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AFITT

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CHAPTER

ONE

OVERVIEW

AFITT is a crystallographic tool for correctly placing small molecules in real-space density. **AFITT** combines our flagship Shape technology with generic forcefields into a new forcefield that fits small molecules into crystallographic density while maintaining excellent chemistry.

AFITT also provides an interface to external refinement programs and tools to validate the refinement including interactive Ramachandran plots and real-space correlation coefficient calculation (RSCC).

CHAPTER

TWO

APPLICATIONS

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

- *FLYNN* for fitting ligands into real-space density.

CHAPTER

THREE

UTILITY PROGRAMS

The following utility programs are also included in this distribution:

- *AlignGrid*: Utility to align proteins with electron-density maps on a single reference
- *RotFit*: Utility to carry out fast automated refitting of side-chains and peptide flips.
- *Rscc*: Utility to perform real-space correlation coefficient and real-space R-factor calculations.
- *WriteDict*: Refinement dictionary generator that properly handles covalent bond restraints between the ligand and the protein

CHAPTER

FOUR

FLYNN

4.1 Overview

Fitting small molecules to electron density is a challenging problem. Small molecules with few rotatable bonds are amenable to hand placement in density. Add a few rotatable bonds, however, and the problem becomes factorially more complicated. Furthermore, unlike protein modeling, many small molecules are relatively unique entities whose conformation cannot be predicted from previous homologies.

FLYNN uses a high-quality conformational analysis and a fast rigid overlay to position ligands in density in conjunction with a combined forcefield to further position these conformations while, at the same time, minimizing ligand strain. FLYNN can automatically locate ligand density and automatically fit fragment cocktails, or, failing that, **FLYNN** can use a supplied bounding box in which to place the ligands of interest.

Ligands are fit to density, however the placements are scored and ranked based on the real space correlation coefficient (RSCC) and optionally protein based docking scores: Piecewise-Linear-Potential (PLP) and Chemscore.

FLYNN reads common map formats such as CCP4, MRC, MAP, CNX/CNS (XPLOR) and MTZ as well as OpenEye's grid formats and a plethora of small molecule, protein and connection table formats.

4.2 Example Commands

The example commands in this section can be run with files found in the `data/1nhu` directory under the top-level installation directory.

4.2.1 Basic Usage

```
> flynn -in 1nhu.ism -map 1nhu_prot.mtz -prot 1nhu_prot.pdb \
          -out 1nhu-poses.pdb
```

Use the ligand specified by **1nhu.ism** and fit it against the density in the mtz file **1nhu_prot.mtz**. Since this is an mtz file and **-autoMTZ** is defaulting to true, the Fdelwt map will automatically be generated and used as the density target. The protein atoms specified in 1nhu_prot.pdb will be used to mask the density before the map is searched for appropriately sized ligand volumes.

4.2.2 Generating Reports

```
> flynn -in 1nhu.ism -map 1nhu_prot.mtz -prot 1nhu_prot.pdb \
          -out 1nhu-poses.pdb -precheck -reporthtml 1nhu.html
```

Performs a preliminary check of the data, ensuring that the ligand can be processed and that the mtz file can be opened. An html file is generated **1nhu.html** with a corresponding image file **1nhu.html.gif**. The html file can be opened with a web browser to view the ligand being fit and any corresponding issues.

The output will be written to 1nhu-poses.pdb in pdb format.

4.2.3 Choosing box regions of density

```
> flynn -in 1nhu.ism -map 1nhu_sigma.mtz -prot 1nhu_prot.ent \
          -out 1nhu_poses.pdb -box 1nhu.pdb -boxpad 2.0
```

This is the same as above except that the density is pruned down to the bounding box specified by **1nhu.pdb** padded by 2.0 Ångströms. Furthermore, if a suitable blob is not found, then the pruned density will be used as is. This is quite effective for regions of density with a high degrees of disorder. It is also useful to select this option when using the supplied interface to **coot**.

4.2.4 Choosing density close to residues

Use the *-residues* and *-distance* flags to indicate residues close near the desired density. Only blobs that are found within *-distance* to the selected residues will be selected. Residues are specified by <residuenumber><chain> separated by commas.

```
> flynn -in 1nhu.ism -map 1nhu_prot.mtz -prot 1nhu_prot.pdb \
          -out 1nhu-poses.pdb -residues 528B,477B
```

4.2.5 Choosing MTZ columns

```
> flynn -in 1nhu.ism -map 1nhu_sigma.mtz -prot 1nhu_prot.ent \
          -out 1nhu_poses.pdb -box 1nhu.pdb -boxpad 2.0 \
          -boxThenBlobs -autoMTZ false -Fobs Frefined1 -Fc FC \
          -Phic PHIC -mtype 2Fo-Fc -autoMTZ false
```

This example shows how to choose a nonstandard column from the MTZ file. the map is generated using **Frefined1** as the observed amplitude column, **FC** as the calculated amplitude column and **PHIC** as the calculated phase column. Furthermore, the regular map **2Fo-Fc** is used. Note that **-autoMTZ** must be set to false for these settings to take effect.

4.2.6 Fragment usage

The **-fragment** flag may be included with any of the above commands. There are three main differences when running in fragment mode:

1. Multiple ligands are fit simultaneously.
2. If the blobs detected for difference ligands overlap, the ligands are assigned to the same blob. (This is for reporting purposes)
3. Ligands are sorted according to the Real Space Correlated Coefficient.

```
> flynn -fragment -in 1nhu.ism -map 1nhu_prot.mtz -prot 1nhu_prot.pdb \
          -out 1nhu-poses.sdf
```

When in fragment mode, it is better to output to a format that supports SD style data (.sdf, .oeb). This makes it much easier to analyze the results in a molecular viewer that supports a sortable spreadsheet. (**VIDA**, **MOE** and so on)

To sort the results using another scoring function, use the **-sortBy** flag.

```
> flynn -sortBy chemscore -in 1nhu.smi ...
```

4.3 Command Line Help

A description of the command line interface can be obtained by executing FLYNN with the *–help* option.

```
> flynn --help
```

will generate the following output:

```
Help functions:
  flynn --help simple      : Get a list of simple parameters
  flynn --help all         : Get a complete list of parameters
  flynn --help <parameter> : Get detailed help on a parameter
  flynn --help html        : Create an html help file for this program
```

4.4 Required Parameters

-in <filename>

File containing a molecule to be fit to density.

File type	Extension
SMILES	.smi .ism .smi.gz .ism.gz
OEBinary	.oeb .oeb.gz
SDF	.sdf .mol .sdf.gz .mol.gz
MOL2	.mol2 .mol2.gz
PDB	.pdb .ent .pdb.gz .ent.gz
MacroModel	.mmod .mmod.gz

-out <filename>

File containing resulting conformations exported in the following formats:

File type	Extension
OEBinary	.oeb .oeb.gz
SDF	.sdf .mol .sdf.gz .mol.gz
MOL2	.mol2 .mol2.gz
PDB	.pdb .ent .pdb.gz .ent.gz
MacroModel	.mmod .mmod.gz

-map <filename>

Input density grid used to fit ligand. Note that **mtz** files have additional settings, see *MTZ File Options*

Grid File type	Extension
MTZ	.mtz
OpenEye	.grd
Grasp	.phi
CCP4	.map .ccp4 .mrc
XPLOR	.xplor xplmap
ASCII Grid	.agd

[Aliases=**-grid**,**-density**]

4.5 Optional Parameters

4.5.1 Input Options

-prot <filename>

Optional protein used to mask density. This model is used to mask away density where the ligand should not be placed. While the protein is not required, it is highly recommended.

File type	Extension
OEBinary	.oeb .oeb.gz
SDF	.sdf .mol .sdf.gz .mol.gz
MOL2	.mol2 .mol2.gz
PDB	.pdb .ent .pdb.gz .ent.gz
MacroModel	.mmod .mmod.gz

-fragment

Fragments are fit taking the input fragment cocktail and, one at a time, fitting each fragment against each region of detected density. Once a fragment has been placed, it is further analyzed to ensure that all possible orientations of the fragment have been sampled. In poor density, several orientations may fit equally well. To break ties, FLYNN scores each pose with the following scores:

o RSCC (real space correlation coefficient) This is a measure of fit to electron density. [Jones-1991]

o PLP Piecewise-linear potential. [Verkhivker-2000]

o Chemscore [Eldridge-1997]

The docking scores are not used to fit the molecule, they are only used to rank the output. Unless highly symmetric molecules are being input, the real space correlation coefficient (RSCC) is the preferred method of ranking results to density.

All scores are annotated to the output ligands using SD data when appropriate (.SD and .OEB output) or using the PDB remark field:

```
Example PDB output

REMARK OpenEye Flynn MMFF/Shape v 2.1.0
REMARK Stereo Variant:      1
REMARK Blob:                1
REMARK Conformer:           1
REMARK Tanimoto Shape:        0.2004
REMARK Tanimoto MMFF/Shape:   0.2034
REMARK Local Strain:          4.9316
REMARK RSCC: 0.529438
REMARK PLP: -51.395416
REMARK Chemscore: -16.288113
```

```
Example SDF output

> <Tanimoto MMFF/SHAPE>
 0.2034

> <Tanimoto Shape>
```

(continues on next page)

(continued from previous page)

```
 0.2004

> <Overlap>
364.767659122018

> <Fit Overlap>
781.301114117834

> <Local Strain>
 4.9316

> <Lambda>
1.600000023842

> <Ref Overlap>
1371.829467773438

> <Stereo>
1

> <Blob>
1

> <Conformer>
1

> <RSCC>
0.529438

> <PLP>
-51.395416

> <Chemscore>
-16.288113
```

To use fragment mode, please add the "-fragment" option to the command line. In future versions of FLYNN, this will most likely become the default setting.

The output of the fragment fitting process is a file for each density region that includes the fragments fit to the region sorted from best-fit to worst fit. For example:

```
> flynn -in fragments.smi -out 2IKO_cocktail.sdf ...
```

would result in the files:

```
2IKO_cocktail_blob001.sdf
2IKO_cocktail_blob002.sdf
2IKO_cocktail_blob003.sdf
```

one for each blob found. The first molecule in the file is the best fit to the density.

To sort using another measure, for instance, PLP, use the sort flag:

```
> flynn -sortBy plp -in fragments.smi -out 2IKO_cocktail.sdf ...
```

When oeb format is used, the blob is also stored in the OEB file. When using VIDA, simply expand the molecule to investigate the blobs density.

-param <parameter filename>

A parameter file is a text file that lists parameter settings to be used during a run. If a parameter is specified both on the command line and in the parameter file, the value specified on the command line is used.

The format of the parameter file is as follows:

- One parameter per line
- For non-list parameters one key-value pair per line.
- For list parameters a key followed by all the values.
- Boolean parameters must be listed as a key followed by true or false.
- The parameter file may not contain the *-param* parameter.
- Lines beginning with # are considered comments

[Aliases=**-com**]

-prefix <file prefix>

Define the default prefix to use for loggging and report file generation.

This -prefix is overridden when using the *-reporthtml* or *-reportfile* command line options.

[Default=flynn]

-manualSearch <filename>

Use the input molecule to generate a box volume. All density inside this box will be used to place the ligand.

[Aliases=**-box**]

-boxpad <number>

Pad the box created with the *-manualSearch* flag by an amount in Ångströms.

[Default=1.0]

-autoThenManualSearch

Automatically search for blobs first, if now suitable blobs are found, use the supplied box to bound density.

[Default=false]

[Aliases=**-blobsThenBox**]

-densityAsIs

Use the supplied density as it is; do not try to find suitable blobs inside the density. Note that the supplied density has to be pretty close to the actual ligand density for this to work

[Default=false]

-distance <value>

Reject blobs whose average distance to the protein is greater than this value.

[Default=4.0]

-ligandAsIs

Do not generate conformations for the ligand; use only the supplied conformations.

-mmff94s

Use the MMFF94s variant of the MMFF94 forcefield (this uses planar aniline nitrogens).

[Default=true]

-ff <forcefield>

Select the forcefield to use for fitting the molecule into density.

Value	Meaning
mmff94	MMFF94
mmff94s	MMFF94s (default)
am1	AM1
am1-sheffield	AM1-Sheffield
pm3	PM3
pm3-sheffield	PM3-Sheffield
mmff94-electrostatics	MMFF94 with electrostatics
mmff94-electrostatics-sheffield	MMFF94 with Sheffield electrostatics

[Default=mmff94s]

-reportfile <filename>

File location for writing the report file. This is a comma separated file containing specifics about the results.

Smiles,Blob,Stereo Variant,Conformer,Tanimoto Shape,Tanimoto MMFF/SHAPE,Local Strain
CC(=O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CCC4=CC(=O)CC[C@]34C)C,1,,,0.4110,0.4296,1.342
CC(=O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CCC4=CC(=O)CC[C@]34C)C,1,,,0.313,0.3704,4.553
CC(=O)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CCC4=CC(=O)CC[C@]34C)C,1,,,0.3265,0.3628,5.223

-resname <name>

Set the output residue name to **<name>**. **<name>** must be less than or equal to three characters in length. This forces the output residue to be named <name> even if the residues structure does not match a known deposited residue.

-chainid <chainid>

Forces the ligand to be placed in the chain <chainid>

-assignClosestChainId

Assign the closest protein chain (within 7 Angstroms) to set the ligand's chain id. Cannot be used with the explicit *-chainid* setting.

[Aliases=**-assignClosestChainID**,**-assignClosestChainid**]

-sortAllChiral <true/false>

If set to true, when multiple chiralities are enumerated, sort all chiralities from best to worst per blob, otherwise sort chiral structures independently. For example, if two blobs are found, then the output will have all chiral structures sorted from best fit to worst fit for the first blob, and then all chiral structures sorted from best fit to worst fit for the second blobs, etc Note that the second blob may contain better fits than the first. (Note: This may interleave chiral structures).

