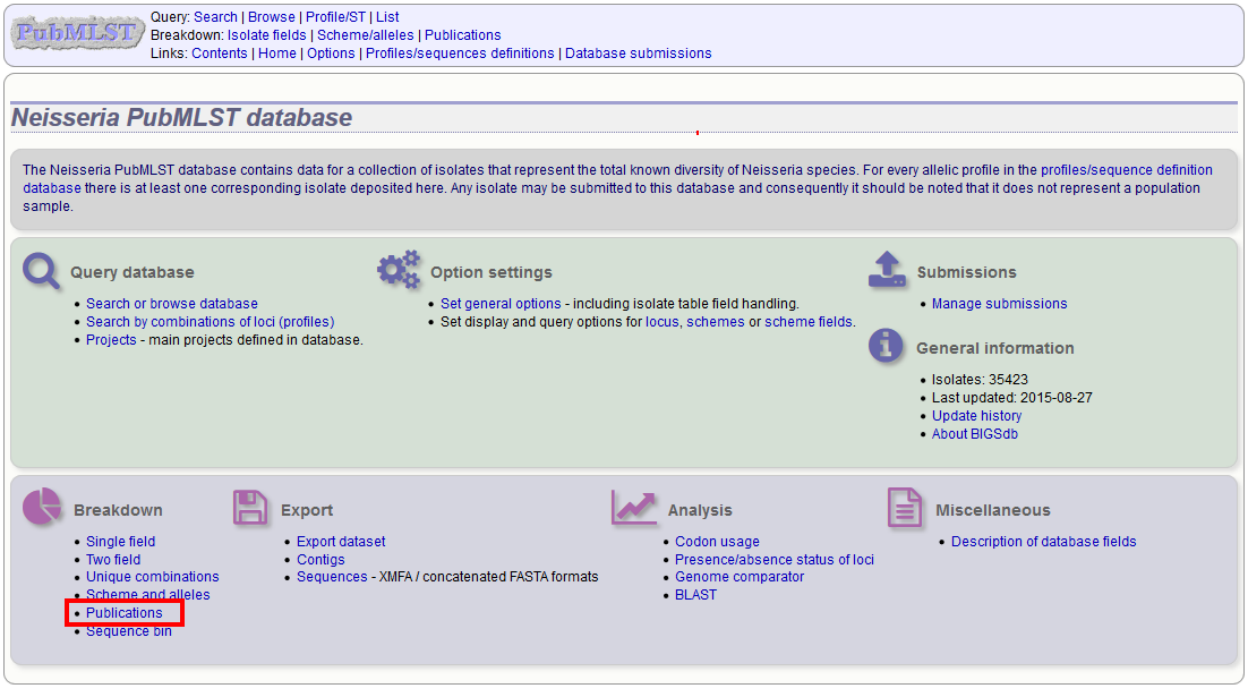


Click 'Submit'.

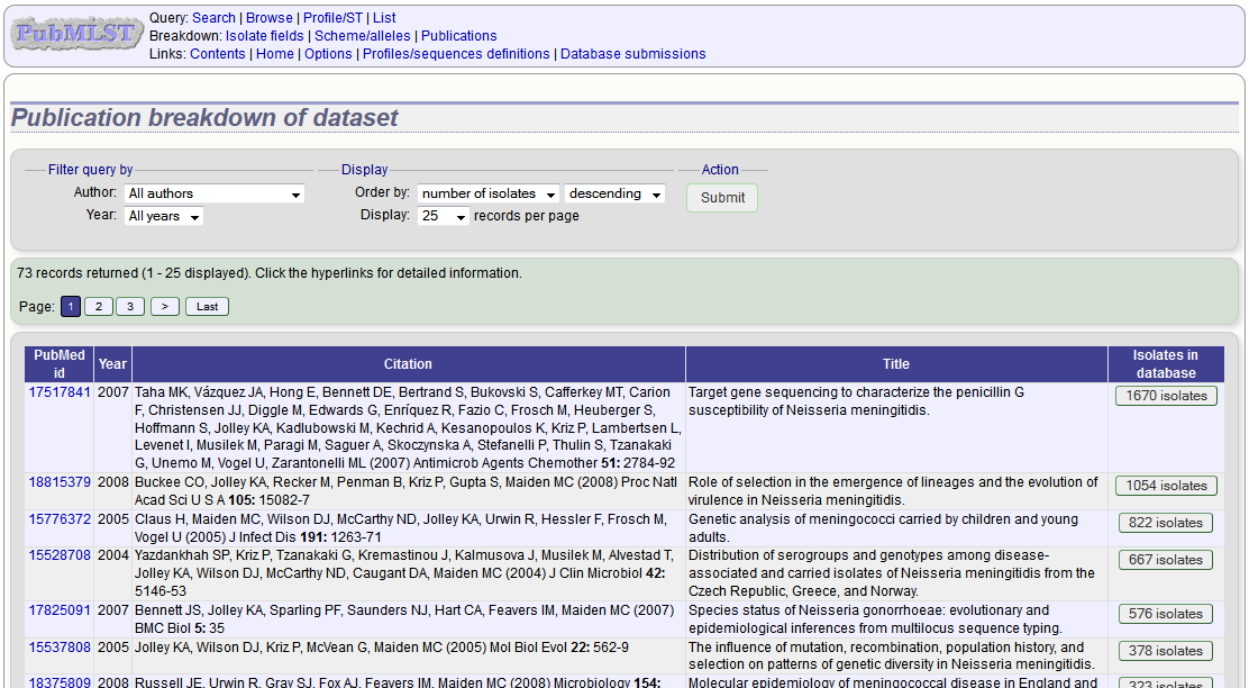


11.12 Retrieving isolates by linked publication

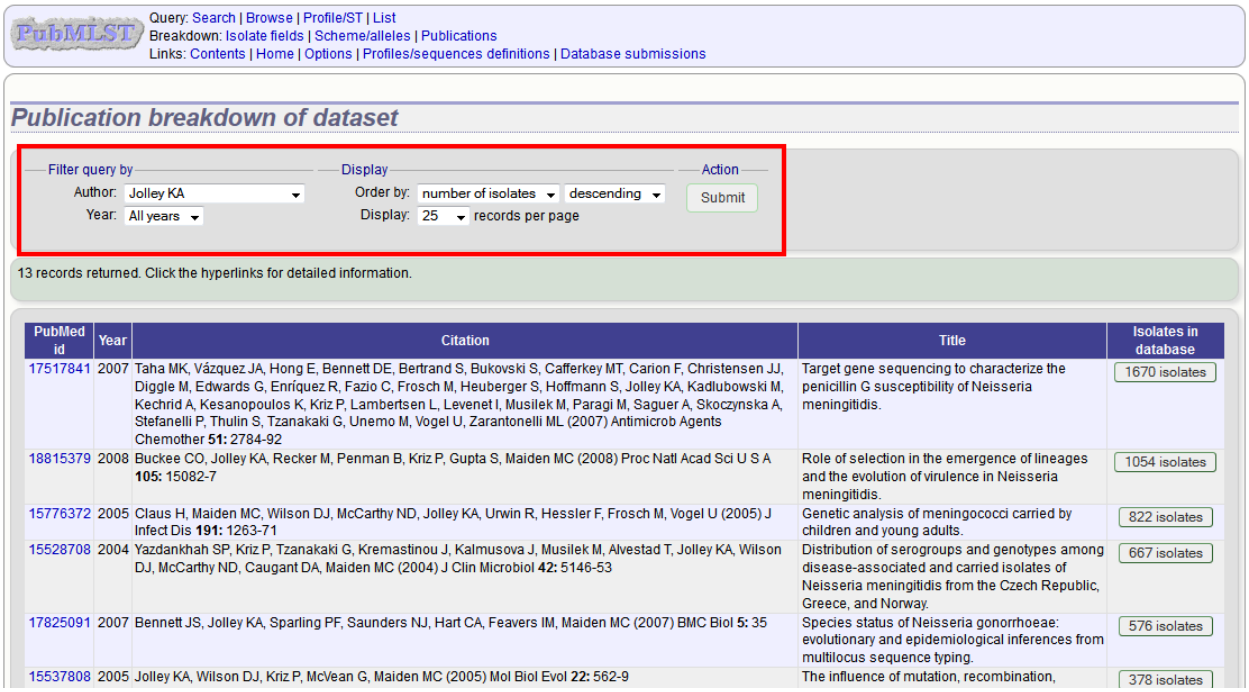
Click ‘Publications’ in the Breakdown section of the contents page.



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

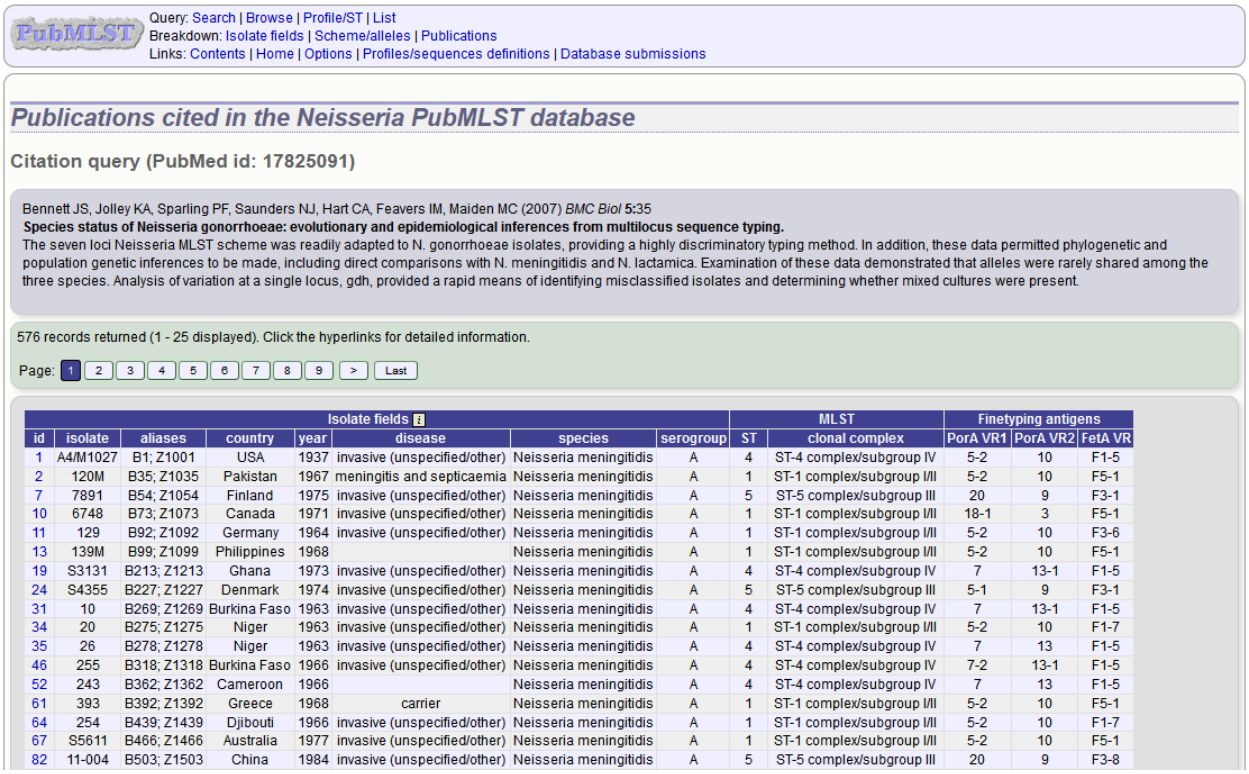


These can be filtered by author and/or year, and the sort order changed.



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

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



PubMLST

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

Publications cited in the Neisseria PubMLST database

Citation query (PubMed id: 17825091)

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.
The seven loci Neisseria MLST scheme was readily adapted to N. gonorrhoeae isolates, providing a highly discriminatory typing method. In addition, these data permitted phylogenetic and population genetic inferences to be made, including direct comparisons with N. meningitidis and N. lactamica. Examination of these data demonstrated that alleles were rarely shared among the three species. Analysis of variation at a single locus, gdh, provided a rapid means of identifying misclassified isolates and determining whether mixed cultures were present.

576 records returned (1 - 25 displayed). Click the hyperlinks for detailed information.

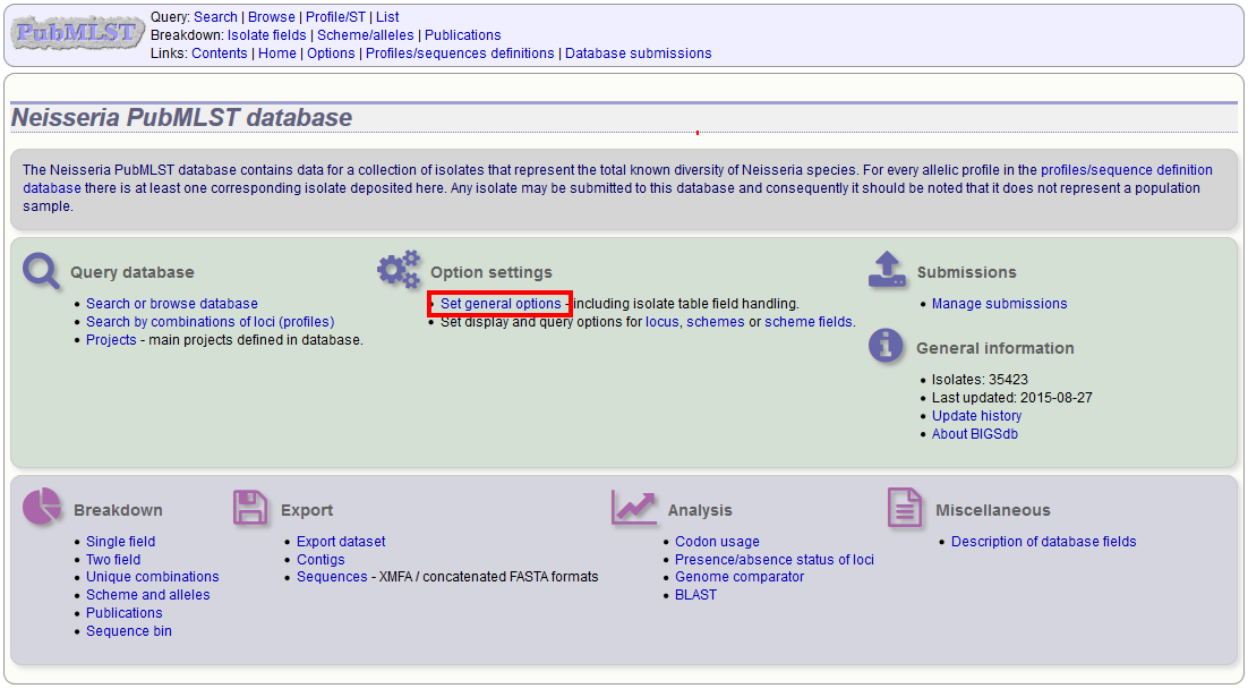
Page: 1 2 3 4 5 6 7 8 9 > Last

Isolate fields								MLST		Finetyping antigens		
id	isolate	aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1	PorA VR2	FetA VR
1	A4/M1027	B1; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	20	9	F3-1
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
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	5-1	9	F3-1
31	10	B269; Z1269	Burkina Faso	1963	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
34	20	B275; Z1275	Niger	1963	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F1-7
35	26	B278; Z1278	Niger	1963	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13	F1-5
46	255	B318; Z1318	Burkina Faso	1966	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7-2	13-1	F1-5
52	243	B362; Z1362	Cameroon	1966		Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13	F1-5
61	393	B392; Z1392	Greece	1968	carrier	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
64	254	B439; Z1439	Djibouti	1966	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F1-7
67	S5611	B466; Z1466	Australia	1977	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
82	11-004	B503; Z1503	China	1984	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	20	9	F3-8

11.13 User-configurable options

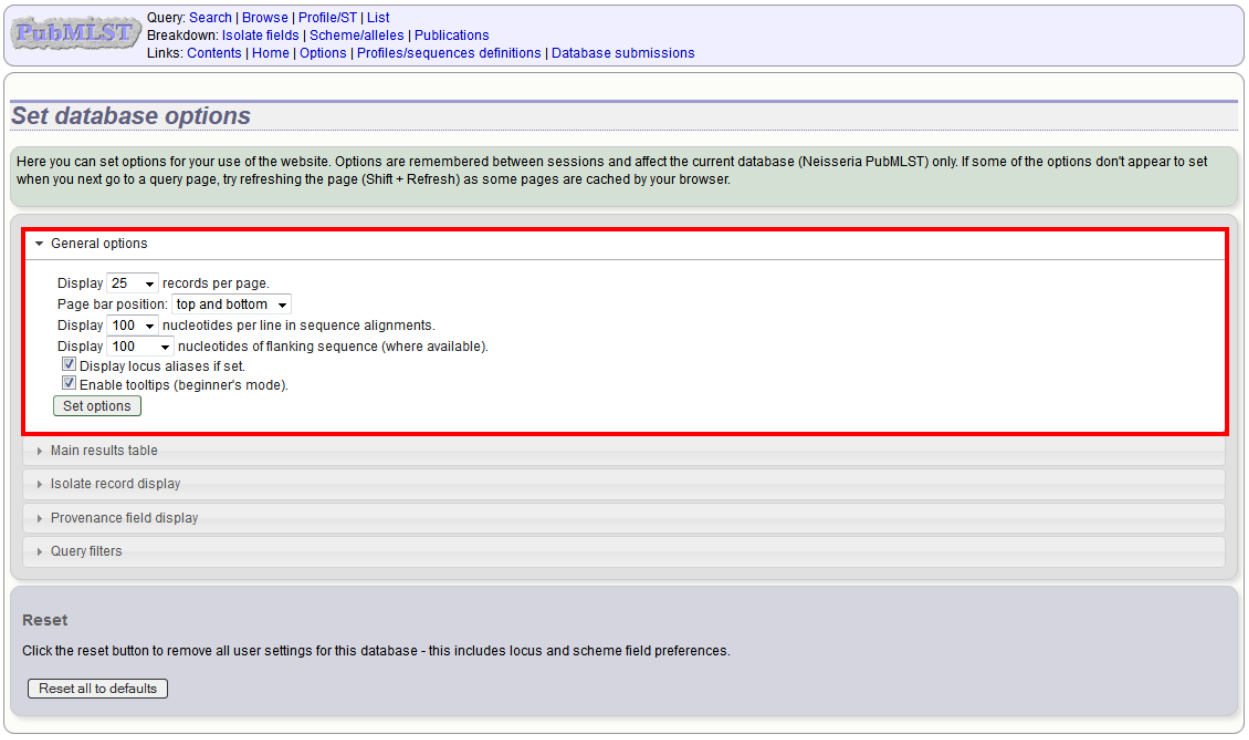
The BIGSdb user interface is configurable in a number of ways. Choices made are remembered between sessions. If the database requires you to log on, the options are associated with your user account, whereas if it is a public database, that you haven't logged in to, the options are associated with a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

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



11.13.1 General options

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



The general tab allows the following options to be modified:

- Records per page

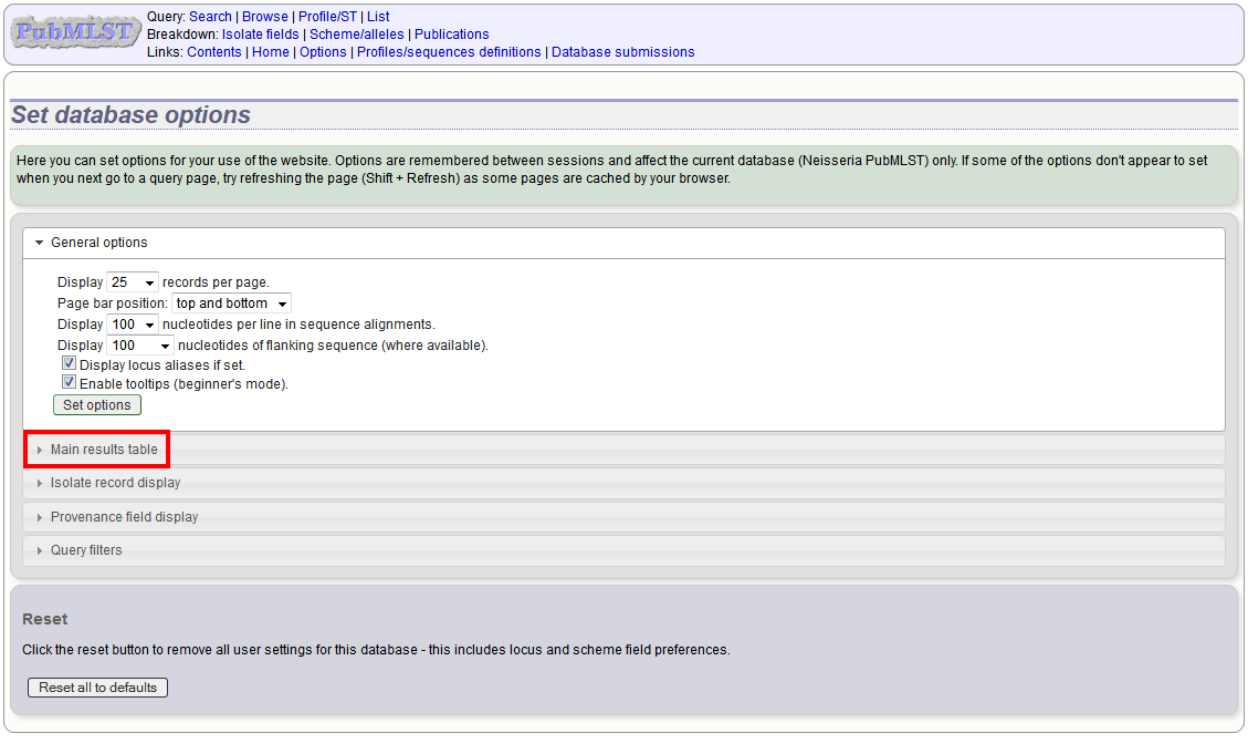
- Page bar position
- Nucleotides per line - Some analyses display sequence alignments. This option allows you to set the width of these alignments so suit your display.
- Flanking sequence length - This sets the length of flanking sequence upstream and downstream of a particular locus that is included whenever a sequence is displayed. Flanking sequences are displayed fainter that the locus sequence.
- Locus aliases - Loci can have multiple names (aliases). Setting this option will display all alternative names in results tables.
- Tooltips (beginner's mode) - Most query forms have help available in the form of information tooltips. These can be switched on/off here. They can also be toggled off by clicking the Toggle: 'i' button at the top-right of the display of some pages.

Click 'Set options' to remember any changes you make.

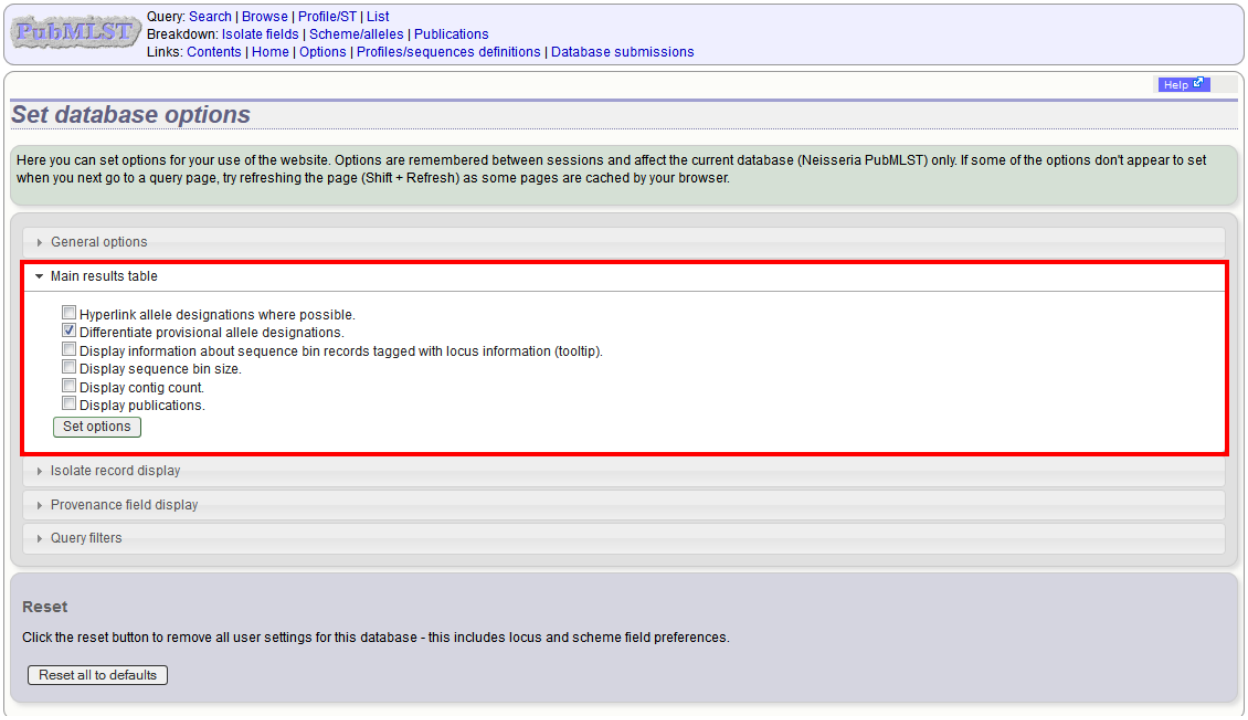
11.13.2 Main results table

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

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



The 'main results table' tab will scroll up.



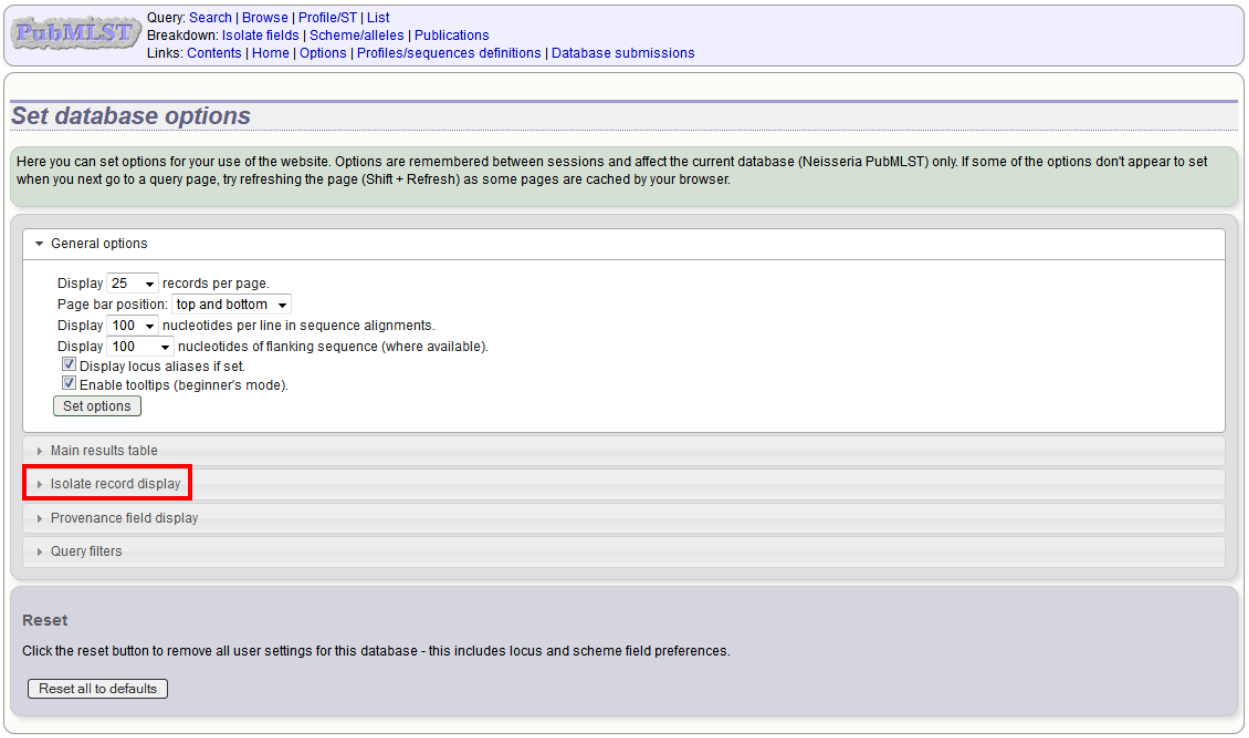
This tab allows the following options to be modified:

- Hyperlink allele designations - Hyperlinks point to an information page about the particular allele definition. Depending on the locus, these may exist on a different website.
- Differentiate provisional allele designations - Allele designations can be set as confirmed or provisional, usually depending on the method of assignment. Selecting this option will display provisional designations in a different colour to confirmed designations.
- Information about sequence bin records - Creates a tooltip that displays details about sequence tags corresponding to a locus.
- Sequence bin records - Displays a tooltip linking to the sequence tag if available.
- Sequence bin size - Displays the size of the sum of all contigs associated with each isolate record.
- Contig count - Displays the number of contigs associated with each isolate record.
- Publications - Displays citations with links to PubMed for each record.

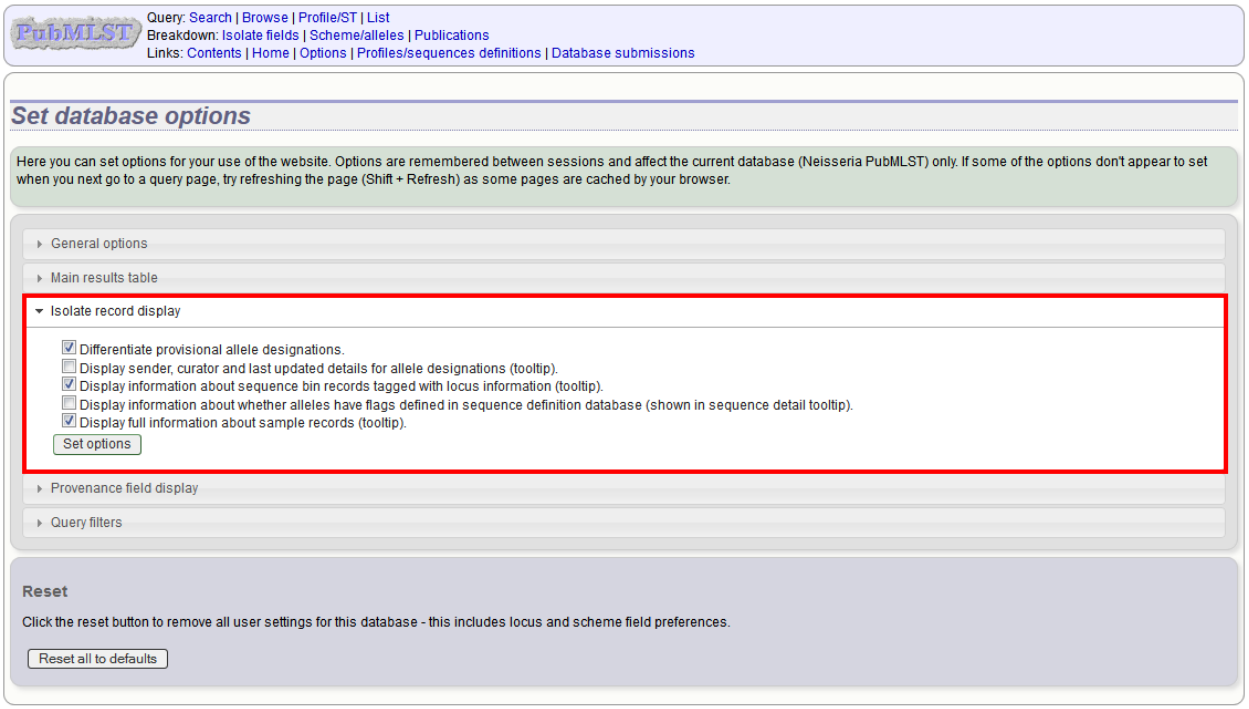
11.13.3 Isolate record display

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

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



The 'Isolate record display' tab will scroll up.



This tab allows the following options to be modified:

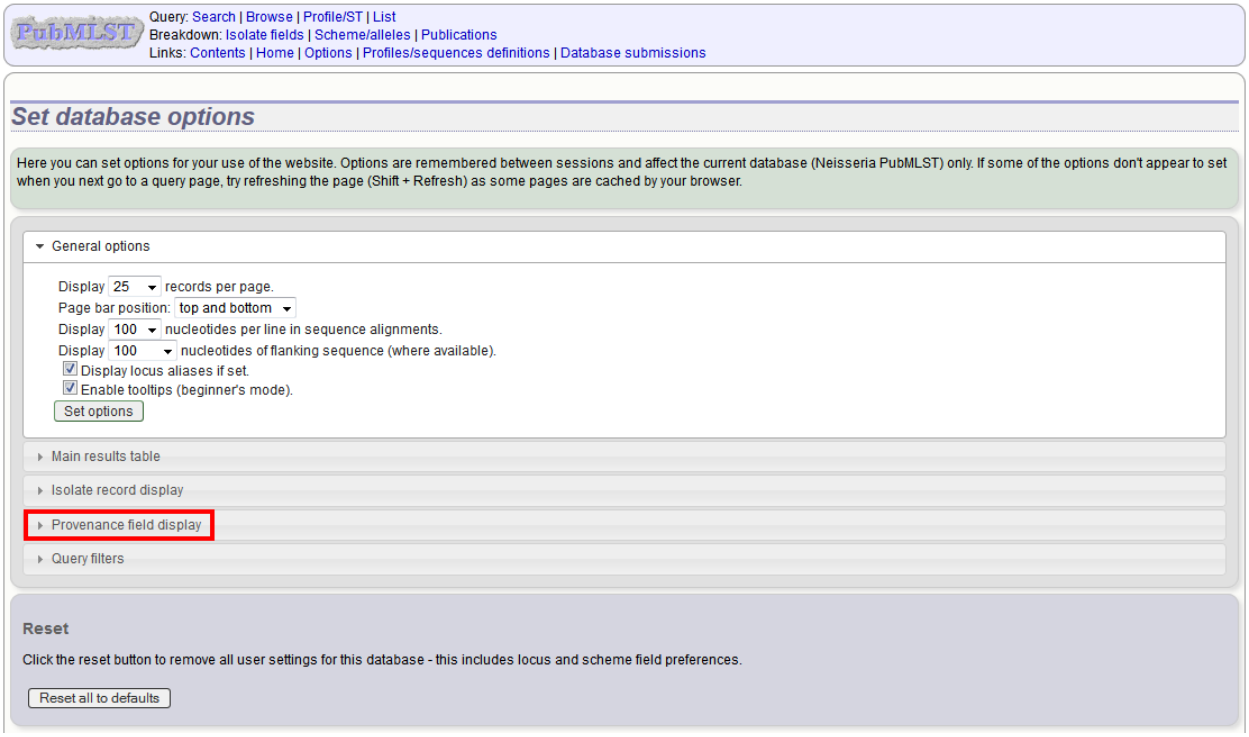
- Differentiate provisional allele designations - Allele designations can be set as confirmed or provisional, usually depending on the method of assignment. Selecting this option will display provisional designations in a different colour to confirmed designations.

- Display sender, curator and last updated records - Displays a tooltip containing sender information next to each allele designation.
- Sequence bin information - Displays a tooltip with information about the position of the sequence if tagged within the sequence bin.
- Allele flags - Displays information about whether alleles have flags defined in sequence definition databases.
- Display full information about sample records - Used when the database is used as part of a basic laboratory information management system (LIMS). This option will display records of samples available for the displayed isolate.

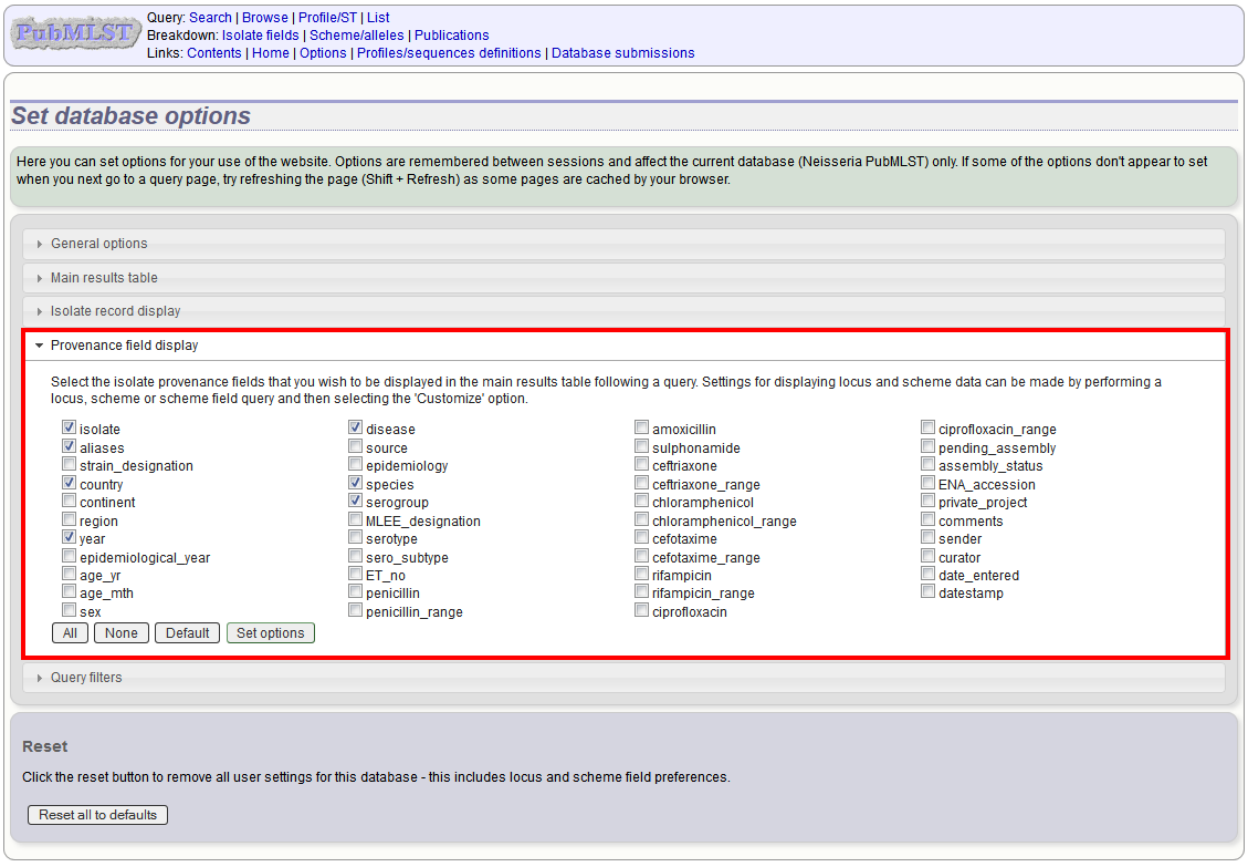
11.13.4 Provenance field display

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

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



The 'Provenance field display' tab will scroll up.



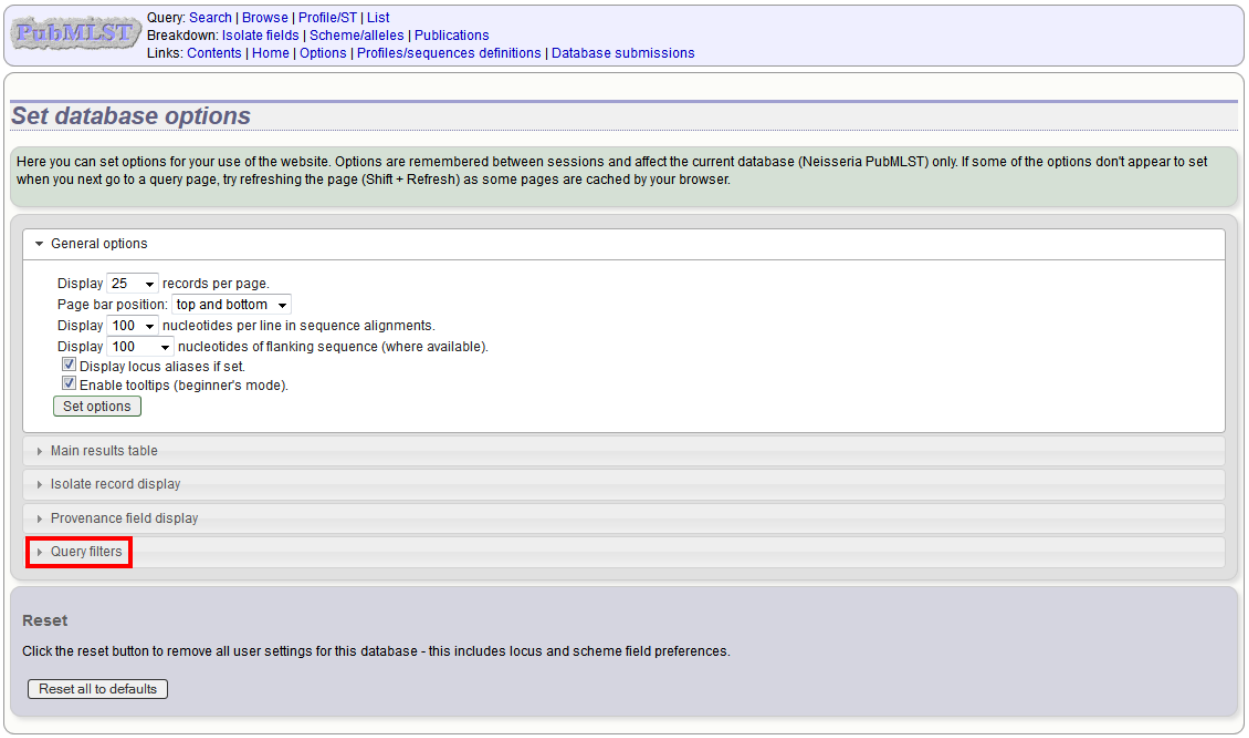
Some fields will be checked by default - these are defined during *database setup* (maindisplay option).

Check any fields that you wish to be displayed and then click 'Set options'. You can return to the default selection by clicking 'Default' followed by 'Set options'.

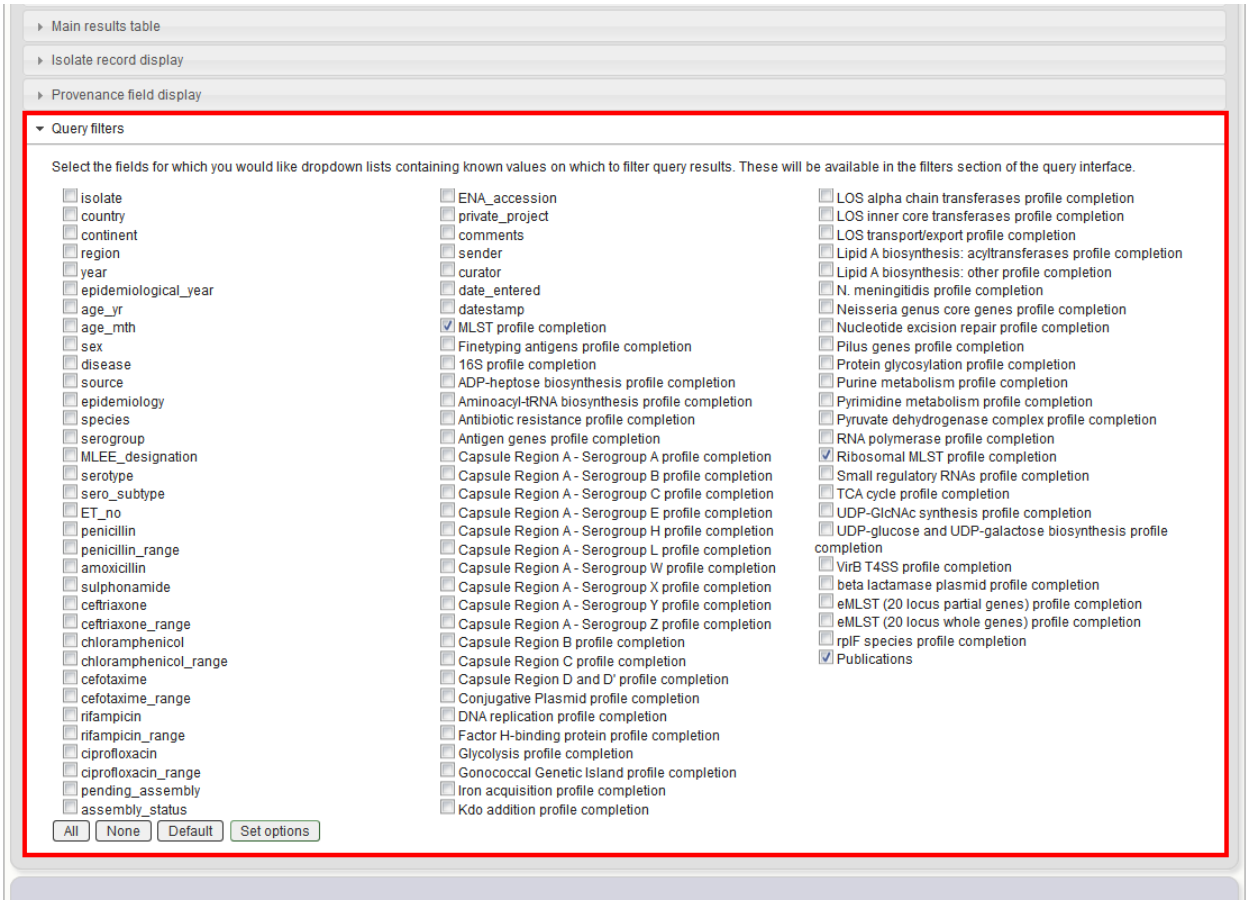
11.13.5 Query filters

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

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



The 'Query filters' tab will scroll up.



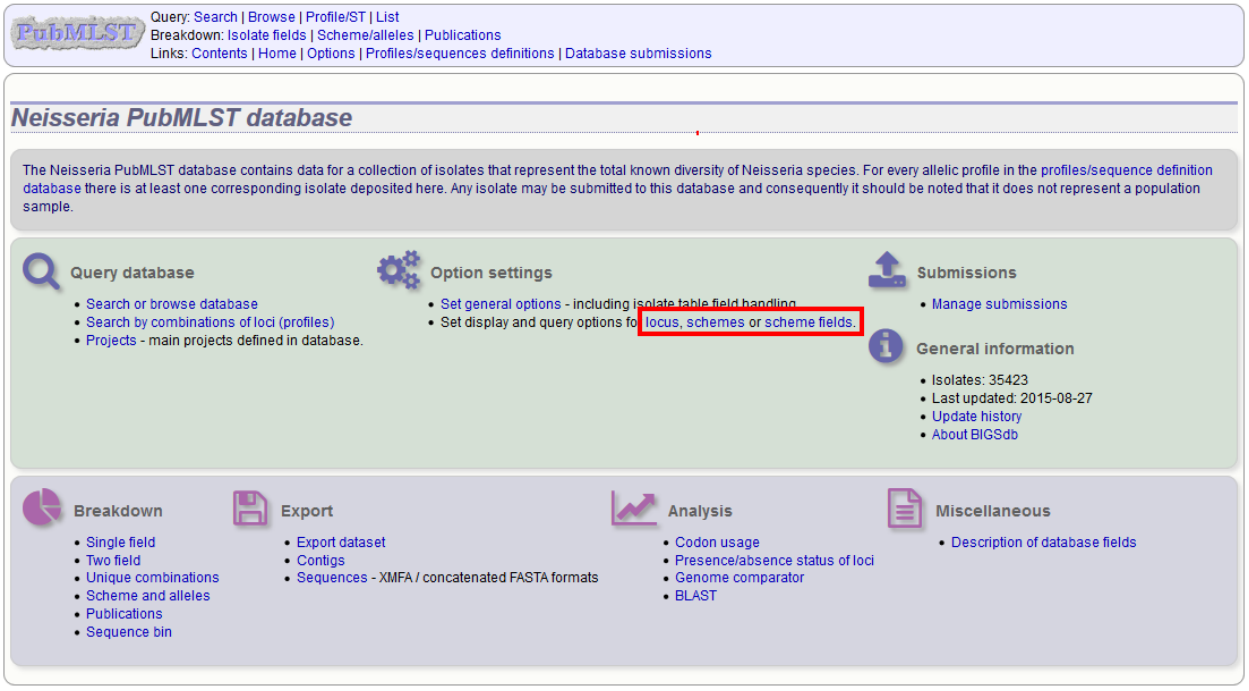
A list of possible filters appears. Click any checkbox for a filter you would like to make available. Click 'Set options' when done. You can return to the default selection by clicking 'Default' followed by 'Set options'.

11.13.6 Modifying locus and scheme display options

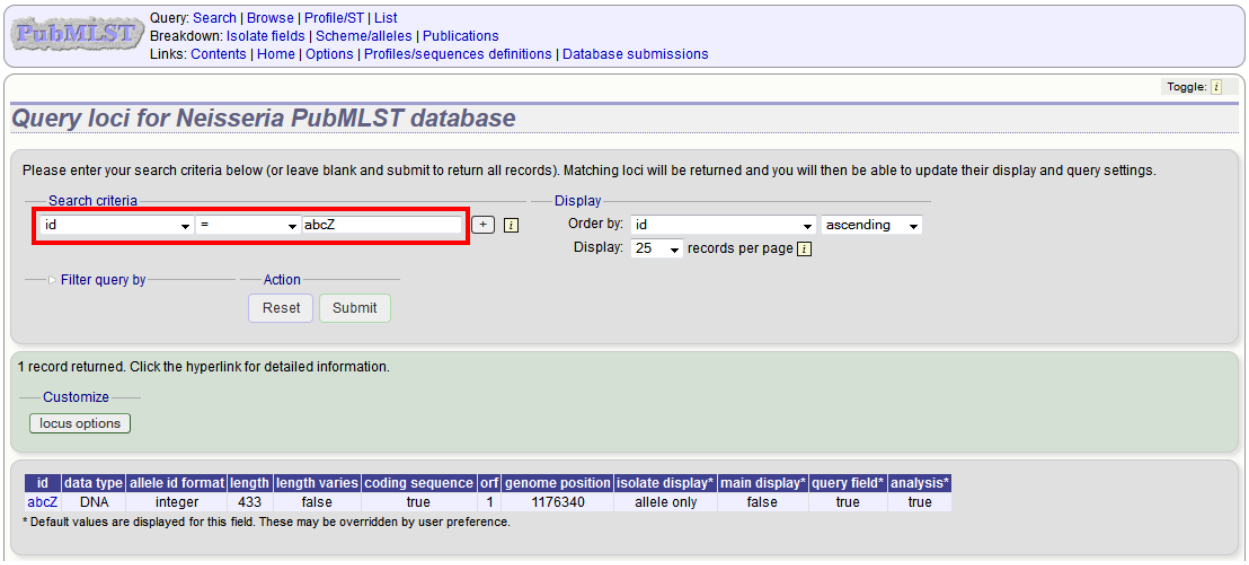
Whether or not loci, schemes or scheme fields are displayed in result tables, isolate records, or within query dropdown boxes can all be set with default options when first defined. These attributes can, however, be overridden by a user, and these selections will be remembered between sessions.

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

Click the appropriate link on the isolate contents page.

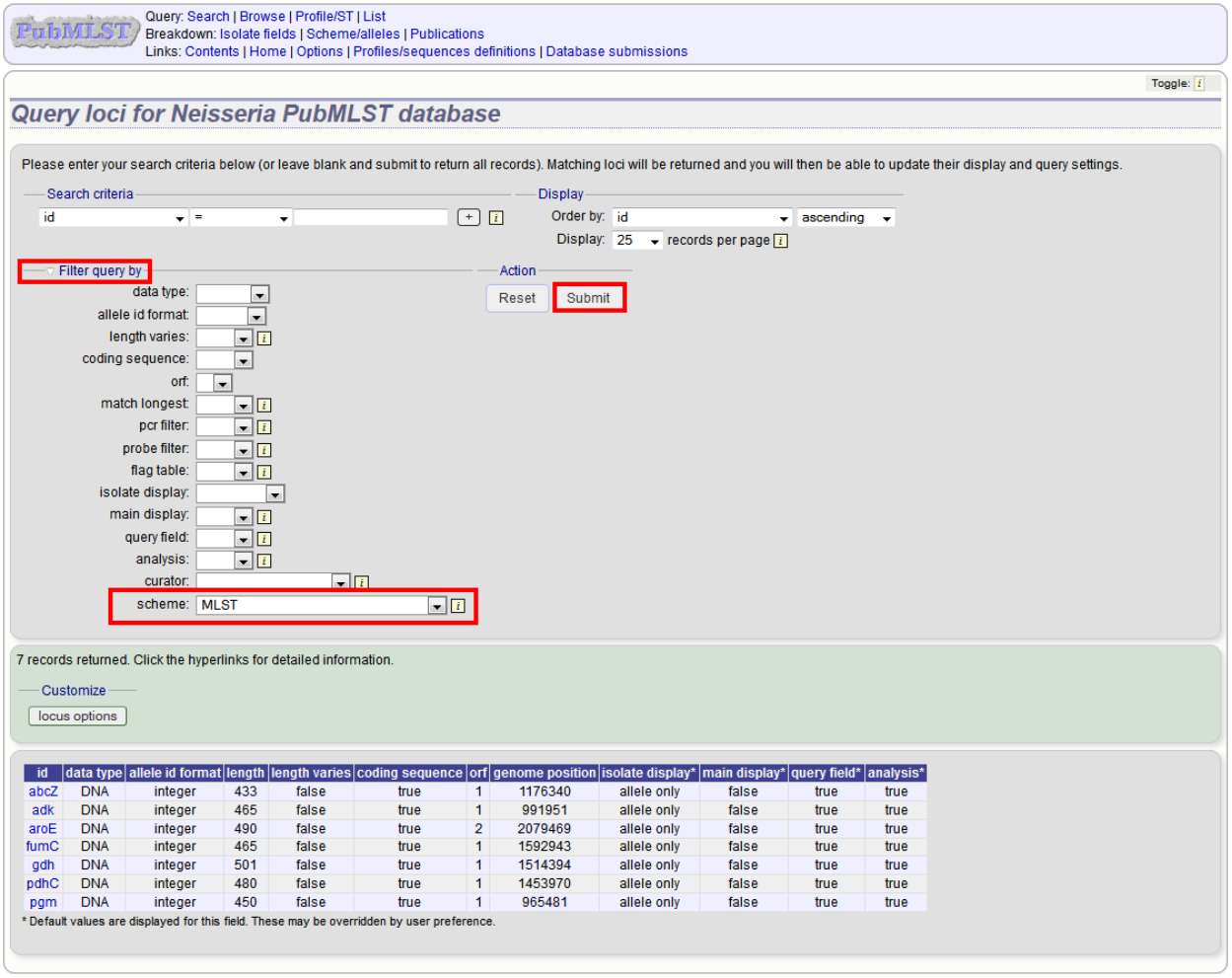


Either select the locus id by querying for it directly.

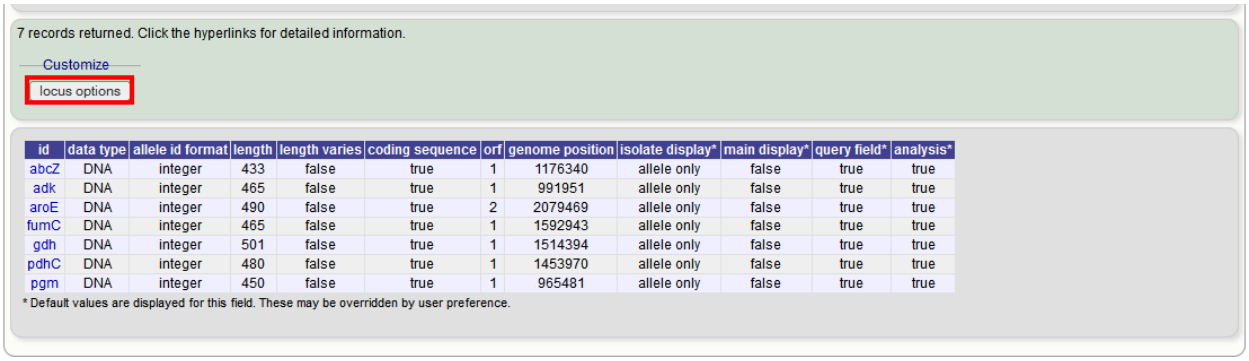


Designations can be queried using *standard operators*.

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



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



id	data type	allele id format	length	length varies	coding sequence	orf	genome position	isolate display*	main display*	query field*	analysis*
abcZ	DNA	integer	433	false	true	1	1176340	allele only	false	true	true
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

* Default values are displayed for this field. These may be overridden by user preference.

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

Possible options for loci are:

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

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

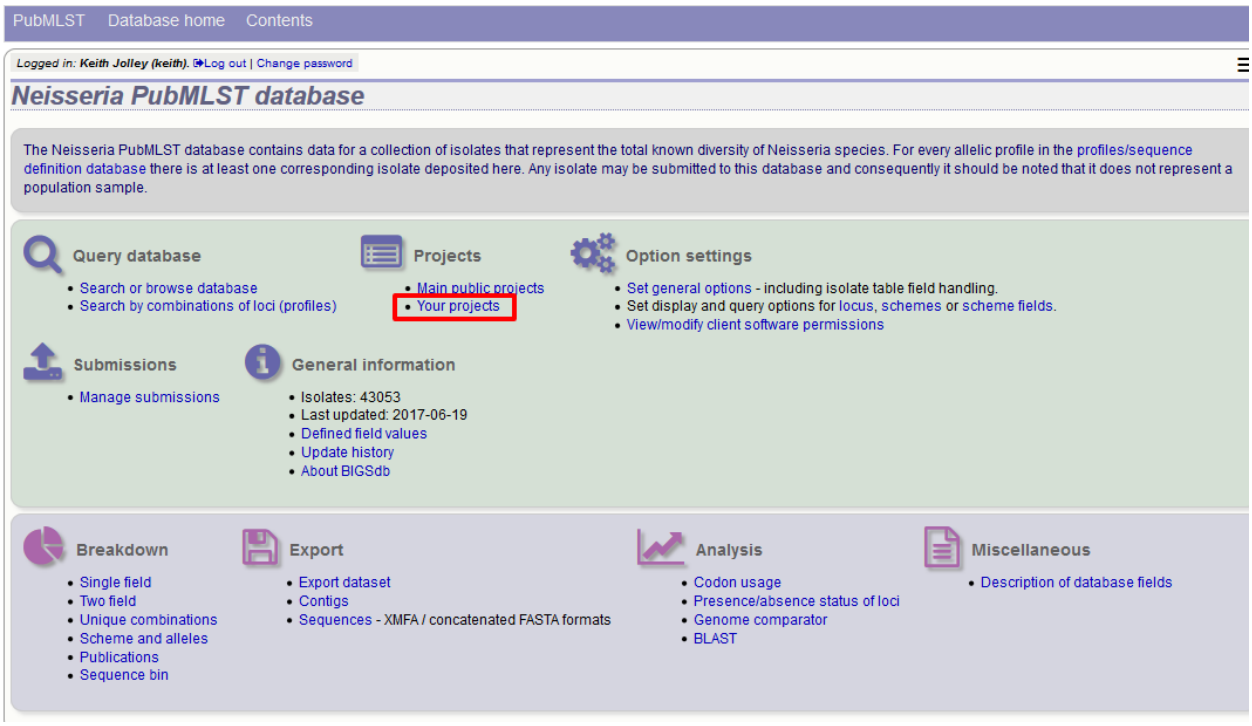
CHAPTER 12

User projects

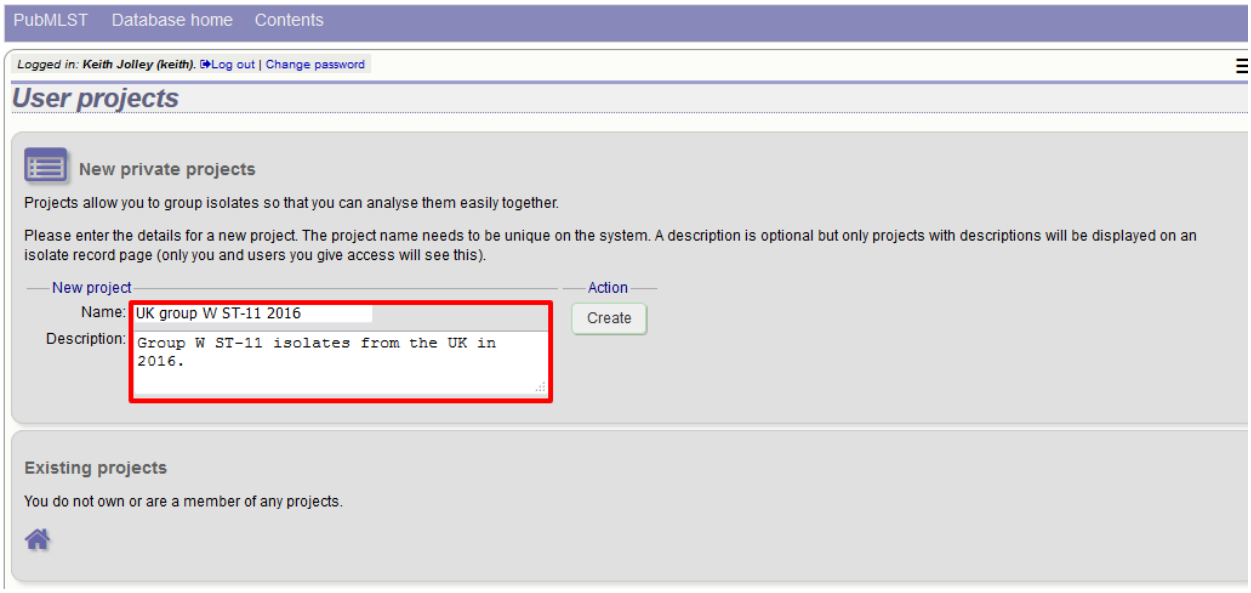
If user projects are enabled, authenticated users are able to set up their own projects in order to group isolates for analysis. If private data and user quotas are enabled, these projects can include private records that can then be shared with other user accounts.

Note: User projects can be enabled by an administrator by setting 'user_projects="yes"' in the *config.xml* file for the database.

To create a new project, go to the isolate database contents page and click 'Your projects'.



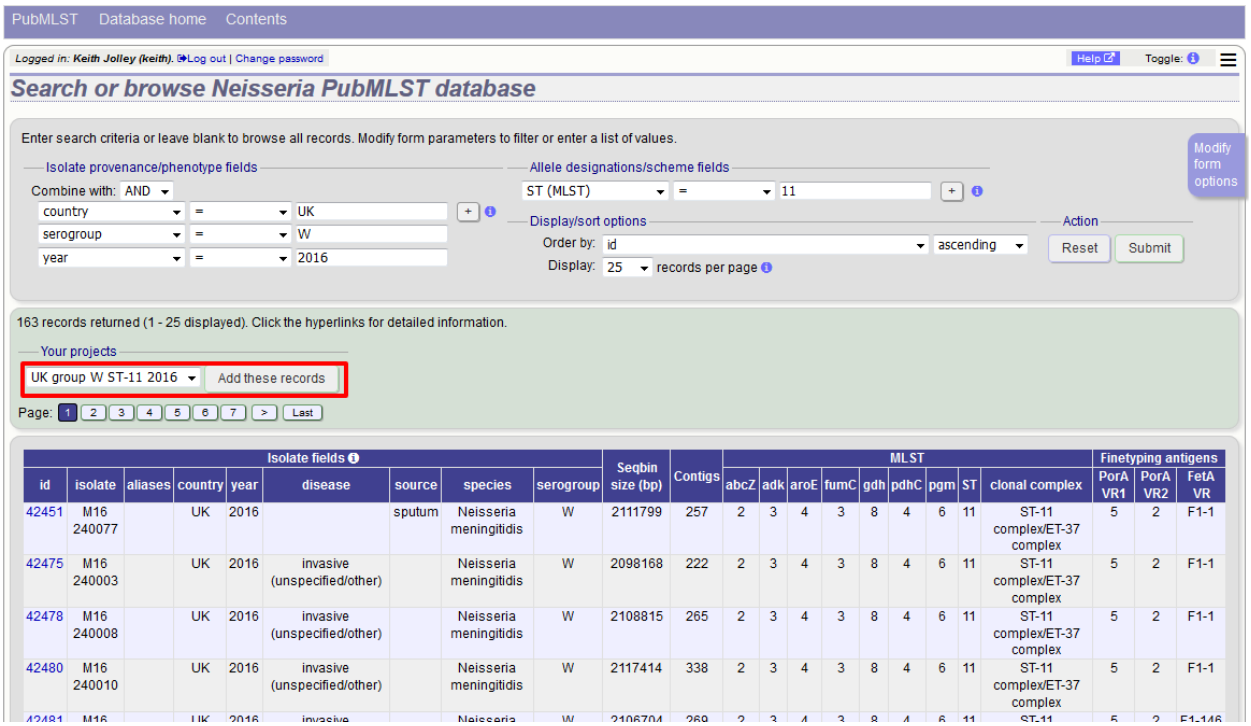
Enter the name of your project (this must be unique on the system - you will be told if the name is already used). You can optionally include a description - if you do this, this will appear within *isolate records* when accessed from your account. Click 'Create'.



You can either add isolates to your project directly following a query or by manually editing a list of ids.

12.1 Adding isolates to a user project following a query

Perform an isolate database query. If you have set up a project, there will be a link in the results header box. Select your project and click 'Add these records'.

