

OpenEye
SCIENTIFIC

# EON

***Release 2026.1.0***

**Cadence Design Systems, Inc.**

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CHAPTER

ONE

# INTRODUCTION

## 1.1 Overview

**EON** is a tool for aligning and scoring a database of molecules based on similarity in molecular shape and electrostatic property. Electrostatic property is described by either charge density (the default option) or potential. The scores are used to rank molecules based on the probability that they share relevant (biological) properties with the query molecule.

**EON** does not require prealigned molecules. The alignment and scoring is done internally with molecular shape and charge density similarity. When **EON** is run in the `-potential` true mode, the aligned geometries are scored with molecular shape and potential similarity.

The inputs into **EON** are a database of molecules in at least one 3D conformation, and a query molecule. The minimal output is a file of the best alignments and shape and electrostatic similarity scores for each of the database molecules to the query.

## 1.2 Applications

The **EON** distribution contains a single application:

*EON*

Aligns and scores molecules in a database file to a query molecule.

CHAPTER

TWO

# EON

## 2.1 Overview

**EON** calculates the electrostatic similarity between two small molecules in the form of an Electrostatic Tanimoto (ET) score. **EON** supports two descriptions of electrostatics: via charge density (by default) and via potential (*-potential* true) Given a query molecule and a set of interesting molecules, **EON** will calculate the Electrostatic Tanimoto between each database molecule and the query. Note, that starting from version 3.0, **EON** does perform an overlay of the input structures using molecular shape and charge density similarity optimization. Since electrostatics calculations require high quality partial charges, **EON** will calculate new partial charges for the input structures using MMFF94. If the user provides an input file that contains structures with higher-quality partial charges, EON can use them as well (*-charges* existing).

**EON** is also dependent on pKa state and formal charges as these have a significant impact on electrostatics. EON now has the ability to adjust both the query and database molecule to a neutral pH model. This feature is on by default, but can be turned off by using appropriate command line flags.

When **EON** is run in *-potential* true mode, the best shape and charge density hits are rescored with shape and potential similarity. In doing so the command line flag *-num_top_scores* (by default equal to 5) controls how many best hits per molecule are being re-scored.

Part of understanding **EON** results is visualization of the electrostatic grids used in the calculation. Although off by default, when writing **EON** results to a binary (OEB) file, ET grids can be attached to each molecule and visualized using the **EON** View mode in **VIDA**. When running with *-writegrid* true, for *-potential* false the charge density grid will be outputted and for *-potential* true the electrostatic PB potential grid will be added to results.

Since **EON** calculations can be time-consuming (approximately 1 molecule per second per CPU for the *-potential* true case), EON can use the same distributed computing technology, Open MPI, that **ROCS** uses to help distribute the workload across a cluster of machines.

## 2.2 Example Commands

**EON** needs an input for a query file and a set of molecules in the database file.

So for example:

```
eon -in database_molecules.oeb.gz -query query.sdf -out EON_hits.oeb
```

will overlay and score all the structures in `database_molecules.oeb.gz` against the molecule in `query.sdf` and place the structures in `EON_hits.oeb` (with ET scores in SD tag data) and a table of results in `eon_hitlist_rpt.csv`.

To keep only the best 100 hits, use:

```
eon -in database_molecules.oeb.gz -query query.sdf -out EON_hits.oeb -maxhits 100
```

Note that the use of an output structure file is mostly for generation of a single file containing structures and tag data such that loading this single file into **VIDA** provides easy analysis of the results. If however, the only real desire is for the numerical scores, simply do not use `-out` command line flag.

```
eon -in database_molecules.oeb.gz -query query.sdf
```

By default, **EON** calculates partial charges using MMFF94. However, if you have structure files that already contain good partial charges in both your dbase file and query file, you can tell **EON** to use them instead:

```
eon -in database_with_charges.mol2 -query query_chg.mol2 -charges existing -fixpka_query␣
↪false -fixpka_dbase false
```

Please note that both *-fixpka_query* and *-fixpka_dbase* should be set to `false` if *-charges* is set to `existing`; otherwise EON will fail.

To prevent continually overwriting output files, the *-prefix* flag allows you to give unique names to these files.

```
eon -in database_molecules.oeb.gz -query query.sdf -prefix FOO
```

will write the hit structures into a file named `FOO_eon.oeb.gz` and the numerical values will be in `FOO_hitlist_rpt.csv`. The parameter file for this run will likewise be named `FOO_parm.txt` and the log file `FOO_log.txt`.

Finally, to create ET grids as used in the calculation and attach them to each output molecule. Note, this only works for OEB output and can be very memory intensive.

```
eon -in database_molecules.oeb.gz -query query.sdf -writegrid true -out EON_results_with_
↪ET_grids.oeb
```

## 2.3 Report File

The **EON** report file format appears as a csv file *eon_hitlist_rpt.csv* with the following fields. Since the names of the query and the hits are of indeterminate length, fixed size fields for these names could result in loss of information. Unfortunately this gives a file that is hard to read in a terminal session, but it can easily be read into a spreadsheet program or into the data manager in **VIDA**.

**Name**
: This is the name of the database molecule.

**SMILES**
: This is the SMILES string of the database molecule.

**Shape Tanimoto**
: This is the shape Tanimoto of the given database molecule with respect to query molecule.

**Charge Tanimoto**
: This is the charge Tanimoto with respect to query molecule. Note, that this field is only output when *-potential* false is used.

**Potential Tanimoto**
: This is the potential Tanimoto with respect to query molecule. Note, that this field is only output when *-potential* true is used.

**Shape + Charge Tanimoto Combo**
: Sum of **Shape Tanimoto** and **Charge Tanimoto**. This is a useful score that takes into account both shape match and (charge) ET match. Note that this field is only output when *-potential* false is used.

**Shape + Potential Tanimoto Combo**
Sum of **Shape Tanimoto** and **Potential Tanimoto**. This is a useful score that takes into account both shape match and (potential) ET match. Note that this field is only output when *-potential* true is used.

## 2.4 Command Line Help

A description of the commandline interface can be obtained by executing **EON** with the *–help* option.

```
prompt> eon --help
```

will generate the following output:

```
Simple parameter list
        -in : Input filename to be processed.
        -out : Output filename to be generated.
        -query : -query filename to be used.

Additional help functions:
  eon --help simple      : Get a list of simple parameters (as seen above)
  eon --help all         : Get a complete list of parameters
  eon --help defaults    : List the defaults for all parameters
  eon --help <parameter> : Get detailed help on a parameter
  eon --help html        : Create an html help file for this program
  eon --help versions    : List the toolkits and versions used in the application
```

## 2.5 Required Parameters

**-query**
Inputs the query or reference molecule.

**-in**

**-dbase**
Inputs file containing one or more 3D molecules to overlay and score against a reference or query molecule.

File format for *-dbase* can be one of:

| File type | Extension |
|---|---|
| OEBinary | .oeb .oeb.gz .oez |
| SDF | .sdf .mol .sdf.gz |
| MOL2 | .mol2 .mol2.gz |

## 2.6 Optional Parameters

### 2.6.1 Execute Options

**-param**
The argument for this flag is the name of a file containing control parameters. The control parameter file acts to either replace or augment the command line interface. All parameters necessary for program execution may be provided in the control parameter file, although any command given explicitly on the command line will supersede options found in the parameter file. The application generates a new parameter file containing the full

set of execution parameters upon every execution. The name of the parameter file is created by combining the prefix base name with the *'.param'* extension.

**-mpi_np** <n>

Specifies the number of processors `n` when the application is run in MPI mode.

**-mpi_hostfile** <filename>

Specifies the name of the file containing processors configuration. For every host this file should contain a line `host_name slots=n` where `n` is the number of processors on the host.

### File Options

**-log**

The argument for this flag specifies the name of the log file. The level of detail for logfile information can be altered using the *-verbose* flag. Generation of an output log may be disabled by providing `nul` as a argument in Windows and `/dev/null` as an argument on Linux and macOS. [default = `prefix` _log.txt]

**-prefix**

The argument for this flag defines the prefix to be used for various information and data files generated. Most important among these is the '*prefix_parm.txt*' file which includes a copy of all the parameters used in the run. The prefix is also used to generate a default log file name if not explicitly specified with the *-log* flag. [default = <app_name>].

**-verbose**

This is a boolean flag that controls the level of detail written to the log file. By default only minimal information is written to the log file. Verbose logging will cause more information to be written to the log file in order to follow behavior during program execution. [default = false]

**-molNames**

This parameter takes a text file containing a list of molecule names (one name per line in the file). If this parameter is set then only molecules in the input file(s) (see parameter *-in*) with names that match those in the text files will be read in.

The general purpose of this flag is to provide an easy mechanism for reading a few specific molecule(s) that are contained in a large file, without having to extract those molecules by hand from the input molecules file. [default = NONE].

**-progress**

Show progress on screen. Options are 'none', 'dots', 'log' and 'percent'. The 'dots' options will displays dots on screen to show molecules completed. The 'log' option will duplicate the log file on screen. The 'percent' option will track progress through the input file. [default = none]

## 2.6.2 EON App Options

**-scdbase**

Treat the database file as a single-conformer input (when the format is not OEB). [Default=true]

**-fixpka_query**

Apply a neutral pH model to the query molecule. It should be set to `false` if *-charges* is set to `existing`; otherwise EON will fail. [Default=true]

**-fixpka_dbase**

Apply a neutral pH model to the database molecules. It should be set to `false` if *-charges* is set to `existing`; otherwise EON will fail. [Default=true]

**-writegrid**

Whether or not to output electrostatic grid when writing to .oeb file. [Default=false]

**-charges**

Specifies charges to be used on the query and the database. Default is to calculate them internally with `mmff`. The option `-charges existing` will use precalculated charges that must be set in the input files. If `existing` is selected and any molecule doesn't have charges then EON will default to `mmff` for those molecules. Both *-fixpka_query* and *-fixpka_dbase* should be set to `false` if *-charges* is set to `existing`; otherwise EON will fail. [Default=mmff]

**-num_top_scores**

When potential mode is engaged, the shape and charge overlay will keep this many best hits, and score them all with potential to choose best combo hit. [Default=5]

**-potential**

Scoring done with shape and potential similarity combo. [Default=false]

**-scoreonly**

Whether or not to score only or do full overlay. [Default=false]

### 2.6.3 EON Hitlist Options

**-besthits** <N>

Keep a hitlist and find best N hits. Zero implies no hitlist, and streaming all scored input in the order of appearance. [Default=500]

**-maxhits** <N>

When this parameter is greater than zero, stop after *N* hits, otherwise find all hits. [Default=0]

**-rankby**

Score to use when ranking the hitlist.

| Value | Meaning |
|---|---|
| ET_pb | Poisson-Boltzmann ET score |
| ET_coul | Coulomb ET score |
| ET_combo | Combined ET score (default) |

[Default=ET_combo]

**-cutoff** <N>

Minimum score to keep. [Default=-1.0]

**-outputquery**

Output query molecule at the beginning of the hits file. [Default=true]

**-sdTags**

Attach score information to output molecules as SD data. [Default=true]

[Aliases=**-sdtags**]

**-nostructs**

Do not output any structures to the hits file. [Default=false]

**-hitsfile** <filename>

Absolute filename for the output hits file. Must be a valid molecule file. Use none for no hit file output. Overrides the name generated from *-prefix*.

**-reportfile** <filename>

Absolute filename for the report file. Use none for no report file output. Overrides the name generated from *-prefix*.

**-oformat** <extension>

Format for the output structure file. Legal values: sdf, mol, mol2, pdb, ent, mmod, oeb, sdf.gz, mol.gz, mol2.gz, pdb.gz, ent.gz, mmod.gz, oeb.gz. [Default=oeb]

**-logfile** <filename>

Absolute filename for the log file. Use - for stdout, none for no log output. Overrides the name generated from *-prefix*.

**-statusfile** <filename>

Write status information to this file. Use none for no status file.

### 2.6.4 ZAP/PB Options

**-salt**

Salt concentration (in mol/L) to use in the PB calculation. [Default=0.04]

**-spacing**

Grid spacing for internal ZAP grid. [Default=0.75]

### 2.6.5 Omega Conformer Options

**-ewindow**

Energy window (kcal/mol) used for conformer selection. [Default=10.0]

**-rms**

RMS threshold used to identify and remove duplicate conformations. [Default=0.3]

**-sampleHydrogens**

Sample hydrogen positions for hydroxyl (OH), thiol (SH), and amine groups during conformer generation. [Default=false]

[Aliases=**-sampleH**,**-samplehydrogens**]

CHAPTER

# THREE

# THEORY

**Electrostatic Charge Density** Starting from version 3.0 EON, incorporates two types of electrostatic description: charge density and potential. The charge density is modeled using partial charges and smearing them with a Gaussian function with a prefactor that is proportional to the partial atomic charge. This method has advantage of fast speed compared to more expensive potential calculations; therefore, it is set as a default behavior of EON.

For two charge distributions A and B:

$$ChargeTanimoto_{A,B} = \frac{O(A,B)}{O(A,A) + O(B,B) - O(A,B)}$$

Charge Tanimoto similarly to potential Tanimoto below behaves for equal and opposite charge distributions similarly

$$ChargeTanimoto_{A,A} = 1.0,$$
$$ChargeTanimoto_{A,-A} = -\frac{1}{3}$$

For hit list ranking, we report a score (Shape + Charge Tanimoto Combo) that is the sum of the Shape Tanimoto (ST) and the Charge Tanimoto.

**Electrostatic Potential**

EON uses a field-based measure of Tanimoto to compare the electrostatic potential of two small molecules. This electrostatic potential is calculated internally using Zap, OpenEye's Poisson-Boltzmann (PB) electrostatics toolkit.

The basic equation for a field Tanimoto is:

$$PotentialTanimoto_{A,B} = \frac{\int A(\vec{r}) * B(\vec{r})}{\int A(\vec{r}) * A(\vec{r}) + \int B(\vec{r}) * B(\vec{r}) - \int A(\vec{r}) * B(\vec{r})}$$

The two boundary cases for Electrostatic Tanimoto occur when B = A:

$$\begin{aligned} PotentialTanimoto_{A,A} &= \frac{\int A(\vec{r}) * A(\vec{r})}{\int A(\vec{r}) * A(\vec{r}) + \int A(\vec{r}) * A(\vec{r}) - \int A(\vec{r}) * A(\vec{r})} \\ &= 1 \end{aligned}$$

and the opposite case, when B = -A:

$$\begin{aligned} PotentialTanimoto_{A,-A} &= \frac{\int A(\vec{r}) * -A(\vec{r})}{\int A(\vec{r}) * A(\vec{r}) + \int -A(\vec{r}) * -A(\vec{r}) - \int A(\vec{r}) * -A(\vec{r})} \\ &= \frac{-\int A(\vec{r}) * A(\vec{r})}{\int A(\vec{r}) * A(\vec{r}) + \int A(\vec{r}) * A(\vec{r}) + \int A(\vec{r}) * A(\vec{r})} \\ &= -\frac{1}{3} \end{aligned}$$

In EON in the potential mode, we report electrostatic potential similarity based on the outer dielectric used in the PB calculation. We use an outer dielectric of 80. The rationale for using a PB electrostatic field is that the external potential

is dampened by orientation of the aqueous solvent. It is a common observation that proteins essentially act to reproduce the aqueous desolvation of well-bound ligands. As a result a PB electrostatic field is more likely to correctly capture the essential elements of binding than that from the Coulombic field.

For hit list ranking, we report a score (Shape + Potential Tanimoto Combo) that is the sum of the Shape Tanimoto (ST) and the PB Electrostatic Potential Tanimoto.

CHAPTER

FOUR

# RELEASE HISTORY

## 4.1 EON 3.1.3

Minor internal improvements have been made.

### 4.1.1 Related Toolkit Information

#### EON TK 3.1.3

#### New Features

- Two new methods, GetJoinRef and SetJoinRef, have been added to OEEonPBOptions to enable PB calculation on complexes in OEEonPBFunc.

#### Zap TK 2.5.3

#### Major Bug Fixes

- Salt concentration implementation in **Zap TK** has been corrected and made robust at higher salt concentrations.
- As a result of the salt concentration improvement, the rotational variation of Zap solvation energy at high salt concentrations has been substantially reduced.

## 4.2 EON 3.1.2

Minor internal improvements have been made.

### 4.2.1 Related Toolkit Information

#### Eon TK 3.1.2

Minor internal improvements have been made.

#### Zap TK 2.5.2

Minor internal improvements have been made.

## 4.3 EON 3.1.1

Minor internal improvements have been made.

### 4.3.1 Related Toolkit Information

#### EON TK 3.1.1

Minor internal improvements have been made.

#### Zap TK 2.5.1

Minor internal improvements have been made.

