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# **screed Documentation**

***Release 0.8-dirty***

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Contents:



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## Basic Documentation

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### 1.1 Notes on this document

This is the default documentation for screed. Some doctests are included in the file ‘example.txt’. The examples in this file are meant for humans only: they will not work in doctests.

### 1.2 Introduction

screed parses FASTA and FASTQ files, generates databases, and lets you query these databases. Values such as sequence name, sequence description, sequence quality, and the sequence itself can be retrieved from these databases.

### 1.3 Getting Going

The following software packages are required to run screed:

- Python 2.4 or newer
- nose (for testing)

#### 1.3.1 Downloading

You will need git to download a copy from the public git repository:

```
git clone git://github.com/ged-lab/screed.git
```

#### 1.3.2 Installing

Assuming you have already downloaded the package, this is how to install:

```
$ python setup.py install
```

To run the optional tests type:

```
$ python -m screed.tests.__main__
```

## 1.4 Quick-Start

### 1.4.1 Reading FASTA/FASTQ files

At the Python prompt, type:

```
>>> import screed
>>> for read in screed.open(filename):
...     print read.name, read.sequence
```

Here, ‘filename’ can be a FASTA or FASTQ file, and can be uncompressed, gzipped, or bz2-zipped.

### 1.4.2 Creating a database from the API

From a Python prompt type:

```
>>> import screed
>>> screed.read_fasta_sequences('screed/tests/test.fa')
```

That command just parsed the FASTA file ‘screed/tests/test.fa’ into a screed-database named ‘screed/tests/test.fa\_screed’. The screed database is independent from the text file it was derived from, so moving, renaming or deleting the ‘screed/tests/test.fa’ file will not affect screed’s operation. To create a screed database from a FASTQ file the syntax is similar:

```
>>> screed.read_fastq_sequences('screed/tests/test.fastq')
```

### 1.4.3 Creating a database from a script

If the screed module is in your PYTHONPATH, you can create a screed db from a FASTQ file at the shell:

```
$ python -m screed.fqdbm <fastq file>
```

Similarly, to create a screed db from a fasta file:

```
$ python -m screed.fadbm <fasta file>
```

where <fast\* file> is the path to a sequence file.

screed natively supports FASTA and FASTQ database creation. If you have a new sequence you want screed to work with, see the section below on Writing Custom Sequence Parsers.

## 1.5 Reading databases

The class ScreedDB is used to read screed databases, regardless of what file format they were derived from (FASTA/FASTQ/hava/etc.). One reader to rule them all!

### 1.5.1 Opening

In the Python environment, import the ScreedDB class and load some databases:



```
>>> from screed import ScreedDB
>>> fadb = ScreedDB('screed/tests/test.fa')
>>> fqdb = ScreedDB('screed/tests/test.fastq')
```

Notice how you didn't need to write the `'_screed'` at the end of the file names? screed automatically adds that to the file name if you didn't.

### 1.5.2 Dictionary Interface

Since screed emulates a read-only dictionary interface, any methods that don't modify a dictionary are supported:

```
>>> fadb.keys()
>>> fqdb.keys()
```

Each record in the database contains 'fields' such as name and sequence information. If the database was derived from a FASTQ file, quality and optional annotation strings are included. Conversely, FASTA-derived databases have a description field.

To retrieve the names of records in the database:

```
>>> names = fadb.keys()
```

Length of the databases are easily found:

```
>>> print len(fadb)
22
>>> print len(fqdb)
125
```

### 1.5.3 Retrieving Records

A record is the standard container unit in screed. Each has 'fields' that vary slightly depending on what kind of file the database was derived from. For instance, a FASTQ-derived screed database has an id, a name, a quality score and a sequence. A FASTA-derived screed database has an id, name, description and a sequence.

Retrieving whole records:

```
>>> records = []
>>> for record in fadb.itervalues():
...     records.append(record)
```

What is returned is a dictionary of fields. The names of fields are keys into this dictionary with the actual information as values. For example:

```
>>> record = fadb[fadb.keys()[0]]
>>> index = record['id']
>>> name = record['name']
>>> description = record['description']
>>> sequence = record['sequence']
```

What this does is retrieve the first record object in the screed database, then retrieve the index, name, description and sequence from the record object using standard dictionary key -> value pairs.