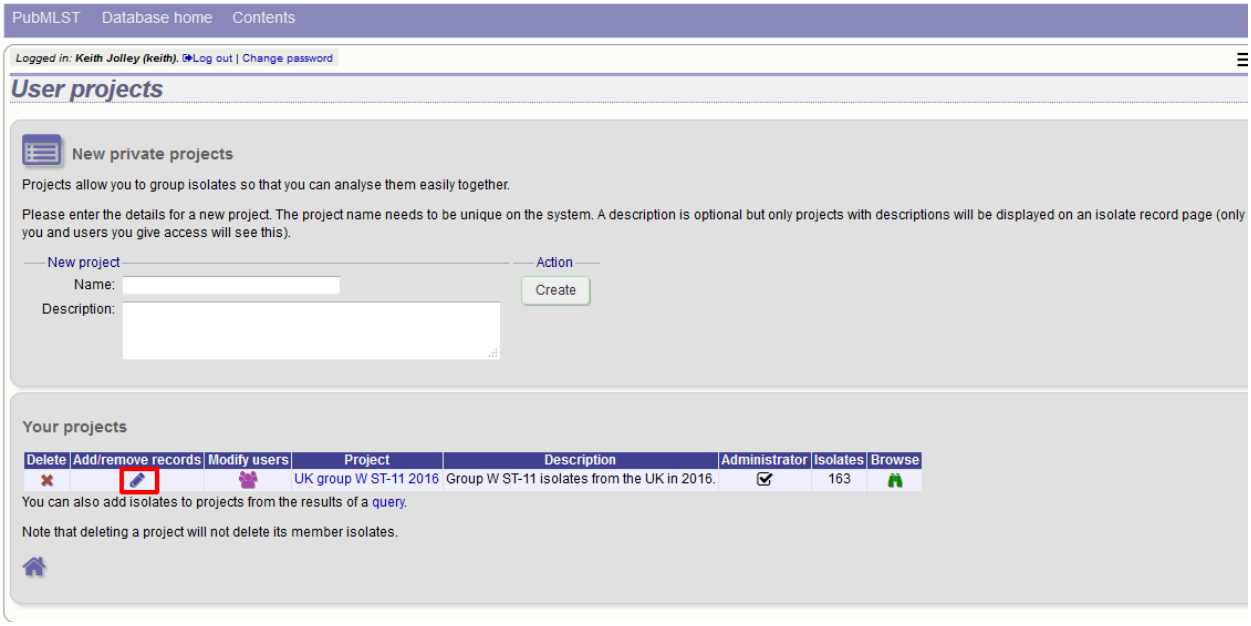


Isolate fields									Seqbin size (bp)	Contigs	MLST								Finetyping antigens		
id	isolate	aliases	country	year	disease	source	species	serogroup			abcZ	adk	aroE	fumC	gdh	pdhC	pgm	ST	clonal complex	PorA VR1	PorA VR2	FetA VR
42451	M16 240077		UK	2016		sputum	Neisseria meningitidis	W	2111799	257	2	3	4	3	8	4	6	11	ST-11 complex/ET-37 complex	5	2	F1-1
42475	M16 240003		UK	2016	invasive (unspecified/other)		Neisseria meningitidis	W	2098168	222	2	3	4	3	8	4	6	11	ST-11 complex/ET-37 complex	5	2	F1-1
42478	M16 240008		UK	2016	invasive (unspecified/other)		Neisseria meningitidis	W	2108815	265	2	3	4	3	8	4	6	11	ST-11 complex/ET-37 complex	5	2	F1-1
42480	M16 240010		UK	2016	invasive (unspecified/other)		Neisseria meningitidis	W	2117414	338	2	3	4	3	8	4	6	11	ST-11 complex/ET-37 complex	5	2	F1-1
42481	M16		UK	2016	invasive		Neisseria	W	2106704	269	2	3	4	3	8	4	6	11	ST-11	5	2	F1-146

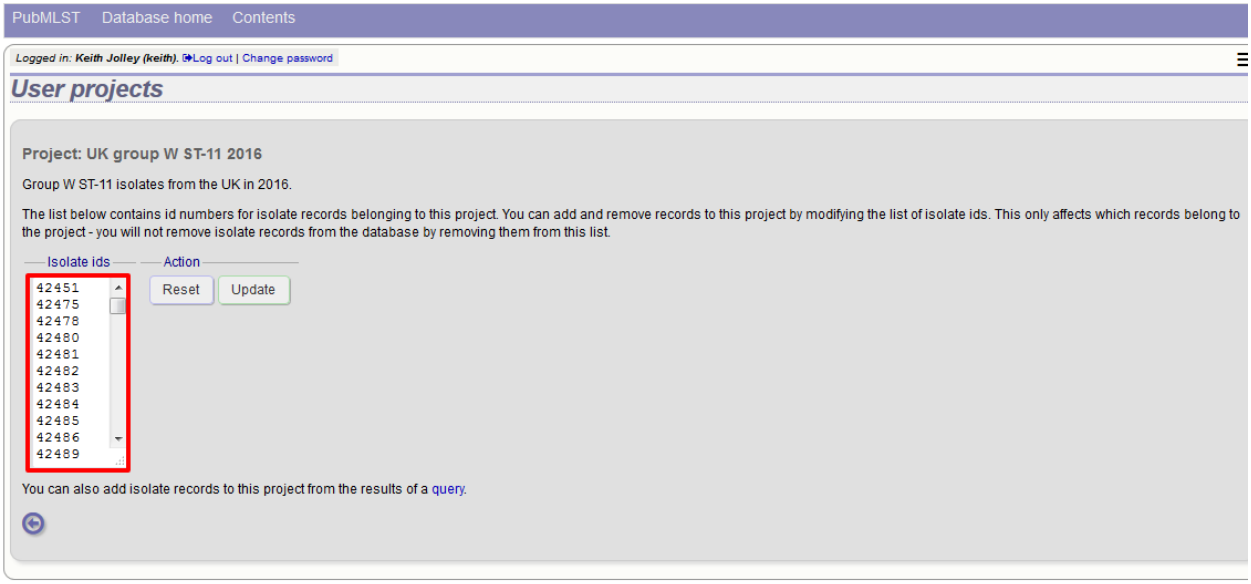
The records will be added to the project. Please note that it doesn't matter whether any of the records have been previously added.

12.2 Adding or removing isolates belonging to a user project by editing a list

From the user projects page, click the 'Add/remove records' link for the project that you wish to modify.

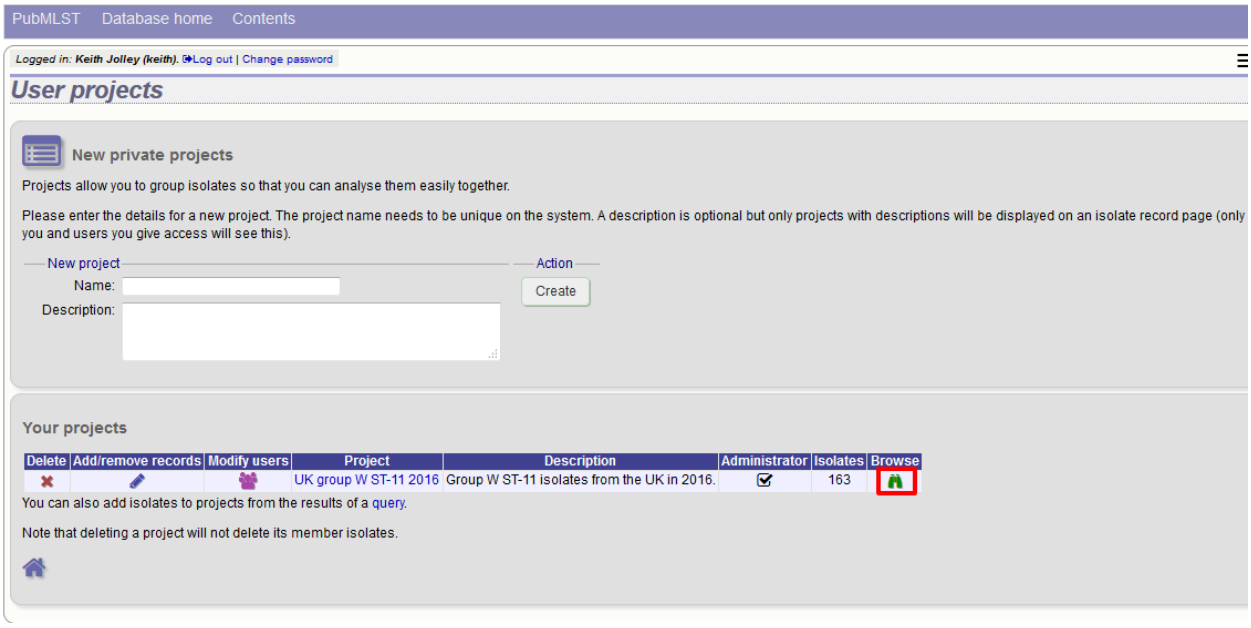


Edit the list of ids of records belonging to the list. You can copy and paste this list if you wish to prepare it in a spreadsheet or text editor. Click 'Update' when finished.

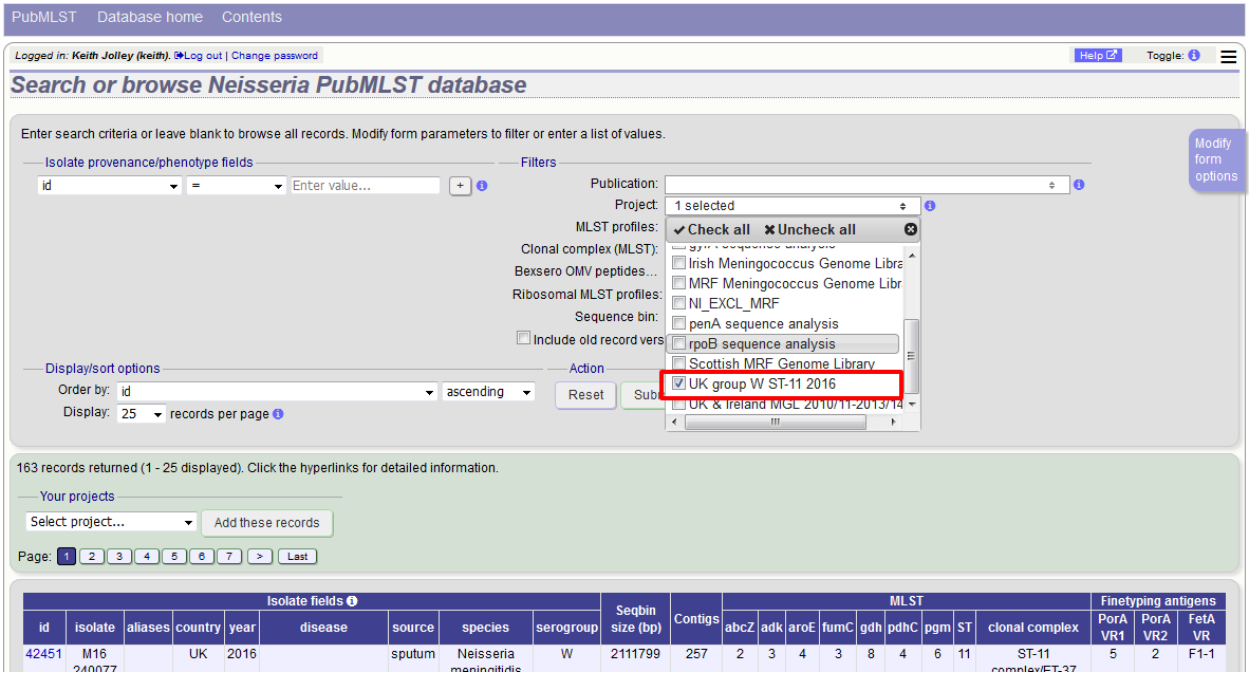


12.3 Accessing project isolates

To browse isolate records belonging to a project, go to the user projects page and click the 'Browse' link for the project.



Alternatively, you can select the project from the *projects filter* on the isolate query page. This would enable you to combine the project with additional search criteria

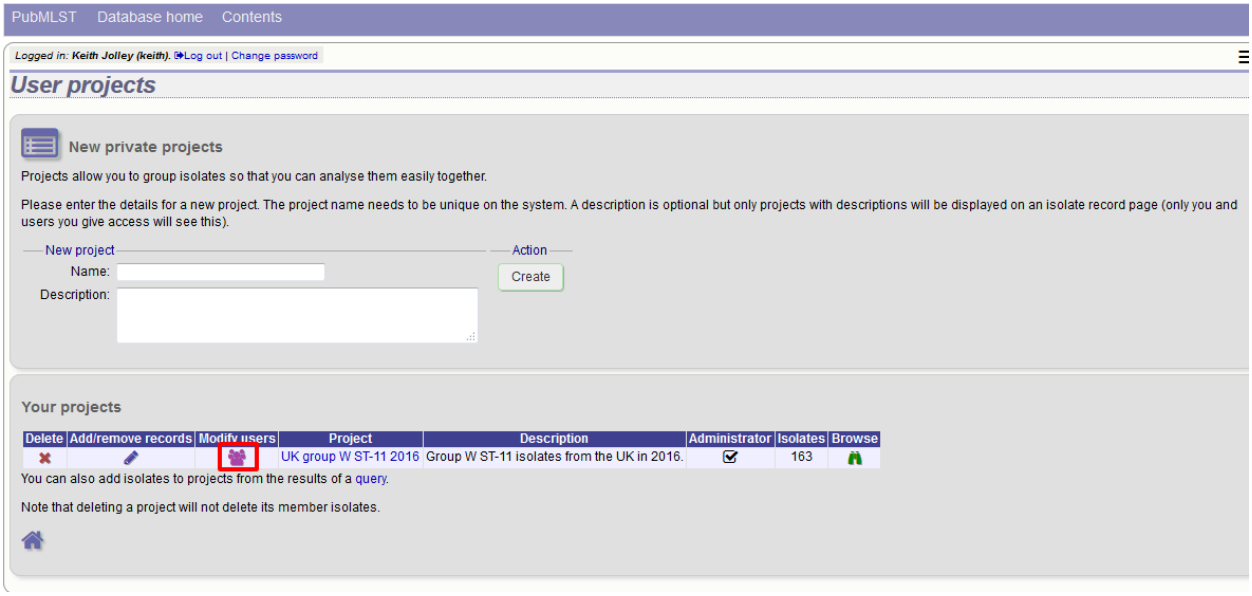


Please note that you will only see your project in the filter list if you are logged in. As a private project, only you will see it.

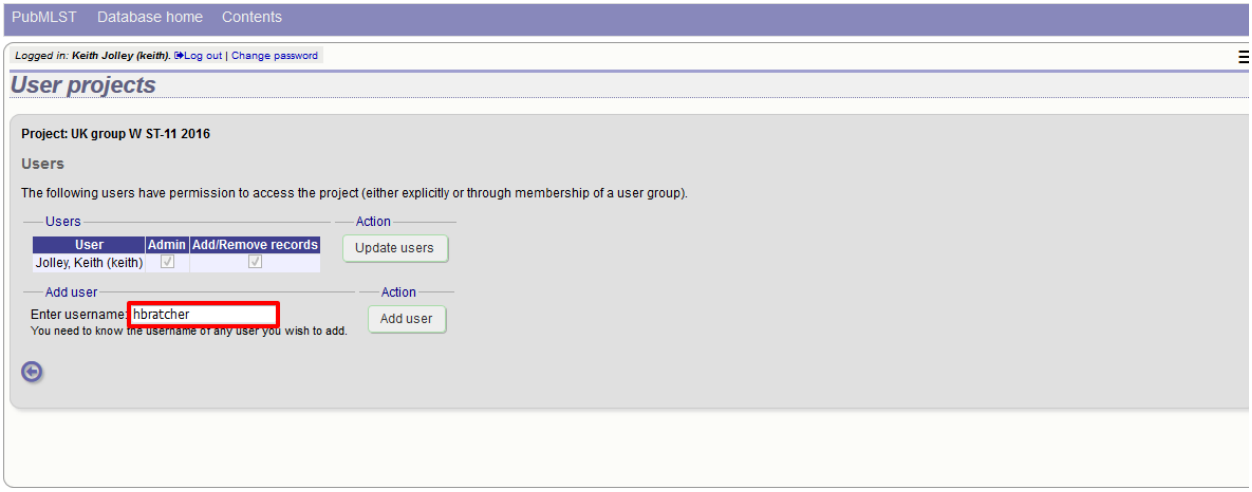
12.4 Allowing other users to share your project

You can share a project that you own with any other user. In order to do this, you must know the username that they use to log in with. They will see the project in their own list of private projects and in the query interface projects filter.

From the user projects page, click the 'Modify users' link for the specified project:

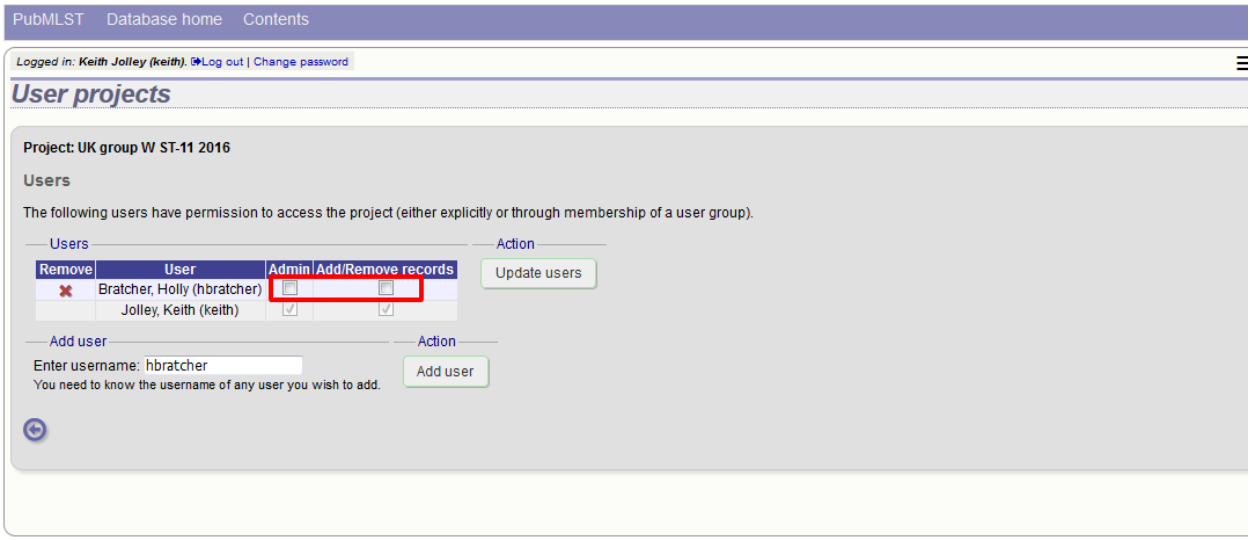


Enter the username of the person you wish to share with and click 'Add user':



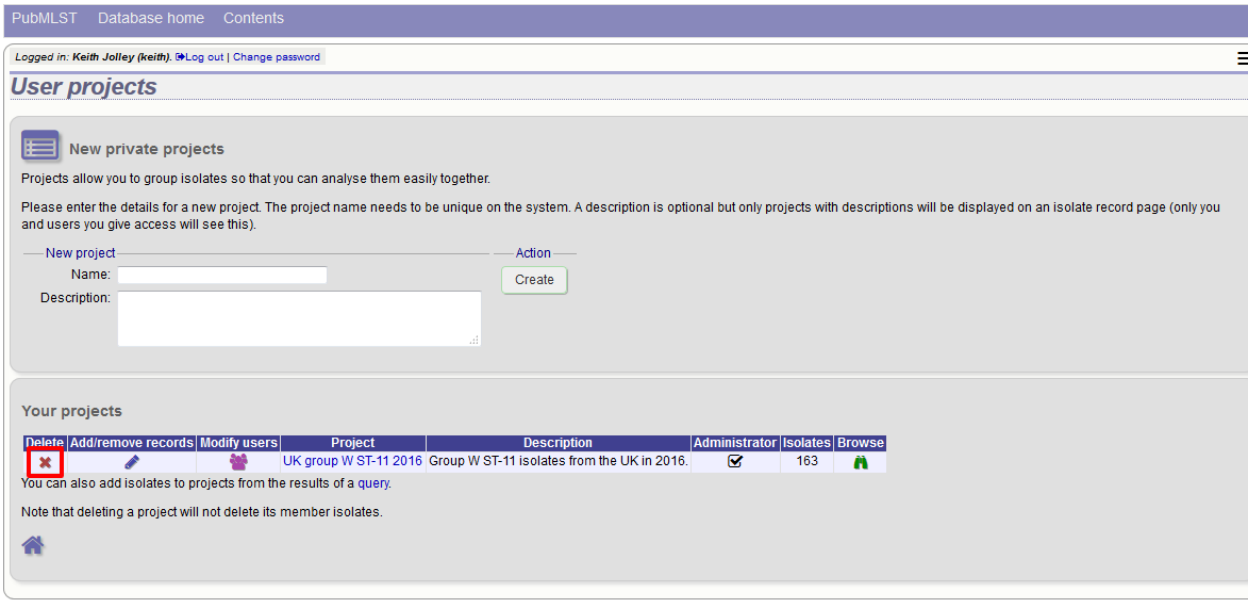
If user groups are in use, you can also share your project with all members of a user group (provided you are also a member of this group) from the same page.

Once a user has been added, you can give them permission to administer (add other users, modify the description or delete) or add/remove records to the project:

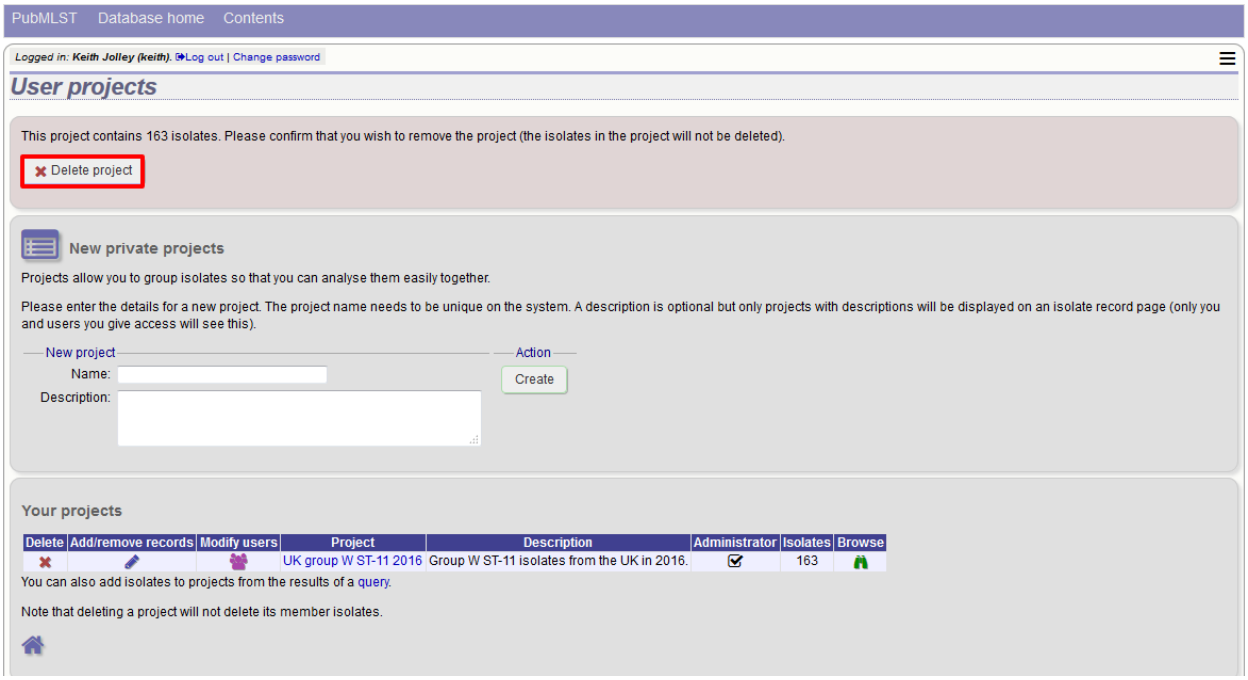


12.5 Deleting a user project

You can delete a project from the user projects page by clicking the 'Delete' link next to the project in question.



If the project contains any isolates you will be asked for confirmation. Click the 'Delete project' button.



If the project contains no isolates, the confirmation page is skipped and the project is removed immediately.

Note: Removing a project does not delete the isolate records belonging to it. A project is simply a means of grouping records.

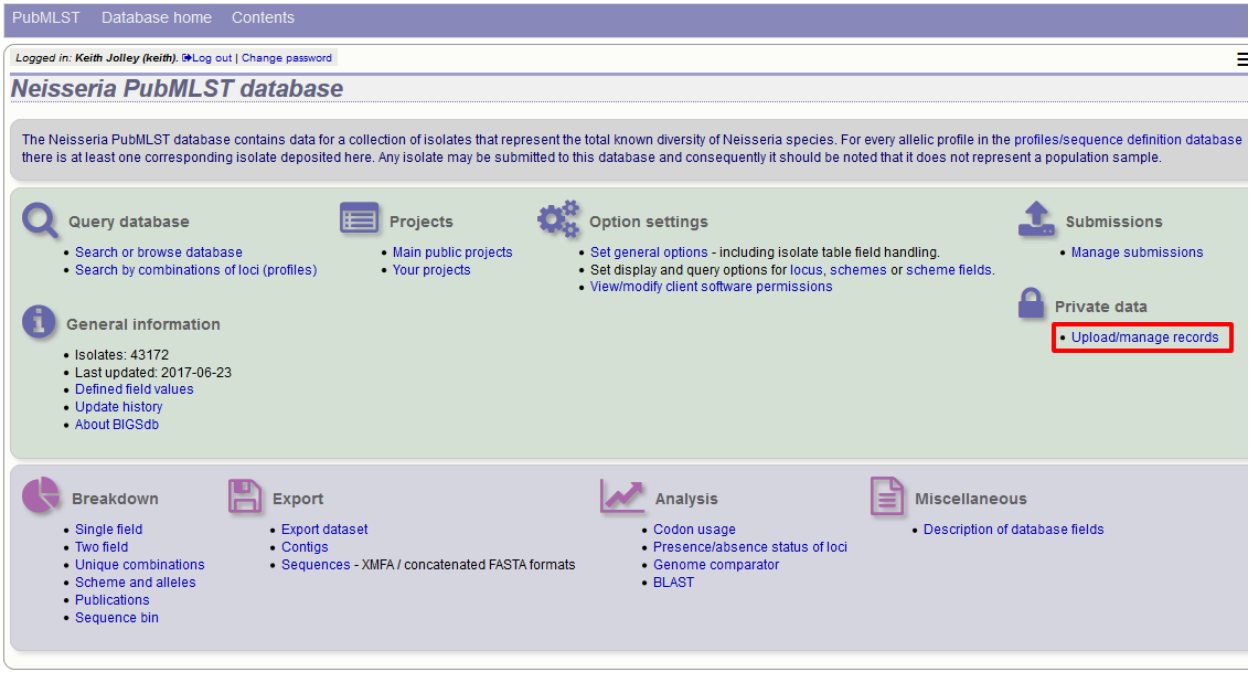
CHAPTER 13

Private records

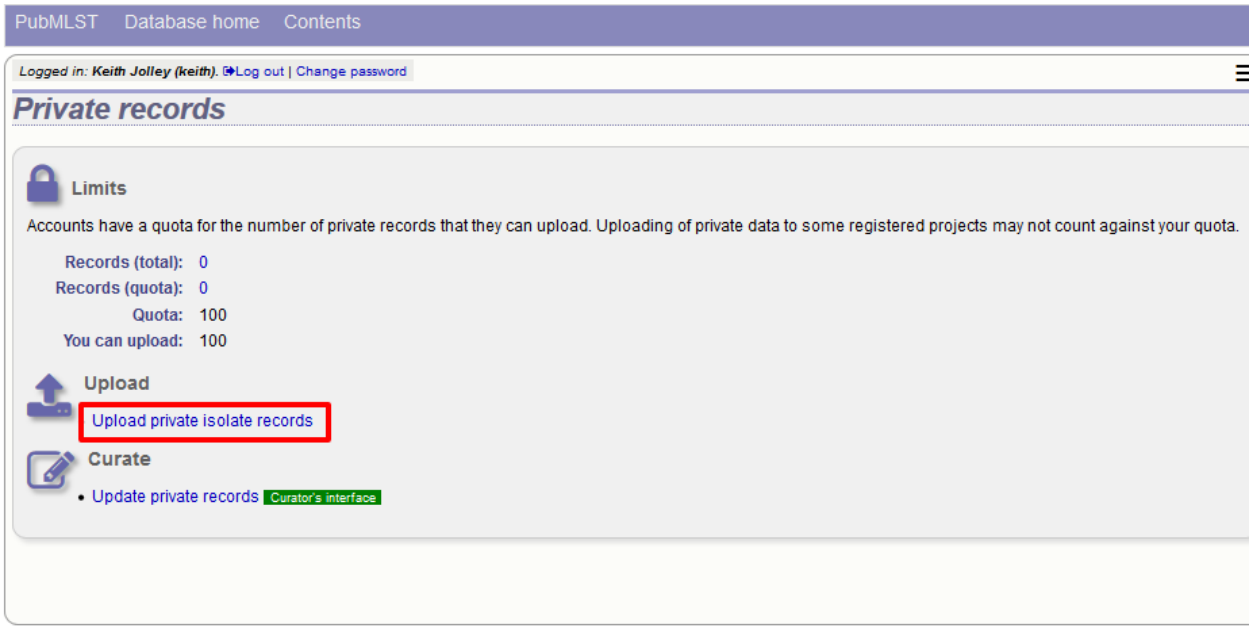
Users with a status of ‘submitter’, ‘curator’, or ‘admin’ can upload private isolate records that will be hidden from public view. A quota needs to be set for the user by an admin before they are able to do this.

13.1 Uploading private records

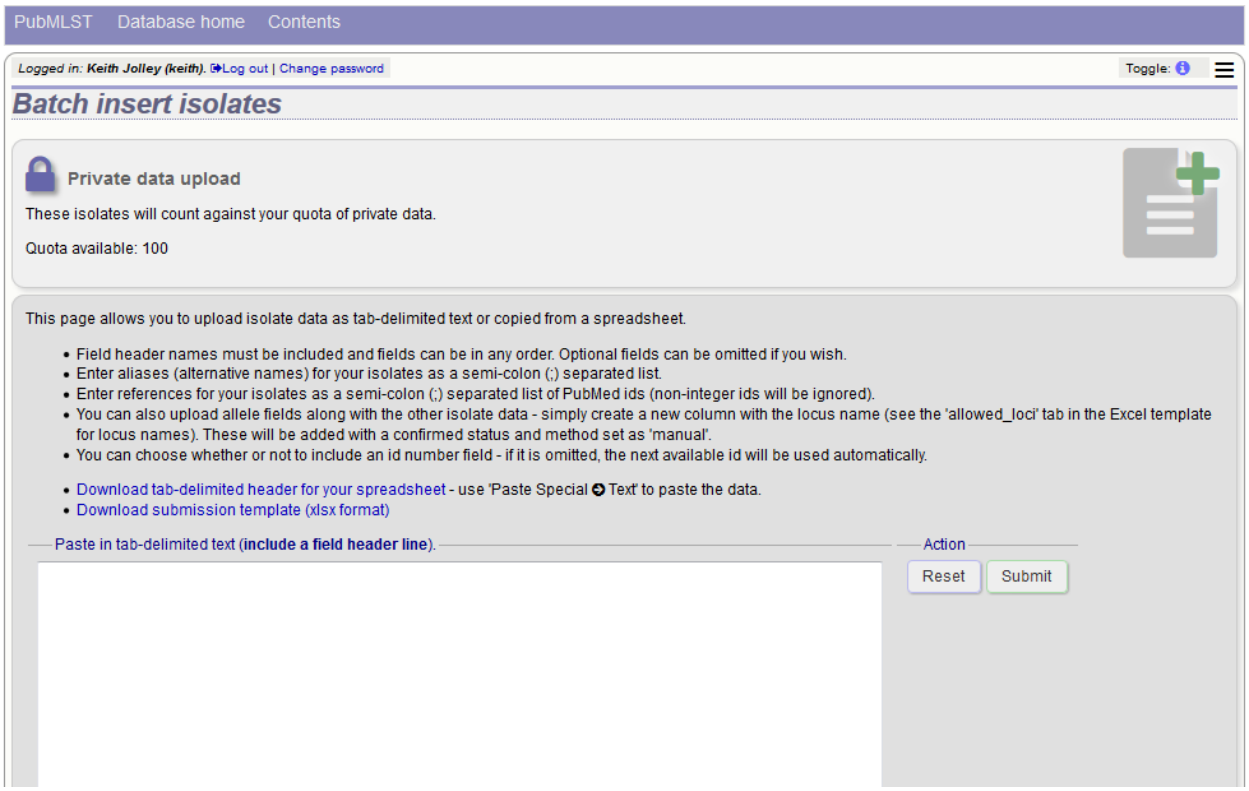
In order to upload private records, you need to make sure that you are logged in. If your account has a quota, there will be a menu item called ‘Private data’. Click the ‘Upload/manage records’ link.



You will see an overview of your quota and links to upload and edit your records. Click the 'Upload private isolate records' link (assuming you have quota available).



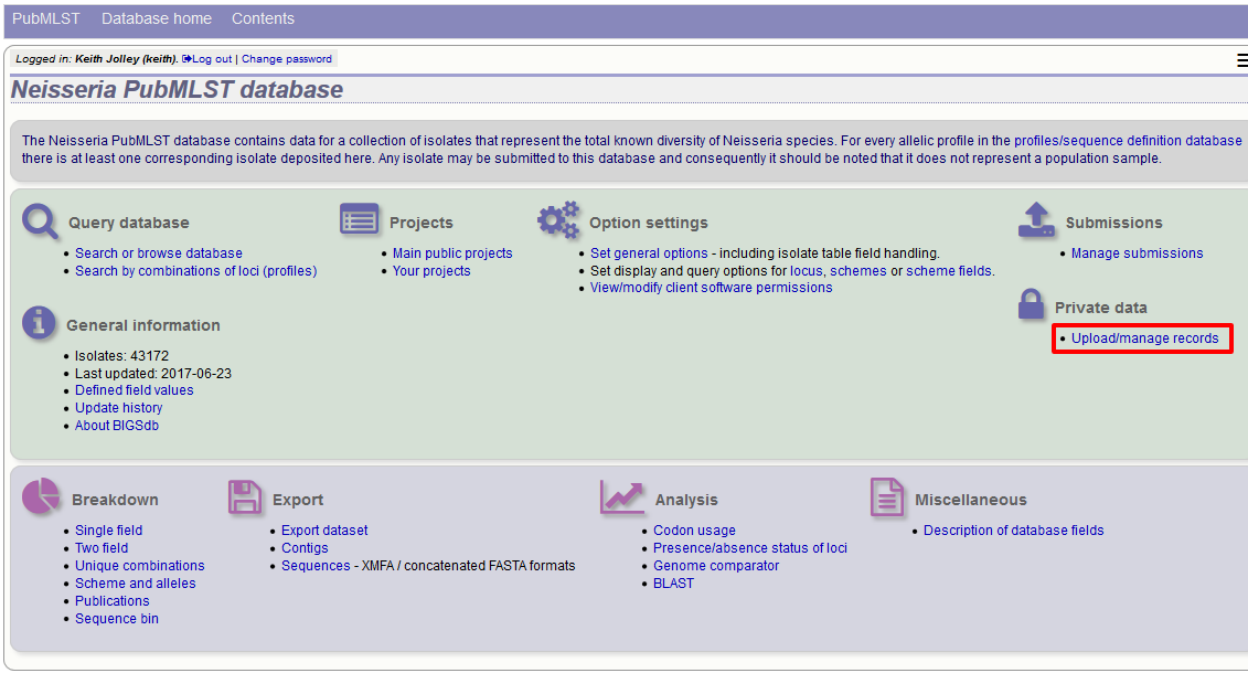
You will then be taken to a curator page that allows you to upload data copy and pasted from a spreadsheet. There is a link to an Excel template that you will need to use to prepare your data - this is the same template used if you were to submit your data to a curator.



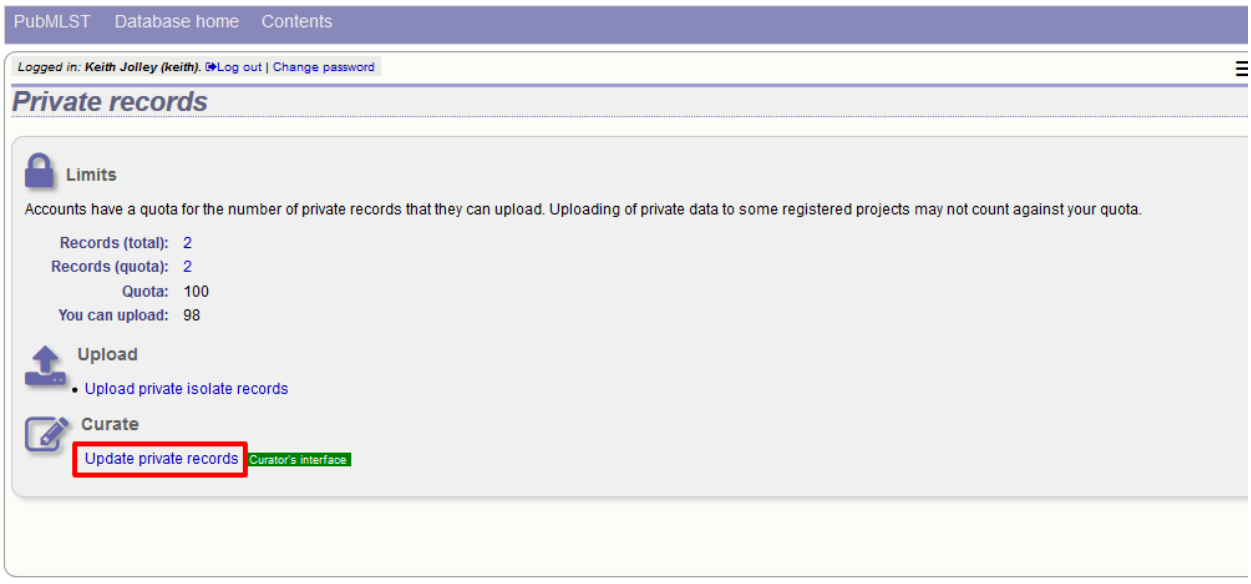
See *batch adding isolate records* for details of the upload process.

13.2 Modifying private records

Click the 'Upload/manage records' link on the contents page.



Now click the 'Update private records' link. You will be taken to the *curators' interface*, where you will be able to use the standard curator tools.



Use the *curators' interface* to make any changes to your isolate records, including *uploading genome data*.

13.3 Sharing access to private records

If *user projects* are enabled on the database, you can share access to your private isolates by adding them in to a user project and then sharing this.

See *user projects* for more details.

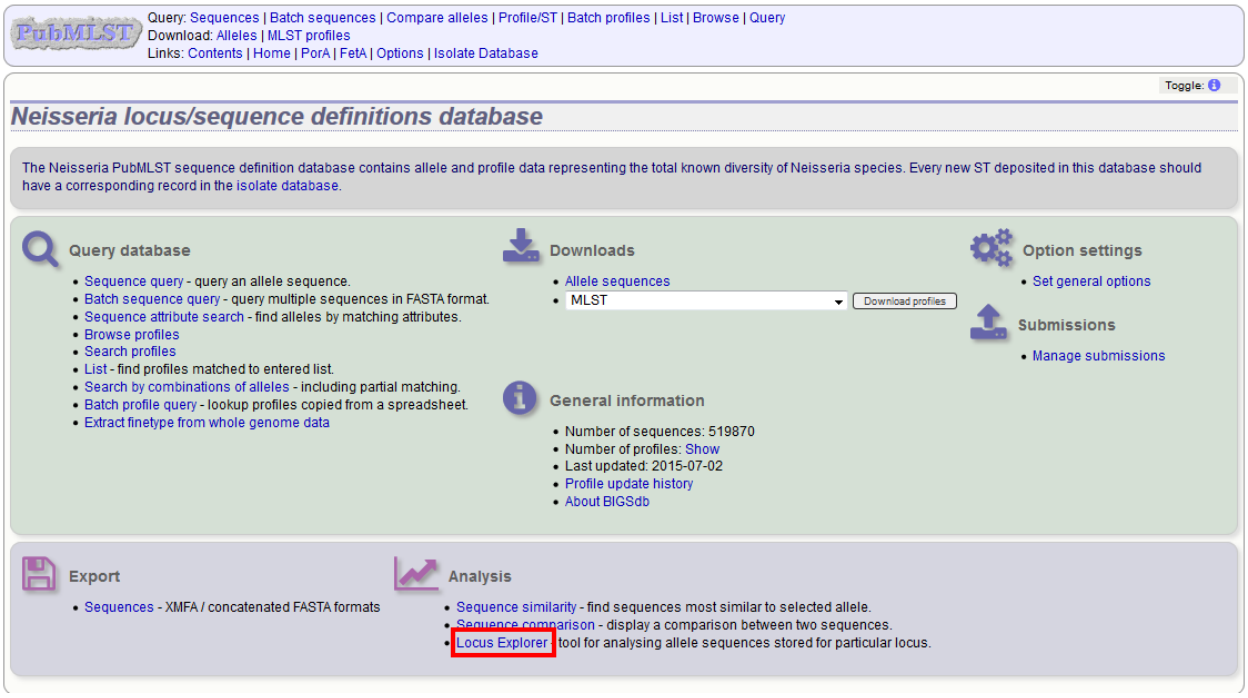
CHAPTER 14

Data analysis plugins

14.1 Locus explorer

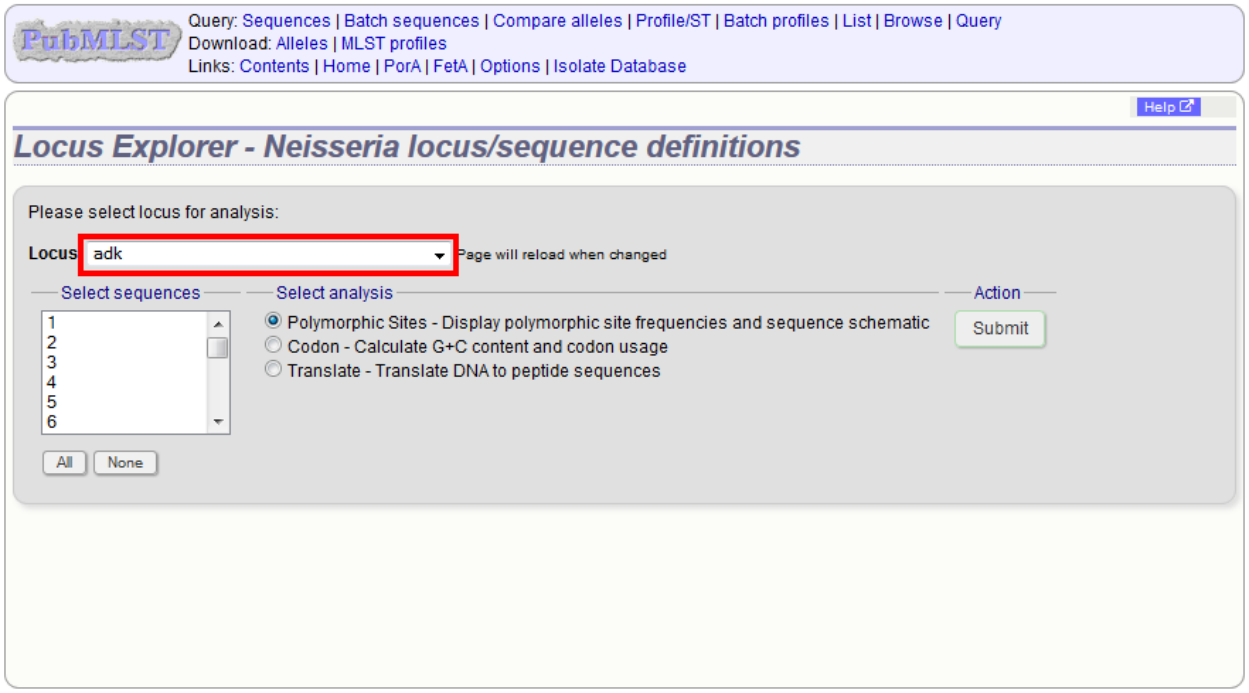
The locus explorer is a sequence definition database plugin. It can create schematics showing the polymorphic sites within a locus, calculate the GC content and generate aligned translated sequences.

Click 'Locus Explorer' from the sequence definition database contents page.

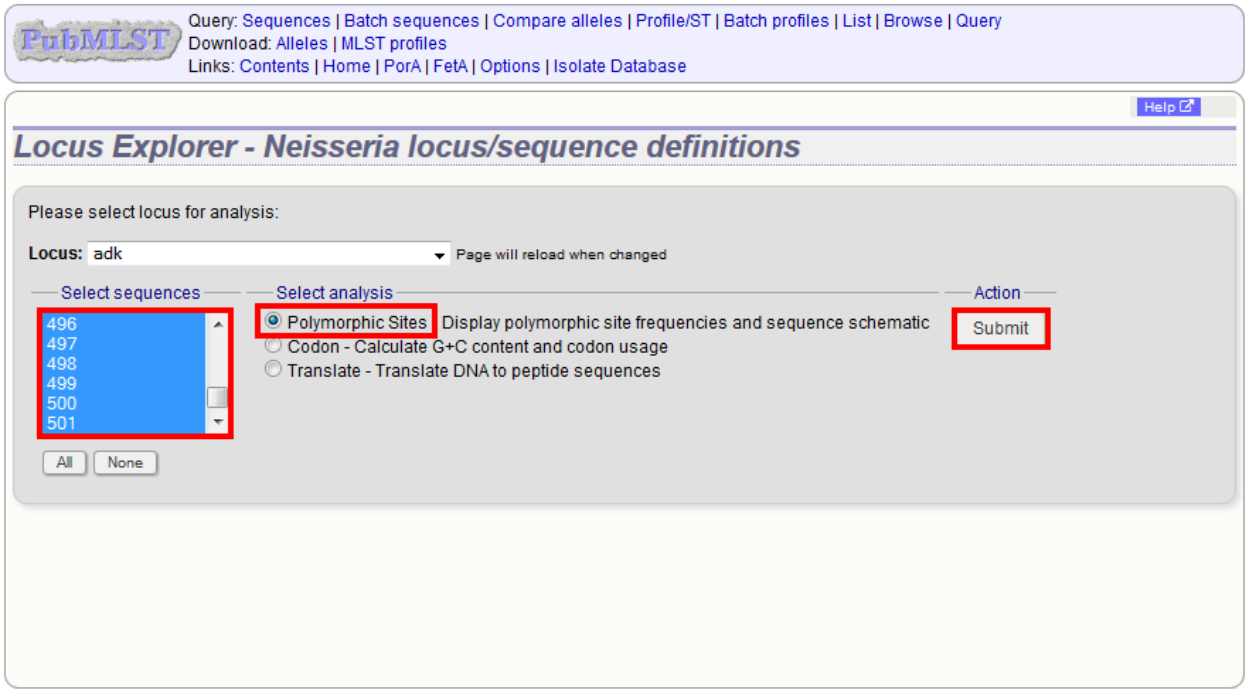


14.1.1 Polymorphic site analysis

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



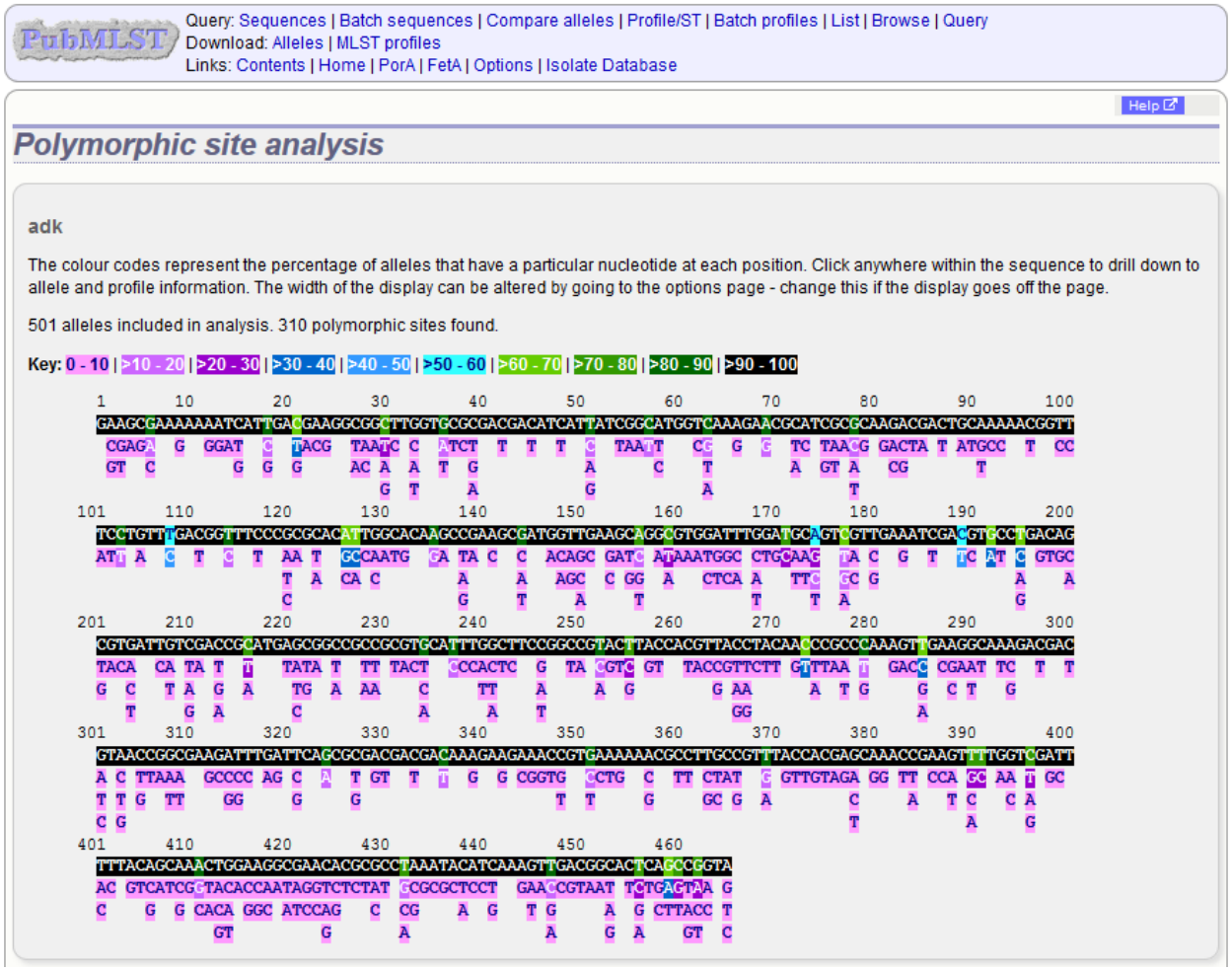
Select the alleles that you would like to include in the analysis. Variable length loci are limited to 2000 sequences or fewer since these need to be aligned. Select 'Polymorphic Sites' in the Analysis selection and click 'Submit'.



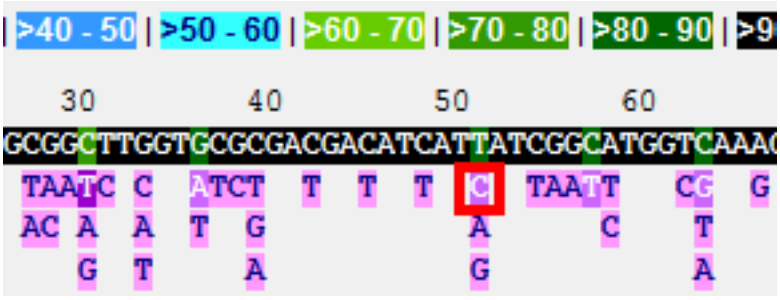
If an alignment is necessary, the job will be submitted to the job queue and the analysis performed. If no alignment is

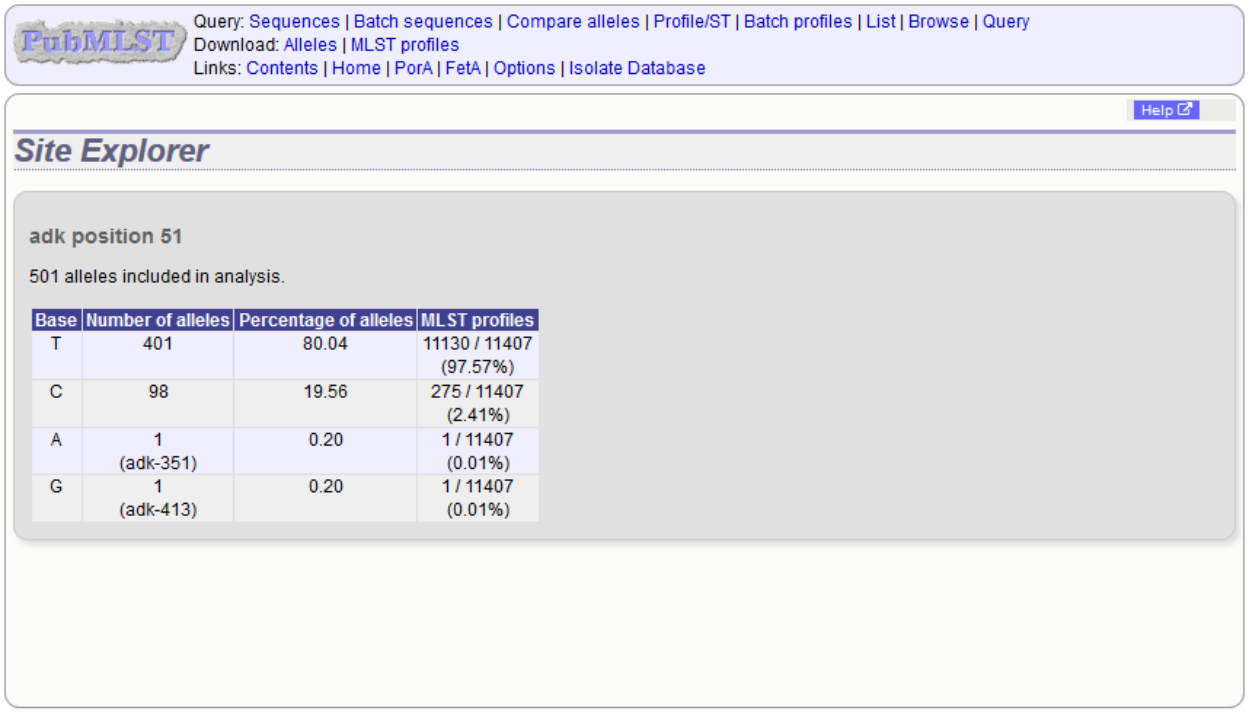
necessary, then the analysis is shown immediately.

The first part of the page shows the schematic.

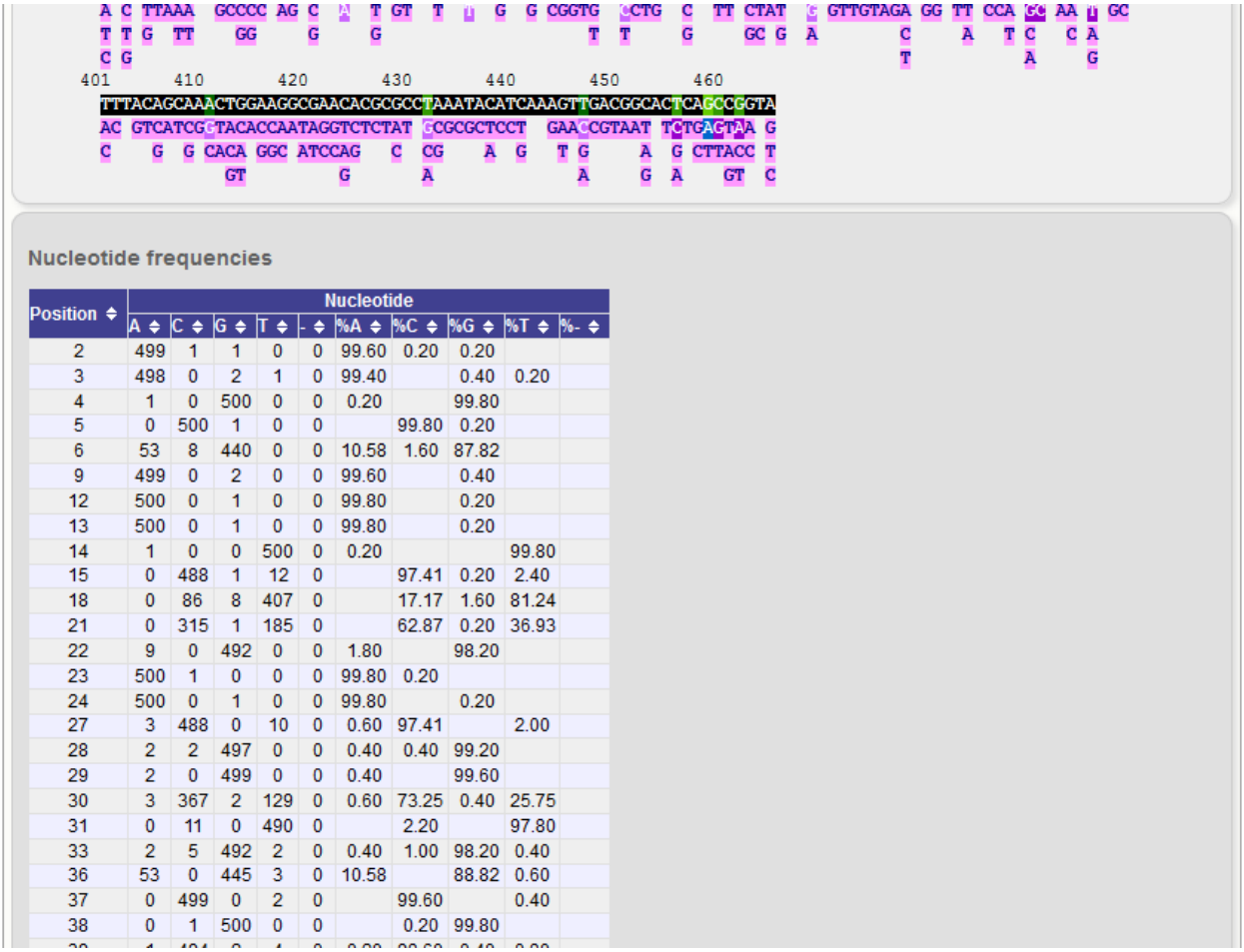


Clicking any of the sequence bases will calculate the exact frequencies of the different nucleotides at that position.





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



Nucleotide frequencies

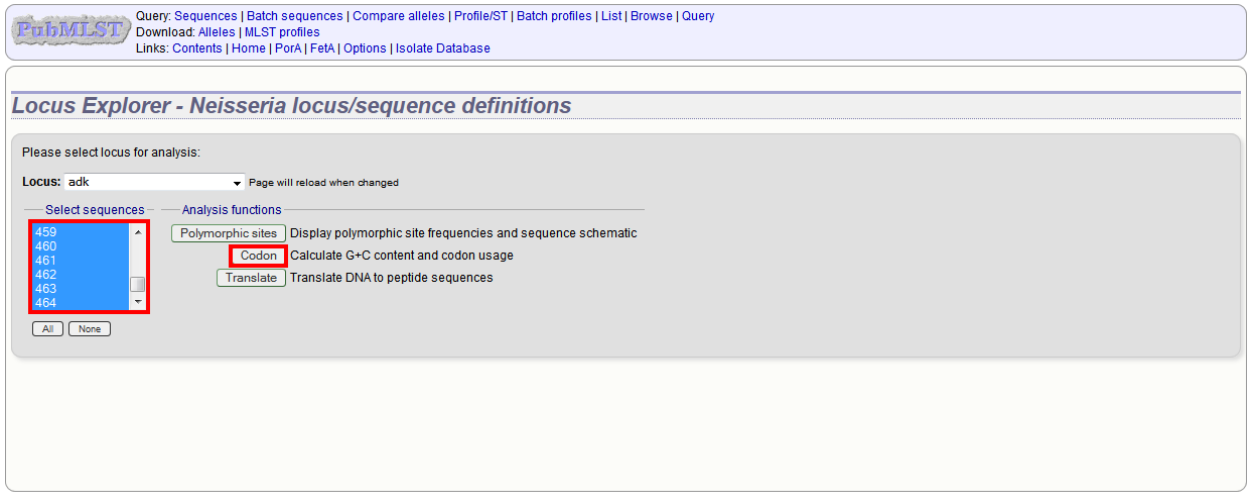
Position	Nucleotide									
	A	C	G	T	-	%A	%C	%G	%T	%-
2	499	1	1	0	0	99.60	0.20	0.20		
3	498	0	2	1	0	99.40		0.40	0.20	
4	1	0	500	0	0	0.20		99.80		
5	0	500	1	0	0		99.80	0.20		
6	53	8	440	0	0	10.58	1.60	87.82		
9	499	0	2	0	0	99.60		0.40		
12	500	0	1	0	0	99.80		0.20		
13	500	0	1	0	0	99.80		0.20		
14	1	0	0	500	0	0.20			99.80	
15	0	488	1	12	0		97.41	0.20	2.40	
18	0	86	8	407	0		17.17	1.60	81.24	
21	0	315	1	185	0		62.87	0.20	36.93	
22	9	0	492	0	0	1.80		98.20		
23	500	1	0	0	0	99.80	0.20			
24	500	0	1	0	0	99.80		0.20		
27	3	488	0	10	0	0.60	97.41		2.00	
28	2	2	497	0	0	0.40	0.40	99.20		
29	2	0	499	0	0	0.40		99.60		
30	3	367	2	129	0	0.60	73.25	0.40	25.75	
31	0	11	0	490	0		2.20		97.80	
33	2	5	492	2	0	0.40	1.00	98.20	0.40	
36	53	0	445	3	0	10.58		88.82	0.60	
37	0	499	0	2	0		99.60		0.40	
38	0	1	500	0	0		0.20	99.80		

See also:

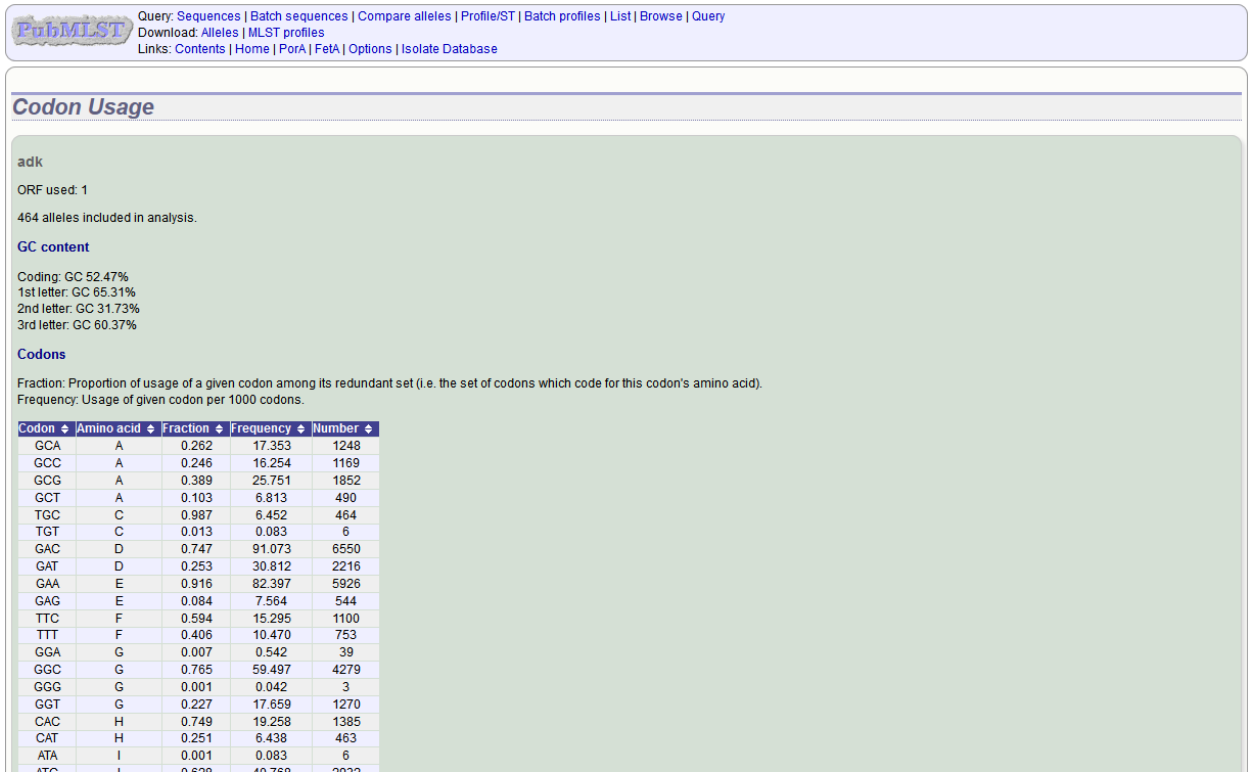
- *Investigating allele differences*.
- *Polymorphism analysis following isolate query*.