## 4.4 EON 3.1.0

### 4.4.1 New Features

- Supported input and output file formats for **EON** have been revised to improve clarity.
- The output csv file now contains additional columns with a rank of hits and best conformer index.
- The Boolean flag `-scoreonly` has been added to the **EON** application to allow passing prealigned molecules that only need to be scored.

### 4.4.2 Bug Fixes

- An issue affecting the **EON** hit list has been fixed. **EON** now properly uses the best conformer for each database molecule based on shape and charge density scores, instead of the first conformer of the molecule, to generate the hit list.
- A bug in combining shape and electrostatics gradients has been fixed.

## 4.5 Eon TK 3.1.0

This is the first commercial release of **Eon TK**.

### 4.5.1 New features

The following classes are available as preliminary API with the first release of this toolkit.

- OEChargeFunc
- OEEonHit
- OEEonHitlistBuilder
- OEEonHitlistOptions
- OEEonOverlapFunc
- OEEonOverlapScore
- OEEonOverlay
- OEEonOverlayResults
- OEEonOverlayScore
- OEEonPBFunc
- OEEonPBOptions
- OEEonPBOverlay
- OEExactChargeFunc

- OEGridChargeFunc

The following functions are available as preliminary API with the first release of this toolkit.

- OEEtGetArch
- OEEtGetLicensee
- OEEtGetPlatform
- OEEtGetRelease
- OEEtGetSite
- OEEtGetVersion
- OEEtIsLicensed

## 4.6 Zap TK 2.5.0

Minor internal improvements have been made.

## 4.7 EON 3.0.0.3

- An issue affecting the **EON** hitlist has been fixed. **EON** now properly uses the best conformer for each database molecule, based on shape and charge density scores, instead of the first conformer of the molecule, in generating the hitlist.

## 4.8 EON 3.0.0.0

### 4.8.1 New Features

- **EON** no longer requires pre-aligned molecules. The alignment and scoring are done internally with molecular shape and charge density similarity. Optionally, via modifying the boolean command line flag *potential* to *true*, rescoring of those alignments with shape and potential similarity is performed.

## 4.9 Zap TK 2.4.7

Minor internal improvements have been made.

## 4.10 EON 2.4.2

Minor internal improvements have been made.

## 4.11 Zap TK 2.4.6

### 4.11.1 New features

- New overloads of GetArea have been added that return solvent accessible surface areas for specific residues.

## 4.12 EON 2.4.1

Minor internal improvements have been made.

## 4.13 Zap TK 2.4.5

Minor internal improvements have been made.

## 4.14 EON 2.4.0

*Fall 2022*

Minor internal improvements have been made.

## 4.15 Zap TK 2.4.4

Minor internal improvements have been made.

## 4.16 EON 2.3.7

*Spring 2022*

- Minor internal improvements have been made.

## 4.17 Zap TK 2.4.3

- Minor internal improvements have been made.

## 4.18 EON 2.3.6

*Fall 2021*

- Minor internal improvements have been made.

## 4.19 Zap TK 2.4.2

*Fall 2021*

- Minor internal improvements have been made.

## 4.20 EON 2.3.5

*July 2021*

Minor internal improvements have been made.

## 4.21 Zap TK 2.4.1

*July 2021*

Minor internal improvements have been made.

## 4.22 EON 2.3.4.0

*Fall 2020*

- Minor internal improvements have been made.

## 4.23 Zap TK 2.4.0

- Minor internal improvements have been made.

## 4.24 EON 2.3.3

*Spring 2020*

- This version of **EON** has been built using **OEToolkits 2020.0**.

## 4.25 EON 2.3.2

*Nov 2019*

- This version of **EON** has been built using **OEToolkits 2019.Oct**. The previous version was built using **OEToolkits 2019.Apr**.

### 4.25.1 Minor bug fixes

- **EON** now fails if *-charges* is set to `existing` and :*-fixpkadbase* or *-fixpkaquery* is `true`. This avoids the problem with `fixpka` incorrectly modifying the molecule but not the charges.

## 4.26 EON 2.3.1

*May 2019*

- This version of **EON** has been built using **OEToolkits 2019.Apr**. The previous version was built using **OEToolkits 2018.Oct**.

### 4.26.1 Minor bug fixes

- EON now fails with an error message if *-charges* is set to `existing` and *-fixpkadbase* or *-fixpkaquery* is true

## 4.27 EON 2.3.0

*November 2018*

- This version of **EON** has been built using **OEToolkits 2018.Oct**. The previous version was built using **OEToolkits 2012.Oct**.

## 4.28 EON 2.2.0

Released June 2013

### 4.28.1 New features

- The default hitlist format has been changed from sdf to oeb for increased functionality and decreased filesize. The output format is adjustable with the *-oformat* parameter.
- The *-spacing* parameter has been added. This parameter can be used to adjust the grid spacing of the Zap/PB calculations.
- An option has been added to allow hydrogen atoms in -OH, -SH, and amines to take part in conformational sampling. This new option can be enabled via the *-sampleHydrogens* parameter. By default, hydrogen atoms are not sampled.
- Now SD tags are prefixed with *EON_*. The tags are optional with the *-sdTags* parameter. Additionally, any existing ROCS tags will not be removed because ROCS and EON tags no longer conflict.

### 4.28.2 Bug fixes

- A bug has been fixed where the multiconformer check was being applied to OEB format files. Additionally, the default for *-scdbase* has been changed from *false* to *true* to prevent inadvertent merging of molecules with other file formats.
- Warnings have been improved for charging failures.
- *-writegrid* will now write out a grid with the same spacing as the actual Zap/PB calculation. Previously the attached grid had tighter spacing which could lead to confusion.

### 4.28.3 Other changes

- PVM (parallel virtual machine) is no longer supported. OpenMPI version 1.6 is supported on all platforms. The *-mpi_np* and *-mpi_hostfile* flags are now used to run EON in MPI mode. These new flags replace the *oempirun* script.
- This will be the last release to support SuSe 10.

## 4.29 EON 2.1.0

Released June 2011

### 4.29.1 Enhancements

- The command line flags for choosing which charges to use have been simplified. There is a single flag `-charges`. The default is still to calculate MMFF charges. To use charges you have precalculated outside EON, first make sure you have charges for both the query and the dbase molecules, then use `-charges existing`.

> **Note**
>
> To use `existing` charges you must provide input files in a format that can store charges. This means input should be in either OEB or MOL2.

- This release adds EON to the set of applications that now use a common script in `openeye/bin` to determine the appropriate architecture and run the appropriate binary.
- On Windows, there is now an installer that installs the documentation and sets up a command prompt to facilitate running the EON command line.

### 4.29.2 Bug Fixes

- Fixed a bug to ensure that SD data present in the database is passed on to the EON hitlist. Note that this is specific to SD data other than ROCS scores. Since EON can modify the conformation, any ROCS scores would no longer be valid so they are removed from the output. Note that the score reported as EON_ShapeTanimoto is the final Shape Tanimoto calculated from the best conformation found inside EON.
- Fixed a bug that caused a crash when trying to write an empty hitlist.
- Fixed a bug that prevented `-salt` from working.
- Adding better error checking and messages for input. All input must be molecules and cannot be shape queries.

## 4.30 EON 2.0.0

Release August 2007

### 4.30.1 Enhancements

This is a significant new release of EON. This release incorporates many internal changes in how Electrostatic Tanimoto is calculated compared to EON 1.1.

- Salt in the PB calculation is now on by default to help moderate large, local charges. This should make EON 2.0 perform much better than 1.1 in the case of molecules with formal charges.
- OpenEye's neutral pH model has been incorporated allowing the setting of a pH model on both the query and database molecules. Since a significant use of EON is similarity searching, having a consistent model between the query and database molecules is very important. However, for the case where the states are well defined, this feature can be turned off.
- Instead of the slow and buggy `-spin` model for searching terminal torsions, EON 2.0 uses technology from OMEGA to only search reasonable torsions and to prevent creation of bad structures while searching for better electrostatic overlap.
- The hitlist is now sorted by default by a new score, ET_combo, which is the sum of the Shape Tanimoto (ST) and the Electrostatic Tanimoto (ET_pb).
- To make visualization of results easier, EON can write out the actual ET grids to the hits file, attached to each hit. This file can be loaded into VIDA 3.0 or later and the grids can be visually compared.
- There are also several changes to the mechanics of running the calculation including a new `-progress` feature and a more detailed PVM log output for PVM jobs.

CHAPTER

# FIVE

# CITATION

**Note**

To cite EON please use the following:

EON 3.1.3.0. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.eyesopen.com.

CHAPTER

SIX

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CHAPTER

SEVEN

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CHAPTER

# EIGHT

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OpenEye Large-Scale Floes 4.2.3. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
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- OEChem TK
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- OEDocking TK
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- FastROCS TK
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- Omega TK
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- Shape TK
- Spicoli TK
- Spruce TK
- Szmap TK
- Szybki TK
- Zap TK
- AFITT Application
- BROOD Application
- OEDocking Application
- EON Application
- OMEGA Application
- PICTO Application
- pKa-Prospector Application
- QUACPAC Application

- ROCS Application
- SiteHopper Application
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- SZMAP Application
- SZYBKI Application
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You can use the version number of the individual Application or Toolkit. For example:

```
SZYBKI Application 2.8.0.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://
↪www.eyesopen.com.

Szybki TK 2.8.0.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.
↪eyesopen.com.
```

The first documentation pages give the product names and version numbers, as in https://docs.eyesopen.com/applications/szybki/index.html and https://docs.eyesopen.com/toolkits/python/szybkitk/index.html.

## 8.4 Publications for Bibliographies

Please also cite these publications if the corresponding product was used in your research.

### 8.4.1 Orion

Sørensen, J., Bannan, C.C., Calabrò, G., Jain, V., Ovanesyan, G., Smith, A., Zhang, S., Bayly, C.I., Darden, T.A., Geballe, M.T., LeBard, D.N., McGann, M., Moon, J.B., Muddana, H.S., Shewmaker, A., LaFon, J., Tolbert, R.W., Skillman, A.G., Nicholls, A. Orion® A Cloud-Native Molecular Design Platform. In *Computational Drug Discovery*. V. Poongavanam and V. Ramaswamy, Eds. Wiley-VCH, 2024; pp. 579–615. DOI: 10.1002/9783527840748.ch24

### 8.4.2 AFITT and FLYNN Applications

Wlodek, S.; Skillman, A.G.; Nicholls, A. Automated Ligand Placement and Refinement with a Combined Force Field and Shape Potential. *Acta Crystallogr., Sect. D: Struct. Biol.* **2006**, *62* (7), 741–749. DOI: 10.1107/s0907444906016076

### 8.4.3 OEDocking Application and Toolkit

Kelley, B.P.; Brown, S.P.; Warren, G.L.; Muchmore, S.W. POSIT: Flexible Shape-Guided Docking For Pose Prediction. *J. Chem. Inf. Model.* **2015**, *55* (8), 1771-1780. DOI: 10.1021/acs.jcim.5b00142

McGann, M. FRED Pose Prediction and Virtual Screening Accuracy. *J. Chem. Inf. Model.* **2011**, *51* (3), 578-596. DOI: 10.1021/ci100436p

McGann, M. FRED and HYBRID Docking Performance on Standardized Datasets. *J. Comput.-Aided Mol. Des.* **2012**, *26* (8), 897-906. DOI: 10.1007/s10822-012-9584-8

### 8.4.4 OMEGA Application and Toolkit

If you are using OMEGA in torsion driving mode, please cite the following two publications.

Hawkins, P.C.D.; Skillman, A.G.; Warren, G.L.; Ellingson, B.A.; Stahl, M.T. Conformer Generation with OMEGA: Algorithm and Validation Using High Quality Structures from the Protein Databank and the Cambridge Structural Database. *J. Chem. Inf. Model.* **2010**, *50* (4), 572-584. DOI: 10.1021/ci100031x

Hawkins, P.C.D. and Nicholls, A. Conformer Generation with OMEGA: Learning from the Data Set and the Analysis of Failures. *J. Chem. Inf. Model.* **2012**, *52* (11), 2919–2936. DOI: /10.1021/ci300314k

If you are using OMEGA in macrocyle mode, please cite the following.

Hawkins, P.C.D. and Wlodek, S. Decisions with Confidence: Application to the Conformation Sampling of Molecules in the Solid State. *J. Chem. Inf. Model.* **2020**, *60* (7), 3518–3533. DOI: /10.1021/acs.jcim.0c00358

### 8.4.5 ROCS Application

Hawkins, P.C.D.; Skillman, A.G.; Nicholls, A. Comparison of Shape-Matching and Docking as Virtual Screening Tools. *J. Med. Chem.* **2007**, *50* (1), 74-82. DOI: 10.1021/jm0603365