[Default=true]

-verbose

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

[Default=false]

4.5.2 MTZ File Options

The allowed MTZ map types and the corresponding column conventions are documented in OEReadMTZ in the **OEChem TK** manual.

-autoMTZ

Automatically try to open the mtz file using the DELWT and FDELWT columns from REFMAC5 mtz files.

See OESystem::OEMTZMapType::Fdelwt for the corresponding difference-map type in **OEChem TK**.

[Default=true]

-Fc <columnname>

Column to use for Fc. *Note, to load arbitrary columns, you can use the* *-Fc** and **-Phic** columns and the **Fc** maptype.*

[Default=FC]

-Fdelwt <columnname>

Column to use for Fdelwt or difference map amplitudes

See OESystem::OEMTZMapType::Fdelwt in **OEChem TK** for map type details.

[Default=DELFWT]

-Fobs <columnname>

Column to use for FObs.

[Default=F]

[Aliases=**-Fo**]

-Phi <columnname>

Column to use for Phi.

[Default=PHI]

-Fwt <columnname>

Column to use for Fwt or regular map amplitudes.

See OESystem::OEMTZMapType::Fwt in **OEChem TK** for map type details.

[Default=FWT]

-Phic <columnname>

Column to use for Phic.

[Default=PHIC]

-Phidelwt <columnname>

Column to use for Phdelwt or difference map phases.

[Default=PHDELWT]

-Phiwt <columnname>

Column to use for Phwt or regular map phases.

[Default=PHWT]

-SigmaA <columnname>

Column to use for SigmaA.

-mtype

The map type to use for fitting. Fo-Fc, Fc, 2Fo-Fc, 3Fo-Fc, Fwt, Fdelwt…

See OEReadMTZ for the full list of map types and their MTZ-column interpretation.

[Default=Fdelwt]

4.5.3 Advanced Options

-ciftype

Specify the format of the refinement dictionary. Legal values for refinement dictionaries are 'refmac', 'phenix' and 'buster'. Refinement dictionaries are always written out using the designation specified in the '-split' command. For best results, use -split when writing out cif files when using FLYNN.

-flipper

Force enumeration of all stereochemical centers. Otherwise, only missing stereo chemistry will be enumerated.

[Default=false]

-overlays

Set the number of initial rigidly fit overlays to optimize into density.

[Default=10]

-precheck

Perform only a preliminary check of the data to see if fitting is possible. (This flag is meaningless without the -reporthtml flag).

[Default=false]

-reporthtml

Generate an html report of the fitting process. This is a useful first step to verify the data. It also includes a 2D image of the ligand that is being fit in order to verify bond orders. All output of FLYNN will be captured in the specified html file.

-residues

Comma separated list of residues to use as distance constraints. If residues are specified, the *-distance* flag will use the residues to reject blobs that are too far away. Note that with a residue list, the distance computed is a minimum distance, not an average distance. Residues must be specified as <residue number><chain id>. For example: 120C,134C. On Windows, double quotes must be added to specify two or more residues, i.e. -residues "120C,134C".

-rms

If the input ligand has 3D coordinates, this calculates the RMS distance to the ligand and records it in the molecule. If -split is on, it also records it in the file name.

[Default=false]

-split

Split the result into different files. Each filename is annotated with the resulting shape score so that when the output directory is listed alphabetically, the best scores will be displayed in order. In the case where the output format is pdb the ligand fitting results are written in REMARK statements at the top of the file.

The splits are labeled as follows outputname_n###_b###_s###_c### where n### is the number of the ordered results, b### is the blob for the result, s### is the stereovariant and c### is the number of the conformer fit as ordered by MMFF/Shape.

[Default=false]

-suppressH

By default FLYNN outputs hydrogens of the resulting poses. Setting this to true will not output hydrogens. It is always recommended to output hydrogrens for ligands in order to keep their chemistry the same as flynn's internal optimizer. Only suppress hydrogens if your refinement package doesn't handle hydrogen names correctly.

[Default=false]

-fix_serial_numbers

Force serial numbers to be unique when writing out the resulting pdb file for use in the refinement package. This is usually caused by adding hydrogens to the ligand outside of the context of the protein and then using it in conjunction with the original PDB structure.

[Default=false]

4.5.4 Fragment Fitting Options

-blobTanimoto

Density is searched for each input ligand. This flag sets the minimum tanimoto overlap for which to consider two blobs the same. When pruning similar blobs, the larger is taken.

[Default=0.45]

[Aliases=**-bt**]

-sortBy

Choose the fragment sorting function, tanimoto, rscc (real space correlation coefficient), plp (piecewise linear potential) or chemscore.

The fragments are fit in the normal fashion (tanimoto), but then re-scored and sorted using the chosen metric.

[Default=rscc]

4.5.5 3D Construction Options

These are advanced conformer generation parameters. Normally, they do not need to be adjusted. Please consult the OMEGA manual for assistance:

-ewindow

Controls the MMFF energy window when generating initial conformations. Normally, this setting does not need to be adjusted, however in some cases large floppy molcules may require an adjustment. This setting is in kcals/mol.

[Default=15.0]

4.6 Usage Notes

4.6.1 Minimum Requirements

At the minimum, FLYNN requires a density file and a the connection table of the ligand - usually derived from a supplied molecule file e.g. .pdb, .sdf, .mol2, .smi. FLYNN automatically searches the density for volumes of unmodeled density that are similar in size to the input ligand. Because of this it is highly recommended that a protein is also input to FLYNN. This makes the job of locating the ligand density less prone to false positives.

Based on analyzing several hundred protein/ligand combinations, the best way to use FLYNN for ligand fitting is described as follows (of course your mileage may vary):

- **Always use a protein:**

  The protein is used to identify modeled density where the ligand cannot be placed. Without this, FLYNN will identify many candidate locations for placing the ligand that will need to be analyzed.

> **Note**
>
> **Working with data from Cryo-electron Microscopy (cryoEM):** FLYNN searches for "blobs" in the density after masking out the protein – it is in these "blobs" that FLYNN attemps to place ligands. For users working with cryoEM data, this means that, e.g., un-modeled density associated with the phospho-lipid membrane in membrane-bound structures will be (mis-)identified as potential binding site(s) for ligands. Our recommendation would be to either use volume segmentation tools to construct a mask for the membrane and mask out this portion of the map prior to feeding the map into FLYNN; or, to simply ignore the ligands placed in to this region (though, if there are many extraneous "blobs" identified in the membrane region, this may cause the program to run for much longer than otherwise necessary). The same general note can be made for regions of the map associated with proteins or other cofactors in a complex that are unmodelled: these regions should be masked out of the map prior to analysis with FLYNN, if possible.

- **Use difference maps for X-ray crystallographic data when appropriate:**

  X-ray reflection data should be refined without a previous ligand conformation or generated without the ligand present. While in many cases, for X-ray data, the same result will be generated, if the ligand is fit to data refined with a previous ligand conformation, FLYNN may be biased towards the density modified by the pre-existing ligand conformation. Similarly, for cryoEM maps, structures used as input to FLYNN should be docked or refined into the map without a ligand present. If the input structure to FLYNN has a ligand present, the "blob" associated with that binding site/pose may be masked out of the map, and new prospective ligand binding poses may not be generated appropriately.

- **use fragment mode for fitting fragments**

  If you have an input cocktail, use the *-fragment* flag. This option simultaneously fits all the cocktails against density and sorts them by best fit.

4.6.2 Types of input ligands

Not all ligands can be successfully fit by FLYNN. Such types include large polypeptides or proteins, very flexible molecules, or simply molecules that contain atoms that are not present in the MMFF94s force-field.

Perhaps the most important property is rotatable bond count. Although FLYNN may be able to generate conformers for molecules with more than 20 rotatable bonds, the results of such an exercise would be dubious at best and should be taken with a grain of salt.

FLYNN will automatically check for unhandled atom types, but will gladly try and fit large molecules or proteins that contain many rotatable bonds usually with disappointing results.

> **Note**
>
> **Dangers of PDB format for ligand input** Many crystallography packages do not enforce writing out connection table or bond order information when outputting pdb files, or worse, strip them out. If bond distances are not correct FLYNN's attempt to automatically assign bond orders and atom types can be suspect. To facilitate this, FLYNN includes a *-precheck* flag that can be used to verify that the input ligand is identified correctly and for validation of the automatic bond order assignments.

4.6.3 Stereochemistry Enumeration

Compounds that contain unspecified or ambiguous definitions of stereochemistry will be preprocessed before conformational sampling to explicitly enumerate stereochemistry. Input molecules that have three dimensional coordinates inherently have stereochemistry specified, but SMILES or two dimensional SD files may have atoms (R/S) or bonds (E/Z) for which the stereochemistry is unknown or unspecified. In the case where the stereochemistry supplied is suspect, FLYNN provides an option that will completely enumerate all stereochemical centers.

The resulting ligands will be sorted based on their best fit to density regardless of the stereochemistry. That is, the best solutions will percolate to the top of the output. See `-sortAllChiral` for more details.

4.6.4 Refinement Dictionaries

Both FLYNN and its companion program WRITEDICT can generate refinement dictionaries. A refinement dictionary is needed to maintain proper ligand geometry when using external reciprocal space refinement programs such as REFMAC5 or CNS X/PLOR.

Refinement dictionaries are a list of geometrical constraints encoding used chemical bonding and molecular conformation information. They are used by various refinement packages to describe standard geometries and constraints that are used during the refinement process. The quality of the post refinement ligand conformations are directly related to the quality of the constraints [Vagin-2004].

FLYNN comes bundled with a refinement dictionary writer named WRITEDICT. WRITEDICT uses the MMFF94 forcefield to derive geometrical constraints for the input ligands or ligand-protein complexes. The output dictionaries enforce, as closely as possible, the input ligand's geometries while allowing the refinement programs to modify the geometry as needed.

WRITEDICT also automatically detects covalent bonds in pdb files and inserts the appropriate PDB LINK records and covalent bond entries in the output refinement dictionary.

4.6.5 REFMAC5 refinement dictionaries

When outputting REFMAC5 refinement dictionaries, WRITEDICT writes out a **.cif** file and a **.pdb** file. The **.pdb** file is written out for two reasons:

- **Inconsistent Hydrogen Naming**

  Some applications write out hydrogen names incorrectly in ways that cause REFMAC5 or visualization programs like coot or WinCoot to be unable to associate the hydrogens in the refinement dictionary with hydrogens in the pdb file. In the worst case, REFMAC5 will crash entirely.

  When necessary, *WRITEDICT* renames and renumbers hydrogens, if they exist, so that REFMAC5 won't crash and so the **.cif** file is consistent with the **.pdb** file.

- **Covalent Bonds**

  WRITEDICT detects covalent bonds and outputs proper LINK records in the **.pdb** file and proper covalent constraints in the **.cif** file. Without using both outputs, REFMAC5 will not detect covalent bonds during refinement.

- **Known residues**

  When WRITEDICT detects a known residue, it may remap the atom names to be canonical with the known residue (this prevents REFMAC5 from failing to refine). These new atom names are saved in the **.pdb** file that WRITEDICT outputs.

- **Input Ligands with no residue information**

  When WRITEDICT analyzes a ligand with no residue information, it assigns the whole ligand to a single residue (by default UNL). If this is not the desired outcome, the ligand must be put into **PDB** or **MOL2** format and the residues must be manually assigned.

It is highly recommended to use WRITEDICT's generated **.pdb** file in conjunction with the **.cif**.

4.6.6 Looking up known residues

WRITEDICT has an internal dictionary of known residues. By default, known residues names are retained when the graph of the known residue is exactly the same as the input residue. When this occurs, writedict can replace REFMAC5's dictionary with the MMFF94 generated dictionary. If the graphs do not match then WRITEDICT relabels the residue with a new residue name since a different dictionary needs to be created.

Options available for residue matching is as follows:

Option	Meaning
exact	Known residue and input residue graphs must match exactly.
substructure	Input residue may be a substructure of the known residue. **Cannot be used with the exact flag.**
fuzzybonds	Bond orders do not need to match
atomname	Atom names must match

Options are set using the *-strict* flag and joined with colons (:).

The default is:

```
-strict substructure:fuzzybonds
```

To reject dictionaries that do not match exactly, use:

```
-strict exact
```

However, the more permissive default setting has been known to generate invalid dictionaries on occasion. It is always safe to force exact matches.

To have WRITEDICT attempt to see if the ligand's residue has already been deposited in RCSB simply add the *-lookup* switch. This forces WRITEDICT to compare (based on the current *-strict* settings) the input residue to all known residues. This is useful if the input is from a 2D connection table, such as smiles or does not contain residue information.

4.6.7 MMFF94 versus MMFF94s forcefields

The MMFF94s forcefield is a variant of MMFF94 that emulates time-averaged structures typically observed during crystallographic structure determination, mainly planar geometries at unstrained delocalized trigonal nitrogen centers. However, there are many theoretical studies that show nitrogen centers are puckered [Halgren-VI-1999].

That being said, due to the prevalence of crystallographic examples where time averaging has occurred, many chemists erroneously consider the time-averaged structure to be correct, hence this variant is available for use.

WRITEDICT approximates the MMFF94s forcefield by enforcing planar aniline nitrogen configurations using the out of plane atom types and parameters from the MMFF94s. See the *-planarAniline* parameter to specify planar constraints.

