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SPRUCE

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CHAPTER

ONE

INTRODUCTION

1.1 Overview

The SPRUCE application provides the facilities to prepare biomolecules (that is, proteins and nucleic acids) for modeling tasks.

1.2 Applications

The **SPRUCE** distribution comprises these applications:

SPRUCE

The *SPRUCE* program is used for biomolecule preparation, from experimental or modeled structures. The process involves, 1) expansion of the asymmetric unit to the biological unit (if structure is from an X-ray crystallography experiment and it is necessary), 2) enumeration (default) or collapse of alternate locations, 3) building missing pieces, for example, partial sidechains, capping chain breaks, and modeling missing loops, 4) placement and optimization of hydrogen atoms including tautomer enumeration of ligands and cofactors, as well as evaluation of those tautomer states in the biomolecule structure.

Superposition

The *Superposition* program is used to superpose biomolecule structures onto a reference structure. Several different superposition methods are included, that are either based on sequence or secondary structure.

1.3 Utility Programs

The following utility programs are also included in this distribution:

LoopDB_Builder

The *LoopDB_Builder* program is used to build a database of known loops from a set of protein structures. This database can then be passed as an option to *SPRUCE* to enable loop modeling of gaps in protein structures.

GetStructure

The *GetStructure* utility program can be used to download biomolecular structure files (PDB, mmCIF, structure factor CIF) for downstream prepping with *SPRUCE*.

Du2pdb

The *Du2pdb* utility program can be used to convert DesignUnit oedu files to PDB file format.

EnumSites

The *EnumSites* program can be used to enumerate sites from prior bio-design units produced by *SPRUCE*. This is particularly useful when enumerating potentially allosteric apo sites, that where not known when the structure was prepared the first time - enumeration ensures that the structure is not re-prepared but just focused into a site of interest.

1.4 Utilizing a Loop Template Database

Included in the SPRUCE product is a large database of loop templates, described further in the Spruce theory section.

To use it during prep:

-loop_db_filename rcsb_spruce.loop_db

The database can be appended to (updated) using the *LoopDB_Builder* utility. This would be in the event that the user has a collection of internal/proprietary structures, or if specific structures are released to the public PDB between OpenEye updates of the database that are crucial for a given target that is less well described by the existing templates.

Loop building will only be done when a loop template database is provided.

For more information, see the theory explanation for the Spruce toolkit and the Iridium chapter of that toolkit.

CHAPTER

TWO

SPRUCE

2.1 Overview

SPRUCE is an application that prepares biomolecular structure files (PDB, mmCIF, oeb, etc.) for downstream modeling applications, such as running a BROOD query, docking a ligand with FRED or HYBRID, predicting poses with POSIT, or for running SZMAP to analyze active-site hydration thermodynamics. SPRUCE first runs a standardization and filter check to determine the quality of the input structure (see OESpruceFilter). The filter will fail the workflow if the structure did not pass the checks. The -allow_filter_error flag will alow one to continue to the preparation workflow even when the structure did not pass the filter. The preparation workflow from an experimental or modeled structure involves, 1) expansion of the asymmetric unit to the biological unit (if structure is from an X-ray crystallography experiment and it is necessary), 2) enumeration (default) or collapse of alternate locations, 3) building missing pieces e.g. partial sidechains, capping chain breaks, and modeling missing loops, 4) placement and optimization of hydrogen atoms including tautomer enumeration of ligands and cofactors, as well as evaluation of those tautomer states in the biomolecule structure. OEReceptors are added to the design units by default so they are ready for docking applications. The generated DU will be checked by a design unit validation function. Parts that are not successfully built in spruce preparation will be logged and styled differently.

Note

Included in the Spruce product is a loop building database which can be used to build missing loops. This database is available for download in a platform-independent format.

See also

- The ReceptorInDU section

2.2 Spruce Output Naming Conventions

Output files generated from Spruce follows a general naming scheme.