## 8.5 OpenEye MMDS Web Service

To cite use of the Macromolecular Data Service (MMDS) web service, please use the syntax:

```
Macromolecular Data Service <version-number>. OpenEye, Cadence Molecular Sciences, Santa␣
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```

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Macromolecular Data Service 1.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
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The MMDS version number appears on the web service's release notes.

CHAPTER

NINE

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| blosc2 | https://github.com/Blosc/python-blosc2 | https://github.com/Blosc/c-blosc2/blob/main/LICENSE.txt |

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| boost | https://www.boost.org/doc/libs/1_71_0/libs/python/doc/html/index.html | https://www.boost.org/LICENSE_1_0.txt |
| boost-cpp | https://www.boost.org/doc/libs/1_71_0/libs/python/doc/html/index.html | https://www.boost.org/LICENSE_1_0.txt |
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| brotlicffi | https://github.com/python-hyper/brotlicffi | https://github.com/python-hyper/brotlicffi?tab=MIT-1-ov-file#readme |
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| bytefmt | https://code.cloudfoundry.org/bytefmt | https://github.com/cloudfoundry/bytefmt/blob/master/LICENSE |
| bzip2 | https://www.bzip.org | https://spdx.org/licenses/bzip2-1.0.6.html |
| c-ares | https://github.com/c-ares/c-ares | https://github.com/c-ares/c-ares/blob/main/LICENSE.md |
| ca-certificates | https://github.com/conda-forge/ca-certificates-feedsto | https://wiki.mozilla.org/CA/Included_Certificates |
| cached-property | https://github.com/pydanny/cached-property | https://github.com/pydanny/cached-property/blob/master/LICENSE |
| cachetools | https://github.com/tkem/cachetools/ | https://github.com/tkem/cachetools/blob/master/LICENSE |
| cairo | https://pycairo.readthedocs.io/en/latest/ | https://github.com/pygobject/pycairo/blob/master/COPYING |
| canvas | https://github.com/Automattic/node-canvas | https://github.com/Automattic/node-canvas |
| cctbx | https://github.com/cctbx/cctbx_project | https://github.com/cctbx/cctbx_project/blob/master/cctbx/LICENSE_2_0.txt |
| celery | https://github.com/celery/celery | https://github.com/celery/celery/blob/master/LICENSE |
| Cerberus | https://docs.python-cerberus.org/en/stable/ | https://docs.python-cerberus.org/en/stable/license.html |
| certifi | https://certifiio.readthedocs.io/en/latest/ | https://wiki.mozilla.org/index.php?title=CA/IncludedCertificates&redirect=no |

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| Name of Project | Website | License URL |
|---|---|---|
| cffi | https://github.com/python-cffi | https://github.com/cffi/cffi/blob/master/COPYRIGHT |
| cftime | https://pypi.org/project/cftime/ | https://github.com/Unidata/cftime/blob/master/LICENSE |
| chardet | https://github.com/chardet/chardet | https://github.com/chardet/chardet/blob/master/LICENSE |
| charset-normalizer | https://github.com/ousret/charset_normalizer | https://github.com/Ousret/charset_normalizer/blob/master/LICENSE |
| ChEMBL Structure Pipeline | https://github.com/chembl/ChEMBL_Structure_Pipeline/tree/master | https://github.com/chembl/ChEMBL_Structure_Pipeline/blob/master/LICENSE |
| choreographer | https://github.com/mazpie/choreographer | https://github.com/mazpie/choreographer/blob/main/LICENSE |
| chunkreader | https://github.com/jackc/chunkreader/v2 | https://github.com/jackc/chunkreader/blob/master/LICENSE |
| click | https://palletsprojects.com/p/click/ | https://github.com/pallets/click/blob/main/LICENSE.rst |
| click-completion | https://github.com/click-contrib/click-completion | https://github.com/click-contrib/click-completion/blob/master/LICENSE |
| click-didyoumean | https://github.com/click-contrib/click-didyoumean | https://github.com/click-contrib/click-didyoumean/blob/master/LICENSE |
| click-plugins | https://github.com/click-contrib/click-plugins | https://github.com/click-contrib/click-plugins/blob/master/LICENSE.txt |

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| Name of Project | Website | License URL |
|---|---|---|
| click-repl | https://github.com/untitaker/click-repl | https://github.com/click-contrib/click-repl/blob/master/LICENSE |
| cloudpickle | https://github.com/cloudpipe/cloudpickle | https://github.com/cloudpipe/cloudpickle/blob/master/LICENSE |
| cmake | https://cmake.org/ | https://cmake.org/licensing/ |
| colorama | https://github.com/tartley/colorama | https://github.com/tartley/colorama/blob/master/LICENSE.txt |
| comm | https://github.com/ipython/comm | https://github.com/ipython/comm/blob/master/LICENSE |
| compose | https://github.com/docker/compose | https://github.com/docker/compose/blob/v2/LICENSE |
| conda-content-trust | https://github.com/conda/conda-content-trust | https://github.com/conda/conda-content-trust/blob/main/LICENSE |
| conda-libmamba-solver | https://github.com/conda/conda-libmamba-solv | https://github.com/conda/conda-libmamba-solv/blob/main/LICENSE |
| conda-pack | https://conda.github.io/conda-pack/ | https://github.com/conda/conda-pack/blob/main/LICENSE.txt |
| conda-package-handling | https://github.com/conda/conda-package-handli | https://github.com/conda/conda-package-handli/blob/main/LICENSE |
| conda-package-streaming | https://anaconda.org/conda-forge/conda-package-stream | https://github.com/conda/conda-package-stream/blob/main/LICENSE |
| conda-token | https://anaconda.org/anaconda/conda-token | https://anaconda.org/anaconda/conda-token |

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| Name of Project | Website | License URL |
|---|---|---|
| conda_package_strear | https://github.com/conda/conda-package-streamtree/main/conda_package_streaming | https://github.com/conda/conda-package-streamtab=License-1-ov-file |
| confuse | https://github.com/beetbox/confuse | https://github.com/beetbox/confuse/blob/main/LICENSE |
| contourpy | https://github.com/contourpy/contourpy | https://github.com/contourpy/contourpy/blob/main/LICENSE |
| cpp-expected | https://github.com/TartanLlama/expected | https://github.com/TartanLlama/expected?tab=CC0-1.0-1-ov-file#readme |
| cpp-peglib | https://github.com/yhirose/cpp-peglib | https://github.com/yhirose/cpp-peglib/blob/master/LICENSE |
| cryptography | https://github.com/pyca/cryptography | https://github.com/pyca/cryptography/blob/main/LICENSE |
| cssselect2 | https://github.com/Kozea/cssselect2/ | https://github.com/Kozea/cssselect2/blob/master/LICENSE |
| cuda-bindings | https://nvidia.github.io/cuda-python/cuda-bindings/latest/install.html | https://github.com/NVIDIA/cuda-python/blob/main/cuda_bindings/LICENSE |
| cuda-pathfinder | https://nvidia.github.io/cuda-python/cuda-pathfinder/latest/ | https://nvidia.github.io/cuda-python/cuda-pathfinder/latest/license.html |
| cudatoolkit | https://developer.nvidia.com/cuda-toolkit | https://docs.nvidia.com/cuda/eula/index.html |
| cuequivariance-ops-cu12 | https://developer.nvidia.com/cuequivariance | https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| cuequivariance-ops-torch-cu12 | https://developer.nvidia.com/cuequivariance | https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE |
| cuequivariance-torch | https://docs.nvidia.com/cuda/cuequivariance/ | https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE |
| cupy-cuda113 | https://cupy.dev/ | https://github.com/cupy/cupy/blob/main/LICENSE |
| cupy-cuda11x | https://cupy.dev/ | https://github.com/cupy/cupy/?tab=MIT-1-ov-file#readme |
| curl | https://curl.se | https://curl.se/docs/copyright.html |
| cycler | https://github.com/matplotlib/cycler | https://github.com/matplotlib/cycler/blob/main/LICENSE |
| cyrus-sasl | https://github.com/cyrusimap/cyrus-sasl | https://github.com/cyrusimap/cyrus-sasl/blob/master/COPYING |
| Cython | https://cython.org | https://www.apache.org/licenses/LICENSE-2.0.html |
| d3 | https://github.com/mbostock/d3 | https://github.com/mbostock/d3/raw/master/LICENSE |
| dataclasses | https://github.com/ericvsmith/dataclasses | https://github.com/ericvsmith/dataclasses/blob/master/LICENSE.txt |
| ddsketch | http://github.com/datadog/sketches-py | https://github.com/DataDog/sketches-py/blob/master/LICENSE |
| debugpy | https://aka.ms/debugpy | https://github.com/microsoft/debugpy/blob/main/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| decimal | https://github.com/shopspring/decimal | https://github.com/shopspring/decimal/blob/master/LICENSE |
| decorator | https://github.com/micheles/decorator | https://github.com/micheles/decorator/blob/master/LICENSE.txt |
| deepdiff | https://github.com/seperman/deepdiff | https://github.com/seperman/deepdiff/blob/master/LICENSE |
| deeptime | https://github.com/deeptime-ml/deeptime | https://github.com/deeptime-ml/deeptime/blob/main/LICENSE.txt |
| defusedxml | https://github.com/tiran/defusedxml | https://github.com/tiran/defusedxml/blob/main/LICENSE |
| dftd3 | https://github.com/dftd3/tad-dftd3 | https://github.com/dftd3/tad-dftd3/blob/main/LICENSE |
| dill | https://github.com/uqfoundation/dill | https://github.com/uqfoundation/dill/blob/master/LICENSE |
| distlib | https://distlib.readthedocs.io/en/latest/ | https://github.com/pypa/distlib/blob/master/LICENSE.txt |
| distro | https://github.com/python-distro/distro | https://github.com/python-distro/distro/blob/master/LICENSE |
| Django | https://www.djangoproject.com/ | https://github.com/django/django/blob/main/LICENSE |
| django-classy-tags | https://github.com/django-cms/django-classy-tags | https://github.com/django-cms/django-classy-tags/blob/master/LICENSE |
| django-cors-headers | https://github.com/adamchainz/django-cors-headers | https://github.com/adamchainz/django-cors-headers/blob/main/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| django-csp | https://github.com/mozilla/django-csp | https://github.com/mozilla/django-csp/blob/main/LICENSE |
| django-extensions | https://github.com/django-extensions/django-extensions | https://github.com/django-extensions/django-extensions/blob/main/LICENSE |
| django-filter | https://github.com/carltongibson/django-filter/tree/master | https://github.com/carltongibson/django-filter/blob/main/LICENSE |
| django-redis | https://github.com/jazzband/django-redis | https://github.com/jazzband/django-redis/blob/master/LICENSE |
| django-taggit | https://github.com/jazzband/django-taggit | https://github.com/jazzband/django-taggit/blob/master/LICENSE |
| django-taggit-serializer | https://github.com/glemmaPaul/django-taggit-serializ | https://github.com/glemmaPaul/django-taggit-serializ blob/master/LICENSE |
| django-taggit-templatetags2 | https://github.com/fizista/django-taggit-templat | https://github.com/fizista/django-taggit-templat blob/master/LICENSE.txt |
| djangorestframework | https://www.django-rest-framewor org/ | https://github.com/encode/django-rest-framewor blob/master/LICENSE.md |
| dkh | https://psicode.org/psi4manual/master/dkh.html | https://github.com/psi4/dkh/blob/master/COPYING.LESSER |
| dm-tree | https://github.com/deepmind/tree | https://github.com/deepmind/tree/blob/master/LICENSE |
| docker-py | https://github.com/docker/docker-py/ | https://github.com/docker/docker-py/blob/master/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| docker-pycreds | https://github.com/shin-/dockerpy-creds | https://github.com/shin-/dockerpy-creds/blob/master/LICENSE |
| docopt | https://docopt.org | https://github.com/docopt/docopt/blob/master/LICENSE-MIT |
| docutils | https://docutils.sourceforge.io | https://docutils.sourceforge.io/COPYING.html |
| drf-dynamic-fields | https://github.com/dbrgn/drf-dynamic-fields | https://github.com/dbrgn/drf-dynamic-fields/blob/master/LICENSE |
| DuckDB | https://duckdb.org/ | https://github.com/duckdb/duckdb?tab=MIT-1-ov-file#readme |
| edgembar | https://rutgerslbsr.gitlab.io/fe-toolkit/edgembar/index.html | https://gitlab.com/RutgersLBSR/fe-toolkit/-/blob/master/LICENSE |
| editdistance | https://github.com/roy-ht/editdistance | https://github.com/roy-ht/editdistance/blob/master/LICENSE |
| eigen | https://eigen.tuxfamily.org/index.php?title=Main_Page | https://eigen.tuxfamily.org/index.php?title=Main_Page#License |
| einops | https://github.com/arogozhnikov/einops | https://github.com/arogozhnikov/einops/blob/master/LICENSE |
| einx | https://github.com/fferflo/einx | https://github.com/fferflo/einx/blob/master/LICENSE |
| entrypoints | https://github.com/takluyver/entrypoints | https://github.com/takluyver/entrypoints/blob/master/LICENSE |
| errors | https://github.com/pkg/errors | https://github.com/pkg/errors/blob/master/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| eslint-plugin | https://github.com/typescript-eslint/typescript-eslint | https://github.com/typescript-eslint/typescript-eslint/raw/master/LICENSE |
| et_xmlfile | https://foss.heptapod.net/openpyxl/et_xmlfile | https://foss.heptapod.net/openpyxl/et_xmlfile/-/blob/branch/default/LICENCE.rst |
| exceptiongroup | https://github.com/agronholm/exceptiongroup | https://github.com/agronholm/exceptiongroup/blob/main/LICENSE |
| execnet | https://execnet.readthedocs.io/en/latest/ | https://github.com/pytest-dev/execnet/blob/master/LICENSE |
| executing | https://github.com/alexmojaki/executing | https://github.com/alexmojaki/executing/blob/master/LICENSE.txt |
| expat | https://libexpat.github.io | https://github.com/libexpat/libexpat/blob/master/expat/COPYING |
| fairscale | https://github.com/facebookresearch/fairscale | https://github.com/facebookresearch/fairscale/blob/main/LICENSE |
| fairseq | https://github.com/pytorch/fairseq | https://github.com/facebookresearch/fairseq/blob/main/LICENSE |
| fastjsonschema | https://github.com/horejsek/python-fastjsonschem | https://github.com/horejsek/python-fastjsonschem/blob/master/LICENSE |
| fastrlock | https://github.com/scoder/fastrlock | https://github.com/scoder/fastrlock/blob/master/LICENSE |
| fftw | https://www.fftw.org | commercial license |

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| Name of Project | Website | License URL |
|---|---|---|
| filebuffer | https://github.com/mattetti/filebuffer | https://github.com/mattetti/filebuffer/blob/master/LICENSE |
| filelock | https://py-filelock.readthedocs.io/en/latest/index.html | https://github.com/tox-dev/py-filelock/blob/main/LICENSE |
| finufft | https://github.com/flatironinstitute/finufft | https://github.com/flatironinstitute/finufft/blob/master/LICENSE |
| Flask | https://flask.palletsprojects.com/en/2.1.x/ | https://flask.palletsprojects.com/en/2.1.x/license/ |
| flatbuffers | https://google.github.io/flatbuffers/ | https://github.com/google/flatbuffers/blob/master/LICENSE.txt |
| flexcache | https://github.com/hgrecco/flexcache | https://github.com/hgrecco/flexcache/blob/main/LICENSE |
| flexparser | https://github.com/hgrecco/flexparser | https://github.com/hgrecco/flexparser/blob/main/LICENSE |
| flit-core | https://github.com/pypa/flit | https://github.com/scientific-python/lazy_loader/blob/main/LICENSE.md |
| FLTK | https://www.fltk.org/index.php | https://www.fltk.org/COPYING.php |
| fmt | https://fmt.dev/latest/index.html | https://github.com/fmtlib/fmt/blob/master/LICENSE.rst |
| font-awesome | https://github.com/FortAwesome/Font-Awesome | https://github.com/FortAwesome/Font-Awesome |
| font-ttf-dejavu-sans-mono | https://dejavu-fonts.github.io | https://dejavu-fonts.github.io/License.html |
| font-ttf-inconsolata | https://fonts.google.com/specimen/Inconsolata | https://scripts.sil.org/cms/scripts/page.php?site_id=nrsi&id=OFL |

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| Name of Project | Website | License URL |
|---|---|---|
| font-ttf-source-code-pro | https://fonts.google.com/specimen/Source+Code+Pro | https://scripts.sil.org/cms/scripts/page.php?site_id=nrsi&id=OFL |
| font-ttf-ubuntu | https://fonts.google.com/specimen/Ubuntu | https://ubuntu.com/legal/font-licence |
| fontconfig | https://www.freedesktop.org/wiki/Software/fontconfig/ | https://gitlab.freedesktop.org/fontconfig/fontconfig/-/blob/main/COPYING |
| fonts-conda-ecosystem | https://anaconda.org/conda-forge/fonts-conda-ecosyster | https://docs.conda.io/en/latest/license.html |
| fonts-conda-forge | https://anaconda.org/conda-forge/fonts-conda-forge/ | https://creativecommons.org/licenses/by/4.0/ |
| fonttools | https://github.com/fonttools/fonttools | https://github.com/fonttools/fonttools/blob/main/LICENSE |
| forcebalance | https://simtk.org/home/forcebalance OR https://github.com/leeping/forcebalance | https://github.com/leeping/forcebalance/blob/master/LICENSE |
| fqdn | https://github.com/ypcrts/fqdn | https://github.com/ypcrts/fqdn?tab=MPL-2.0-1-ov-file#readme |
| freetype | https://freetype.org | https://freetype.org/license.html |
| freetype-py | https://github.com/rougier/freetype-py | https://github.com/rougier/freetype-py?tab=License-1-ov-file#readme |
| fribidi | https://github.com/fribidi/fribidi | https://github.com/fribidi/fribidi/blob/master/COPYING |
| frozendict | https://github.com/Marco-Sulla/python-frozendict | https://github.com/Marco-Sulla/python-frozendict/blob/master/LICENSE.txt |
| frozenlist | https://github.com/aio-libs/frozenlist | https://github.com/aio-libs/frozenlist/blob/master/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| fsmlite | https://github.com/tkem/fsmlite | https://github.com/tkem/fsmlite/blob/master/LICENSE |
| fsspec | https://github.com/fsspec/filesystem_spec | https://github.com/fsspec/filesystem_spec/blob/master/LICENSE |
| funcy | https://github.com/Suor/funcy | https://github.com/Suor/funcy/blob/master/LICENSE |
| gast | https://github.com/serge-sans-paille/gast/ | https://github.com/serge-sans-paille/gast/blob/master/LICENSE |
| gau2grid | https://github.com/dgasmith/gau2grid | https://github.com/dgasmith/gau2grid/blob/master/LICENSE |
| gax-go | https://github.com/googleapis/gax-go/v2 | https://github.com/googleapis/gax-go/blob/main/LICENSE |
| gdk-pixbuf | https://gitlab.gnome.org/GNOME/gdk-pixbuf | https://gitlab.gnome.org/GNOME/gdk-pixbuf/-/blob/master/COPYING |
| gemmi | https://gemmi.readthedocs.io/en/latest/ | https://github.com/project-gemmi/gemmi/blob/master/LICENSE.txt |
| genproto | https://google.golang.org/genproto/googleapis | https://github.com/googleapis/go-genproto/blob/main/LICENSE |