4.6.8 FLYNN and writing CIF Files

When FLYNN is run, CIF dictionary files are always written as output. Because the dictionary files are not conformation independent, they are written as if the molecules were split into separate files whether or not the user specifies FLYNN's *-split* flag. (See the split flag in *Advanced Options* below for more details). These files are numbered, however, so that the file with the lowest number corresponds to the best scored fit ligand.

For example, consider using the *-sortBy plp* flag and getting the following output:

1nhu-poses_n001_b001_s01_c003.pdb 1nhu-poses_n002_b001_s01_c000.pdb 1nhu-poses_n003_b001_s01_c001.pdb 1nhu-poses_n004_b001_s01_c002.pdb

This indicates that the best fit to density (c000) has the second best PLP score (n001). By default the files are sorted by RSCC.

FLYNN CIF output consists of the following files:

1. a CIF file
2. a PDB file (in case atom names were remapped) or links were added.
3. an OEB file that contains the original molecule with annotations

It is safest, however, to run WRITEDICT on the output ligand and protein complex. The CIF files generated by FLYNN are primarily useful for adjusting torsions and geometries in various ligand building programs, such as coot.

4.6.9 Results on The Gold Test Set

Included in the FLYNN distribution is a copy of the protein+ligand complexes that have structures factors available from the *Electron Density Server* [Kleywegt-2004].

Along with this data set is a simple python script that can be used to fit ligands to the test data set. OpenEye has prepared the input test set as follows:

1. The Structure Factors and protein complexes were downloaded from **EDS**.
2. The ligands were separated from the proteins.
3. The protein was re-refined using the original mtz file to remove ligand bias.

A simple directory structure was created as follows:

- **pdbcode/protein.pdb** - the re-refined protein
- **pdbcode/ligand.pdb** - the original ligand
- **pdbcode/protein.mtz** - the re-refined difference map density.

The following python script was used to run FLYNN on all of the proteins. (This script is also included in the FLYNN distribution):

```
##############################################################################################
## Copyright (C) OpenEye Scientific 2007,2008,2009,2010,2011
##############################################################################################
## This script analyzes the Gold dataset shipped with the flynn distribution
import os,sys
command = "../../../bin/flynn -in %(CODE)s/ligand.pdb -map %(CODE)s/protein.mtz " \
          "-prot %(CODE)s/protein.pdb -out %(CODE)s_results.sdf " \
          "-verbose -rms -reportfile %(CODE)s.log %(REDIRECT)s %(CODE)s.out"
if sys.platform == "win32":
  REDIRECT = "2>"
else:
```

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```
  REDIRECT = "&>"
RMS = []
for file in os.listdir("."):
   print file
   if os.path.isdir(file) and len(file) == 4:
       code = file
       CMD = command % {"CODE":code, "REDIRECT": REDIRECT}
       print CMD
       os.system(CMD)
       index = None
       rmses = []
       for line in open("%s.log"%code):
          if index is None:
             index = line.strip().split(",").index("RMSD")
          else:
             rmses.append( float(line.strip().split(",")[index]) )
       if rmses:
           print "\t===>Lowest RMS", min(rmses)
```

The results of FLYNN are shown in Figure *Gold Test Set Results*. The mean RMS to the crystal structure is 0.676 Angstroms.

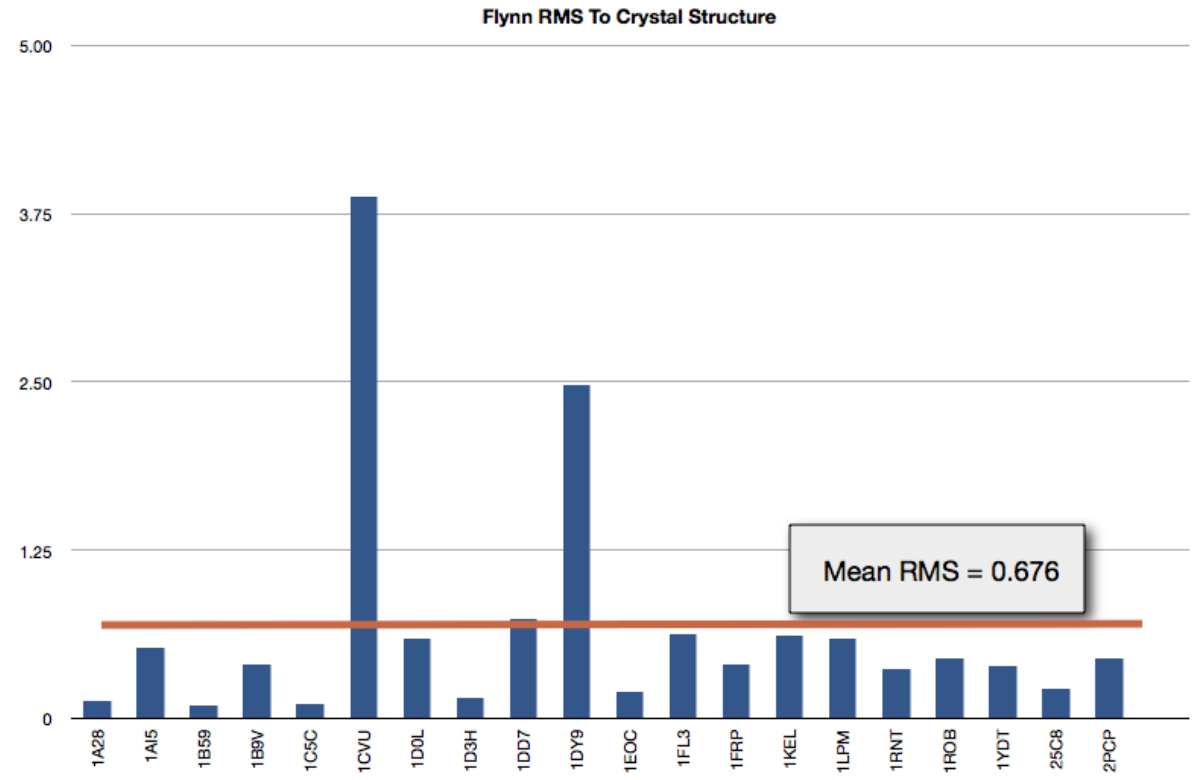


Fig. 1: **Gold Test Set Results**

CHAPTER

FIVE

COOT INTEGRATION

5.1 Overview

Due to its command line nature, AFITT-CL tools (such as FLYNN) can be integrated with other crystallographic applications such as Coot (and WinCoot). OpenEye supplies a simple script that allows users of Coot to use FLYNN directly from the Coot GUI.

This script adds "Fit Ligand…" option, a "Make cif…" and a "Fit sidechains…" options to the extensions menu.

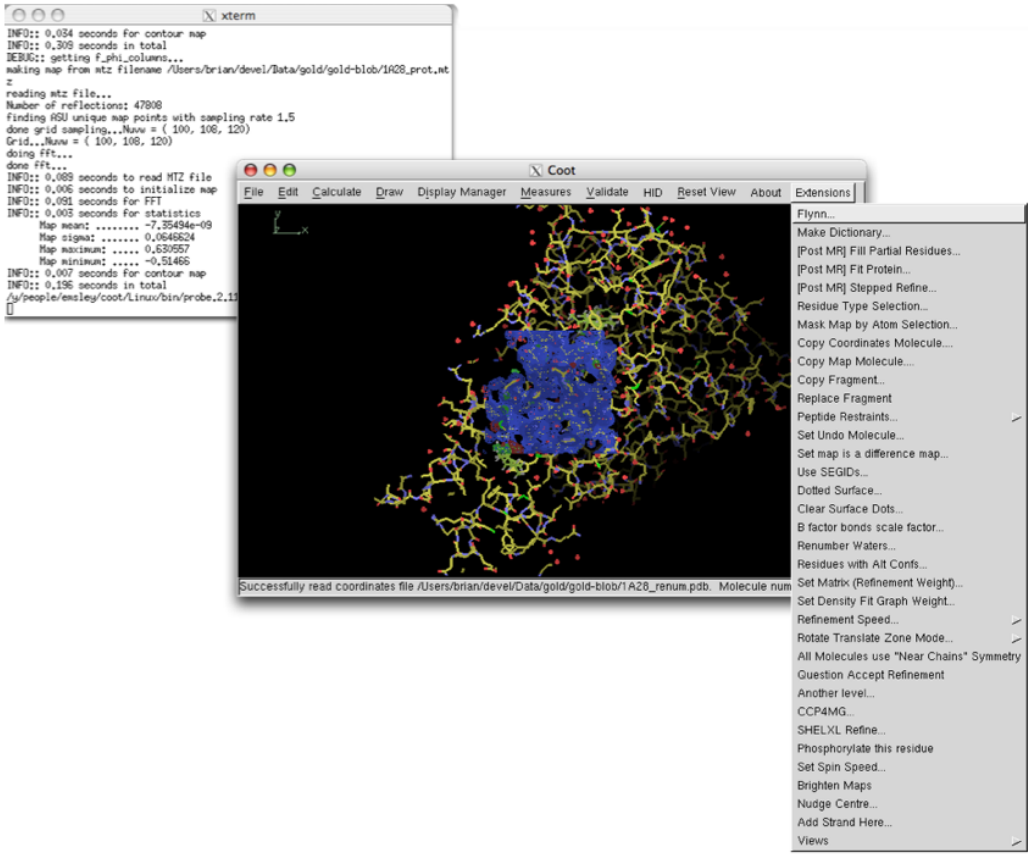


Fig. 1: **Coot Integration**

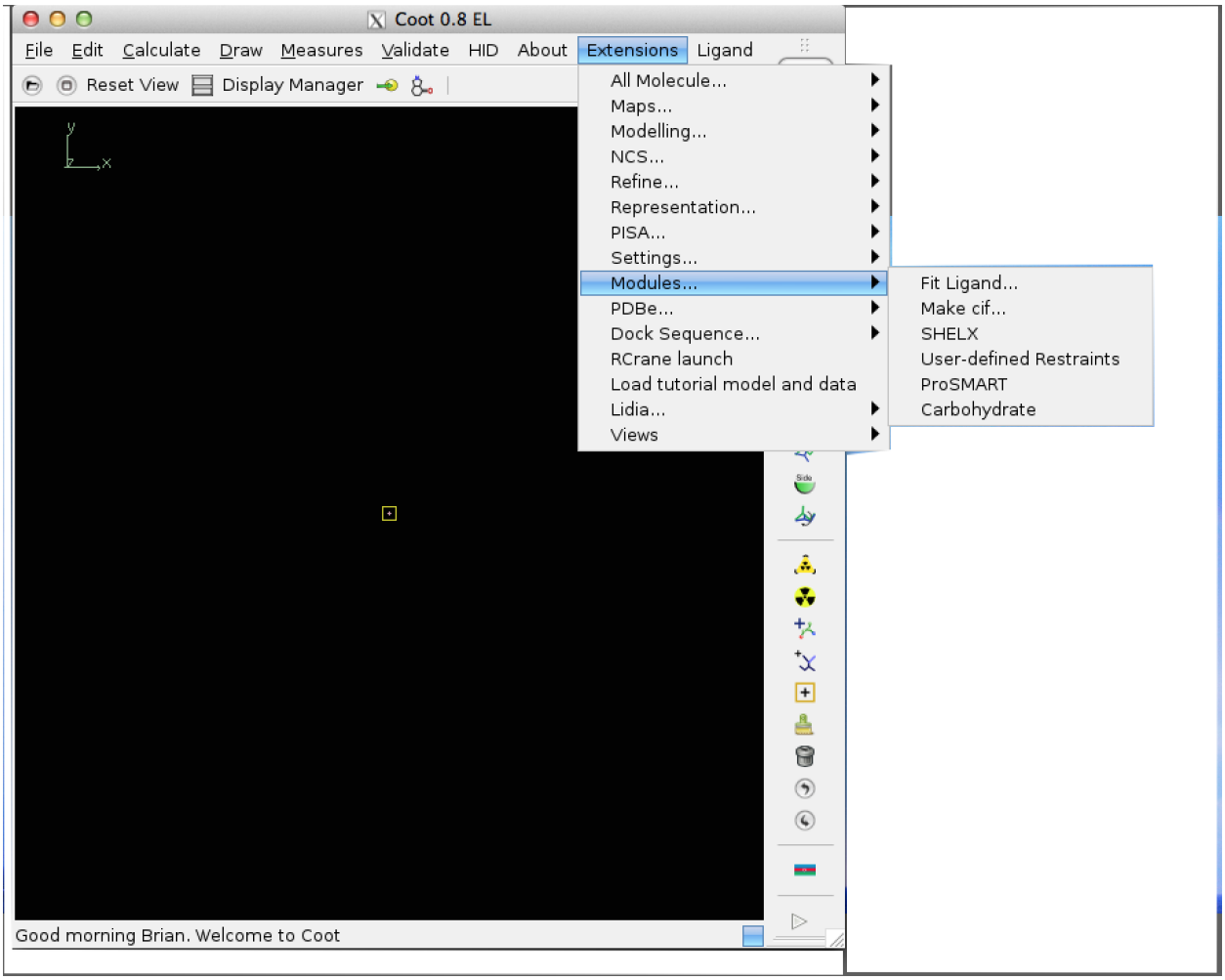


Fig. 2: **COOT 0.8 Integration**

5.2 Using FLYNN

Activating the "Fit Ligand…" menu option from the Extensions menu opens up the FLYNN dialog:

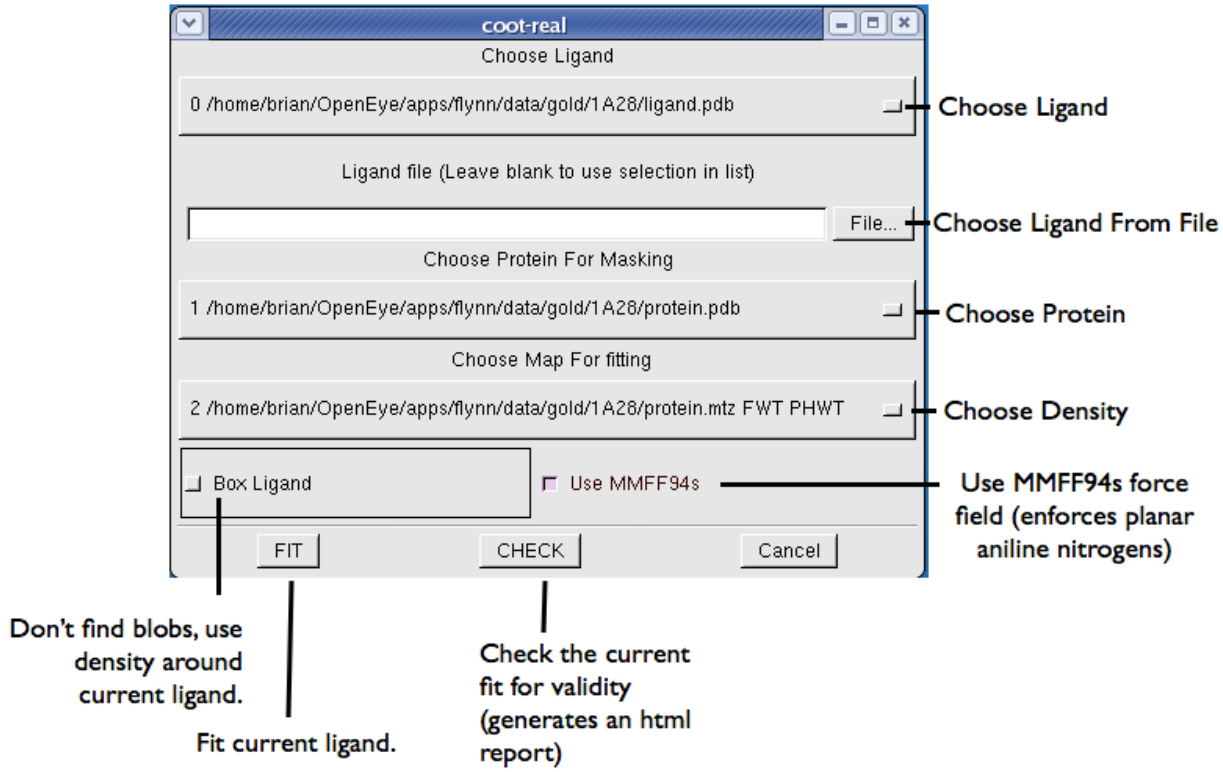


Fig. 3: **FLYNN Dialog to fit a ligand**

To use the FLYNN dialog, select the Ligand to fit from the pull-down menu. Next select the Protein and then the desired map file.

If the map is a difference map, click on the "Difference Map" to optimize the analysis. Then click on Fit.

The output of FLYNN will appear in the console window used to start coot. When FLYNN is complete, coot will automatically load the resulting ligands.

5.2.1 FLYNN Advanced Options

FLYNN's coot interface includes access to some of the advanced options contained in the application.

`-Box`

Unlike the AFITT GUI interface, coot does not have a method to select density blobs to be used for fitting. If the density is poor, flynn can use the input ligand as a bounding box to fit to the surrounding density.

`-Check`

Running check runs flynn without performing any fitting operation. When the check is completed, an html report is generated and opened in a webbrowser (if available). Since coot only display's single bonds, the report includes a depiction of the ligand being fit in order to verify that the ligand being analyzed is actually correct.

The report also indicates any problems or issues with the ligand or the map being fit against.

`-MMFF94s`

This option uses the MMFF94s variant of the MMFF94 forcefield to enforce planar aniline configurations. See the FLYNN *Advanced Options* command line flags for more details

5.3 Using WriteDict

Activating the "Make Dictionary…" menu option opens up the WriteDict dialog:

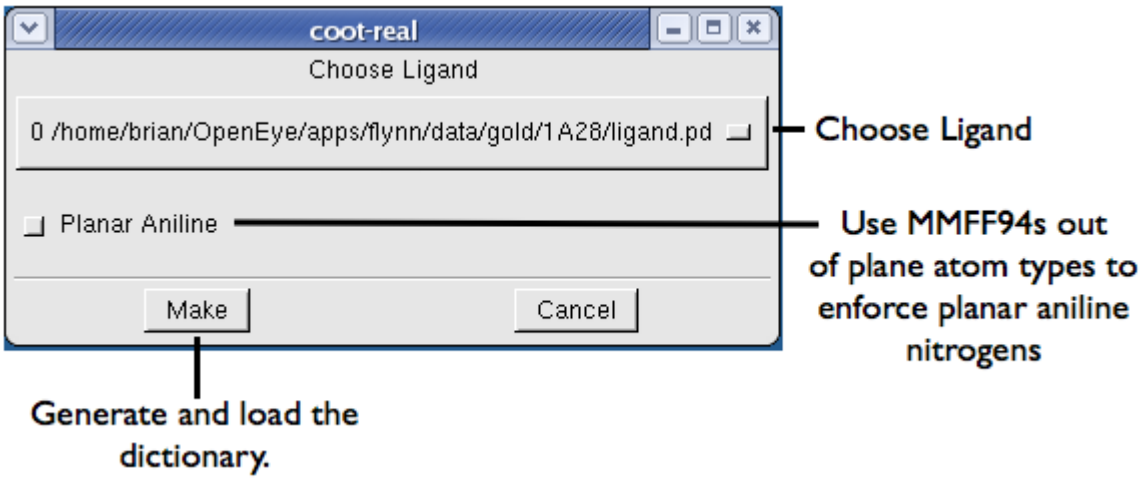


Fig. 4: **Writedict Dialog**

To use the WriteDict dialog, simply select the protein or ligand from the pull-down menu and click "ok". *Coot* will automatically open up the resulting dictionary and pdb files generated by WriteDict.

Note that new ".pdb" files are generated when using writedict, this is because hydrogen may have been relabeled and covalent *LINK* records may have been inserted into the *pdb* file.

5.3.1 WriteDict Advanced Options

FLYNN's coot interface includes access to some of the advanced options contained in the application.

5.3.2 planarAniline option

Similar to FLYNN's *MMFF94s* option, this enforces planar aniline nitrogen configurations. Note that since this is an approximation of the *MMFF94s* forcefield using planar constraints, it is not called *MMFF94s*. See the *WriteDict command line flags* for more details.

5.4 Using RotFit

Activating the "Fit Sidechains…" menu option opens up the ROTFIT dialog:

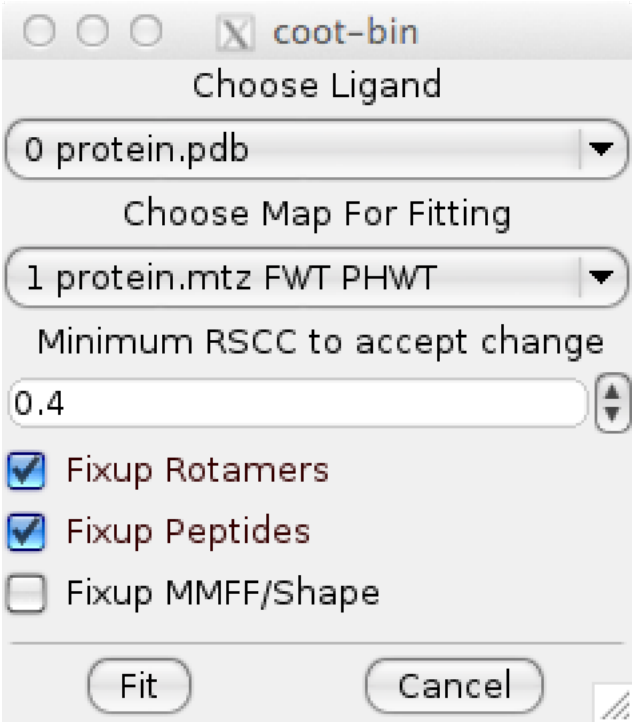


Fig. 5: **Writedict Dialog**

To use the ROTFIT dialog, a protein and mtz map must be loaded into coot. The ROTFIT interface deduces the appropriate regular and difference map to use and currently cannot handle non standard or unique column names.

5.4.1 ROTFIT options

ROTFIT is a program that fits protein side-chains into the surrounding density. It utilizes both regular and difference density to place side-chains appropriately searching both rotamers and peptide flips in addition to an optional full MMFF94-driven optimization into density.

Fixup Rotamer

Rotamer fixups selects from the probable rotamer sets to find the rotamer that best matches the surrounding density.

Fixup Pep-flip

Peptide flips are enumerated and the one that best matches the surrounding density is selected.

Fixup MMFF/Shape

Full MMFF/Shape minimization is performed on compatible residues attempting to fit the residue into the locally surrounding density.

5.5 Installing Coot Interface

5.5.1 Coot

The coot script file “flynn.scm” is included in your FLYNN distribution in the “etc” directory. The following steps are required to integrate FLYNN with coot.

The current default version of COOT is 0.9.5, to install another version please look for the files with the appropriate extension.

1. Install coot (at least version 0.3.3)
2. Install flynn and writedict somewhere in your path. If you can't run FLYNN from the command line, neither can Coot.
3. Place *flynn.scm* to the coot extensions directory. This is the directory where the files *extensions.scm* and *coot.scm* are located.

   This directory may be one of the following:

   /usr/local/coot/scheme /usr/local/xtal/coot64/share/coot/scheme/ /my_coot_installation/share/coot/scheme/ /ccp4-7.0/share/coot/scheme/ for the cpp4 installation

   on OSX the install for Coot 0.7/0.8 is most likely
   /Library/Coot/share/coot/scheme/

   Typing **which coot** may help locate these directories.
4. Copy *flynn.scm* to the extension list in *coot.scm* which is in the same directory as *extensions.scm*. Please use the appropriate file for your version of coot.

   To accomplish this, change the following code in *coot.scm* for coot 0.7