{StructureID}_{ChainIDs}[alt{AltCode}]__DU__{LigandCode}_{ChainID}-{ResidueNumber}.oedu

The scheme can be prefixed by the user using the *-prefix* input parameter. The user can also control the output to a single file using the *-out*, and additionally, set *-warts* to append "_#" to the user specified output name.

Example of a structure without an alternate location, 2 files generate due to two ligand sites detected:

```
4ICL_AB__DU__T27_A-601.oedu
```

```
4ICL_AB__DU__14N_A-607.oedu
```

Example with an alternate location code:

`1XDN_AaltA__DU__ATP_A-501.oedu`

For apo structures, the residue named is the one closest to the center of the marked binding site. That is unless the user has provided a binding site residue to indicate the binding site, in which case that is used in the title and filename. Apo pocket example:

`1HHP_AB__DU__apo_ASP_A-25.oedu`

Peptidic ligand example, where the ligand section is named slightly differently following the scheme chainID-StartingResidueNumber-1LetterCodes-EndingResidueNumber. Only standard residue get 1 letter codes, whereas non-standard residue will have 3 letter codes separated by dashes.

`4OBD_AB__DU__E-2-PGNFFQNRP-10.oedu`

2.3 Example Commands

The simplest way to run **SPRUCE** is by passing in an input biomolecular structure file (PDB or mmCIF) as the only argument.

```
prompt> spruce -in 3fly.cif.gz
```

Here, **SPRUCE** will correctly split and prepare `3fly.cif.gz` with the *-in* parameter and the standard set of default options. The output will generally be a set of OEDesignUnit (.oedu) files, depending on the number of ligands and biological units in the asymmetric unit. In this case a single design unit file is produced (`3FLY_A__DU__FLY_A-361.oedu`).

There are also many options that can be invoked from **SPRUCE** on the command line. For instance, several options are available to help **SPRUCE** determine the ligand based on molecular features like the number of residues in a peptidic ligand:

So for example:

```
prompt> spruce -in 4obd.cif.gz -max_lig_residues 20
```

will correctly split and prepare `4obd.cif.gz`, based on the *-max_lig_residues* which sets the maximum number of residues that can still be considered a ligand (required for larger, peptidic ligands like those in 4OBD).

Alternatively, one may want to prepare a biomolecular structure file based on the structure of a similar reference system. For instance, one may construct an OEDesignUnit with a set of site residues defined using a reference that includes a ligand:

```
prompt> spruce -ref 4OBD.oedu -in 1hhp.cif
```

Here, an mmCIF file (`1hhp.cif`) is prepared using the site defined in the output OEDesignUnit file prepared using the *-ref* option and an output .oedu file from the example above.

This could also have been done by specifying a site residue, for example (note the blank character for the insert code):

```
prompt> spruce -site_residue "ASP:25: :A" -in 1hhp.cif
```

To calculate the Iridium classification as a metric of structure quality, one must provide the map file that corresponds to experiment from which the biomolecular structure was derived:

```
prompt> spruce -map 3rox_validation_2fo-fc_map_coef.cif.gz -in 3rox.cif.gz
```

Here a set of OEDesignUnit files will be produced from `3rox.cif.gz`, where each oedu file will include its own Iridium score taken from a calculation on the density passed in through the *-map* option

(`3rox_validation_2fo-fc_map_coef.cif.gz`). The Iridium score can be extracted from any OEDesignUnit file using the **spruce TK** API, but it will also be reported in the **spruce** application's output.

> **Note**
>
> The *-map* option accepts structure factor CIF files (`.cif`, `.cif.gz`) as provided by *GetStructure* and the RCSB, as well as legacy MTZ files (`.mtz`).

Several options in **SPRUCE** are available to help control how the system is prepared. For instance by default, **spruce** calculates partial charges and adds any hydrogen atoms missing from the experimental structure. However, if you have a have a downstream application that does not require certain time-consuming computations, like calculating partial charges or adding missing hydrogen atoms, you can tell **SPRUCE** to turn these features off:

```
prompt> spruce -protonate false -charge_radii false -in 3tpp.cif.gz
```

Here, **SPRUCE** will not add partial charges or hydrogen atoms to the output structures during the preparation process of `3tpp.cif.gz` by using the boolean options *-protonate* and *-charge_radii*, both of which are set to `true` by default.