### 1.5.4 Retrieving Partial Sequences (slicing)

screed supports the concept of retrieving a ‘slice’ or a subset of a sequence string. The motivation is speed: if you have a database entry with a very long sequence string but only want a small portion of the string, it is faster to retrieve only the portion than to retrieve the entire string and then perform standard Python string slicing.

By default, screed’s FASTA database creator sets up the ‘sequence’ column to support slicing. For example, if you have an entry with name ‘someSeq’ which has a 10K long sequence, and you want a slice of the sequence spanning positions 4000 to 4080:

```
>>> seq = db['someSeq'].sequence
>>> slice = seq[4000:4080]
```

This is much faster than say:

```
>>> seq = str(db['someSeq'].sequence)
>>> slice = seq[4000:4080]
```

Because deep down, less information is being read off the disk. The `str()` method above causes the entire sequence to be retrieved as a string. Then Python slicing is done on the string ‘seq’ and the subset stored in ‘slice’.

### 1.5.5 Retrieving Via Index

Sometimes you don’t care what the name of a sequence is; you’re only interested in its position in the database. In these cases, retrieval via index is the method you’ll want to use:

```
>>> record = fqdb.loadRecordByIndex(5)
```

An index is like an offset into the database. The order records were kept in the FASTA or FASTQ file determines the index in their resulting screed database. The first record in a sequence file will have an index of 0, the second, an index of 1 and so on.

## 1.6 Writing Custom Sequence Parsers

screed is built to be adaptable to new kinds of file sequence formats. Included with screed are parsers for handling FASTA and FASTQ sequence file types, though if you need screed to work with a new format, all you need to do is write a new parser.

### 1.6.1 Field Roles

Each field in a screed database is assigned a role. These roles describe what kind of information is stored in their field. Right now there are only 4 different roles in a screed database: the text role, the sliceable role, the indexed key role and the primary key role. All roles are defined in the file: `screed/DBConstants.py`

The text role (`DBConstants._STANDARD_TEXT`) is the role most fields in a database will have. This role tells screed that the associated field is storing standard textual data. Nothing special.

The sliceable role (`DBConstants._SLICEABLE_TEXT`) is a role that can be assigned to long sequence fields. screed’s default FASTA parser defines the ‘sequence’ field with the sliceable role. When screed retrieves a field that has the sliceable role, it builds a special data structure that supports slicing into the text.

The indexed key role (`DBConstants._INDEXED_TEXT_KEY`) is associated with exactly one of the fields in a screed database. In screed’s FASTA and FASTQ parsers, this role is fulfilled by the ‘name’ field. This field is required because it is the field screed tells sqlite to index when creating the database and it is the field used for name look-ups when querying a screed database.

The primary key role (`DBConstants._PRIMARY_KEY_ROLE`) is a role automatically associated with the 'id' field in each database. This field is always created with each screed database and always holds this role. You as a user of screed won't need to worry about this one.

## 1.6.2 General Parsing Function Format

`create_db` is the function central to the creation of screed databases. This function accepts a file path, a tuple of field names and roles, and an iterator function. The file path describes where the screed database should go, the tuple contains the names of fields and their associated roles and the iterator function yields records in a dictionary format.

This sub-section describes general steps for preparing and using screed with a custom sequence parser. Though they don't have to be, future sequence parsers should be located in the `seqparse.py` file for convenience. These steps will be described in the context of working from the Python shell.

First import the `create_db` function:

```
>>> from screed import create_db
```

The `create_db` class handles the formatting of screed databases and provides a simple interface for storing sequence data.