```
(define load-all-scheme
  (lambda (use-gui?)
    (let ((pre-list (list "filter.scm"
                          "coot-utils.scm"))
          (post-list (list "coot-lsq.scm"
                           "shelx.scm"
```

   to look like this:

```
(define load-all-scheme
  (lambda (use-gui?)
    (let ((pre-list (list "filter.scm"
           "coot-utils.scm"))
           (post-list (list "coot-lsq."
                            "shelx.scm"
                            "flynn.scm"
```

5. Finally, make the following changes to *extensions.scm*

   For coot 0.3.3 to 0.5 near the top of the file, change:

```
(if (defined? 'coot-main-menubar)
   (let ((menu (coot-menubar-menu "Extensions")))
```

   to become:

```
(if (defined? 'coot-main-menubar)
   (let ((menu (coot-menubar-menu "Extensions")))
     (add-simple-coot-menu-menuitem menu "Flynn..."
       (lambda () (do-flynn-gui)))
     (add-simple-coot-menu-menuitem menu "Make Dictionary..."
       (lambda () (do-flynn-gendict-gui)))
```

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```
    (add-simple-coot-menu-menuitem menu "Fit Sidechains..."
       (lambda () (do-flynn-fitsidechains-gui)))
```

For coot 0.6.x, near the top of the file, change:

```
(if (defined? 'coot-main-menubar)
    ;; ---------------------------------------------
    ;;           extensions
    ;; ---------------------------------------------
    ;;
   (let ((menu (coot-menubar-menu "Extensions")))
```

to become:

```
(if (defined? 'coot-main-menubar)
     ;; ---------------------------------------------
     ;;           extensions
     ;; ---------------------------------------------
     ;;
  (let ((menu (coot-menubar-menu "Extensions")))
     (add-simple-coot-menu-menuitem menu "Flynn..."
       (lambda () (do-flynn-gui)))
     (add-simple-coot-menu-menuitem menu "Make Dictionary..."
       (lambda () (do-flynn-gendict-gui)))
    (add-simple-coot-menu-menuitem menu "Fit Sidechains..."
       (lambda () (do-flynn-fitsidechains-gui)))
```

For coot 0.8 you should make the change to the "Modules" section as shown below:

```
;; ------------------------------------------------------------------------
;;     Modules
;; ------------------------------------------------------------------------

(add-simple-coot-menu-menuitem
 submenu-modules "Fit Ligand..."
 (lambda ()
   (do-flynn-gui)))

(add-simple-coot-menu-menuitem
 submenu-modules "Make cif..."
 (lambda ()
   (do-flynn-gendict-gui)))

(add-simple-coot-menu-menuitem
 submenu-modules "Fit sidechains..."
 (lambda ()
   (do-flynn-fitsidechains-gui)))
```

5.5.2 WinCoot 0.9.4.1+

WinCoot does not support writing extensions in GUILE. Extensions may be written in PYTHON, however.

The WinCoot scheme script file *flynn.py* is included in your FLYNN distribution in the *Data/wincoot* directory. The following steps are required to integrate FLYNN with *WinCoot*.

1. Install *WinCoot* (at least version 0.9.4.1)
2. Install flynn and writedict somewhere in your path. If you can't run FLYNN from the command line, neither can *WinCoot*.
3. Place this file *flynn.py* in the coot extensions directory where *extensions.py* is located.