14.1.2 Codon usage

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



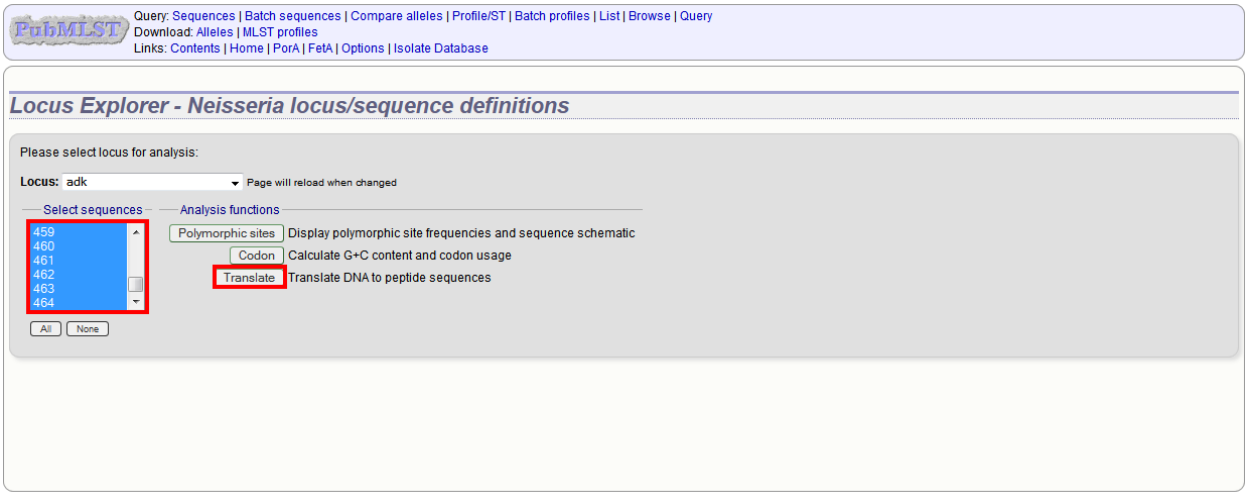
The GC content of the alleles will be determined and a table of the codon frequencies displayed.



14.1.3 Aligned translations

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

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



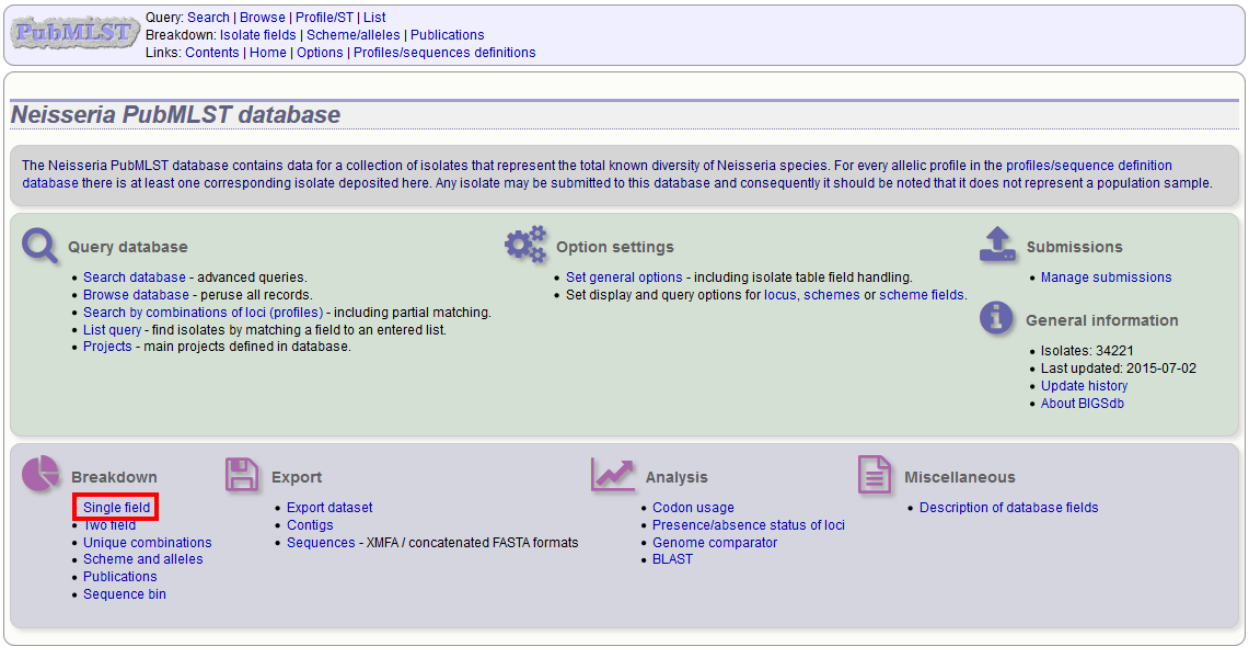
An aligned amino acid sequence will be displayed.

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

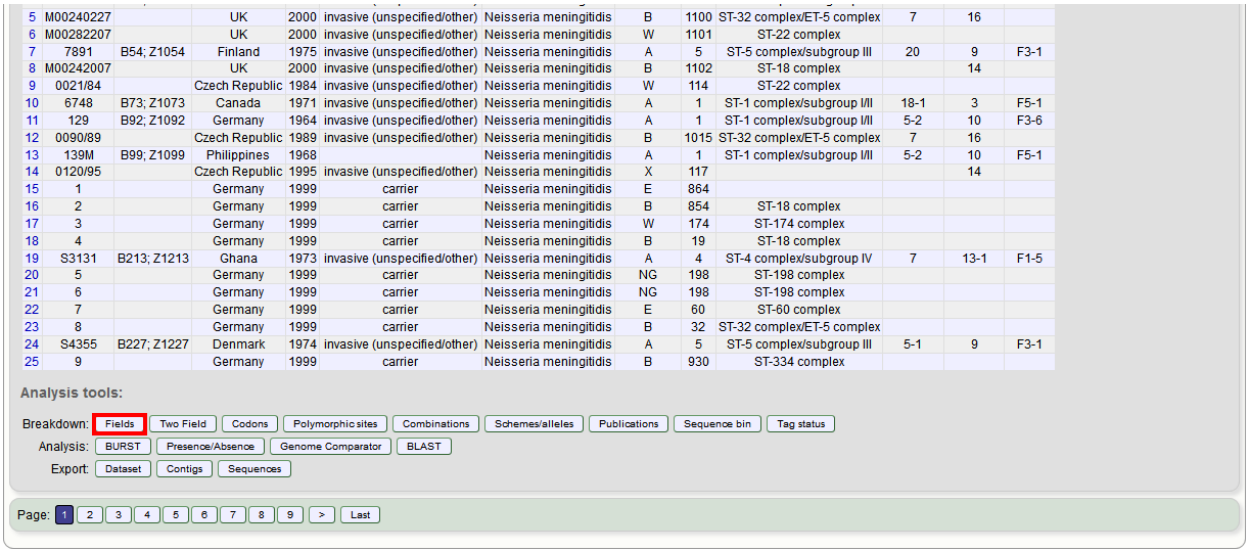
14.2 Field breakdown

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

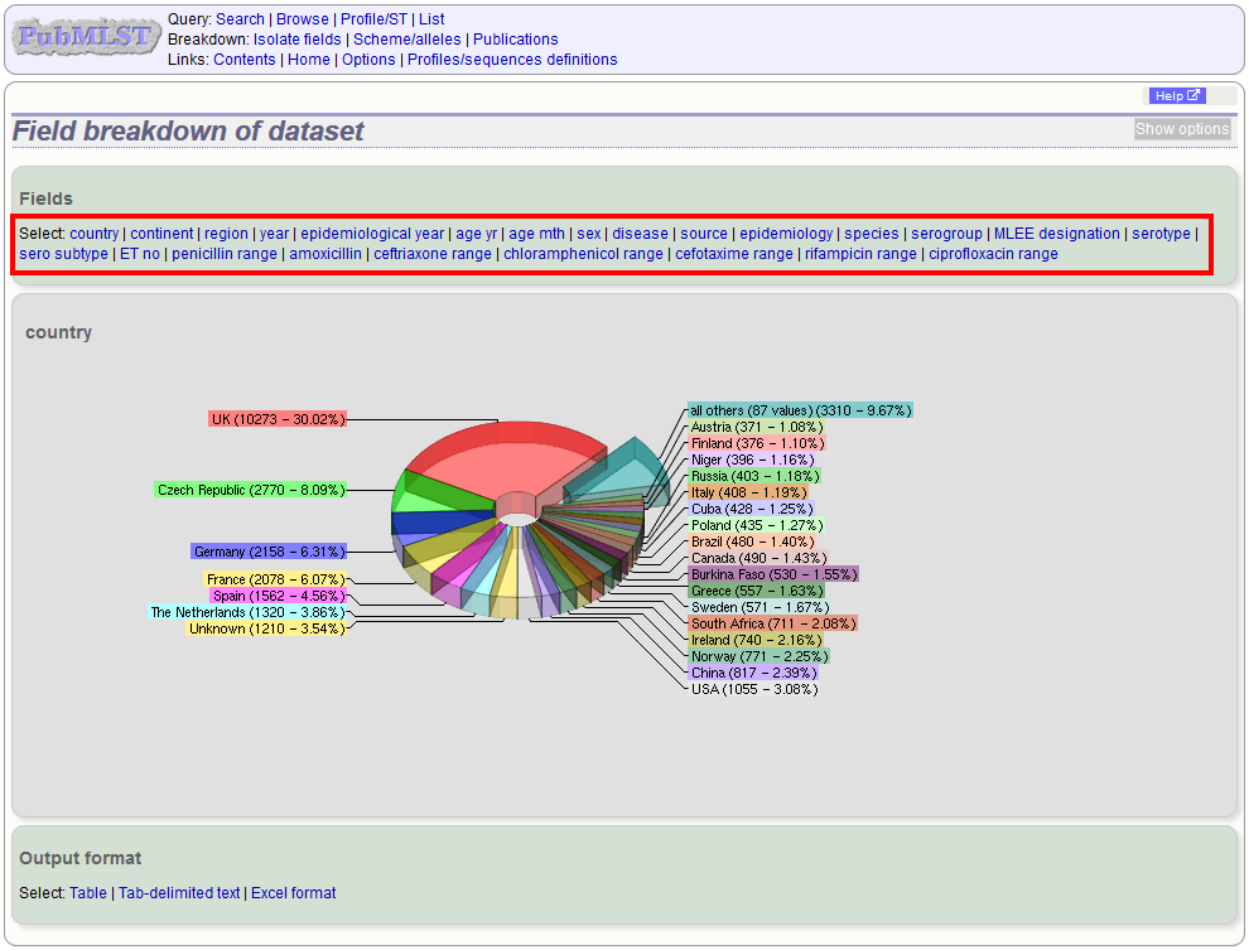
The breakdown function can be selected for the whole database by clicking the 'Single field' link in the Breakdown section of the main contents page.



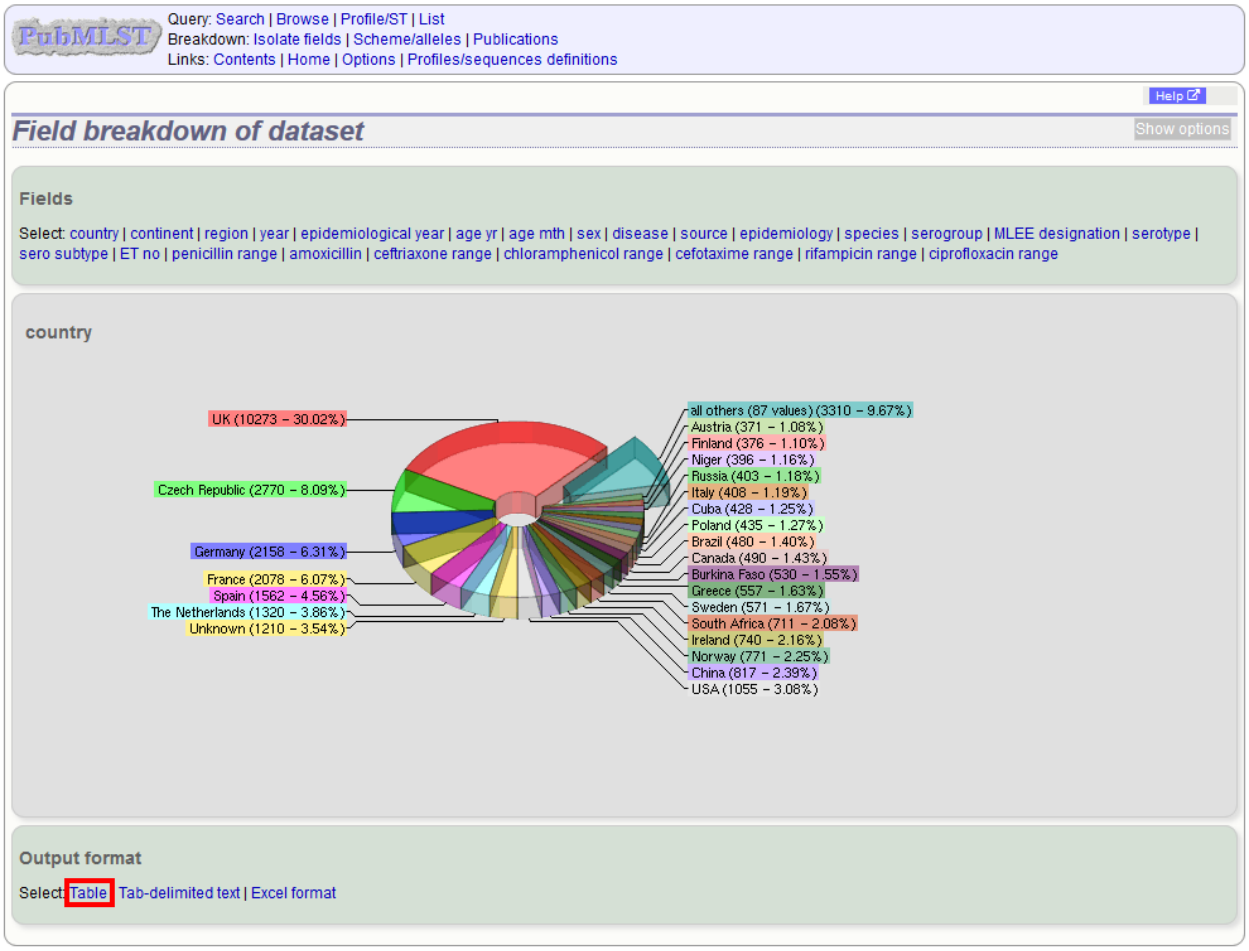
Alternatively, a breakdown can be displayed of the dataset returned from a query by clicking the 'Fields' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.



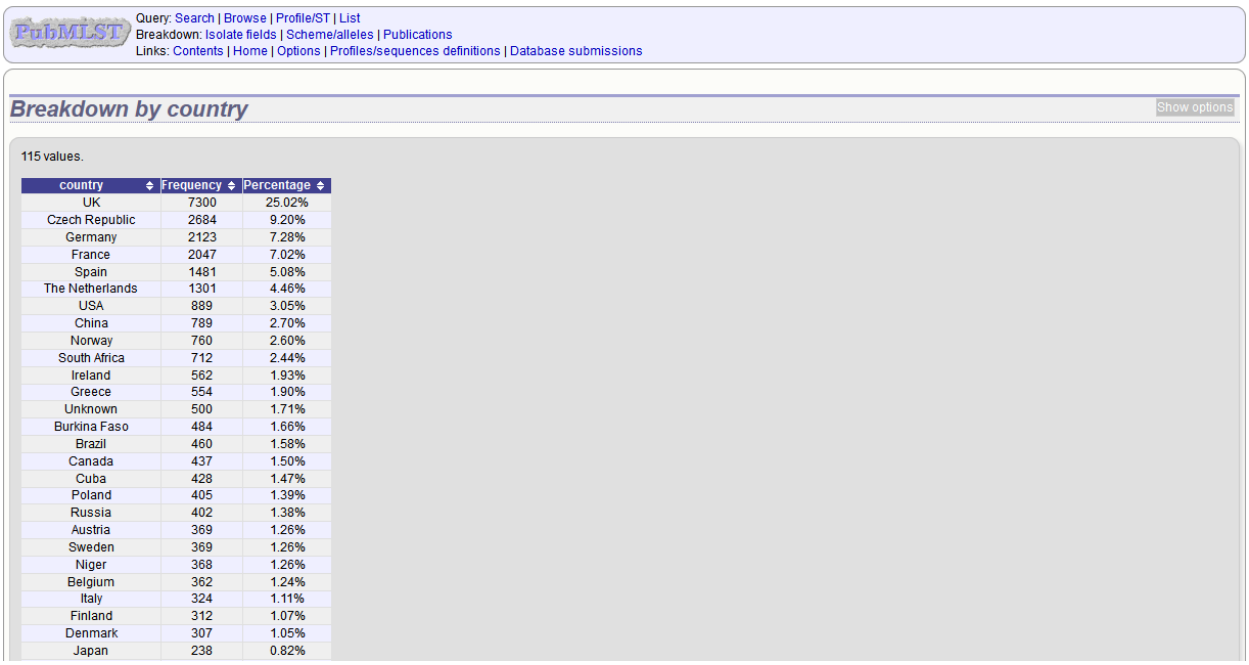
A series of charts will be displayed. Pick the field to display from the list at the top.



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

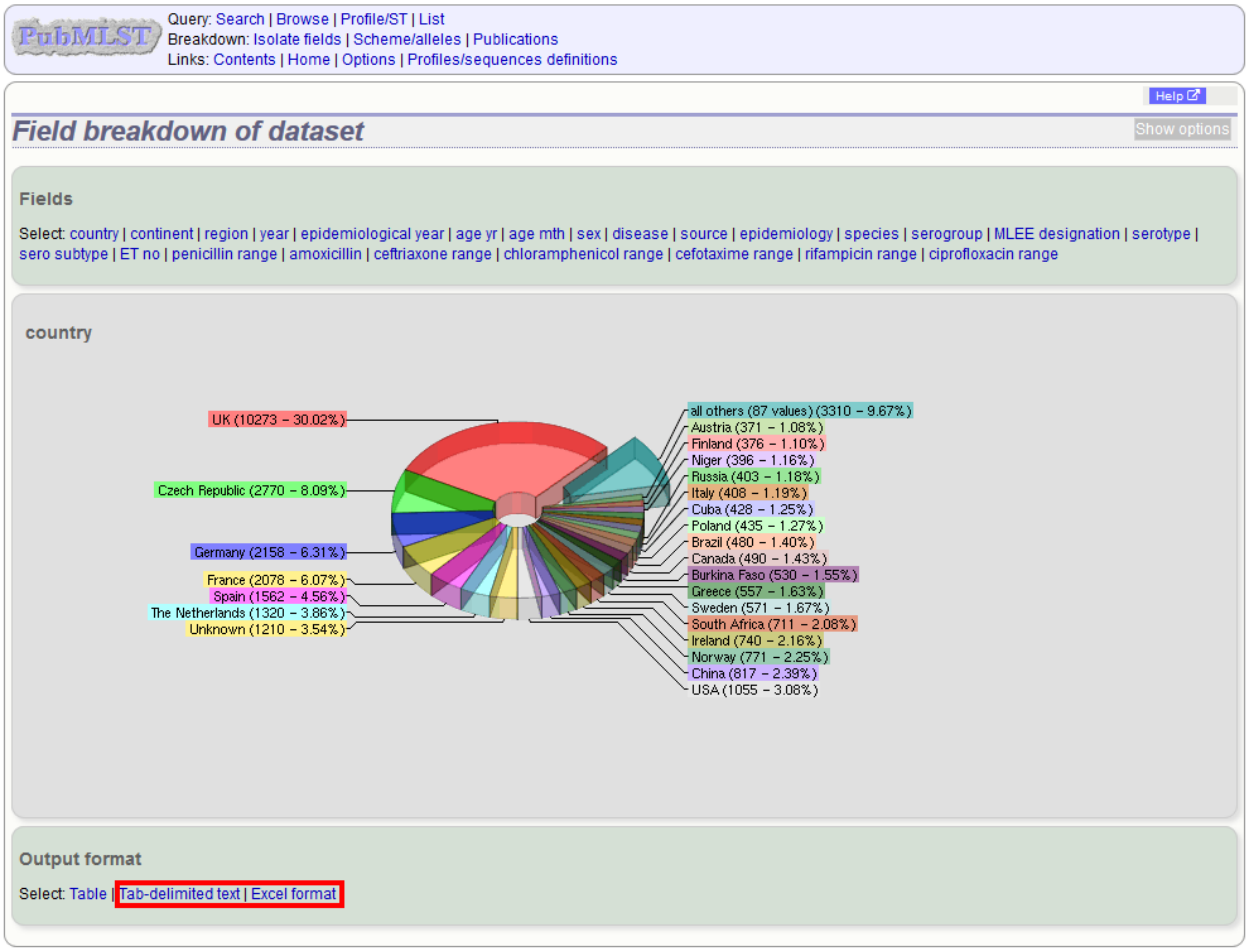


This displays a table that can be ordered by clicking the appropriate header.



country	Frequency	Percentage
UK	7300	25.02%
Czech Republic	2684	9.20%
Germany	2123	7.28%
France	2047	7.02%
Spain	1481	5.08%
The Netherlands	1301	4.46%
USA	889	3.05%
China	789	2.70%
Norway	760	2.60%
South Africa	712	2.44%
Ireland	562	1.93%
Greece	554	1.90%
Unknown	500	1.71%
Burkina Faso	484	1.66%
Brazil	460	1.58%
Canada	437	1.50%
Cuba	428	1.47%
Poland	405	1.39%
Russia	402	1.38%
Austria	369	1.26%
Sweden	369	1.26%
Niger	368	1.26%
Belgium	362	1.24%
Italy	324	1.11%
Finland	312	1.07%
Denmark	307	1.05%
Japan	238	0.82%

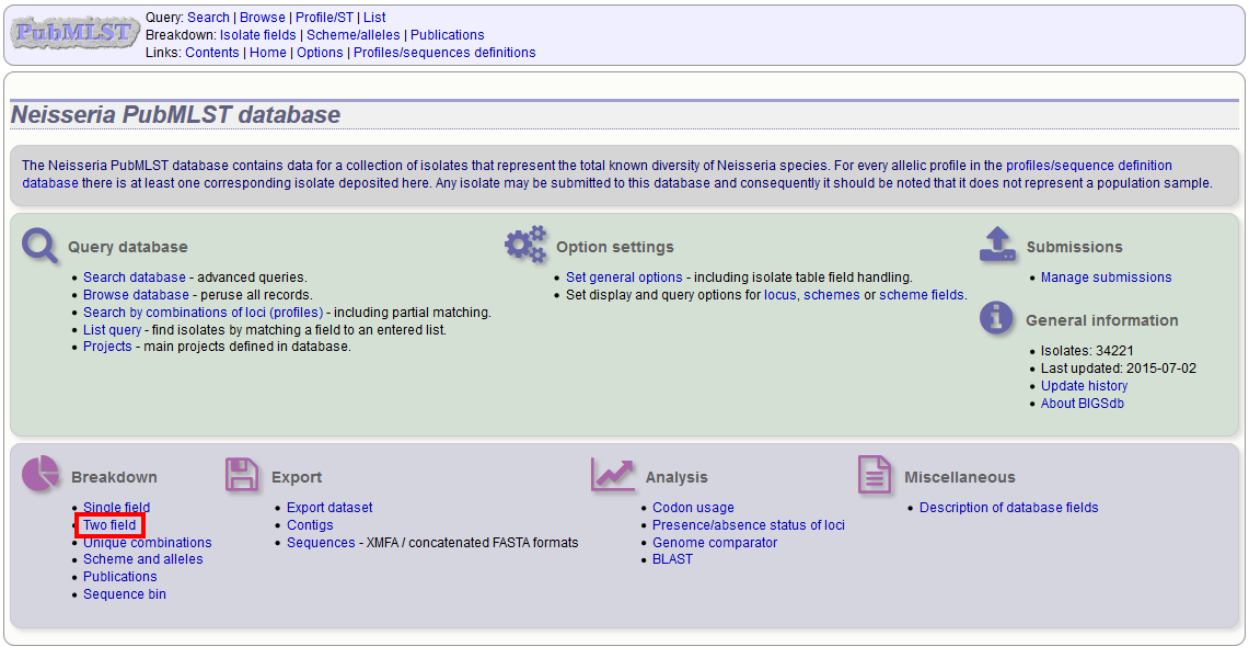
The data can also be downloaded in tab-delimited text or Excel formats by clicking the appropriate links.



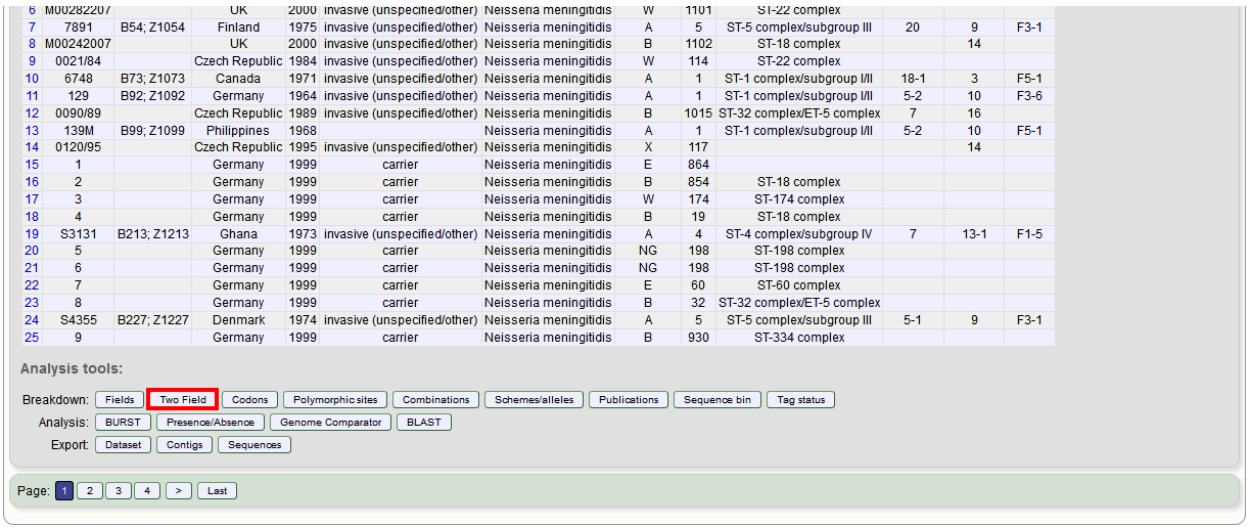
14.3 Two field breakdown

The two field breakdown plugin displays a table breaking down one field against another, e.g. breakdown of serogroup by year.

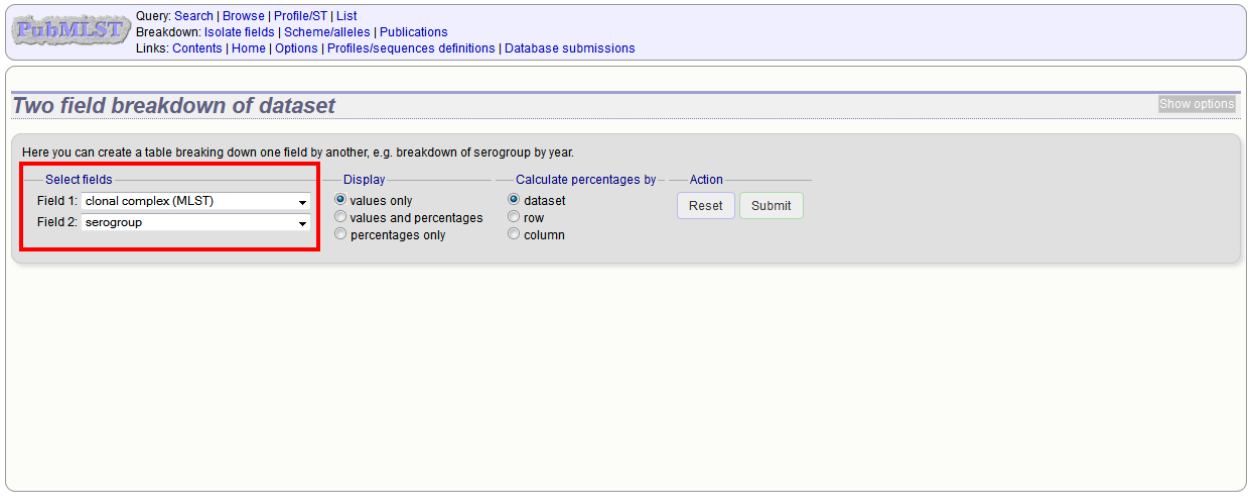
The analysis can be selected for the whole database by clicking the 'Two field breakdown' link on the main contents page.



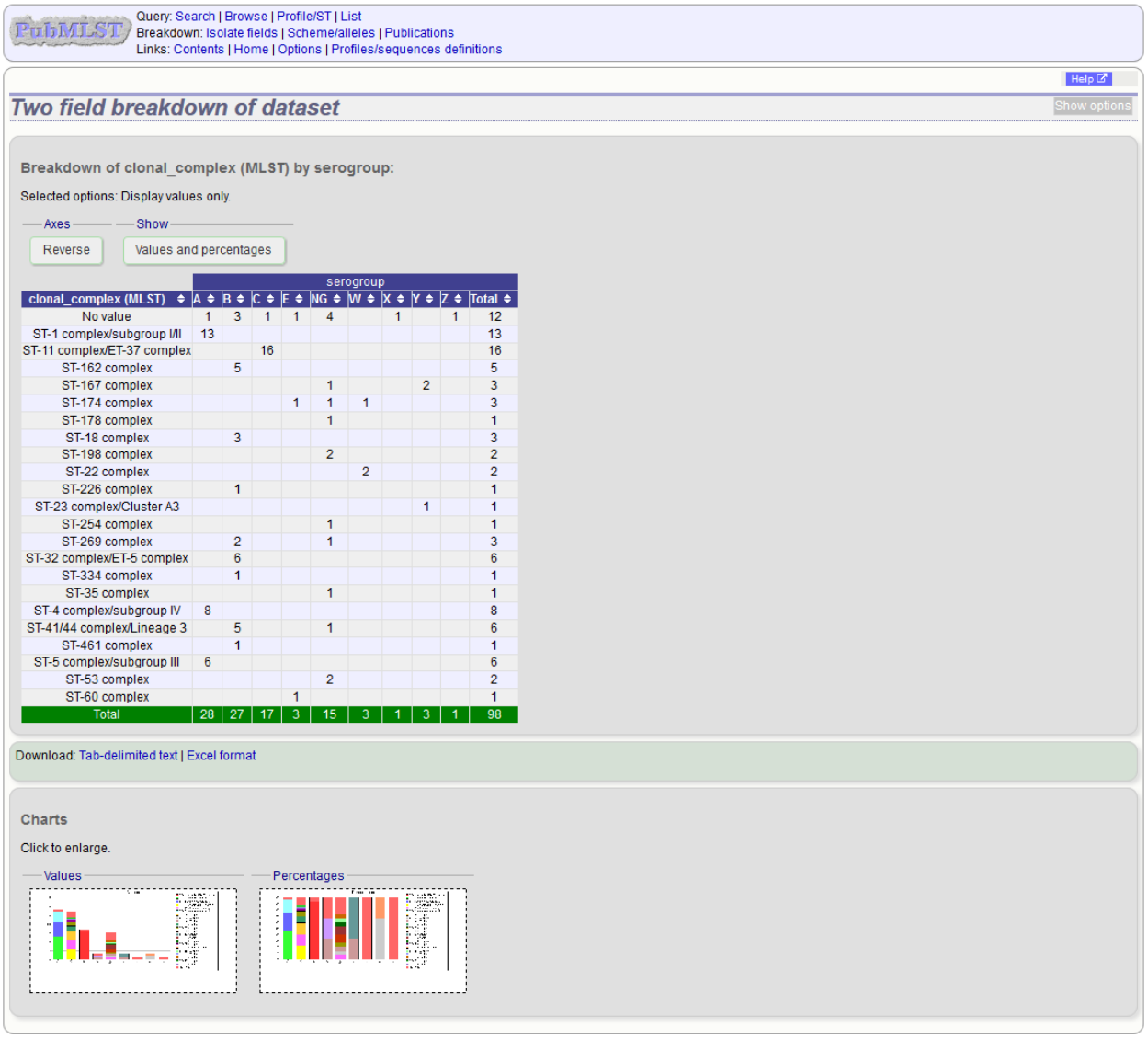
Alternatively, a two field breakdown can be displayed of the dataset returned from a query by clicking the 'Two field' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.



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



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.



	serogroup									
clonal_complex (MLST)	A	B	C	E	NG	W	X	Y	Z	Total
No value	1	3	1	1	4		1		1	12
ST-1 complex/subgroup I/II	13									13
ST-11 complex/ET-37 complex			16							16
ST-162 complex		5								5
ST-167 complex					1			2		3
ST-174 complex				1	1	1				3
ST-178 complex					1					1
ST-18 complex		3								3
ST-198 complex					2					2
ST-22 complex						2				2
ST-226 complex		1								1
ST-23 complex/Cluster A3								1		1
ST-254 complex					1					1
ST-269 complex		2			1					3
ST-32 complex/ET-5 complex		6								6
ST-334 complex		1								1
ST-35 complex					1					1
ST-4 complex/subgroup IV	8									8
ST-41/44 complex/Lineage 3		5			1					6
ST-461 complex		1								1
ST-5 complex/subgroup III	6									6
ST-53 complex					2					2
ST-60 complex				1						1
Total	28	27	17	3	15	3	1	3	1	98

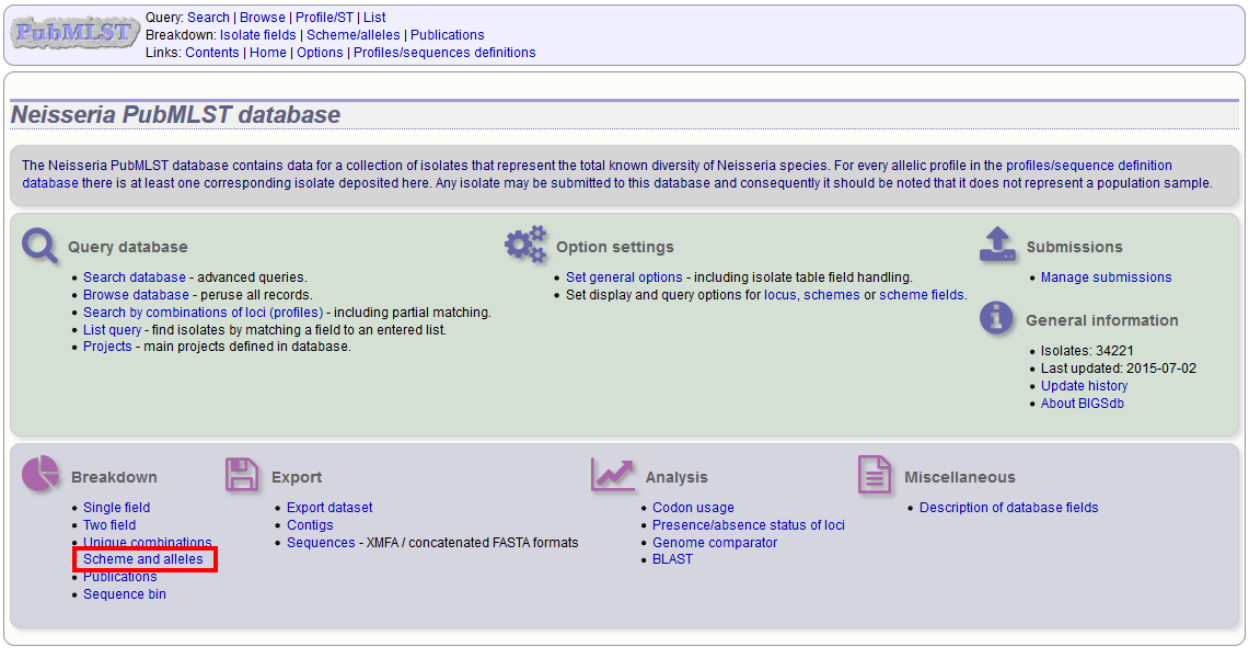
The table values can be exported in a format suitable for copying in to a spreadsheet by clicking 'Download as tab-delimited text' underneath the table.

Note: The job will be submitted to the offline job queue if the query returns 10,000 or more isolates. In this case, the buttons to reverse the axes or to change whether values or percentages are shown will not be available.

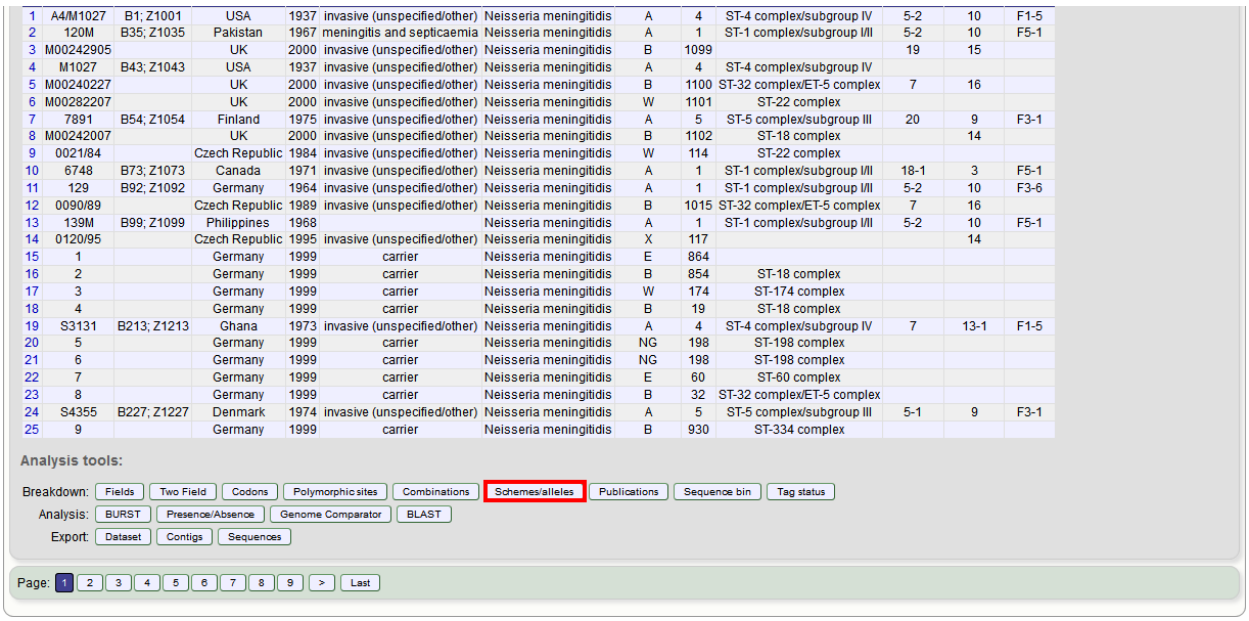
14.4 Scheme and allele breakdown

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

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

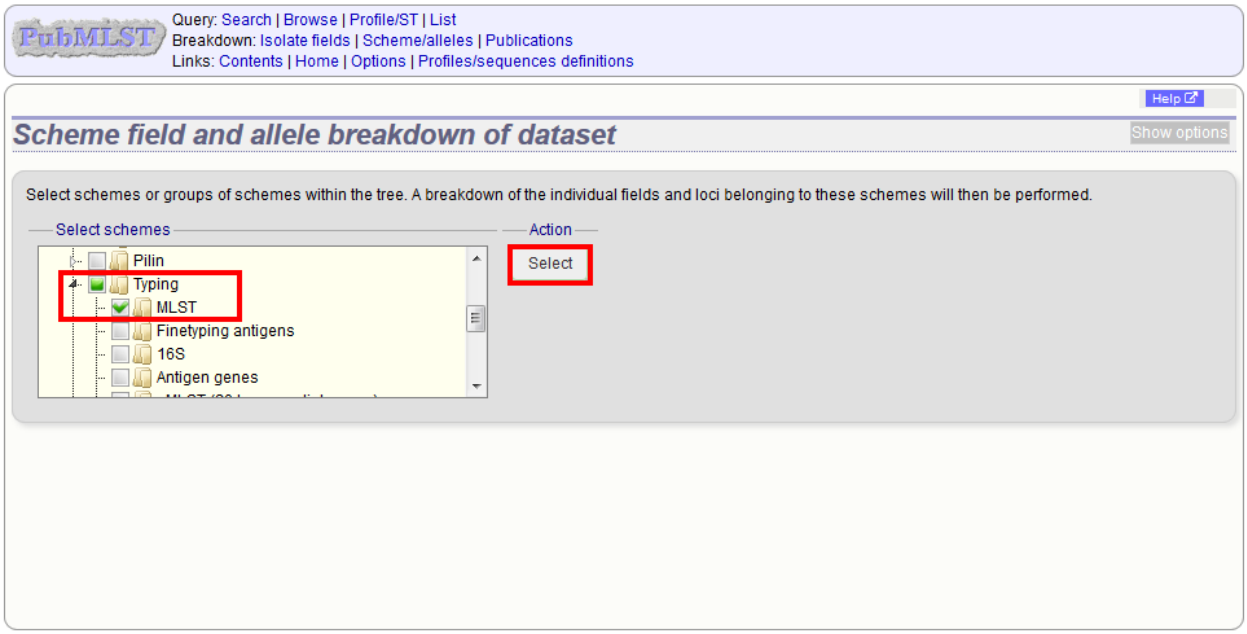


Alternatively, a breakdown can be displayed of the dataset returned from a query by clicking the 'Schemes/alleles' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

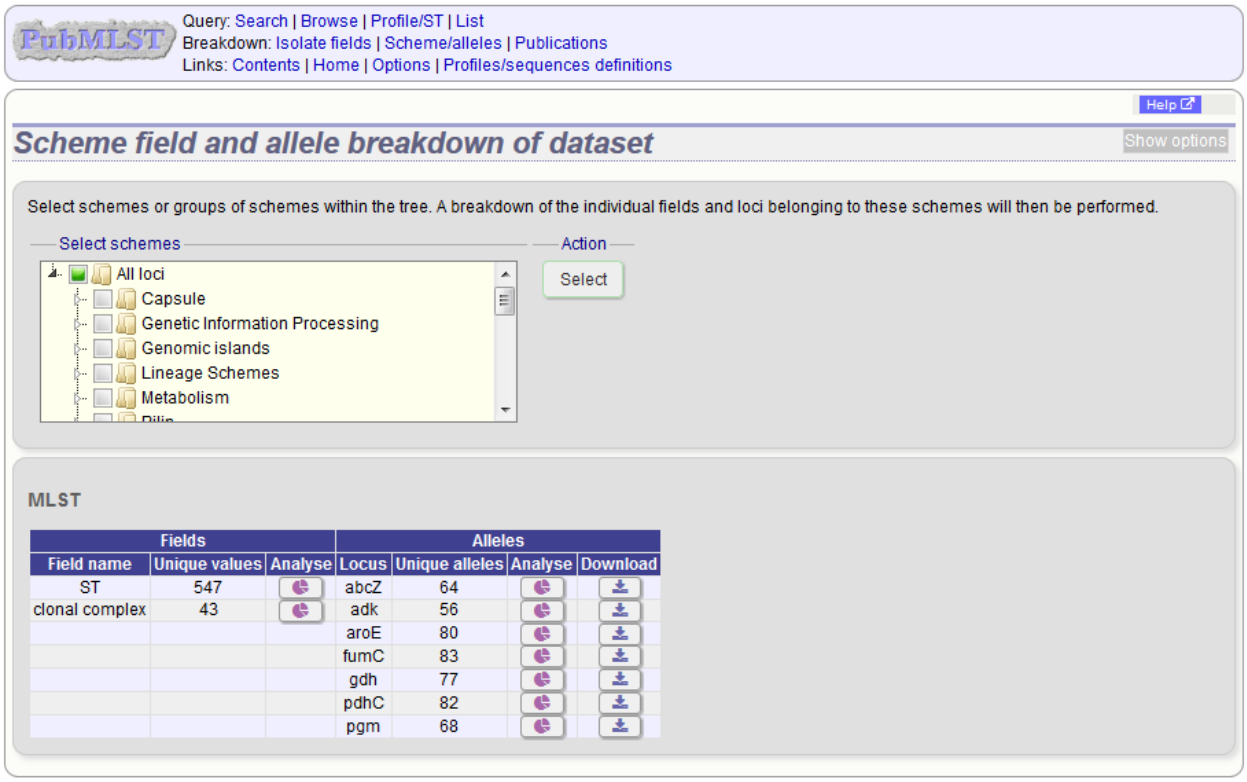


1	A4/M1027	B1; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
3	M00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	B	1099		19	15	
4	M1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV			
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	B	1100	ST-32 complex/ET-5 complex	7	16	
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	B	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	B	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	X	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	B	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	B	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
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	B	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	B	930	ST-334 complex			

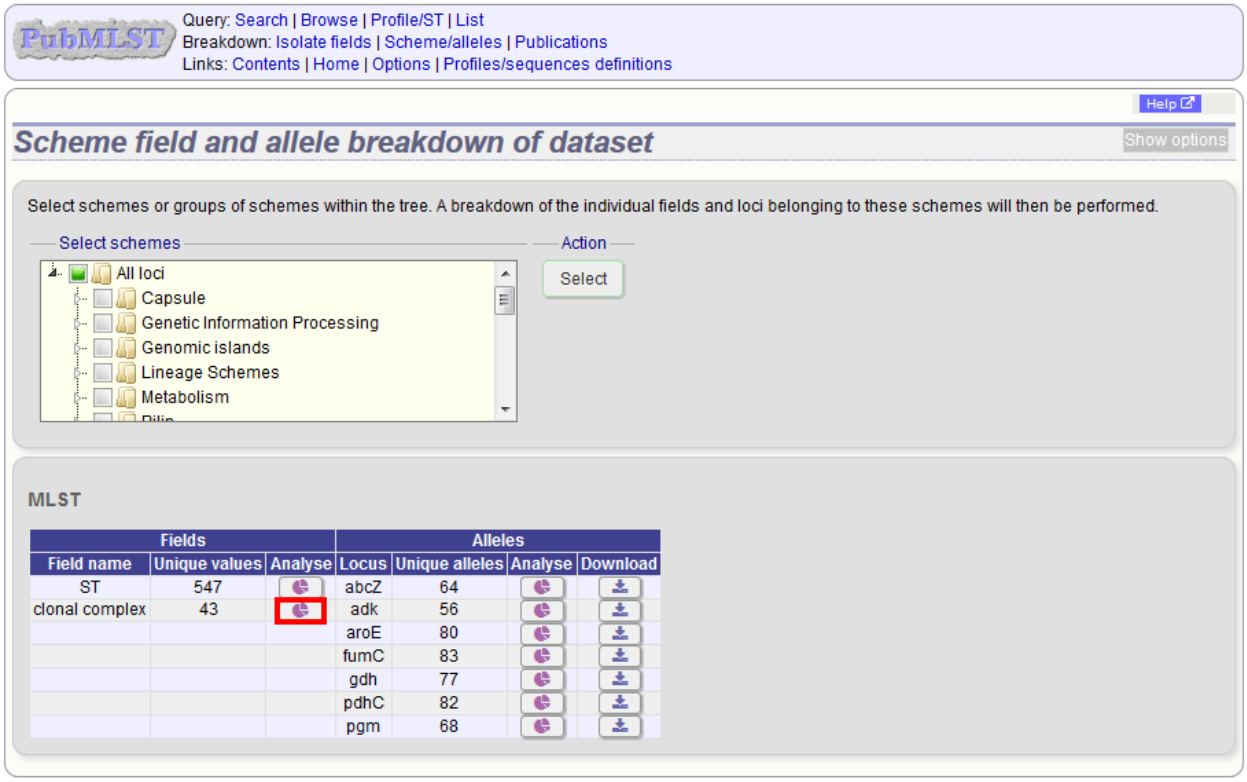
A scheme tree is shown. Select any combination of schemes to analyse. Click 'Select'.



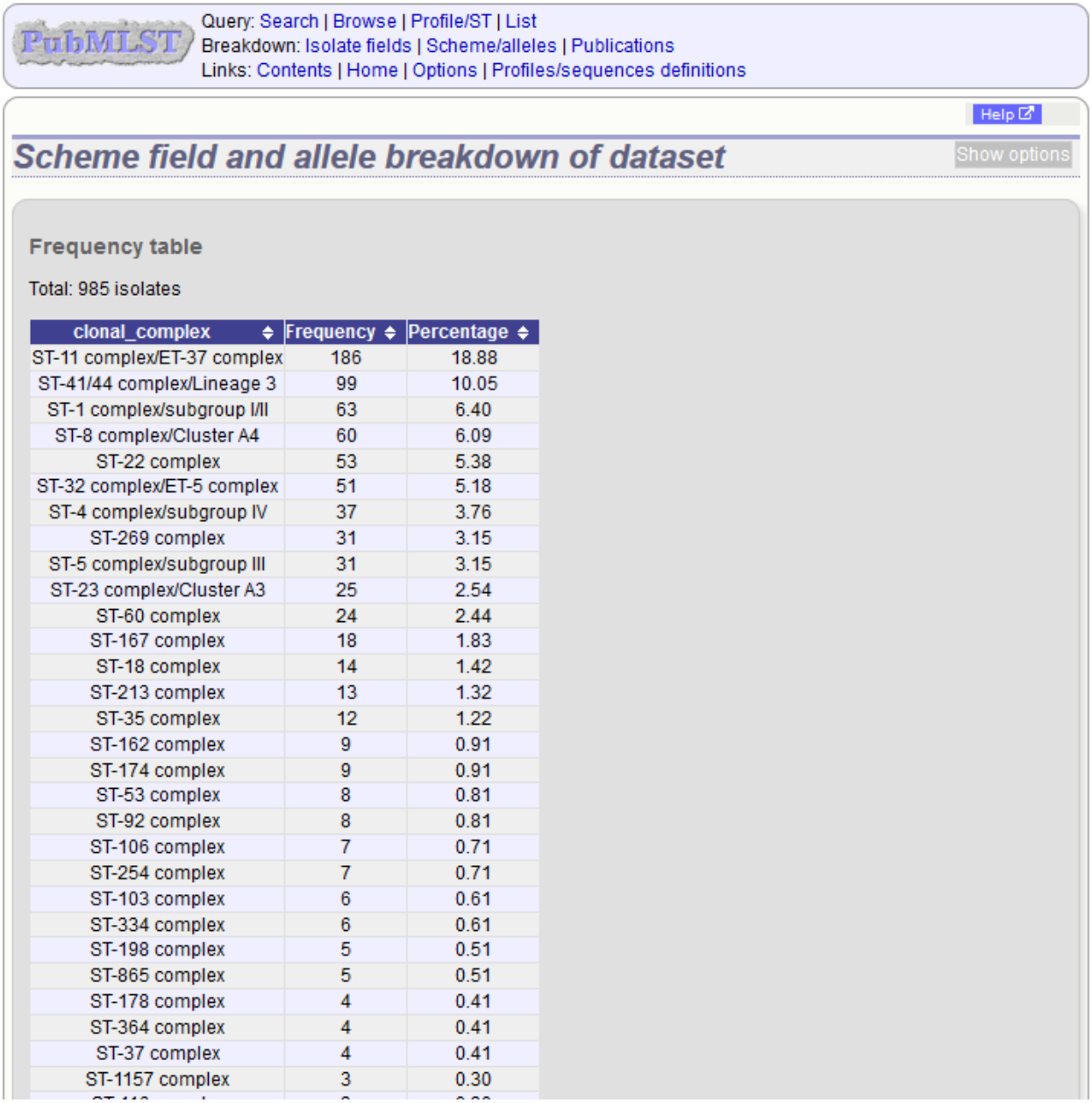
A table showing the number of unique values for each locus and scheme field will be displayed.



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



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



clonal_complex	Frequency	Percentage
ST-11 complex/ET-37 complex	186	18.88
ST-41/44 complex/Lineage 3	99	10.05
ST-1 complex/subgroup I/II	63	6.40
ST-8 complex/Cluster A4	60	6.09
ST-22 complex	53	5.38
ST-32 complex/ET-5 complex	51	5.18
ST-4 complex/subgroup IV	37	3.76
ST-269 complex	31	3.15
ST-5 complex/subgroup III	31	3.15
ST-23 complex/Cluster A3	25	2.54
ST-60 complex	24	2.44
ST-167 complex	18	1.83
ST-18 complex	14	1.42
ST-213 complex	13	1.32
ST-35 complex	12	1.22
ST-162 complex	9	0.91
ST-174 complex	9	0.91
ST-53 complex	8	0.81
ST-92 complex	8	0.81
ST-106 complex	7	0.71
ST-254 complex	7	0.71
ST-103 complex	6	0.61
ST-334 complex	6	0.61
ST-198 complex	5	0.51
ST-865 complex	5	0.51
ST-178 complex	4	0.41
ST-364 complex	4	0.41
ST-37 complex	4	0.41
ST-1157 complex	3	0.30

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

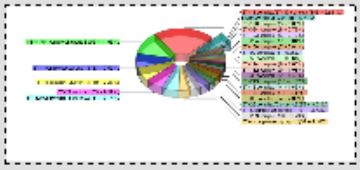
ST-92 complex	8	0.81
ST-106 complex	7	0.71
ST-254 complex	7	0.71
ST-103 complex	6	0.61
ST-334 complex	6	0.61
ST-198 complex	5	0.51
ST-865 complex	5	0.51
ST-178 complex	4	0.41
ST-364 complex	4	0.41
ST-37 complex	4	0.41
ST-1157 complex	3	0.30
ST-116 complex	3	0.30
ST-1494 complex (lactamica)	3	0.30
ST-4240/6688 complex	3	0.30
ST-624 complex (lactamica)	3	0.30
ST-1136 complex	2	0.20
ST-1540 complex (lactamica)	2	0.20
ST-212 complex	2	0.20
ST-461 complex	2	0.20
ST-613 complex (lactamica)	2	0.20
ST-750 complex	2	0.20
ST-226 complex	1	0.10
ST-282 complex	1	0.10
ST-595 complex (lactamica)	1	0.10
ST-640 complex (lactamica)	1	0.10

Download: Tab-delimited text

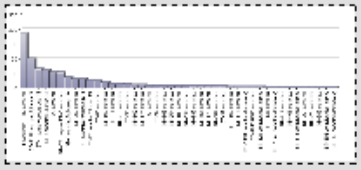
Charts

Click to enlarge.

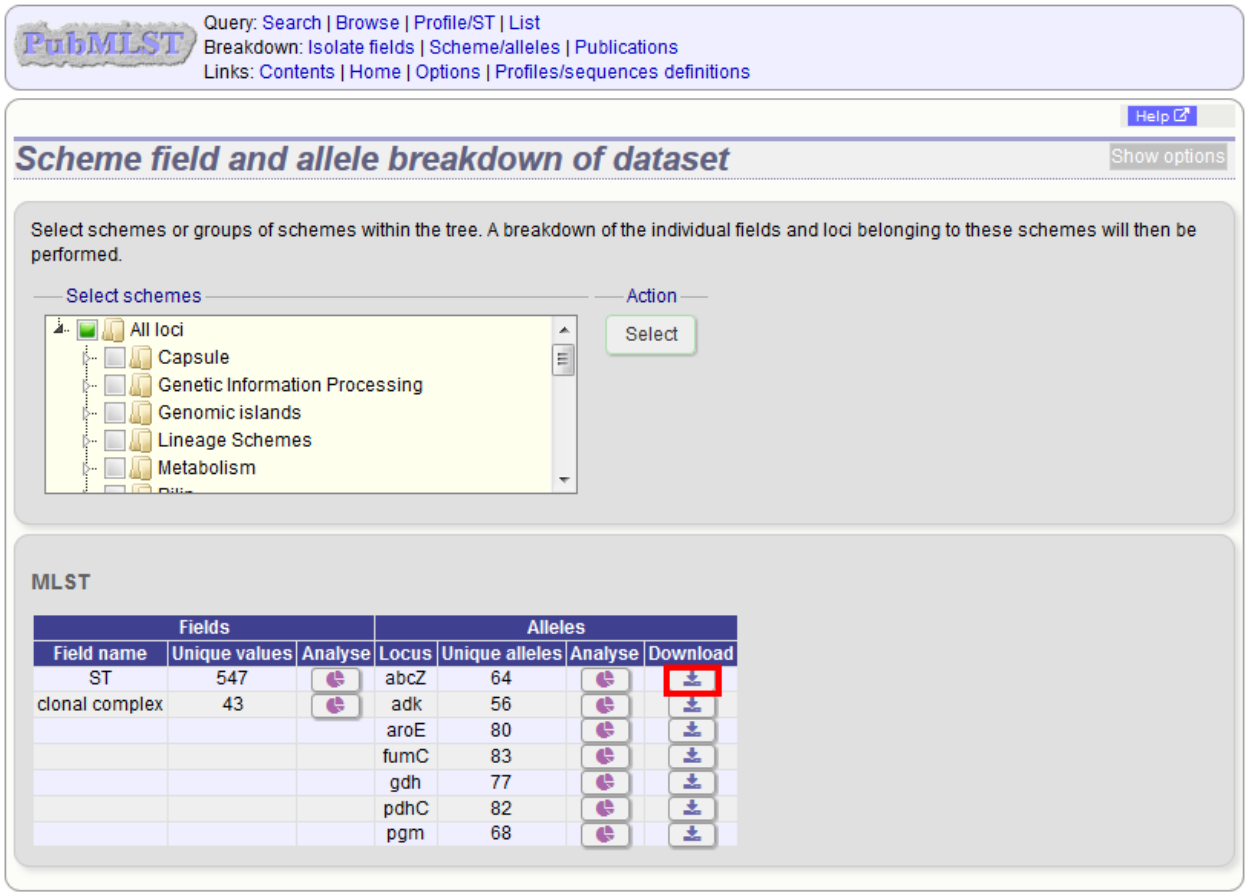
Pie chart



Bar chart



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



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

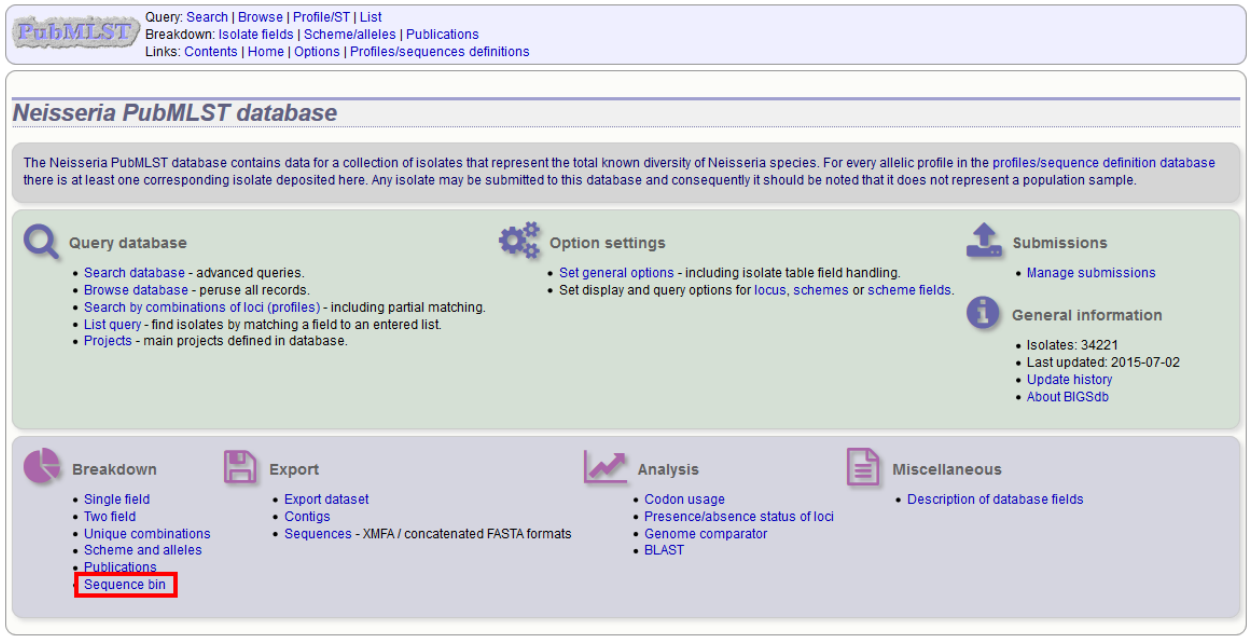
```
>2
TTTGATACCGTTGCCGAAGGTTTGGGTGAAATTCGCGATTTATTGCGCCGTTACCACCGC
GTCGGCCATGAGTTGGAAAACGGTTCGGGTGAGGCTTTGTTGAAAGAACTCAACGAATTA
CAACTTGAAATCGAAGCGAAGGACGGCTGGAAGCTGGATGCGGCAGTCAAGCAGACTTTG
GGGGAACTCGGTTTGCCGGAAAACGAAAAAATCGGCAACCTTTCCGGCGGTCAGAAAAAG
CGTGTCGCCTTGGCGCAGGCTTGGGTGCAGAAGCCCGACGTATTGCTGCTGGACGAACCG
ACCAACCATTTGGATATCGACGCGATTATTTGGCTGGAAAATCTGCTCAAAGCGTTTGAA
GGCAGCTTGGTTGTGATTACCCACGACCGCCGTTTTTTGGACAATATCGCCACGCGGATT
GTCGAACTCGATC
>1
TTTGATACTGTTGCCGAAGGTTTGGGCGAAATTCGCGATTTATTGCGCCGTTATCATCAT
GTCAGCCATGAGTTGGAAAATGGTTCGAGTGAGGCCTTATTGAAAGAGCTCAACGAATTG
CAACTTGAGATCGAAGCGAAGGACGGCTGGAAGTTGGATGCGGCGGTGAAGCAGACTTTG
GGCGAACTCGGTTTGCCGGAAAACGAAAAAATCGGCAACCTCTCCGGCGGTCAGAAAAAG
CGCGTCGCCTTGGCGCAGGCTTGGGTGCAGAAGCCCGACGTATTGCTGCTCGATGAACCG
ACCAACCATTTGGACATCGACGCGATTATTTGGTTGGAAAACCTGCTCAAAGCGTTTGAA
GGCAGCCTGGTTGTGATTACCCACGACCGCCGTTTTTTGGACAATATCGCCACGCGGATT
GTCGAACTCGATC
>4
TTTGATACCGTTGCCGAAGGTTTGGGCGAAATTCGTGATTTATTGCGCCGTTATCATCAT
GTCAGCCATGAGTTGGAAAATGGTTCGAGTGAGGCTTTGTTGAAAGAACTCAACGAATTG
CAACTTGAAATCGAAGCGAAGGACGGCTGGAAACTGGATGCGGCAGTCAAGCAGACTTTG
GGGGAACTCGGTTTGCCGGAAAATGAAAAAATCGGCAACCTTTCCGGCGGTCAGAAAAAG
CGCGTCGCCTTGGCTCAGGCTTGGGTGCAAAAGCCCGACGTATTGCTGCTGGACGAGCCG
ACCAACCATTTGGATATCGACGCGATTATTTGGCTGGAAAATCTGCTCAAAGCGTTTGAA
```

```
GGCAGCTTGGTTGTGATTACCCACGACCGCCGTTTTTTGGACAATATCGCCACGCGGATT
GTCGAACTCGATC
```

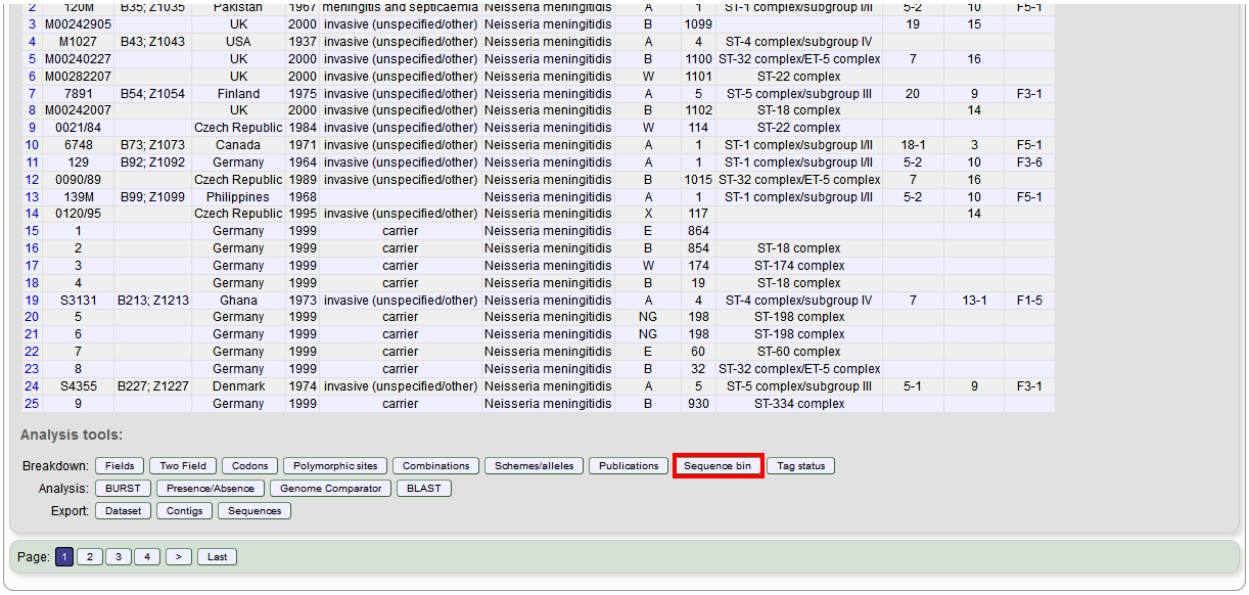
14.5 Sequence bin breakdown

The sequence bin breakdown plugin calculates statistics based on the number and length of contigs in the sequence bin as well as the number of loci tagged for an isolate record.