Next the database fields and roles must be specified. The fields tell screed the names and order of the data fields inside each record. For instance, lets say our new sequence has types 'name', 'bar', and 'baz', all text. The tuple will be:

```
>>> fields = (('name', DBConstants._INDEXED_TEXT_KEY),
              ('bar', DBConstants._STANDARD_TEXT),
              ('baz', DBConstants._STANDARD_TEXT))
```

Notice how 'name' is given the indexed key role and bar and baz are given text roles? If, for instance, you know 'baz' fields can be very long and you want to be able to retrieve slices of them, you could specify fields as:

```
>>> fields = (('name', DBConstants._INDEXED_TEXT_KEY),
              ('bar', DBConstants._STANDARD_TEXT),
              ('baz', DBConstants._SLICEABLE_TEXT))
```

All screed databases come with an 'id' field, which is a sequential numbering order starting at 0 for the first record, 1 for the second, and so on. The names and number of the other fields are arbitrary with one restriction: one and only one of the fields must fulfill the indexed key role.

Next, you need to setup an iterator function that will return records in a dictionary format. Have a look at the 'fastq\_iter', 'fasta\_iter', or 'hava\_iter' functions in the `screed/fastq.py`, `screed/fasta.py`, and `screed/hava.py` files, respectively for examples on how to write one of these. If you don't know what an iterator function is, the documentation on the Python website gives a good description: <http://docs.python.org/library/stdtypes.html#iterator-types>.

Once the iterator function is written, it needs to be instantiated. In the context of the built-in parsing functions, this means opening a file and passing the file handle to the iterator function:

```
>>> seqfile = open('path_to_seq_file', 'rb')
>>> iter_instance = myiter(seqfile)
```

Assuming that your iterator function is called 'myiter', this sets up an instance of it ready to use with `create_db`.

Now the screed database is created with one command:

```
>>> create_db('path_to_screed_db', fields, iter_instance)
```

If you want the screed database saved at 'path\_to\_screed\_db'. If instead you want the screed database created in the same directory and with a similar file name as the sequence file, its OK to do this:

```
>>> create_db('path_to_seq_file', fields, iter_instance)
```

`create_db` will just append ‘\_screed’ to the end of the file name and make a screed database at that file path so the original file won’t be overwritten.

When you’re done the sequence file should be closed:

```
>>> seqfile.close()
```

### 1.6.3 Using the Built-in Sequence Iterator Functions

This section shows how to use the ‘fastq\_iter’ and ‘fasta\_iter’ functions for returning records from a sequence file.

These functions both take a file handle as the only argument and then return a dictionary for each record in the file containing names of fields and associated data. These functions are primarily used in conjunction with the `db_create()` function, but they can be useful by themselves.

First, import the necessary module and open a text file containing sequences. For this example, the ‘fastq\_iter’ function will be used:

```
>>> import screed.fastq
>>> seqfile = open('path_to_seqfile', 'rb')
```

Now, the ‘fastq\_iter’ can be instantiated and iterated over:

```
>>> fq_instance = screed.fastq(seqfile)
>>> for record in fq_instance:
...     print record.name
```

That will print the name of every sequence in the file. If instead you want to accumulate the sequences:

```
>>> sequences = []
>>> for record in fq_instance:
...     sequences.append(record.sequence)
```

These iterators are the core of screed’s sequence modularity. If there is a new sequence format you want screed to work with, all it needs is its own iterator.

### 1.6.4 Error checking in parsing methods

The existing FASTA/FASTQ parsing functions contain some error checking, such as making sure the file can be opened and checking correct data is being read. Though screed doesn’t enforce this, it is strongly recommended to include error checking code in your parser. To remain non-specific to one file sequence type or another, the underlying screed library can’t contain error checking code of this kind. If errors are not detected by the parsing function, they will be silently included into the database being built and could cause problems much later when trying to read from the database.

## 1.7 File formats as understood by screed

While the screed database remains non-specific to file formats, the included FASTA and FASTQ parsers expect specific formats. These parsers attempt to handle the most common attributes of sequence files, though they can not support all features.

### 1.7.1 FASTQ

The FASTQ parsing function is `read_fastq_sequences()` and is located in the `screed` module.

The first line in a record must begin with '@' and is followed by a record identifier (a name). An optional annotations string may be included after a space on the same line.

The second line begins the sequence line(s) which may be line wrapped. `screed` defines no limit on the length of sequence lines and no length on how many sequence lines a record may contain.