To prevent continually over-writing output files, the *-prefix* input parameter. allows you to give unique names to these files.

```
prompt> spruce -in 3fly.cif.gz -prefix FOO
```

will write the output structure into a file named `FOO_3FLY_A__DU__FLY_A-361.oedu`.

Finally, to help **spruce** identify ligands in the biomolecular structure file, use the *-ligand_names* flag as in this example with `3b3n.cif.gz`.

```
prompt> spruce -ligand_names JI2 -in 3b3n.cif.gz
```

2.4 Command Line Help

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

```
prompt> spruce --help
```

will generate the following output:

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

2.5 Required Parameters

-in <filename>

File containing one or more 3D biomolecules that will be split into known components and fully prepared for downstream modeling.

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

File type	Extension
OEBinary	.oeb .oeb.gz
PDB	.pdb .ent .pdb.gz .ent.gz
mmCIF	.cif .cif.gz

[keyless parameter 1]

2.6 Optional Parameters

2.6.1 Input Options

-ligand_names <names>

If multiple ligands are in the structure but only a specific ones are desired, they can be specified here. Examples are either the three letter code "LIG", or in case of a peptide "VAL-GLU-TYS-PHE-ALA". Multiple different ligands, should be separated by commas, "LIG,GIL,INH".

See also

- OEStructureMetadata in the **Spruce TK** manual.
- OEHeterogenMetadata in the **Spruce TK** manual.

-map <filename>

Input electron density map from X-ray crystallography, to be used for Iridium score calculation. Accepted formats are structure factor CIF files (`.cif`, `.cif.gz`) and legacy MTZ files (`.mtz`). Structure factor CIF files are the current format provided by the RCSB; MTZ files are supported for backward compatibility.

-metadata <filename>

Metadata json file containing OEStructureMetadata. Using this can be a way to indicate desired ligands, tautomers to use for ligands, structure sequence etc., as well as structure title for output file names. The -generate_tautomers option should be set to false and -opt_expt_protons to true to only consider the desired ligands. More details along with an example metadata file can be found at Creating OEDesignUnits Using Provided Metadata. The OESpruce::OEStructureMetadataToJson fucntion can be used to create an appropriate json file as well.

See also

- OEStructureMetadata in the **Spruce TK** manual.
- OESequenceMetadata in the **Spruce TK** manual.
- OEHeterogenMetadata in the **Spruce TK** manual.

-ref <filename>

Reference OEDesignUnit indicating the proper biological unit and relevant binding site.

-site_residue <residue identifier>

Input option to specify a binding site using a single residue specification if apo (or holo). The format

is "name:num:insert code:chainid", e.g. "ASP:25: :A" indicating Aspartic acid 25 in chain A. Note: A blank/whitespace character is used for the insert code, which is a typical use case.

> **See also**
>
> - OEMakeDesignUnits in the **Spruce TK** manual. This API exposes the `siteResidue` argument.
> - OEMakeBioDesignUnits in the **Spruce TK** manual.

-add_receptors

Option to add OEReceptors onto the design units

[Default=true]

> **See also**
>
> - OEDocking::OEMakeReceptor in the **OEDocking TK** manual. This API takes an OEDesignUnit argument.

2.6.2 Output Options

-out <out>

Write to a user specified file. Enforces *.oedu format. Can be used with *-warts* to write multiple files, one per design unit.

-warts

Option to add warts "_#" to the user supplied filename, when writing multiple design units.

[Default=false]

-prefix <prefix>

Prefix used to name output files, default is blank

-log <logfile>

The argument for this flag specifies the name of the log file. This overrides any specified prefix. The default will be spruce_output.log, if no prefix is specified.