The function can be selected by clicking the 'Sequence bin' link on the Breakdown section of the main contents page.



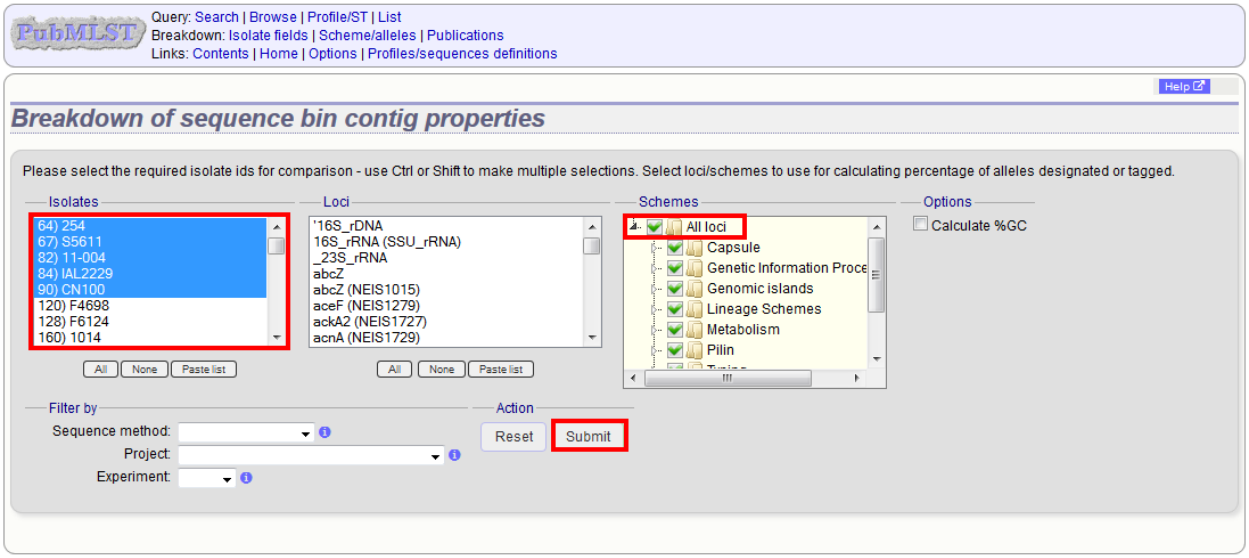
Alternatively, it can be accessed following a query by clicking the 'Sequence bin' button in the Breakdown list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.



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.

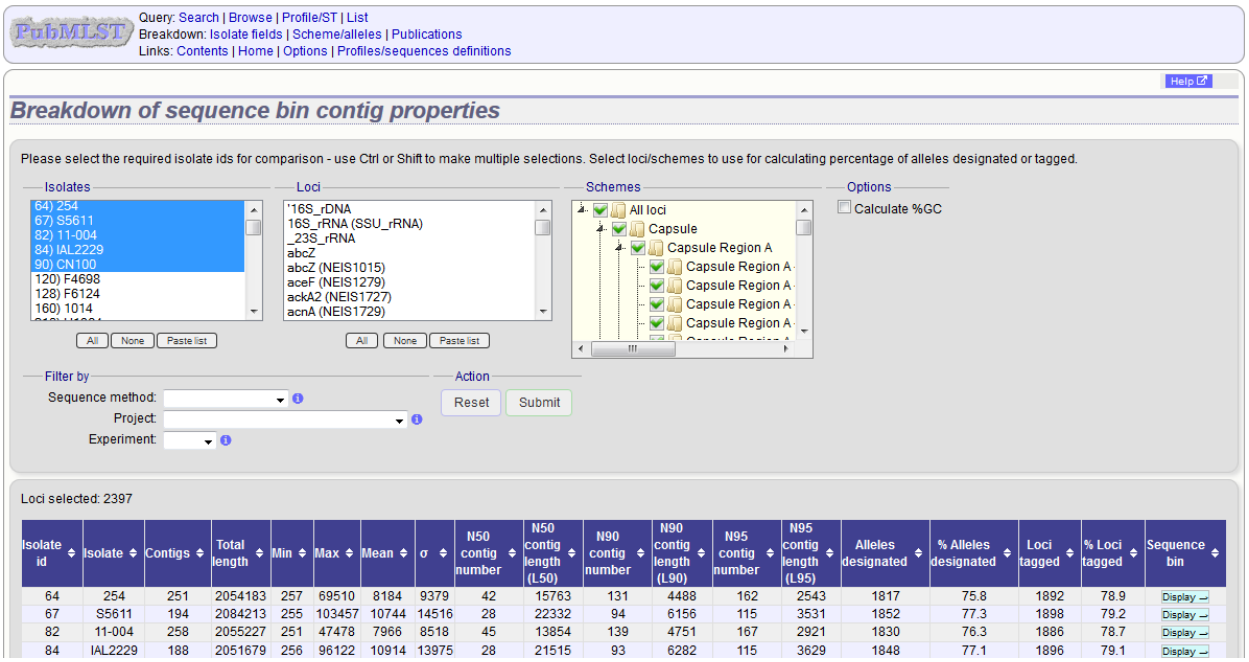
There is also an option to determine the mean G+C content of the sequence bin of each isolate.

Click submit.



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

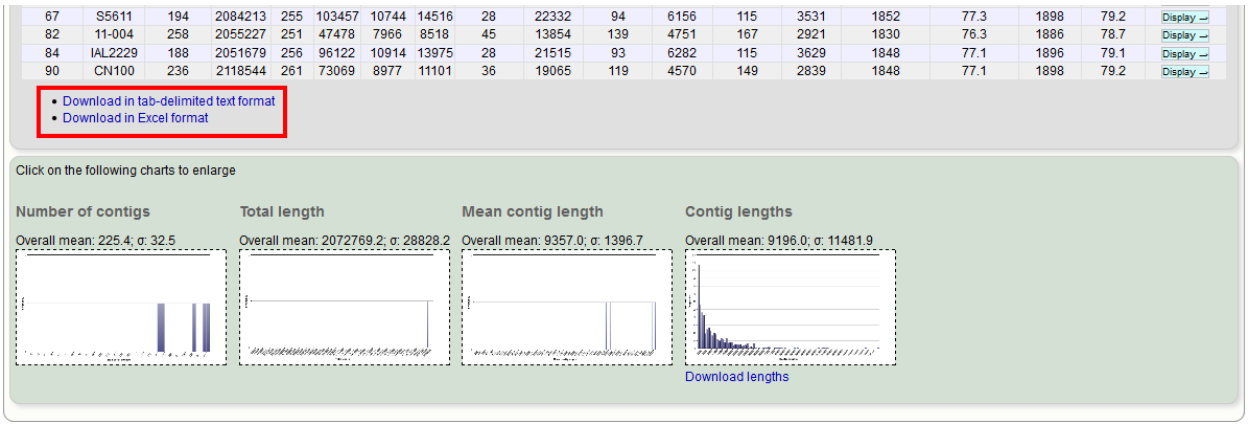
A table of sequence bin stats will be generated.



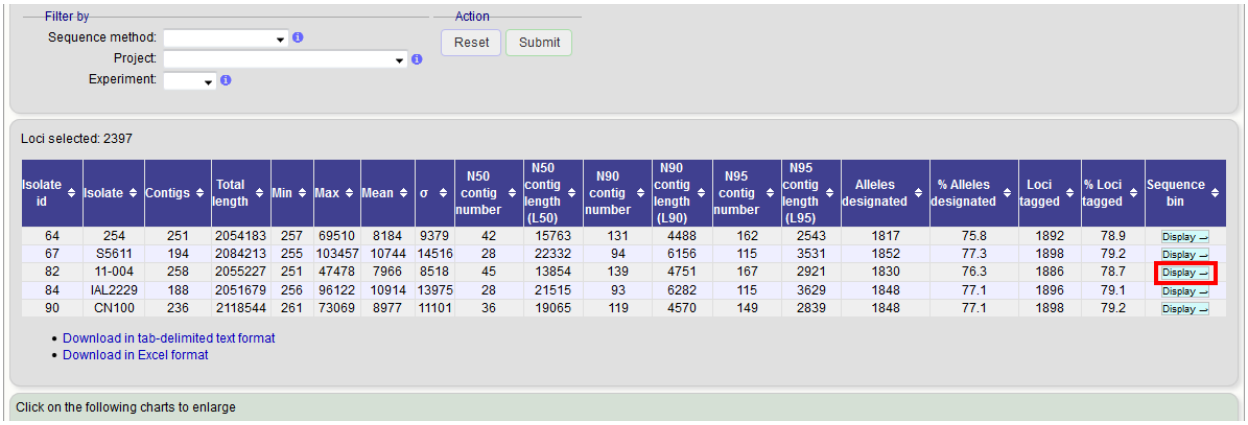
Isolate id	Isolate	Contigs	Total length	Min	Max	Mean	σ	N50 contig number	N50 contig length (L50)	N90 contig number	N90 contig length (L90)	N95 contig number	N95 contig length (L95)	Alleles designated	% Alleles designated	Loci tagged	% Loci tagged	Sequence bin
64	254	251	2054183	257	69510	8184	9379	42	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

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.



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

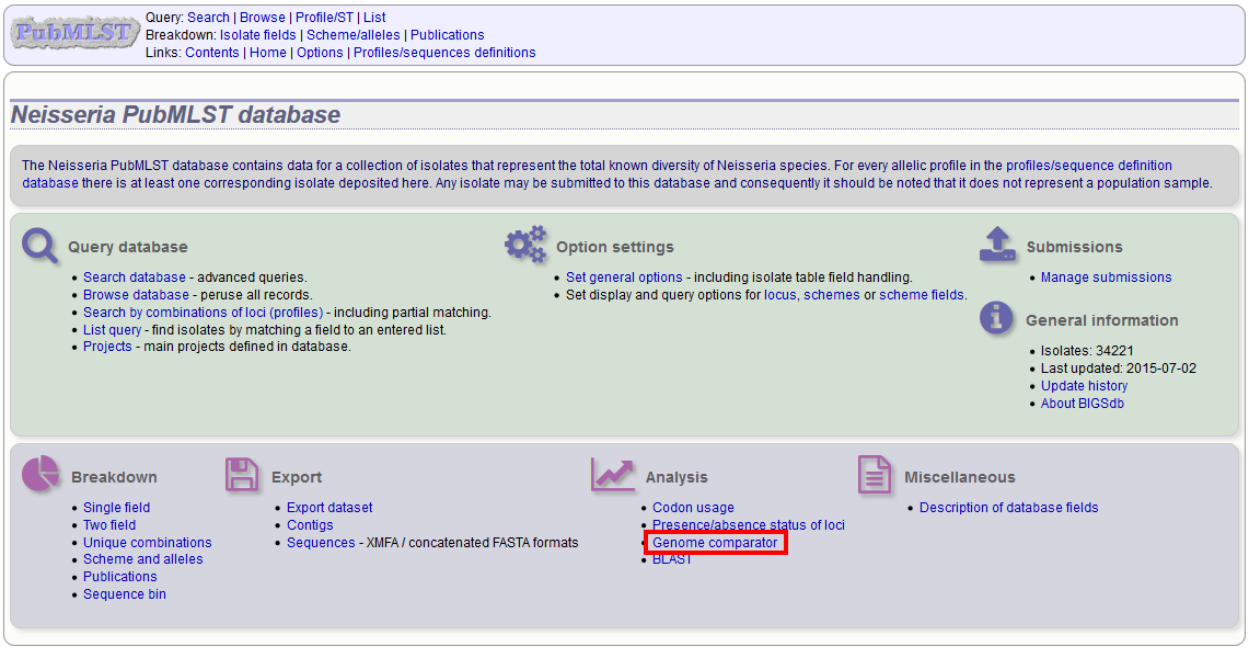


14.6 Genome comparator

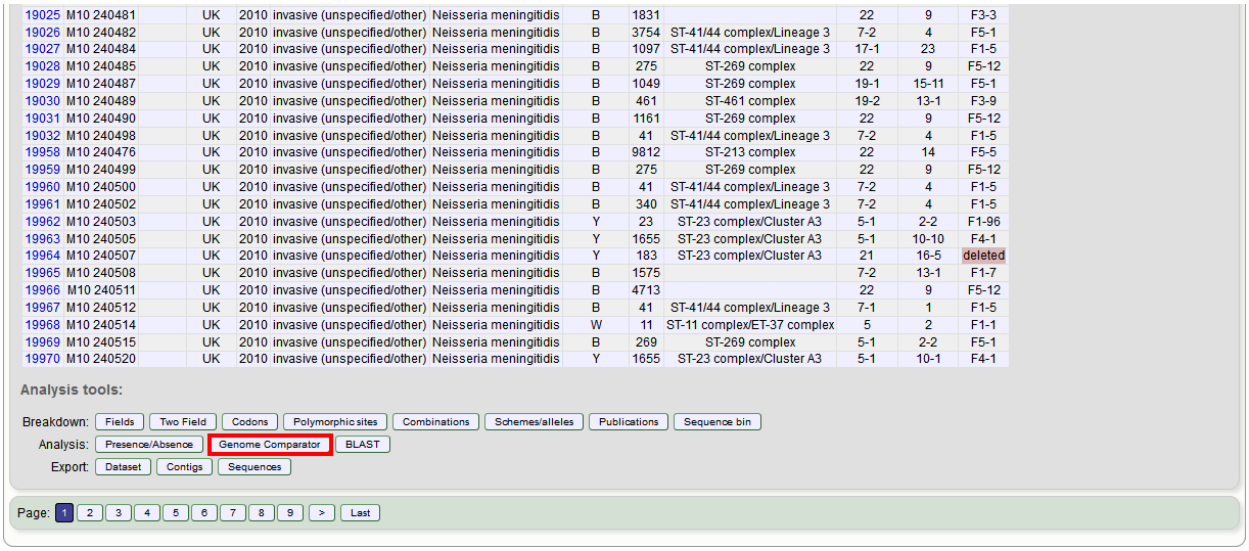
Genome Comparator is an optional plugin that can be enabled for specific databases. It is used to compare whole genome data of isolates within the database using either the database defined loci or the coding sequences of an annotated genome as the comparator.

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

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

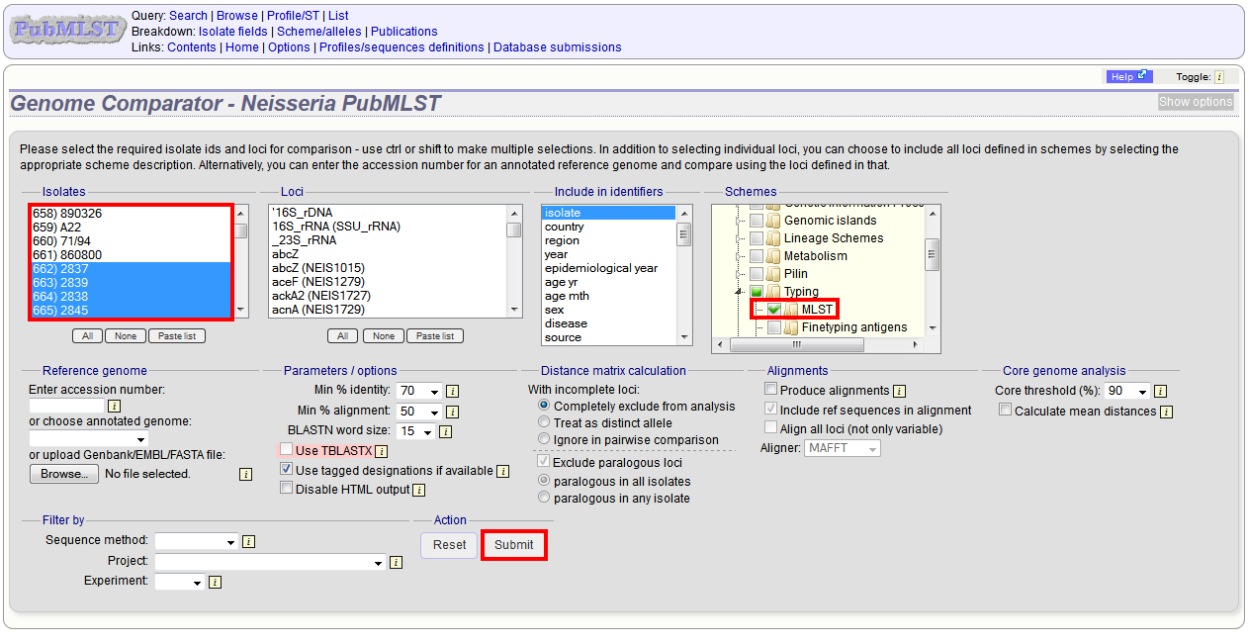


Alternatively, it can be accessed following a query by clicking the 'Genome Comparator' button at the bottom of the results table. Isolates with sequence data returned in the query will be automatically selected within the Genome Comparator interface.



14.6.1 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.

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.

Job status viewer

Status

Job id:	BIGSdb_27748_1405410063_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

Output

Analysis against defined loci

Allele numbers are used where these have been defined, otherwise sequences will be marked as 'New#1, 'New#2' etc. Missing alleles are marked as 'X'. Truncated alleles (located at end of contig) are marked as 'T'.

Locus	644 (L93/4286)	662 (2837)	663 (2839)	664 (2838)	665 (2845)	666 (2843)	667 (2842)	669 (2846)	670 (2840)	671 (2844)	672 (2847)	698 (FAM18)
abcZ	2	2	2	2	2	2	2	7	2	2	2	2
adk	3	3	3	3	3	3	3	3	3	3	3	3
aroE	4	19	4	4	4	4	4	4	19	19	19	4
fumC	3	3	3	3	24	23	23	3	3	3	3	3
gdh	8	8	8	8	8	8	8	8	8	8	8	8
pdhC	4	4	4	4	4	6	6	4	4	4	4	4
pgm	6	6	6	6	6	6	6	6	6	6	6	6

Loci with sequence differences among isolates:

Variable loci: 4

Locus	644 (L93/4286)	662 (2837)	663 (2839)	664 (2838)	665 (2845)	666 (2843)	667 (2842)	669 (2846)	670 (2840)	671 (2844)	672 (2847)	698 (FAM18)
abcZ	2	2	2	2	2	2	2	7	2	2	2	2
aroE	4	19	4	4	4	4	4	4	19	19	19	4
fumC	3	3	3	3	24	23	23	3	3	3	3	3
pdhC	4	4	4	4	4	6	6	4	4	4	4	4

Exactly matching loci

These loci are identical in all isolates.

Matches: 3

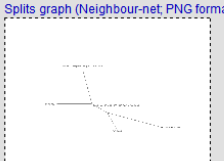
Locus	644 (L93/4286)	662 (2837)	663 (2839)	664 (2838)	665 (2845)	666 (2843)	667 (2842)	669 (2846)	670 (2840)	671 (2844)	672 (2847)	698 (FAM18)
adk	3	3	3	3	3	3	3	3	3	3	3	3
gdh	8	8	8	8	8	8	8	8	8	8	8	8
pgm	6	6	6	6	6	6	6	6	6	6	6	6

Unique strains

Unique strains: 5

Strain 1	Strain 2	Strain 3	Strain 4	Strain 5
644 (L93/4286)	662 (2837)	666 (2843)	665 (2845)	669 (2846)
663 (2839)	670 (2840)	667 (2842)		
664 (2838)	671 (2844)			
698 (FAM18)	672 (2847)			

- Text output file
- Excel format
- Distance matrix (Nexus format) - Suitable for loading in to SplitsTree. Distances between taxa are calculated as the number of loci with different allele sequences
- Splits graph (Neighbour-net; PNG format)



(click to enlarge)

- Splits graph (Neighbour-net; SVG format) - This can be edited in Inkscape or other vector graphics editors
- Locus presence frequency
- Locus presence frequency chart (PNG format)

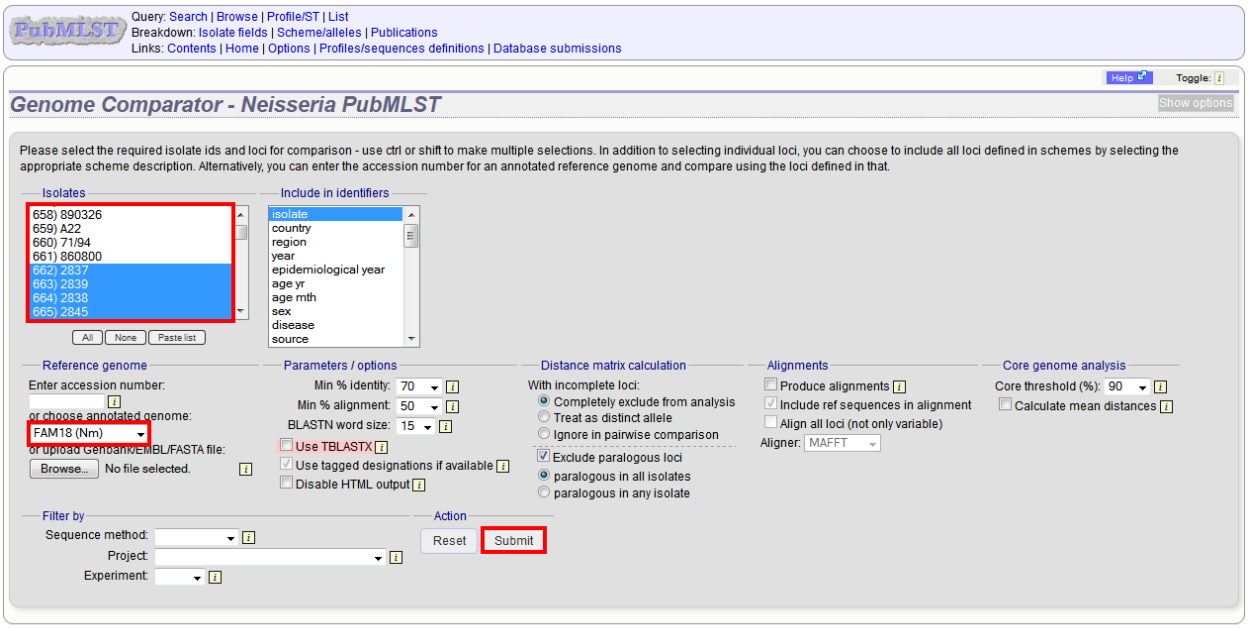
(click to enlarge)

- Tar file containing output files

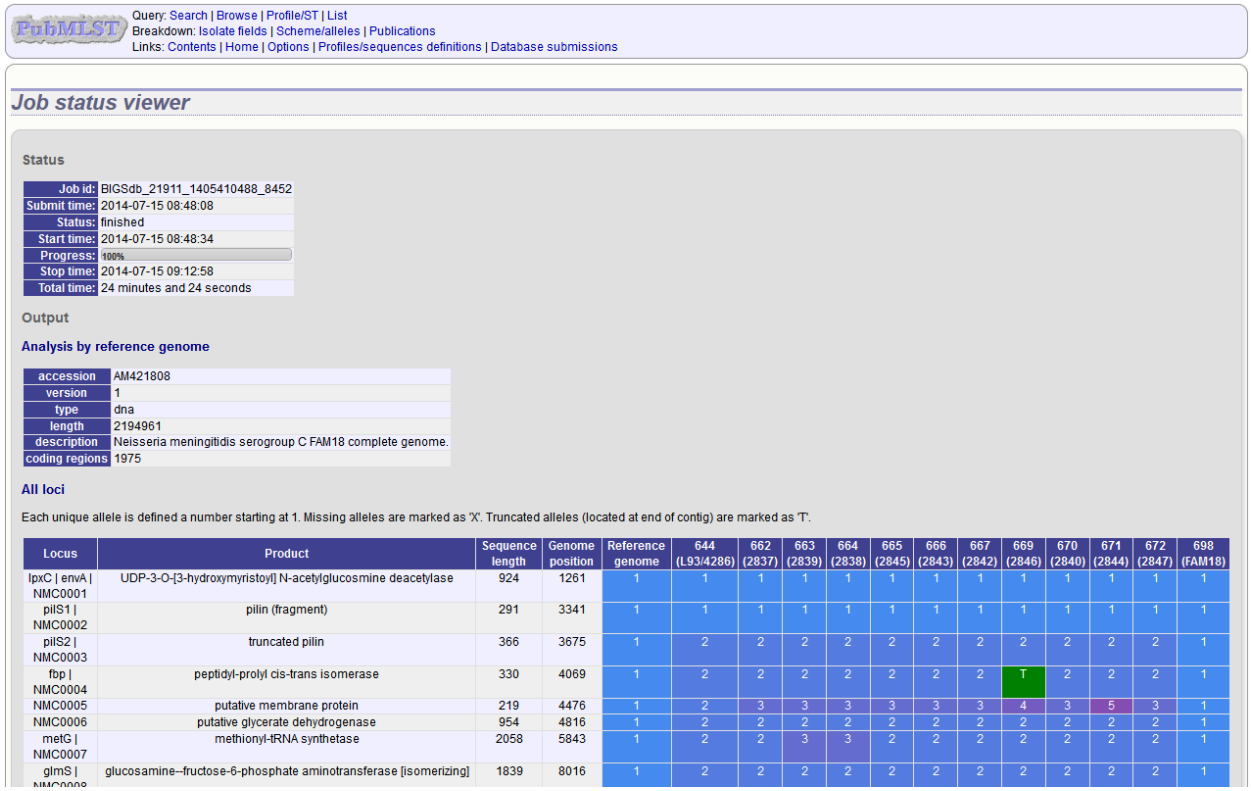
Please note that job results will remain on the server for 7 days.

14.6.2 Analysis using annotated reference genome

Select the isolate genomes that you wish to analyse and then either enter a Genbank accession number for the reference genome, or select from the list of reference genomes (this list will only be present if the administrator has *set it up*). Selecting reference genomes will hide the locus and scheme selection forms.



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.



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

Job status viewer

Status

Job id:	BIGSdb_21911_1405410488_8452
Submit time:	2014-07-15 08:48:08
Status:	finished
Start time:	2014-07-15 08:48:34
Progress:	100%
Stop time:	2014-07-15 09:12:58
Total time:	24 minutes and 24 seconds

Output

Analysis by reference genome

accession	AM421808
version	1
type	dna
length	2194961
description	Neisseria meningitidis serogroup C FAM18 complete genome.
coding regions	1975

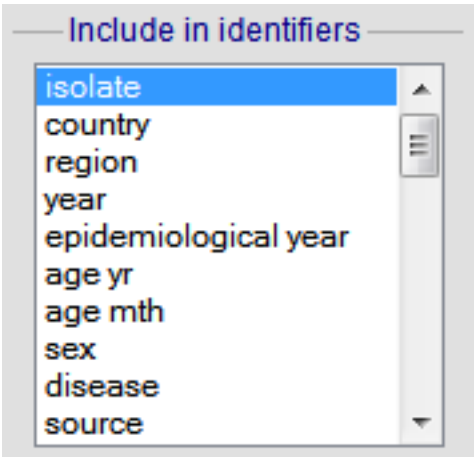
All loci

Each unique allele is defined a number starting at 1. Missing alleles are marked as 'X'. Truncated alleles (located at end of contig) are marked as 'T'.

Locus	Product	Sequence length	Genome position	Reference genome	644 (L93/4286)	662 (2837)	663 (2839)	664 (2838)	665 (2845)	666 (2843)	667 (2842)	669 (2846)	670 (2840)	671 (2844)	672 (2847)	698 (FAM18)
lpxC | envA | NMC0001	UDP-3-O-[3-hydroxymyristoyl] N-acetylglucosmine deacetylase	924	1261	1	1	1	1	1	1	1	1	1	1	1	1	1
pilS1 | NMC0002	pilin (fragment)	291	3341	1	1	1	1	1	1	1	1	1	1	1	1	1
pilS2 | NMC0003	truncated pilin	366	3675	1	2	2	2	2	2	2	2	2	2	2	2	1
fbp | NMC0004	peptidyl-prolyl cis-trans isomerase	330	4069	1	2	2	2	2	2	2	2	T	2	2	2	1
NMC0005	putative membrane protein	219	4476	1	2	3	3	3	3	3	3	4	3	5	3	1
NMC0006	putative glycerate dehydrogenase	954	4816	1	2	2	2	2	2	2	2	2	2	2	2	1
metG | NMC0007	methionyl-tRNA synthetase	2058	5843	1	2	2	3	3	2	2	2	2	2	2	2	1
glmS | NMC0008	glucosamine--fructose-6-phosphate aminotransferase [isomerizing]	1839	8016	1	2	2	2	2	2	2	2	2	2	2	2	1

14.6.3 Include in identifiers fieldset

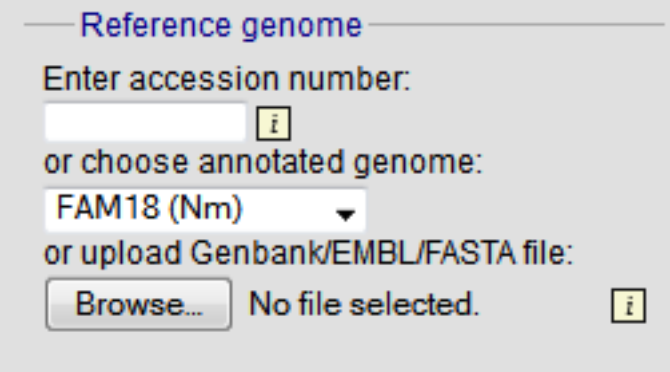
This selection box allows you to choose which isolate provenance fields will be included in the results table. This does not affect the output of the alignments as taxa names are limited in length by the alignment programs.



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

14.6.4 Reference genome fieldset

This section allows you to choose a reference genome to use as the source of comparator sequences.

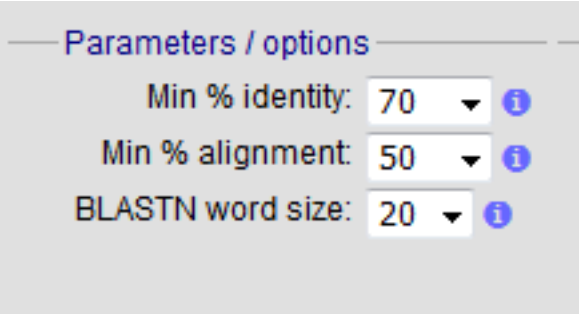


There are three possibilities here:

1. Enter accession number - Enter a Genbank accession number of an annotated reference and Genome Comparator will automatically retrieve this from Genbank.
2. Select from list - The administrator may have selected some genomes to offer for comparison. If these are present, simply select from the list.
3. Upload genome - Click 'Browse' and upload your own reference. This can either be in Genbank, EMBL or FASTA format. Ensure that the filename ends in the appropriate file extension (.gb, .embl, .fas) so that it is recognized.

14.6.5 Parameters/options fieldset

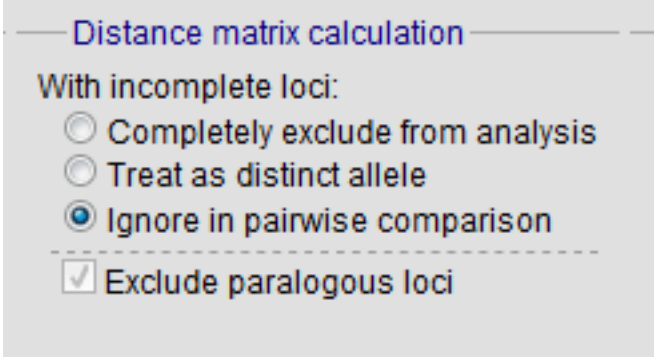
This section allows you to modify BLAST parameters. This affects sensitivity and speed.



- Min % identity - This sets the threshold identity that a matching sequence has to be in order to be considered (default: 70%). Only the best match is used.
- Min % alignment - This sets the percentage of the length of reference allele sequence that the alignment has to cover in order to be considered (default: 50%).
- BLASTN word size - This is the length of the initial identical match that BLAST requires before extending a match (default: 20). Increasing this value improves speed at the expense of sensitivity. The default value gives good results in most cases. The default setting used to be 15 but the new default of 20 is almost as good (there was 1 difference among 2000 loci in a test run) but the analysis runs twice as fast.

14.6.6 Distance matrix calculation fieldset

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



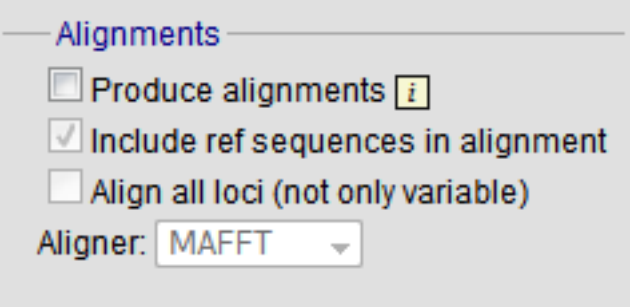
For incomplete loci, i.e. those that continue beyond the end of a contig so are incomplete you can:

- Completely exclude from analysis - Any locus that is incomplete in at least one isolate will be removed from the analysis completely. Using this option means that if there is one bad genome with a lot of incomplete sequences in your analysis, a large proportion of the loci may not be used to calculate distances.
- Treat as a distinct allele - This treats all incomplete sequences as a specific allele 'I'. This varies from any other allele, but all incomplete sequences will be treated as though they were identical.
- Ignore in pairwise comparison (default) - This is probably the best option. In this case, incomplete alleles are only excluded from the analysis when comparing the particular isolate that has it. Other isolates with different alleles will be properly included. The effect of this option will be to shorten the distances of isolates with poorly sequenced genomes with the others.

Paralogous loci, i.e. those with multiple good matches, can be excluded from the analysis (default). This is the safest option since there is no guarantee that differences seen between isolates at paralogous loci are real if the alternative matches are equally good. NB: Loci are also only classed as paralogous when the alternative matches identify different sequences, otherwise multiple contigs of the same sequence region would result in false positives.

14.6.7 Alignments fieldset

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



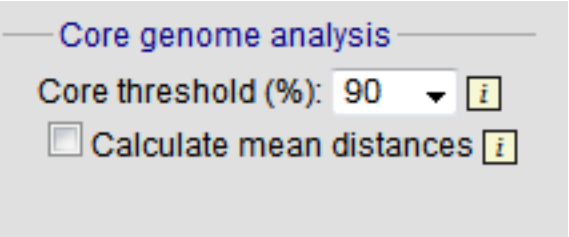
Available options are:

- 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 isused otherwise.

14.6.8 Core genome analysis fieldset

This section enables you to modify the inclusion threshold used to calculate whether or not a locus is part of the core genome (of the dataset).



The default setting of 90% means that a locus is counted as core if it appears within 90% or more of the genomes in the dataset.

There is also an option to calculate the mean distance among sequences of the loci. Selecting this will also select the option to produce alignments.

14.6.9 Filter fieldset

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

Available options are:

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

14.6.10 Understanding the output

14.6.10.1 Distance matrix

The distance matrix is simply a count of the number of loci that differ between each pair of isolates. It is generated in NEXUS format which can be used as the input file for SplitsTree. This can be used to generate NeighborNet, Split

decomposition graphs and trees offline. If 200 isolates or fewer are included in the analysis, a Neighbor network is automatically generated from this distance matrix.

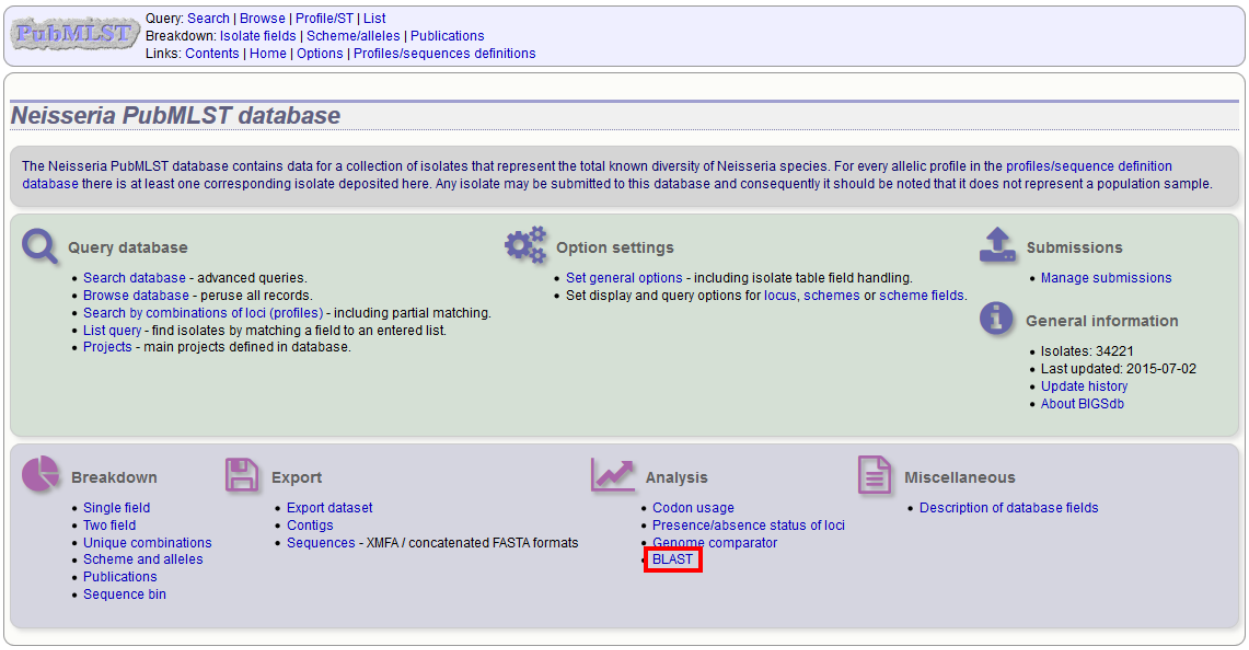
14.6.10.2 Unique strains

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

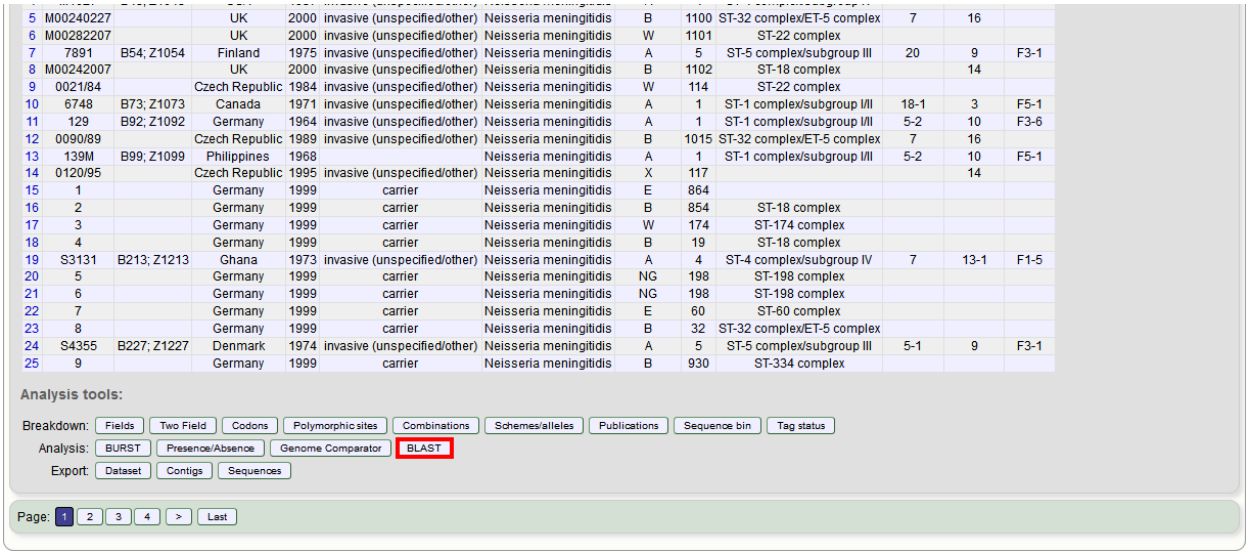
14.7 BLAST

The BLAST plugin enables you to BLAST a sequence against any of the genomes in the database, displaying a table of matches and extracting matching sequences.

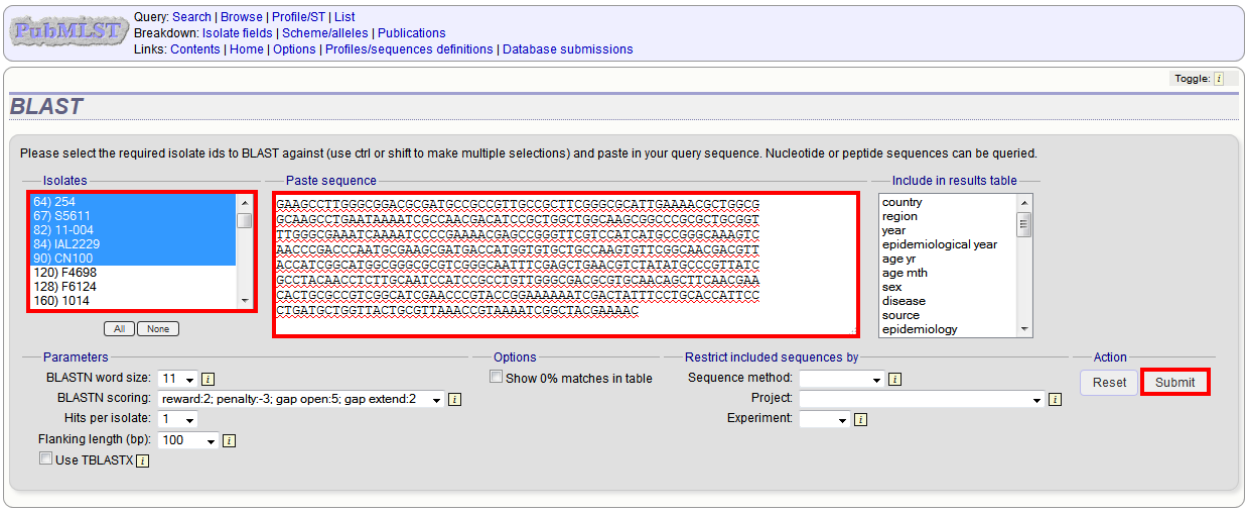
The function can be accessed by selecting the 'BLAST' link on the Analysis section of the main contents page.



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.

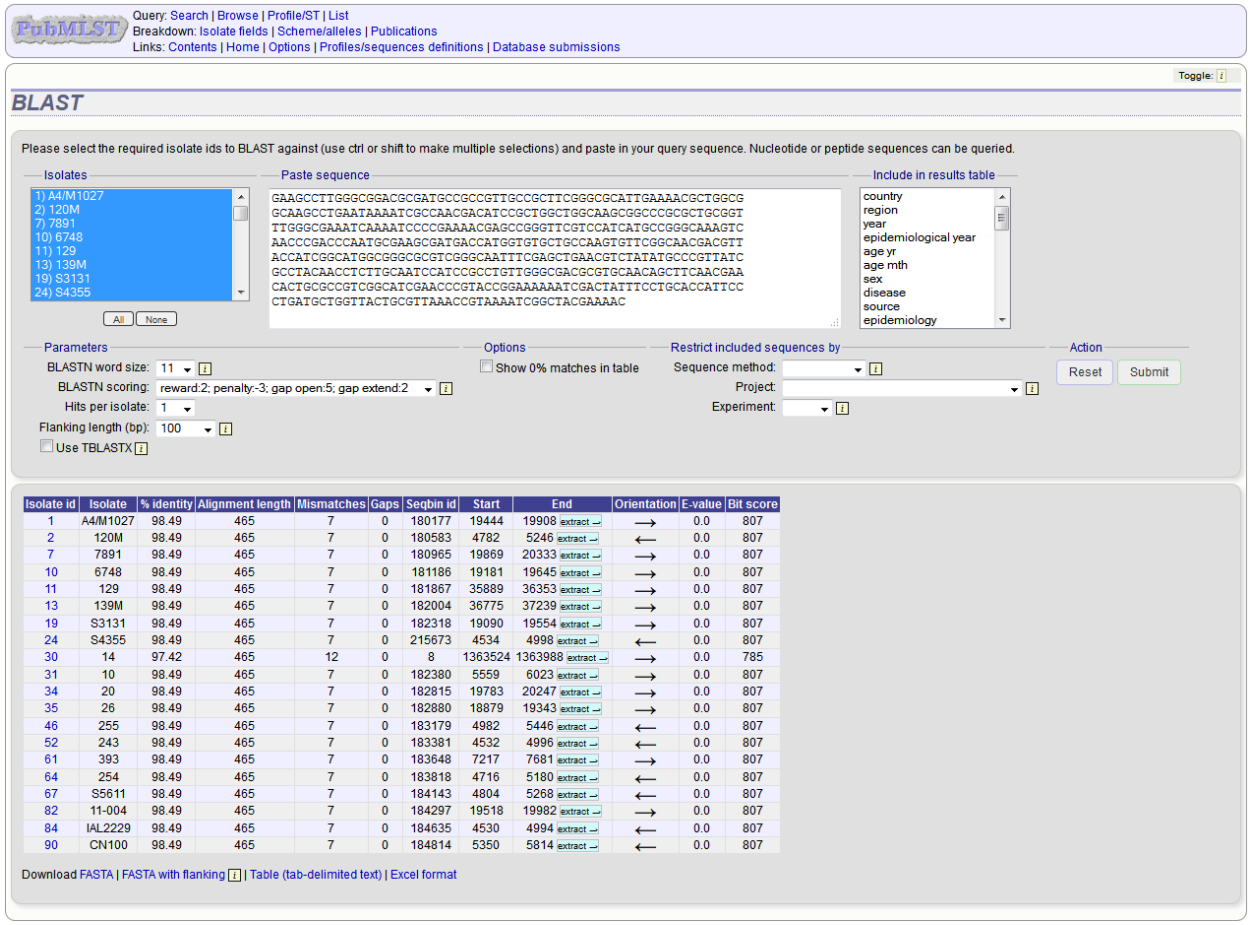


Select the isolate records to analyse - these will be pre-selected if you accessed the plugin following a query. Paste in a sequence to query - this be either a DNA or peptide sequence.

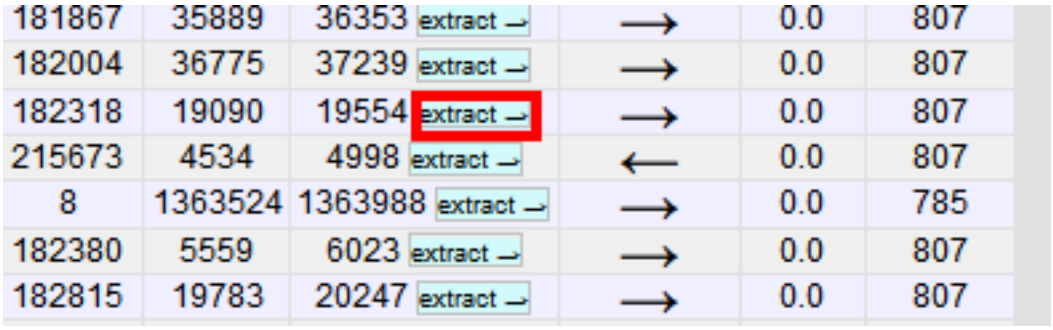


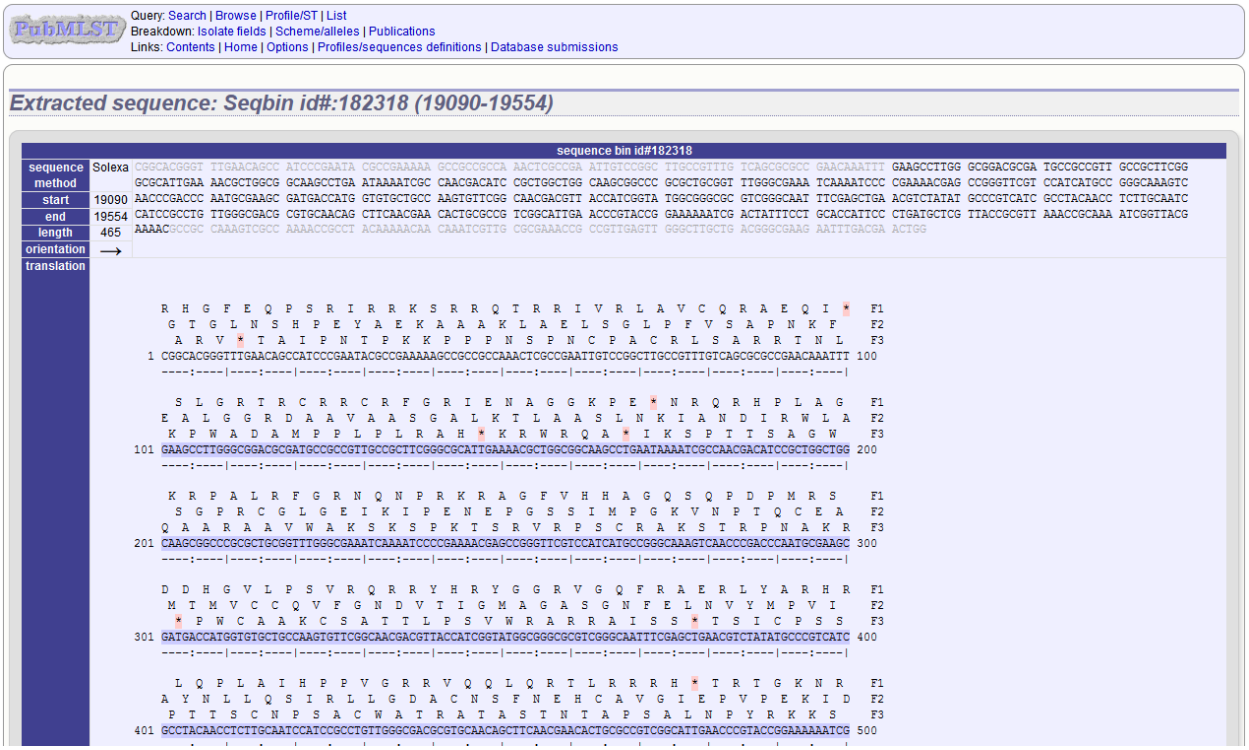
Click submit.

A table of BLAST results will be displayed.

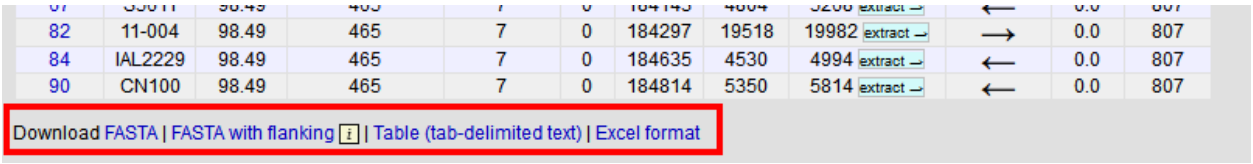


Clicking any of the 'extract' buttons will display the matched sequence along with a translated sequence and flanking sequences.



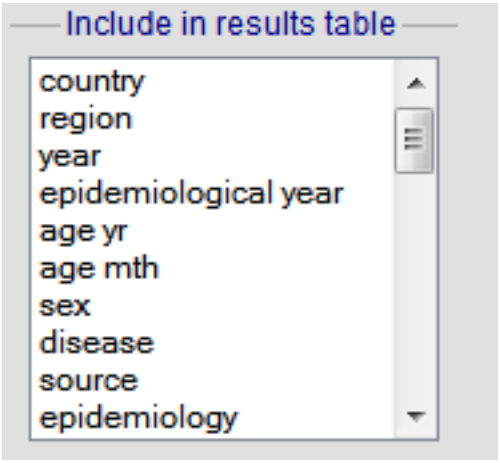


At the bottom of the results table are links to export the matching sequences in FASTA format, (optionall) including flanking sequnces. You can also export the table in tab-delimited text or Excel formats.



14.7.1 Include in results table fieldset

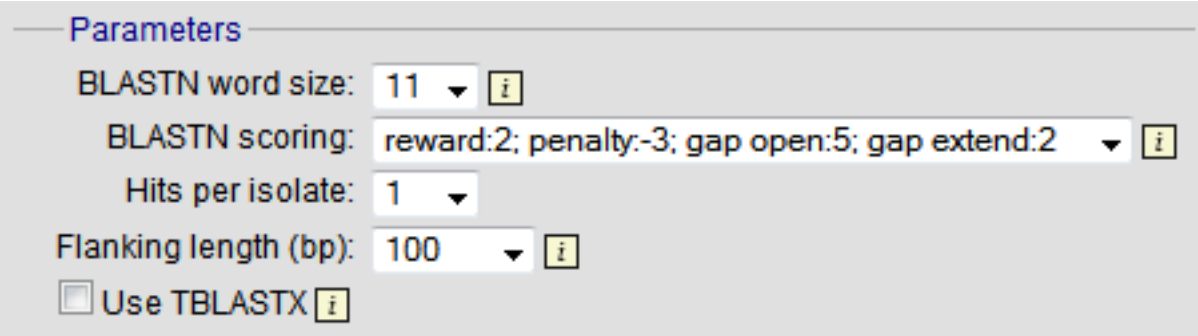
This selection box allows you to choose which isolate provenance fields will be included in the results table.



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

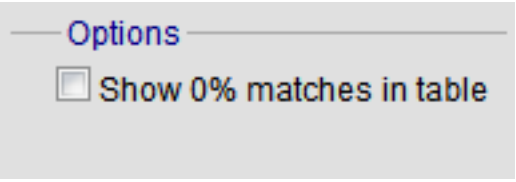
14.7.2 Parameters fieldset

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



- BLASTN word size - This is the length of the initial identical match that BLAST requires before extending a match (default: 11). Increasing this value improves speed at the expense of sensitivity.
- BLASTN scoring - This is a dropdown box of combinations of identical base rewards; mismatch penalties; and gap open and extension penalties. BLASTN has a constrained list of allowed values which reflects the available options in the list.
- Hits per isolate - By default, only the best match is shown. Increase this value to the number of hits you'd like to see per isolate.
- Flanking length - Set the size of the upstream and downstream flanking sequences that you'd like to include.
- Use TBLASTX - This compares the six-frame translation of your nucleotide query sequence against the six-frame translation of the contig sequences. This is significantly slower than using BLASTN.

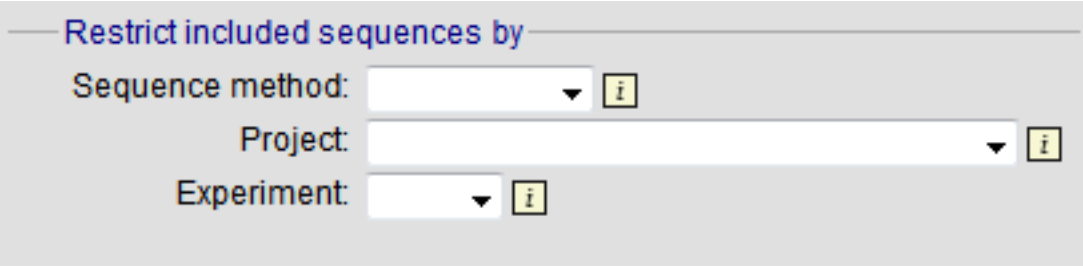
14.7.3 No matches



Click this option to create a row in the table indicating that a match was not found. This can be useful when screening a large number of isolates.

14.7.4 Filter fieldset

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



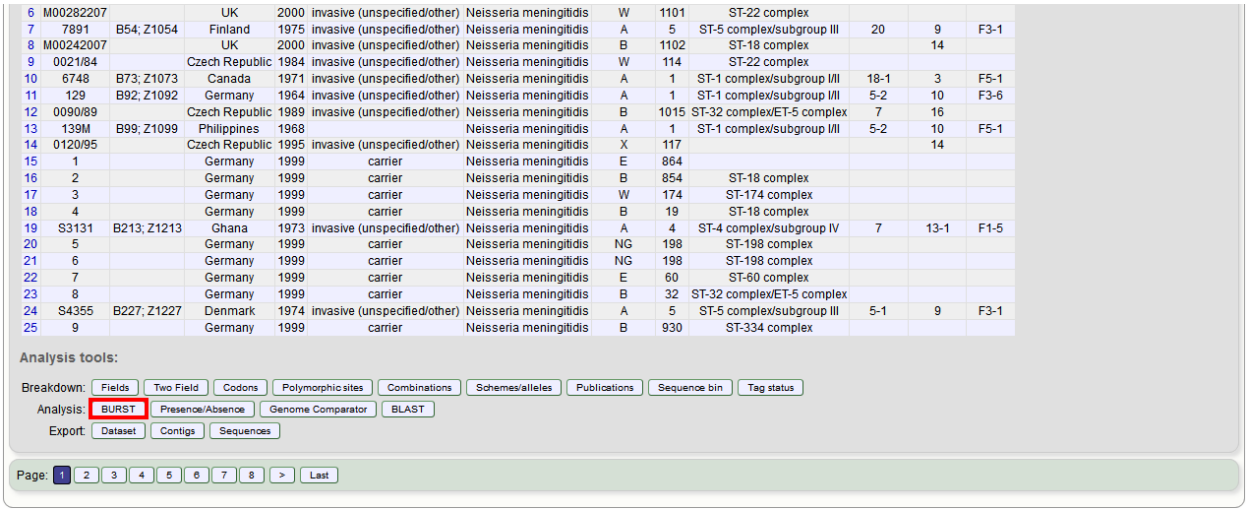
Available options are:

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

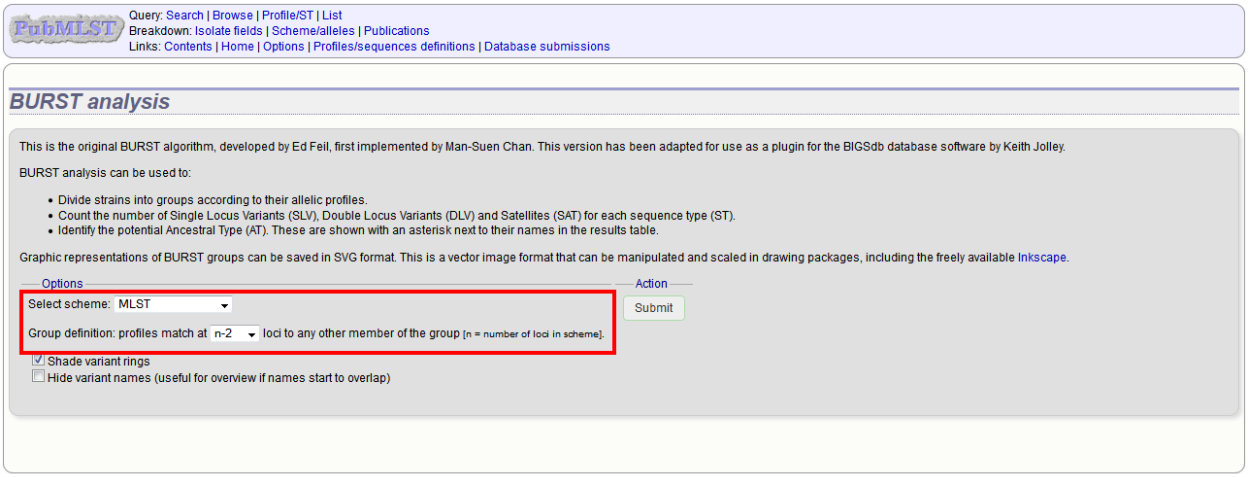
14.8 BURST

BURST is an algorithm used to group MLST-type data based on a count of the number of profiles that match each other at specified numbers of loci. The analysis is available for both sequence definition database and isolate database schemes that have primary key fields set. The algorithm has to be *specifically enabled* by an administrator. Analysis is limited to 1000 or fewer records.

The plugin can be accessed following a query by clicking the 'BURST' button in the Analysis list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.



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

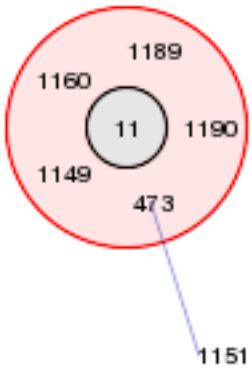


Modifying the group definition affects the size of groups and how they link together. By default, the definition is n-2 (where n is the number of loci), so for example on a 7 locus MLST scheme groups contain STs that match at 5 or more loci to any other member of the group.

Click Submit.

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

group: 2				
ST	Frequency	SLV	DLV	SAT
11*	37	5		1
473	1	2	4	
1149	19	1	4	1
1151	1	0	1	5
1160	1	2	3	1
1189	1	1	4	1
1190	1	1	4	1

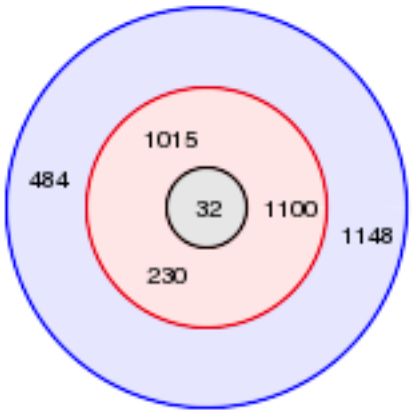


SVG file (right click to save)

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

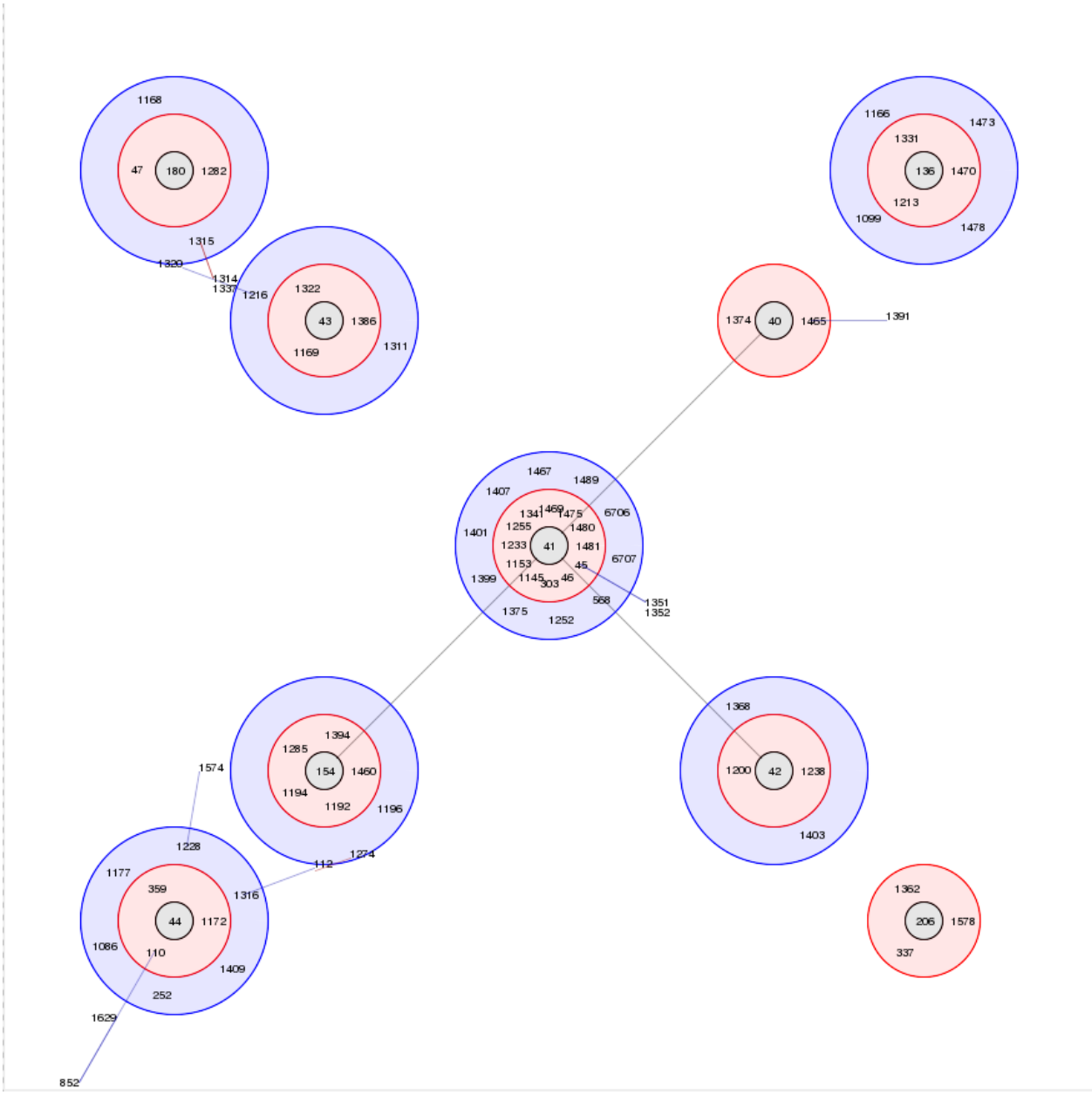
shown in a blue circle.