   Typically, this directory is C:\WinCoot\lib\python-2.7\site-packages\coot.
4. Add *flynn.py* to the extension list in *coot_load_modules.py*. (same directory as above) *before extensions.py*

   For example:

   ```
   ...
   "get_recent_pdbe.py",
   "flynn.py",
   "extensions.py",
   ...
   ```
5. Modify the file named enhanced_ligand.py

   To add Flynn and MakeDict, find the last menu item in enhanced_ligand.py and add the following menu items below it:

   ```
   add_simple_coot_menu_menuitem(menu, "Use Flynn to Fit Ligand...", lambda func:␣
   ↪do_flynn_gui())
   add_simple_coot_menu_menuitem(menu, "Use WriteDict to generate CIF...", lambda␣
   ↪func: do_writedict_gui())
   ```

   For example, if "Display Ligand Distortions" is the last menu time, it would look like this:

   ```
   add_simple_coot_menu_menuitem(menu, "Display Ligand Distortions", lambda func:␣
   ↪display_ligand_distortions_func())
   add_simple_coot_menu_menuitem(menu, "Use Flynn to Fit Ligand...", lambda func:␣
   ↪do_flynn_gui())
   add_simple_coot_menu_menuitem(menu, "Use WriteDict to generate CIF...", lambda␣
   ↪func: do_writedict_gui())
   ```

   This results in the Ligand menu being updated to include Flynn's functionality

5.5.3 WinCoot 0.3.3 to 0.8.9.2

WinCoot does not support writing extensions in GUILE. Extensions may be written in PYTHON, however.

The WinCoot scheme script file *flynn.py* is included in your FLYNN distribution in the *utilities/flynn/wincoot* directory. The following steps are required to integrate FLYNN with *WinCoot*.

1. Install *WinCoot* (at least version 0.3.3)
2. Install flynn and writedict somewhere in your path. If you can't run FLYNN from the command line, neither can *WinCoot*.
3. Place this file *flynn.py* in the coot extensions directory where *extensions.py* is located.

   Typically, this directory is *C:WinCootsharecootscheme*.

4. Add *flynn.py* to the extension list in *coot_load_modules+gui.py*. (same directory as extensions.py) *before extensions.py*

   For example:

```
"coot-gui.py",
"flynn.py",
"extensions.py",
```

5. Add the following lines to the file named extensions.scm (this will be in your coot distribution)

   The easiest place to put this right after the line

```
menu = coot_menubar_menu("Extensions")
```

   here are the lines to add:

```
add_simple_coot_menu_menuitem(menu, "Fit Ligand...", do_flynn_gui)
add_simple_coot_menu_menuitem(menu, "Make CIF...", do_writedict_gui)
add_simple_coot_menu_menuitem(menu, "Fit Sidechains...",
  do_fitsidechains_gui)
```

CHAPTER

SIX

UTILITIES

6.1 AlignGrid

6.1.1 Overview

The **AlignGrid** utility aligns proteins with electron-density maps on a single reference.

6.1.2 Example Commands

```
> aligngrid -grid input.ccp4 -query protein1.pdb \
            -target protein2.pdb -out output.ccp4
```

Take the input grid in ccp4 format and protein. Align protein1 to protein2 and rotate and translate the input grid using the same alignment outputting the result to *output.ccp4*.

6.1.3 Command Line Help

A description of the command line interface can be obtained by executing **AlignGrid** with the *–help* option.

```
> aligngrid --help
```

will generate the following output:

```
Help functions:
  aligngrid --help simple      : Get a list of simple parameters
  aligngrid --help all         : Get a complete list of parameters
  aligngrid --help <parameter> : Get detailed help on a parameter
  aligngrid --help html        : Create an html help file for this program
```

6.1.4 Required Parameters

-grid

Input density grid. This is the grid that is to be rotated and translated into the new reference frame.

[Aliases=**-density**]

-out

The output grid in any writable format. These include **.ccp4**, **.map** and **.grd**

-protein

The query protein that corresponds to the input grid.

[Aliases=**-query**]

`-target`

The target protein that the grid and query protein will be aligned toward.

6.1.5 Optional Parameters

`-outprot`

An optional file to output the query protein after it is translated and rotated into the new reference frame.

`-padding`

When writing out a **.grd** file, this indicates the added extents (in Ångströms around the protein when outputting the density. [Default=4.0]

[Aliases=**-pad**]

`-scale`

The final map spacing in Ångströms. [Default=1.0]

`-verbose`

Triggers copious logging output. [Default=false]

The allowed MTZ map types and the corresponding column conventions are documented in OEReadMTZ in the **OEChem TK** manual.

`-autoMTZ`

Automatically try to open the mtz file using the DELWT and FDELWT columns from REFMAC5 mtz files.

See OESystem::OEMTZMapType::Fdelwt for the corresponding difference-map type in **OEChem TK**.

[Default=true]

`-Fc` <columnname>

Column to use for Fc. *Note, to load arbitrary columns, you can use the* *-Fc** and **-Phic** columns and the **Fc** maptype.*

[Default=FC]

`-Fdelwt` <columnname>

Column to use for Fdelwt or difference map amplitudes

See OESystem::OEMTZMapType::Fdelwt in **OEChem TK** for map type details.

[Default=DELFWT]

`-Fobs` <columnname>

Column to use for FObs.

[Default=F]

[Aliases=**-Fo**]

`-Phi` <columnname>

Column to use for Phi.

[Default=PHI]

`-Fwt` <columnname>

Column to use for Fwt or regular map amplitudes.

See OESystem::OEMTZMapType::Fwt in **OEChem TK** for map type details.

[Default=FWT]

-Phic <columnname>

Column to use for Phic.

[Default=PHIC]

-Phidelwt <columnname>

Column to use for Phdelwt or difference map phases.

[Default=PHDELWT]

-Phiwt <columnname>

Column to use for Phwt or regular map phases.

[Default=PHWT]

-mtype

The map type to use for fitting. Fo-Fc, Fc, 2Fo-Fc, 3Fo-Fc, Fwt, Fdelwt...

See OEReadMTZ for the full list of map types and their MTZ-column interpretation.

[Default=Fdelwt]

6.2 RotFit

6.2.1 Overview

RotFit is a side-chain fitting tool that quickly fits sidechains to the surrounding density. Currently only a MTZ file can be used for density Side chains can be fit using several techniques:

1. Using the most probably rotamers and ranking based on real space correlation (RSCC) to the density.
2. pep-flipping the rotamer and ranking on RSCC.
3. Full MMFF/Shape fitting in to the density.

By default **RotFit** searches the rotamers and pep-flips.

For **RotFit** to apply a changed residue, their has to have an increase in RSCC and be above a minium value (currently 0.4). Additionally, the RSCC must be greater by a minimum amount (0.05).

6.2.2 Example Commands

6.2.3 Command Line Help

A description of the command line interface can be obtained by executing ROTFIT with the *–help* option.

```
> rotfit --help
```

will generate the following output:

```
Help functions:
  rotfit --help simple      : Get a list of simple parameters
  rotfit --help all         : Get a complete list of parameters
  rotfit --help defaults    : List the defaults for all parameters
  rotfit --help <parameter> : Get detailed help on a parameter
  rotfit --help html        : Create an html help file for this program
  rotfit --help versions    : List the toolkits and versions used in the application
```

6.2.4 Required Parameters

-in <proteinfile>

Input protein structure. The side chains of this protein will be optimized.

[Aliases=**-prot**,**-protein**]

-map <mtz file>

The input MTZ file to fit side chains against.

[Aliases=**-grid**,**-density**]

-out <protein>

The protein structure with optimized side chains will be outputted to this file.

-param <parameter filename>

A parameter file is a text file that lists parameter settings to be used during a run. If a parameter is specified both on the command line and in the parameter file, the value specified on the command line is used.

The format of the parameter file is as follows:

- One parameter per line.
- For non-list parameters one key-value pair per line.
- For list parameters a key followed by all the values.
- Boolean parameters must be listed as a key followed by true or false.
- The parameter file may not contain the *-param* parameter.
- Lines beginning with # are considered comments.

[Aliases=**-com**]

-verbose <true or false>

Ouptuts copious extra information.

[Default=false]

6.2.5 Optional Parameters

-fixup_rotamers <true or false>

Search the most probable rotamers and choose the one that fits best to the surrounding density.

[Default=true]

[Aliases=**-fixup-rotamers**]

-fixup_pepflips <true or false>

Search the pep-flips and pick the one that fits best to the surrounding density.

[Default=false]

[Aliases=**-fixup-pepflips**]

-fixup_shapefit_residues <true or false>

Use MMFF/Shape to fit the residue into the surrounding density. Normally it is best to use **-fixup_rotamers** in conjunction with this flag.

[Default=false]

[Aliases=**-fixup-shapefit-residues**]

-minimum_rscc <number>

For a give residue if the best tested RSCC of any conformation is below this value the residue will not be modified. This prevents optimization from happenening when the is no density anywhere near the side chain.

[Default=0.4]

-minimum_rscc_increase <number>

For a given residue if the best tested RSCC of any conformation is not this much better than the starting conformation, then the residue will not be modified.

[Default=0.05]

[Aliases=**-increase**]

-autoMTZ <true or false>

Automatically try to open the mtz file using the DELWT and FDELWT columns from REFMAC5 mtz files.

See OEReadMTZ and OESystem::OEMTZMapType::Fdelwt in **OEChem TK** for map and column conventions.

[Default=true]

-Fc <columnname>

Column to use for Fc. *Note, to load arbitrary columns, you can use the* *-Fc** and **-Phic** columns and the **Fc** maptype.*

[Default=FC]

-Fdelwt <columnname>

Column to use for Fdelwt or difference map amplitudes

See OESystem::OEMTZMapType::Fdelwt in **OEChem TK** for map type details.

[Default=DELFWT]

-Fobs <columnname>

Column to use for FObs.

[Default=F]

[Aliases=**-Fo**]

-Phi <columnname>

Column to use for Phi.

[Default=PHI]

-Fwt <columnname>

Column to use for Fwt or regular map amplitudes.

See OESystem::OEMTZMapType::Fwt in **OEChem TK** for map type details.

[Default=FWT]

-Phic <columnname>

Column to use for Phic.

[Default=PHIC]

-Phidelwt <columnname>

Column to use for Phdelwt or difference map phases.

[Default=PHDELWT]

-Phiwt <columnname>

Column to use for Phwt or regular map phases.

[Default=PHWT]

-SigmaA <columnname>

Column to use for SigmaA.

6.3 Rscc

6.3.1 Overview

RSCC is a real-space fit calculation tool both real-space correlation coefficient (rscc) and real-space R-factor (rsr). By default this tool calculates rscc. RSCC was designed to be a standalone tool using the same code that is used for ligand fitting by AFITT.

6.3.2 Example Commands

6.3.3 Command Line Help

6.3.4 Required Parameters

-in <molecule file>

Input molecule(s) to be scored against the density

[Aliases=**-prot**]

-mtz <mtz file>

Input MTZ file to be used for calculations. Currently only MTZ format is supported.

[Aliases=**-density**,**-map**]

6.3.5 Optional Parameters

-clamp_at_level

Set an electron density contour sigma level (positive) to be used for calculating rsr values. [Default=0.0]

[Aliases=**-level**]

-flatten

Flatten B-factors (20.0) of the input molecule. This flag is to be used with the –scatter flag. [Default=false]

-rsr

Use rsr instead of rscc. [Default=false]

-scatter

Calculate Fc (calculated) density from the input molecule. [Default=false]

-verbose

This triggers copious logging of output to the screen. [Default=false]

6.4 WriteDict

6.4.1 Overview

WriteDict is a comprehensive refinement dictionary generator that properly handles covalent bond restraints between the ligand and the protein.

6.4.2 Example Commands

The basic usage of writedict is to take an input structure and generate the corresponding .pdb and .cif files for input into COOT or REFMAC5.

```
> writedict -in 1nhu.ism -out 1nhu_out
```

This creates the files *1nhu_out.cif* and *1nhu_out.pdb*. The pdb is always created since the atom names may be remapped from the input. Since the input contains no residue information, the ligand is placed in residue "UNL".

To add your own residue names for unmapped residues:

```
> writedict -in 1nhu.ism -out 1nhu_out -residues 153
```

Note that if the given residue name (153) does not map to the known residue 153 the next residue name in the unmapped residue list will be used. Since none are specified it will go to the standard defaults: "UNL,UN1,UN2…"

Note

When doing whole complexes, renaming residues gets quite complicated since you may not know which residues will map before you run WRITEDICT.

```
> writedict -in 1nhu.ism -out 1nhu_out -residues LIG -nolookup
```

Force the residue to be named LIG. (It will also indicate an invalid dictionary)

```
Warning: LIG   1: Known Residue, but does not map to previous residue: LIG from: RCSB
Warning: LIG   1: previous smiles c1ccc2c(c1)CC3=C(NN=C23)c4ccncc4
Warning: LIG   1: current  smiles c1ccc(cc1)CC(C(=O)[O-
↪])N(Cc2cccc(c2)C(F)(F)F)C(=O)c3ccc(cc3Cl)Cl
Warning: LIG: Keeping residue name (dictionary may be invalid)
Warning: LIG: Adding new residue dictionary
Warning: LIG: already in dictionary from: RCSB but with different structure.
Warning: LIG: c1ccc2c(c1)CC3=C(NN=C23)c4ccncc4
Warning: LIG: c1ccc(cc1)CC(C(=O)[O-])N(Cc2cccc(c2)C(F)(F)F)C(=O)c3ccc(cc3Cl)Cl
Warning: LIG: Overwriting existing residue (dictionary may be invalid)
```

To ensure planarAniline constraints consistent with the MMFF94s forcefield, use the *-planarAniline* flag.

```
> writedict -in 1nhu.ism -out 1nhu_out -planarAniline
```

6.4.3 Command Line Help

A description of the command line interface can be obtained by executing WRITEDICT with the *–help* option.

```
> writedict --help
```

will generate the following output:

```
Help functions:
  writedict --help simple      : Get a list of simple parameters
  writedict --help all         : Get a complete list of parameters
  writedict --help <parameter> : Get detailed help on a parameter
  writedict --help html        : Create an html help file for this program
```

6.4.4 Required Parameters

-in <filename>

File containing a molecule to be fit to density.