-settings_file <settingsfile>

(Alias: -settings)

The argument for this flag specifies the name of the settings file. This overrides any specified prefix. The default will be spruce_settings.param, if no prefix is specified.

-verbose

Triggers copious logging output.

[Default=false]

-write_biounits

Option to write intermediate Bio-DesignUnits, which can be used with *enumsites* to site to potential allosteric sites later.

[Default=false]

2.6.3 Split Parameters

`-altloc` <method>

Parameter determining how alternate locations are handled. The *primary* option, collapses alternate locations, whereas the *enumerate* option attempts to set detected alternate locations, A, B, etc.

[Default=enumerate]

See also

- OESpruce::OEDesignUnitSplitOptions::SetAlternateLocationHandling in the **Spruce TK** manual.

`-cofactor_codes` <codes>

Mechanism to define 3 letter codes that should be recognized as co-factors if not done automatically, e.g. "ATP", or "ATP,NAD"

See also

- OESpruce::OEDesignUnitSplitOptions::SetCofactorCodes in the **Spruce TK** manual.

`-excipient_codes`

Mechanism to define 3 letter codes that should be recognized as excipients if not done automatically, e.g. "GOL", or "GOL,DMS"

See also

- OESpruce::OEDesignUnitSplitOptions::SetExcipientCodes in the **Spruce TK** manual.

`-lipid_codes` <codes>

Mechanism to define 3 letter codes that should be recognized as lipids if not done automatically, e.g. "PGR", or "PGR,CHL"

See also

- OESpruce::OEDesignUnitSplitOptions::SetLipidCodes in the **Spruce TK** manual.

`-make_packing_residues`

Option to generate packing residues, both for visualization, but also for Iridium classification

[Default=true]

See also

- OESpruce::OEDesignUnitSplitOptions::SetMakePackingResidues in the **Spruce TK** manual.

`-min_lig_atoms`

Parameter determining the min number of atoms a ligand molecule can have. A reason to lower this number would be for small fragments that need to be classified as ligands

[Default=8]

See also

- OESpruce::OEDesignUnitSplitOptions::SetMinLigAtoms in the **Spruce TK** manual.

`-max_lig_atoms`

Parameter determining the max number of atoms a ligand molecule can have. A reasons to increase this number could be for peptidic ligands

[Default=100]

See also

- OESpruce::OEDesignUnitSplitOptions::SetMaxLigAtoms in the **Spruce TK** manual.

`-max_lig_residues`

Parameter determining the max number of residues a ligand molecule can have. A reasons to increase this number could be for peptidic ligands

[Default=5]

See also

- OESpruce::OEDesignUnitSplitOptions::SetMaxLigResidues in the **Spruce TK** manual.

`-max_sys_atoms`

Parameter limiting the max number of atoms in the entire system that spruce will allow for processing. If this limit is reached e.g. due to a large systems or symmetry expansion resulting in a larger than expected system, spruce will stop processing and return false.

[Default=50,000]

See also

- OESpruce::OEDesignUnitSplitOptions::SetMaxSystemAtoms in the **Spruce TK** manual.

`-target`

Parameter telling the system what the "target" is. This is particularly helpful for systems containing both protein and nucleic acids, where the automated system does not correctly identify the nucleic acid as the target of interest. Allowed values are protein or nucleic.

[Default=protein]

See also

- OESpruce::OEDesignUnitSplitOptions::SetTargetComponentID in the **Spruce TK** manual.

2.6.4 Enumerate Sites Parameters

`-add_interactions`

Option to add OEInteractionHints to the design unit(s)

[Default=true]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetAddInteractionHints in the **Spruce TK** manual.

`-add_style`

Option to add visualization style to the design unit(s)

[Default=true]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetAddStyle in the **Spruce TK** manual.

`-collapse_nonsite_alts`

Option to deduplicate structures with different alternate locations if those alternate locations are far from the binding site

[Default=true]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetCollapseNonSiteAlts in the **Spruce TK** manual.