| geometric | https://openbase.com/python/geometric | https://openbase.com/python/geometric |
| giflib | https://giflib.sourceforge.net | https://github.com/mirrorer/giflib/blob/master/COPYING |
| gitdb | https://github.com/gitpython-developers/gitdb | https://github.com/gitpython-developers/gitdb/blob/master/LICENSE |
| GitPython | https://github.com/gitpython-developers/GitPython | https://github.com/gitpython-developers/GitPython/blob/main/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| glib | https://docs.gtk.org/glib/ | https://gitlab.gnome.org/GNOME/glib/-/blob/main/LICENSES/LGPL-2.1-or-later.txt |
| GLM Library | https://github.com/g-truc/glm | https://github.com/g-truc/glm/blob/master/manual.md#section0 |
| gls | https://github.com/jtolds/gls | https://github.com/jtolds/gls/blob/master/LICENSE |
| gmpy2 | https://github.com/aleaxit/gmpy | https://github.com/gmpy2/gmpy2/blob/master/COPYING.LESSER |
| go-cleanhttp | https://github.com/hashicorp/go-cleanhttp | https://github.com/hashicorp/go-cleanhttp/blob/master/LICENSE |
| go-connections | https://github.com/docker/go-connections | https://github.com/docker/go-connections/blob/master/LICENSE |
| go-cpio | https://github.com/cavaliercoder/go-cpio | https://github.com/cavaliercoder/go-cpio/blob/master/LICENSE |
| go-getter | https://github.com/hashicorp/go-getter | https://github.com/hashicorp/go-getter/blob/master/LICENSE |
| go-homedir | https://github.com/mitchellh/go-homedir | https://github.com/mitchellh/go-homedir/blob/master/LICENSE |
| go-ini | https://github.com/go-ini/ini | https://github.com/go-ini/ini/blob/master/LICENSE |
| go-jmespath | https://github.com/jmespath/go-jmespath | https://github.com/jmespath/go-jmespath/blob/master/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| go-junit-report | https://github.com/jstemmer/go-junit-report | https://github.com/jstemmer/go-junit-report/blob/master/LICENSE |
| go-netrc | https://github.com/bgentry/go-netrc/netrc | https://github.com/bgentry/go-netrc/blob/master/LICENSE |
| go-ole | https://github.com/go-ole/go-ole | https://github.com/go-ole/go-ole/blob/master/LICENSE |
| go-pg | https://github.com/go-pg/pg | https://github.com/go-pg/pg/blob/master/LICENSE |
| go-redis | https://github.com/go-redis/redis/v8 | https://github.com/go-redis/redis/blob/master/LICENSE |
| go-rendezvous | https://github.com/dgryski/go-rendezvous | https://github.com/dgryski/go-rendezvous/blob/master/LICENSE |
| go-safetemp | https://github.com/hashicorp/go-safetemp | https://github.com/hashicorp/go-safetemp/blob/master/LICENSE |
| go-sysconf | https://github.com/tklauser/go-sysconf | https://github.com/tklauser/go-sysconf/blob/master/LICENSE |
| go-testing-interface | https://github.com/mitchellh/go-testing-interface | https://github.com/mitchellh/go-testing-interface/blob/master/LICENSE |
| go-units | https://github.com/docker/go-units | https://github.com/docker/go-units/blob/master/LICENSE |
| go-version | https://github.com/hashicorp/go-version | https://github.com/hashicorp/go-version/blob/master/LICENSE |
| go-zglob | https://github.com/mattn/go-zglob | https://github.com/mattn/go-zglob/blob/master/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| go.opencensus | https://go.opencensus.io | https://github.com/census-instrumentatio opencensus-go/blob/master/LICENSE |
| gobrake.v2 | https://gopkg.in/airbrake/gobrake.v2 | https://github.com/airbrake/gobrake/blob/v2.0.9/LICENSE |
| goconvey | https://github.com/smartystreets/goconvey | https://github.com/smartystreets/goconvey/blob/master/LICENSE.md |
| golden-layout | https://github.com/deepstreamIO/golden-layout | https://github.com/deepstreamIO/golden-layout/raw/master/LICENSE |
| google-auth | https://google-auth.readthedocs.io/en/master/ | https://github.com/GoogleCloudPlatform google-auth-library-p blob/master/LICENSE |
| google-auth-oauthlib | https://github.com/googleapis/google-auth-library-p | https://github.com/googleapis/google-auth-library-p blob/main/LICENSE |
| google-cloud-go | https://cloud.google.com/go | https://github.com/googleapis/google-cloud-go/blob/main/LICENSE |
| google-cloud-go/storage | https://cloud.google.com/go/storage | https://github.com/googleapis/google-cloud-go/blob/main/LICENSE |
| google-pasta | https://github.com/google/pasta | https://github.com/google/pasta/blob/master/LICENSE |
| google.golang.org/api | https://google.golang.org/api | https://github.com/googleapis/google-api-go-client/blob/main/LICENSE |
| gopsutil | https://github.com/shirou/gopsutil | https://github.com/shirou/gopsutil/blob/master/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| gorilla websocket | https://github.com/gorilla/websocket | https://github.com/gorilla/websocket/blob/master/LICENSE |
| gpytorch | https://gpytorch.ai | https://github.com/cornellius-gp/gpytorch?tab=MIT-1-ov-file#readme |
| graphite2 | https://github.com/silnrsi/graphite | https://github.com/silnrsi/graphite/blob/master/LICENSE |
| graphviz | https://graphviz.org/ | https://graphviz.org/license/ |
| greenlet | https://greenlet.readthedocs.io/en/latest/ | https://github.com/python-greenlet/greenlet/blob/master/LICENSE |
| groupcache | https://github.com/golang/groupcache | https://github.com/golang/groupcache/blob/master/LICENSE |
| grpc | https://google.golang.org/grpc | https://github.com/grpc/grpc-go/blob/master/LICENSE |
| grpc-cpp | https://github.com/grpc/grpc | https://github.com/grpc/grpc/blob/master/LICENSE |
| grpcio | https://github.com/grpc/grpc.io/blob/main/LICENSE | https://github.com/grpc/grpc.io/blob/main/LICENSE |
| gtk2 | https://gitlab.gnome.org/GNOME/gtk | https://gitlab.gnome.org/GNOME/gtk/-/blob/main/COPYING |
| gts | https://sourceforge.net/projects/gts/ | https://www.gnu.org/licenses/lgpl-3.0.html |
| h11 | https://github.com/python-hyper/h11 | https://github.com/python-hyper/h11/blob/master/LICENSE.txt |
| h2 | https://github.com/python-hyper/h2 | https://github.com/python-hyper/h2?tab=MIT-1-ov-file#readme |

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| h5py | https://www.h5py.org | https://docs.h5py.org/en/stable/licenses.html |
| harfbuzz | https://github.com/harfbuzz/harfbuzz | https://github.com/harfbuzz/harfbuzz/blob/main/COPYING |
| hdbscan | https://hdbscan.readthedocs.io/en/latest/ | https://github.com/scikit-learn-contrib/hdbscan/blob/master/LICENSE |
| hdf4 | https://www.hdfgroup.org/solutions/hdf4/ | https://github.com/HDFGroup/hdf4/blob/master/COPYING |
| hdf5 | https://www.hdfgroup.org/solutions/hdf5/ | https://github.com/HDFGroup/hdf5/blob/master/COPYING |
| he | https://github.com/mathiasbynens/he | https://github.com/mathiasbynens/he/raw/master/LICENSE-MIT.txt |
| hpack | https://github.com/python-hyper/hpack | https://github.com/python-hyper/hpack?tab=MIT-1-ov-file#readme |
| html-loader | https://github.com/webpack-contrib/html-loader | https://github.com/webpack-contrib/html-loader/raw/master/LICENSE |
| html5lib | https://github.com/html5lib/html5lib-python | https://github.com/html5lib/html5lib-python/blob/master/LICENSE |
| htslib | https://www.htslib.org | https://github.com/samtools/htslib/blob/develop/LICENSE |
| httpcore | https://www.encode.io/httpcore/ | https://github.com/encode/httpcore/blob/master/LICENSE.md |
| httpx | https://github.com/encode/httpx | https://github.com/encode/httpx/blob/master/LICENSE.md |

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| Name of Project | Website | License URL |
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| humanize | https://github.com/jmoiron/humanize | https://github.com/jmoiron/humanize/blob/master/LICENCE |
| hydra-core | https://github.com/facebookresearch/hydra | https://github.com/facebookresearch/hydra/blob/main/LICENSE |
| hyperframe | https://github.com/python-hyper/hyperframe | https://github.com/python-hyper/hyperframe?tab=MIT-1-ov-file#readme |
| icu | https://github.com/unicode-org/icu | https://github.com/unicode-org/icu/blob/main/icu4c/LICENSE |
| idna | https://github.com/kjd/idna | https://github.com/kjd/idna/blob/master/LICENSE.md |
| ihm | https://github.com/ihmwg/python-ihm | https://github.com/ihmwg/python-ihm/blob/main/LICENSE |
| imageio | https://github.com/imageio/imageio | https://github.com/imageio/imageio/blob/master/LICENSE |
| imagesize | https://github.com/shibukawa/imagesize_py | https://github.com/shibukawa/imagesize_py/blob/master/LICENSE.rst |
| ImmuneBuilder | https://github.com/oxpig/ImmuneBuilder/tree/main | https://github.com/oxpig/ImmuneBuilder/blob/main/LICENSE |
| importlib-metadata | https://github.com/python/importlib_metadata | https://github.com/python/importlib_metadata/blob/main/LICENSE |
| importlib_metadata | https://github.com/python/importlib_metadata | https://github.com/python/importlib_metadata/blob/main/LICENSE |

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| Name of Project | Website | License URL |
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| importlib_resources | https://github.com/python/importlib_resources | https://github.com/python/importlib_resources/blob/main/LICENSE |
| InChI | https://iupac.org/who-we-are/divisions/division-details/inchi/ | https://iupac.org/wp-content/uploads/2021/06/iupac-inchi-license_2020.pdf |
| inflection | https://github.com/jinzhu/inflection | https://github.com/jinzhu/inflection/blob/master/LICENSE |
| ini.v1 | https://gopkg.in/ini.v1 | https://github.com/go-ini/ini/blob/v1.66.2/LICENSE |
| iniconfig | https://github.com/pytest-dev/iniconfig | https://github.com/pytest-dev/iniconfig/blob/main/LICENSE |
| innersvg-polyfill | https://github.com/dnozay/innersvg-polyfill | https://github.com/dnozay/innersvg-polyfill/raw/master/LICENSE |
| intel-openmp | https://github.com/hermitcore/libomp_oss | https://github.com/hermitcore/libomp_oss/blob/hermit/LICENSE.txt |
| ipykernel | https://ipython.org | https://ipython.org |
| ipython | https://ipython.org | https://github.com/ipython/ipython/blob/master/LICENSE |
| ipython-genutils | http://ipython.org | https://github.com/ipython/ipython_genutils/blob/master/COPYING.md |
| ipython_pygments_le | https://github.com/ipython/ipython-pygments-lex | https://github.com/ipython/ipython-pygments-lex blob/main/LICENSE |
| ipywidgets | http://jupyter.org | https://github.com/jupyter-widgets/ipywidgets/blob/main/LICENSE |

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| Name of Project | Website | License URL |
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| isodate | https://github.com/gweis/isodate/ | https://github.com/gweis/isodate/blob/master/LICENSE |
| isoduration | https://github.com/bolsote/isoduration | https://github.com/bolsote/isoduration?tab=ISC-1-ov-file#readme |
| itsdangerous | https://palletsprojects.com/p/itsdangerous/ | https://itsdangerous.palletsprojects.com/en/2.1.x/license/ |
| jax | https://github.com/google/jax | https://github.com/google/jax/blob/main/LICENSE |
| jaxlib | https://github.com/google/jax | https://github.com/google/jax/blob/main/LICENSE |
| jaxtyping | https://github.com/patrick-kidger/jaxtyping | https://github.com/patrick-kidger/jaxtyping?tab=License-1-ov-file#readme |
| jedi | https://jedi.readthedocs.io/en/latest/ | https://github.com/davidhalter/jedi/blob/master/LICENSE.txt |
| Jinja2 | https://palletsprojects.com/p/jinja/ | https://github.com/pallets/jinja/blob/main/LICENSE.rst |
| jmespath | https://github.com/jmespath/jmespath.py | https://github.com/jmespath/jmespath.py/blob/develop/LICENSE.txt |
| joblib | https://joblib.readthedocs.io/en/latest/ | https://github.com/joblib/joblib/blob/master/LICENSE.txt |
| jpeg | https://www.ijg.org | https://www.ijg.org/files/README |
| json5 | https://github.com/dpranke/pyjson5 | https://github.com/dpranke/pyjson5/blob/main/LICENSE |
| jsonfield | https://github.com/dmkoch/django-jsonfield/ | https://github.com/rpkilby/jsonfield/blob/master/LICENSE |

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| jsonpatch | https://github.com/stefankoegl/python-json-patch | https://github.com/stefankoegl/python-json-patch/blob/master/LICENSE |
| jsonpickle | https://github.com/jsonpickle/jsonpickle | https://github.com/jsonpickle/jsonpickle/blob/main/LICENSE |
| jsonpointer | https://github.com/stefankoegl/python-json-pointer | https://github.com/stefankoegl/python-json-pointer/blob/master/LICENSE.txt |
| jsonschema | https://github.com/python-jsonschema/jsonschema | https://github.com/python-jsonschema/jsonschema/blob/master/COPYING |
| jsonschema-specifications | https://github.com/python-jsonschema/jsonschema-specificat | https://github.com/python-jsonschema/jsonschema-specificat blob/main/COPYING |
| jstat | https://github.com/jstat/jstat | https://www.opensource.org/licenses/mit-license.php |
| jupyter-client | https://jupyter.org | https://github.com/jupyter/jupyter_client/blob/main/COPYING.md |
| jupyter-core | https://jupyter.org | https://github.com/jupyter/jupyter_core/blob/master/COPYING.md |
| jupyter-events | https://github.com/jupyter/jupyter_events | https://github.com/jupyter/jupyter_events/blob/main/LICENSE |
| jupyter-lsp | https://github.com/jupyter-lsp/jupyterlab-lsp | https://github.com/jupyter-lsp/jupyterlab-lsp |
| jupyter-serverhttp://jupyter.or | https://github.com/jupyter-server/jupyter_server/blob/main/LICENSE | |
| jupyter_client | http://jupyter.org | https://github.com/jupyter/jupyter_client/blob/main/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| jupyter_core | http://jupyter.org | https://github.com/jupyter/jupyter_core/blob/master/LICENSE |
| jupyter_server | https://github.com/jupyter-server/jupyter_server | https://github.com/jupyter-server/jupyter_server/blob/main/LICENSE |
| jupyter_server_termin | https://github.com/jupyter-server/jupyter_server_terminals | https://github.com/jupyter-server/jupyter_server_terminals/blob/main/LICENSE |
| jupyterlab | https://github.com/jupyterlab/jupyterlab | https://github.com/jupyterlab/jupyterlab/blob/main/LICENSE |
| jupyterlab-pygments | http://jupyter.org | https://github.com/jupyterlab/jupyterlab_pygments/blob/main/LICENSE |
| jupyterlab-widgets | http://jupyter.org | https://github.com/jupyter-widgets/ipywidgets/blob/master/LICENSE |
| jupyter-lab_pygments | https://github.com/jupyterlab/jupyterlab_pygments | https://github.com/jupyterlab/jupyterlab_pygments?tab=BSD-3-Clause-1-ov-file#readme |
| jupyterlab_server | https://github.com/jupyterlab/jupyterlab_server | https://github.com/jupyterlab/jupyterlab_server/blob/main/LICENSE |
| jupyterlab_widgets | https://github.com/jupyter-widgets/ipywidgets | https://github.com/jupyter-widgets/ipywidgets?tab=BSD-3-Clause-1-ov-file#readme |
| kaleido | https://github.com/plotly/Kaleido | https://github.com/plotly/Kaleido/blob/master/LICENSE.txt |
| keras | https://github.com/keras-team/keras | https://github.com/keras-team/keras/blob/master/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| Keras-Preprocessing | https://github.com/keras-team/keras-preprocessing | https://github.com/keras-team/keras-preprocessing/blob/master/LICENSE |
| keras-tuner | https://github.com/keras-team/keras-tuner | https://github.com/keras-team/keras-tuner/blob/master/LICENSE |
| keyring | https://github.com/jaraco/keyring | https://github.com/jaraco/keyring/blob/main/LICENSE |
| keyutils | https://github.com/sassoftware/python-keyutils | https://github.com/sassoftware/python-keyutils/blob/master/LICENSE |
| kiwisolver | https://kiwisolver.readthedocs.io/en/latest/ | https://github.com/nucleic/kiwi/blob/main/LICENSE |
| kombu | https://kombu.readthedocs.io | https://github.com/celery/kombu/blob/master/LICENSE |
| krb5 | https://web.mit.edu/kerberos/ | https://github.com/krb5/krb5/blob/master/src/lib/gssapi/LICENSE |
| kt-legacy | https://github.com/haifeng-jin/kt-legacy | https://github.com/haifeng-jin/kt-legacy/blob/main/LICENSE |
| lark | https://github.com/lark-parser/lark | https://github.com/lark-parser/lark?tab=MIT-1-ov-file#readme |
| lazy_loader | https://github.com/scientific-python/lazy_loader | https://github.com/scientific-python/lazy_loader/blob/main/LICENSE.md |
| lcms2 | https://www.littlecms.com | https://github.com/sk1project/python-lcms2/blob/master/LICENSE |
| legacy-cgi | https://github.com/jackrosenthal/legacy-cgi | https://github.com/jackrosenthal/legacy-cgi?tab=License-1-ov-file#readme |

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| lerc | https://github.com/Esri/lerc | https://github.com/Esri/lerc/blob/master/LICENSE |
| libarchive | http://www.libarchive.org | https://raw.githubusercontent.com/libarchive/libarchive/master/COPYING |
| libblas | https://www.netlib.org/blas/ | https://www.netlib.org/blas/#_licensing |
| libbrotlicommon | https://github.com/google/brotli | https://github.com/google/brotli/blob/master/LICENSE |
| libbrotlidec | https://github.com/google/brotli | https://github.com/google/brotli/blob/master/LICENSE |
| libbrotlienc | https://github.com/google/brotli | https://github.com/google/brotli/blob/master/LICENSE |
| libcblas | https://anaconda.org/conda-forge/libcblas | N/A |
| libclang | https://github.com/sighingnow/libclang | https://github.com/sighingnow/libclang/blob/master/LICENSE.TXT |
| libcurl | https://curl.se/libcurl/ | https://curl.se/docs/copyright.html |
| libcxx | https://github.com/llvm-mirror/libcxx | https://github.com/llvm-mirror/libcxx/blob/master/LICENSE.TXT |
| libdb | https://www.oracle.com/technology/software/products/berkeley-db/index.html | https://github.com/berkeleydb/libdb/blob/master/LEGAL |
| libdeflate | https://github.com/ebiggers/libdeflate | https://github.com/ebiggers/libdeflate/blob/master/COPYING |
| libedit | https://thrysoee.dk/editline/ | http://www.netbsd.org/Goals/redistribution.html |
| libev | https://software.schmorp.de/pkg/libev.html | https://software.schmorp.de/pkg/libev.html |

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| libexpat | https://libexpat.github.io/ | https://github.com/libexpat/libexpat?tab=MIT-1-ov-file#readme |
| libffi | https://github.com/libffi/libffi | https://github.com/libffi/libffi/blob/master/LICENSE |
| libgcc | https://gcc.gnu.org/onlinedocs/gccint/Libgcc.html | https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html |
| libgcrypt | https://gnupg.org/software/index.html | https://git.gnupg.org/cgi-bin/gitweb.cgi?p=libgcrypt.git;a=blob;f=COPYING.LIB;hb=HEAD |
| libgd | https://libgd.github.io | https://libgd.github.io/manuals/2.2.1/files/license-txt.html |