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



SVG file (right click to save)

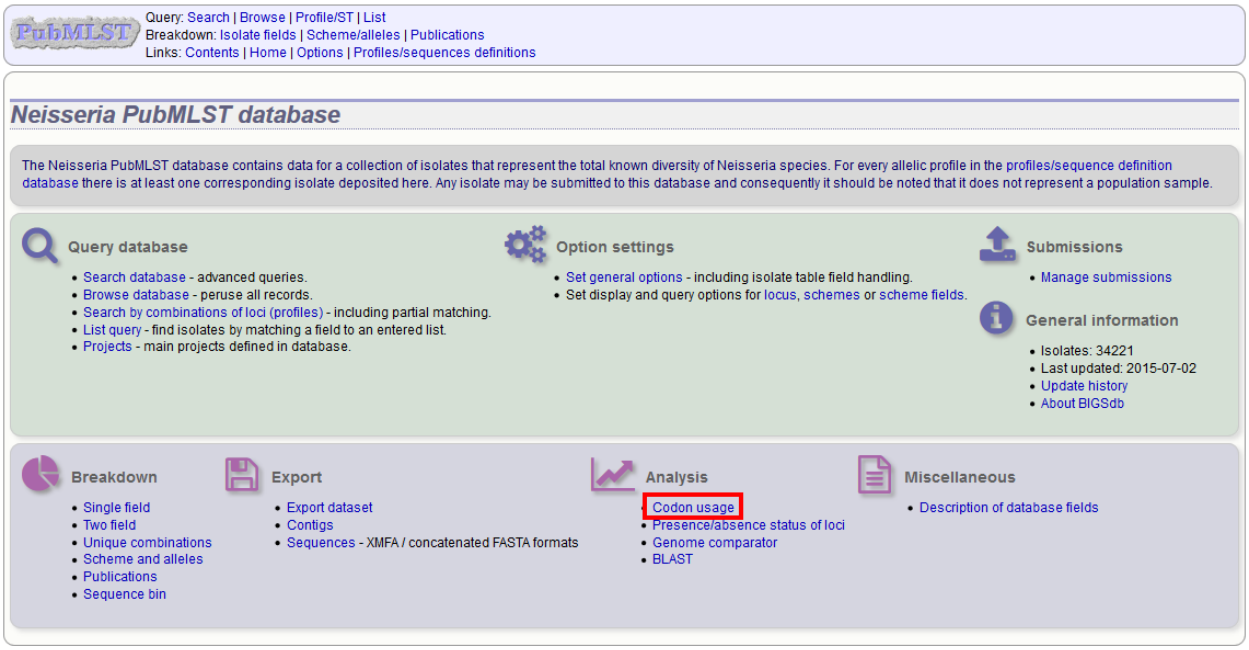
Groups can get very large, where linked profiles form sub-groups and an attempt is made to depict these.



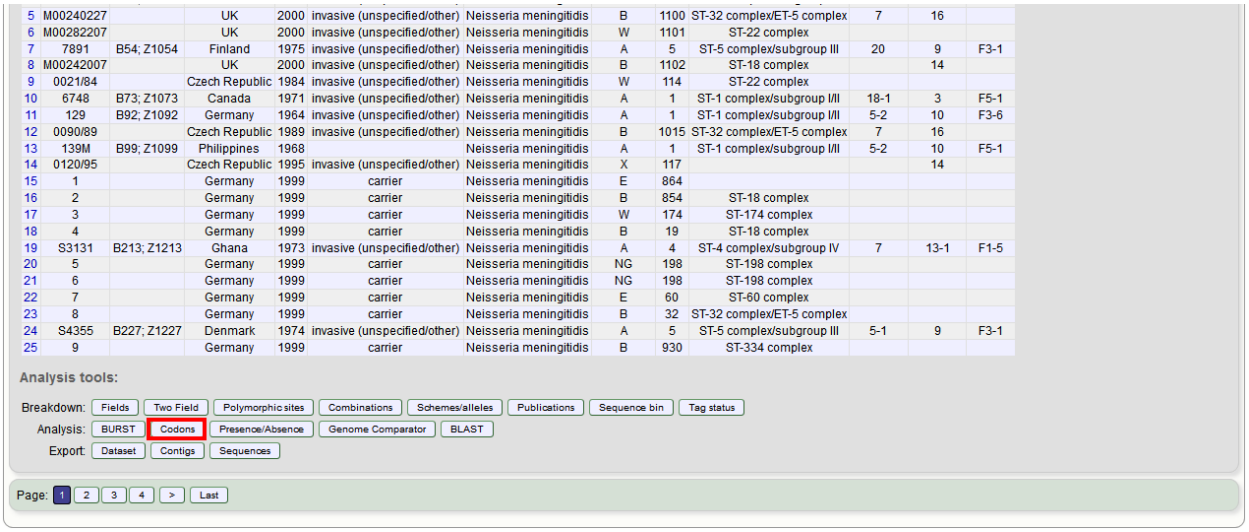
14.9 Codon usage

The codon usage plugin for isolate databases calculates the absolute and relative synonymous codon usage by isolate and by locus.

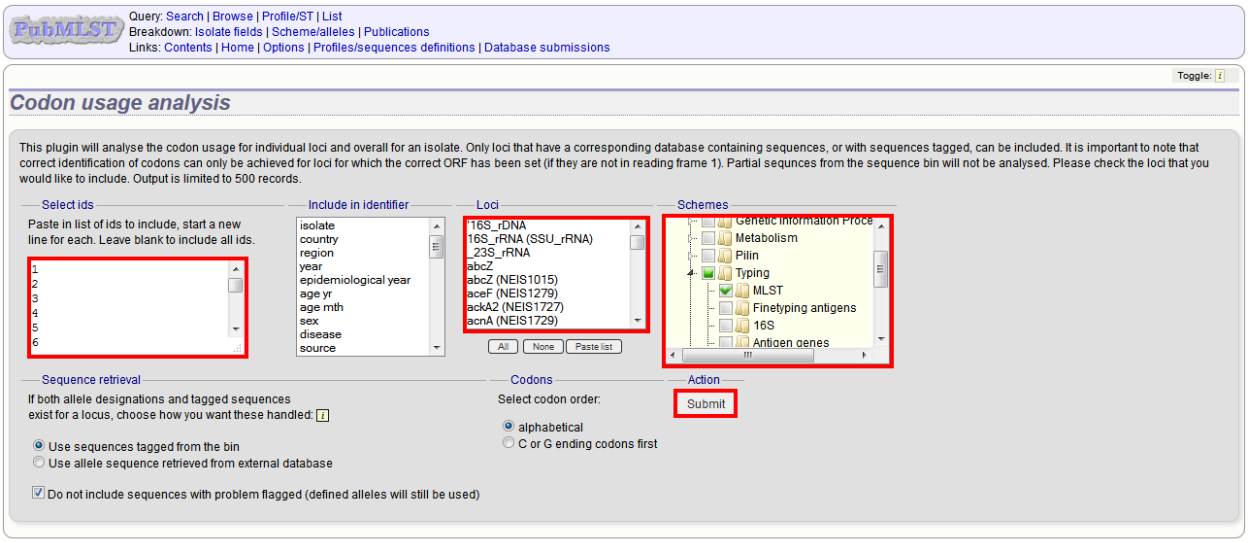
The function can be selected by clicking the 'Codon usage' link in the Analysis section of the main contents page.



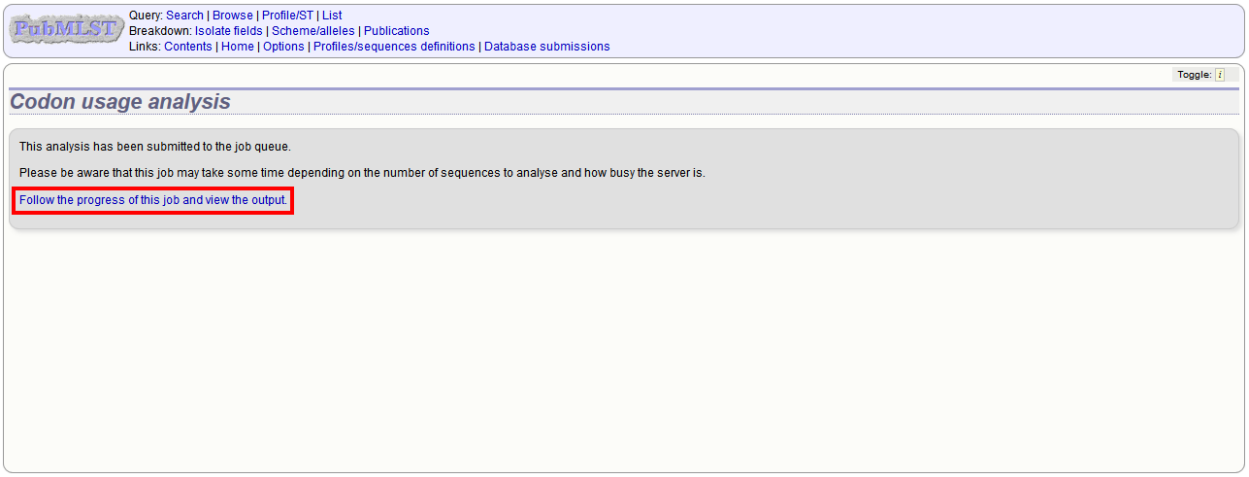
Alternatively, it can be accessed following a query by clicking the 'Codons' button in the Analysis list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.



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



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.



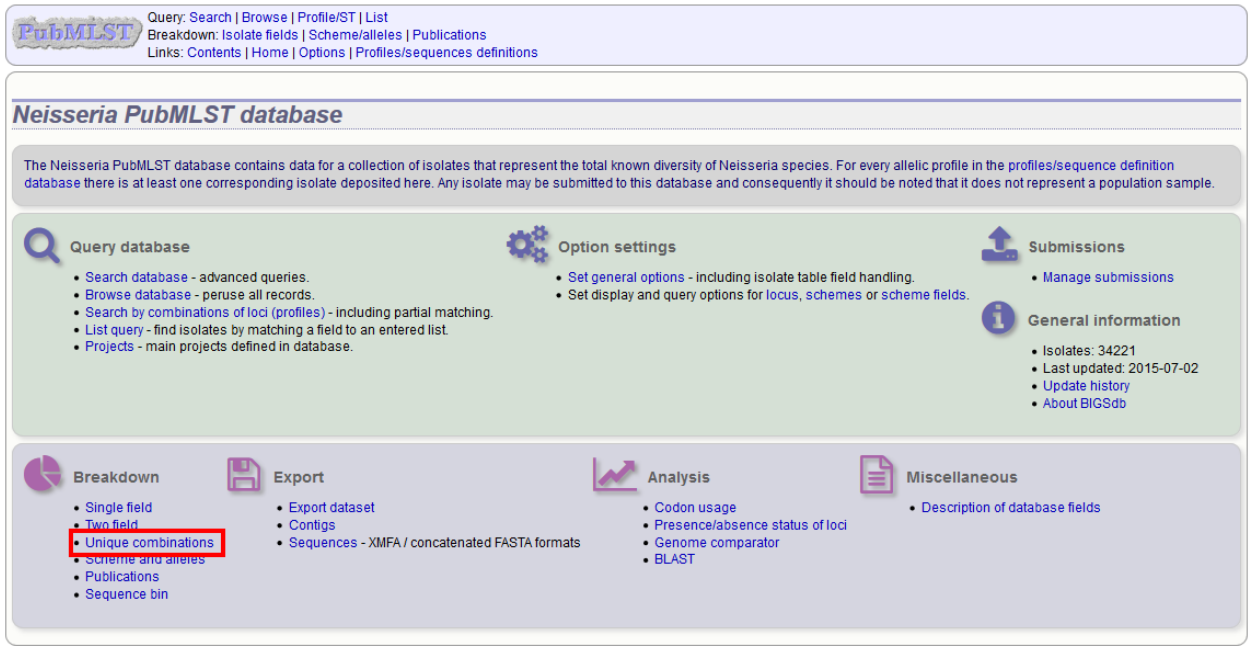
Four tab-delimited text files will be created.

- 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

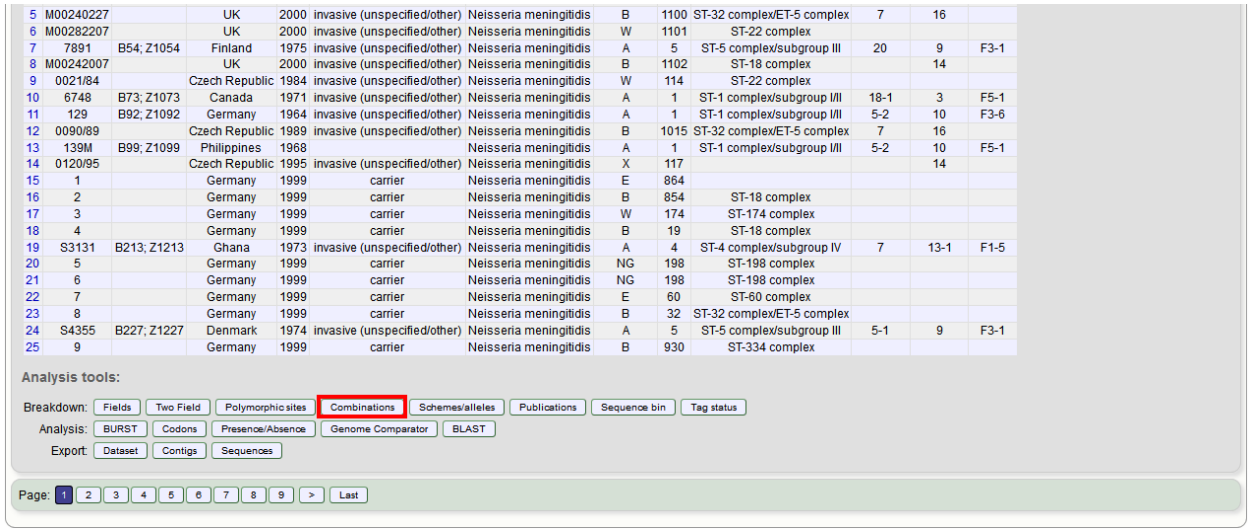
14.10 Unique combinations

The Unique Combinations plugin calculates the frequencies of unique file combinations within an isolate dataset. Provenance fields, composite fields, allele designations and scheme fields can be combined.

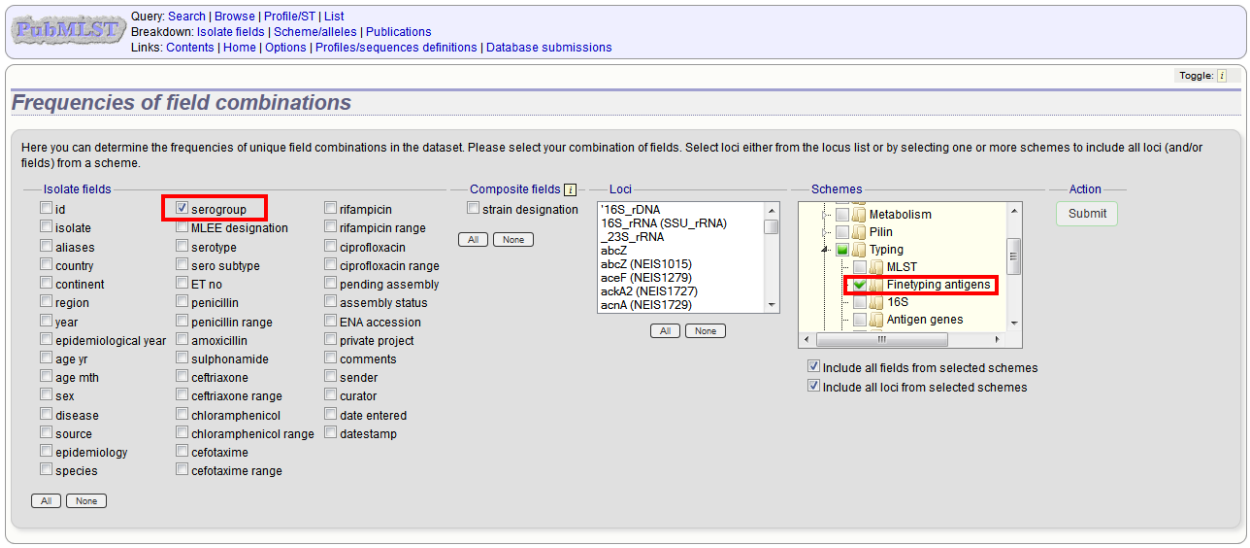
The function can be selected by clicking the 'Unique combinations' link in the Breakdown section of the main contents page. This will run the analysis on the entire database.



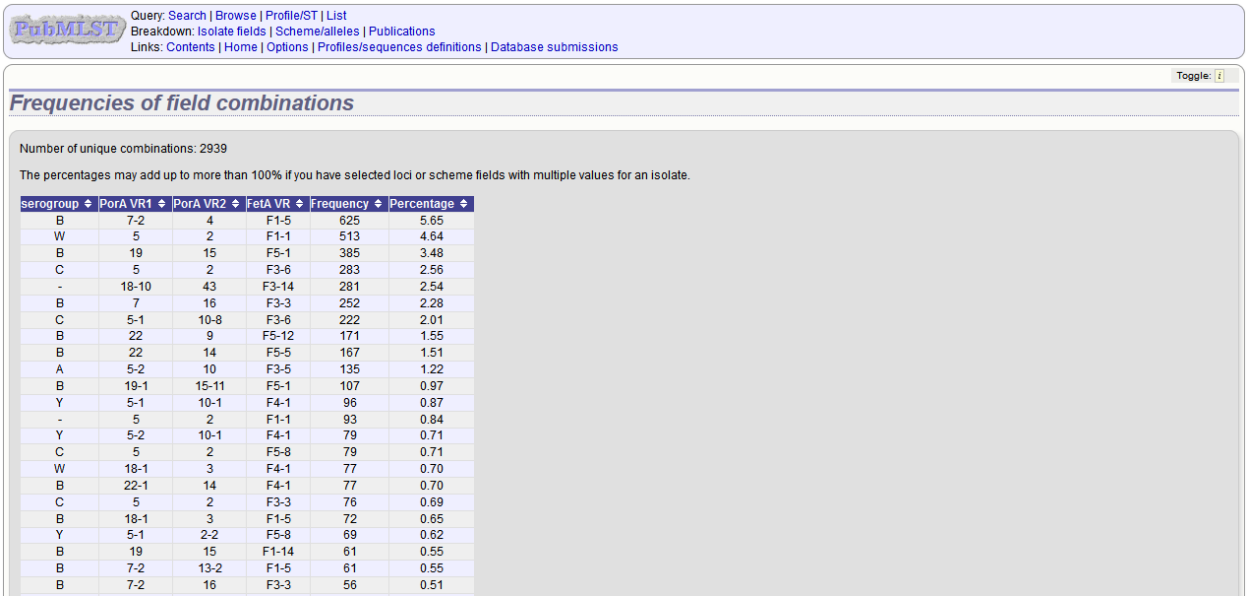
Alternatively, it can be accessed following a query by clicking the 'Combinations' button in the Breakdown list at the bottom of the results table. This will run the analysis on the dataset returned from the query. Please note that the list of functions here may vary depending on the setup of the database.



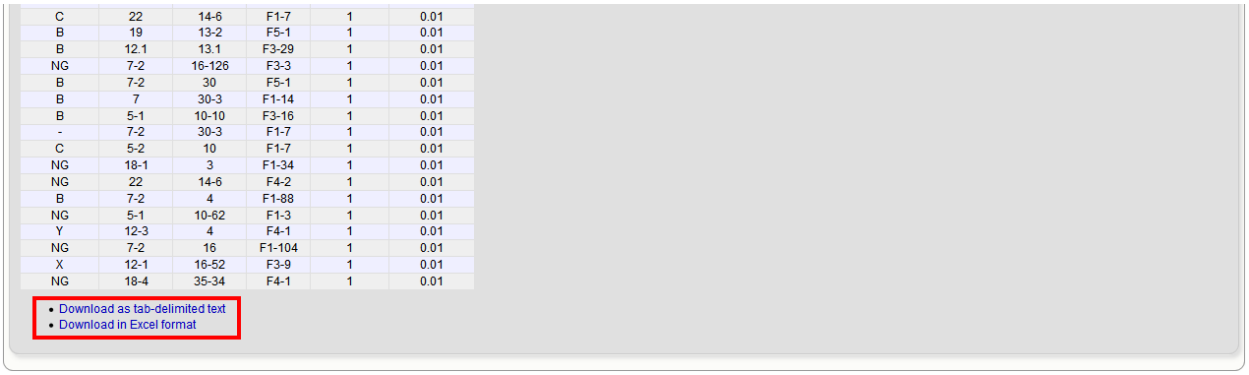
Select the combination of fields to analyse, e.g. serogroup and finetyping antigens.



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.



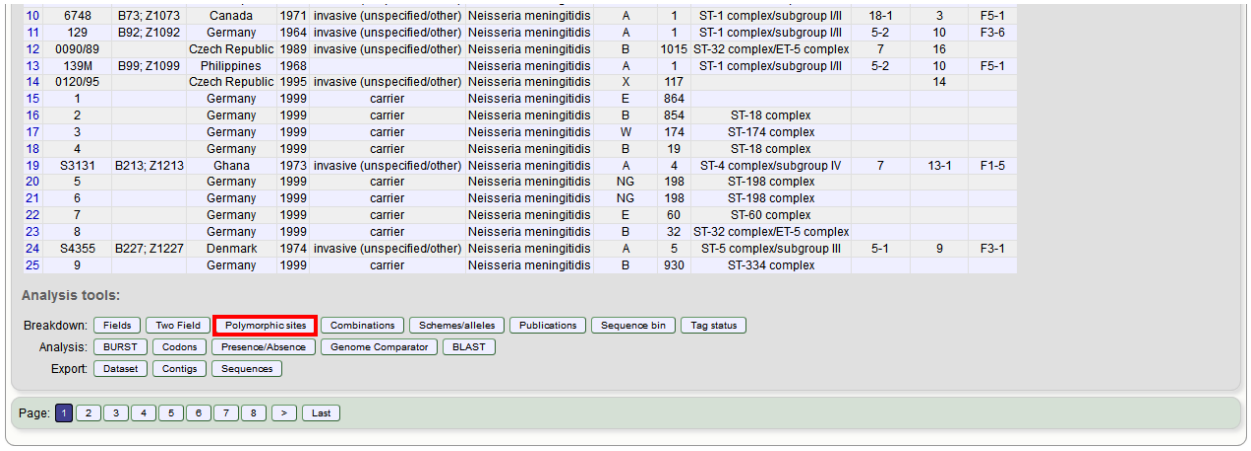
The table can be downloaded in tab-delimited text or Excel formats by clicking the links at the bottom of the page.



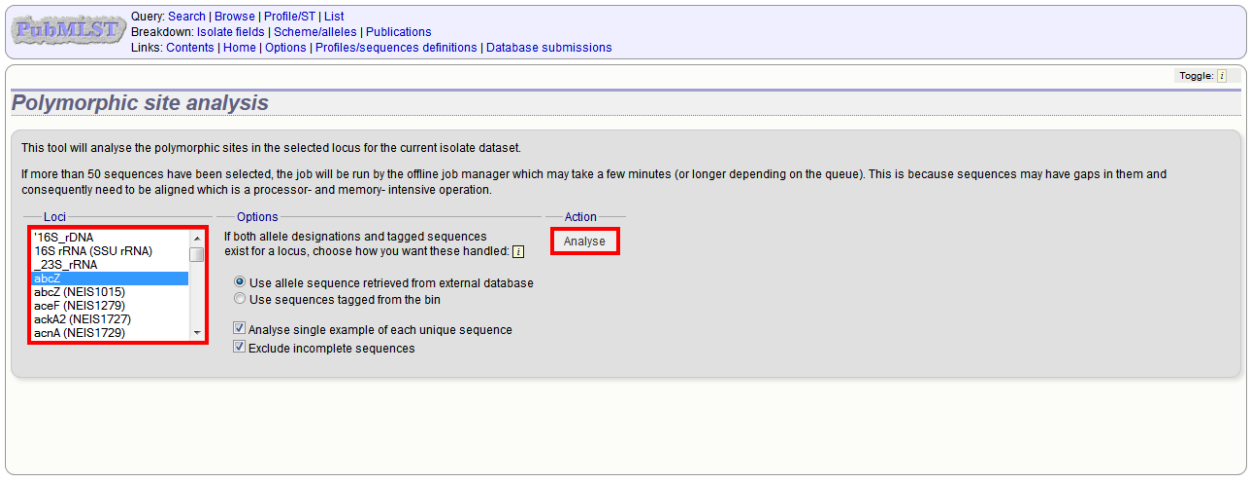
14.11 Polymorphisms

The Polymorphisms plugin generates a *Locus Explorer* polymorphic site analysis on the alleles designated in an isolate dataset following a query.

The analysis is accessed by clicking the 'Polymorphic sites' button in the Breakdown list at the bottom of a results table following a query.

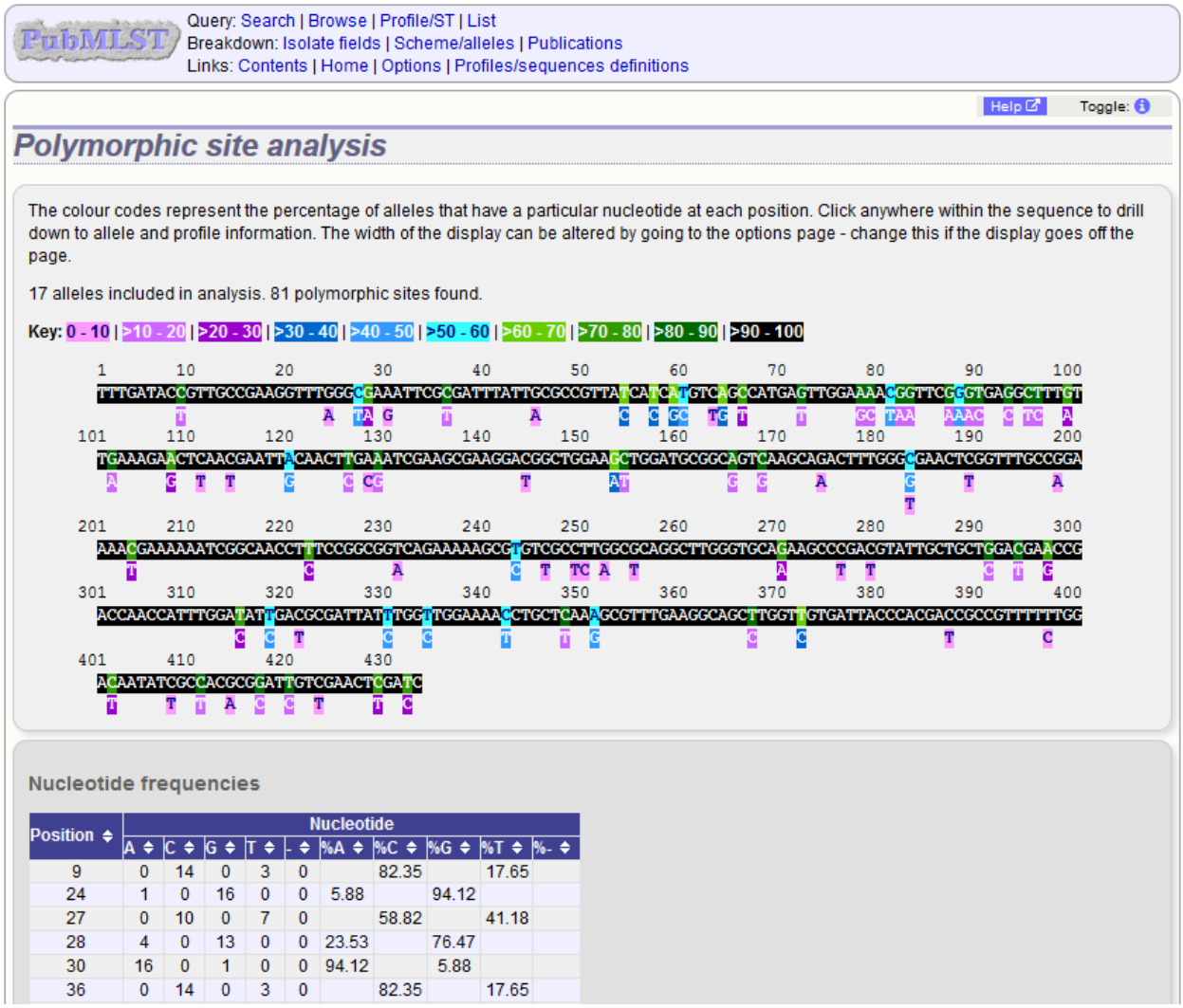


Select the locus that you would like to analyse from the list.



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.

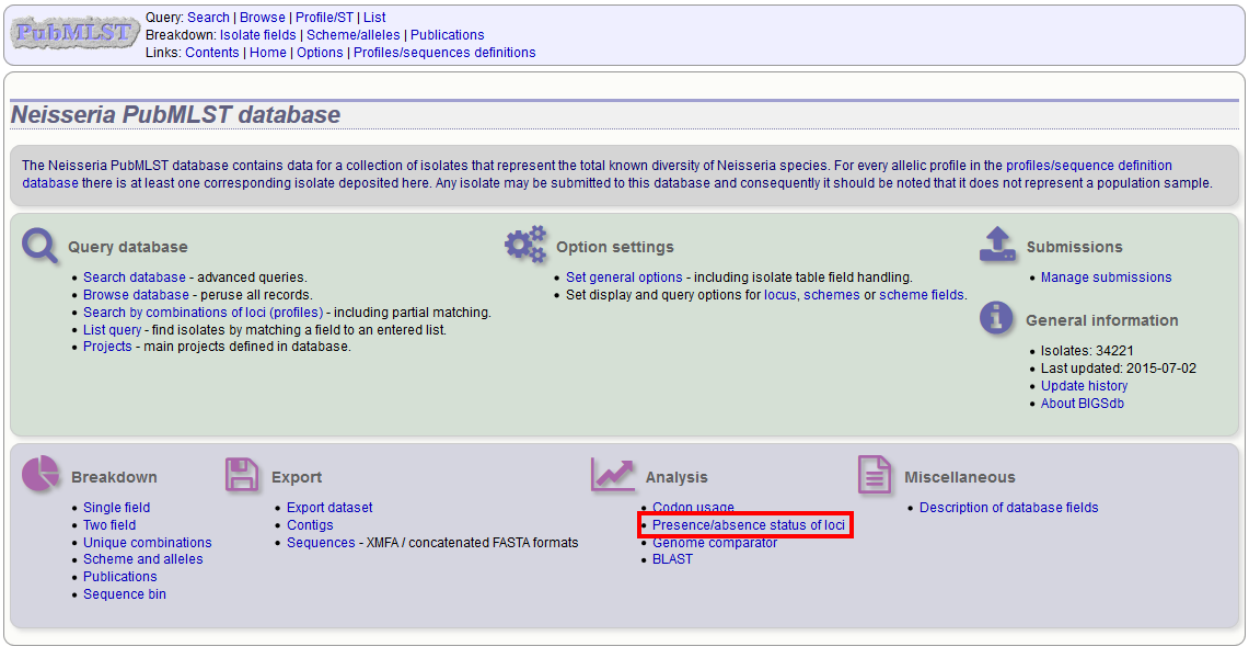


Position	Nucleotide									
	A	C	G	T	-	%A	%C	%G	%T	%-
9	0	14	0	3	0		82.35		17.65	
24	1	0	16	0	0	5.88		94.12		
27	0	10	0	7	0		58.82		41.18	
28	4	0	13	0	0	23.53		76.47		
30	16	0	1	0	0	94.12		5.88		
36	0	14	0	3	0		82.35		17.65	

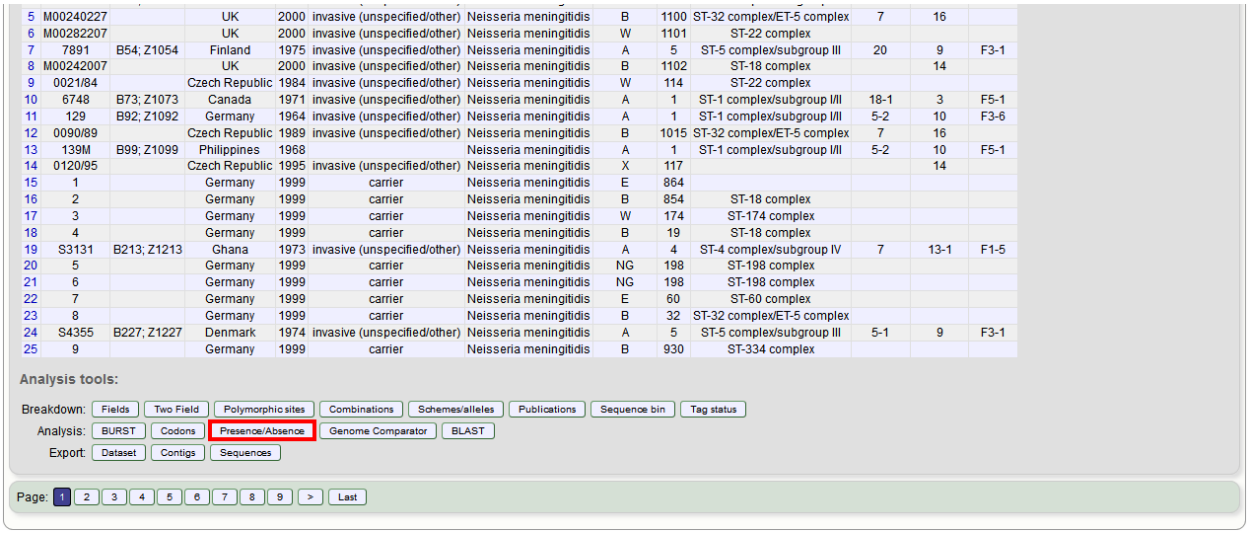
14.12 Presence/absence

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

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

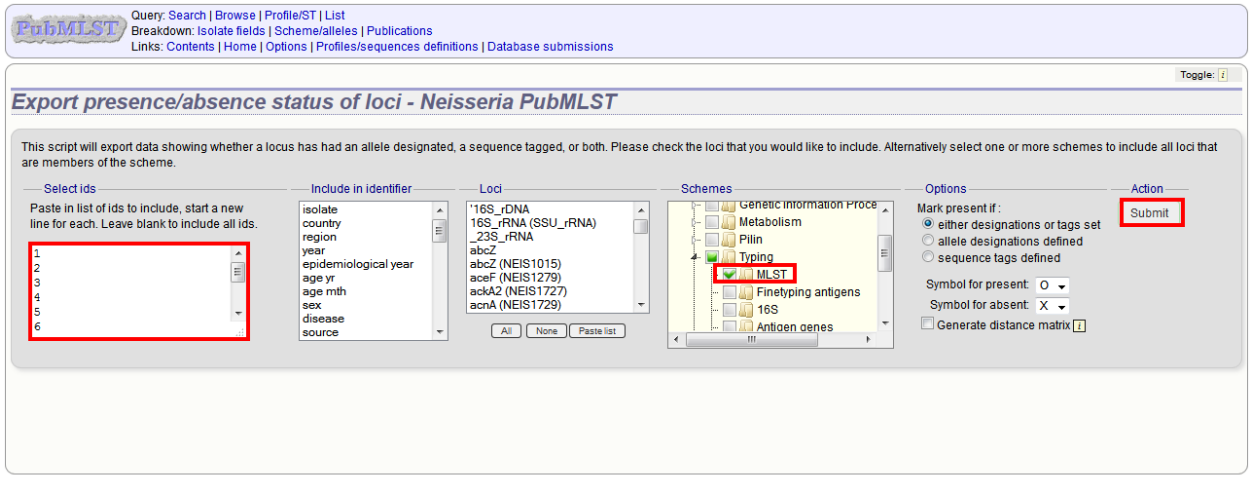


Alternatively, it can be accessed following a query by clicking the 'Presence/Absence' button in the Analysis list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.

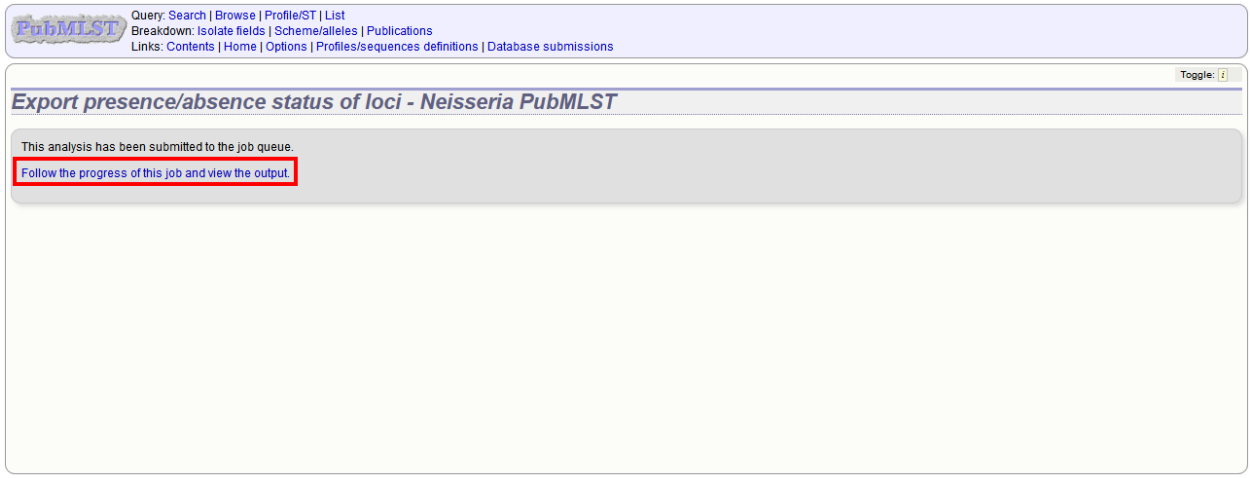


5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	B	1100	ST-32 complex/ET-5 complex	7	16	
6	M00282207		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	W	1101	ST-22 complex			
7	7891	B54; Z1054	Finland	1975	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5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

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.



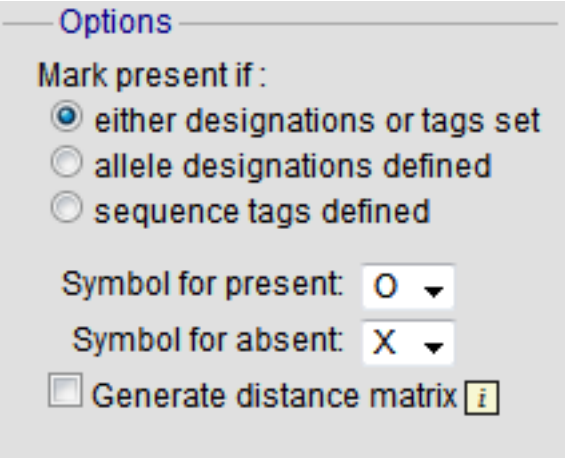
When complete, a single text file will have been generated.

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	O	O	O	O	O	O	O
2	O	O	O	O	O	O	O
3	O	O	O	O	O	O	O
4	O	O	O	O	O	O	O
5	O	O	O	O	O	O	O
6	O	O	O	O	O	O	O
7	O	O	O	O	O	O	O
8	O	O	O	O	O	O	O
9	O	O	O	O	O	O	O
10	O	O	O	O	O	O	O

14.12.1 Options

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

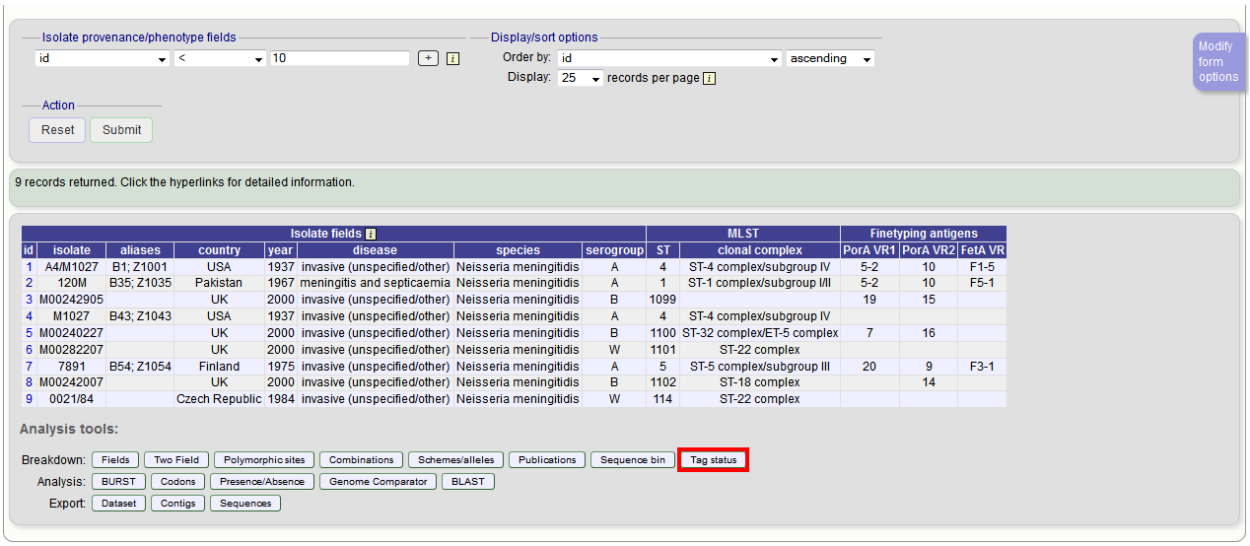


With these you can change the symbols used and whether designations, or tags, or both are counted.

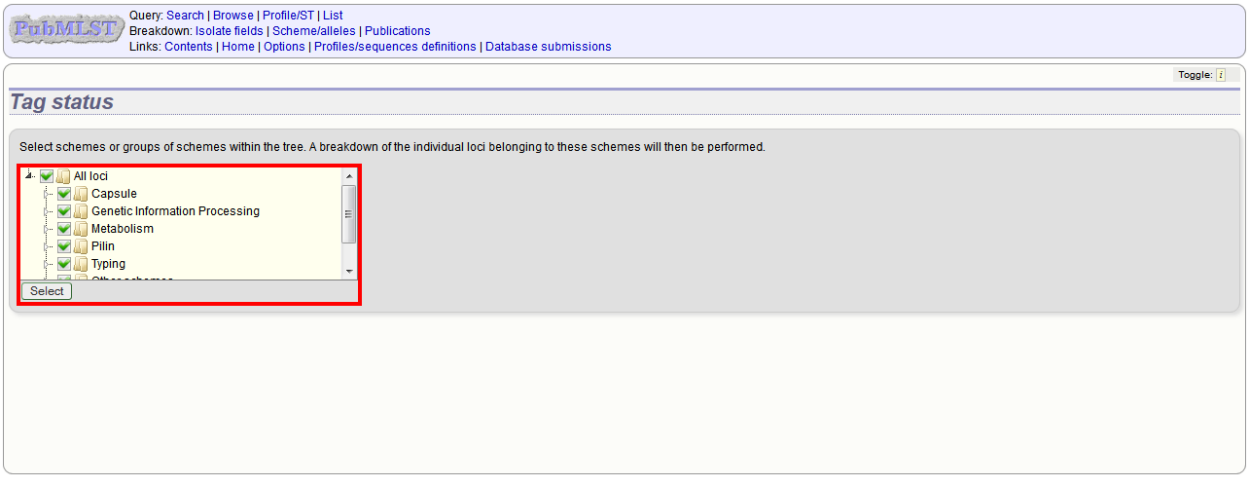
You can also choose to generate a distance matrix based on presence/absence.

14.13 Tag status

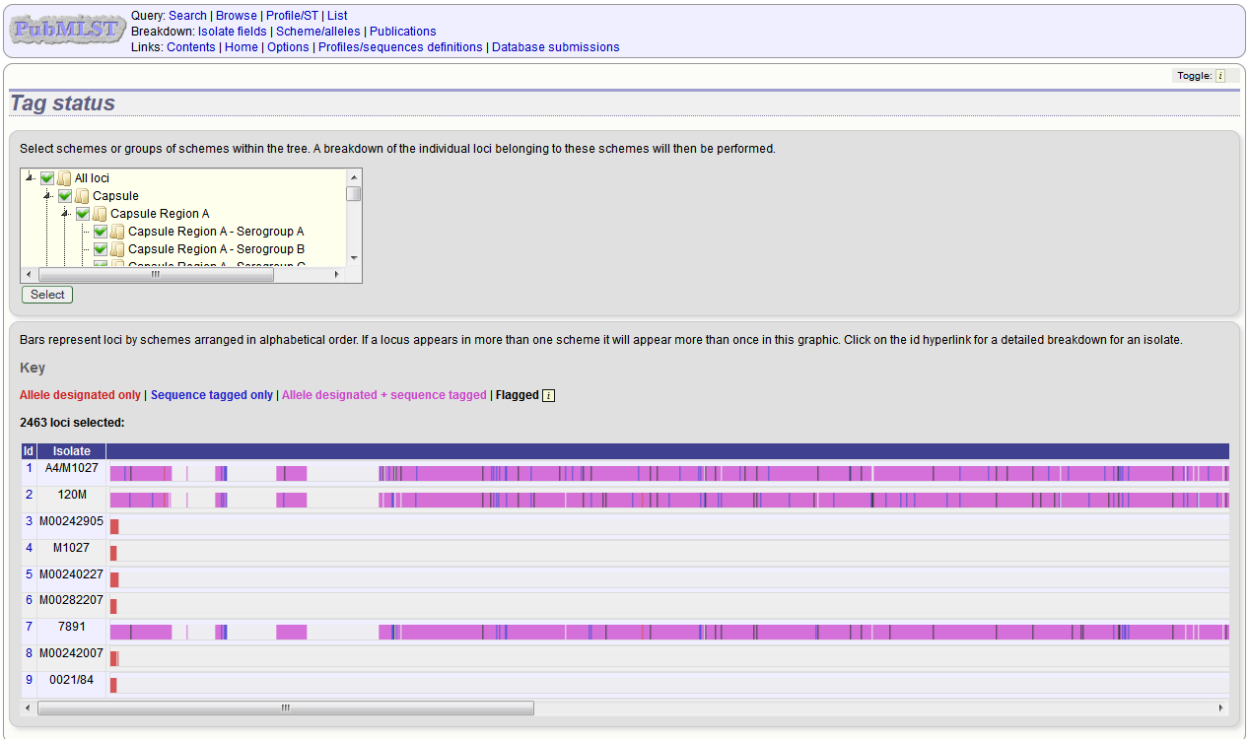
The tag status plugin displays a graphical representation of the status of loci designations or tags for isolate data. It is accessed following a query by clicking the 'Tag status' button in the Breakdown section at the bottom of the results table.



Select the loci you would like to analyse.



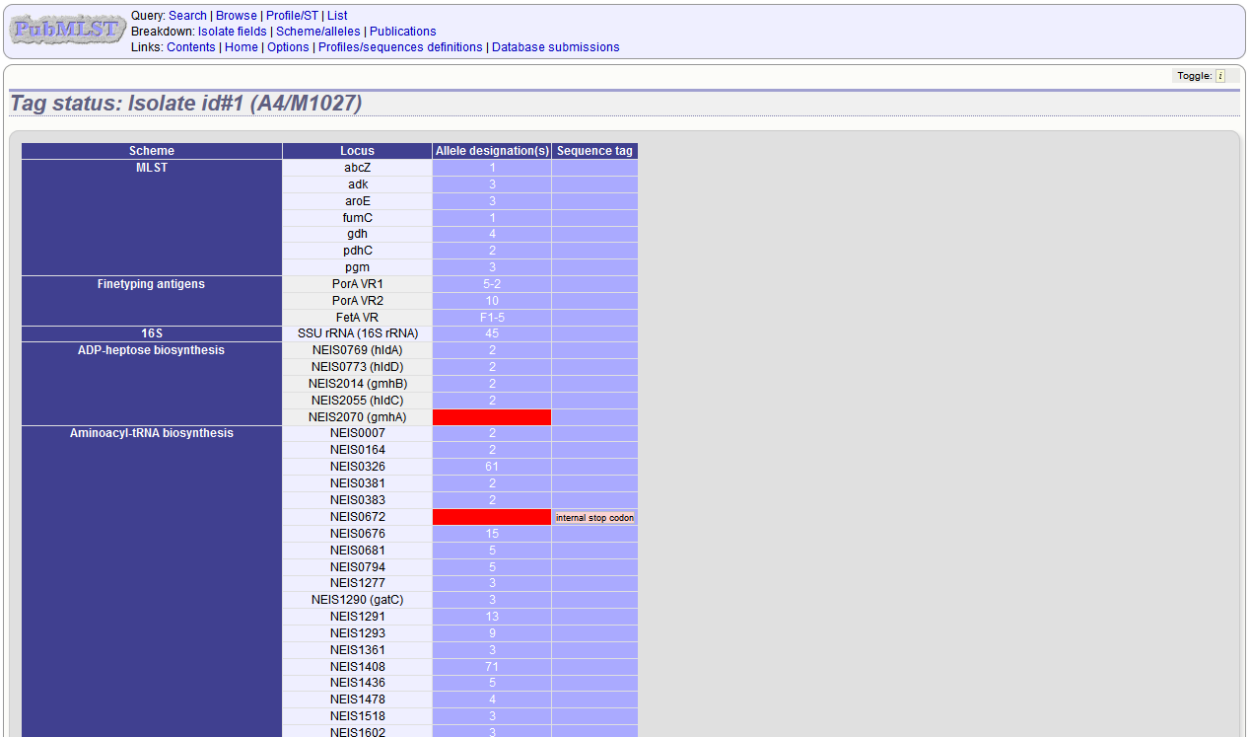
You should see a series of bars representing loci. The colour of these bars designates whether they have an allele designation only, a sequence tag only, both designations or tags, or whether they have flags set.



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

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

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



Scheme	Locus	Allele designation(s)	Sequence tag
MLST	abcZ	1	
	adk	3	
	aroE	3	
	fumC	1	
	gdh	4	
	pdhC	2	
	pgm	3	
Finetyping antigens	PorA VR1	5-2	
	PorA VR2	10	
	FetA VR	F1-5	
16S	SSU rRNA (16S rRNA)	45	
ADP-heptose biosynthesis	NEIS0769 (hldA)	2	
	NEIS0773 (hldD)	2	
	NEIS2014 (gmhB)	2	
	NEIS2055 (hldC)	2	
	NEIS2070 (gmhA)		
Aminoacyl-tRNA biosynthesis	NEIS0007	2	
	NEIS0164	2	
	NEIS0326	61	
	NEIS0381	2	
	NEIS0383	2	
	NEIS0672		internal stop codon
	NEIS0676	15	
	NEIS0681	5	
	NEIS0794	5	
	NEIS1277	3	
	NEIS1290 (gatC)	3	
	NEIS1291	13	
	NEIS1293	9	
	NEIS1361	3	
	NEIS1408	71	
	NEIS1436	5	
	NEIS1478	4	
	NEIS1518	3	
	NEIS1602	3	

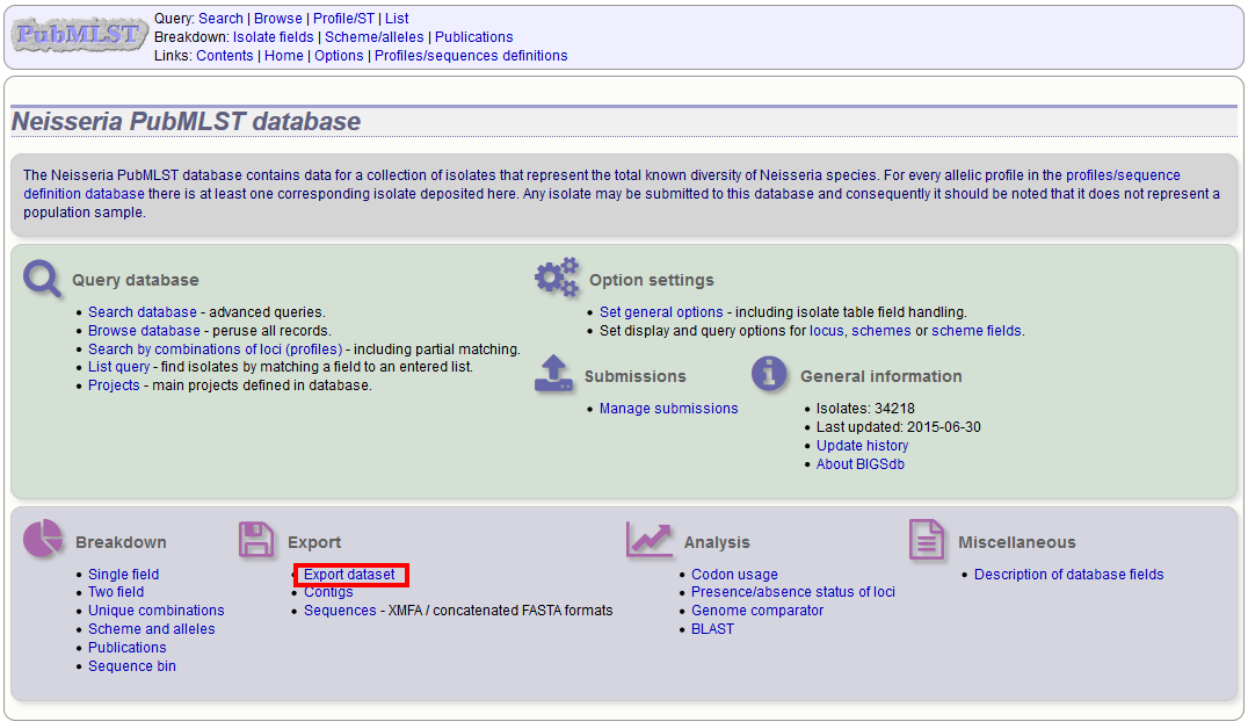
There is a column each for allele designations and sequence tags. If an allele designation is defined, the allele identifier is displayed. Cells shaded in blue show that the designation or tag is present, whereas red indicates thet they are absent.

CHAPTER 15

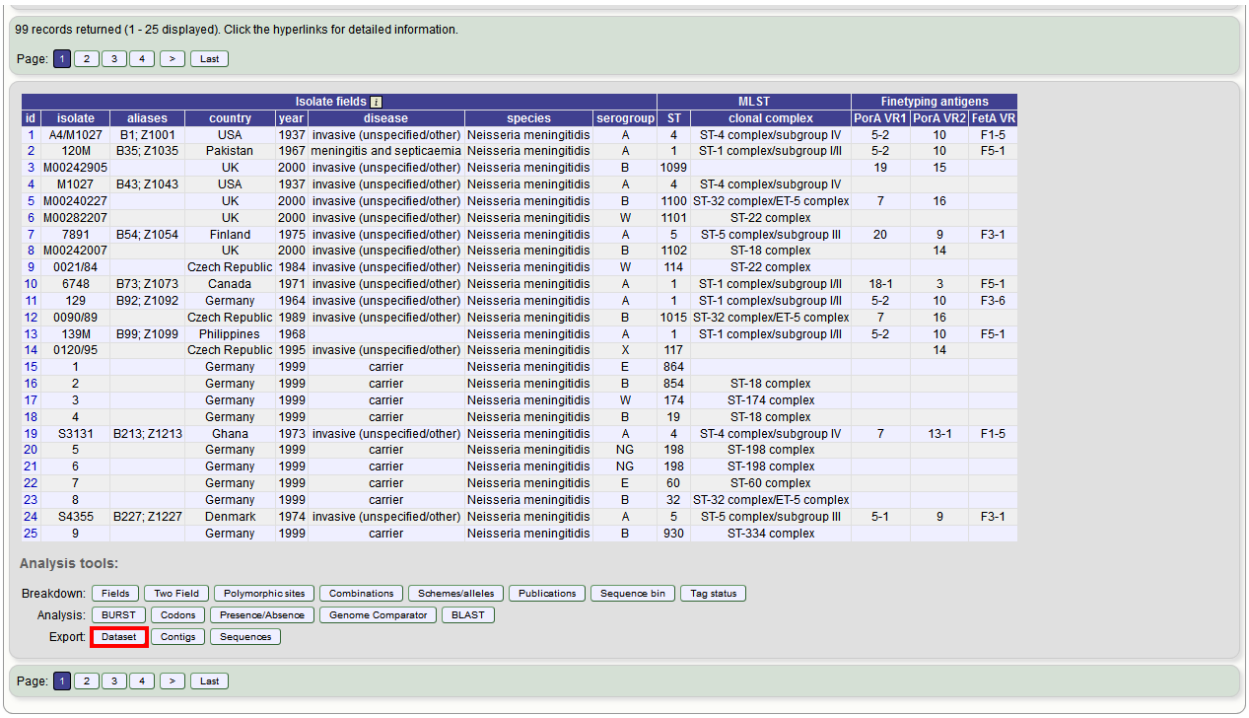
Data export plugins

15.1 Isolate record export

You can export the entire isolate recordset by clicking the 'Export dataset' link in the Export section of the main contents page.



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.



99 records returned (1 - 25 displayed). Click the hyperlinks for detailed information.

Page: 1 2 3 4 > Last

Isolate fields								MLST		Finetyping antigens		
id	isolate	aliases	country	year	disease	species	serogroup	ST	clonal complex	PorA VR1	PorA VR2	FetA VR
1	A4/M1027	B1; Z1001	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	5-2	10	F1-5
2	120M	B35; Z1035	Pakistan	1967	meningitis and septicaemia	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
3	M00242905		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	B	1099		19	15	
4	M1027	B43; Z1043	USA	1937	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV			
5	M00240227		UK	2000	invasive (unspecified/other)	Neisseria meningitidis	B	1100	ST-32 complex/ET-5 complex	7	16	
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	B	1102	ST-18 complex		14	
9	0021/84		Czech Republic	1984	invasive (unspecified/other)	Neisseria meningitidis	W	114	ST-22 complex			
10	6748	B73; Z1073	Canada	1971	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	18-1	3	F5-1
11	129	B92; Z1092	Germany	1964	invasive (unspecified/other)	Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F3-6
12	0090/89		Czech Republic	1989	invasive (unspecified/other)	Neisseria meningitidis	B	1015	ST-32 complex/ET-5 complex	7	16	
13	139M	B99; Z1099	Philippines	1968		Neisseria meningitidis	A	1	ST-1 complex/subgroup I/II	5-2	10	F5-1
14	0120/95		Czech Republic	1995	invasive (unspecified/other)	Neisseria meningitidis	X	117			14	
15	1		Germany	1999	carrier	Neisseria meningitidis	E	864				
16	2		Germany	1999	carrier	Neisseria meningitidis	B	854	ST-18 complex			
17	3		Germany	1999	carrier	Neisseria meningitidis	W	174	ST-174 complex			
18	4		Germany	1999	carrier	Neisseria meningitidis	B	19	ST-18 complex			
19	S3131	B213; Z1213	Ghana	1973	invasive (unspecified/other)	Neisseria meningitidis	A	4	ST-4 complex/subgroup IV	7	13-1	F1-5
20	5		Germany	1999	carrier	Neisseria meningitidis	NG	198	ST-198 complex			
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	B	32	ST-32 complex/ET-5 complex			
24	S4355	B227; Z1227	Denmark	1974	invasive (unspecified/other)	Neisseria meningitidis	A	5	ST-5 complex/subgroup III	5-1	9	F3-1
25	9		Germany	1999	carrier	Neisseria meningitidis	B	930	ST-334 complex			

Analysis tools:

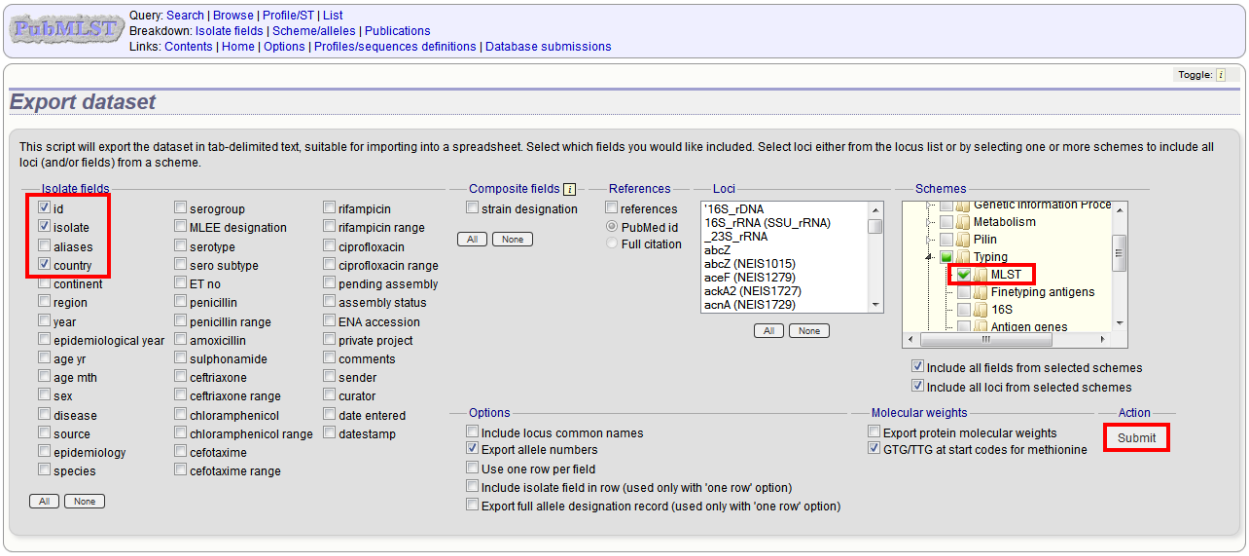
Breakdown: Fields | Two Field | Polymorphic sites | Combinations | Schemes/alleles | Publications | Sequence bin | Tag status

Analysis: BURST | Codons | Presence/Absence | Genome Comparator | BLAST

Export: Dataset | Contigs | Sequences

Page: 1 2 3 4 > Last

Select the isolate fields and schemes to include.



PubMLST

Query: Search | Browse | Profile/ST | List

Breakdown: Isolate fields | Scheme/alleles | Publications

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

Toggle:

Export dataset

This script will export the dataset in tab-delimited text, suitable for importing into a spreadsheet. Select which fields you would like included. Select loci either from the locus list or by selecting one or more schemes to include all loci (and/or fields) from a scheme.

Isolate fields

- id
- isolate
- aliases
- country
- continent
- region
- year
- epidemiological 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
- assembly status
- ENA accession
- private project
- comments
- sender
- curator
- date entered
- datestamp

All | None

Composite fields

- strain designation

All | None

References

- references
- PubMed id
- Full citation

Loci

'16S_rDNA
16S_rRNA (SSU_rRNA)
_23S_rRNA
abcZ
abcZ (NEIS1015)
aceF (NEIS1279)
ackA2 (NEIS1727)
acnA (NEIS1729)

All | None

Schemes

- Genetic information Proce
- Metabolism
- Pilin
- Typing
- MLST
- Finetyping antigens
- 16S
- Antigen genes

Include all fields from selected schemes

Include all loci from selected schemes

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)

Molecular weights

- Export protein molecular weights
- GTG/TTG at start codes for methionine

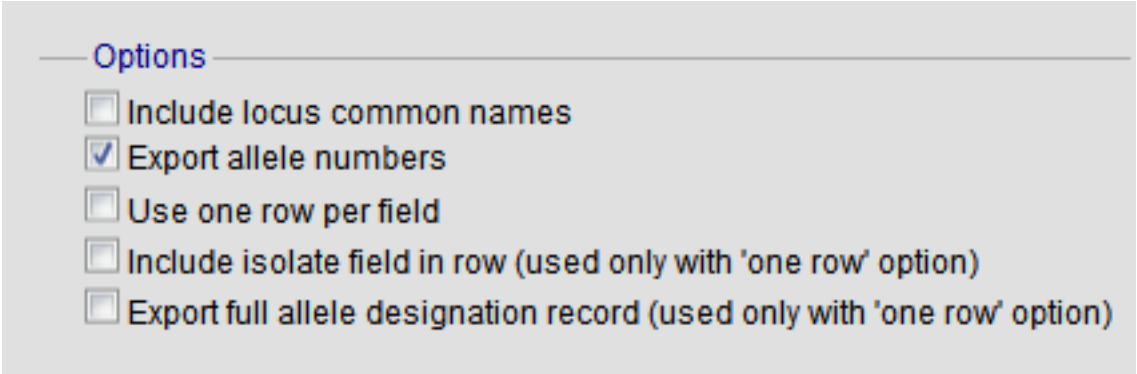
Action

Submit

Click Submit.

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

15.1.1 Advanced options

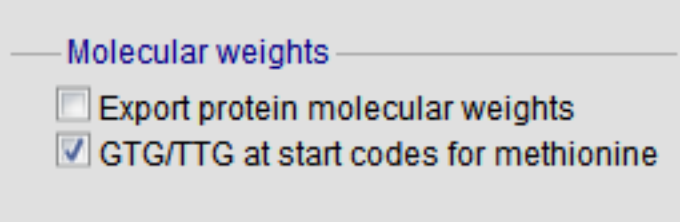


The options fieldset has the following options.

- Include locus common names - any common name for the locus is displayed in parentheses following the primary name.
- Export allele numbers - the allele designation is included for any locus included.
- Use one row per field - this is an alternative output format where instead of each locus and field having a separate column, each field is export on a separate row.
- Include isolate field in row - the name of the isolate is included as a separate column when exporting in 'one row per field' fomrmat.
- Export full allele designation record - export sender, curator and datestamp information as separate rows when exporting allele designation data.