`-duplicate_removal`

Option to deduplicate identical structures resulting from symmetry operations

[Default=true]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetDuplicateRemoval in the **Spruce TK** manual.

`-enum_cofactors_sites`

Option to generate design units with sites based on components classified as co-factors

[Default=false]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetEnumerateCofactorSites in the **Spruce TK** manual.

-restrict_to_refsite

Option to skip generating design units for sites identified, that do not match a provided reference design unit

[Default=true]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetRestrictToRefSite in the **Spruce TK** manual.

-site_size <value>

Distance from the ligand used to determine the size of the site

[Default=5.0 (angstroms)]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetSiteSize in the **Spruce TK** manual.

-superpose

Option to superpose generated design units, if multiple. If a reference is provided, the first generated design unit will be superposed onto the reference structure, and subsequent structures onto that one.

[Default=true]

See also

- OESpruce::OEMakeDesignUnitOptions::SetSuperpose in the **Spruce TK** manual.

-superpose_method <method>

The method to use for superposition

Method	Description
global	Global Sequence Alignment to identify CA pairs
site	Global Sequence Alignment to identity CA pairs - focusing on the subset in active site
ddm	Superposition using the Distance Difference Matrix method (DDM)
sse	Superposition using an overlap of Secondary Structure Elements (SSE)
weighted	Superposition weighting residues by B-factor or occupancy
sitehopper	Superposition based on binding site similarities (sitehopper)
GlobalSequence	Alias for global — Global Sequence Alignment to identify CA pairs
DDMatrix	Alias for ddm — Superposition using the Distance Difference Matrix method
SiteSequence	Alias for site — Global Sequence Alignment focusing on the active site

See also

- OESpruce::OEMakeDesignUnitOptions::SetSuperpositionMethod in the **Spruce TK** manual.

2.6.5 Build Parameters

`-build_cterm_caps`

Option to cap broken c-termini in protein chains

[Default=true]

See also

- OESpruce::OEDesignUnitBuildOptions::SetCapCTermini in the **Spruce TK** manual.

`-build_nterm_caps`

Option to cap broken n-termini in protein chains

[Default=true]

See also

- OESpruce::OEDesignUnitBuildOptions::SetCapNTermini in the **Spruce TK** manual.

`-build_loops`

Option to build loops for gaps in the protein structure

[Default=true]

See also

- OESpruce::OEDesignUnitBuildOptions::SetBuildLoops in the **Spruce TK** manual.

`-build_sidechains`

Option to build missing or partial protein sidechains

[Default=true]

See also

- OESpruce::OEDesignUnitBuildOptions::SetBuildSidechains in the **Spruce TK** manual.

`-enum_pockets`

Option to detect pockets and generate design units from them

[Default=false]

2.6.6 Sidechain Build Parameters

-sc_delete_clashing_solvent

Option to allow build steps to remove clashing solvent

[Default=true]

> **See also**
>
> - OESpruce::OESidechainBuilderOptions::SetDeleteClashingSolvent in the **Spruce TK** manual.

-rot_coverage <value>

Coverage of rotamer libraries to use, a lower number can be used to speed up side chain re-building skipping lower probability side-chain rotamers.

[Default=100.0]

> **See also**
>
> - OESpruce::OESidechainBuilderOptions::SetRotamerCoverage in the **Spruce TK** manual.

-rot_library <value>

Rotamer library used for building sidechains and loops. Allowed values are 'richardson2016', 'dunbrack', 'richardson'.

[Default=richardson2016]

> **See also**
>
> - OESpruce::OESidechainBuilderOptions::SetRotamerLibrary in the **Spruce TK** manual.

2.6.7 Loop Build Parameters

-build_with_crystalpacking

Include packing residues when building loops

[Default=false]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetUsePackingResidues in the **Spruce TK** manual.

-loop_db_filename <filename>

Database containing loop templates

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetLoopDBFilename in the **Spruce TK** manual.

`-crop_length` <value>

Anchor residues on the protein to crop back for a better fit, results in longer loops being built

[Default=1]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetCropLength in the **Spruce TK** manual.