After the sequence line(s) comes a '+' character on a new line. Some FASTQ formats require the first line to be repeated after the '+' character, but since this adds no new information to the record, `read_fastq_sequences()` will ignore this if it is included.

The quality line(s) is last. Like the sequence line(s) this may be line wrapped. `read_fastq_sequences()` will raise an exception if the quality and sequence strings are of unequal length. `screed` performs no checking for valid quality scores.

### 1.7.2 FASTA

The FASTA parsing function is `read_fasta_sequences()` and is also located in the `screed` module.

The first line in a record must begin with '>' and is followed with the sequence's name and an optional description. If the description is included, it is separated from the name with a space. Note that though the FASTA format doesn't require named records, `screed` does. Without a unique name, `screed` can't look up sequences by name.

The second line begins the line(s) of sequence. Like the FASTQ parser, `read_fasta_sequences()` allows any number of lines of any length.

## 1.8 FASTA <-> FASTQ Conversion

@CTB this doesn't work?

As an extra nicety, `screed` can convert FASTA files to FASTQ and back again.

### 1.8.1 FASTA to FASTQ

The function used for this process is called 'ToFastq' and is located in the `screed` module. It takes the path to a `screed` database as the first argument and a path to the desired FASTQ file as the second argument. There is also a shell interface if the `screed` module is in your PYTHONPATH:

```
$ python -m screed.dump_to_fastq <path to fasta db> <converted fastq file>
```

The FASTA name attribute is directly dumped from the file. The sequence attribute is also dumped pretty much directly, but is line wrapped to 80 characters if it is longer.

Any description line in the FASTA database is stored as a FASTQ annotation string with no other interpretation done.

Finally, as there is no quality or quality score in a FASTA file, a default one is generated. The generation of the quality follows the Sanger FASTQ conventions. The score is 1 (ASCII: "'") meaning a probability of about 75% that the read is incorrect (1 in 4 chance). This PHRED quality score is calculated from the Sanger format:  $Q = -10\log(p)$  where  $p$  is the probability of an incorrect read. Obviously this is a very rough way of providing a quality score and it is only intended to fill in the requirements of a FASTQ file. Any application needing a true measurement of the quality should not rely on this automatic conversion.

## 1.8.2 FASTQ to FASTA

The function used for this process is called ‘toFasta’ and is located in the screed module. It takes the path to a screed database as the first argument and a path to the desired FASTA file as the second argument. Like the ToFastq function before, there is a shell interface to ToFasta if the screed module is in your PYTHONPATH:

```
$ python -m screed.dump_to_fasta <path to fastq db> <converted fasta file>
```

As above, the name and sequence attributes are directly dumped from the FASTQ database to the FASTA file with the sequence line wrapping to 80 characters.

If it exists, the FASTQ annotation tag is stored as the FASTA description tag. As there is no equivalent in FASTA, the FASTQ quality score is ignored.

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## screed examples

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### 2.1 Basic Usage

Load screed, index the database, and return a dictionary-like object:

```
>>> import screed
>>> db = screed.read_fasta_sequences('../screed/tests/test.fa')
```

Get the list of sequence names, sort alphabetically, and look at the first one:

```
>>> names = db.keys()
>>> names.sort()
>>> names[0]
u'ENSMICT000000000730'
```

Retrieve that record:

```
>>> r = db[names[0]]
>>> print r.keys()
[u'description', u'id', u'name', u'sequence']
```

Print out the internal ID number and the name:

```
>>> print r.id
13
>>> print r.name
ENSMICT000000000730
```





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## The screed developer documentation

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This section of the documentation is for people who are contributing (or would like to contribute to) the screed project codebase, either by contributing code or by helping improve the documentation.

Please note that this project is released with a *Contributor Code of Conduct*. By participating in the development of this project you agree to abide by its terms.

Contents:

### 3.1 Coding guidelines and code review checklist

This document is for anyone who want to contribute code to the screed project, and describes our coding standards and code review checklist.

---

#### 3.1.1 Coding standards

All plain-text files should have line widths of 80 characters or less unless that is not supported for the particular file format.