15.1.2 Molecular weight calculation

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

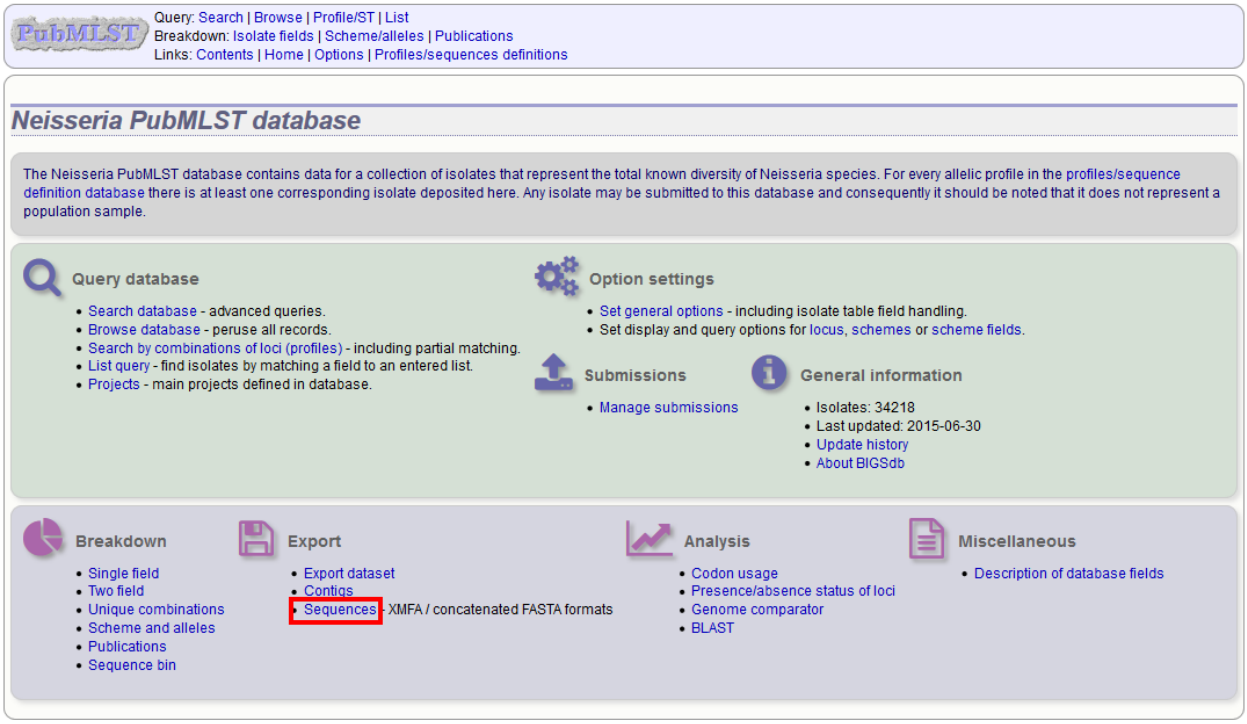


Click the 'Export protein molecular weight' checkbox. Additional columns (or rows depending on the output format) will be created to include the molecular weight data.

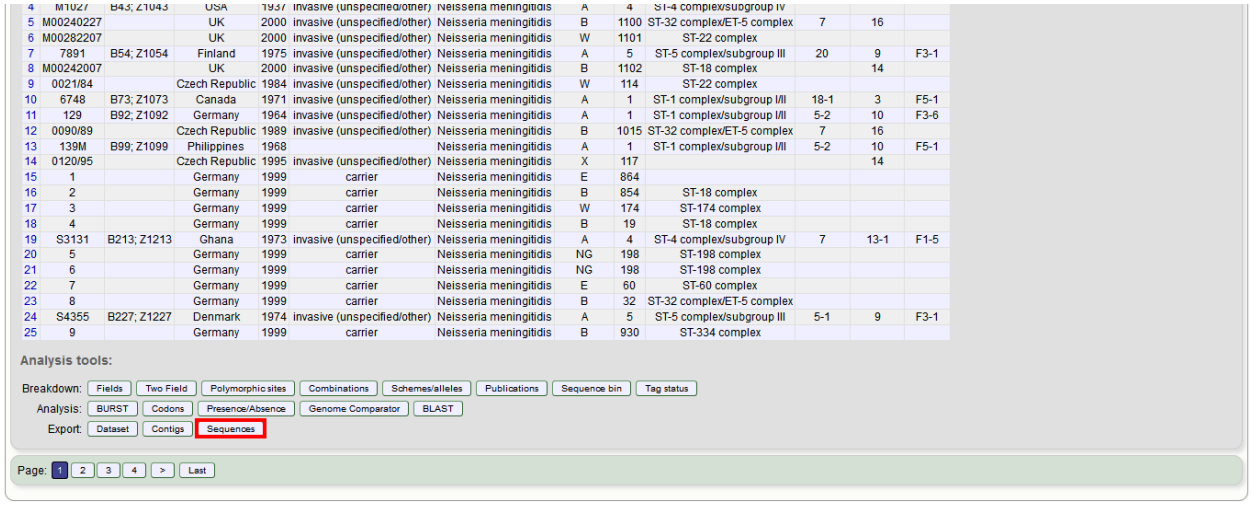
15.2 Sequence export

You can export the sequences for any set of loci designated in isolate records, or belonging to scheme profiles in the sequence definition database.

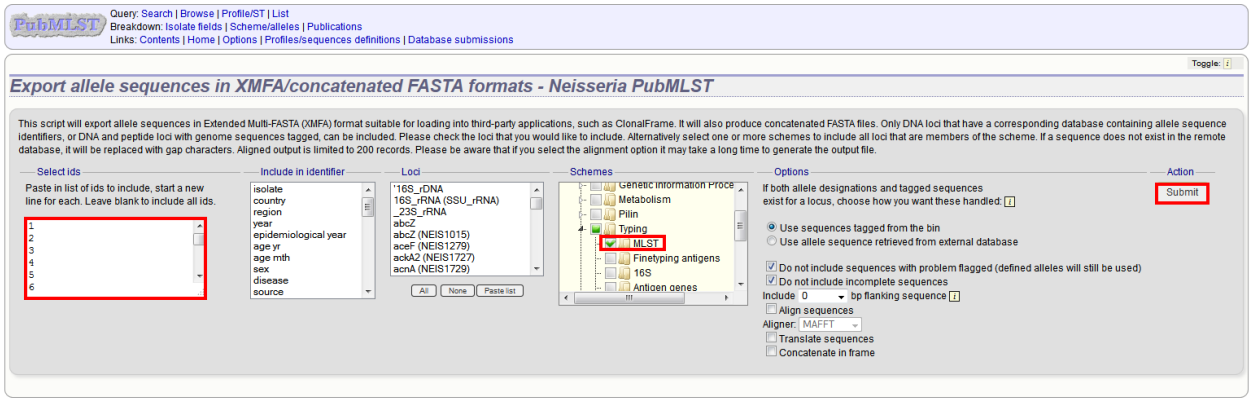
The sequence export function can be accessed by clicking the 'Sequences' link in the Export section of the contents page.



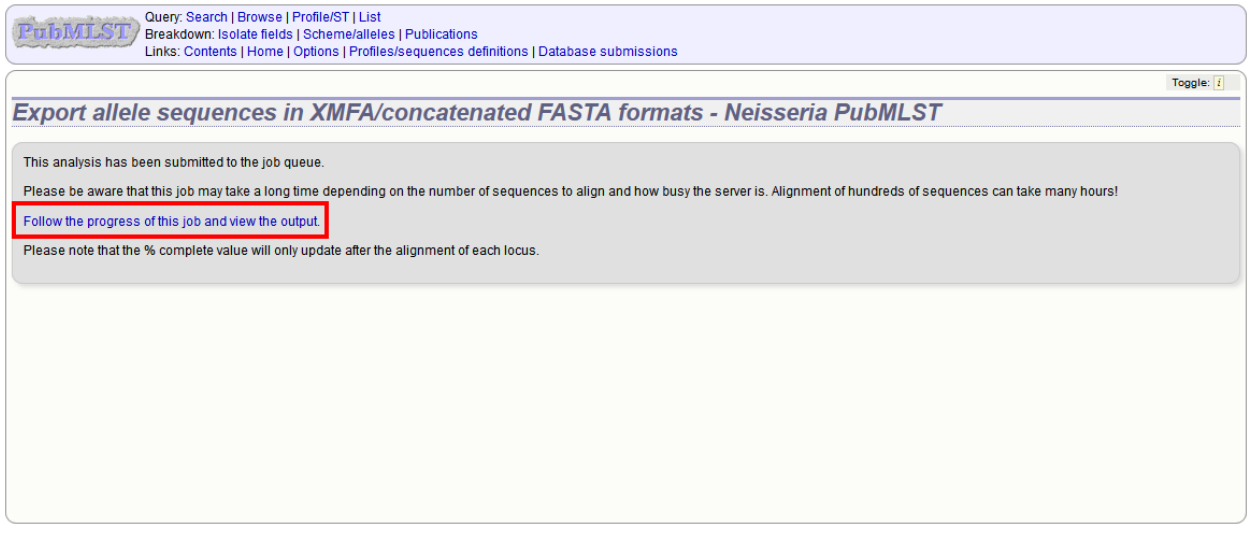
Alternatively, you can access this function by clicking the 'Sequences' button in the Export list at the bottom of the results table. Please note that the list of functions here may vary depending on the setup of the database.



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.

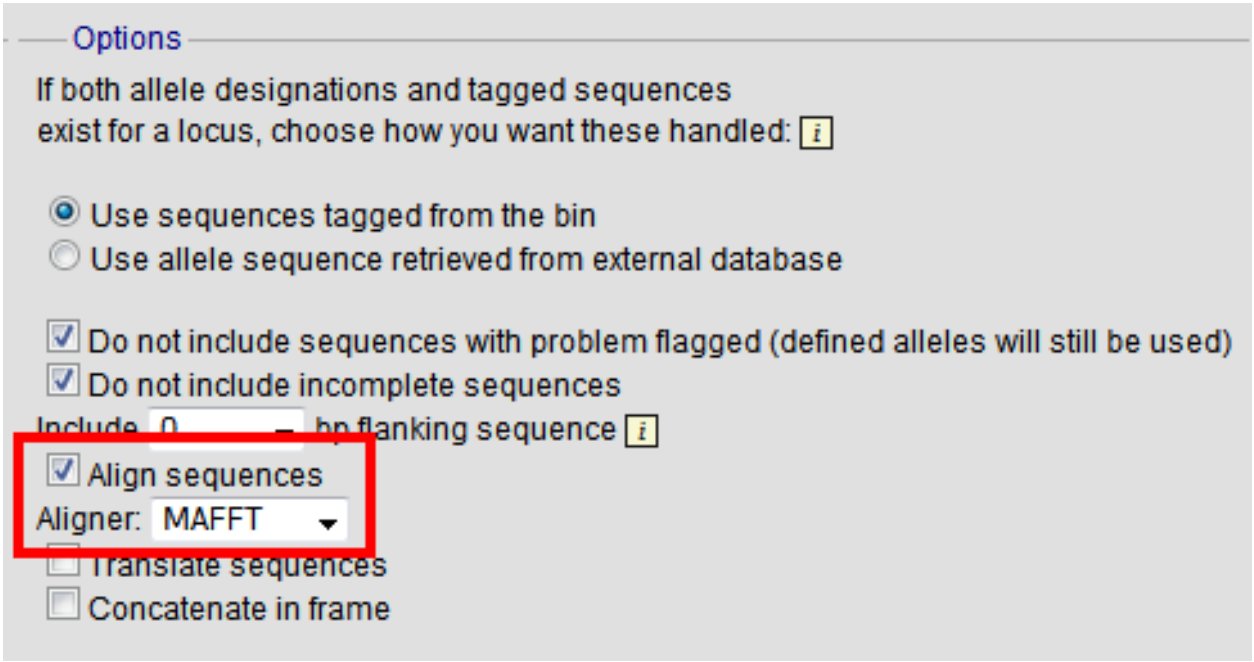


The job will be submitted to the job queue. Click the link to follow the progress and download the resulting files.

Sequences will be export in XMFA and FASTA file formats.

15.2.1 Aligning sequences

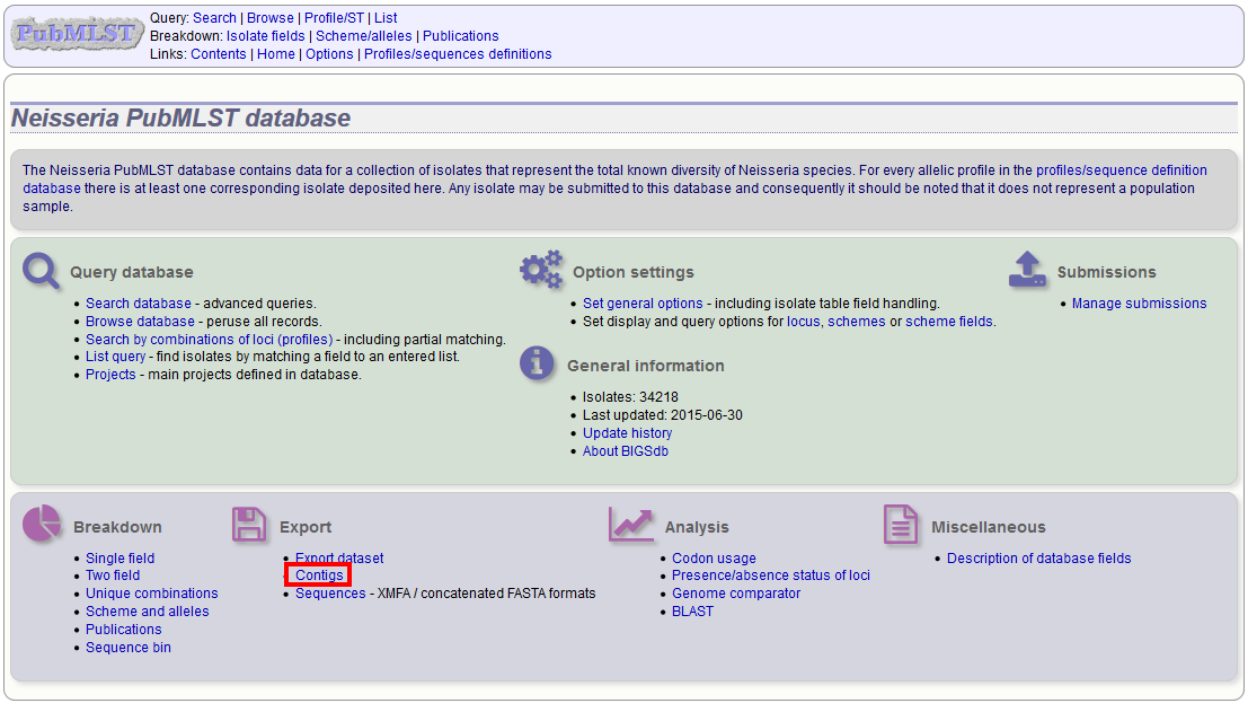
By default, sequences will be exported unaligned - this is very quick since no processing is required. You can choose to align the sequences by checking the 'Align sequences' checkbox.



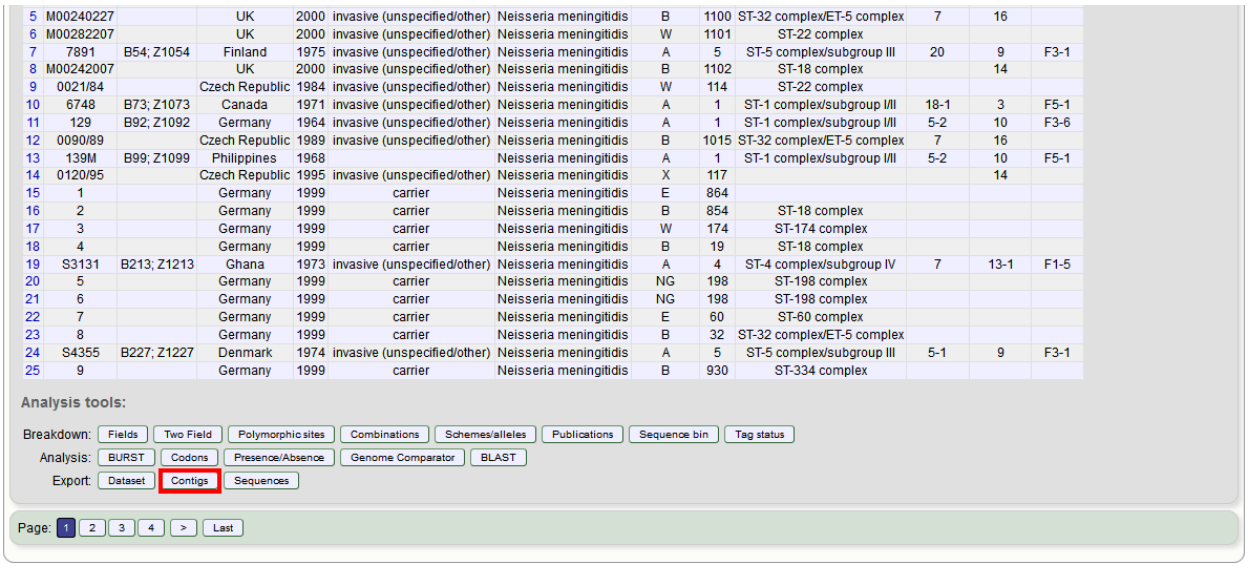
You can also choose to use MUSCLE or MAFFT as the aligner. MAFFT is the default choice and is usually much quicker than MUSCLE. Both produce comparable results.

15.3 Contig export

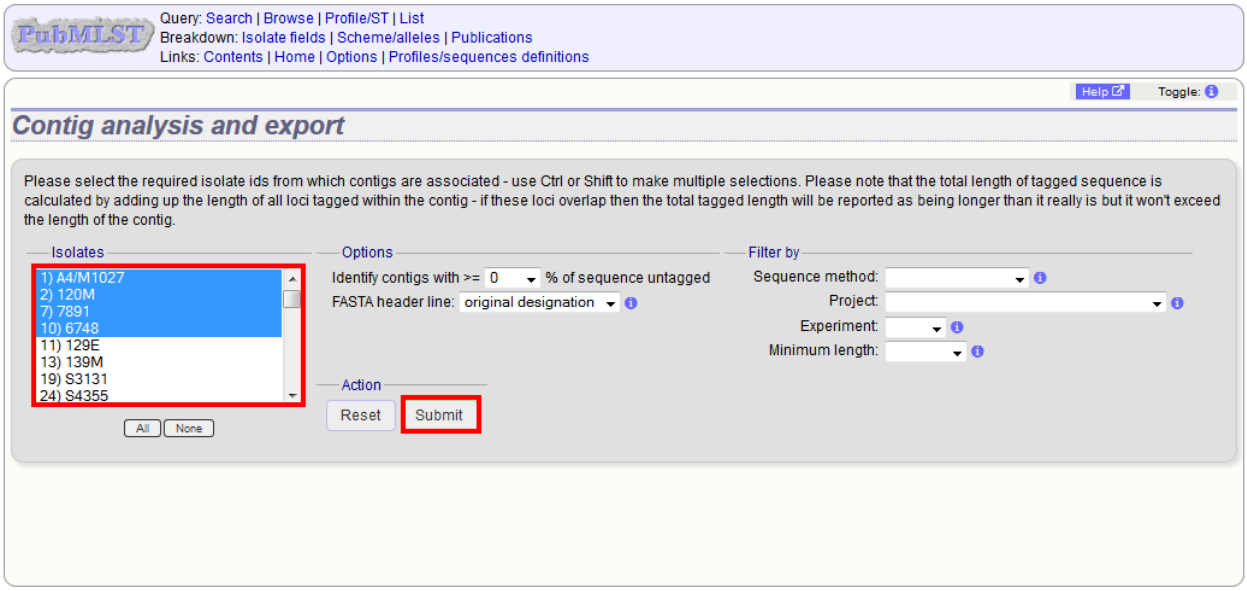
The contig export plugin can be accessed by clicking the 'Contigs' link in the Export section of the contents page of isolate databases.



Alternatively, it can be accessed following a query by clicking the 'Contigs' button in the Export section at the bottom of the results table.

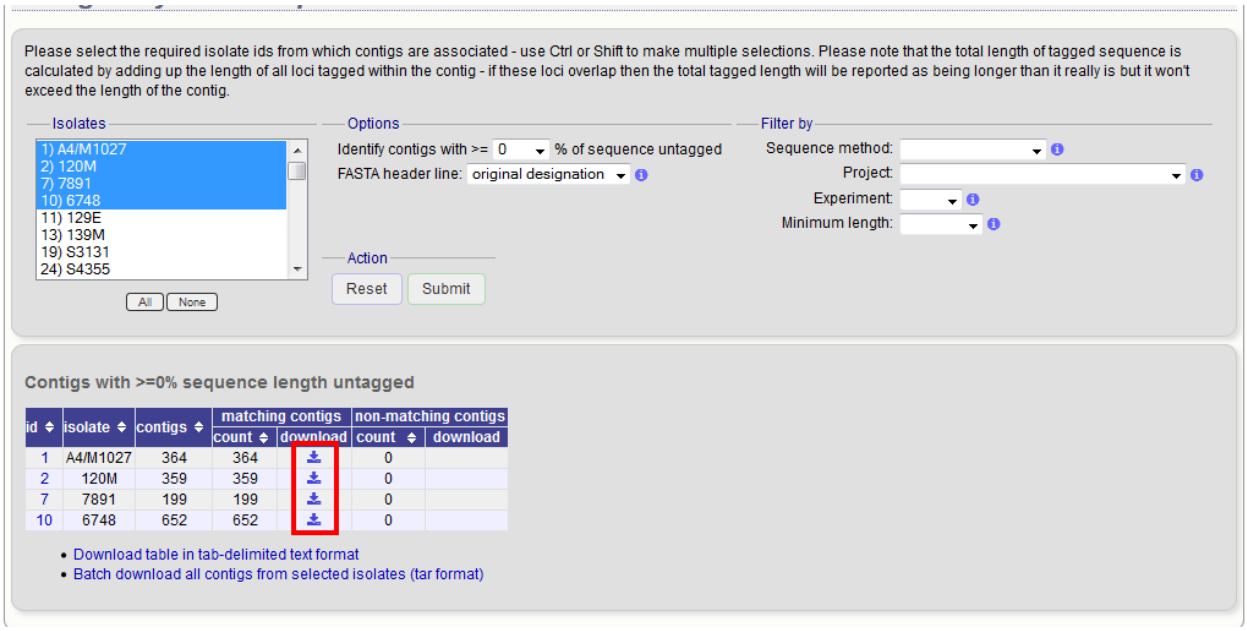


Select the isolates for which you wish to export contig data for. If the export function was accessed following a query, isolates returned in the query will be pre-selected.

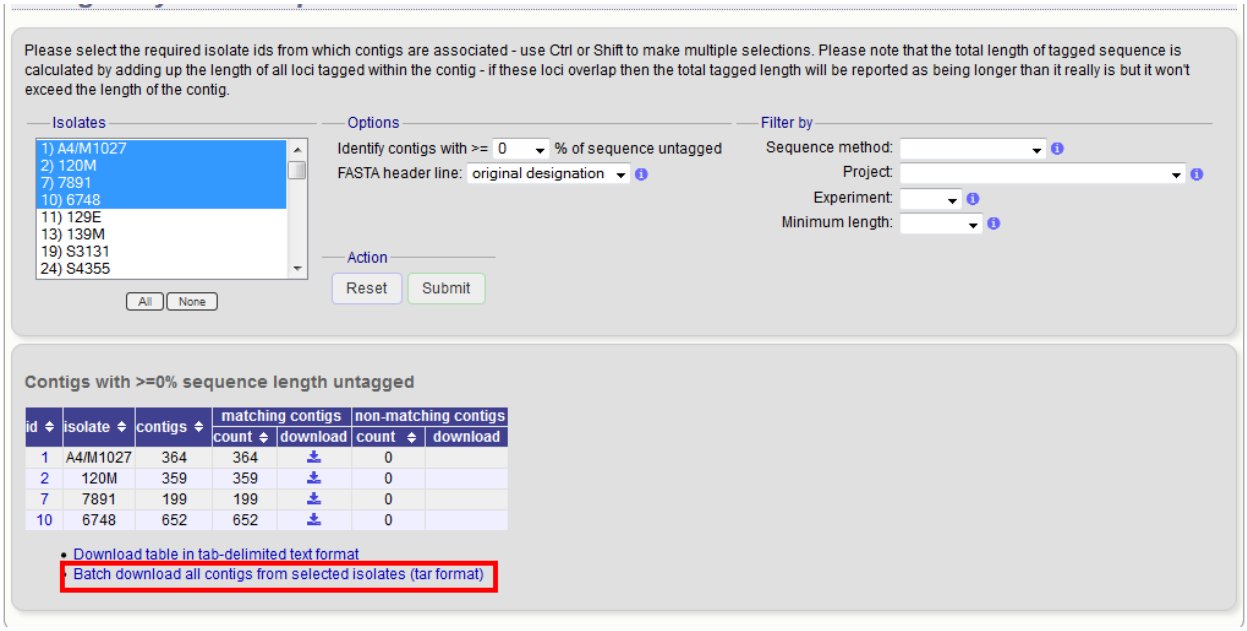


At its simplest, press submit.

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



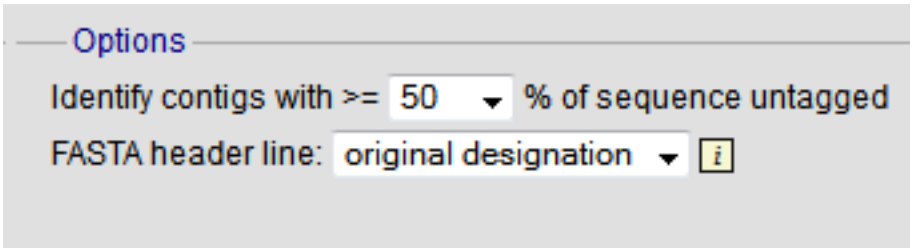
You can also download all the data in a tar file by clicking the 'Batch download' link.



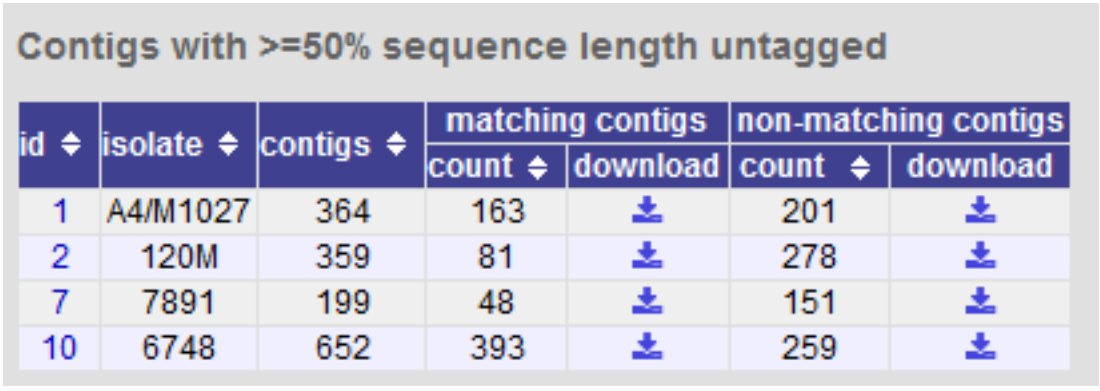
15.3.1 Filtering by tagged status of contigs

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.



The resulting table has two download links for each isolate, one for contigs matching the condition, and one for contigs that don't match.

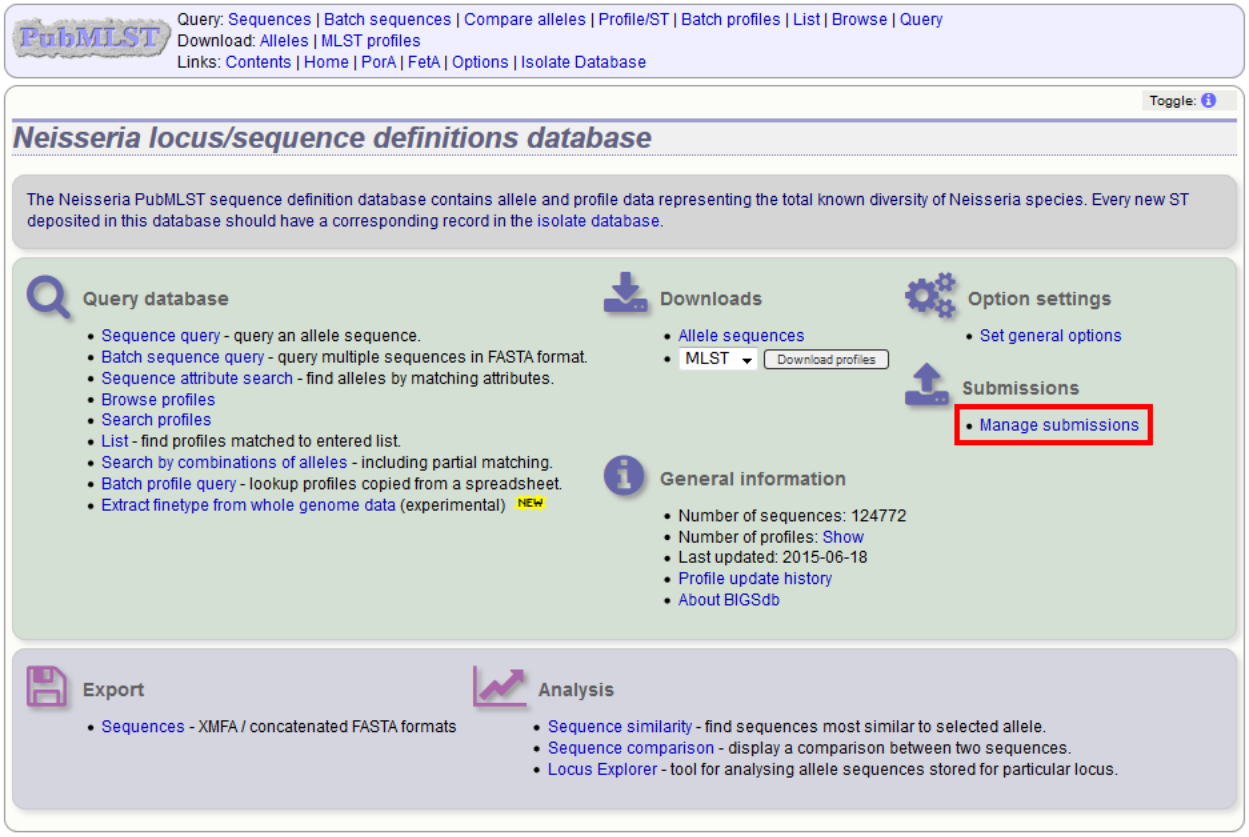


CHAPTER 16

Submitting data using the submission system

The automated submission system allows users to submit data (new alleles, profiles, or isolates) to the database curators for assignment and upload to the database. The submission system is enabled on a per-database basis so will not always be available.

If the system is enabled, new submissions can be made by clicking the 'Manage submissions' link on the database front page.



16.1 Registering a user account

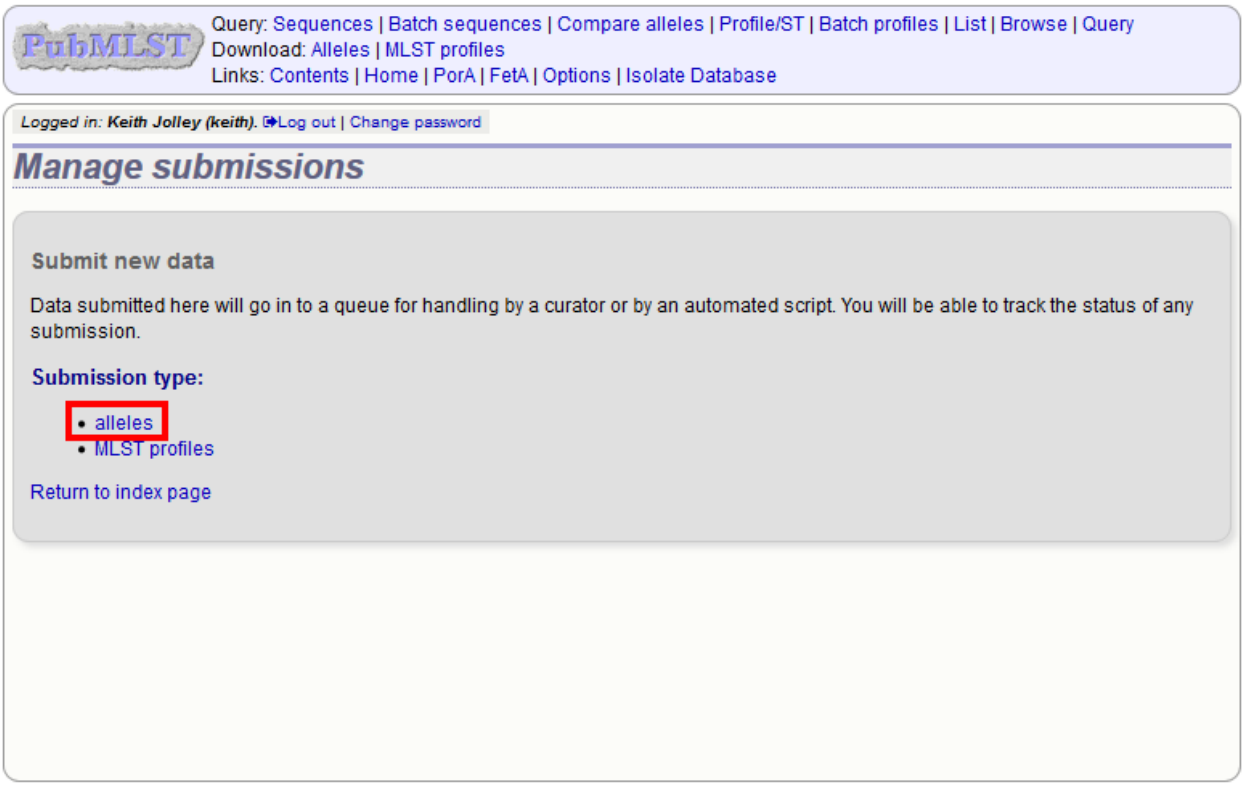
You must have an account for the appropriate database in order to use the submission system. On systems utilizing site-wide databases, such as PubMLST, this can be done automatically via the web. Other sites may require you to contact a curator to set this up.

16.2 Allele submission

New allele data can only be submitted from within the appropriate sequence definition database. Submissions consist of one or more new allele sequences for a single locus. You will need to create separate submissions for each locus - this is because different loci may be handled by different curators.

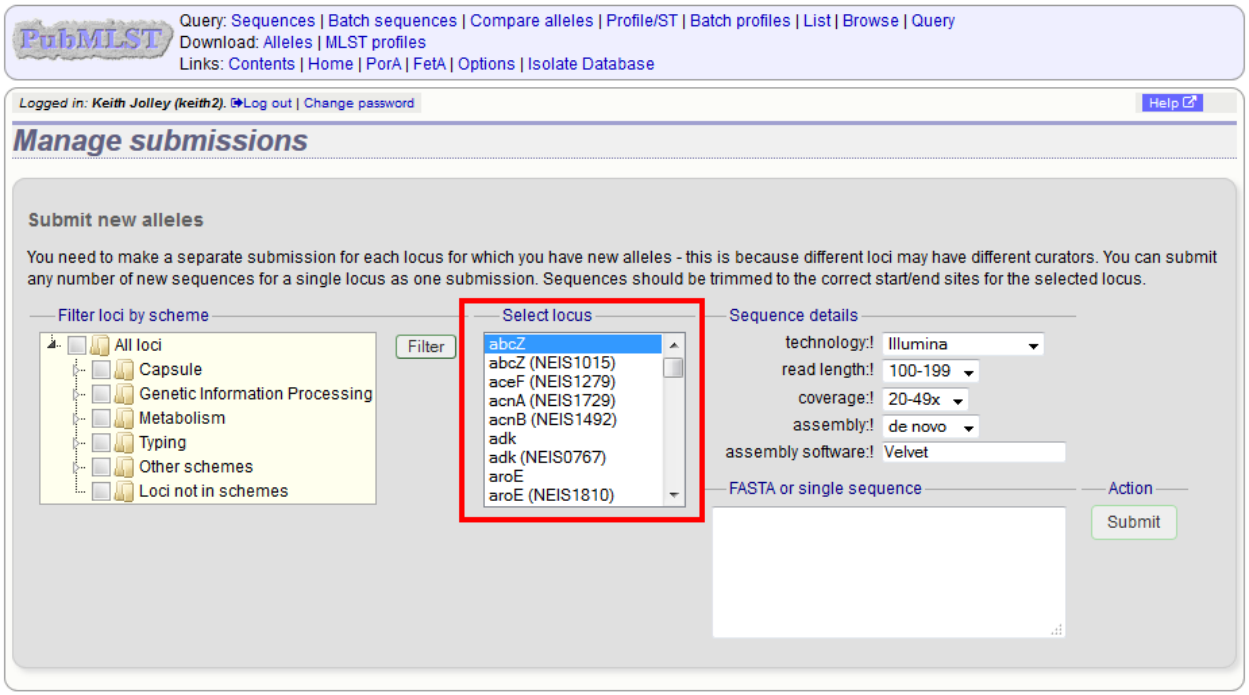
16.2.1 Start

Click the 'alleles' link under submission type on the submission management page.

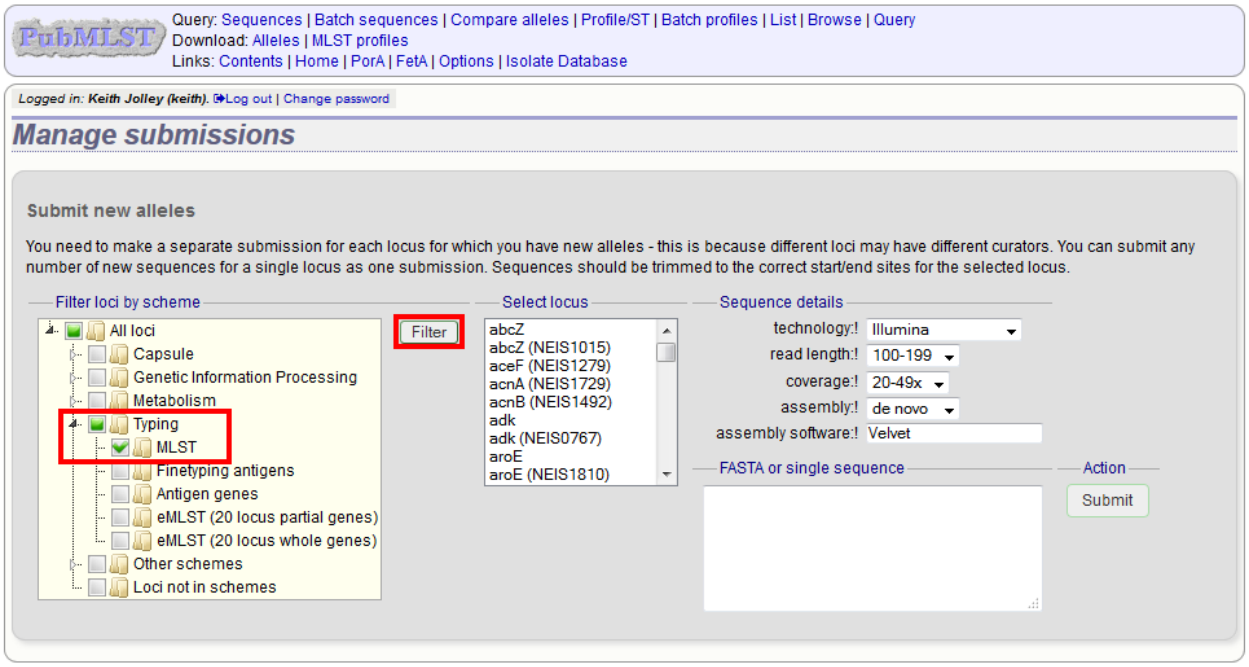


16.2.2 Select the submission locus

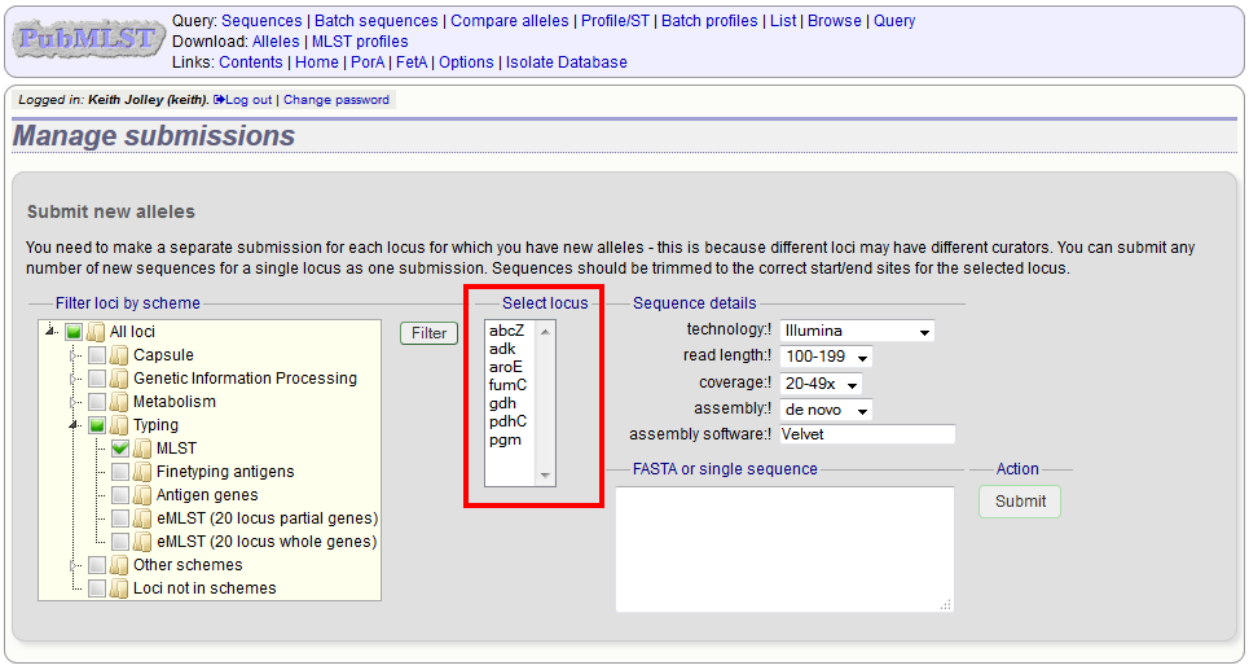
Select the locus from the locus list box:



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'.



The locus list is now constrained making selection easier.



16.2.3 Enter details of sequencing method

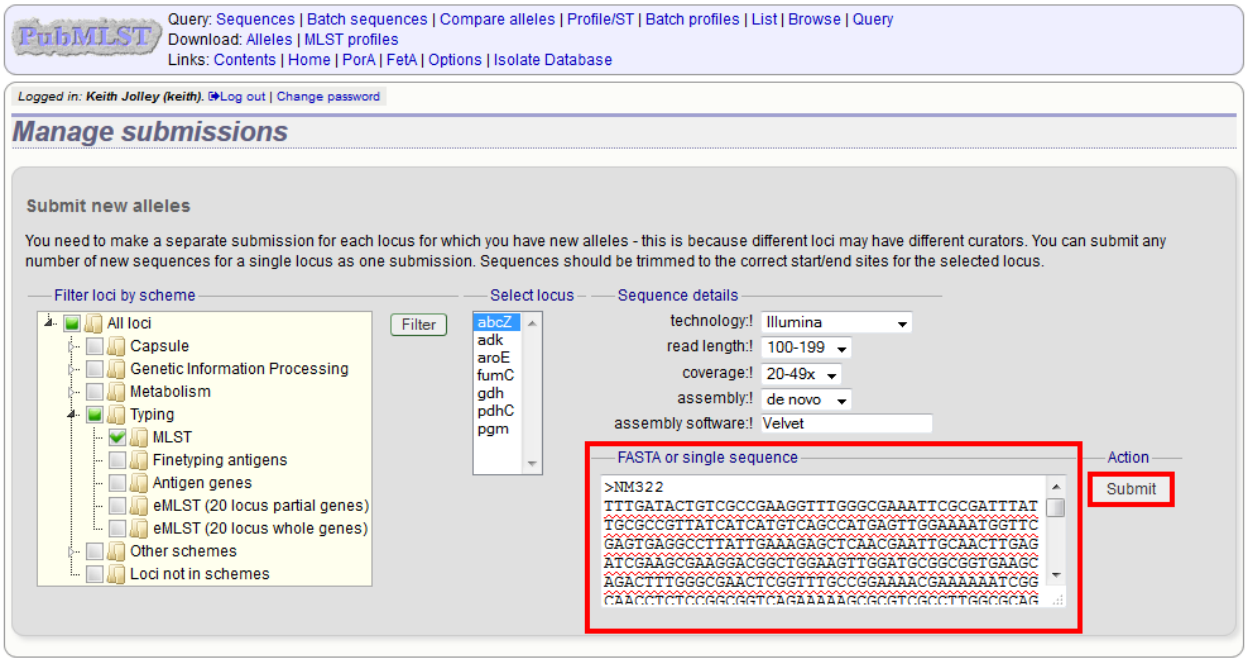
There are a number of fields that must be filled in so that the curator knows how the sequence was obtained:

- technology - the sequncing platform used, allowed values are:

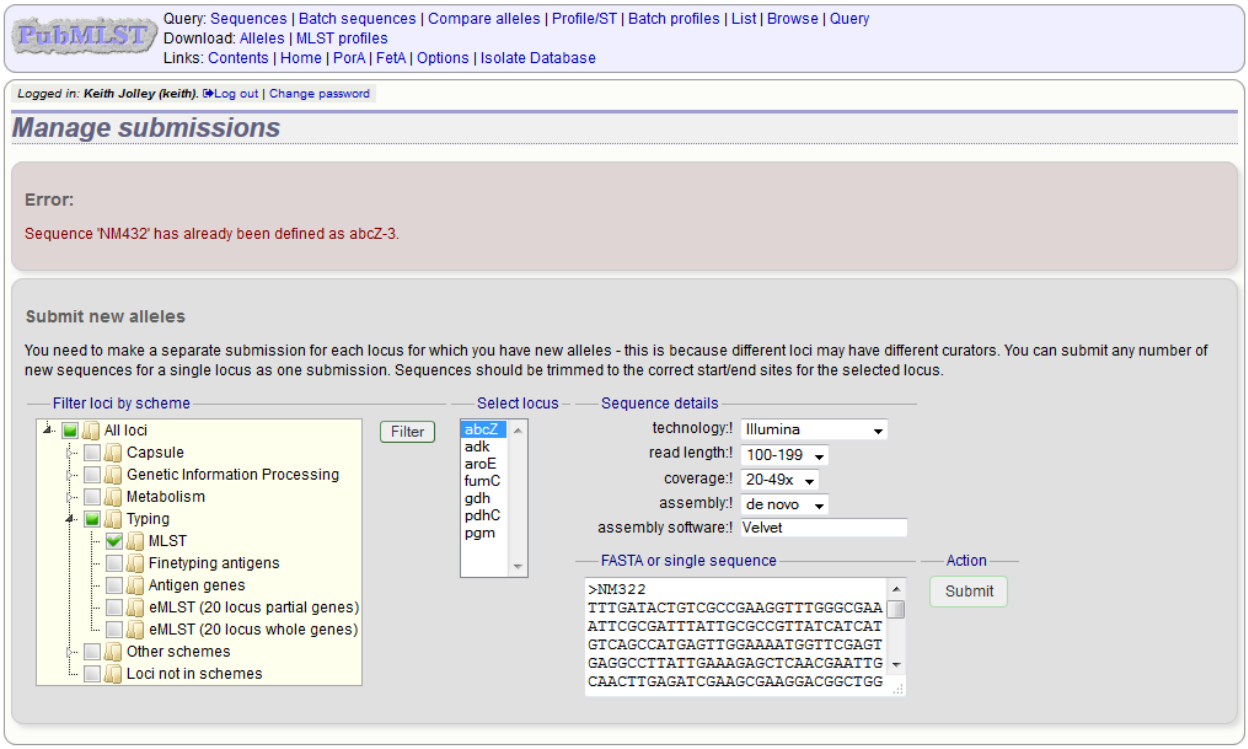
  - 454
  - Illumina
  - Ion Torrent
  - PacBio
  - Oxford Nanopore
  - Sanger
  - Solexa
  - SOLiD
  - other
  - unknown
- read length - this is the length of sequencing reads. This is a required field for Illumina data, and not relevant to Sanger sequencing. Allowed values are:
  - <100
  - 100-199
  - 200-299
  - 300-499
  - >500
- coverage - the mean number of reads covering each nucleotide position of the sequence. This is not relevant to Sanger sequencing, Allowed values are:
  - <20x
  - 20-49x
  - 50-99x
  - >100x
- assembly - the means of generating the submitted sequence from the sequencing reads. Allowed values are:
  - de novo
  - mapped
- assembly software - this is a free text field where you should enter the name of the software used to generate the submitted sequence.

16.2.4 Paste in sequence(s)

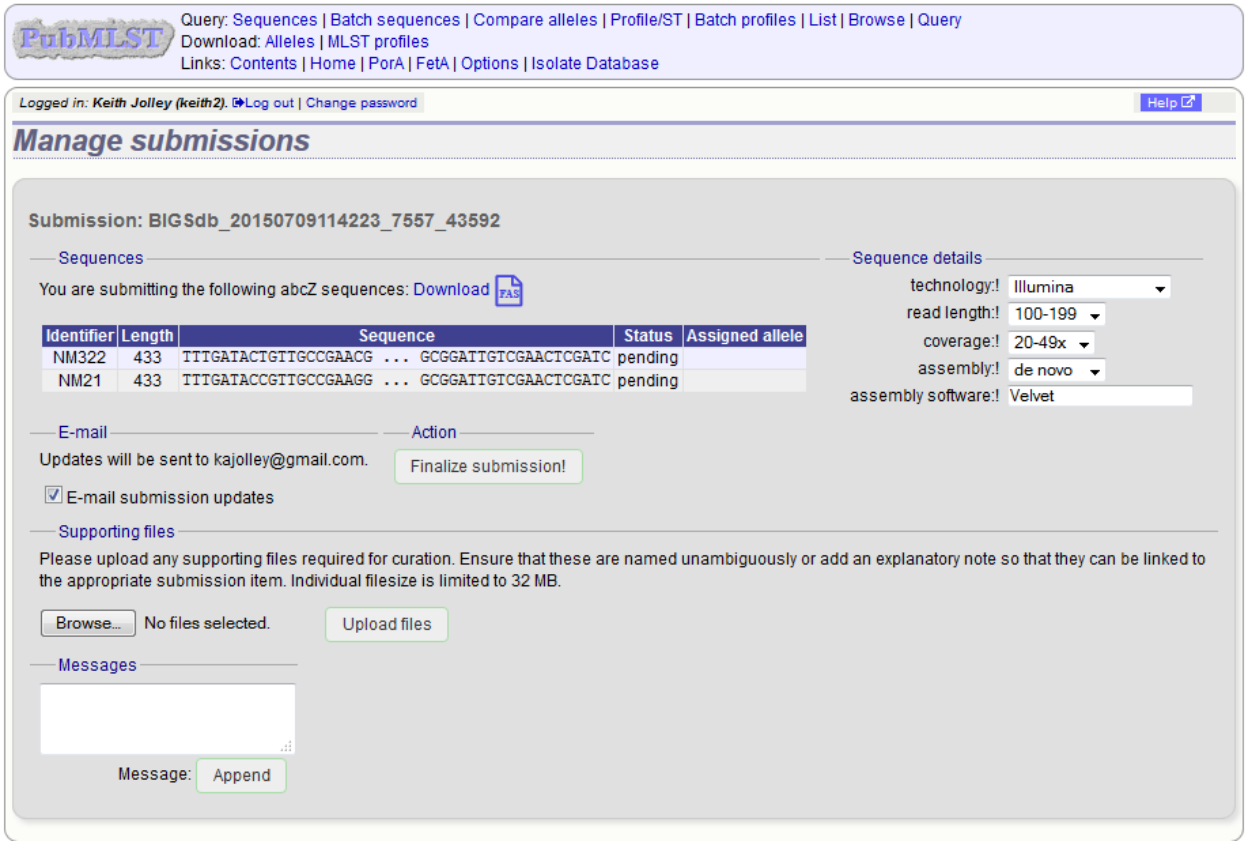
Paste in the new variant sequences to the box. This can either be a stand- alone sequence or multiple sequences in FASTA format. The sequences must be trimmed to the start and end points of the loci - check existing allele definitions if in doubt. The submission is likely to be rejected if sequences are not trimmed. Click submit.



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.

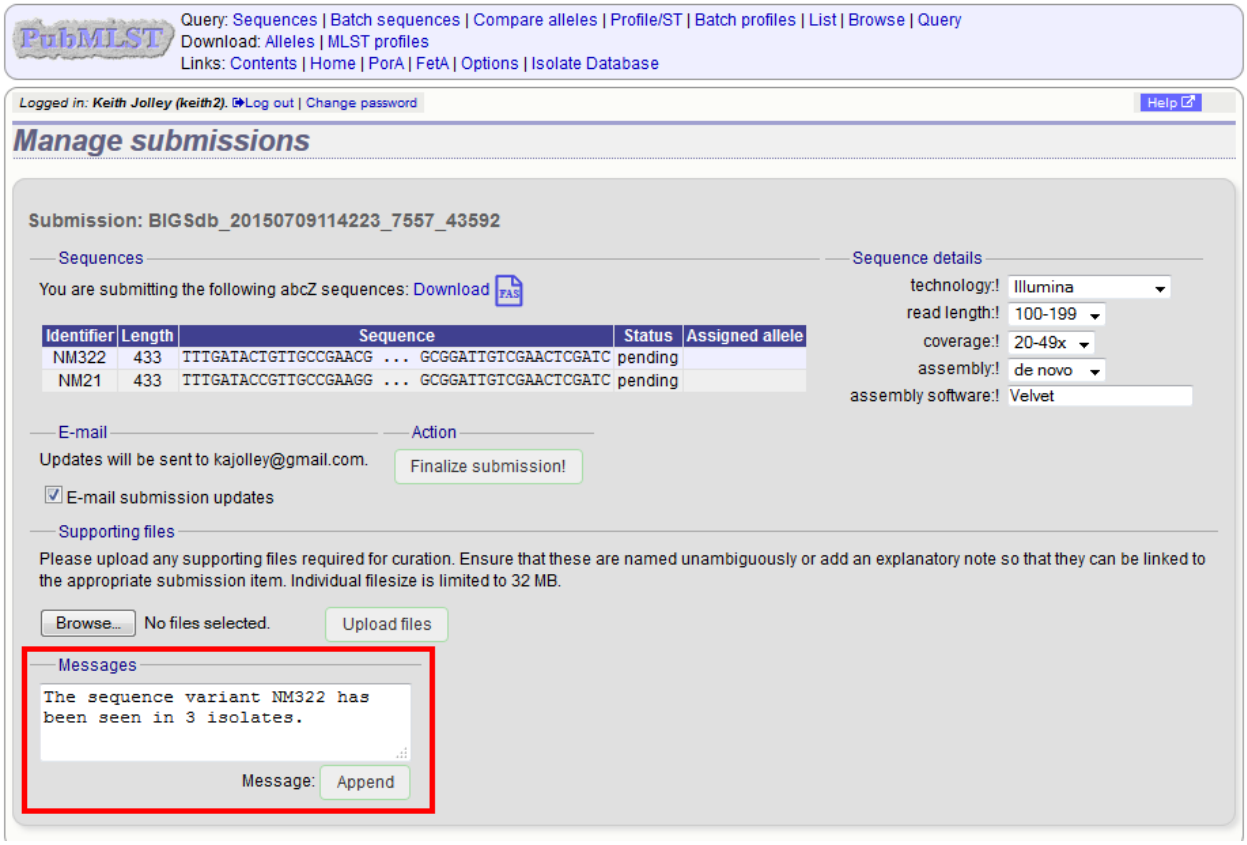


Assuming the preliminary checks have passed you will then be able to add additional information to your submission.

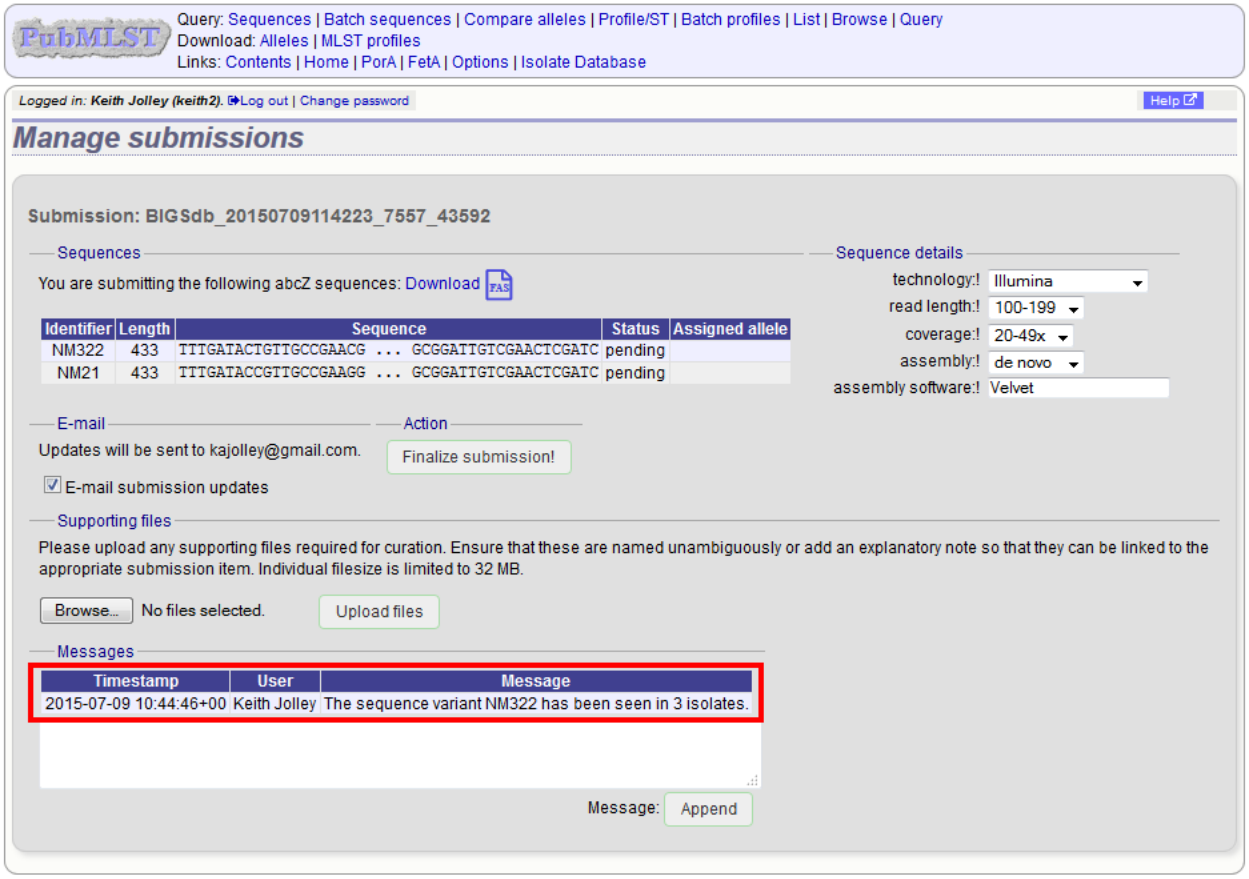


16.2.5 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Append'.



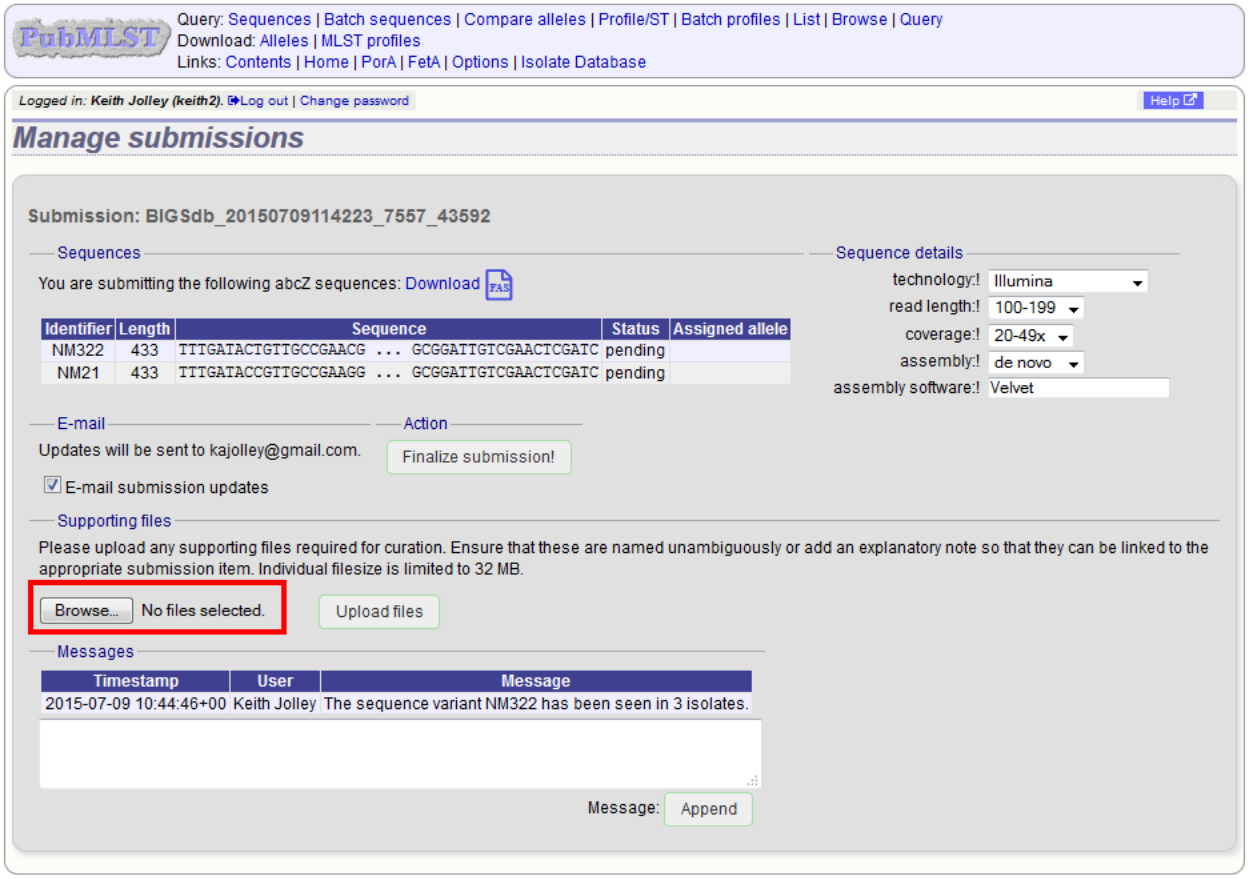
The message will be attached. A curator may respond to the message and attach their own, with the full conversation becoming part of the submission record.



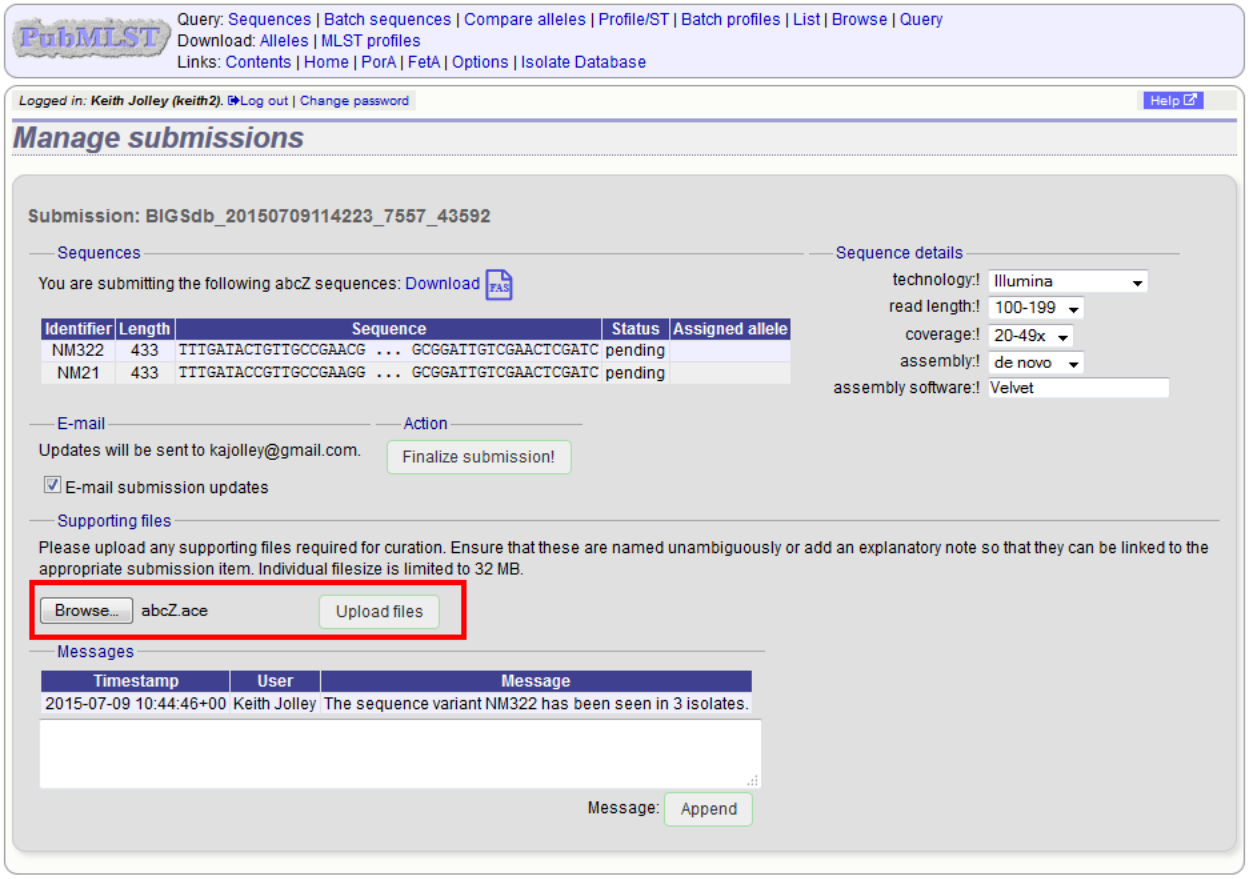
16.2.6 Add supporting files

Some submissions will require the attachment of supporting files. This will depend on the policies of the individual databases. Sequences determined by Sanger sequencing should normally have forward and reverse trace files attached.