`-transform_threshold` <value>

Number of loops to allow through the sidechain clash checker. No matter this number, will process all with an identical sequence to target.

[Default=25]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetTransformThreshold in the **Spruce TK** manual.

`-strict_proline_match`

Fuzzy matches in the loop database have to have proline in exact locations of sequence.

[Default=true]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetStrictProlineMatch in the **Spruce TK** manual.

`-loop_distance_buffer` <value>

Fuzzy matches in the loop database has to have distance between anchor atoms correct, +/- buffer distance

[Default=1.0]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetConnectBufferDistance in the **Spruce TK** manual.

`-bb_clash_threshold` <value>

Loops from the database where more than the threshold fraction of the backbone atoms clash, are rejected

[Default=0.25]

See also

- OESpruce::OELoopBuilderOptions::SetBackboneClashRejectThreshold in the **Spruce TK** manual.

`-loop_clash_threshold` <value>

Loops from the database where more than the threshold fraction of the loops atoms in addition to the backbone clashing ones clash, are rejected

[Default=0.2]

See also

- OESpruce::OELoopBuilderOptions::SetLoopClashRejectThreshold in the **Spruce TK** manual.

`-opt_shell` <value>

Include atoms within this distance in the loop optimization, larger distance results in slower optimization

[Default=15.0]

See also

- OESpruce::OELoopBuilderOptions::SetOptimizationShell in the **Spruce TK** manual.

`-opt_tolerance` <value>

Tolerance for the loop optimization, smaller numbers result in slower optimization

[Default=0.001]

See also

- OESpruce::OELoopBuilderOptions::SetOptimizationTolerance in the **Spruce TK** manual.

`-opt_stage1_iter_multiplier` <value>

Number of steps per number of residues in the loop for the first stage optimizer

[Default=5]

See also

- OESpruce::OELoopBuilderOptions::SetOptimizationStage1IterMultiplier in the **Spruce TK** manual.

`-opt_stage2_iter_multiplier` <value>

Number of steps per number of residues in the loop for the second stage optimizer

[Default=10]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetOptimizationStage2IterMultiplier in the **Spruce TK** manual.

`-incl_solvation` <value>

Include simple solvation model when building loops

[Default=true]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetOptimizationUseSolventModel in the **Spruce TK** manual.

`-incl_SA_term` <value>

Include solvent accessible surface area term when ranking the loops

[Default=true]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetOptimizationInclSurfaceAreaTerm in the **Spruce TK** manual.

`-max_eval_loops` <value>

Maximum number of loops to connect and minimize

[Default=5]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetOptimizationMaxLoops in the **Spruce TK** manual.

`-build_disulfidebridges` <value>

Allow the loop builder to build disulfide brides during loop modeling (if possible)

[Default=true]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetAllowBuildDisulfideBridges in the **Spruce TK** manual.

`-build_tails`

Option to build missing terminal residues from sequence database

[Default=false]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetBuildTails in the **Spruce TK** manual.

`-seqalign_gap_penalty` <value>
: Gap penalty for sequence alignment during loop building

  [Default=-10]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetSeqAlignGapPenalty in the **Spruce TK** manual.

`-seqalign_extend_penalty` <value>
: Gap extension penalty for sequence alignment during loop building

  [Default=-2]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetSeqAlignExtendPenalty in the **Spruce TK** manual.

`-reject_clashing_loops_postminimization`
: Reject loops that clash after minimization

  [Default=true]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetRejectClashingLoopsPostMinimization in the **Spruce TK** manual.

`-delete_existing_residues`
: Delete existing residues in the loop region before building

  [Default=false]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetDeleteExistingResidues in the **Spruce TK** manual.

2.6.8 Cap Build Parameters

`-cap_delete_clashing_solvent`
: Option to allow build steps to remove clashing solvent

  [Default=true]

> **See also**
>
> - OESpruce::OECapBuilderOptions::SetDeleteClashingSolvent in the **Spruce TK** manual.