[Aliases=**-prot**]

File type	Extension
SMILES	.smi .ism .smi.gz .ism.gz
OEBinary	.oeb .oeb.gz
SDF	.sdf .mol .sdf.gz .mol.gz
MOL2	.mol2 .mol2.gz
PDB	.pdb .ent .pdb.gz .ent.gz
MacroModel	.mmod .mmod.gz

-out <filename prefix>

This specifies a prefix for outputting the refinement dictionary **.cif** or **.xplor** and the **pdb** file. The pdb file (and pdb.oeb) is always output and should be used for purposes of refinement since WRITEDICT sometimes corrects faulty hydrogen atom names and will include LINK records in the pdb if covalent bonds are detected.

The log file will also be written using this prefix as <*filename prefix*>.*log*.

-prefix <filename prefix>

Alias for *-out*

6.4.5 Optional Parameters

-assignCCP4

If true then CCP4 atom types will be assigned to the output pdb file.

[Default=true]

-includeRotors

Set to true if the output should include rotor torsion terms. If this is set to false, refinement programs will not be able to modify any rotors.

[Default=true]

-suppressH

If true, no hydrogens are output.

[Default=false]

-dictionary_type

Selects the output refinement dictionary format:

Value	Meaning
0 / refmac	REFMAC5 dictionary (default)
1 / xplor	CNS/CNX (XPLOR) dictionary
2 / phenix	PHENIX dictionary
3 / buster	BUSTER dictionary

[Default=refmac]

[Aliases=**-type**]

`-planarAniline`

Use the MMFF94s variant of the MMFF94 forcefield. This forcefield emulates time-averages structures observed in crystallographic and other structure determination methods.

The MMFF94s forcefield is a variant of MMFF94 that emulates time-averages structures typically observed during crystallographic structure determination, mainly planar geometries at unstrained delocalized trigonal nitrogen centers. However, there are many theoretical studies that show puckering at nitrogen centers. (see MMFF VI. in JCICS)

That being said, due to the prevalence of crystallographic studies, many chemist erroneously consider the time-averaged structure to be correct, hence this variant is available for use.

[Default=true]

[Aliases=**-mmff94s**]

`-strict`

Change the known residue matching mode.

Options available for residue matching is as follows:

Option	Meaning
exact	Known residue and input residue graphs must match exactly.
substructure	Input residue may be a substructure of the known residue. **Cannot be used with the exact flag.**
fuzzybonds	Bond orders do not need to match
atomname	Atom names must match

Options are separated by colons. The default settings are set to limit the number of REFMAC5 issues. -strict exact:substructure will find more matches, but increases the risk of REFMAC5 rejecting the dictionary.

[Default=substructure:fuzzybonds]

`-lookup`

Attempts to lookup residues from the internal dictionary store using the current -strict status. This is useful to find out if a residue has already been deposited in the RCSB.

If -lookup is not set, mismatching residues will be given new names. [Default=false]

`-forceExistingResidueNames`

Force WRITEDICT to use the given residues, even if they do not match the deposited residues from the RCSB.

[Default=false]

[Aliases=**-nolookup**,**-force**]

`-writeFullDict`

If true then all refinement dictionaries are created for all residues. If false only residues that are unknown or are in the set of replaceable residues or covalently bound to a ligand are output. Setting this to true can confuse REFMAC5.

{default=false]

`-residues`

Comma-separated list of default residue names to assign to unknown components.

[Aliases=**-resnames**,**-res**]

-split

Split separate molecules (and bonded covalent structures) into different dictionaries. [Default=false]

-fix_serial_numbers

Fix serial numbers if there are duplicates in the input files. [Default=false]

-fixResidueHydrogens

If a residue has more hydrogens than the known dictionary entry, remove them. [Default=false]

-fixups

Set fixups for known bugs in refinement packages. Accepts a comma-separated list. Supported value: `REFMAC560117_MODRES` (fixes LINK issues in CCP4 6.2.0 REFMAC5.6.0117; should be used with `MAKE CONNECTIVITY YES`).

-verbose

Output copious information of how writedict operates. [Default=false]

CHAPTER

SEVEN

THEORY

Current methods of ligand fitting that are based on either topological analysis of electron density [Menéndez-Velázquez-2003] global optimization of position and conformation of a ligand in a density blob [Diller-1999] interatomic distance matrix [Koch-1974] [Cascarano-1991] or on varying torsion dihedral angles of shape-matched ligand conformations [Oldfield-2001] are unable to prevent creation of high energy, sometimes even chemically unrealistic, ligand models. As a result, there are a number of PDB ligands with unlikely, very high-energy structures [Perola-2004]. For example, the PDB structure of an inhibitor of RNA polymerase in *1nhu* has significant repulsion between the two methylene groups.

FLYNN is composed of two main components, location of ligand density and ligand fitting. Location of density generally works well with clean density but there are times when ligand density is unclear or not well resolved. In the latter cases, the user should supply a bounding box or simply just input the ligand density by itself and use the density as is.

By default, FLYNN samples bioactive conformations [Boström-2001] [Boström-2003] of the input ligand, however, there are times when it might be desirable to input the ligand and use it as is (see section *Required Parameters* for more details).

Once the location of the ligand in the map and the conformations have been selected, FLYNN then adapts the initial conformations to the ligand density using a modern force-field, MMFF94 [Halgren-I-1996] [Halgren-II-1996] [Halgren-III-1996] [Halgren-IV-1996] [Halgren-V-1996] [Halgren-VI-1999] [Halgren-VII-1999]

The potential function being used to adapt the ligand is

$$V = V_{ff} + \lambda V_{shape}$$

where V_{ff} represents the internal energy of the ligand and V_{shape} is the overlap between the ligand and the electron density. λ is a mixing parameter that represents the degree to which the shape of the density dominates the combined potential during the current optimization step [Wlodek-2006].

The strain placed on the ligand is bounded while the function is optimized producing high-quality fits with low-strain ligand conformations.

7.1 Fragment Fitting

Fragments are fit taking the input fragment cocktail and, one at a time, fitting each fragment against each region of detected density. Once a fragment has been placed, it is further analyzed to ensure that all possible orientations of the fragment have been sampled. In poor density, several orientations may fit equally well. To break ties, FLYNN scores each pose with the following scores:

o RSCC (real space correlation coefficient) This is a measure of fit to electron density (higher is better). [Jones-1991]

o PLP Piecewise-linear potential (lower is better). [Verkhivker-2000]

o Chemscore (lower is better). [Eldridge-1997]

The docking scores are not used to fit the molecule, they are only used to rank the output. Unless highly symmetric molecules are being input, the real space correlation coefficient (RSCC) is the preferred method of ranking results to density.

To use fragment mode, please add the "-fragment" option to the command line. In future versions of FLYNN, this will most likely become the default setting.

The output of the fragment fitting process is a file for each density region that includes the fragments fit to the region sorted from best-fit to worst fit. For example:

```
prompt> flynn -in fragments.smi -out 2IKO_cocktail.sdf ...
```

would result in the files:

```
2IKO_cocktail_blob001.sdf
2IKO_cocktail_blob002.sdf
2IKO_cocktail_blob003.sdf
```

one for each blob found. By default, the first molecule in the file is the best fit to the density (RSCC):

$$RSCC = \frac{\Sigma|p_{obs} - <p_{obs}>|\Sigma|p_{calc} - <p_{calc}>|}{(\Sigma|p_{obs} - <p_{obs}>|^2 \Sigma|p_{calc} - <p_{calc}>|^2)^{\frac{1}{2}}}$$ [Jones-1991]

where obs refers to the experimental electron density and calc refers to the calculated electron density sampled from grid points around the residue being scored. The experimental density is usually the sigma weighted difference map when loading an MTZ map. The calculated density is generated by simulating scattering of the ligand conformation with bfactors set to 20.

To sort using another measure, for instance, PLP, use the sort flag:

```
prompt> flynn -sortBy plp -in fragments.smi -out 2IKO_cocktail.sdf ...
```

Note

The *-sortBy* flag can be used in non-fragment mode as well.

CHAPTER

EIGHT

RELEASE HISTORY

8.1 FLYNN 3.0.4

Minor internal improvements have been made.

8.2 FLYNN 3.0.3

Minor internal improvements have been made.

8.3 FLYNN 3.0.2

Minor internal improvements have been made.

8.4 AFITT 3.0.1

Minor internal improvements have been made.

8.5 AFITT 3.0.0

8.5.1 New Features

- **FLYNN** can now handle maps from cryo-electron microscopy (cryo-EM) natively. Maps from cryo-EM in the *.mrc*, *.ccp4*, or *.map* file formats can be input using the *-map* map command-line parameter, alongside the protein structure file (*-prot*) docked/refined into the map and the 2D or 3D ligand information for the molecule to be modeled (*-in*).

8.6 AFITT 2.6.5

- An issue was fix that caused a ligand to sometimes have a set of incorrect protein residue names assigned.

8.7 AFITT 2.6.4

Minor internal improvements have been made.

8.8 AFITT 2.6.3

Minor internal improvements have been made.

8.9 AFITT 2.6.2

Fall 2022

Minor internal improvements have been made.

8.10 AFITT 2.6.1

Spring 2022

- Multiple typos were fixed in **Flynn** command line help.
- Multiple typos were fixed in **WriteDict** command line help.

8.11 AFITT 2.6.0

Fall 2021

8.11.1 New features

- The REFMAC dictionary writer now inlcudes molecule coordinates in the CIF keys _chem_comp_atom.{x,y,z}.

8.12 AFITT 2.5.3

July 2021

8.12.1 Minor Bug Fixes

- Minor deprecation warnings have been removed.

8.12.2 Documentation Changes

- Updated documentation to support newer WinCoot version (0.9.4.1 and beyond)

8.13 AFITT 2.5.2.0

Fall 2020

- Minor internal improvements have been made.

8.14 AFITT 2.5.1

Spring 2020

- This version of **AFITT** has been built using **OEToolkits 2020.0**.
- The **AFITT** GUI is not available as part of the 2020.0 release.

8.15 AFITT 2.5.0

Nov 2019

- This is the first inclusion of **AFITT** applications in the **OpenEye Applications** bundle. They have been built using **OEToolkits 2019.Oct**.
- The **AFITT** GUI is not available as part of the **2019.Nov** release.

8.16 AFITT-CL 2.4.1

March 2017

8.16.1 Platform Support

- Support has been added for Ubuntu 16, OSX 10.10, OSX 10.11, and OSX 10.12.
- OSX 10.7, OSX 10.8, OSX 10.9, SuSe 11, and Redhat 5 x86 are no longer supported.

8.16.2 Coot Support

- Support has been added for Coot 0.8.
- Coot versions 0.6 and earlier are no longer supported.

8.16.3 Bug Fixes

- A bug in WRITEDICT that caused inappropriate bond lengths to be written for some cyclic systems has been fixed. Originally, WRITEDICT outputted the MMFF bond potential minimum as the bond length. However, for aromatic rings this value is inappropriately large since MMFFs angle and torsion potentials also affect the bond length significantly. In these cases, the equilibrium bond lengths are used by WRITEDICT.
- A bug that caused PDB remark data that was more than 72 characters long to be clipped from the refined output has been fixed. Practically, this only occurred when the input and output file formats were both PDB.
- On Windows, the default "save" location has been changed from C:Program Files (x86)AFITT 2.4.0 to the Users Home directory.
- Previously, if an older version of AFITT was installed on Windows, users could not overwrite the old preferences. This issue has been fixed.
- A crash that occurred on Windows 10 after selecting the Refmac option without a locally installed copy of Refmac has been fixed.
- The AFITT suite ships with a simple Python-based do_gold.py test script, to make sure AFITT-CL (FLYNN) is functioning as intended. This script analyzes the Gold dataset (protein+ligand complexes) available from the Electron Density Server (EDS) and included with the distribution. The do_gold.py test script has been modified to run correctly with either Python 2 or Python 3.

8.17 AFITT-CL 2.4.0

November 2014

- Add helper programs to allow ligand forcefields during refinement for PHENIX and BUSTER
- Updated PHENIX support, including covalent bond support
- Alter the protein masking to not remove density that may be created by hydrogen or covalent bonds. This was causing density very close to the protein to be truncated and hard to find automatically.

8.17.1 Platform Support

- Added support for RedHat 7, Ubuntu 14 and OSX 10.9
- Dropped support for RedHat 5 32 bit, Ubuntu 10 and OSX 10.6
- This will be the last release for SuSe 11

8.17.2 FLYNN

- Alter the protein masking to not remove density that may be created by hydrogen or covalent bonds. This was causing density very close to the protein to be truncated and hard to find automatically.
- -box is now called -manualSearch (-box still works)
- -blobsThenBox is now called -autoThenManualSearch for clarity (-blobsThenBox still works)
- -ciftype now follows the new writedict convention (accepts both numeric and more readable names such as "refmac", "xplor")
- -ciftype parameter is now in the correct parameter section (Advanced not Fragment)
- FLYNN always fixes serial numbers when writing CIF output to better enable use in workflow situations. These can be caused when hydrogens are added to ligands outside the context of the protein for instance.