| libglib | https://github.com/PolMine/libglib | https://github.com/PolMine/libglib/blob/master/include/glib-2.0/glib.h |
| libiconv | https://www.gnu.org/software/libiconv/ | https://www.gnu.org/software/libiconv/#downloading |
| libint | https://tinyurl.com/yvw97wbw | https://tinyurl.com/yvw97wbw |
| liblapack | http://www.netlib.org/lapack/ | https://www.netlib.org/lapack/LICENSE.txt |
| liblapacke | https://anaconda.org/conda-forge/liblapacke | https://www.netlib.org/lapack/LICENSE.txt |
| liblzma | https://tukaani.org/xz/ | https://git.tukaani.org/?p=xz.git;a=blob;f=COPYING.0BSD |
| libmamba | https://medium.com/@QuantStack/open-software-packag | https://github.com/mamba-org/mamba/blob/main/LICENSE |

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| libmambapy | https://www.anaconda.com/blog/a-faster-conda-for-a-g | https://github.com/conda/conda-libmamba-solv blob/main/LICENSE |
| libnetcdf | https://www.unidata.ucar.edu/software/netcdf/ | https://www.unidata.ucar.edu/software/netcdf/copyright.html |
| libnghttp2 | https://github.com/nghttp2/nghttp2 | https://github.com/nghttp2/nghttp2/blob/master/COPYING |
| libnsl | https://github.com/thkukuk/libnsl | https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html |
| libopenblas | https://www.openblas.net/ | https://github.com/xianyi/OpenBLAS/blob/develop/LICENSE |
| libpng | https://www.libpng.org/pub/png/libpng.html | https://www.libpng.org/pub/png/src/libpng-LICENSE.txt |
| libpq | https://www.postgresql.org/ | https://www.postgresql.org/about/licence/ |
| librsvg | https://gitlab.gnome.org/GNOME/librsvg | https://gitlab.gnome.org/GNOME/librsvg/-/blob/main/COPYING.LIB |
| libsolv | https://github.com/openSUSE/libsolv | https://github.com/openSUSE/libsolv/blob/master/LICENSE.BSD |
| libsqlite | https://github.com/mackyle/sqlite | https://github.com/mackyle/sqlite?tab=License-1-ov-file#readme |
| libssh2 | https://github.com/libssh2/libssh2 | https://github.com/libssh2/libssh2/blob/master/COPYING |
| libstdcxx | https://gcc.gnu.org/ | https://gcc.gnu.org/onlinedocs/libstdc++/manual/license.html |

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| libtiff | https://www.libtiff.org/ | https://www.libtiff.org/misc.html |
| libtrust | https://github.com/docker/libtrust | https://github.com/docker/libtrust/blob/master/LICENSE |
| libuuid | https://sourceforge.net/projects/libuuid/ | https://sourceforge.net/p/libuuid/code/ci/master/tree/COPYING |
| libuv | https://github.com/libuv/libuv | https://github.com/libuv/libuv/blob/v1.x/LICENSE |
| libwebp | https://chromium.googlesource.com/?format=HTML | https://chromium.googlesource.com/chromium/src/third_party/+/refs/heads/main/libwebp/LICENSE |
| libwebp-base | https://chromium.googlesource.com/?format=HTML | https://chromium.googlesource.com/chromium/src/third_party/+/refs/heads/main/libwebp/LICENSE |
| libxc | https://www.tddft.org/programs/libxc/ | https://gitlab.com/libxc/libxc/-/blob/master/COPYING |
| libxcb | https://xcb.freedesktop.org | https://github.com/freedesktop/xcb-libxcb/blob/master/COPYING |
| libxcrypt | https://github.com/besser82/libxcrypt | https://github.com/besser82/libxcrypt?tab=LGPL-2.1-1-ov-file#readme |
| libxml2 | https://git.gnome.org/browse/libxml2/ | https://gitlab.gnome.org/GNOME/libxml2/-/blob/master/Copyright |
| libxmlsec1 | https://github.com/lsh123/xmlsec | https://github.com/lsh123/xmlsec/blob/master/README |
| libxslt | https://gitlab.gnome.org/GNOME/libxslt/-/wikis/home | https://gitlab.gnome.org/GNOME/libxslt/-/blob/master/Copyright |

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| libzlib | https://zlib.net | https://zlib.net/zlib_license.html |
| lightning-utilities | https://github.com/Lightning-AI/utilities | https://github.com/Lightning-AI/utilities?tab=Apache-2.0-1-ov-file#readme |
| lime | https://github.com/marcotcr/lime | https://github.com/marcotcr/lime/blob/master/LICENSE |
| linear-operator | https://github.com/cornellius-gp/linear_operator | https://github.com/cornellius-gp/linear_operator?tab=MIT-1-ov-file#readme |
| lit | http://llvm.org | https://releases.llvm.org/14.0.0/LICENSE.TXT |
| llvm-openmp | https://github.com/llvm-mirror/openmp | https://github.com/llvm-mirror/openmp/blob/master/LICENSE.txt |
| llvmlite | http://llvmlite.readthedocs.io | https://github.com/numba/llvmlite/blob/main/LICENSE |
| loader-utils | https://github.com/webpack/loader-utils | https://github.com/webpack/loader-utils/raw/master/LICENSE |
| logistro | https://github.com/geopozo/logistro | https://github.com/geopozo/logistro?tab=MIT-1-ov-file#readme |
| logomaker | https://logomaker.readthedocs.io/en/latest/ | https://github.com/jbkinney/logomaker/blob/master/LICENSE |
| logrus | https://github.com/sirupsen/logrus | https://github.com/sirupsen/logrus/blob/master/LICENSE |
| logrus-airbrake-hook.v2 | https://gopkg.in/gemnasium/logrus-airbrake-hook.v2 | https://github.com/gemnasium/logrus-airbrake-hook/blob/v2.1.2/LICENSE |
| lxml | https://lxml.de | https://lxml.de/index.html#license |

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| lz4-c | https://www.lz4.org/ | https://github.com/lz4/lz4/blob/dev/LICENSE |
| lzo | https://www.oberhumer.com/opensource/lzo/ | https://www.oberhumer.com/opensource/gpl.html |
| mamba | https://github.com/mamba-org/mamba | https://github.com/mamba-org/mamba?tab=BSD-3-Clause-1-ov-f readme |
| markdown | https://github.com/evilstreak/markdown-js | https://www.opensource.org/licenses/mit-license.php |
| markdown-it-py | https://github.com/executablebooks/markdown-it-py | https://github.com/executablebooks/markdown-it-py/blob/master/LICENSE |
| markupsafe | https://github.com/pallets/markupsafe/tree/main/src/markupsafe | https://github.com/pallets/markupsafe/tree/main?tab=BSD-3-Clause-1-ov-f |
| MarkupSafe | https://palletsprojects.com/p/markupsafe/ | https://github.com/pallets/markupsafe/blob/main/LICENSE.rst |
| mashumaro | https://github.com/Fatal1ty/mashumaro | https://github.com/Fatal1ty/mashumaro |
| matplotlib | https://matplotlib.org | https://matplotlib.org/stable/users/project/license.html |
| matplotlib-base | https://matplotlib.org | https://matplotlib.org/stable/users/project/license.html |
| matplotlib-inline | https://github.com/ipython/matplotlib-inline | https://github.com/ipython/matplotlib-inline/blob/master/LICENSE |
| mda-xdrlib | https://github.com/MDAnalysis/mda-xdrlib | https://github.com/MDAnalysis/mda-xdrlib/blob/main/LICENSE |

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| mda_xdrlib | https://github.com/MDAnalysis/mda-xdrlib | https://github.com/MDAnalysis/mda-xdrlib?tab=License-1-ov-file#readme |
| mdtraj | https://www.mdtraj.org/ | https://www.mdtraj.org/1.9.8.dev0/index.html#license |
| mdurl | https://github.com/markdown-it/mdurl | https://github.com/markdown-it/mdurl/blob/master/LICENSE |
| menuinst | https://github.com/conda/menuinst | https://github.com/conda/menuinst/blob/main/LICENSE.txt |
| mergo | https://github.com/imdario/mergo | https://github.com/imdario/mergo/blob/master/LICENSE |
| mistune | https://github.com/lepture/mistune | https://github.com/lepture/mistune/blob/master/LICENSE |
| mkl | https://github.com/rust-math/intel-mkl-src | https://github.com/rust-math/intel-mkl-src/blob/master/License.txt |
| mkl-fft | https://github.com/IntelPython/mkl_fft | https://github.com/IntelPython/mkl_fft/blob/master/LICENSE.txt |
| mkl-random | https://github.com/IntelPython/mkl_random | https://github.com/IntelPython/mkl_random/blob/master/LICENSE.txt |
| mkl-service | https://github.com/IntelPython/mkl-service | https://github.com/IntelPython/mkl-service/blob/master/LICENSE.txt |
| mkl_fft | http://github.com/IntelPython/mkl_fft | https://github.com/IntelPython/mkl_fft?tab=BSD-3-Clause-1-ov-f readme |

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| Name of Project | Website | License URL |
|---|---|---|
| mkl_random | http://github.com/IntelPython/mkl_random | https://github.com/IntelPython/mkl_random?tab=BSD-3-Clause-1-ov-f readme |
| ml-dtypes | https://github.com/jax-ml/ml_dtypes | https://github.com/jax-ml/ml_dtypes/blob/main/LICENSE |
| ml_dtypes | https://github.com/jax-ml/ml_dtypes | https://github.com/jax-ml/ml_dtypes/blob/main/LICENSE |
| modelcif | https://github.com/ihmwg/python-modelcif | https://github.com/ihmwg/python-modelcif/blob/main/LICENSE |
| molecupy | https://molecupy.readthedocs.io/en/latest/ | https://github.com/samirelanduk/atomium/blob/master/LICENSE |
| moment | https://github.com/moment/moment | https://github.com/moment/moment/raw/master/LICENSE |
| moment-precise-range-plugin | https://github.com/codebox/moment-precise-rang | https://github.com/codebox/moment-precise-rang raw/master/LICENSE.md |
| more-itertools | https://github.com/more-itertools/more-itertools | https://github.com/more-itertools/more-itertools/blob/master/LICENSE |
| mpiplus | https://github.com/choderalab/mpiplus | https://github.com/choderalab/mpiplus/blob/main/LICENSE |
| mpmath | http://mpmath.org/ | https://github.com/mpmath/mpmath/blob/master/LICENSE |
| mrcfile | https://github.com/ccpem/mrcfile | https://github.com/ccpem/mrcfile/blob/master/LICENSE.txt |

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| Name of Project | Website | License URL |
|---|---|---|
| msgpack | https://msgpack.org/ | https://github.com/msgpack/msgpack-python/blob/main/COPYING |
| multidict | https://github.com/aio-libs/multidict | https://github.com/aio-libs/multidict/blob/master/LICENSE |
| multierr | https://go.uber.org/multierr | https://github.com/uber-go/multierr/blob/master/LICENSE.txt |
| multiprocess | https://github.com/uqfoundation/multiprocess | https://github.com/uqfoundation/multiprocess/blob/master/LICENSE |
| munkres | https://software.clapper.org/munkres/ | https://github.com/bmc/munkres/blob/master/LICENSE.md |
| myesui uuid | https://github.com/myesui/uuid | https://pkg.go.dev/github.com/myesui/uuid?tab=licenses |
| namex | https://github.com/bcgov/namex | https://github.com/bcgov/namex/blob/main/LICENSE |
| narwhals | https://github.com/narwhals-dev/narwhals | https://github.com/narwhals-dev/narwhals?tab=MIT-1-ov-file#readme |
| nbclassic | http://jupyter.org | https://github.com/jupyter/nbclassic/blob/main/LICENSE |
| nbclient | https://jupyter.org | https://github.com/jupyter/nbclient/blob/main/LICENSE |
| nbconvert | https://jupyter.org | https://github.com/jupyter/nbconvert/blob/main/LICENSE |
| nbformat | http://jupyter.org | https://github.com/jupyter/nbformat/blob/main/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| ncurses | https://invisible-island.net/ncurses/ | https://invisible-island.net/ncurses/ncurses-license.html |
| ndfes | https://rutgerslbsr.gitlab.io/fe-toolkit/ | https://gitlab.com/RutgersLBSR/fe-toolkit/-/blob/master/LICENSE |
| ndindex | https://quansight-labs.github.io/ndindex/ | https://github.com/Quansight-Labs/ndindex?tab=MIT-1-ov-file#readme |
| nest-asyncio | https://github.com/erdewit/nest_asyncio | https://github.com/erdewit/nest_asyncio/blob/master/LICENSE |
| nest_asyncio | https://github.com/erdewit/nest_asyncio | https://github.com/erdewit/nest_asyncio?tab=BSD-2-Clause-1-ov-f readme |
| netcdf-fortran | https://www.unidata.ucar.edu/software/netcdf/ | https://www.unidata.ucar.edu/software/netcdf/copyright.html |
| netCDF4 | http://github.com/Unidata/netcdf4-python | https://github.com/Unidata/netcdf4-python/blob/master/LICENSE |
| nettle | https://git.lysator.liu.se/nettle/nettle | https://git.lysator.liu.se/nettle/nettle/-/blob/master/AUTHORS?ref_type=heads |
| networkx | https://networkx.org | https://github.com/networkx/networkx/blob/main/LICENSE.txt |
| nfpm | https://github.com/goreleaser/nfpm | https://github.com/goreleaser/nfpm/blob/master/LICENSE.md |
| ng-tags-input | https://github.com/mbenford/ngTagsInput | https://github.com/mbenford/ngTagsInput |
| ng-toast | https://github.com/tameraydin/ngToast | https://github.com/tameraydin/ngToast |

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| Name of Project | Website | License URL |
|---|---|---|
| ngdraggable | https://github.com/fatlinesofcode/ngDraggable | https://github.com/fatlinesofcode/ngDraggable/raw/master/LICENSE.txt |
| ngVue | https://github.com/ngVue/ngVue | https://github.com/ngVue/ngVue/raw/master/LICENSE |
| nh3 | https://nh3.readthedocs.io/en/latest/ | https://github.com/messense/nh3/blob/main/LICENSE |
| nlohmann_json | https://github.com/nlohmann/json | https://github.com/nlohmann/json?tab=MIT-1-ov-file#readme |
| nlopt | https://nlopt.readthedocs.io/en/latest/NLopt_Python_Reference/ | https://nlopt.readthedocs.io/en/latest/NLopt_License_and_Copyright/ |
| nodejs | https://nodejs.org/en/ | https://raw.githubusercontent.com/nodejs/node/master/LICENSE |
| nomkl | https://github.com/conda-forge/nomkl-feedstock | https://github.com/conda-forge/nomkl-feedstock/blob/main/LICENSE.txt |
| notebook | http://jupyter.org | https://github.com/jupyter/notebook/blob/main/LICENSE |
| notebook-shim | https://github.com/jupyter/notebook_shim | https://github.com/jupyter/notebook_shim |
| notebook_shim | http://jupyter.org | https://github.com/jupyter/notebook_shim/blob/main/LICENSE |
| numba | https://numba.pydata.org | https://github.com/numba/numba/blob/main/LICENSE |
| numcpus | https://github.com/tklauser/numcpus | https://github.com/tklauser/numcpus/blob/master/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| numexpr | https://github.com/pydata/numexpr | https://github.com/pydata/numexpr/blob/master/LICENSE.txt |
| numpy | https://numpy.org | https://github.com/numpy/numpy/blob/main/LICENSE.txt |
| numpy-base | https://numpy.org | https://github.com/numpy/numpy/blob/main/LICENSE.txt |
| numpydoc | https://numpydoc.readthedocs.io/en/latest/index.html | https://github.com/numpy/numpydoc/blob/main/LICENSE.txt |
| nvidia-cublas-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cublas-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cuda-cupti-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cuda-cupti-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cuda-nvrtc-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cuda-nvrtc-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cuda-runtime-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cuda-runtime-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cudnn-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/deeplearning/cudnn/sla/index.html |
| nvidia-cudnn-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/deeplearning/cudnn/sla/index.html |

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| Name of Project | Website | License URL |
|---|---|---|
| nvidia-cuEquivariance | https://github.com/NVIDIA/cuEquivariance | https://github.com/NVIDIA/cuEquivariance/blob/main/LICENSES/LICENSE |
| nvidia-cufft-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cufft-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cufile-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html# |
| nvidia-curand-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-curand-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cusolver-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cusolver-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cusparse-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cusparse-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-cusparselt-cu12 | https://docs.nvidia.com/cuda/cusparselt/index.html | https://docs.nvidia.com/cuda/cusparselt/license.html |
| nvidia-ml-py | https://pypi.org/project/nvidia-ml-py/ | https://pypi.org/project/nvidia-ml-py/ |
| nvidia-nccl-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/hpc-sdk/eula/index.html |
| nvidia-nccl-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/hpc-sdk/eula/index.html |
| nvidia-nvjitlink-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |

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| Name of Project | Website | License URL |
|---|---|---|
| nvidia-nvshmem-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-nvtx-cu11 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| nvidia-nvtx-cu12 | https://developer.nvidia.com/cuda-zone | https://docs.nvidia.com/cuda/eula/index.html |
| Oat++ | https://oatpp.io/ | https://github.com/oatpp/oatpp/blob/master/LICENSE |
| oauthlib | https://github.com/oauthlib/oauthlib | https://github.com/oauthlib/oauthlib/blob/master/LICENSE |
| ocl-icd | https://github.com/OCL-dev/ocl-icd | https://github.com/OCL-dev/ocl-icd/blob/master/COPYING |
| ocl-icd-system | https://github.com/conda-forge/ocl-icd-system-feedst | https://github.com/conda-forge/ocl-icd-system-feedst blob/main/LICENSE.txt |
| olefile | https://www.decalage.info/python/olefileio | https://olefile.readthedocs.io/en/latest/License.html |
| omegaconf | https://github.com/omry/omegaconf | https://github.com/omry/omegaconf/blob/master/LICENSE |
| OmegaFold | https://github.com/HeliXonProtein/OmegaFold/tree/main | https://github.com/HeliXonProtein/OmegaFold/blob/main/LICENSE |
| omnicanvas | https://omnicanvas.readthedocs.io/en/latest/ | https://github.com/samirelanduk/omnicanvas/blob/master/LICENSE |
| OpenFF | https://openforcefield.org/ | https://github.com/openforcefield/openff-forcefields |
| openff-amber-ff-ports | https://github.com/openforcefield/openff-amber-ff-ports | https://github.com/openforcefield/openff-amber-ff-ports blob/main/LICENSE |

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| Name of Project | Website | License URL |
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| openff-forcefields | https://openforcefield.org | https://github.com/openforcefield/openff-forcefields/blob/master/LICENSE |
| openff-fragmenter | https://github.com/openforcefield/openff-fragmenter | https://github.com/openforcefield/openff-fragmenter/blob/main/LICENSE |
| openff-interchange | https://github.com/openforcefield/openff-interchange | https://github.com/openforcefield/openff-interchange/blob/main/LICENSE |
| openff-models | https://github.com/openforcefield/openff-models | https://github.com/openforcefield/openff-models/blob/main/LICENSE |
| openff-nagl | https://docs.openforcefield.org/projects/nagl/en/latest/?badge=latest | https://github.com/openforcefield/openff-nagl/blob/main/LICENSE |
| openff-nagl-models | https://github.com/openforcefield/openff-nagl-models | https://github.com/openforcefield/openff-nagl-models/blob/main/LICENSE |