Vim user can set the indentation with:

```
set expandtab
set shiftwidth=4
set softtabstop=4
```

We are a pure Python project and [PEP 8](#) is our standard. The `'pep8'` and `'autopep8'` Makefile targets are helpful.

Code and documentation must have its spelling checked. Vim users can run:

```
:setlocal spell spelllang=en_us
```

Use `/s` and `/S` to navigate between misspellings and `z=` to suggest a correctly spelled word. `zg` will add a word as a good word.

GNU *aspell* can also be used to check the spelling in a single file:

```
aspell check --mode $filename
```

### 3.1.2 Code Review

Please read [11 Best Practices for Peer Code Review](#).

See also [Code reviews: the lab meeting for code](#) and [the PyCogent coding guidelines](#).

### 3.1.3 Checklist

Copy and paste the following into a pull request comment when it is ready for review:

- [ ] Is it mergable?
- [ ] Did it pass the tests?
- [ ] If it introduces new functionality, is it tested?
- [ ] Is it well formatted? Look at `'make pep8'`, `'make diff_pylint_report'`, and `'make doc'` output. Use `'make format'` and manual fixing as needed.
- [ ] Is it documented in the ChangeLog?
- [ ] Was a spellchecker run on the source code and documentation after changes were made?

**Note** that after you submit the comment you can check and uncheck the individual boxes on the formatted comment; no need to put x or y in the middle.

## 3.2 Release Documentation

### 3.2.1 Introduction

This is the release documentation for releasing a new version of screed. This document is meant for screed release managers. Michael R. Crusoe and C. Titus Brown have released screed in the past. Jake Fenton is the first to release screed using this checklist.

### 3.2.2 Getting Started

1. Start with a clean checkout:

```
cd `mktemp -d`  
git clone git@github.com:ged-lab/screed.git  
cd screed
```

2. Install/update versioneer:

```
pip install versioneer  
versioneer-installer
```

If there is a new version of versioneer:

```
git diff  
./setup.py versioneer  
git commit -p -m "new version of versioneer.py"  
# or abandon the changes  
git checkout -- versioneer.py screed/_version.py screed/__init.py \  
MANIFEST.in
```

3. Review the git logs since the previous release and that ChangeLog reflects the major changes:

```
git log --minimal --patch \  
    'git describe --tags --always --abbrev=0'..HEAD
```

4. Review the issue list for any existing bugs that won't be fixed in the release and ensure they're documented in `doc/known-issues.txt`
5. Verify that the build is clean: <http://ci.ged.msu.edu/job/screed/>
6. Set the new version number and release candidate:

```
new_version=1.1  
rc=rc3
```

Tag the release candidate with the new version prefixed by the letter 'v':

```
git tag v${new_version}-${rc}  
git push --tags git@github.com:ged-lab/screed.git
```

7. Test the release candidate:

```
cd ..  
virtualenv testenv1  
virtualenv testenv2  
virtualenv testenv3  
virtualenv testenv4  
  
# first we test the tag  
cd testenv1  
source bin/activate  
pip install nose  
git clone --depth 1 --branch v${new_version}-${rc} \  
    https://github.com/ged-lab/screed.git  
cd screed  
make install  
nosetests screed --attr '!known_failing'  
make test  
python -c 'import screed; print screed.__version__' # double-check  
version number  
  
# Test via pip  
cd ../../testenv2  
source bin/activate  
pip install nose  
pip install -e  
git+https://github.com/ged-lab/screed.git@v${new_version}-${rc}#egg=screed  
cd src/screed  
make dist  
make install  
nosetests screed --attr '!known_failing'  
python -c 'import screed; print screed.__version__'  
cp dist/screed*tar.gz ../../testenv3  
  
# test if the dist made in testenv2 is complete enough to build another  
# functional dist  
  
cd ../../testenv3  
source bin/activate  
pip install nose  
pip install screed*tar.gz
```

```
nosetests screed --attr '!known_failing'
python -c 'import screed; print screed.__version__'
tar xzf screed.tar.gz
cd screed*
make dist
make test
```