8.17.3 WRITEDICT

- AFITT now Post-processes equilibrium angles to see if they are compatible with geometric forcefields. If they are not, replace them with fully MMFF optimized angles. This mostly affects 6-5 aromatic systems, but is a general fix ensuring the geometric force-field will work properly given the constraints in the CIF dictionary.
- Writedict now properly fail if the input protein has duplicate serial numbers. Most refinement programs cannot handle this state.
- Prevent duplication of CRYST1 records in the writedict output.
- Always output disulfide bridges if input
- Never rename standard residues hydrogens, this was causing Markly naming violations.
- Fix phenix covalent link output when covalently linking two residues of the same residue type.
- WRITEDICT no longers fails if input standard residues have alternate conformations with different graphs.
- WRITEDICT now defaults to MMFF94s
- WRITEDICT now understands human readable names for the dictionary type, i.e. -type refmac as opposed to -type 0
- WRITEDICT now has a -fix_serial_numbers flag that corrects duplicate serial numbers in the resulting pdb output

8.17.4 ROTFIT

- Added rotfit rotamer driving command line program. This used to live entirely in the GUI.

8.18 AFITT-CL 2.3.0

July 2013

8.18.1 Other

Note: Last release for SUSE Linux Enterprise 10.

8.18.2 WRITEDICT

- Hydrogen naming is now consistent with RSCB standards.
- added -prefix flag for controlling report and logging generation

8.18.3 FLYNN

- Optimization fixes for molecules with high strain.
- Better default ligand density location.
- Optional PM3 and AM1 ligand minimization (see the -ff flag).
- Fixed symmetry operations on cubic lattices.
- added -prefix flag for controlling report and logging generation.

8.18.4 COOT Integration

- Better error message when the ligand and protein are set to the same coordinates
- Added ability to choose both chain id and residue name for the fit ligand.

8.19 AFITT-CL 2.2.0

August 2012

8.19.1 WRITEDICT

- Updated to support REFMAC 5.6 and 5.7 (CCP4 6.3.0)
- Monomers updated to current RCSB and CCP4 releases.
- PDB LINK records are validated to be in the correct order. This validation is required for REFMAC 5.6 and up.

8.19.2 FLYNN

- Bugfixes and general speedups applied to internal optimizer.
- A memory leak in the optimzer was fixed.

8.20 AFITT-CL 2.1.1

December 2011

8.20.1 WRITEDICT

- Added PHENIX suppoert
- Monomers in CIF files are given IUPAC names when possible
- Updated dictionaries to support REFMAC5 in CCP4 6.2.0

8.20.2 FLYNN

- Added PHENIX suppoert
- Fixed issues where ligands fit in poor density could be overstrained.

8.21 AFITT-CL 2.1.0

July 2011

8.21.1 WRITEDICT

- Updated internal REFMAC and RCSB to current versions.
- When remapping dictionaries, WRITEDICT now indicates where the matching monomer was sourced.
- Moved "lookup" out of the -strict settings to a new flag "-lookup" adding this switch will search for a matching monomer from the internal libraries using the current -strict settings.
- -force options added. WRITEDICT will output the residue name even if it doesn't match the internal list of known monomers.
- Various corrections to aniline nitrogen dictionaries.

8.21.2 FLYNN

- FLYNN now sorts the output fits based on real space correlation coefficient if applicable (RSCC)
- FLYNN now can automatically fit fragment cocktails. (use -fragment flag)
- FLYNN adds additional scores to all ligands besides the default MMFF Tanimoto/Shape, these are RSCC (Real space correlation coefficient), PLP (Piecewise-linear potential, requires protein) and Chemscore (requires protein).
- -resname now forces the ligand to use the given residue name even if it conflicts with the internal monomer library.
- -chainid Output the ligands with the given chain id.

8.22 AFITT-CL 2.0.1

September 2010

Package renamed from FLYNN to AFITT-CL. None of the internal programs have been renamed. AFITT and AFITT-CL will be released simultaneously with the same version numbers from this point forward.

8.22.1 WRITEDICT

- Added correct dictionary creation including connection table. This is required for newer versions of *coot*
- CIF dictionaries properly encode all LINK records.
- CIF dictionaries now encode proper planarity for guanine and no longer have duplicate planar atoms when using MMFF94s.
- CIF Dictionaries now look up known non-peptide residues. If the residue is not consistent with the known dictionary, the residue name is changed and a new MMFF94 derived dictionary is generated.
- Updated COOT integration to 0.6+

8.22.2 FLYNN

- Enhanced automatic density location. Blobs are now slightly larger than before making better targets for fitting.
- Added experimental fragment fitting. See the documentation for more information about this command line option. For version 2.0.1 this requires the fragment feature of the FLYNN license. This requirement will be removed when this feature is considered non-experimental. If you are interested in helping us test this feature, please contact business@eyesopen.com for more details.
- Refinement dictionaries are always written out for the ligand. Please note that these are written as if the -split flag is set to true. Refer to the documentation or type "flynn –help" at the command line for more details.
- Updated COOT integration to 0.6+

8.23 FLYNN 2.0.0

February 2010

- Internal Release used with collaborators. Used for testing new dictionary formats.

CHAPTER

NINE

CITATION

Note

To cite AFITT or FLYNN please use the following:

AFITT 3.0.4.0. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.eyesopen.com/.

Wlodek, S., Skillman A.G., Nicholls A., **Automated ligand placement and refinement with a combined force field and shape potential**, Acta Cryst., Vol. D62, pp. 741-749, 2006

CHAPTER

TEN

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CHAPTER

ELEVEN

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For more information, please contact OpenEye Support.

12.1 Orion®

To cite use of Orion, please use the following:

```
Orion <version-number>. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.
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```

For example:

```
Orion 2025.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.eyesopen.com.
```

The version number for Orion appears in the product's release notes, for example, https://docs.eyesopen.com/orion-user-interface/releasenotes/index.html.

12.2 Orion Floes

To cite use of an Orion-based floe package, please use the following:

```
OpenEye <package-name> <version-number>. OpenEye, Cadence Molecular Sciences, Santa Fe,␣
↪NM. http://www.eyesopen.com.
```

For example:

```
OpenEye Large-Scale Floes 4.2.3. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
↪http://www.eyesopen.com.
```

The version number for a floe package is displayed on the first page of the package's release notes. For example: https://docs.eyesopen.com/floe/modules/large_scale_floes/docs/source/releasenotes_2025_1.html.

12.3 Toolkits and Applications

To cite OpenEye toolkits or applications used in your work, please use the following:

```
OpenEye Toolkits [or Applications] <version-number>. OpenEye, Cadence Molecular Sciences,
↪ Santa Fe, NM. http://www.eyesopen.com.
```

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```
OpenEye Toolkits 2024.2.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.
↪eyesopen.com.
```

The Applications and Toolkits are released as a package, multiple times per year. The first part of the version number designates the calendar year. The version number appears on the summary document for the package.

If you want to cite an individual application or toolkit, you can use the syntax:

```
<product name> <version-number>. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
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```

where <*product name*> is:

- Bioisostere TK
- OEChem TK
- OEDepict TK
- OEDocking TK
- OEFF TK
- Eon TK
- FastROCS TK
- Grapheme TK
- GraphSim TK
- Lexichem TK
- OEMedChem TK
- MolProp TK
- Omega TK
- Quacpac TK
- 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
- SPRUCE Application
- SZMAP Application
- SZYBKI Application
- VIDA Application

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.

12.4 Publications for Bibliographies

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

12.4.1 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

12.4.2 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

12.4.3 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

12.4.4 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

12.4.5 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

12.5 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␣
↪Fe, NM. http://www.eyesopen.com.
```