| openff-toolkit | https://openforcefield.org | https://github.com/openforcefield/openff-toolkit/blob/master/LICENSE |
| openff-toolkit-base | https://openforcefield.org | https://github.com/openforcefield/openff-toolkit/blob/master/LICENSE |
| openff-units | https://github.com/openforcefield/openff-units | https://github.com/openforcefield/openff-units/blob/main/LICENSE |
| openff-utilities | https://github.com/openforcefield/openff-utilities | https://github.com/openforcefield/openff-utilities/blob/main/LICENSE |
| openjpeg | https://github.com/uclouvain/openjpeg | https://github.com/uclouvain/openjpeg/blob/master/LICENSE |

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| openldap | https://www.openldap.org/software/repo.html | https://git.openldap.org/openldap/openldap/-/blob/master/LICENSE |
| OpenMM | https://openmm.org | https://docs.openmm.org/7.1.0/userguide/library.html#license |
| openmmtools | https://github.com/choderalab/openmmtools | https://github.com/choderalab/openmmtools/blob/main/LICENSE |
| openmoltools | https://github.com/choderalab/openmoltools | https://github.com/choderalab/openmoltools/blob/master/LICENSE |
| openpyxl | https://openpyxl.readthedocs.io/en/stable/ | https://foss.heptapod.net/openpyxl/openpyxl/-/blob/branch/3.0/LICENCE.rst |
| openssl | https://www.openssl.org | https://github.com/openssl/openssl/blob/master/LICENSE.txt |
| opt-einsum | https://github.com/dgasmith/opt_einsum | https://github.com/dgasmith/opt_einsum/blob/master/LICENSE |
| opt_einsum | https://github.com/dgasmith/opt_einsum | https://github.com/dgasmith/opt_einsum/blob/main/LICENSE |
| OptKing | https://github.com/psi-rking/optking | https://github.com/psi-rking/optking/blob/master/LICENSE |
| optree | https://optree.readthedocs.io/en/latest/ | https://github.com/metaopt/optree/blob/main/LICENSE |
| oscrypto | https://github.com/wbond/oscrypto | https://github.com/wbond/oscrypto/blob/master/LICENSE |
| overrides | https://github.com/mkorpela/overrides | https://github.com/mkorpela/overrides/blob/main/LICENSE |

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| packaging | https://github.com/pypa/packaging | https://github.com/pypa/packaging/blob/main/LICENSE |
| packmol | https://leandro.iqm.unicamp.br/m3g/packmol/home.shtml | https://github.com/m3g/packmol/blob/master/LICENSE |
| packmol_memgen | http://cpclab.uni-duesseldorf.de/ | https://gitlab.com/cbjh/memgen/py-memgen/-/blob/main/LICENSE |
| pandas | https://pandas.pydata.org | https://github.com/pandas-dev/pandas/blob/main/LICENSE |
| pandocfilters | http://github.com/jgm/pandocfilters | https://github.com/jgm/pandocfilters/blob/master/LICENSE |
| panedr | https://github.com/MDAnalysis/panedr | https://github.com/MDAnalysis/panedr/blob/master/LICENSE.txt |
| pango | https://pango.gnome.org | https://gitlab.gnome.org/GNOME/pango/-/blob/main/COPYING |
| ParmEd | https://parmed.github.io/ParmEd/html/index.html | https://github.com/ParmEd/ParmEd#license |
| parser | https://github.com/typescript-eslint/typescript-eslint | https://github.com/typescript-eslint/typescript-eslint/raw/master/LICENSE |
| parso | https://parso.readthedocs.io/en/latest/ | https://github.com/davidhalter/parso/blob/master/LICENSE.txt |
| pathos | https://github.com/uqfoundation/pathos | https://github.com/uqfoundation/pathos/blob/master/LICENSE |
| patsy | https://patsy.readthedocs.io/en/latest/ | https://github.com/pydata/patsy/blob/master/LICENSE.txt |

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| pbkdf2 | https://golang.org/x/crypto/pbkdf2 | https://cs.opensource.google/go/x/crypto/+/master:LICENSE |
| pbr | https://docs.openstack.org/pbr/latest/ | https://opendev.org/openstack/pbr/src/branch/master/LICENSE |
| pcmsolver | https://pcmsolver.readthedocs.io/en/stable/ | https://github.com/PCMSolver/pcmsolver/blob/master/LICENSE |
| pcre | https://www.pcre.org | https://www.pcre.org/licence.txt |
| pcre2 | https://www.pcre.org | https://github.com/PCRE2Project/pcre2/blob/master/LICENCE |
| pdb4amber | https://github.com/Amber-MD/pdb4amber | https://github.com/Amber-MD/pdb4amber/blob/master/LICENSE |
| pdbfixer | https://github.com/openmm/pdbfixer | https://github.com/openmm/pdbfixer/blob/master/LICENSE |
| pexpect | https://pexpect.readthedocs.io/ | https://github.com/pexpect/pexpect/blob/master/LICENSE |
| pgconn | https://github.com/jackc/pgconn | https://github.com/jackc/pgconn/blob/master/LICENSE |
| pgio | https://github.com/jackc/pgio | https://github.com/jackc/pgio/blob/master/LICENSE |
| pgpassfile | https://github.com/jackc/pgpassfile | https://github.com/jackc/pgpassfile/blob/master/LICENSE |
| pgproto3 | https://github.com/jackc/pgproto3/v2 | https://github.com/jackc/pgproto3/blob/master/LICENSE |
| pgtype | https://github.com/jackc/pgtype | https://github.com/jackc/pgtype/blob/master/LICENSE |
| pgx | https://github.com/jackc/pgx/v4 | https://github.com/jackc/pgx/blob/v4.0.1/LICENSE |

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| Name of Project | Website | License URL |
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| phonopy | https://github.com/phonopy/phono3py | https://github.com/phonopy/phono3py/blob/develop/LICENSE |
| pickleshare | https://github.com/pickleshare/pickleshare | https://github.com/pickleshare/pickleshare/blob/master/LICENSE |
| Pillow | https://python-pillow.org | https://github.com/python-pillow/Pillow/blob/main/LICENSE |
| Pint | https://pint.readthedocs.io/en/stable/ | https://github.com/hgrecco/pint/blob/master/LICENSE |
| pip | https://pip.pypa.io/ | https://github.com/pypa/pip/blob/main/LICENSE.txt |
| pip-licenses | https://github.com/raimon49/pip-licenses | https://github.com/raimon49/pip-licenses/blob/master/LICENSE |
| pixman | https://pixman.org | https://cgit.freedesktop.org/pixman/tree/COPYING |
| pkginfo | https://launchpad.net/pkginfo | https://bazaar.launchpad.net/~tseaver/pkginfo/trunk/view/head:/LICENSE.txt |
| pkgutil-resolve-name | https://github.com/graingert/pkgutil-resolve-name | https://github.com/graingert/pkgutil-resolve-name?tab=License-1-ov-file#readme |
| pkgutil_resolve_name | https://github.com/graingert/pkgutil-resolve-name | https://github.com/graingert/pkgutil-resolve-name?tab=License-1-ov-file#readme |
| platformdirs | https://github.com/platformdirs/platformdirs | https://github.com/platformdirs/platformdirs/blob/main/LICENSE |

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| Name of Project | Website | License URL |
|---|---|---|
| plotly | https://plotly.com/python/ | https://github.com/plotly/plotly.py/blob/master/LICENSE.txt |
| plotly-orca | https://github.com/plotly/orca | https://github.com/plotly/orca/blob/master/LICENSE |
| plotly.js | https://github.com/plotly/plotly.js | https://github.com/plotly/plotly.js/raw/master/LICENSE |
| pluggy | https://pluggy.readthedocs.io/en/stable/index.html | https://github.com/pytest-dev/pluggy/blob/main/LICENSE |
| pooch | https://github.com/fatiando/pooch | https://github.com/fatiando/pooch/blob/main/LICENSE.txt |
| portalocker | https://github.com/WoLpH/portalocker | https://github.com/wolph/portalocker/blob/develop/LICENSE |
| pox | https://github.com/uqfoundation/pox | https://github.com/uqfoundation/pox/blob/master/LICENSE |
| ppft | https://github.com/uqfoundation/ppft | https://github.com/uqfoundation/ppft/blob/master/LICENSE |
| pq | https://github.com/lib/pq | https://github.com/lib/pq/blob/master/LICENSE.md |
| ProDy | http://www.csb.pitt.edu/ProDy | https://github.com/prody/ProDy/blob/master/LICENSE.rst |
| prometheus-client | https://github.com/prometheus/client_python | https://github.com/prometheus/client_python/blob/master/LICENSE |
| prometheus_client | https://github.com/prometheus/client_python | https://github.com/prometheus/client_python/blob/master/LICENSE |
| prompt-toolkit | https://python-prompt-toolkit.readthedocs.io/en/stable/ | https://github.com/prompt-toolkit/python-prompt-toolkit/blob/master/LICENSE |

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|---|---|---|
| prompt_toolkit | https://github.com/prompt-toolkit/python-prompt-toolki | https://github.com/prompt-toolkit/python-prompt-toolki tab=BSD-3-Clause-1-ov-f readme |
| propcache | https://github.com/aio-libs/propcache | https://github.com/aio-libs/propcache?tab=Apache-2.0-1-ov-file#readme |
| protobuf | https://google.golang.org/protobuf | https://github.com/protocolbuffers/protobuf-go/blob/master/LICENSE |
| psi4 | https://psicode.org | https://github.com/psi4/psi4/blob/master/COPYING.LESSER |
| psutil | https://psutil.readthedocs.io/en/latest/ | https://github.com/giampaolo/psutil/blob/master/LICENSE |
| psycopg2 | https://psycopg.org/ | https://github.com/psycopg/psycopg2/blob/master/LICENSE |
| PTable | https://github.com/kxxoling/PTable | https://github.com/kxxoling/PTable/blob/master/COPYING |
| pthread-stubs | https://xcb.freedesktop.org | https://github.com/freedesktop/xcb-pthread-stubs/blob/master/COPYING |
| ptyprocess | https://ptyprocess.readthedocs.io/en/latest/ | https://github.com/pexpect/ptyprocess/blob/master/LICENSE |
| pure-eval | http://github.com/alexmojaki/pure_eval | http://github.com/alexmojaki/pure_eval/blob/master/LICENSE.txt |
| pure_eval | http://github.com/alexmojaki/pure_eval | https://github.com/alexmojaki/pure_eval?tab=MIT-1-ov-file#readme |

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| py | https://py.readthedocs.io/en/latest/ | https://github.com/pytest-dev/py/blob/master/LICENSE |
| py-cpuinfo | https://github.com/workhorsy/py-cpuinfo | https://github.com/workhorsy/py-cpuinfo/blob/master/LICENSE |
| pyasn1 | https://github.com/etingof/pyasn1 | https://github.com/etingof/pyasn1/blob/master/LICENSE.rst |
| pyasn1-modules | https://github.com/etingof/pyasn1-modules | https://github.com/etingof/pyasn1-modules/blob/master/LICENSE.txt |
| pyasn1_modules | https://pyasn1.readthedocs.io/en/latest/contents.html | https://github.com/pyasn1/pyasn1-modules?tab=BSD-2-Clause-1-ov-file#readme |
| pybind11 | http://pybind11.readthedocs.io/en/stable/ | https://github.com/pybind/pybind11/blob/master/LICENSE |
| pybind11-abi | https://github.com/pybind/pybind11 | https://github.com/pybind/pybind11/blob/master/LICENSE |
| pybind11_global | http://pybind11.readthedocs.io/en/stable/ | https://github.com/pybind/pybind11/blob/master/LICENSE |
| pycairo | https://pycairo.readthedocs.io/en/latest/index.html | https://github.com/pygobject/pycairo/blob/master/COPYING |
| pycosat | https://github.com/conda/pycosat | https://github.com/conda/pycosat/blob/main/LICENSE |
| pycparser | https://github.com/eliben/pycparser | https://github.com/eliben/pycparser/blob/master/LICENSE |
| pydantic | https://pydantic-docs.helpmanual.io | https://github.com/samuelcolvin/pydantic/blob/master/LICENSE |

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| pydantic-core | https://github.com/pydantic/pydantic-core | https://github.com/pydantic/pydantic-core |
| pyedr | https://github.com/MDAnalysis/panedr | https://github.com/MDAnalysis/panedr/blob/master/LICENSE.txt |
| pyEMMA | http://github.com/markovmodel/PyEMMA | https://github.com/markovmodel/PyEMMA/blob/devel/LICENSE.txt |
| Pygments | https://pygments.org | https://github.com/pygments/pygments/blob/master/LICENSE |
| pygments | https://pygments.org/ | https://github.com/pygments/pygments?tab=BSD-2-Clause-1-ov-file#readme |
| pygraphviz | https://pygraphviz.github.io | https://github.com/pygraphviz/pygraphviz/blob/main/LICENSE |
| pygtop | https://pygtop.readthedocs.io/en/latest/ | https://github.com/samirelanduk/pygtop/blob/master/LICENSE |
| pyHanko | https://github.com/MatthiasValvekens/pyHanko | https://github.com/MatthiasValvekens/pyHanko/blob/master/LICENSE |
| pyhanko-certvalidator | https://github.com/MatthiasValvekens/certvalidator | https://github.com/MatthiasValvekens/certvalidator/blob/master/LICENSE |
| PyJWT | https://github.com/jpadilla/pyjwt | https://github.com/jpadilla/pyjwt/blob/master/LICENSE |
| pymbar | https://pymbar.org | https://github.com/choderalab/pymbar/blob/master/LICENSE |
| pynvml | https://github.com/gpuopenanalytics/pynvml | https://github.com/gpuopenanalytics/pynvml/blob/master/LICENSE.txt |

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| pyOpenSSL | https://pyopenssl.org/ | https://github.com/pyca/pyopenssl/blob/main/LICENSE |
| pyparsing | https://pyparsing-docs.readthedocs.io/en/latest/ | https://github.com/pyparsing/pyparsing/blob/master/LICENSE |
| PyPDF3 | https://github.com/sfneal/PyPDF3 | https://github.com/sfneal/PyPDF3/blob/master/LICENSE |
| pyrsistent | http://github.com/tobgu/pyrsistent/ | https://github.com/tobgu/pyrsistent/blob/master/LICENSE.mit |
| pysam | https://github.com/pysam-developers/pysam | https://github.com/pysam-developers/pysam/blob/master/COPYING |
| PySocks | https://github.com/Anorov/PySocks | https://github.com/Anorov/PySocks/blob/master/LICENSE |
| pytables | https://www.pytables.org | https://github.com/PyTables/PyTables/blob/master/LICENSE.txt |
| python | https://www.python.org/ | https://docs.python.org/3/license.html |
| python-bidi | https://github.com/MeirKriheli/python-bidi | https://github.com/MeirKriheli/python-bidi/blob/master/COPYING |
| python-constraint | https://github.com/python-constraint/python-constraint | https://github.com/python-constraint/python-constraint/blob/master/LICENSE |
| python-dateutil | https://dateutil.readthedocs.io | https://github.com/dateutil/dateutil/blob/master/LICENSE |
| python-json-logger | http://github.com/madzak/python-json-logger | https://github.com/madzak/python-json-logger/blob/master/LICENSE |

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| python-pptx | https://github.com/scanny/python-pptx | https://github.com/scanny/python-pptx/blob/master/LICENSE |
| python-ldap | https://www.python-ldap.org/ | https://github.com/python-ldap/python-ldap/blob/python-ldap-3.4.0/LICENCE |
| python3-saml | https://github.com/onelogin/python3-saml | https://github.com/onelogin/python3-saml/blob/master/LICENSE |
| python_abi | https://github.com/conda-forge/python_abi-feedstock | https://github.com/conda-forge/python_abi-feedstock/blob/main/LICENSE.txt |
| pytorch-lightning | https://github.com/Lightning-AI/pytorch-lightning | https://github.com/Lightning-AI/pytorch-lightning/blob/master/LICENSE |
| pytz | https://pythonhosted.org/pytz | https://git.launchpad.net/pytz/tree/LICENSE.txt |
| pytz-deprecation-shim | https://github.com/pganssle/pytz-deprecation-shim | https://github.com/pganssle/pytz-deprecation-shim/blob/master/LICENSE |
| PyWavelets | https://github.com/PyWavelets/pywt | https://github.com/PyWavelets/pywt/blob/master/LICENSE |
| PyYAML | https://pyyaml.org/ | https://github.com/yaml/pyyaml/blob/master/LICENSE |
| pyyml | No longer available | No longer available |
| pyzmq | https://pyzmq.readthedocs.io/en/latest/ | https://github.com/zeromq/pyzmq/blob/main/COPYING.BSD |
| qcelemental | https://github.com/MolSSI/QCElemental | https://github.com/MolSSI/QCElemental/blob/master/LICENSE |

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| qcengine | https://github.com/MolSSI/QCEngine | https://github.com/MolSSI/QCEngine/blob/master/LICENSE |
| qrcode | https://github.com/lincolnloop/python-qrcode | https://github.com/lincolnloop/python-qrcode/blob/main/LICENSE |
| ramda | https://github.com/ramda/ramda | https://github.com/ramda/ramda/raw/master/LICENSE.txt |
| rapidjson | https://rapidjson.org/ | https://github.com/Tencent/rapidjson/blob/master/license.txt |
| rdkit | https://www.rdkit.org | https://github.com/rdkit/rdkit/blob/master/license.txt |
| re2 | https://github.com/google/re2 | https://github.com/google/re2/blob/main/LICENSE |
| readme-renderer | https://github.com/pypa/readme_renderer | https://github.com/pypa/readme_renderer/blob/main/LICENSE |
| redis-py | https://github.com/andymccurdy/redis-py | https://github.com/redis/redis-py/blob/master/LICENSE |
| referencing | https://github.com/python-jsonschema/referencing | https://github.com/python-jsonschema/referencing |
| regex | https://github.com/mrabarnett/mrab-regex | https://github.com/mrabarnett/mrab-regex/blob/hg/LICENSE.txt |
| reportlab | https://www.reportlab.com | https://www.reportlab.com/dev/docs/faq/#1.3 |
| reproc | https://github.com/DaanDeMeyer/reproc | https://github.com/DaanDeMeyer/reproc/blob/main/LICENSE |
| reproc-cpp | https://github.com/DaanDeMeyer/reproc | https://github.com/DaanDeMeyer/reproc/blob/main/LICENSE |

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| requests | https://requests.readthedocs.io | https://github.com/psf/requests/blob/main/LICENSE |
| requests-oauthlib | https://github.com/requests/requests-oauthlib | https://github.com/requests/requests-oauthlib/blob/master/LICENSE |
| requests-toolbelt | https://toolbelt.readthedocs.org | https://github.com/requests/toolbelt/blob/master/LICENSE |
| resumable | https://github.com/stevvooe/resumable | https://github.com/stevvooe/resumable/blob/master/LICENSE |
| retrying | https://github.com/rholder/retrying | https://github.com/rholder/retrying/blob/master/LICENSE |
| rfc3339-validator | https://github.com/naimetti/rfc3339-validator | https://github.com/naimetti/rfc3339-validator/blob/master/LICENSE |
| rfc3339_validator | https://github.com/naimetti/rfc3339-validator | https://github.com/naimetti/rfc3339-validator?tab=MIT-1-ov-file#readme |
| rfc3986 | https://rfc3986.readthedocs.io/en/latest/ | https://github.com/python-hyper/rfc3986/blob/main/LICENSE |
| rfc3986-validator | https://github.com/naimetti/rfc3986-validator | https://github.com/naimetti/rfc3986-validator/blob/master/LICENSE |
| rfc3987-syntax | https://github.com/willynilly/rfc3987-syntax | https://github.com/willynilly/rfc3987-syntax?tab=MIT-1-ov-file#readme |
| rich | https://github.com/Textualize/rich | https://github.com/Textualize/rich/blob/master/LICENSE |

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| rich-argparse | https://github.com/hamdanal/rich-argparse | https://github.com/hamdanal/rich-argparse/blob/main/LICENSE |
| rlPyCairo | https://pypi.org/project/rlPyCairo/ | https://hg.reportlab.com/hg-public/rlPyCairo/file/tip/rlPyCairo/LICENSE.txt |
| RocksDict | https://github.com/rocksdict/RocksDict | https://github.com/rocksdict/RocksDict?tab=MIT-1-ov-file#readme |
| roman-numerals | https://github.com/AA-Turner/roman-numerals | https://github.com/AA-Turner/roman-numerals?tab=License-1-ov-file#readme |