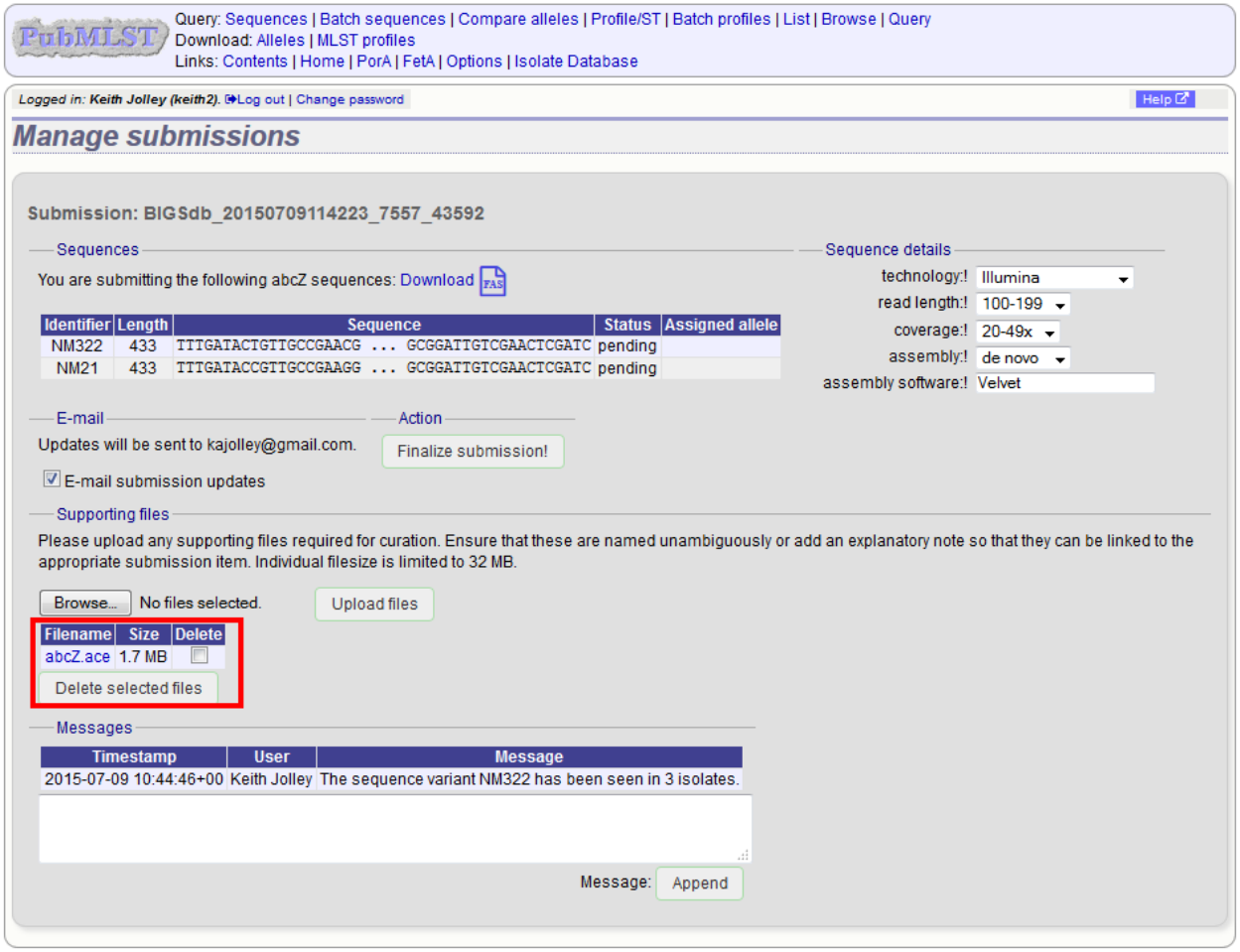
Files can be added to the submission by clicking the 'Browse' button in the 'Supporting files' section.



Select the file in the selection box, then click ‘Upload files’.



The file will be uploaded and shown in a table.

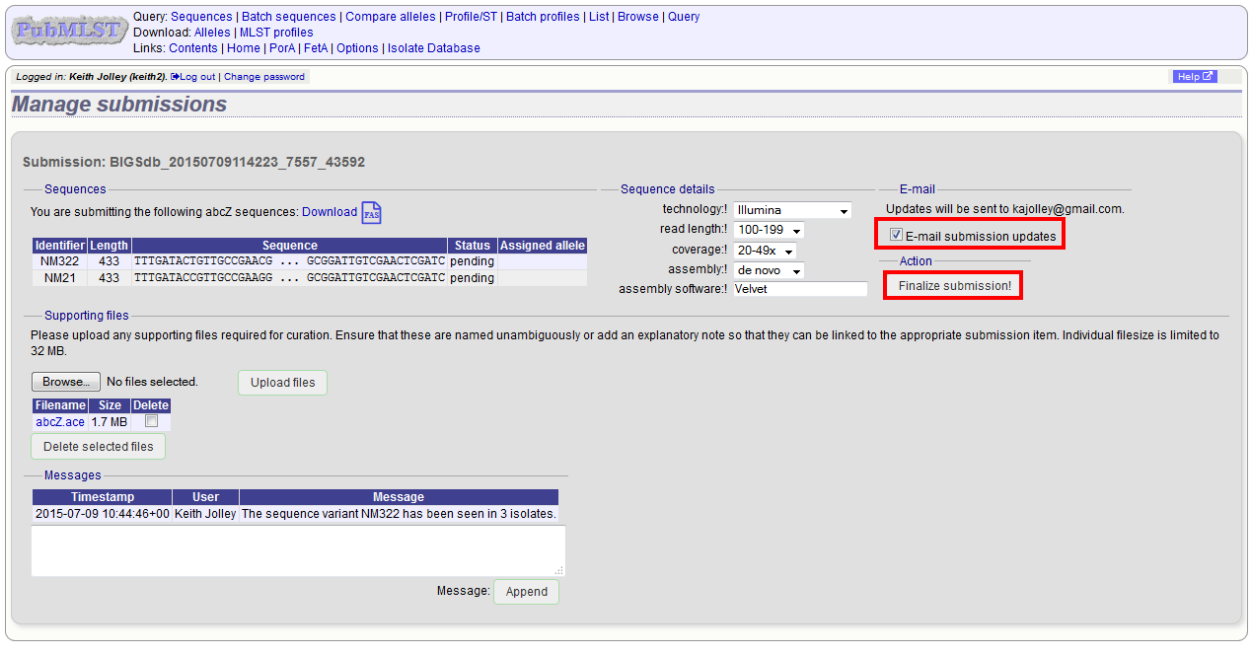


Files can be removed from the submission by checking the appropriate 'Delete' box and clicking 'Delete selected files'.

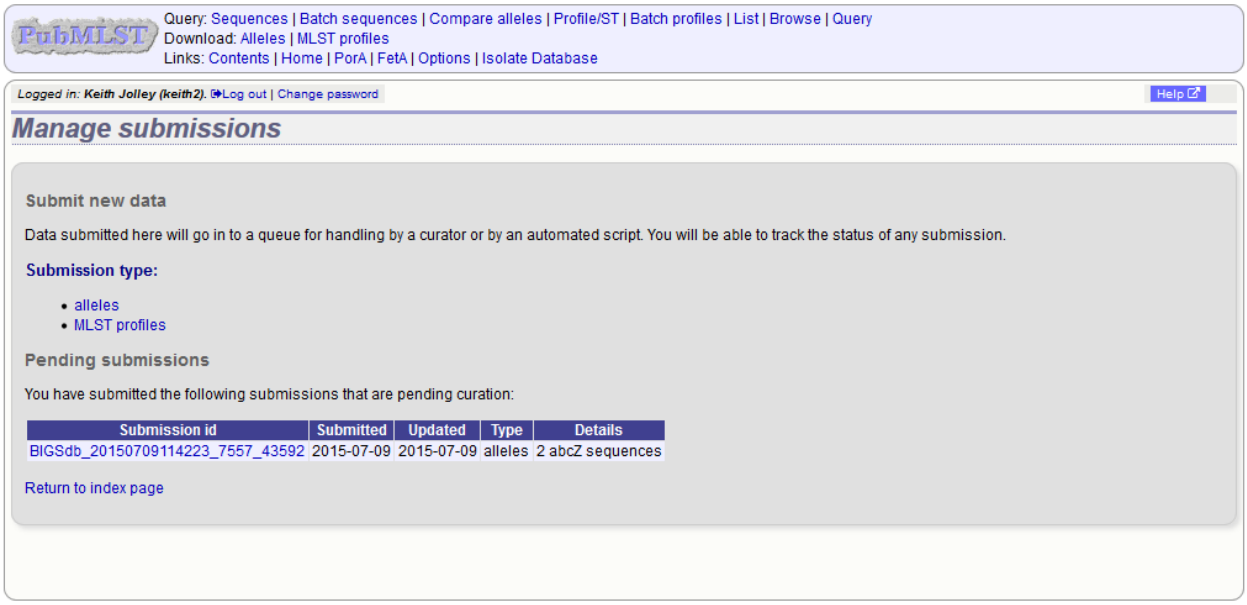
16.2.7 Finalize submission

Make sure the 'E-mail submission updates' box is checked if you wish to receive E-mail notification of the result of your submission. This setting is remembered between submissions.

Click 'Finalize submission!'.



Your submission will then be listed under 'Pending submissions' on your submission page.

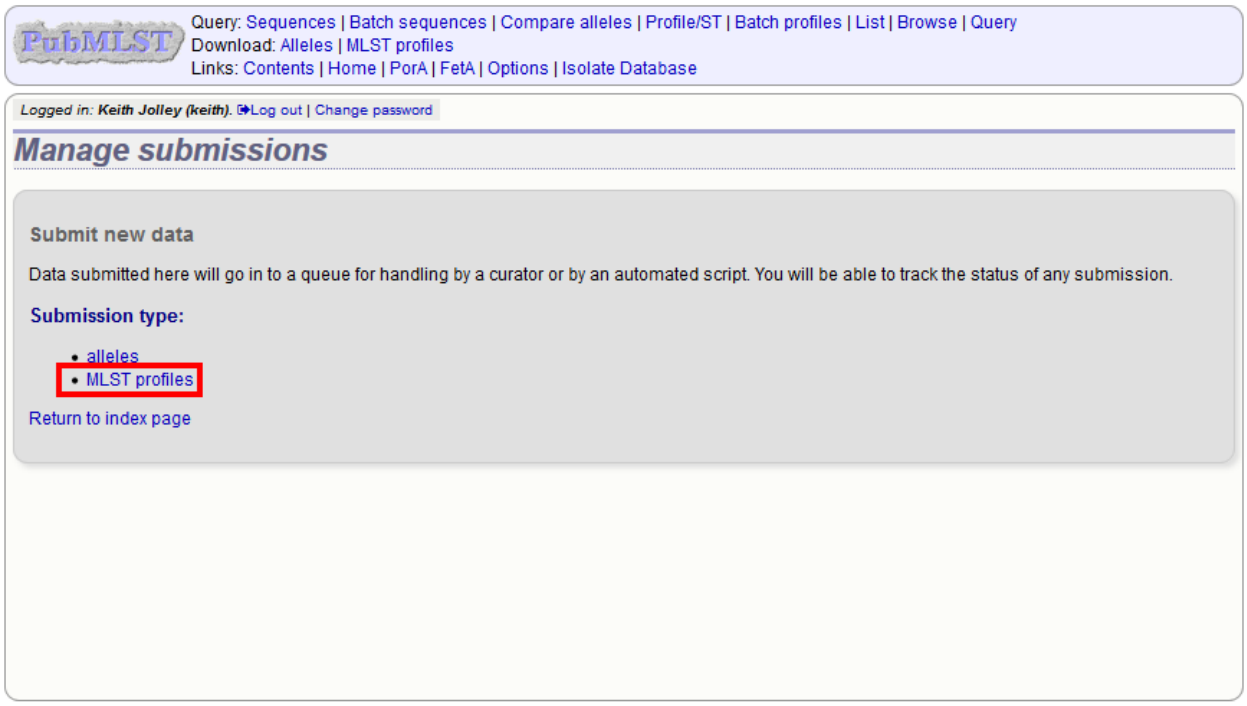


16.3 Profile submission

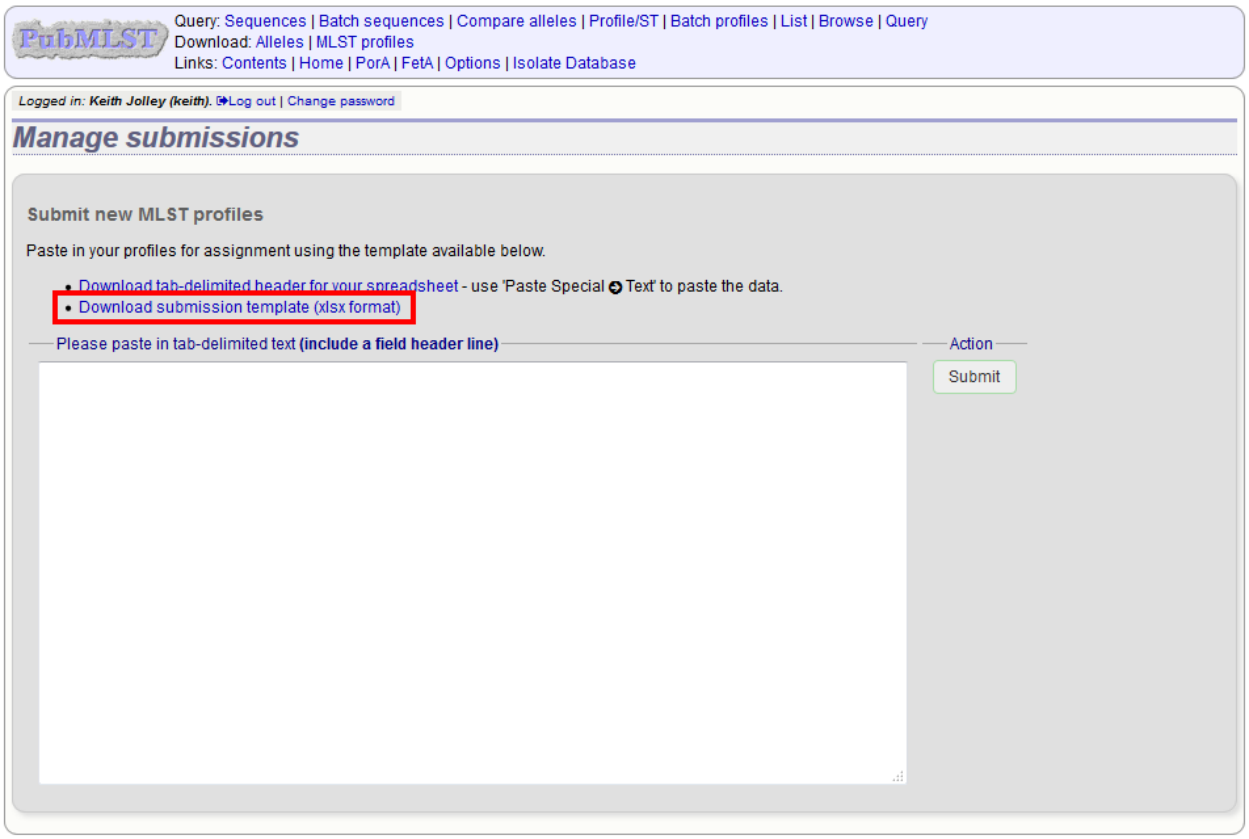
16.3.1 Start

Note: Most MLST databases on PubMLST.org require you to submit an isolate record for each new ST that you wish to be defined. In these cases, you should add the isolate name to the id field of your profile submission and make a corresponding *isolate submission* containing the allelic profile.

Click the appropriate profiles link under submission type on the submission management page.



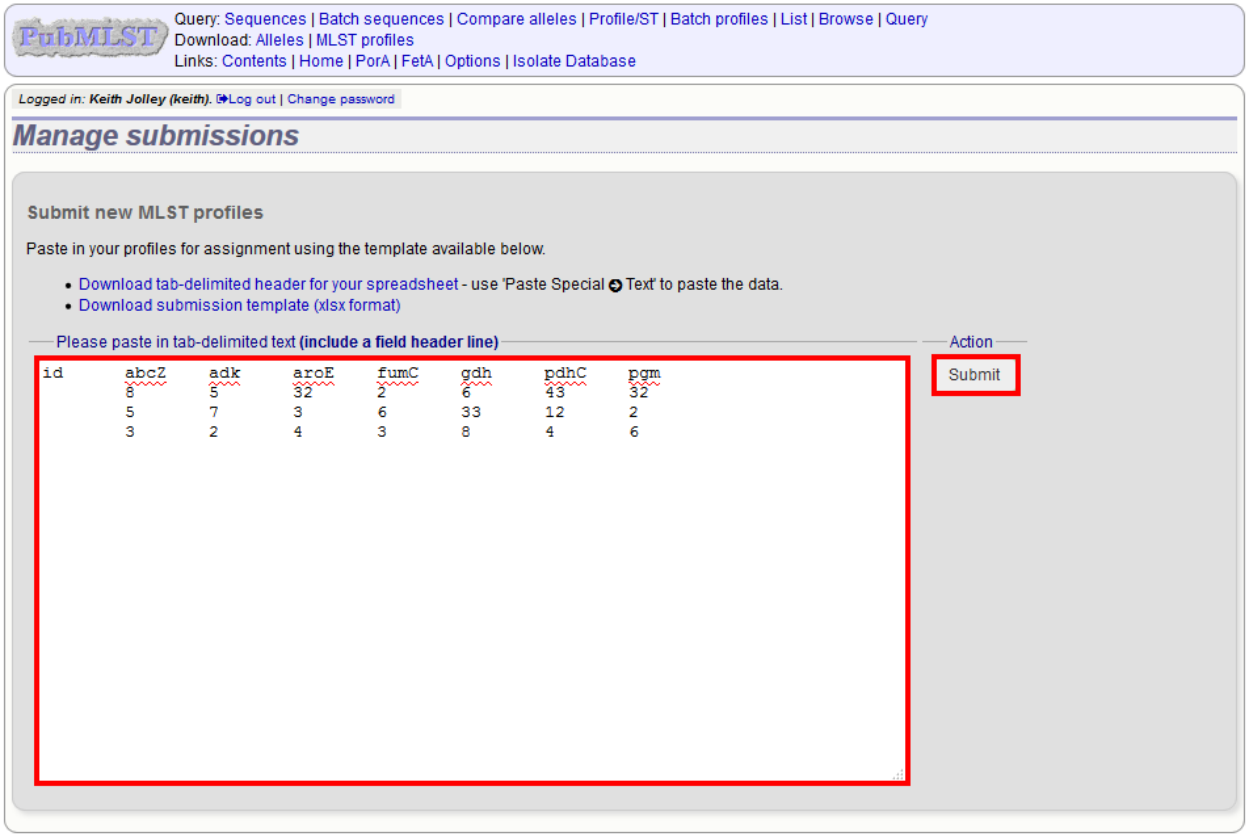
Download the Excel submission template.



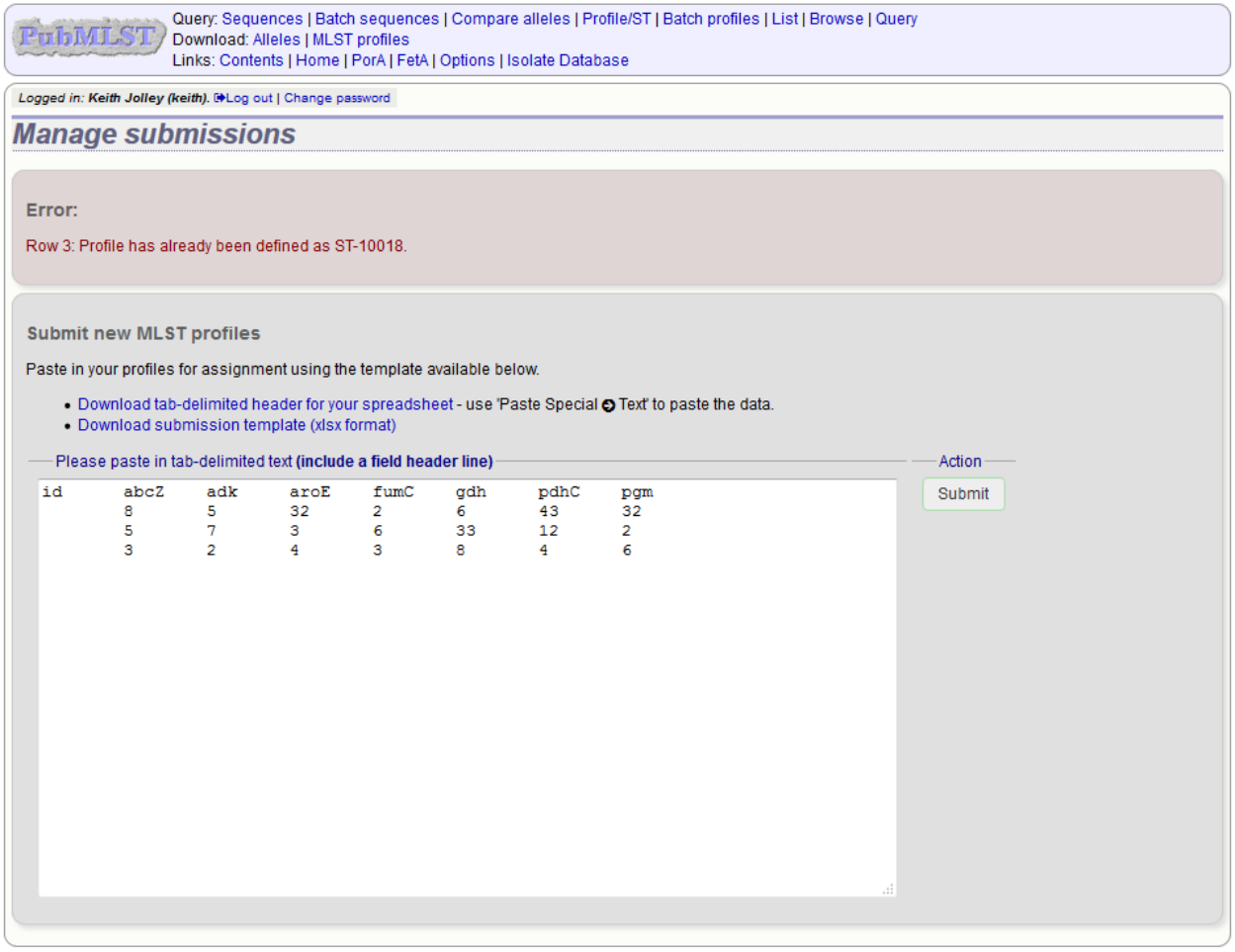
16.3.2 Paste in profile(s)

Fill in the template. The first column 'id' can be used to enter an identifier that is meaningful to you - it is used to report back the results but is not uploaded to the database. It can be left blank, or the entire column can be removed - in which case individual profiles will be identified by row number.

Copy and paste the entire contents of the submission worksheet. Click submit.



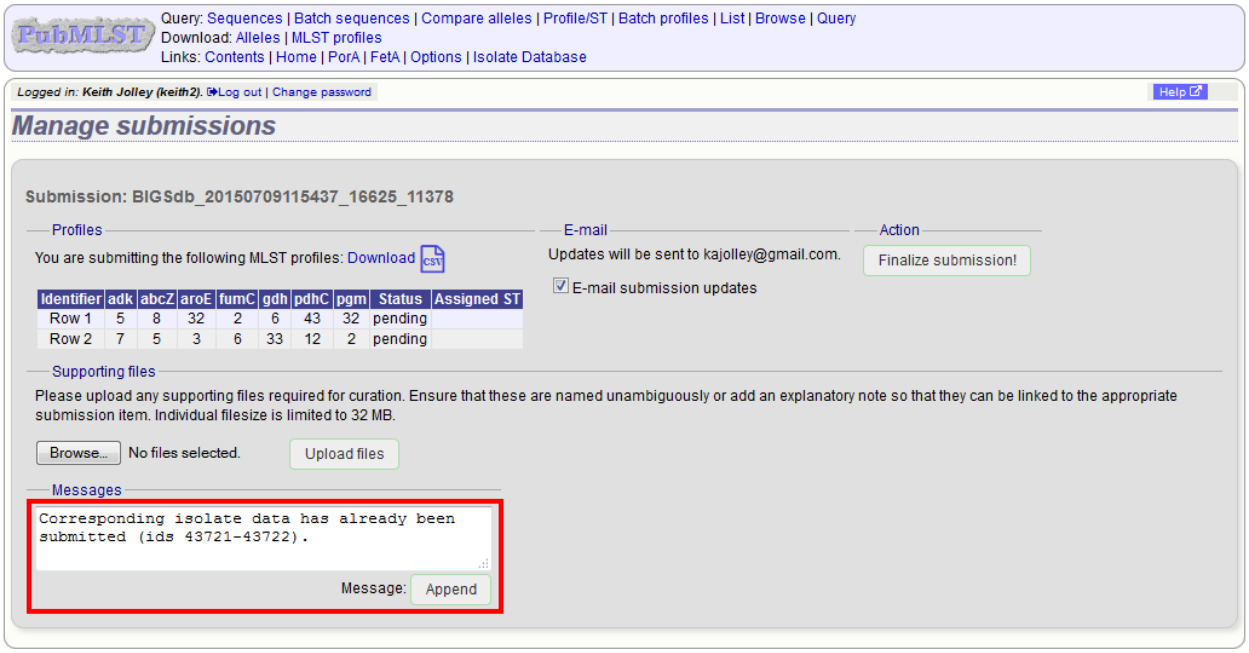
Some basic checks will be performed. These include whether the profile has already been assigned and whether each allele identifier exists. The submission cannot proceed if the checks fail.



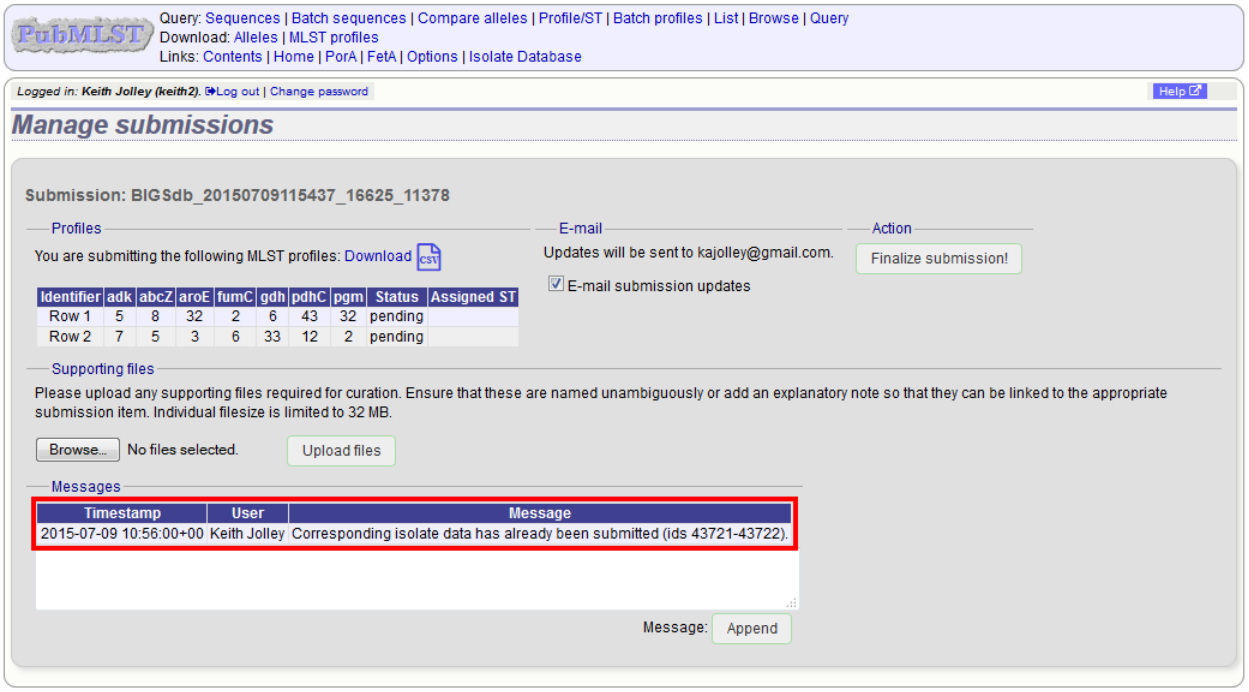
Provided the checks pass, you will then be able to add additional information to your submission

16.3.3 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Append'.



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.



16.3.4 Add supporting files

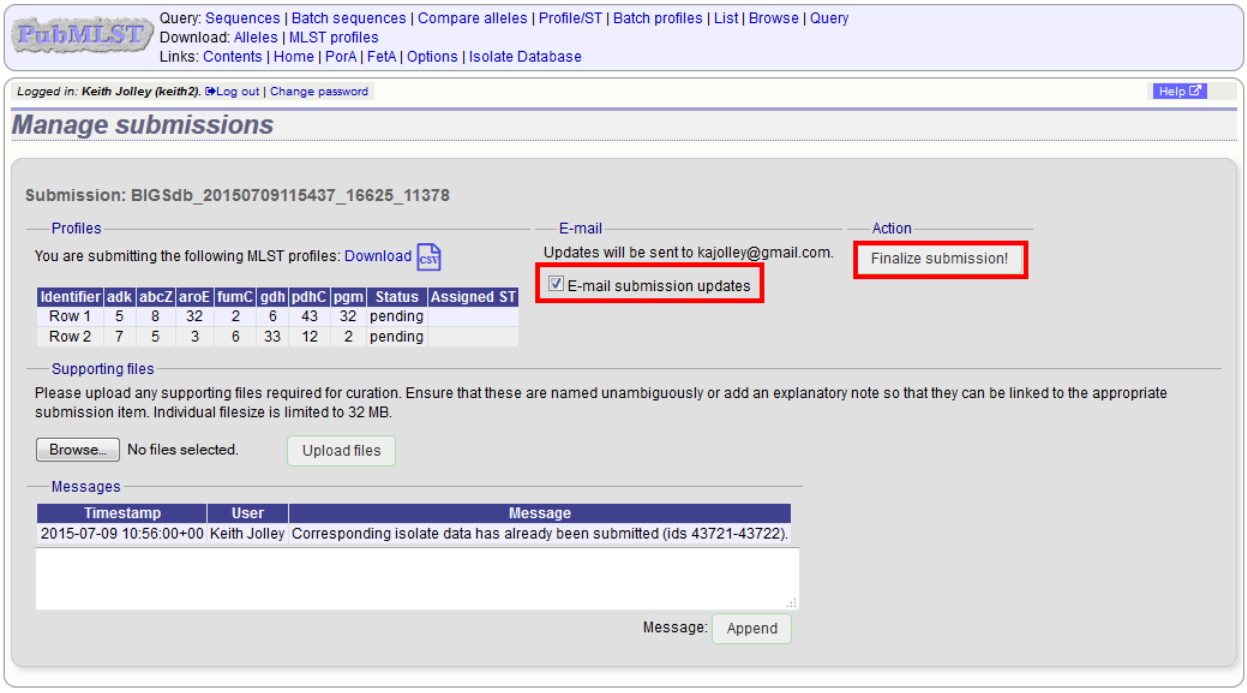
Some submissions may require the attachment of supporting files. These files can be added to the submission by clicking the 'Browse' button in the 'Supporting files' section.

Select the file in the selection box, then click 'Upload files'.

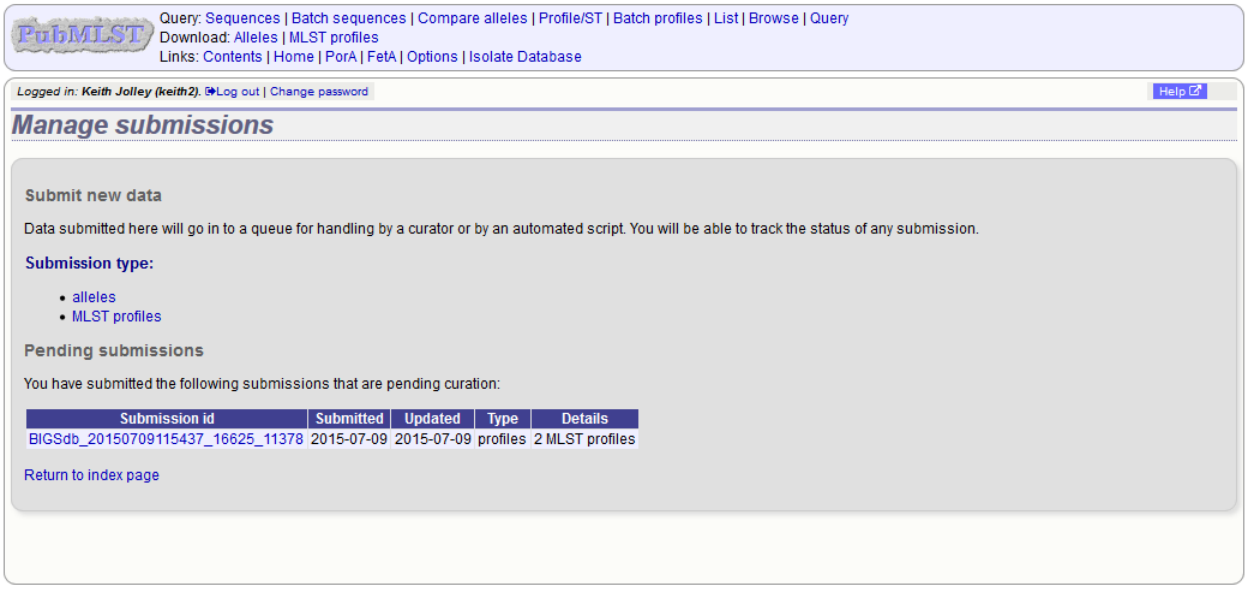
16.3.5 Finalize submission

Make sure the 'E-mail submission updates' box is checked if you wish to receive E-mail notification of the result of your submission. This setting is remembered between sessions.

Click 'Finalize submission!'.



Your submission will then be listed under 'Pending submissions' on your submission page.

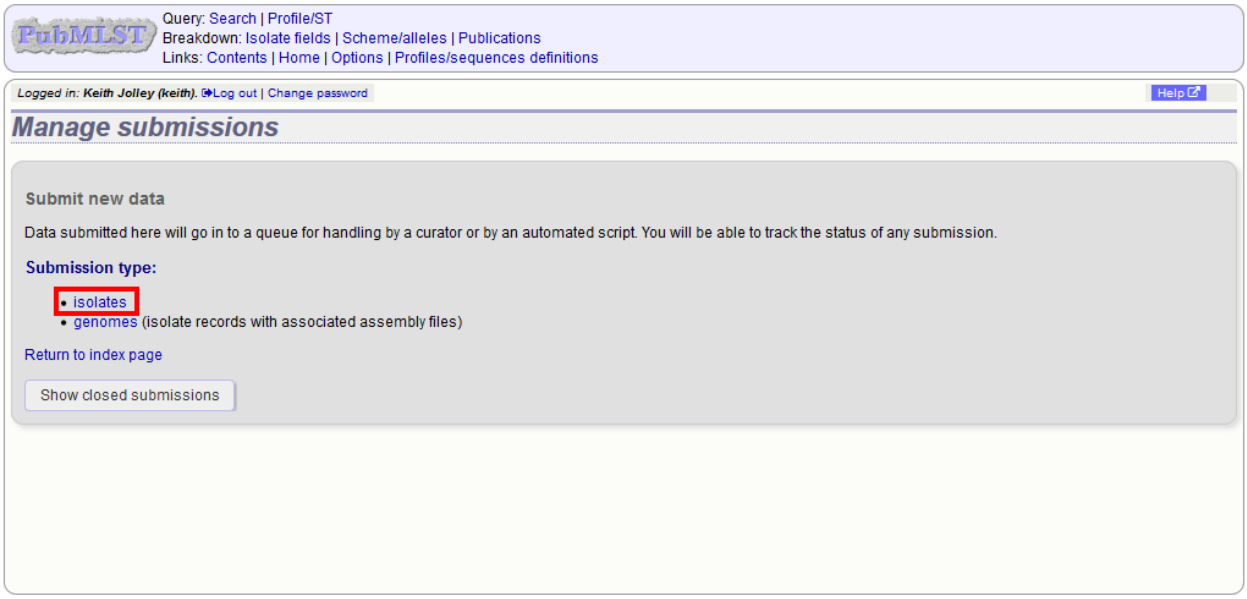


16.4 Isolate submission

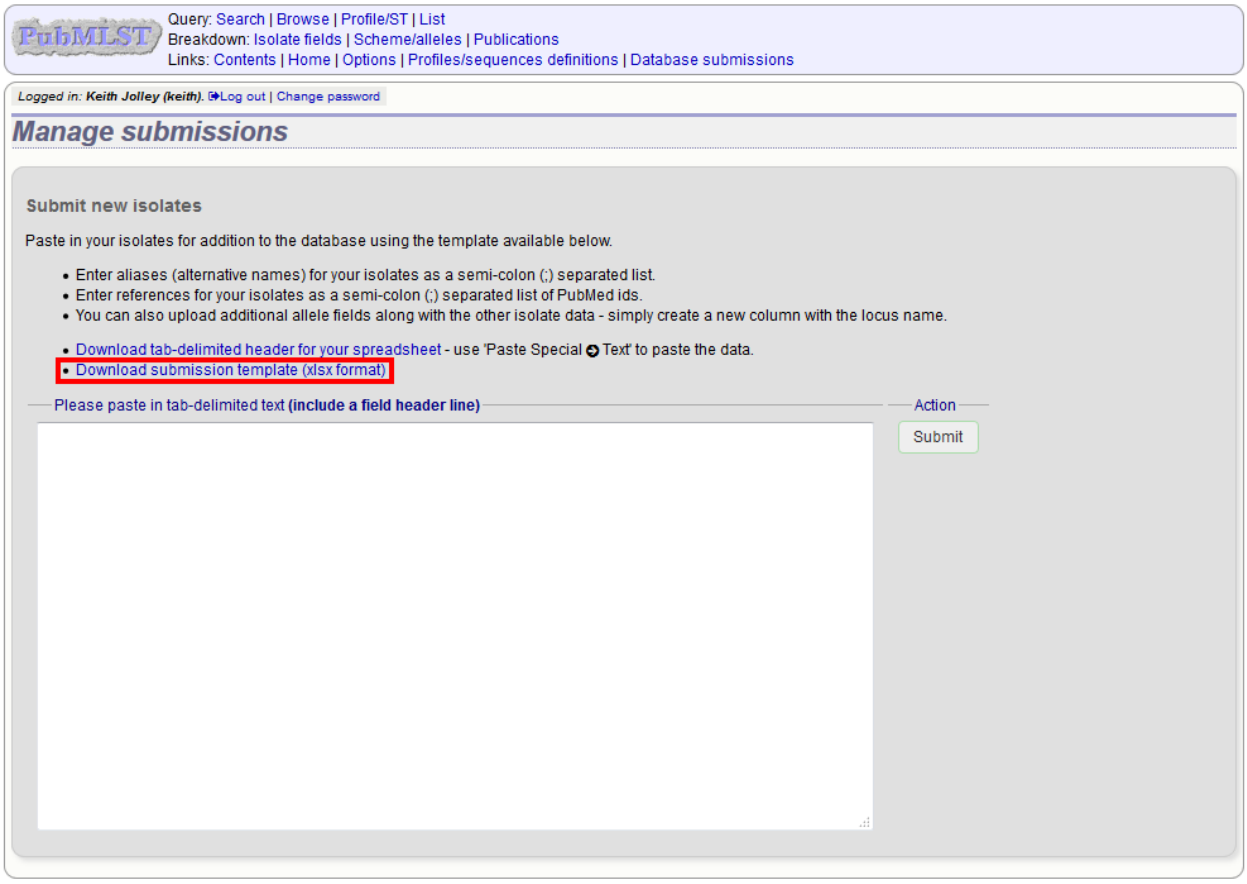
New isolate data can only be submitted from within the appropriate isolate database. You may be required to submit isolate data if you would like to get a new MLST sequence type defined, but this depends on individual database policy.

16.4.1 Start

Click the 'isolates' link under submission type on the submission management page.



Download the Excel submission template.

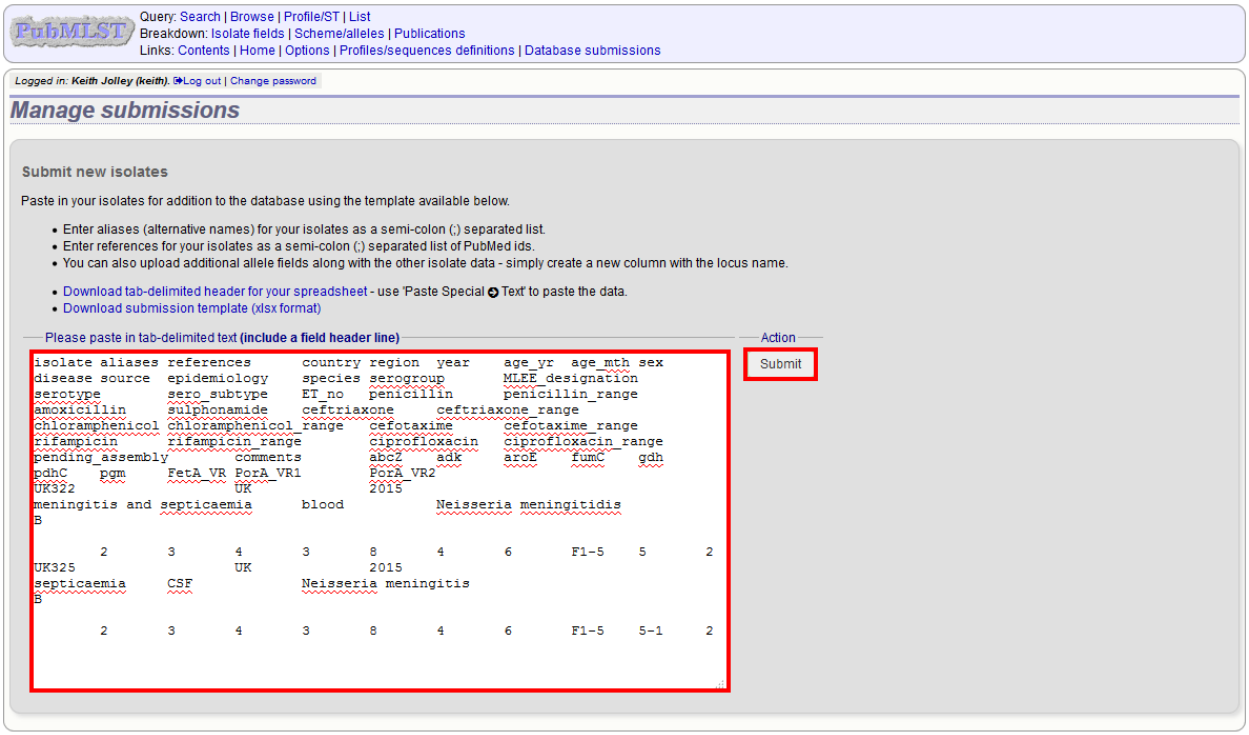


16.4.2 Paste in isolate data

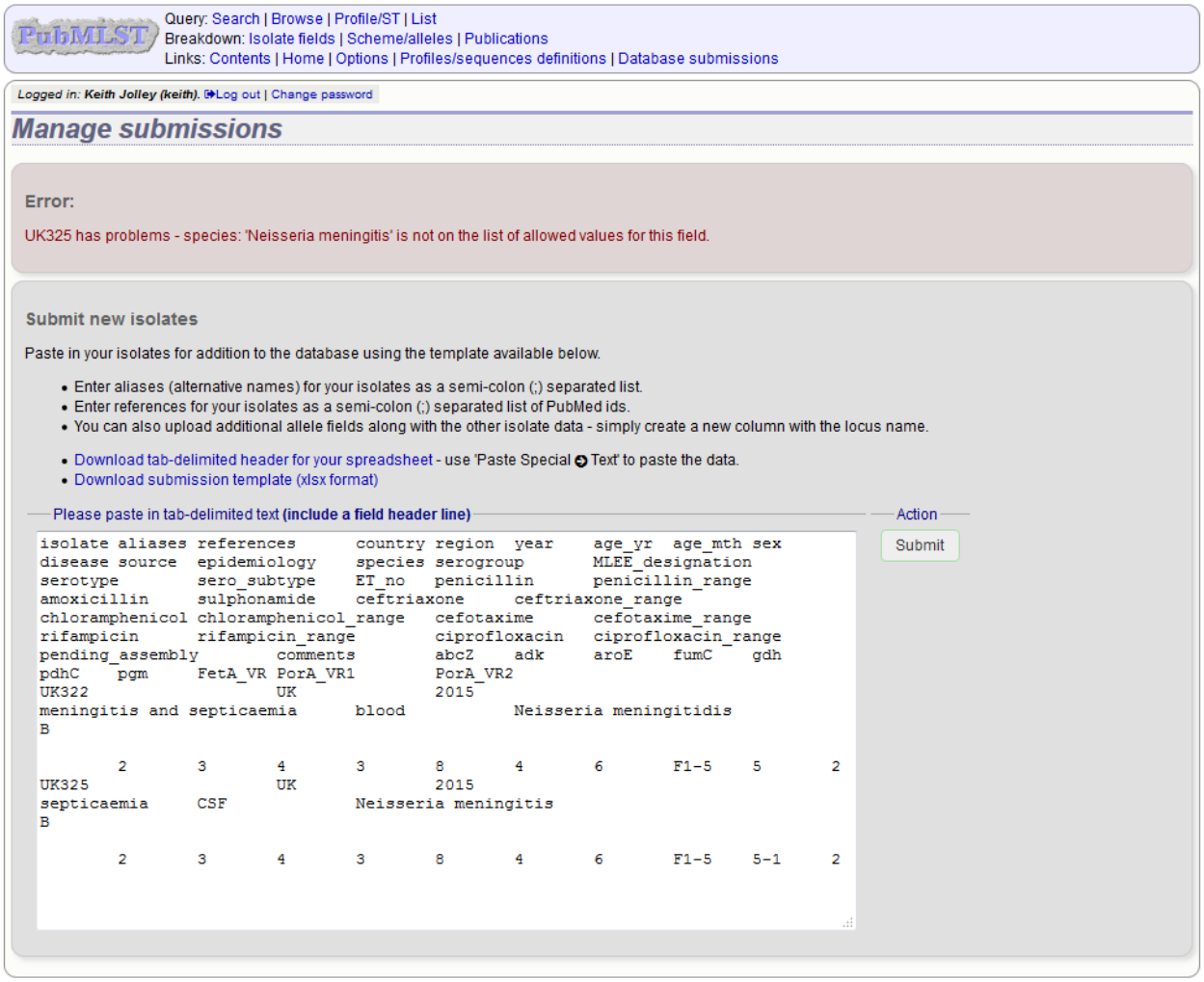
Fill in the template. Some fields are required and cannot be left blank. Check the 'Description of database fields' link on the database contents page to see a description of the fields and allowed values where these have been defined. Where allowed values have been set, the template will have dropdown boxes (although these require newer versions of Excel to work).

Some databases may have hundreds of loci defined, and most will not have a column in the template. You can add new columns for any loci that have been defined and for which you would like to include allelic information for. These locus names must be the primary locus identifier. A list of loci can be found in the 'allowed_loci' tab of the Excel submission template.

Copy and paste the entire contents of the submission worksheet. Click submit.



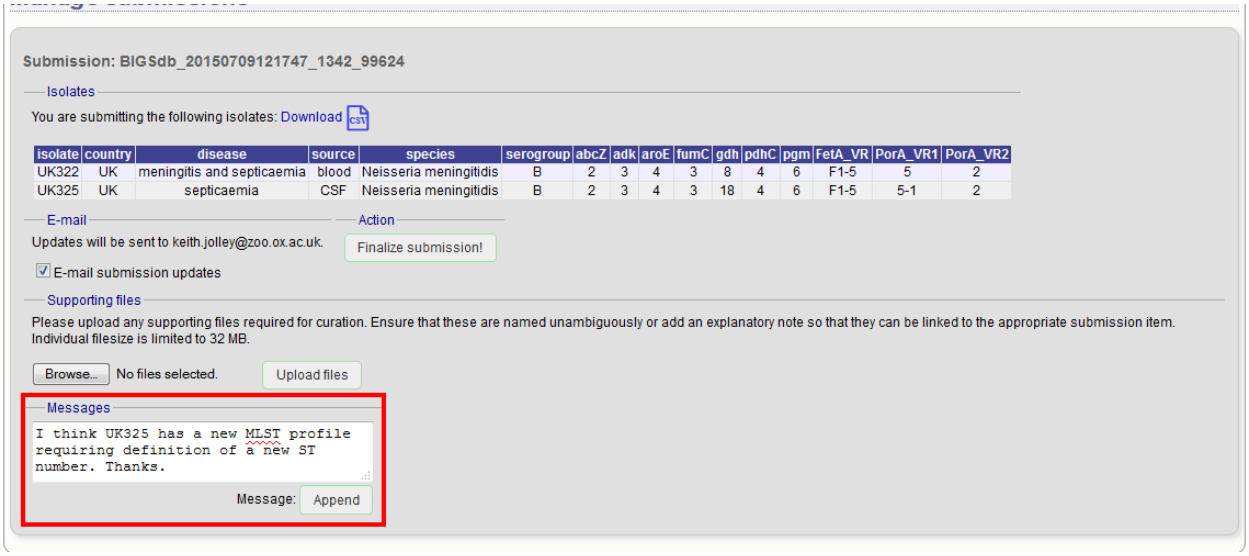
Some basic checks will be performed. These include checking all field values conform to allowed lists or data types. The submission cannot proceed if any checks fail.



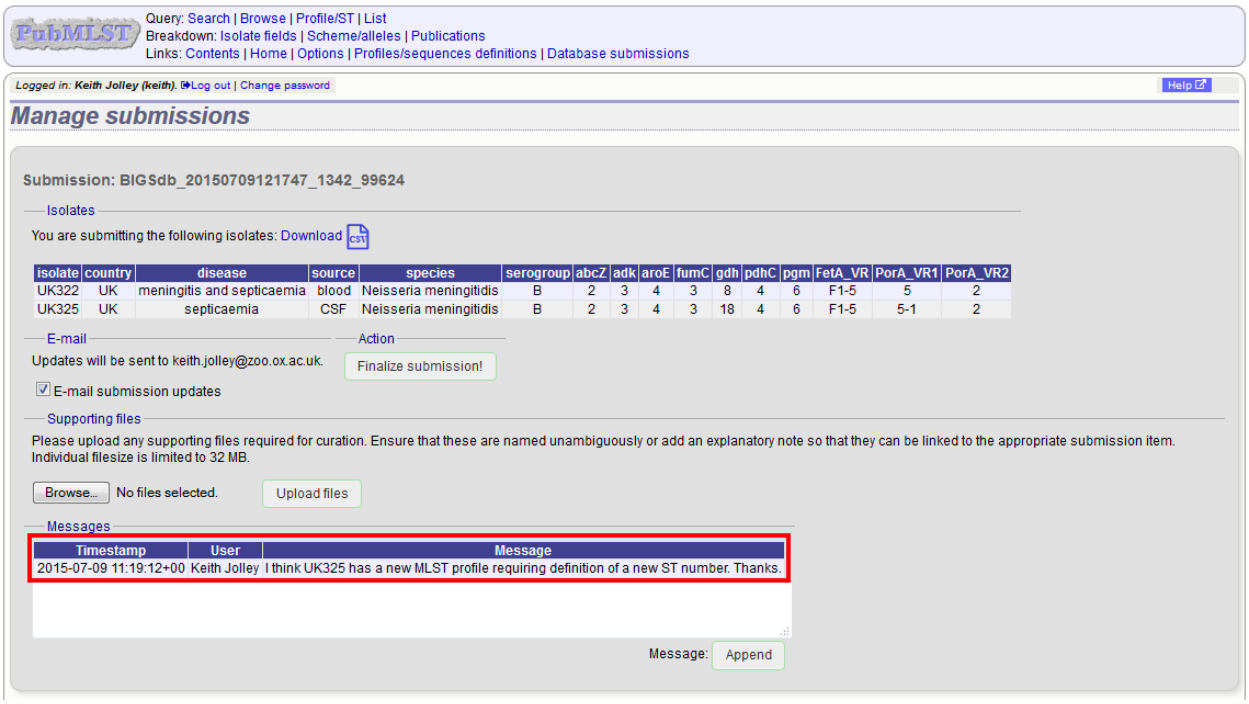
Provided the checks pass, you will then be able to add additional information to your submission.

16.4.3 Add message to curator

If you wish to enter a message to the curator, enter this in the messages box and click 'Append'.



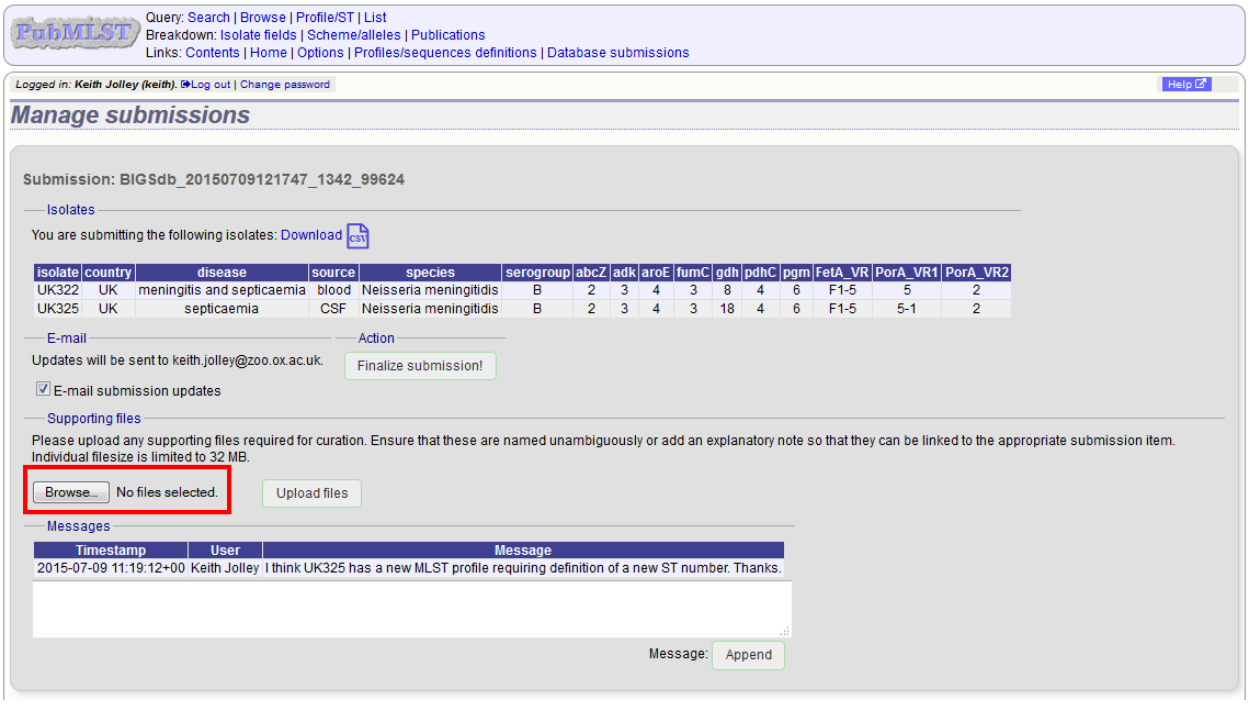
The message will be attached. A curator may respond to the message and attach their own, with the full conversation becoming part of the submission record.



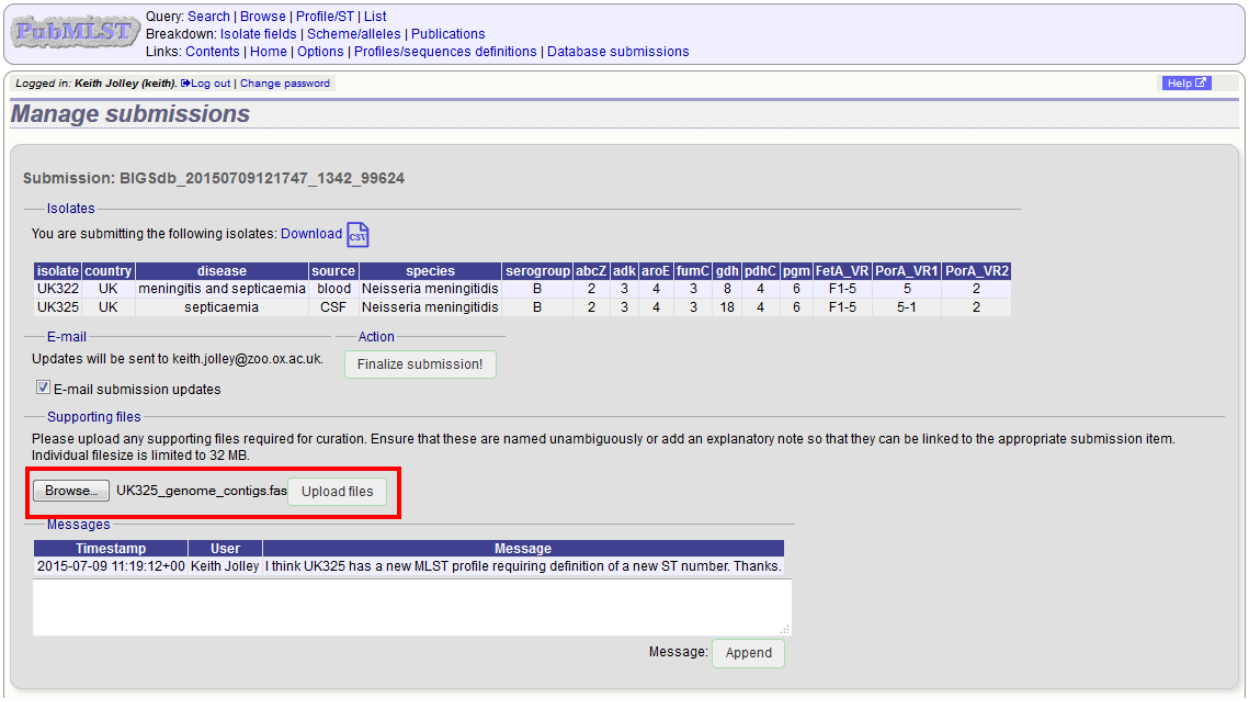
16.4.4 Add supporting files

You can add any files required to support the submission. You may, for example, wish to include a genome sequence for an isolate record (contigs in FASTA format). If you are doing this, make sure that the filename can be unambiguously linked to the appropriate isolate record and *add a message*.

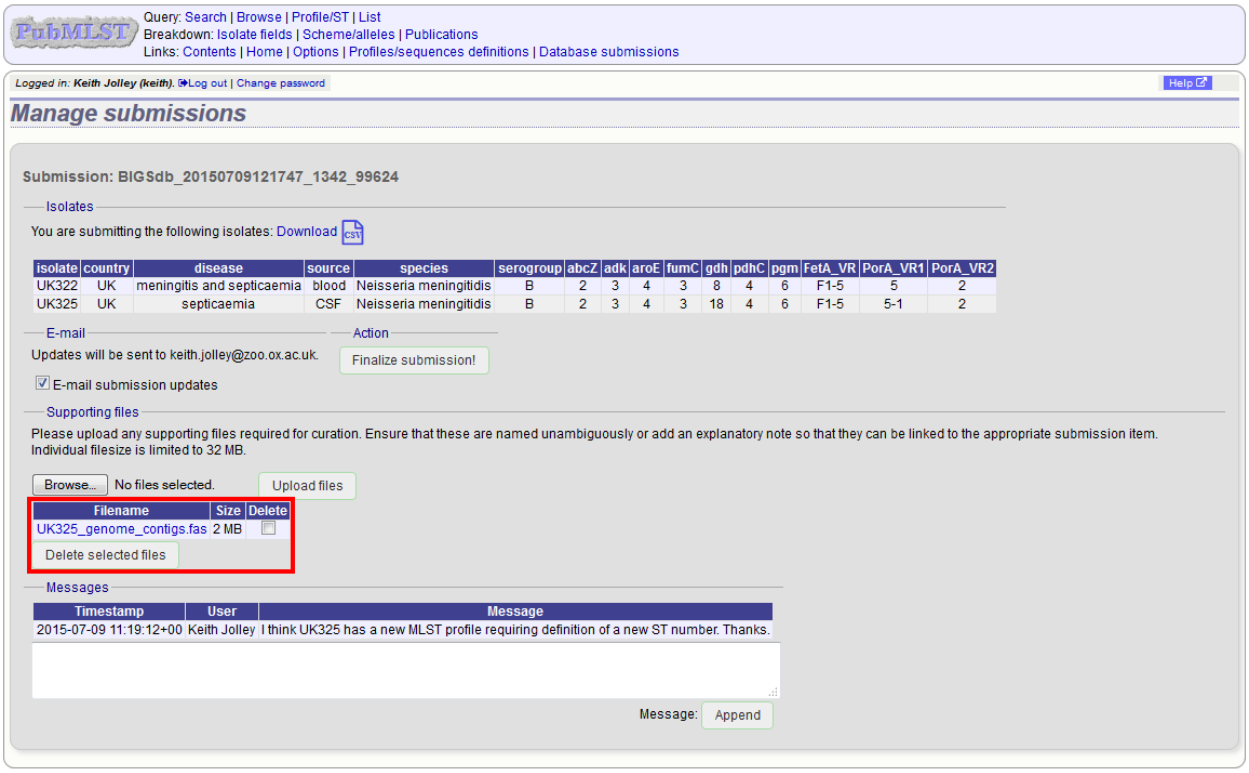
Files can be added to the submission by clicking the 'Browse' button in the 'Supporting files' section.



Select the file in the selection box, then click 'Upload files'.



The file will be uploaded and shown in a table.

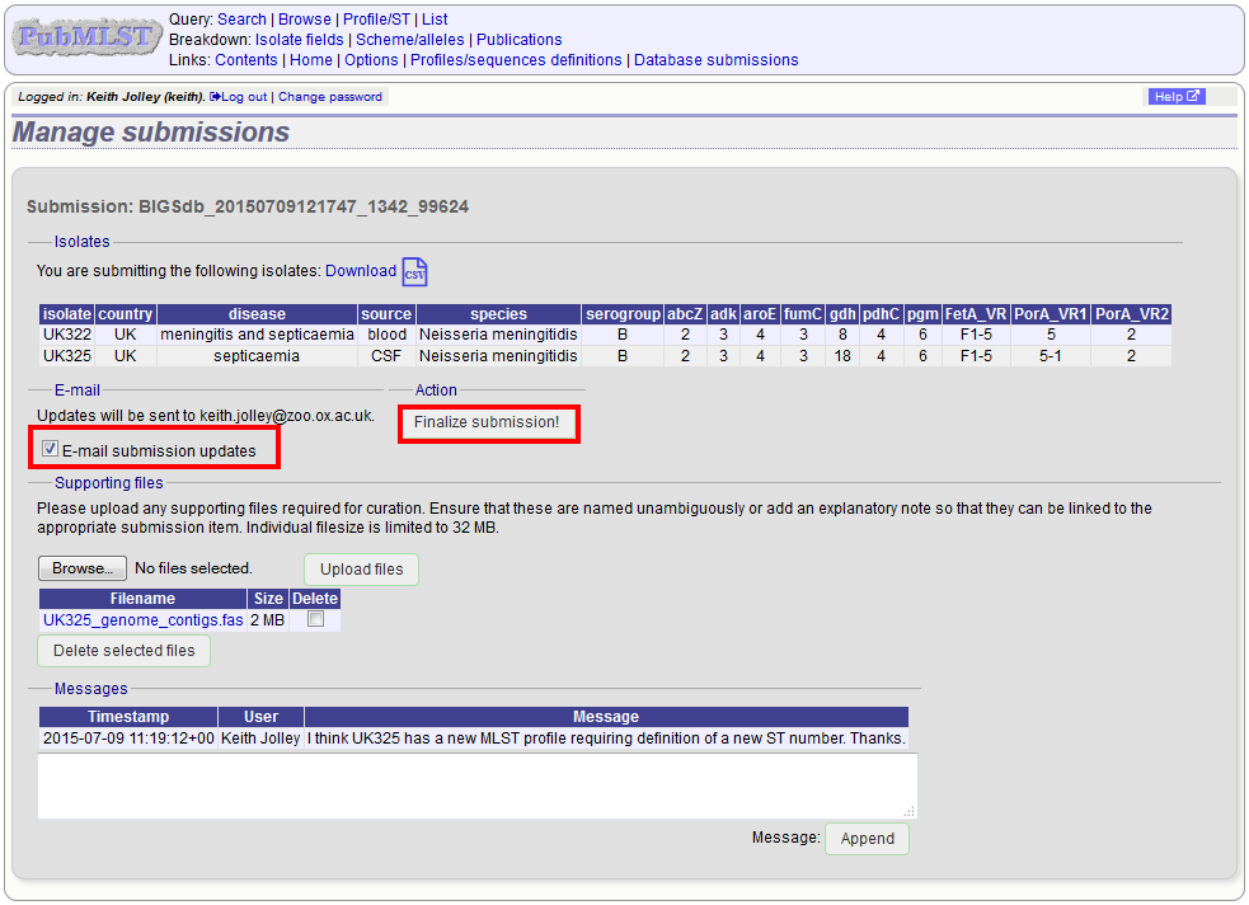


Files can be removed from the submission by checking the appropriate 'Delete' box and clicking 'Delete selected files'.