For example:

```
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

THIRTEEN

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Table 1: Licensed Technology

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_openmp_mutex	https://github.com/conda-forge/_openmp_mutex-feedstock	https://github.com/conda-forge/_openmp_mutex-feedstock/blob/main/LICENSE.txt
ablang2	https://github.com/TobiasHeOl/AbLang2	https://github.com/TobiasHeOl/AbLang2/blob/main/LICENSE
abseil-cpp	https://github.com/abseil/abseil-cpp	https://github.com/abseil/abseil-cpp/blob/master/LICENSE
absl-py	https://github.com/abseil/abseil-py	https://github.com/abseil/abseil-py/blob/main/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
aiohappyeyeballs	https://github.com/aio-libs/aiohappyeyeballs	https://github.com/aio-libs/aiohappyeyeballs/blob/main/LICENSE
aiohttp	https://docs.aiohttp.org/en/stable/	https://github.com/aio-libs/aiohttp/blob/master/LICENSE.txt
aiosignal	https://github.com/aio-libs/aiosignal	https://github.com/aio-libs/aiosignal/blob/master/LICENSE
Amazon Linux 2	https://aws.amazon.com/amazon-linux-2	N/A
AmberUtils	http://ambermd.org	N/A
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angular	https://github.com/angular/angular.js	https://github.com/angular/angular.js/raw/master/LICENSE.md
angular-animate	https://github.com/angular/angular.js	https://github.com/angular/angular.js/raw/master/LICENSE.md
angular-cache	https://github.com/jmdobry/angular-cache	https://github.com/jmdobry/angular-cache/raw/master/LICENSE
angular-cookies	https://github.com/angular/angular.js	https://github.com/angular/angular.js/raw/master/LICENSE.md

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Table 1 – continued from previous page

Name of Project	Website	License URL
angular-loggly-logger	https://github.com/ajbrown/angular-loggly-logger	https://github.com/ajbrown/angular-loggly-logger/raw/master/LICENSE.md
angular-mocks	https://github.com/angular/angular.js	https://raw.githubusercontent.com/angular/angular.js/master/LICENSE
angular-resource	https://github.com/angular/angular.js	https://raw.githubusercontent.com/angular/angular.js/master/LICENSE
angular-toggle-switch	https://github.com/cgarvis/angular-toggle-switch	https://github.com/cgarvis/angular-toggle-switch/blob/master/LICENSE
angular-ui-grid	https://github.com/angular-ui/ui-grid	https://github.com/angular-ui/ui-grid
angular-ui-router	https://github.com/angular-ui/ui-router	https://github.com/angular-ui/ui-router/raw/master/LICENSE
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antlr4-python3-runtime	http://www.antlr.org OR https://pypi.org/project/antlr4-python3-runtin	https://github.com/conda-forge/antlr4-python3-runtin/blob/master/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
anyio	https://github.com/agronholm/anyio	https://github.com/agronholm/anyio/blob/master/LICENSE
appdirs	http://github.com/ActiveState/appdirs	http://github.com/ActiveState/appdirs/blob/master/LICENSE.txt
appengine	https://google.golang.org/appengine	https://github.com/golang/appengine/blob/master/LICENSE
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arpack	https://www.caam.rice.edu/software/ARPACK/	https://www.caam.rice.edu/software/ARPACK/
arrow	https://github.com/arrow-py/arrow	https://github.com/arrow-py/arrow?tab=Apache-2.0-1-ov-file#readme
ascii85	https://github.com/huandu/node-ascii85	https://github.com/huandu/node-ascii85/raw/master/LICENSE
ase	https://wiki.fysik.dtu.dk/ase/	https://wiki.fysik.dtu.dk/ase/development/licenseinfo.html#license-info
asgiref	https://github.com/django/asgiref/	https://github.com/django/asgiref/blob/main/LICENSE

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assertions go-render	https://github.com/smartystreets/assertions/internal/go-render/render	https://github.com/smartystreets/assertions/blob/master/internal/go-render/LICENSE
assertions oglmatchers	https://github.com/smartystreets/assertions/internal/oglematchers	https://github.com/smartystreets/assertions/blob/master/internal/oglematchers/LICENSE
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async-timeout	https://github.com/aio-libs/async-timeout	https://github.com/aio-libs/async-timeout/blob/master/LICENSE
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Name of Project	Website	License URL
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babel	https://babel.pocoo.org/ OR https://github.com/python-babel/babel	https://github.com/python-babel/babel/blob/master/LICENSE OR https://babel.pocoo.org/en/latest/license.html#babel-license
Babel	https://github.com/python-babel/babel	https://github.com/python-babel/babel/blob/master/LICENSE
backcall	https://github.com/takluyver/backcall	https://github.com/takluyver/backcall/blob/master/LICENSE
backports	https://github.com/brandon-rhodes/backports	https://github.com/brandon-rhodes/backports/blob/master/LICENSE.TXT
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base62	https://github.com/kare/base62	https://github.com/kare/base62/blob/main/LICENSE
beautifulsoup4	https://www.crummy.com/software/BeautifulSoup/	https://www.crummy.com/software/BeautifulSoup/

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biotite	https://github.com/biotite-dev/biotite/blob/master/README.rst	https://github.com/biotite-dev/biotite/blob/master/LICENSE.rst
bitarray	https://github.com/ilanschnell/bitarray	https://github.com/ilanschnell/bitarray/blob/master/LICENSE
bitset	https://github.com/willf/bitset	https://github.com/willf/bitset/blob/master/LICENSE
blas	https://www.netlib.org/blas/	https://www.netlib.org/blas/#_licensing
bleach	https://github.com/mozilla/bleach	https://github.com/mozilla/bleach/blob/main/LICENSE
blessings	https://github.com/erikrose/blessings	https://github.com/erikrose/blessings/blob/master/LICENSE
blinker	https://pythonhosted.org/blinker/	https://github.com/pallets-eco/blinker/blob/master/LICENSE
bokeh	https://github.com/bokeh/bokeh	https://github.com/bokeh/bokeh/blob/branch-4.0/LICENSE.txt
blosc	https://github.com/Blosc/python-blosc	https://github.com/Blosc/python-blosc/blob/master/LICENSE.txt
blosc2	https://github.com/Blosc/python-blosc2	https://github.com/Blosc/c-blosc2/blob/main/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
boltons	https://github.com/mahmoud/boltons	https://github.com/mahmoud/boltons/blob/master/LICENSE
Boltz	https://boltz.bio	https://github.com/jwohlwend/boltz/blob/main/LICENSE
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
bootstrap-vue	https://github.com/bootstrap-vue/bootstrap-vue	https://github.com/bootstrap-vue/bootstrap-vue/raw/master/LICENSE
boto3	https://github.com/boto/boto3	https://github.com/boto/boto3/blob/develop/LICENSE
botocore	https://github.com/boto/botocore	https://github.com/boto/botocore/blob/develop/LICENSE.txt
Bottleneck	https://bottleneck.readthedocs.io/en/latest/index.html	https://bottleneck.readthedocs.io/en/latest/license.html
Brotli	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
brotli-bin	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
brotli-python	http://python-hyper.org/projects/brotlipy/en/latest/	https://github.com/python-hyper/brotlicffi/blob/main/LICENSE
brotlicffi	https://github.com/python-hyper/brotlicffi	https://github.com/python-hyper/brotlicffi?tab=MIT-1-ov-file#readme
brotlipy	https://github.com/python-hyper/brotlicffi	https://github.com/python-hyper/brotlicffi/blob/main/LICENSE

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Name of Project	Website	License URL
bson	http://github.com/py-bson/bson	https://github.com/py-bson/bson/blob/master/LICENSE_APACHE
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
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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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Name of Project	Website	License URL
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
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
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
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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-range	https://github.com/codebox/moment-precise-range 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
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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
sphinxcontrib-htmlhelp	https://github.com/sphinx-doc/sphinxcontrib-htmlhel	https://github.com/sphinx-doc/sphinxcontrib-htmlhel blob/master/LICENSE

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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
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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Name of Project	Website	License URL
tiffile	https://github.com/cgohlke/tiffile/	https://github.com/cgohlke/tiffile/blob/master/LICENSE
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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Name of Project	Website	License URL		
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		
triton	https://github.com/openai/triton/	https://github.com/openai/triton/blob/main/LICENSE		
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		
urllib3	https://urllib3.readthedocs.io/	https://github.com/urllib3/urllib3/blob/main/LICENSE.txt		
vine	https://github.com/celery/vine	https://github.com/celery/vine/blob/master/LICENSE		
vue	https://github.com/vuejs/vue	https://github.com/vuejs/vue/raw/master/LICENSE		
wadler_lindig	https://github.com/patrick-kidger/wadler_lindig	https://github.com/patrick-kidger/wadler_lindig?tab=Apache-2.0-1-ov-file#readme		
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		
webcolors	https://github.com/ubernostrum/webcolors	https://github.com/ubernostrum/webcolors?tab=BSD-3-Clause-1-ov-file#readme		
webencodings	https://github.com/gsnedders/python-webencodings	https://github.com/gsnedders/python-webencodings blob/master/LICENSE		
websocket-client	https://github.com/websocket-client/websocket-client.git	https://github.com/websocket-client/websocket-client/blob/master/LICENSE		
Werkzeug	https://palletsprojects.com/p/werkzeug/	https://werkzeug.palletsprojects.com/en/2.1.x/license/		
westpa	http://github.com/westpa/westpa	https://github.com/westpa/westpa/blob/westpa2/LICENSE		
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
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
wsutil	https://github.com/yhat/wsutil	https://github.com/yhat/wsutil/blob/master/LICENSE
x/lint	https://golang.org/x/lint	https://github.com/golang/lint/blob/master/LICENSE
x/mod	https://golang.org/x/mod/semver	https://cs.opensource.google/go/x/mod/+/master:LICENSE
x/net	https://golang.org/x/net	https://cs.opensource.google/go/x/net/+/master:LICENSE
x/oauth2	https://golang.org/x/oauth2	https://cs.opensource.google/go/x/oauth2/+/master:LICENSE
x/sys	https://golang.org/x/sys	https://cs.opensource.google/go/x/sys/+/master:LICENSE
x/text	https://golang.org/x/text	https://cs.opensource.google/go/x/text/+/master:LICENSE
x/tools	https://golang.org/x/tools	https://cs.opensource.google/go/x/tools/+/master:LICENSE
x/xerrors	https://golang.org/x/xerrors	https://cs.opensource.google/go/x/xerrors/+/master:LICENSE
xgboost	https://github.com/dmlc/xgboost	https://github.com/dmlc/xgboost/blob/master/LICENSE
xhtml2pdf	http://github.com/xhtml2pdf/xhtml2pdf	https://github.com/xhtml2pdf/xhtml2pdf/blob/master/LICENSE.txt

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Name of Project	Website	License URL
xlrd	https://github.com/python-excel/xlrd	https://github.com/python-excel/xlrd/blob/master/LICENSE
xlsxwriter	https://github.com/jmcnamara/XlsxWriter	https://github.com/jmcnamara/XlsxWriter/blob/main/LICENSE.txt
xmlsec	https://github.com/mehcode/python-xmlsec	https://github.com/mehcode/python-xmlsec/blob/master/LICENSE
xmltodict	https://github.com/martinblech/xmltodict	https://github.com/martinblech/xmltodict/blob/master/LICENSE
xorg-kbproto	https://gitlab.freedesktop.org/xorg/proto/kbproto	https://gitlab.freedesktop.org/xorg/proto/kbproto/-/blob/master/COPYING
xorg-libice	https://gitlab.freedesktop.org/xorg/lib/libice	https://gitlab.freedesktop.org/xorg/lib/libice/-/blob/master/COPYING
xorg-libsm	https://gitlab.freedesktop.org/xorg/lib/libsm	https://gitlab.freedesktop.org/xorg/lib/libsm/-/blob/master/COPYING
xorg-libx11	https://gitlab.freedesktop.org/xorg/lib/libx11	https://gitlab.freedesktop.org/xorg/lib/libx11/-/blob/master/COPYING
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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Name of Project	Website	License URL
xorg-libxext	https://gitlab.freedesktop.org/xorg/lib/libxext	https://gitlab.freedesktop.org/xorg/lib/libxext/-/blob/master/COPYING
xorg-libxrender	https://gitlab.freedesktop.org/xorg/lib/libxrender	https://gitlab.freedesktop.org/xorg/lib/libxrender/-/blob/master/COPYING
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
xz	https://github.com/ulikunitz/xz	https://github.com/ulikunitz/xz/blob/master/LICENSE
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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Name of Project	Website	License URL
yarl	https://github.com/aio-libs/yarl/	https://github.com/aio-libs/yarl/blob/master/LICENSE
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
click-option-group	https://github.com/click-contrib/click-option-group	https://github.com/click-contrib/click-option-group/blob/master/LICENSE

13.1 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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You should have received a copy of the GNU General Public License along with GCC (see below). If not, see Licenses GNU Project .

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.

13.1.1 GCC RUNTIME LIBRARY EXCEPTION

```
Version 3.1, 31 March 2009

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Everyone is permitted to copy and distribute verbatim copies of this license document,␣
↪but changing it is not allowed.

This GCC Runtime Library Exception ("Exception") is an additional permission under␣
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↪notice placed by the copyright holder
of the file stating that the file is governed by GPLv3 along with this Exception.

When you use GCC to compile a program, GCC may combine portions of certain GCC header␣
↪files and runtime libraries with
the compiled program. The purpose of this Exception is to allow compilation of non-GPL␣
↪(including proprietary) programs
to use, in this way, the header files and runtime libraries covered by this Exception.

0. Definitions.

A file is an "Independent Module" if it either requires the Runtime Library for␣
↪execution after a Compilation Process,
or makes use of an interface provided by the Runtime Library, but is not otherwise based␣
↪on the Runtime Library.

"GCC" means a version of the GNU Compiler Collection, with or without modifications,␣
↪governed by version 3 (or a specified
later version) of the GNU General Public License (GPL) with the option of using any␣
↪subsequent versions published by the FSF.

"GPL-compatible Software" is software whose conditions of propagation, modification and␣
↪use would permit combination with
GCC in accord with the license of GCC.

"Target Code" refers to output from any compiler for a real or virtual target processor␣
↪architecture, in executable
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-
↪compatible software, or if it is
done without using any work based on GCC. For example, using non-GPL-compatible Software␣
↪to optimize any GCC intermediate
representations would not qualify as an Eligible Compilation Process.

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You have permission to propagate a work of Target Code formed by combining the Runtime␣
↪Library with Independent Modules,
even if such propagation would otherwise violate the terms of GPLv3, provided that all␣
↪Target Code was generated by
Eligible Compilation Processes. You may then convey such a combination under terms of␣
↪your choice, consistent with the
licensing of the Independent Modules.

2. No Weakening of GCC Copyleft.

The availability of this Exception does not imply any general presumption that third-
↪party software is unaffected by
the copyleft requirements of the license of GCC.
```

See also

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

13.1.2 GNU GENERAL PUBLIC LICENSE

```
                    GNU GENERAL PUBLIC LICENSE
                       Version 3, 29 June 2007

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   The licenses for most software and other practical works are designed
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  Developers that use the GNU GPL protect your rights with two steps:
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authors' sake, the GPL requires that modified versions be marked as
changed, so that their problems will not be attributed erroneously to
authors of previous versions.

  Some devices are designed to deny users access to install or run
modified versions of the software inside them, although the manufacturer
can do so.  This is fundamentally incompatible with the aim of
protecting users' freedom to change the software.  The systematic
pattern of such abuse occurs in the area of products for individuals to
use, which is precisely where it is most unacceptable.  Therefore, we
have designed this version of the GPL to prohibit the practice for those
products.  If such problems arise substantially in other domains, we
stand ready to extend this provision to those domains in future versions
of the GPL, as needed to protect the freedom of users.

  Finally, every program is threatened constantly by software patents.
States should not allow patents to restrict development and use of
software on general-purpose computers, but in those that do, we wish to
avoid the special danger that patents applied to a free program could
make it effectively proprietary.  To prevent this, the GPL assures that
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patents cannot be used to render the program non-free.

  The precise terms and conditions for copying, distribution and
modification follow.

                    TERMS AND CONDITIONS

  0. Definitions.

  "This License" refers to version 3 of the GNU General Public License.

  "Copyright" also means copyright-like laws that apply to other kinds of
works, such as semiconductor masks.

  "The Program" refers to any copyrightable work licensed under this
License.  Each licensee is addressed as "you".  "Licensees" and
"recipients" may be individuals or organizations.

  To "modify" a work means to copy from or adapt all or part of the work
in a fashion requiring copyright permission, other than the making of an
exact copy.  The resulting work is called a "modified version" of the
earlier work or a work "based on" the earlier work.

  A "covered work" means either the unmodified Program or a work based
on the Program.

  To "propagate" a work means to do anything with it that, without
permission, would make you directly or secondarily liable for
infringement under applicable copyright law, except executing it on a
computer or modifying a private copy.  Propagation includes copying,
distribution (with or without modification), making available to the
public, and in some countries other activities as well.

  To "convey" a work means any kind of propagation that enables other
parties to make or receive copies.  Mere interaction with a user through
a computer network, with no transfer of a copy, is not conveying.

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to the extent that it includes a convenient and prominently visible
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tells the user that there is no warranty for the work (except to the
extent that warranties are provided), that licensees may convey the
work under this License, and how to view a copy of this License.  If
the interface presents a list of user commands or options, such as a
menu, a prominent item in the list meets this criterion.

  1. Source Code.

  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
interfaces specified for a particular programming language, one that
is widely used among developers working in that language.

  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
packaging a Major Component, but which is not part of that Major
Component, and (b) serves only to enable use of the work with that
Major Component, or to implement a Standard Interface for which an
implementation is available to the public in source code form.  A
"Major Component", in this context, means a major essential component
(kernel, window system, and so on) of the specific operating system
(if any) on which the executable work runs, or a compiler used to
produce the work, or an object code interpreter used to run it.

  The "Corresponding Source" for a work in object code form means all
the source code needed to generate, install, and (for an executable
work) run the object code and to modify the work, including scripts to
control those activities.  However, it does not include the work's
System Libraries, or general-purpose tools or generally available free
programs which are used unmodified in performing those activities but
which are not part of the work.  For example, Corresponding Source
includes interface definition files associated with source files for
the work, and the source code for shared libraries and dynamically
linked subprograms that the work is specifically designed to require,
such as by intimate data communication or control flow between those
subprograms and other parts of the work.

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the terms of this License in conveying all material for which you do
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  You may convey a work based on the Program, or the modifications to
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terms of section 4, provided that you also meet all of these conditions:

   a) The work must carry prominent notices stating that you modified
   it, and giving a relevant date.

   b) The work must carry prominent notices stating that it is
   released under this License and any conditions added under section
   7.  This requirement modifies the requirement in section 4 to
   "keep intact all notices".
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    c) You must license the entire work, as a whole, under this
    License to anyone who comes into possession of a copy.  This
    License will therefore apply, along with any applicable section 7
    additional terms, to the whole of the work, and all its parts,
    regardless of how they are packaged.  This License gives no
    permission to license the work in any other way, but it does not
    invalidate such permission if you have separately received it.

    d) If the work has interactive user interfaces, each must display
    Appropriate Legal Notices; however, if the Program has interactive
    interfaces that do not display Appropriate Legal Notices, your
    work need not make them do so.

  A compilation of a covered work with other separate and independent
works, which are not by their nature extensions of the covered work,
and which are not combined with it such as to form a larger program,
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beyond what the individual works permit.  Inclusion of a covered work
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  6. Conveying Non-Source Forms.

  You may convey a covered work in object code form under the terms
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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,
or household purposes, or (2) anything designed or sold for incorporation
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,
in accord with this section must be in a format that is publicly
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but do not include claims that would be infringed only as a
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