| roman-numerals-py | https://github.com/AA-Turner/roman-numerals | https://github.com/AA-Turner/roman-numerals?tab=License-1-ov-file#readme |
| rotary-embedding-torch | https://github.com/lucidrains/rotary-embedding-tor | https://github.com/lucidrains/rotary-embedding-tor blob/main/LICENSE |
| rpds-py | https://github.com/crate-py/rpds | https://github.com/crate-py/rpds |
| rpmpack | https://github.com/google/rpmpack | https://github.com/google/rpmpack/blob/master/LICENSE |
| rsa | https://stuvel.eu/rsa | https://github.com/sybrenstuvel/python-rsa/blob/main/LICENSE |
| ruamel-yaml | https://sourceforge.net/p/ruamel-yaml/code/ci/default/tree/ | https://sourceforge.net/p/ruamel-yaml/code/ci/default/tree/LICENSE |
| ruamel.yaml.clib | https://sourceforge.net/p/ruamel-yaml-clib/code/ci/default/tree/ | https://sourceforge.net/p/ruamel-yaml-clib/code/ci/default/tree/LICENSE |

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| s3transfer | https://github.com/boto/s3transfer | https://github.com/boto/s3transfer/blob/develop/LICENSE.txt |
| sacrebleu | https://github.com/mjpost/sacrebleu | https://github.com/mjpost/sacrebleu/blob/master/LICENSE.txt |
| sapiens | https://github.com/Merck/Sapiens | https://github.com/Merck/Sapiens/blob/main/LICENSE |
| sasl | https://mellium.im/sasl | https://github.com/mellium/sasl/blob/main/LICENSE |
| scikit-gstat | https://mmaelicke.github.io/scikit-gstat/ | https://github.com/mmaelicke/scikit-gstat/blob/main/LICENSE |
| scikit-image | https://scikit-image.org | https://scikit-image.org/docs/dev/license.html |
| scikit-learn | https://scikit-learn.org/stable/ | https://github.com/scikit-learn/scikit-learn/blob/main/COPYING |
| scikit-learn-extra | https://github.com/scikit-learn-contrib/scikit-learn-extra | https://github.com/scikit-learn-contrib/scikit-learn-extra/blob/main/LICENSE |
| scikit-network | https://github.com/sknetwork-team/scikit-network | https://github.com/sknetwork-team/scikit-network?tab=License-1-ov-file#readme |
| scipy | https://scipy.org | https://github.com/scipy/scipy/blob/main/LICENSE.txt |
| seaborn | https://seaborn.pydata.org | https://github.com/mwaskom/seaborn/blob/master/LICENSE |
| seaborn-base | https://seaborn.pydata.org | https://github.com/mwaskom/seaborn/blob/master/LICENSE |

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| semver | https://github.com/Masterminds/semver/v3 | https://github.com/Masterminds/semver/blob/v3.0.3/LICENSE.txt |
| Send2Trash | https://github.com/arsenetar/send2trash | https://github.com/arsenetar/send2trash/blob/master/LICENSE |
| sentry-sdk | https://github.com/getsentry/sentry-python | https://github.com/getsentry/sentry-python/blob/master/LICENSE |
| setproctitle | https://github.com/dvarrazzo/py-setproctitle | https://github.com/dvarrazzo/py-setproctitle/blob/master/LICENSE |
| setuptools | https://github.com/pypa/setuptools | https://github.com/pypa/setuptools/blob/main/LICENSE |
| setuptools-scm | https://github.com/pypa/setuptools_scm/ | https://github.com/pypa/setuptools_scm/blob/main/LICENSE |
| sh | https://github.com/amoffat/sh | https://github.com/amoffat/sh/blob/develop/LICENSE.txt |
| shellingham | https://github.com/sarugaku/shellingham | https://github.com/sarugaku/shellingham/blob/master/LICENSE |
| simdjson | https://github.com/simdjson/simdjson/tree/master | https://github.com/simdjson/simdjson/blob/master/LICENSE |
| simint | https://www.bennyp.org/research/simint/ | https://github.com/simint-chem/simint-generator/blob/master/LICENSE |
| simplejson | https://github.com/simplejson/simplejson | https://github.com/simplejson/simplejson/blob/master/LICENSE.txt |
| six | https://github.com/benjaminp/six | https://github.com/benjaminp/six/blob/master/LICENSE |

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| smirnoff99frosst | https://github.com/openforcefield/smirnoff99frosst | https://github.com/openforcefield/smirnoff99Frosst/blob/master/LICENSE |
| smmap | https://github.com/gitpython-developers/smmap | https://github.com/gitpython-developers/smmap/blob/master/LICENSE |
| snappy | https://github.com/google/snappy | https://github.com/google/snappy/blob/main/COPYING |
| sniffio | https://github.com/python-trio/sniffio | https://github.com/python-trio/sniffio/blob/master/LICENSE.MIT |
| snowballstemmer | https://github.com/snowballstem/snowball | https://github.com/snowballstem/snowball/blob/master/COPYING |
| soupsieve | https://github.com/facelessuser/soupsieve | https://github.com/facelessuser/soupsieve/blob/main/LICENSE.md |
| spdlog | https://github.com/gabime/spdlog | https://github.com/gabime/spdlog?tab=License-1-ov-file#readme |
| spglib | https://spglib.readthedocs.io/ | https://github.com/spglib/spglib/blob/develop/COPYING |
| sphinx | https://github.com/sphinx-doc/sphinx | https://github.com/sphinx-doc/sphinx/blob/5.x/LICENSE |
| sphinxcontrib-applehelp | https://github.com/sphinx-doc/sphinxcontrib-applehe | https://github.com/sphinx-doc/sphinxcontrib-applehe blob/master/LICENSE |
| sphinxcontrib-devhelp | https://github.com/sphinx-doc/sphinxcontrib-devhelp | https://github.com/sphinx-doc/sphinxcontrib-devhelp blob/master/LICENSE |
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| sphinxcontrib-jsmath | https://github.com/sphinx-doc/sphinxcontrib-jsmath | https://github.com/sphinx-doc/sphinxcontrib-jsmath/blob/master/LICENSE |
| sphinxcontrib-qthelp | https://github.com/sphinx-doc/sphinxcontrib-qthelp | https://github.com/sphinx-doc/sphinxcontrib-qthelp/blob/master/LICENSE |
| sphinxcontrib-serializinghtml | https://github.com/sphinx-doc/sphinxcontrib-serializ | https://github.com/sphinx-doc/sphinxcontrib-serializ blob/master/LICENSE |
| SQLAlchemy | https://www.sqlalchemy.org | https://docs.sqlalchemy.org/en/14/copyright.html |
| SQLAlchemy | https://www.sqlalchemy.org/ | https://github.com/sqlalchemy/sqlalchemy?tab=MIT-1-ov-file#readme |
| sqlite | https://sqlite.org/index.html | https://sqlite.org/copyright.html |
| sqlparse | https://github.com/andialbrecht/sqlparse | https://github.com/andialbrecht/sqlparse/blob/master/LICENSE |
| stack-data | http://github.com/alexmojaki/stack_data | https://github.com/alexmojaki/stack_data/blob/master/LICENSE.txt |
| stack_data | http://github.com/alexmojaki/stack_data | https://github.com/alexmojaki/stack_data?tab=MIT-1-ov-file#readme |
| starfile | https://github.com/alisterburt/starfile | https://github.com/teamtomo/starfile/blob/main/LICENSE |
| statsmodels | https://github.com/statsmodels/statsmodels | https://github.com/statsmodels/statsmodels/blob/main/LICENSE.txt |
| structlog | https://www.structlog.org/ | https://github.com/hynek/structlog/blob/main/LICENSE |

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| streamlit | https://github.com/streamlit/streamlit | https://github.com/streamlit/streamlit/blob/develop/LICENSE |
| svglib | https://github.com/deeplook/svglib | https://github.com/deeplook/svglib/blob/master/LICENSE.txt |
| sympy | https://sympy.org | https://github.com/sympy/sympy/blob/master/LICENSE |
| tables | https://www.pytables.org/ | https://github.com/PyTables/PyTables/blob/master/LICENSE.txt |
| tabulate | https://github.com/astanin/python-tabulate | https://github.com/astanin/python-tabulate/blob/master/LICENSE |
| tbb | https://github.com/oneapi-src/oneTBB | https://github.com/oneapi-src/oneTBB/blob/master/LICENSE.txt |
| tenacity | https://github.com/jd/tenacity | https://github.com/jd/tenacity/blob/master/LICENSE |
| tensorboard | https://github.com/tensorflow/tensorboard | https://github.com/tensorflow/tensorboard/blob/master/LICENSE |
| tensorboard-data-server | https://github.com/tensorflow/tensorboard | https://github.com/tensorflow/tensorboard/blob/master/LICENSE |
| tensorboard-plugin-wit | https://github.com/pair-code/what-if-tool | https://github.com/PAIR-code/what-if-tool/blob/master/LICENSE |
| tensorboardX | https://github.com/lanpa/tensorboardX | https://github.com/lanpa/tensorboardX/blob/master/LICENSE |
| tensorflow | https://github.com/tensorflow/tensorflow | https://github.com/tensorflow/tensorflow/blob/master/LICENSE |

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| tensorflow-estimator | https://github.com/tensorflow/estimator | https://github.com/tensorflow/estimator/blob/master/LICENSE |
| tensorflow-io-gcs-filesystem | https://github.com/tensorflow/io | https://github.com/tensorflow/io/blob/master/LICENSE |
| tensorflow-probability | https://github.com/tensorflow/probability | https://github.com/tensorflow/probability/blob/main/LICENSE |
| termcolor | https://github.com/hugovk/termcolor | https://github.com/hugovk/termcolor/blob/main/COPYING.txt |
| terminado | https://github.com/jupyter/terminado | https://github.com/jupyter/terminado/blob/main/LICENSE |
| testpath | https://github.com/jupyter/testpath | https://github.com/jupyter/testpath/blob/master/LICENSE |
| textangular | https://github.com/fraywing/textAngular | https://github.com/fraywing/textAngular |
| texttable | https://github.com/foutaise/texttable/ | https://github.com/foutaise/texttable/?tab=MIT-1-ov-file#readme |
| tf_keras | https://github.com/keras-team/keras-io | https://github.com/keras-team/keras-io/blob/master/LICENSE |
| tf_keras | https://github.com/keras-team/keras-io | https://github.com/keras-team/keras-io/blob/master/LICENSE |
| threadpoolctl | https://github.com/joblib/threadpoolctl | https://github.com/joblib/threadpoolctl/blob/master/LICENSE |
| three | https://github.com/mrdoob/three.js | https://github.com/mrdoob/three.js/raw/master/LICENSE |

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| tinycss2 | https://github.com/Kozea/tinycss2/ | https://github.com/Kozea/tinycss2/blob/master/LICENSE |
| tinyxml2 | https://github.com/leethomason/tinyxml2 | https://github.com/leethomason/tinyxml2/blob/master/LICENSE.txt |
| tk | https://www.tcl.tk/ | https://www.tcl.tk/software/tcltk/license.html |
| toml | https://github.com/toml-lang/toml | https://github.com/toml-lang/toml/blob/main/LICENSE |
| tomli | https://github.com/hukkin/tomli | https://github.com/hukkin/tomli/blob/master/LICENSE |
| toolz | https://github.com/pytoolz/toolz | https://github.com/pytoolz/toolz/blob/master/LICENSE.txt |
| torch | https://pytorch.org/ | https://pypi.org/project/torch/#license |
| torch-geometric | https://pyg.org/ | https://github.com/pyg-team/pytorch_geometric?tab=MIT-1-ov-file#readme |
| torcheval | https://github.com/pytorch/torcheval | https://github.com/pytorch/torcheval?tab=License-1-ov-file#readme |
| torchmetrics | https://github.com/Lightning-AI/torchmetrics | https://github.com/Lightning-AI/torchmetrics?tab=Apache-2.0-1-ov-file#readme |
| tornado | https://www.tornadoweb.org | https://github.com/tornadoweb/tornado/blob/master/LICENSE |

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| tqdm | https://github.com/tqdm/tqdm | https://github.com/tqdm/tqdm/blob/master/LICENCE | | |
| tracy | https://github.com/gear-genomics/tracy | https://github.com/gear-genomics/tracy/blob/main/LICENSE | | |
| traitlets | https://github.com/ipython/traitlets | https://github.com/ipython/traitlets/blob/main/COPYING.md | | |
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| truststore | https://github.com/sethmlarson/trus | https://github.com/sethmlarson/truststore/blob/main/LICENSE | | |
| truststore | https://github.com/sethmlarson/truststore | https://github.com/sethmlarson/truststore/blob/main/LICENSEtruststore | https://github.com/sethmlarson/truststore | https://github.com/sethmlarson/truststore/blob/main/LICENSE |
| ts-jest | https://github.com/kulshekhar/ts-jest | https://github.com/kulshekhar/ts-jest/raw/master/LICENSE.md | | |
| ts-loader | https://github.com/TypeStrong/ts-loader | https://github.com/TypeStrong/ts-loader/raw/master/LICENSE | | |
| twine | https://github.com/pypa/twine | https://github.com/pypa/twine/blob/main/LICENSE | | |
| twinj uuid | https://github.com/twinj/uuid | https://github.com/twinj/uuid/blob/master/LICENSE | | |
| types | https://github.com/babel/babel | https://github.com/babel/babel/raw/master/LICENSE | | |
| types-python-dateutil | https://github.com/python/typeshed | https://github.com/python/typeshed?tab=License-1-ov-file#readme | | |
| types-requests | https://pypi.org/project/types-requests/ | https://github.com/python/typeshed/blob/main/LICENSE | | |

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| Name of Project | Website | License URL |
|---|---|---|
| typescript | https://github.com/Microsoft/TypeScript | https://github.com/Microsoft/TypeScript/raw/master/LICENSE.txt |
| typing-inspection | https://github.com/pydantic/typing-inspection | https://github.com/pydantic/typing-inspection?tab=MIT-1-ov-file#readme |
| typing-utils | https://github.com/bojiang/typing_utils | https://github.com/bojiang/typing_utils?tab=Apache-2.0-1-ov-file#readme |
| typing_extensions | https://github.com/python/typing | https://github.com/python/typing/blob/master/LICENSE |
| typing_utils | https://github.com/bojiang/typing_utils | https://github.com/bojiang/typing_utils?tab=Apache-2.0-1-ov-file#readme |
| tzdata | https://github.com/python/tzdata | https://github.com/python/tzdata/blob/master/LICENSE |
| tzlocal | https://github.com/regebro/tzlocal | https://github.com/regebro/tzlocal/blob/master/LICENSE.txt |
| umf | https://github.com/oneapi-src/unified-memory-fram | https://github.com/oneapi-src/unified-memory-fram tab=License-1-ov-file#readme |
| umi-tools | https://github.com/CGATOxford/UMI-tools | https://github.com/CGATOxford/UMI-tools/blob/master/LICENSE |
| unicodedata2 | https://github.com/fonttools/unicodedata2 | https://github.com/fonttools/unicodedata2/blob/master/LICENSE |
| uri-template | https://gitlab.linss.com/open-source/python/uri-template | https://gitlab.linss.com/open-source/python/uri-template/-/blob/main/LICENSE |
| uritools | https://github.com/tkem/uritools/ | https://github.com/tkem/uritools/blob/master/LICENSE |

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| Name of Project | Website | License URL | | |
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| urllib3 | https://urllib3.readthedocs.io/ | https://github.com/urllib3/urllib3/blob/main/LICENSE.txt | | |
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| wadler_lindig | https://github.com/patrick-kidger/wadler_lindig | https://github.com/patrick-kidger/wadler_lindig?tab=Apache-2.0-1-ov-file#readmewcwidth | https://github.com/jquast/wcwidth | https://github.com/jquast/wcwidth/blob/master/LICENSE |
| wandb | https://github.com/wandb/wandb | https://github.com/wandb/wandb/blob/main/LICENSE | | |
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| wheel | https://github.com/pypa/wheel | https://github.com/pypa/wheel/blob/main/LICENSE.txt | | |

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| Name of Project | Website | License URL |
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| widgetsnbextension | https://github.com/jupyter-widgets/ipywidgets#readme | https://github.com/jupyter-widgets/ipywidgets/blob/main/LICENSE |
| wrapt | https://github.com/GrahamDumpleton/wrapt | https://github.com/GrahamDumpleton/wrapt/blob/develop/LICENSE |
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| x/text | https://golang.org/x/text | https://cs.opensource.google/go/x/text/+/master:LICENSE |
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| xlsxwriter | https://github.com/jmcnamara/XlsxWriter | https://github.com/jmcnamara/XlsxWriter/blob/main/LICENSE.txt |
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| xorg-libxau | https://gitlab.freedesktop.org/xorg/lib/libxau | https://gitlab.freedesktop.org/xorg/lib/libxau/-/blob/master/COPYING |
| xorg-libxdmcp | https://gitlab.freedesktop.org/xorg/lib/libxdmcp | https://gitlab.freedesktop.org/xorg/lib/libxdmcp/-/blob/master/COPYING |

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| xorg-libxt | https://gitlab.freedesktop.org/xorg/lib/libxt | https://gitlab.freedesktop.org/xorg/lib/libxt/-/blob/master/COPYING |
| xorg-renderproto | https://gitlab.freedesktop.org/xorg/proto/renderproto | https://gitlab.freedesktop.org/xorg/proto/renderproto/-/blob/master/COPYING |
| xorg-xextproto | https://gitlab.freedesktop.org/xorg/proto/xextproto | https://gitlab.freedesktop.org/xorg/proto/xextproto/-/blob/master/COPYING |
| xorg-xproto | https://gitlab.freedesktop.org/xorg/proto/xproto | https://gitlab.freedesktop.org/xorg/proto/xproto/-/blob/master/COPYING |
| xxhash | https://github.com/cespare/xxhash/v2 | https://github.com/cespare/xxhash/blob/main/LICENSE.txt |
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| yaml | https://pyyaml.org/ | https://github.com/yaml/pyyaml/blob/master/LICENSE |
| yaml-cpp | https://github.com/jbeder/yaml-cpp | https://github.com/jbeder/yaml-cpp/blob/master/LICENSE |
| yaml.v2 | https://gopkg.in/yaml.v2 | https://github.com/go-yaml/yaml/blob/v2.4.0/LICENSE |
| yaml.v3 | https://gopkg.in/yaml.v3 | https://github.com/go-yaml/yaml/blob/v3/LICENSE |

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|---|---|---|
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| yaspin | https://github.com/pavdmyt/yaspin | https://github.com/pavdmyt/yaspin/blob/master/LICENSE |
| yfiles | https://www.yworks.com/products/yfiles | commercial license |
| yml | https://pypi.org/project/yml/ | N/A |
| zap | https://go.uber.org/zap | https://github.com/uber-go/zap/blob/master/LICENSE.txt |
| zipp | https://github.com/jaraco/zipp | https://github.com/jaraco/zipp/blob/main/LICENSE |
| zlib | https://zlib.net/ | https://zlib.net/zlib_license.html |
| zstandard | https://github.com/indygreg/python-zstandard | https://github.com/indygreg/python-zstandard/blob/main/LICENSE |
| zstd | https://facebook.github.io/zstd/ | https://github.com/facebook/zstd/blob/dev/LICENSE |
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## 9.1 GCC

On the Linux platform, The OpenEye toolkits are linked with the GCC libraries using an eligible compilation process under the terms of the GCC RUNTIME LIBRARY EXCEPTION (see below).

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Per GPLv3, section 6d, the source for GCC is available for download from the following location: GNU. The GCC library components included here are from version gcc-4.9.3 and are built using the standard instructions at Installing GCC.

### 9.1.1 GCC RUNTIME LIBRARY EXCEPTION