8. Publish the new release on the testing PyPI server. You will need to change your PyPI credentials as documented here: <https://wiki.python.org/moin/TestPyPI>. You may need to re-register:

```
python setup.py register --repository test
```

Now, upload the new release:

```
python setup.py sdist upload -r test
```

Test the PyPI release in a new virtualenv:

```
cd ../../testenv4
source bin/activate
pip install -U setuptools
pip install nose
pip install -i https://testpypi.python.org/pypi --pre --no-clean screed
nosetests screed --attr '!known_failing'
python -c 'import screed; print screed.__version__'
cd build/screed
./setup.py nosetests --attr '!known_failing'
```

9. Do any final testing (acceptance tests, etc.) Note that the acceptance tests for screed are to run the khmer automated tests with the new version of screed installed and then to run the khmer acceptance tests.
10. Make sure any release notes are merged into doc/release-notes/.

### 3.2.3 Notes on this document

This is the procedure for cutting a new release of screed. It has been adapted from the release documentation for the khmer project, found at <http://khmer.readthedocs.org/en/v1.1/release.html>.

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## Release notes for past versions of screed

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Contents:

### 4.1 Release v0.5

We are proud to announce the release of screed v0.5. screed is a database engine capable of storing and retrieving short-read sequence data. screed is designed to be fast and adaptable to different sequence file formats. This marks the first release of screed which we consider stable and complete.

**Features:**

- Read sequence data from FASTA/FASTQ files into screed databases
- Save screed databases back to FASTA/FASTQ files
- Lookup sequence data by index (offset) or name
- Native support for sequence substring slicing
- Convert between FASTA <-> FASTQ file formats

screed is written entirely in Python and uses the Sqlite database for backend storage. screed can be downloaded from the public git repository: <http://github.com/acr/screed.git>

screed is licensed under the BSD license which can be viewed in the doc/LICENSE.txt file.



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## Known Issues

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This document details the known issues in the current release of screed. All issues for screed are tracked at <https://github.com/ged-lab/khmer/labels/screed>

### 5.1 List of known issues

Screed does not support gzip file streaming. This is an issue with Python 2.x and will likely *not* be fixed in future releases. <https://github.com/ged-lab/khmer/issues/700>

Screed is overly tolerant of spaces in fast{q,a} which is against spec. <https://github.com/ged-lab/khmer/issues/108>

Screed records cannot be sliced requiring un-Pythonic techniques to achieve the same behavior This will be included in a future release. <https://github.com/ged-lab/khmer/issues/768>

Screed self-tests do not use a temporary directory which causes tests run from package-based installs to fail <https://github.com/ged-lab/khmer/issues/748>





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## Contributor Code of Conduct

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As contributors and maintainers of this project, we pledge to respect all people who contribute through reporting issues, posting feature requests, updating documentation, submitting pull requests or patches, and other activities.

We are committed to making participation in this project a harassment-free experience for everyone, regardless of level of experience, gender, gender identity and expression, sexual orientation, disability, personal appearance, body size, race, age, or religion.

Examples of unacceptable behavior by participants include the use of sexual language or imagery, derogatory comments or personal attacks, trolling, public or private harassment, insults, or other unprofessional conduct.

Project maintainers have the right and responsibility to remove, edit, or reject comments, commits, code, wiki edits, issues, and other contributions that are not aligned to this Code of Conduct. Project maintainers or contributors who do not follow the Code of Conduct may be removed from the project team.

Instances of abusive, harassing, or otherwise unacceptable behavior may be reported by emailing [khmer-project@idyll.org](mailto:khmer-project@idyll.org) which only goes to C. Titus Brown and Michael R. Crusoe. To report an issue involving either of them please email [Judi Brown Clarke, Ph.D.](#) the Diversity Director at the BEACON Center for the Study of Evolution in Action, an NSF Center for Science and Technology.

This Code of Conduct is adapted from the [Contributor Covenant](#), version 1.0.0, available at <http://contributor-covenant.org/version/1/0/0/>



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## Indices and tables

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- *genindex*
- *modindex*
- *search*