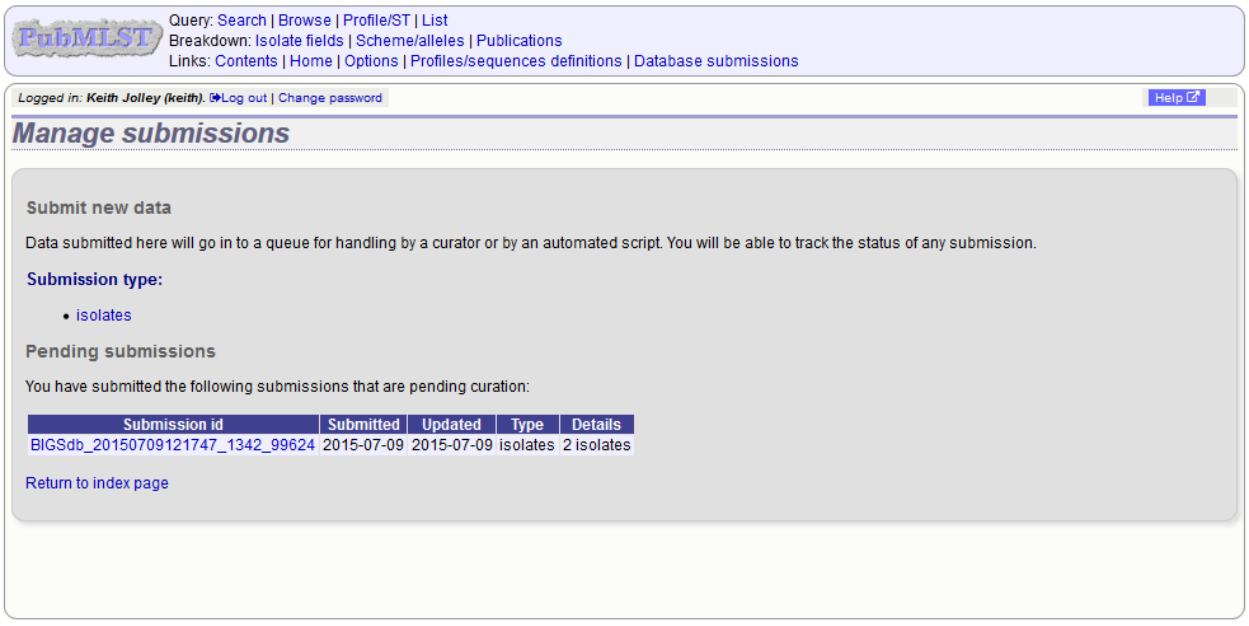
16.4.5 Finalize submission

Make sure the 'E-mail submission updates' box is checked if you wish to receive E-mail notification of the result of your submission. This setting is remembered between sessions.

Click 'Finalize submission!'.



Your submission will then be listed under 'Pending submissions' on your submission page.

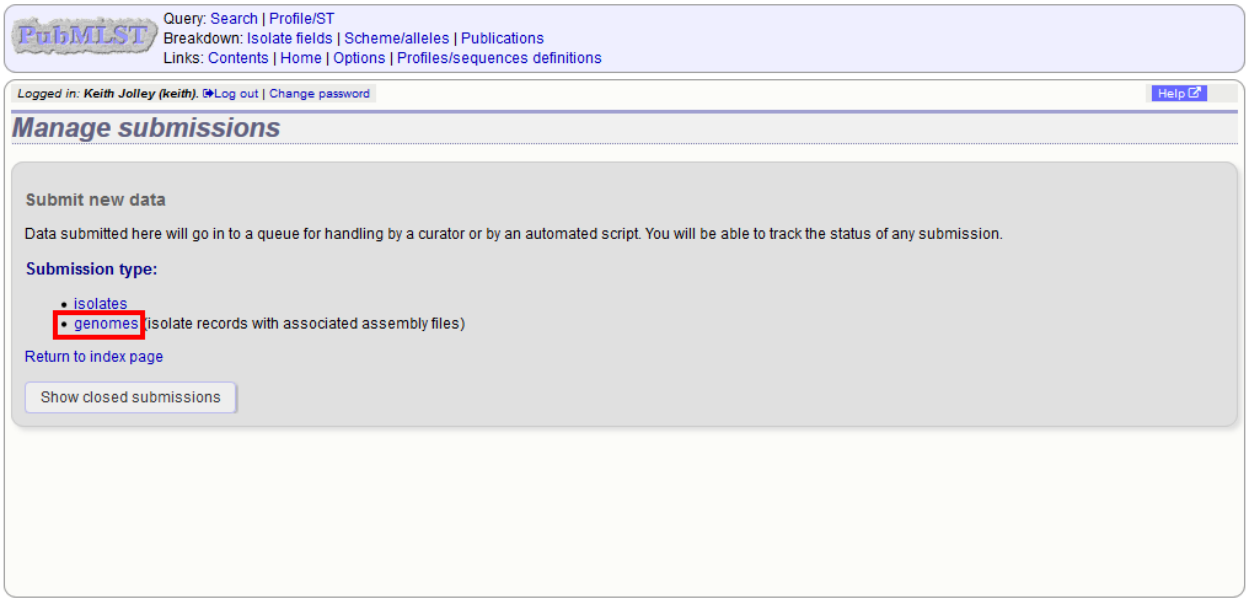


16.5 Genome submission

Submitting genomes uses the same process as standard *isolate submission*. The only difference is that there are a couple of extra required fields in the submission table:

- assembly_filename - this is the name of the FASTA file containing the assembly contigs. This must be uploaded as a supporting file - you will not be able to finalize the submission until every isolate record has a matching contig file.
- sequence_method - the sequencing technology used to generate the sequences. The allowed values are listed on the submission page.

To start the submission, click the 'genomes' link under submission type on the submission management page.



Then follow the steps for *isolate submission*, uploading the contigs files as supporting files.

16.6 Removing submissions from your notification list

Once a submission has been closed by a curator, the results will be displayed in your 'Manage submissions' area. You can remove submissions once you have noted the result by clicking the 'Remove' link.

Alternatively, submissions will be removed automatically a specified period of time after closure. By default, this time is 90 days, but this can vary depending on the site configuration.

_restful_api:

CHAPTER 17

RESTful Application Programming Interface (API)

The REST API allows third-party applications to retrive data stored within BIGSdb databases or to send new submissions to database curators. To use the REST API, your application will make a HTTP request and parse the response. The response format is JSON (except for routes that request a FASTA or CSV file).

Access to protected resources, i.e. those requiring an account, can be accessed via the API using *OAuth authentication*.

17.1 Passing additional/optional parameters

If you are using a method called with GET, optional parameters can be passed as arguments to the query URL by adding a '?' followed by the first argument and its value (separated by a '='). Additional parameters are separated by a '&', e.g.

http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates?page=2&page_size=100

Methods called with POST require their arguments to be sent as JSON within the post body.

17.2 Paging using request headers

Paging of results can be selected using query parameters as described above. In this case, methods that support paging will include a paging object in the JSON response. This will contain links to the next page, last page etc.

The API also supports paging using request headers. The following request headers are supported:

- X-OFFSET
- X-PER-PAGE

e.g.

```
curl -i -H "X-PER-PAGE:10" -H "X-OFFSET:0" http://rest.pubmlst.org/db/pubmlst_
↪neisseria_isolates/isolates
```

If either of these headers are used, the paging object is no longer returned as part of the JSON response. The response will include the following headers:

- X-OFFSET
- X-PER-PAGE
- X-TOTAL-PAGES

17.3 Resources

- *GET / or /db* - List site resources
- *GET /db/{database}* - List database resources
- *GET /db/{database}/classification_schemes* - List classification schemes
- *GET /db/{database}/classification_schemes/{classification_scheme_id}* - Retrieve classification scheme information and groups
- *GET /db/{database}/classification_schemes/{classification_scheme_id}/groups/{group_id}* - List isolates belonging to a classification scheme group
- *GET /db/{database}/loci* - List loci
- *GET /db/{database}/loci/{locus}* - Retrieve locus record
- *GET /db/{database}/loci/{locus}/alleles* - Retrieve list of alleles defined for a locus
- *GET /db/{database}/loci/{locus}/alleles_fasta* - Download alleles in FASTA format
- *GET /db/{database}/loci/{locus}/alleles/{allele_id}* - Retrieve full allele information
- *POST /db/{database}/loci/{locus}/sequence* - Query sequence to identify allele
- *POST /db/{database}/sequence* - Query sequence to identify allele without specifying locus
- *GET /db/{database}/schemes* - List schemes
- *GET /db/{database}/schemes/{scheme_id}* - Retrieve scheme information
- *GET /db/{database}/schemes/{scheme_id}/fields/{field}* - Retrieve information about scheme field
- *GET /db/{database}/schemes/{scheme_id}/profiles* - List allelic profiles defined for scheme
- *GET /db/{database}/schemes/{scheme_id}/profiles_csv* - Download allelic profiles in CSV (tab-delimited) format
- *GET /db/{database}/schemes/{scheme_id}/profiles/{profile_id}* - Retrieve allelic profile record
- *GET /db/{database}/isolates* - Retrieve list of isolate records
- *POST /db/{database}/isolates/search* - Search isolate database
- *GET /db/{database}/isolates/{isolate_id}* - Retrieve isolate record
- *GET /db/{database}/isolates/{isolate_id}/allele_designations* - Retrieve list of allele designations
- *GET /db/{database}/isolates/{isolate_id}/allele_designations/{locus}* - Retrieve full allele designation record
- *GET /db/{database}/isolates/{isolate_id}/allele_ids* - Retrieve allele identifiers
- *GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_designations* - Retrieve scheme allele designation records

- *GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_ids* - Retrieve list of scheme allele identifiers
- *GET /db/{database}/isolates/{isolate_id}/contigs* - Retrieve list of contigs
- *GET /db/{database}/isolates/{isolate_id}/contigs_fasta* - Download contigs in FASTA format
- *GET /db/{database}/contigs/{contig_id}* - Retrieve contig record
- *GET /db/{database}/fields* - Retrieve list of isolate provenance field descriptions
- *GET /db/{database}/field/{field}* - Retrieve values set for a provenance field
- *GET /db/{database}/users/{user_id}* - Retrieve user information
- *GET /db/{database}/projects* - Retrieve list of projects
- *GET /db/{database}/projects/{project_id}* - Retrieve project information
- *GET /db/{database}/projects/{project_id}/isolates* - Retrieve list of isolates belonging to a project
- *GET /db/{database}/submissions* - Retrieve list of submissions
- *POST /db/{database}/submissions* - Create new submission
- *GET /db/{database}/submissions/{submission_id}* - Retrieve submission record
- *DELETE /db/{database}/submissions/{submission_id}* - Delete submission record
- *GET /db/{database}/submissions/{submission_id}/messages* - Retrieve submission correspondence
- *POST /db/{database}/submissions/{submission_id}/messages* - Add submission correspondence
- *GET /db/{database}/submissions/{submission_id}/files* - retrieve list of supporting files uploaded for submission
- *POST /db/{database}/submissions/{submission_id}/files* - Upload submission supporting file
- *GET /db/{database}/submissions/{submission_id}/files/{filename}* - Download submission supporting file
- *DELETE /db/{database}/submissions/{submission_id}/files/{filename}* - Delete submission supporting file

17.3.1 GET / or /db - List site resources

Required route parameters: None

Optional query parameters: None

Example request URI: http://rest.pubmlst.org/

Response: List of resource groupings (ordered by name). Groups may consist of paired databases for sequence definitions and isolate data, or any set of related resources. Each group contains:

- name [string] - short name (usually a single word)
- description [string] - fuller description
- databases [array] - list of database objects, each consists of three key/value pairs:
  - name [string] - name of database config
  - description [string] - short description of resource
  - href [string] - URI to access resource

17.3.2 GET /db/{database} - List database resources

These will vary depending on whether the resource is an isolate or a sequence definition database.

Required route parameter: database [string] - Database configuration name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates

Response: Object containing a subset of the following key/value pairs:

- *fields* [string] - URI to isolate provenance field information
- *isolates* [string] - URI to isolate records
- *schemes* [string] - URI to list of schemes
- *loci* [string] - URI to list of loci
- *projects* [string] - URI to list of projects

17.3.3 GET /db/{database}/classification_schemes - List classification schemes

Required route parameter: database [string] - Database configuration name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/classification_schemes

Response: Object containing:

- records [int] - Number of classification schemes.
- classification_schemes [array] - List of *URIs to classificaton schemes*.

17.3.4 GET /db/{database}/classification_schemes/{classification_scheme_id} - Retrieve classification scheme information and groups

Sequence definition databases only.

Required route parameters:

- database [string] - Database configuration name
- classification_scheme_id [integer] - Classification scheme id number

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/classification_schemes/1

Response: Object containing some or all of:

- id [integer] - Classification scheme id
- name [text] - Name of classification scheme
- description [text] - Description of classification scheme
- relative_threshold [boolean] - True if a *relative thresold* is used
- inclusion_threshold [integer] - The threshold for number of loci difference used to group
- groups [array] (sequence definition databases only) - list of group objects consisting of:

  - id [integer] - group id
  - profiles [array] - list of *URIs to profiles* belonging to the group

17.3.5 GET /db/{database}/classification_schemes/{classification_scheme_id}/groups/{group_id} - List isolates belonging to a classification scheme group

Isolate databases only.

Required route parameters:

- database [string] - Database configuration name
- classification_scheme_id [integer] - Classification scheme id number
- group_id [integer] - Group id number

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/classification_schemes/4/groups/65

Response: Object containing of:

- records [integer] - Number of isolates
- isolates [array] - List of *URIs to isolate records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.6 GET /db/{database}/loci - List loci

Required route parameter: database [string] - Database configuration name

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci

Response: Object containing:

- records [integer] - Number of loci
- loci [array] - List of *URIs to defined locus records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.

- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.7 GET /db/{database}/loci/{locus} - Retrieve locus record

Provides information about a locus, including links to allele sequences (in seqdef databases).

Required route parameters:

- database [string] - Database configuration name
- locus [string] - Locus name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ

Response: Object containing a subset of the following key/value pairs:

- id [string] - locus name
- data_type [string] - 'DNA' or 'peptide'
- allele_id_format [string] - 'integer' or 'text'
- allele_id_regex [string] - regular expression constraining allele ids
- common_name [string]
- aliases [array] - list of alternative names of the locus
- length_varies [boolean]
- length [integer] - length if alleles are of a fixed length
- coding_sequence [boolean]
- orf [integer] - 1-6
- schemes [array] - list of scheme objects, each consisting of:
  - scheme [string] - URI to scheme information
  - description [string]
- min_length [integer] (seqdef databases) - minimum length for variable length loci
- max_length [integer] (seqdef databases) - maximum length for variable length loci
- alleles [string] (seqdef databases) - *URI to list of allele records*
- alleles_fasta [string] (seqdef databases) - *URI to FASTA file of all alleles of locus*
- curators [array] (seqdef databases) - list of *URIs to user records* of curators of the locus
- publications [array] (seqdef databases) - list of PubMed id numbers of papers describing the locus
- full_name [string] (seqdef databases)
- product [string] (seqdef databases)

- description [string] (seqdef databases)
- extended_attributes [array] (seqdef databases) - list of extended attribute objects. Each consists of a subset of the following fields:
  - field [string] - field name
  - value_format [string] - 'integer', 'text', or 'boolean'
  - value_regex [string] - regular expression constraining value
  - description [string] - description of field
  - length [integer] - maximum length of field
  - required [boolean]
  - allowed_values [array] - list of allowed values
- genome_position [integer] (isolate databases)

17.3.8 GET /db/{database}/loci/{locus}/alleles - Retrieve list of alleles defined for a locus

Required route parameters:

- database [string] - Database configuration name
- locus [string] - Locus name

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.
- added_after [date] - Include only alleles added after specified date (ISO 8601 format).
- updated_after [date] - Include only alleles last modified after specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles

Response: Object containing:

- records [int] - Number of alleles.
- last_updated [date] - Latest allele addition/modification date (ISO 8601 format).
- alleles [array] - List of *URIs to defined allele records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.9 GET /db/{database}/loci/{locus}/alleles_fasta - Download alleles in FASTA format

Required route parameters:

- database [string] - Database configuration name
- locus [string] - Locus name

Optional parameters:

- added_after [date] - Include only alleles added after specified date (ISO 8601 format).
- updated_after [date] - Include only alleles last modified after specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles_fasta

Response: FASTA format file of allele sequences

17.3.10 GET /db/{database}/loci/{locus}/alleles/{allele_id} - Retrieve full allele information

Required route parameters:

- database [string] - Database configuration name
- locus [string] - Locus name
- allele_id [string] - Allele identifier

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/loci/abcZ/alleles/5

Response: Object containing the following key/value pairs:

- locus [string] - *URI to locus description*
- allele_id [string] - allele identifier
- sequence [string] - sequence
- status [string] - either 'Sanger trace checked', 'WGS: manual extract', 'WGS: automated extract', or 'unchecked'
- sender [string] - *URI to user details* of sender
- curator [string] - *URI to user details* of curator
- date_entered [string] - record creation date (ISO 8601 format)
- datestamp [string] - last updated date (ISO 8601 format)

17.3.11 POST /db/{database}/loci/{locus}/sequence - Query sequence to identify allele

Required route parameters:

- database [string] - Database configuration name
- locus [string] - Locus name

Required additional parameters (JSON-encoded in POST body):

- sequence [string] - Sequence string

Optional parameters: None

Response: Object containing the following key/value pairs:

- exact_matches [array] - list of match objects, each consisting of:
  - allele_id
  - href - *URI to allele record*.

Note: This method currently only supports exact matches. Whitespace is removed from the sequence and it is capitalized before querying the database.

17.3.12 POST /db/{database}/sequence - Query sequence to identify allele without specifying locus

Required route parameters:

- database [string] - Database configuration name

Required additional parameters (JSON-encoded in POST body):

- sequence [string] - Sequence string

Optional parameters: None

Response: Object containing the following key/value pairs:

- exact_matches [array] - list of match objects, each consisting of:
  - locus [string] - locus name
  - allele_id [string] - allele identifier
  - href - *URI to allele record*.

Note: This method currently only supports exact matches. Whitespace is removed from the sequence and it is capitalized before querying the database.

17.3.13 GET /db/{database}/schemes - List schemes

Required route parameter: database [string] - Database configuration name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes

Response:

- records [integer] - Number of schemes
- schemes [array] - list of scheme objects, each containing:
  - scheme [string] - *URI to scheme information*
  - description [string]

17.3.14 GET /db/{database}/schemes/{scheme_id} - Retrieve scheme information

Includes links to allelic profiles (in seqdef databases, if appropriate). **Required route parameters:**

- database [string] - Database configuration name
- scheme_id [integer] - Scheme id number

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1

Response: Object containing a subset of the following key/value pairs:

- id [integer]
- description [string]
- locus_count [integer] - number of loci belonging to scheme
- loci [array] - list of *URIs to locus descriptions*
- has_primary_key_field [boolean]
- fields [array] - list of *URIs to scheme field descriptions*
- primary_key_field [string] - *URI to primary key field description*
- profiles [string] - URI to list of profile definitions (only seqdef databases)
- profiles_csv [string] - URI to tab-delimited file of all scheme profiles
- curators [array] (seqdef databases) - list of *URIs to user records* of curators of the scheme

17.3.15 GET /db/{database}/schemes/{scheme_id}/fields/{field} - Retrieve information about scheme field

Required route parameters:

- database [string] - Database configuration name
- scheme_id [integer] - Scheme id number
- field [string] - Field name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/fields/ST

Response: Object containing the following key/value pairs:

- field [string] - field name
- type [string] - data type of field (integer or text)
- primary_key [boolean] - true if field is the scheme primary key

17.3.16 GET /db/{database}/schemes/{scheme_id}/profiles - List allelic profiles defined for scheme

Required route parameters:

- database [string] - Database configuration name
- scheme_id [integer] - Scheme id

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.
- added_after [date] - Include only profiles added after specified date (ISO 8601 format).
- updated_after [date] - Include only profiles last modified after specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles

Response: Object containing:

- records [int] - Number of profiles
- last_updated [date] - Latest profile addition/modification date (ISO 8601 format).
- profiles [array] - List of *URIs to defined profile records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

Note: This method also supports content negotiation. If the request accepts header includes TSV or CSV, then the call is redirected to */db/{database}/schemes/{scheme_id}/profiles_csv*.

17.3.17 GET /db/{database}/schemes/{scheme_id}/profiles_csv - Download allelic profiles in CSV (tab-delimited) format

Required route parameters:

- database [string] - Database configuration name
- scheme_id [integer] - Scheme id

Optional parameters:

- added_after [date] - Include only profiles added after specified date (ISO 8601 format).
- updated_after [date] - Include only profiles last modified after specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles_csv

Response: Tab-delimited text file of allelic profiles

17.3.18 GET /db/{database}/schemes/{scheme_id}/profiles/{profile_id} - Retrieve allelic profile record

Required route parameters:

- database [string] - Database configuration name
- scheme_id [integer] - Scheme id
- profile_id [string/integer] - Profile id

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/schemes/1/profiles/11

Response: Object containing the following key/value pairs:

- *primary_key_term* [string/integer] - The field name is the primary key, e.g. ST. The value is the primary key value (primary_id used as an argument).
- alleles [object] - *list of URIs to allele descriptions*
- *other_scheme_fields* [string/integer] - Each scheme field will have its own value if defined. The field name is the name of the field.
- sender [string] - *URI to user details* of sender
- curator [string] - *URI to user details* of curator
- date_entered [string] - record creation date (ISO 8601 format)
- datestamp [string] - last updated date (ISO 8601 format)

17.3.19 GET /db/{database}/isolates - Retrieve list of isolate records

Required route parameter: database [string] - Database configuration name

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.
- added_after [date] - Include only isolates added after specified date (ISO 8601 format).
- updated_after [date] - Include only isolates last modified after specified date (ISO 8601 format).

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates

Response: Object containing:

- records [int] - Number of isolates
- isolates [array] - List of *URIs to isolate records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.20 GET /db/{database}/isolates/{isolate_id} - Retrieve isolate record

Required route parameters:

- database [string] - Database configuration name
- isolate_id [integer] - Isolate identifier

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1

Response: Object containing some or all of the following key/value pairs:

- provenance [object] - set of key/value pairs. Keys are defined by calling the */fields route* route. The fields will vary by database but will always contain the following:
  - id [integer]
  - sender [string] - *URI to user details* of sender
  - curator [string] - *URI to user details* of curator
  - date_entered [string] - record creation date (ISO 8601 format)
  - datestamp [string] - last updated date (ISO 8601 format)
- publications [array] (seqdef databases) - list of PubMed id numbers of papers that refer to the isolate
- sequence_bin [object] - consists of the following key/value pairs:
  - contigs_fasta [string] - *URI to FASTA file containing all the contigs belonging to this isolate*
  - contigs [string] - *URI to list of contig records*
  - contig_count [integer] - number of contigs
  - total_length [integer] - total length of contigs
- allele_designations [object] - consists of the following key/value pairs:
  - allele_ids - *URI to list of all allele_id values* defined for the isolate
  - designation_count - number of allele designations defined for the isolate
  - full_designations - *URI to list of full allele designation records*
- schemes [array] - list of scheme objects, each containing some of the following:
  - description [string] - description of scheme
  - loci_designated_count [integer] - number of loci within scheme that have an allele designated for this isolate.
  - allele_ids [string] - *URI to list of all allele_id values defined for this scheme* for this isolate
  - full_designations [string] - *URI to list of full allele designation records* for this isolate
  - fields [object] - consisting of key/value pairs where the key is the name of each scheme field
  - classification_schemes [object] - consisting of key/value pairs, where each key is the name of the classification scheme and the value is an object consisting of:
    - href [string] - *URI to classification scheme description*
    - groups [array] - list of group objects consisting of:
      - group [integer] - group id
      - records [integer] - number of isolates in group

        - isolates [string] - URI to classification group record containing URIs to member isolate records
- projects [array] - list of project objects, each containing the following:
  - id [string] - *URI to project information*
  - description [string] - description of project
- new_version [string] - URI to newer version of record
- old_version [string] - URI to older version of record

17.3.21 GET /db/{database}/isolates/{isolate_id}/allele_designations - Retrieve list of allele designation records

Required route parameters:

- database [string] - Database configuration name
- isolate_id [integer] - Isolate identifier

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_designations

Response: Object containing:

- records [int] - Number of allele designations
- allele_designations [array] - List of *URIs to allele designation records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.22 GET /db/{database}/isolates/{isolate_id}/allele_designations/{locus} - Retrieve full allele designation record

Required route parameters:

- database [string] - Database configuration name
- isolate_id [integer] - Isolate identifier
- locus [string] - Locus name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_designations/BACT000065

Response: List of allele_designation objects (there may be multiple designations for the same locus), each containing:

- locus [string] - *URI to locus description*
- allele_id [string]
- method [string] - either 'manual' or 'automatic'
- status [string] - either 'confirmed' or 'provisional'
- comments [string]
- sender [string] - *URI to user details* of sender
- curator [string] - *URI to user details* of curator
- datestamp [string] - last updated date (ISO 8601 format)

17.3.23 GET /db/{database}/isolates/{isolate_id}/allele_ids - Retrieve allele identifiers

Required route parameters:

- database [string] - Database configuration name
- isolate_id [integer] - Isolate identifier

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/allele_ids

Response: Object containing:

- records [int] - Number of allele id objects
- allele_ids [array] - List of allele id objects, each consisting of a key/value pair where the key is the locus name. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.24 GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_designations - Retrieve scheme allele designation records

Required route parameters:

- database [string] - Database configuration name
- isolate_id [integer] - Isolate identifier
- scheme_id [integer] - Scheme identifier

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/schemes/1/allele_designations

Response:

- records [int] - Number of allele designation objects
- allele_designations [array] - List of *allele designation objects* for each locus in the specified scheme that has been designated.

17.3.25 GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele_ids - Retrieve list of scheme allele identifiers

Required route parameters:

- database [string] - Database configuration name
- isolate_id [integer] - Isolate identifier
- scheme_id [integer] - Scheme identifier

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/schemes/1/allele_ids

Response:

- records [int] - Number of allele id objects
- allele_ids [array] - List containing allele id objects for each locus in the specified scheme that has been designated. Each allele_id object contains a key which is the name of the locus with a value that may be either a string, integer or array of strings or integers (required where there are multiple designations for a locus). The data type depends on the allele_id_format set for the specific locus.

17.3.26 GET /db/{database}/isolates/{isolate_id}/contigs - Retrieve list of contigs

Required route parameters:

- database [string] - Database configuration name
- isolate_id [integer] - Isolate identifier

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/contigs

Response: Object containing:

- records [int] - Number of contigs
- contigs [array] - List of *URIs to contig records* Pages are 100 records by default. Page size can be modified using the page_size parameter.
- **paging [object] - Some or all of the following:**
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.27 GET /db/{database}/isolates/{isolate_id}/contigs_fasta - Download contigs in FASTA format

Required route parameters:

- database [string] - Database configuration name
- isolate_id [integer] - Isolate identifier

Optional parameter:

- header [string] - either 'original_designation' or 'id' (default is 'id'). This selects whether the FASTA header lines contain the originally uploaded FASTA headers or the sequence bin id numbers.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/1/contigs_fasta?header=original_designation

Response: FASTA format file of isolate contig sequences

17.3.28 POST /db/{database}/isolates/search - Search isolate database

Required route parameters:

- database [string] - Database configuration name

Optional parameters (appended to URI):

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.

Query parameters (JSON-encoded in POST body):

You must include at least one query parameter.

Flattened parameter names in the following forms are supported:

- field.{field} - key/value pairs for provenance fields. Supported field names can be found by calling the */fields route*. The fields will vary by database.
- locus.{locus} - key/value pairs of locus and its allele designation. Supported locus names can be found by calling the */loci route*.

- scheme.{scheme_id}.{scheme_field} - key/value pairs of scheme fields and their values. Supported field names can be determined by following routes from the */schemes route*.

Parameters have to be flattened rather than using nested attributes to support passing via OAuth.

Example method call using curl: The following searches for *Neisseria* ST-11 isolates from Europe in 2015 (MLST is scheme#1 in this database).

```
curl -s -H "Content-Type: application/json" -X POST \
"http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/isolates/search" \
-d '{"field.continent":"europe","field.year":2015,"scheme.1.ST":11}'
```

Response: Object containing:

- records [int] - Number of isolates
- isolates [array] - List of *URIs to isolate records*. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.29 GET /db/{database}/contigs/{contig_id} - Retrieve contig record

Required route parameters:

- database [string] - Database configuration name
- contig_id [integer] - Contig identifier

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/contigs/180062

Response: Contig object consisting of the following key/value pairs:

- id [integer] - contig identifier
- isolate_id [integer] - isolate identifier
- sequence [string] - contig sequence
- length [integer] - length of contig sequence
- method [string] - sequencing method
- sender [string] - *URI to user details* of sender
- curator [string] - *URI to user details* of curator
- date_entered [string] - record creation date (ISO 8601 format)
- datestamp [string] - last updated date (ISO 8601 format)
- loci [array] - list of sequence tag objects consisting of:
  - locus [string] - *URI to locus description*

  - locus_name [string]
  - start [integer]
  - end [integer]
  - direction [string] - forward/reverse
  - complete [boolean] - true/false

17.3.30 GET /db/{database}/fields - Retrieve list of isolate provenance field descriptions

Required route parameters:

- database [string] - Database configuration name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/fields

Response: Array of field objects, each consisting of some or all of the following key/value pairs:

- name [string] - name of field
- type [string] - data type (int, text, date, float)
- length [integer] - maximum length of field
- required [boolean] - true if field value is required
- min [integer] - minimum value for integer values
- max [integer] - maximum value for integer values
- regex [string] - regular expression that constrains the allowed value of the field
- comments [string]
- allowed values [array] - list of allowed values for the field
- values [string] - URI to list of used field values

17.3.31 GET /db/{database}/fields/{field} - Retrieve values set for a provenance field

Required route parameters:

- database [string] - Database configuration name
- field [string] - Provenance metadata field name

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/fields/country

Response: Object containing:

- records [int] - Number of values

- values [array] - List of values used in isolate records. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.32 GET /db/{database}/users/{user_id} - Retrieve user information

Users may be data submitters or curators.

Required route parameters:

- database [string] - Database configuration name
- user_id [integer] - User id number

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/users/2

Response: Object containing the following key/value pairs:

- id [integer] - user id number
- first_name [string]
- surname [string]
- affiliation [string] - institutional affiliation
- email [string] - E-mail address

17.3.33 GET /db/{database}/projects - Retrieve list of projects

Required route parameter: database [string] - Database configuration name

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/projects

Response:

- projects [array] - List of project objects, each containing:
  - project [string] - *URI to project information*
  - description [string]
  - isolate_count [integer] - number of isolates in project

17.3.34 GET /db/{database}/projects/{project_id} - Retrieve project information

Required route parameters:

- database [string] - Database configuration name
- project_id [integer] - Project id number

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/projects/3

Response: Object containing a subset of the following key/value pairs:

- id [integer]
- description [string]
- isolates [string] - *URI to list of URIs of member isolate records*.

17.3.35 GET /db/{database}/projects/{project_id}/isolates - Retrieve list of isolates belonging to a project

Required route parameter:

- database [string] - Database configuration name
- project_id [integer] - Project id number

Optional parameters:

- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/projects/3/isolates

Response: Object containing:

- records [int] - Number of isolates in the project
- isolates [array] - List of URIs to isolate records. Pages are 100 records by default. Page size can be modified using the page_size parameter.
- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.36 GET /db/{database}/submissions - retrieve list of submissions

Required route parameter: database [string] - Database configuration name

Optional parameters:

- type [string] - either 'alleles', 'profiles' or 'isolates'

- status [string] - either 'closed' or 'pending'
- page [integer]
- page_size [integer]
- return_all [integer] - Set to non-zero value to disable paging.

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_isolates/submissions

Response: Object containing:

- records [int] - Number of submissions
- submissions [array] - List of *URIs to submission records*
- paging [object] - Some or all of the following:
  - previous - URI to previous page of results
  - next - URI to next page of results
  - first - URI to first page of results
  - last - URI to last page of results
  - return_all - URI to page containing all results (paging disabled)

17.3.37 POST /db/{database}/submissions - create new submission

Required route parameter: database [string] - Database configuration name

Required additional parameters (JSON-encoded in POST body):

- type [string] - either:
  - alleles (sequence definition databases only)
  - profiles (sequence definition databases only)
  - isolates (isolate databases only)
  - genomes (isolate databases only)

  The following are required with the specified database type:

  Allele submissions
- locus [string] - name of locus
- technology [string] - name of sequencing technology: either '454', 'Illumina', 'Ion Torrent', 'PacBio', 'Oxford Nanopore', 'Sanger', 'Solexa', 'SOLiD', or 'other'
- read_length [string] - read length of sequencing: either '<100', '100-199', '200-299', '300-499', '>500', or any positive integer (only required for Illumina)
- coverage [string] - mean coverage of sequencing: either '<20x', '20-49x', '50-99x', '>100x', or any positive integer (only required for Illumina)
- assembly [string] - assembly method: either 'de novo' or 'mapped'
- software [string] - name of assembly software
- sequences [string] - either single raw sequence or multiple sequences in FASTA format

  Profile submissions
- scheme_id [int] - scheme id number

- profiles [string] - tab-delimited profile data - this should include a header line containing the name of each locus

  Isolate submissions

- isolates [string] - tab-delimited isolate data - this should include a header line containing each field or locus included

  Genome submissions

- isolates [string] - tab-delimited isolate data - this should include a header line containing each field or locus included as well as for 'assembly_filename' and 'sequence_method'. The 'sequence_method' should be either '454', 'Illumina', 'Ion Torrent', 'PacBio', 'Oxford Nanopore', 'Sanger', 'Solexa', 'SOLiD', or 'other'. Following submission, contig files should be uploaded with the same names as set for 'assembly_filename'. This can be done using the *file upload route*.

Optional parameters:

- message [string] - correspondence to the curator
- email [int] - set to 1 to enable E-mail updates (E-mails will be sent to the registered user account address).

Response: Object containing:

- submission - *URI to submission record*

  For genome submissions, the response object will also contain:

- missing_files [array] - List of filenames that need to be uploaded to complete the submission. These filenames are defined in the 'assembly_filename' field of the isolate record upload. The files should contain the contig assemblies.
- message [string] - 'Please upload missing contig files to complete submission.'

17.3.38 GET /db/{database}/submissions/{submission_id} - Retrieve submission record

Required route parameters:

- database [string] - Database configuration name
- submission_id [string] - Submission id

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740

Response: Object containing some of the following:

- id [string] - Submission id
- type [string] - Either 'alleles', 'profiles', 'isolates'
- date_submitted [string] - Submission date (ISO 8601 format)
- datestamp [string] - Last updated date (ISO 8601 format)
- submitter [string] - *URI to user details* of submitter
- curator [string] - *URI to user details* of curator
- status [string] - either 'started', 'pending', or 'closed'
- outcome [string] - either 'good' (data uploaded), 'bad' (data rejected), or 'mixed' (parts of submission accepted)
- correspondence [array] - List of correspondence objects in time order. Each contains:

  - user [string] *URI to user details* of user
  - timestamp [string]
  - message [string]

Allele submissions

- locus [string] - name of locus
- technology [string] - name of sequencing technology: either '454', 'Illumina', 'Ion Torrent', 'PacBio', 'Oxford Nanopore', 'Sanger', 'Solexa', 'SOLiD', or 'other'
- read_length [string] - read length of sequencing: either '<100', '100-199', '200-299', '300-499', '>500', or any positive integer (only required for Illumina)
- coverage [string] - mean coverage of sequencing: either '<20x', '20-49x', '50-99x', '>100x', or any positive integer (only required for Illumina)
- assembly [string] - assembly method: either 'de novo' or 'mapped'
- software [string] - name of assembly software
- seqs [array] - List of sequence objects each containing:
  - seq_id [string] - Sequence identifier
  - assigned_id [string] - Allele identifier if uploaded to the database (otherwise undefined)
  - status [string] - Either 'pending', 'assigned', or 'rejected'
  - sequence [string]

Profile submissions

- scheme [string] - *URI to scheme information*
- profiles [array] - List of profile record objects. Each contains:
  - profile_id [string] - Record identifier
  - assigned_id [string] - Profile identifier if uploaded to the database (otherwise undefined)
  - status [string] - Either 'pending', 'assigned', or 'rejected'
  - designations [object] containing key/value pairs for each locus containing the allele identifier

Isolate submissions

- isolates [array] - List of isolate record objects. Each contains key/value pairs for included fields.

17.3.39 DELETE /db/{database}/submissions/{submission_id} - Delete submission record

You must be the owner and the record must be closed.

Required route parameters:

- database [string] - Database configuration name
- submission_id [string] - Submission id

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740

Response: message [string] - 'Submission deleted.'

17.3.40 GET /db/{database}/submissions/{submission_id}/messages - Retrieve submission correspondence

Required route parameters:

- database [string] - Database configuration name
- submission_id [string] - Submission id

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740/messages

Response: Array of correspondence objects in time order. Each contains:

- user [string] *URI to user details* of user
- timestamp [string]
- message [string]

17.3.41 POST /db/{database}/submissions/{submission_id}/messages - Add submission correspondence

Required route parameters:

- database [string] - Database configuration name
- submission_id [string] - Submission id

Required additional parameter (JSON-encoded in POST body):

- message [string] - Message text

Optional parameters: None

Response: message [string] - 'Message added.'

17.3.42 GET /db/{database}/submissions/{submission_id}/files - Retrieve list of supporting files uploaded for submission

Required route parameters:

- database [string] - Database configuration name
- submission_id [string] - Submission id

Optional parameters: None

Example request URI: http://rest.pubmlst.org/db/pubmlst_neisseria_seqdef/submissions/BIGSdb_20151013081836_14559_14740/files

Response: Array of URIs to files

17.3.43 POST /db/{database}/submissions/{submission_id}/files - Upload submission supporting file

Required route parameters:

- database [string] - Database configuration name
- submission_id [string] - Submission id

Required additional parameters (JSON-encoded in POST body):

- filename [string] - Name of file to store within submission
- upload [base64 encoded data] - Raw file data

Optional parameters: None

Response: message [string] - 'File uploaded.'

17.3.44 GET /db/{database}/submissions/{submission_id}/files/{filename} - Download submission supporting file

Required route parameters:

- database [string] - Database configuration name
- submission_id [string] - Submission id
- filename [string] - Name of file

Optional parameters: None

Response: File download

17.3.45 DELETE /db/{database}/submissions/{submission_id}/files/{filename} - Delete submission supporting file

Required route parameters:

- database [string] - Database configuration name
- submission_id [string] - Submission id
- filename [string] - Name of file

Optional parameters: None

Response: message [string] - 'File deleted.'

17.4 Authentication

Protected resources, i.e. those requiring a user to log in, can be accessed via the API using OAuth (1.0A) authentication (see IETF RFC5849 for details). Third-party client software has to be registered with the BIGSdb site before they can access authenticated resources. The overall three-legged flow works as follows:

1. *Developer signs up* and gets a consumer key and consumer secret specific to their application.
2. Application *gets a request token* and directs user to authorization page on BIGSdb.

3. BIGSdb *asks user for authorization* for application to access specific resource using their credentials. A verifier code is provided.
4. The application exchanges the request token and OAuth verifier code for an *access token and secret* (these do not expire but may be revoked by the user or site admin).
5. Application uses access token/secret to *request session token* (this is valid for 12 hours).
6. All calls to *access protected resources* are signed using the session token/secret and consumer key/secret.

It is recommended that application developers use an OAuth library to generate and sign requests.

17.4.1 Developer sign up to get a consumer key

Application developers should apply to the site administrator of the site running BIGSdb. The administrator can *generate a key and secret* using a script - both of these will need to be used by the application to sign requests.

The client id is usually a 24 character alphanumeric string. The secret is usually a 42 character alphanumeric (including punctuation) string, e.g.

- **client_id:** efKXmqp2D0EBlMBkZaGC2lPf
- **client_secret:** F$M)_+fQ2AFFB2YBDfF9fpHF^qSWJdmmN%L4Fxf5Gur3

17.4.2 Getting a request token

- **Relative URL:** /db/{database}/oauth/get_request_token
- **Supported method:** GET

The application uses the consumer key to obtain a request token. The request token is a temporary token used to initiate user authorization for the application and will expire in 60 minutes. The request needs to contain the following parameters and to be signed using the consumer secret:

- oauth_consumer_key
- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_timestamp (UNIX timestamp - seconds since Jan 1 1970) - this must be within 600 seconds of the current time.
- oauth_callback ('oob' for desktop applications)
- oauth_nonce (random string)
- oauth_version ('1.0')

If the application has been registered and has been granted permission to access the specific resource, a JSON response will be returned containing the following parameters:

- **oauth_token**
  - This is the request token. It is usually a 32 character alphanumeric string.
  - e.g. fKFm0WNhCfbEX8zQm6qhDA8K23FOWDGE
- **oauth_token_secret**

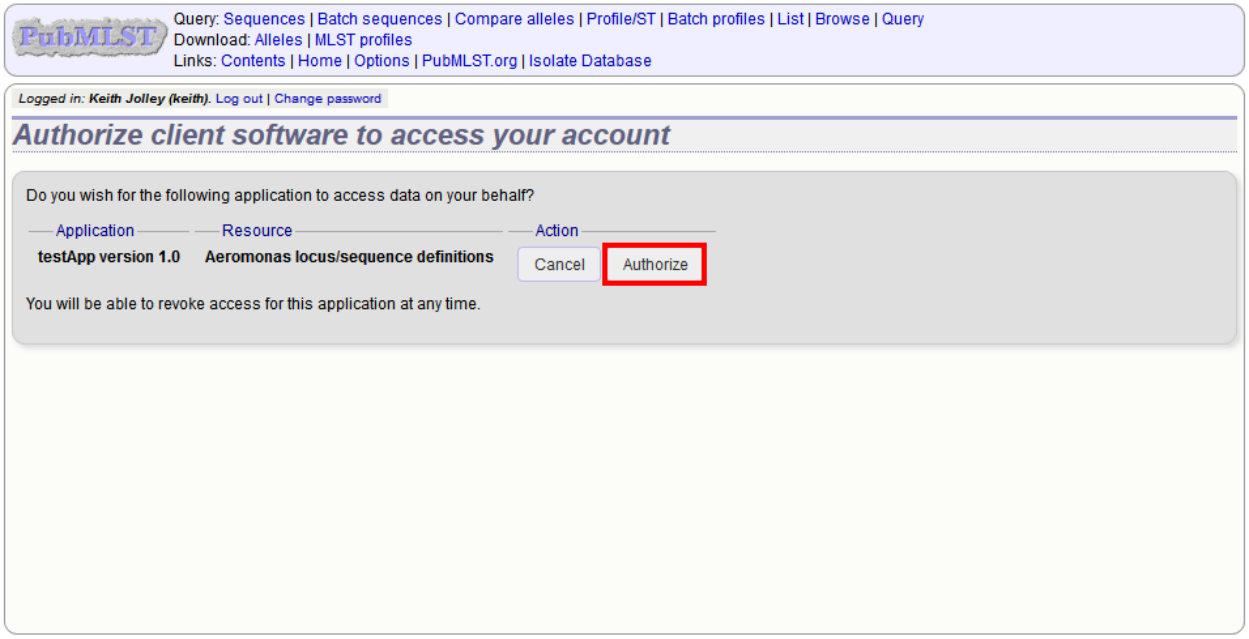
  - This is the secret associated with the request token. It is usually a 32 character alphanumeric string.
  - e.g. aZ0fncP7i5w5jlebdK5zyQ4vrRRVcdnv

- **oauth_callback_confirmed**
  - This parameter is always set to true.

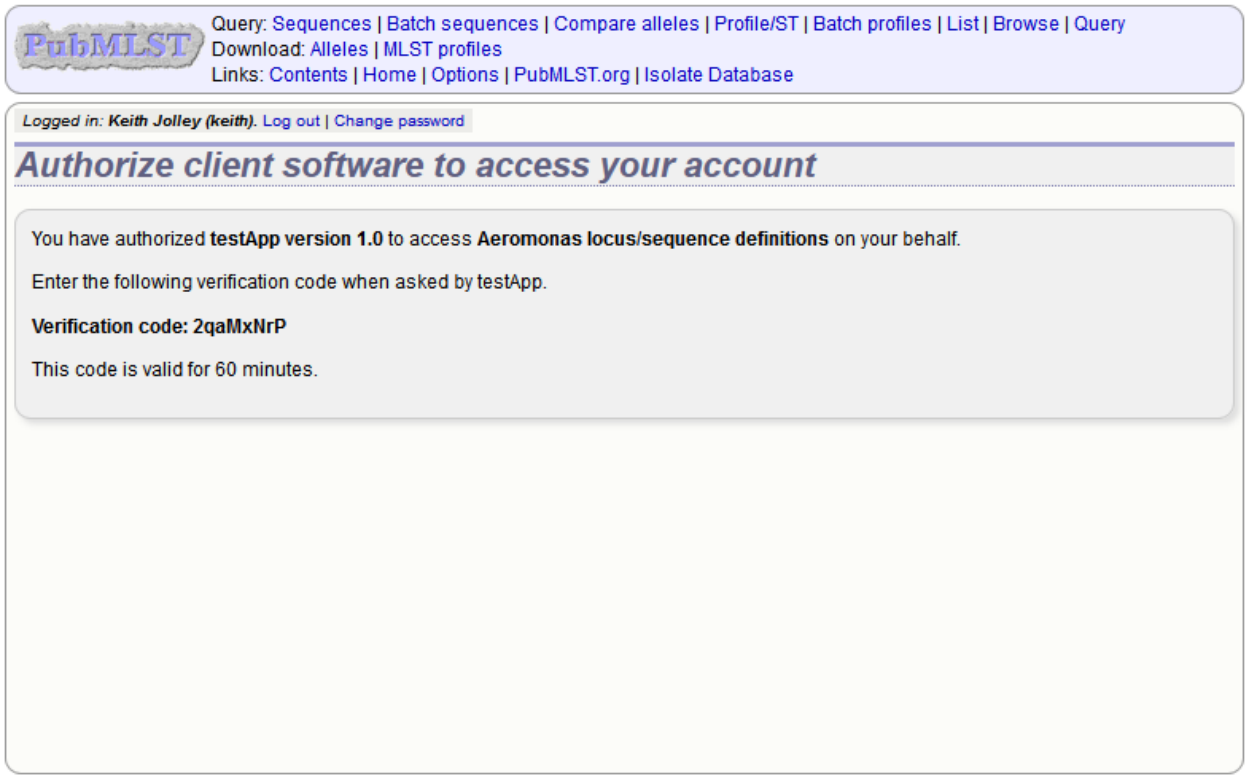
17.4.3 Getting user authorization

Once a request token has been obtained, this can be used by the end user to grant permission to access a specific resource to the application. The application should direct the user to the client authorization page (authorizeClient) specific to a database within BIGSdb, e.g. http://pubmlst.org/cgi-bin/bigsdb/bigsdb.pl?db=pubmlst_neisseria_seqdef&page=authorizeClient&oauth_token=fKFm0WNhCfbEX8zQm6qhDA8K23FOWDGE

The user will be asked if they wish to grant access to the application on their behalf:



If they authorize the access, they will be presented with a verifier code. This should be entered in to the client application which will use this together with the request token to request an access token.



The verifier code is valid for 60 minutes.

17.4.4 Getting an access token

- **Relative URL:** /db/{database}/oauth/get_access_token
- **Supported method:** GET

The application uses the request token, verifier code and its consumer key to obtain an access token. The access token does not expire but can be revoked by both the end user or the site admininstrator. The request needs to contain the following parameters and to be signed using the consumer secret and request token secret:

- oauth_consumer_key
- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_token (request token)
- oauth_timestamp (UNIX timestamp - seconds since Jan 1 1970) - this must be within 600 seconds of the current time.
- oauth_nonce (random string)
- oauth_version ('1.0')

If the application has been registered and has been granted permission to access the specific resource, a JSON response will be returned containing the following parameters:

- **oauth_token**
  - This is the access token. It is usually a 32 character alphanumeric string.
  - e.g. SDrC74ZVl5SYSqY8lWZqrRxnyDnNGVFO
- **oauth_token_secret**
  - This is the secret associated with the access token. It is usually a 32 character alphanumeric string.
  - e.g. tYI2SPzgiO02IRVzW4JR1ez6Vvm4gVyv

17.4.5 Getting a session token

- **Relative URL:** /db/{database}/oauth/get_session_token
- **Supported method:** GET

The application uses the access token and its consumer key to obtain a session token. The session token is valid for 12 hours before it expires. The request needs to contain the following parameters and to be signed using the consumer secret and access token secret:

- oauth_consumer_key
- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_token (access token)
- oauth_timestamp (UNIX timestamp - seconds since Jan 1 1970) - this must be within 600 seconds of the current time.
- oauth_nonce (random string)
- oauth_version ('1.0')

If the application has been registered and has been granted permission to access the specific resource, a JSON response will be returned containing the following parameters:

- **oauth_token**
  - This is the session token. It is usually a 32 character alphanumeric string.
  - e.g. H8CjIS8Ikq6hwCUqUfF1l4pTaCYl8Ljw
- **oauth_token_secret**
  - This is the secret associated with the session token. It is usually a 32 character alphanumeric string.
  - e.g. RfponbaNPO7tkZ2miHFISk0pMndePNfJ

17.4.6 Accessing protected resources

- **Supported method:** GET

The application uses the session token and its consumer key to access a protected resource. The request needs to contain the following parameters and to be signed using the consumer secret and session token secret:

- oauth_consumer_key

- oauth_request_method ('GET')
- oauth_request_url (request URL)
- oauth_signature_method ('HMAC-SHA1')
- oauth_signature
- oauth_token (session token)
- oauth_timestamp (UNIX timestamp - seconds since Jan 1 1970) - this must be within 600 seconds of the current time.
- oauth_nonce (random string)
- oauth_version ('1.0')

CHAPTER 18

Frequently asked questions (FAQs)

18.1 General

1. **What is the minimum specification of hardware required to run BIGSdb?**

   The software will run on fairly modest hardware - a number of PubMLST mirrors have been set up on virtual machines with 1 processor core and 4 GB RAM. This should be considered an absolute minimum specification though. For an installation with only local users, the following minimum is recommended:

   - 4 processor cores
   - 16 GB RAM
   - 50 GB partition for temporary files
   - 100 GB partition for databases

   As usual, the more RAM that is available the better. Ideally you would want enough RAM that the whole database(s) can reside in memory (an approximation is roughly twice the total size of your contigs), although this is not absolutely required.

   Offline jobs, such as *Genome Comparator* will use multiple cores (depending on the settings in bigsdb.conf), so if you want to run multiple jobs in parallel then you may want more cores (and memory). Tagging of new genomes using the offline *autotagger* is usually run in multi-threaded mode so the more cores available the faster this will be.

   As a comparison, the PubMLST site is run on two machines - separate web and database servers. All offline jobs and tagging of genomes is performed on the database server. These have the following specification:

   - web server: 40 cores, 128GB RAM
   - database server: 64 cores, 1TB RAM, 3TB RAID 10 local storage

2. **Why might icons be missing when using Internet Explorer?**

   This can occur if you have Compatibility Mode enabled. BIGSdb generates valid HTML5 and Compatibility Mode should not be used. Please ensure this is not enabled in the Internet Explorer tools section.

18.2 Installation

1. **BIGSdb is accumulating files in various temp directories - is this normal and how do I clean them out?**

   See: *Periodically delete temporary files*.

2. **BIGSdb is complaining of an invalid script path - what does this mean?**

   In your database config.xml file system tag are two attributes - script_path_includes and curate_path_includes. These contain regexes that the web url to your script (bigsdb.pl and bigscurate.pl respectively) must match. This prevents somebody from accessing a private database using an instance of bigsdb.pl that is not in a protected directory if you're using apache authentication.

   So, if you access the script from http://localhost/cgi-bin/bigsdb/bigsdb.pl then you can set script_path_includes to something like "/bigsdb/" (which is the default), or "/cgi-bin/" or just "/" if you don't care about this check.

18.3 Administration

1. **How can I make some isolates public but not others?**

   The easiest way to do this is to set up two or more separate configuration directories that refer to the database. The URLs to access these will differ by the value of the 'db' attribute, which refers to the name of the configuration directory (in /etc/bigsdb/dbases/). The database view accessed by each of these configurations can be different as can the access restrictions.

   Example:

   We have a database 'bigsdb_test' that contains data, only some of which we wish to make publicly available. The isolates to make public are all members of a project. First we can make a view of the isolates table that contains only isolates within this project.

   For isolates in project id 3, create a database view by logging in to psql as the postgresql user. We will name this view 'public'.:

```
sudo su postgres
psql bigsdb_test

CREATE VIEW public AS SELECT * FROM isolates WHERE id IN (SELECT isolate_id
  FROM project_members WHERE project_id=3);
GRANT SELECT ON public TO apache;
```

   Create a private configuration that can access everything in the database in /etc/bigsdb/dbases/test_private. This will be accessible from http://IP_ADDRESS/cgi-bin/bigsdb/bigsdb.pl?db=test_private.

   The important attributes to set in the system tag of the config.xml file in this directory are::

```
view="isolates"
read_access="authenticated_users"
```

   This means that anyone with an account can log in and view all the isolates (because the view is set to the isolates table).

   Now create a public configuration in /etc/bigsdb/dbases/test_public. This will be accessible from http://IP_ADDRESS/cgi-bin/bigsdb/bigsdb.pl?db=test_public. It is better to create a symlink to the private config.xml and then override the attributes that are different. So create a symlink to the private config file:

```
cd /etc/bigsdb/dbases/test_public
sudo ln -s ../test_private/config.xml .
```

You can now override the view and access settings. Within /etc/bigsdb/dbases/test_public, create a file called system.overrides and add the following:

```
view="public"
read_access="public"
```

See also *Restricting particular configurations to specific user accounts*.

CHAPTER 19

Appendix

19.1 Query operators

Various query forms have operators for use with field values. Available operators are:

- =
  - Exact match (case-insensitive).
- contains
  - Match to a partial string (case-insensitive), e.g. searching for clonal complex 'contains' st-11 would return all STs belonging to the ST-11 complex.
- starts with
  - Match to values that start with the search term (case-insensitive).
- ends with
  - Match to values that end with the search term (case-sensitive).
- >
  - Greater than the search term.
- >=
  - Greater than or equal the search term.
- <
  - Less than the search term.
- <=
  - Less than or equal the search term.
- NOT
  - Match to values that do not equal the search term (case-insensitive).

- NOT contain
  - Match to values that do not contain the search term (case-insensitive).

19.2 Sequence tag flags

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

- ambiguous read
  - Genome sequence contains ambiguous nucleotides in coding sequence.
- apparent misassembly
  - Sequence has a region of very high identity to existing allele in one region but looks completely different in another.
- atypical
  - Catch-all term for a sequence that is unusual compared to other alleles of locus.
- contains IS element
  - Coding sequence is interrupted by insertion sequence.
- downstream fusion
  - No stop codon present resulting in translation continuing.
- frameshift
  - Frameshift in sequence relative to other alleles, not resulting in internal stop codon.
- internal stop codon
  - Frameshift in sequence relative to other alleles, resulting in internal stop codon.
- no start codon
  - No apparent start codon in immediate vicinity of usual start.
- no stop codon
  - No stop codon in immediate vicinity of usual stop.
- phase variable: off
  - Coding sequence has a homopolymeric run with a frameshift resulting in a stop codon preventing complete translation.
- truncated
  - Coding sequence is unusually short resulting in a truncated protein (not the same as running off the end of a contig).
- upstream fusion
  - No apparent start codon in immediate vicinity of usual start, likely due to a gene fusion (sequence is transcribed together with upstream coding sequence).

19.3 Allele sequence flags

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

- atypical
  - Catch-all term for a sequence that is unusual compared to other alleles of locus.
- contains IS element
  - Coding sequence is interrupted by insertion sequence.
- downstream fusion
  - No stop codon present resulting in translation continuing.
- frameshift
  - Frameshift in sequence relative to other alleles, not resulting in internal stop codon.
- internal stop codon
  - Frameshift in sequence relative to other alleles, resulting in internal stop codon.
- no start codon
  - No apparent start codon in immediate vicinity of usual start.
- no stop codon
  - No stop codon in immediate vicinity of usual stop.
- phase variable: off
  - Coding sequence has a homopolymeric run with a frameshift resulting in a stop codon preventing complete translation.
- truncated
  - Coding sequence is unusually short resulting in a truncated protein (not the same as running off the end of a contig).
- upstream fusion
  - No apparent start codon in immediate vicinity of usual start, likely due to a gene fusion (sequence is transcribed together with upstream coding sequence).

CHAPTER 20

Database schema

- Sequence definition database
- Isolate database

Index

A

access
    control lists, 44
    restricting, 44
adding
    classification groups, 90
    isolates, 145
    locus, 54, 57, 58, 64, 95
    MLST scheme, 88
    schemes, 69
allele
    breakdown, 308
allele definition
    records, 221
allele designations
    count, 257
    query, 256
    status, 259
allele sequence
    identify, 225
allele sequences
    adding, 122
alleles, 3
    list query, 235
API authentication
    access token, 415
    accessing protected resources, 416
    consumer key, 413
    request token, 413
    session token, 416
    user authorization, 414
API resources
    add submission correspondence, 411
    create new submission, 408
    DELETE /db/{database}/submissions/{submission_id}, 410
    DELETE /db/{database}/submissions/{submission_id}/files/{filename}, 412
    delete submission record, 410
    delete submission supporting file, 412
    download alleles in FASTA format, 393
    download allelic profiles in CSV (tab-delimited) format, 397
    download contigs in FASTA format, 403
    download submission supporting file, 412
    GET /, 389
    GET /db, 389
    GET /db/{database}, 389
    GET /db/{database}/classification_schemes, 390
    GET /db/{database}/classification_schemes/{classification_scheme_id 390
    GET /db/{database}/classification_schemes/{classification_scheme_id 391
    GET /db/{database}/contigs/{contig_id}, 404
    GET /db/{database}/fields, 405
    GET /db/{database}/fields/{field}, 405
    GET /db/{database}/isolates, 398
    GET /db/{database}/isolates/{isolate_id}, 398
    GET /db/{database}/isolates/{isolate_id}/allele_designations, 400
    GET /db/{database}/isolates/{isolate_id}/allele_designations/{locus}, 400
    GET /db/{database}/isolates/{isolate_id}/allele_ids, 401
    GET /db/{database}/isolates/{isolate_id}/contigs, 402
    GET /db/{database}/isolates/{isolate_id}/contigs_fasta, 403
    GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele 401
    GET /db/{database}/isolates/{isolate_id}/schemes/{scheme_id}/allele 402
    GET /db/{database}/loci, 391
    GET /db/{database}/loci/{locus}, 392
    GET /db/{database}/loci/{locus}/alleles, 393
    GET /db/{database}/loci/{locus}/alleles/{allele_id}, 394
    GET /db/{database}/loci/{locus}/alleles_fasta, 393
    GET /db/{database}/projects, 406

GET /db/{database}/projects/{project_id}, 406
GET /db/{database}/projects/{project_id}/isolates, 407
GET /db/{database}/schemes, 395
GET /db/{database}/schemes/{scheme_id}, 395
GET /db/{database}/schemes/{scheme_id}/fields/{field}, 396
GET /db/{database}/schemes/{scheme_id}/profiles, 396
GET /db/{database}/schemes/{scheme_id}/profiles/{profile_id}, 397
GET /db/{database}/schemes/{scheme_id}/profiles_csv, 397
GET /db/{database}/submissions, 407
GET /db/{database}/submissions/{submission_id}, 409
GET /db/{database}/submissions/{submission_id}/files, 411
GET /db/{database}/submissions/{submission_id}/files/{filename}, 412
GET /db/{database}/submissions/{submission_id}/messages, 411
GET /db/{database}/users/{user_id}, 406
list allelic profiles defined for scheme, 396
list classification schemes, 390
list database resources, 389
list loci, 391
list schemes, 395
list site resources, 389
POST /db/{database}/isolates/search, 403
POST /db/{database}/loci/{locus}/sequence, 394
POST /db/{database}/sequence, 395
POST /db/{database}/submissions, 408
POST /db/{database}/submissions/{submission_id}/files, 411
POST /db/{database}/submissions/{submission_id}/messages, 411
query allele sequence, 394
query allele sequence without specifying locus, 395
retrieve allele identifiers, 401
retrieve classification scheme information and groups, 390, 391
retrieve contig record, 404
retrieve full allele designation record, 400
retrieve full allele information, 394
retrieve information about scheme field, 396
retrieve isolate record, 398
retrieve list of allele designations, 400
retrieve list of alleles defined for a locus, 393
retrieve list of contigs, 402
retrieve list of isolate provenance field descriptions, 405
retrieve list of isolate records, 398
retrieve list of isolates belonging to a project, 407
retrieve list of projects, 406
retrieve list of scheme allele identifiers, 402
retrieve list of submissions, 407
retrieve list of supporting files uploaded for submission, 411
retrieve locus record, 392
retrieve project information, 406
retrieve scheme allele designation records, 401
retrieve scheme information, 395
retrieve specific allelic profile record, 397
retrieve submission correspondence, 411
retrieve submission record, 409
retrieve user information, 406
retrieve values set for a provenance field, 405
search isolate database, 403
upload submission supporting file, 411
auto
allele definer, 204
stop, 207
automated assignment
scheme profiles, 89
autotagger, 201
stop, 207

B

batch profile definitions
query, 245
BLAST, 326
breakdown
allele, 308
provenance field, 301
scheme, 308
sequence bin, 315
two-field, 305
browse
scheme profiles, 237
BURST, 331

C

caching
schemes, 47
classification groups, 4
adding, 90
client authorization
RESTful interface, 119
client databases, 80
clustering
core genome, 93
codon usage, 334
Locus Explorer, 299
composite fields, 107
configuration
export, 116
configuration settings
validation, 115

core genome
clustering, 93
count
allele designations, 257
sequence tags, 260

D

defining
exemplar alleles, 203

E

exemplar alleles
defining, 203
export
configuration, 116
extended attributes
locus, 66
provenance fields, 110

F

filters, 264

G

Genome Comparator, 317
genome filtering, 98
in silico hybridization, 101
in silico PCR, 98
groups
scheme, 76

H

hosts
mapping, 47

I

identify
allele sequence, 225
sequence type, 227
in silico hybridization, 101
in silico PCR, 98
isolate
records, 217
isolate aliases, 158
isolate record
options, 274
isolates
adding, 145

L

linking remote contigs, 167
list query
alleles, 235
loci, 3
modifying display, 279
locus
adding, 54, 57, 58, 64, 95
copying existing record, 62
extended attributes, 66
Locus Explorer, 295
codon usage, 299
polymorphic sites, 295
translated sequences, 300
locus positions
setting, 102

M

main results table
options, 273
mapping
hosts, 47
MLST, 4
MLST scheme
adding, 88
mod_perl, 47
modifying display
loci, 279
schemes, 279

O

offline curation
auto allele definer, 204
autotagger, 201
options, 271
isolate record, 274
main results table, 273
provenance fields, 276
query, 277

P

partitioning
sets, 49
passwords
setting, 44
first user, 45
performance
caching schemes, 47
mod_perl, 47
permissions, 39
locus curation, 42
scheme curation, 42
plugins
enabling, 46
polymorphic sites
Locus Explorer, 295
polymorphisms, 339
profile
records, 223

profiles, 4
projects, 173
provenance field
    breakdown, 301
provenance fields
    extended attributes, 110
    options, 276
publications, 160

Q

query
    allele designations, 256
    batch profile definitions, 245
    options, 277
    scheme profiles, 238
    sequence tags, 261
    ST definitions from allelic profiles, 242

R

records
    allele definition, 221
    isolate, 217
    profile, 223
    sequence bin, 224
    sequence tag, 222
RESTful interface
    client authorization, 119
rule-based queries, 86

S

scheme
    breakdown, 308
    groups, 76
scheme profiles
    automated assignment, 89
    browse, 237
    query, 238
schemes, 4
    adding, 69
    caching, 47
    modifying display, 279
sequence bin
    breakdown, 315
    records, 224
sequence similarity
    determining, 248
sequence tag
    records, 222
    status, 344
sequence tags, 4
    count, 260
    query, 261
sequence type
    identify, 227
sets, 5
    partitioning, 49
ST definitions from allelic profiles
    query, 242
stop
    auto allele definer, 207
    autotagger, 207

T

translated sequences
    Locus Explorer, 300
two-field
    breakdown, 305

U

unique combinations, 337
updates
    disabling, 46
uploading contigs, 162
user groups, 39
user projects, 281
user types, 39
users
    adding, 121