```
Version 3.1, 31 March 2009

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↪(including proprietary) programs
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0. Definitions.

A file is an "Independent Module" if it either requires the Runtime Library for␣
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"GCC" means a version of the GNU Compiler Collection, with or without modifications,␣
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"Target Code" refers to output from any compiler for a real or virtual target processor␣
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form or suitable for input to an assembler, loader, linker and/or execution phase.␣
↪Notwithstanding that, Target Code
does not include data in any format that is used as a compiler intermediate␣
↪representation, or used for producing a
compiler intermediate representation.
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The "Compilation Process" transforms code entirely represented in non-intermediate␣
↪languages designed for human-written
code, and/or in Java Virtual Machine byte code, into Target Code. Thus, for example, use␣
↪of source code generators and
preprocessors need not be considered part of the Compilation Process, since the␣
↪Compilation Process can be understood
as starting with the output of the generators or preprocessors.

A Compilation Process is "Eligible" if it is done using GCC, alone or with other GPL-
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done without using any work based on GCC. For example, using non-GPL-compatible Software␣
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```

**See also**

- http://www.gnu.org/licenses/gcc-exception.html

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                       Version 3, 29 June 2007

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the interface presents a list of user commands or options, such as a
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  The "source code" for a work means the preferred form of the work
for making modifications to it.  "Object code" means any non-source
form of a work.
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  A "Standard Interface" means an interface that either is an official
standard defined by a recognized standards body, or, in the case of
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  The "System Libraries" of an executable work include anything, other
than the work as a whole, that (a) is included in the normal form of
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Component, and (b) serves only to enable use of the work with that
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"Major Component", in this context, means a major essential component
(kernel, window system, and so on) of the specific operating system
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  The "Corresponding Source" for a work in object code form means all
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work) run the object code and to modify the work, including scripts to
control those activities.  However, it does not include the work's
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which are not part of the work.  For example, Corresponding Source
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the work, and the source code for shared libraries and dynamically
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parts of the aggregate.

  6. Conveying Non-Source Forms.

  You may convey a covered work in object code form under the terms
of sections 4 and 5, provided that you also convey the
machine-readable Corresponding Source under the terms of this License,
in one of these ways:

  a) Convey the object code in, or embodied in, a physical product
  (including a physical distribution medium), accompanied by the
  Corresponding Source fixed on a durable physical medium
  customarily used for software interchange.

  b) Convey the object code in, or embodied in, a physical product
  (including a physical distribution medium), accompanied by a
  written offer, valid for at least three years and valid for as
  long as you offer spare parts or customer support for that product
  model, to give anyone who possesses the object code either (1) a
  copy of the Corresponding Source for all the software in the
  product that is covered by this License, on a durable physical
  medium customarily used for software interchange, for a price no
  more than your reasonable cost of physically performing this
  conveying of source, or (2) access to copy the
  Corresponding Source from a network server at no charge.

  c) Convey individual copies of the object code with a copy of the
  written offer to provide the Corresponding Source.  This
  alternative is allowed only occasionally and noncommercially, and
  only if you received the object code with such an offer, in accord
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   with subsection 6b.

   d) Convey the object code by offering access from a designated
   place (gratis or for a charge), and offer equivalent access to the
   Corresponding Source in the same way through the same place at no
   further charge.  You need not require recipients to copy the
   Corresponding Source along with the object code.  If the place to
   copy the object code is a network server, the Corresponding Source
   may be on a different server (operated by you or a third party)
   that supports equivalent copying facilities, provided you maintain
   clear directions next to the object code saying where to find the
   Corresponding Source.  Regardless of what server hosts the
   Corresponding Source, you remain obligated to ensure that it is
   available for as long as needed to satisfy these requirements.

   e) Convey the object code using peer-to-peer transmission, provided
   you inform other peers where the object code and Corresponding
   Source of the work are being offered to the general public at no
   charge under subsection 6d.

  A separable portion of the object code, whose source code is excluded
from the Corresponding Source as a System Library, need not be
included in conveying the object code work.

  A "User Product" is either (1) a "consumer product", which means any
tangible personal property which is normally used for personal, family,
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into a dwelling.  In determining whether a product is a consumer product,
doubtful cases shall be resolved in favor of coverage.  For a particular
product received by a particular user, "normally used" refers to a
typical or common use of that class of product, regardless of the status
of the particular user or of the way in which the particular user
actually uses, or expects or is expected to use, the product.  A product
is a consumer product regardless of whether the product has substantial
commercial, industrial or non-consumer uses, unless such uses represent
the only significant mode of use of the product.

  "Installation Information" for a User Product means any methods,
procedures, authorization keys, or other information required to install
and execute modified versions of a covered work in that User Product from
a modified version of its Corresponding Source.  The information must
suffice to ensure that the continued functioning of the modified object
code is in no case prevented or interfered with solely because
modification has been made.

  If you convey an object code work under this section in, or with, or
specifically for use in, a User Product, and the conveying occurs as
part of a transaction in which the right of possession and use of the
User Product is transferred to the recipient in perpetuity or for a
fixed term (regardless of how the transaction is characterized), the
Corresponding Source conveyed under this section must be accompanied
by the Installation Information.  But this requirement does not apply
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if neither you nor any third party retains the ability to install
modified object code on the User Product (for example, the work has
been installed in ROM).

  The requirement to provide Installation Information does not include a
requirement to continue to provide support service, warranty, or updates
for a work that has been modified or installed by the recipient, or for
the User Product in which it has been modified or installed.  Access to a
network may be denied when the modification itself materially and
adversely affects the operation of the network or violates the rules and
protocols for communication across the network.

  Corresponding Source conveyed, and Installation Information provided,
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**See also**

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