`-allow_truncate`

Option to allow terminal residue to converted to cap, if cap will otherwise clash

[Default=true]

> **See also**
>
> - OESpruce::OECapBuilderOptions::SetAllowTruncate in the **Spruce TK** manual.

2.6.9 Prep Parameters

`-charge_radii`

Option to assign partial charge and radii

[Default=true]

> **See also**
>
> - OESpruce::OEDesignUnitPrepOptions::SetAssignPartialChargesAndRadii in the **Spruce TK** manual.

`-protonate`

Option add and optimize protons in the system

[Default=true]

> **See also**
>
> - OESpruce::OEDesignUnitPrepOptions::SetProtonate in the **Spruce TK** manual.

`-strict_protonate`

Option to use strict protonation, disabling tautomer generation for heterogens

[Default=false]

2.6.10 Protonation Parameters

`-generate_tautomers`

Option to generate and use tautomers in the hydrogen network optimization

[Default=true]

> **See also**
>
> - OESpruce::OEProtonateDesignUnitOptions::SetGenerateTautomers in the **Spruce TK** manual.

-het_group_nbr_dist <value>
: Distance between heterogens used to determine optimization clusters for protonation

[Default=3.5 (angstroms)]

> **See also**
>
> - OESpruce::OEProtonateDesignUnitOptions::SetHetGroupNbrDist in the **Spruce TK** manual.

-opt_expt_protons
: Option to optimize hydrogens assigned in the experiment.

[Default=false]

> **See also**
>
> - OESpruce::OEProtonateDesignUnitOptions::SetOptimizeExpProtons in the **Spruce TK** manual.

-flip_bias_scale
: Bias scale for flippable groups (e.g. HIS/ASN/GLN) during hydrogen placement

[Default=1.0]

> **See also**
>
> - OESpruce::OEProtonateDesignUnitOptions::SetPlaceHydrogensOptions in the **Spruce TK** manual.

2.6.11 Biological Unit Extraction Parameters

-bu_superpose
: Option to superpose the biological units

[Default=false]

> **See also**
>
> - OESpruce::OEBioUnitExtractionOptions::SetSuperpose in the **Spruce TK** manual.

-max_bu_atoms
: Option to limit the size of BUs processed based on number of atoms

[Default=50,000]

> **See also**
>
> - OESpruce::OEBioUnitExtractionOptions::SetMaxAtoms in the **Spruce TK** manual.

`-max_bu_parts`

Option to limit the size of BUs processed based on number of parts

[Default=24]

> **See also**
>
> - OESpruce::OEBioUnitExtractionOptions::SetMaxParts in the **Spruce TK** manual.

`-min_align_score`

Option to specify minimum sequence alignment score

[Default=200]

> **See also**
>
> - OESpruce::OEBioUnitExtractionOptions::SetMinScore in the **Spruce TK** manual.

`-pref_author_record`

Option where the author BIOMT record is preferred over the software generated one

[Default=true]

> **See also**
>
> - OESpruce::OEBioUnitExtractionOptions::SetPreferAuthorRecord in the **Spruce TK** manual.

2.6.12 Enumerate Pocket Parameters

`-pocketMask`

Option to set the subset of design unit components to be used for pocket finding. Multiple components can be combined as a comma separated string to create the input.

[Default=true]

`-min_pocket_surf_area`

Option to set minimum surface area of detected pocket.

[Default=150.0]

> **See also**
>
> - OESpruce::OEPocketOptions::SetMinSurfaceArea in the **Spruce TK** manual.

-max_pocket_surf_area

Option to set maximum surface area of detected pocket.

[Default=3000.0]

> **See also**
>
> - OESpruce::OEPocketOptions::SetMaxSurfaceArea in the **Spruce TK** manual.

-pocket_burial_factor

Option to set the factor used to distinguish pockets from the general surface.

[Default=1.4]

> **See also**
>
> - OESpruce::OEPocketOptions::SetBurialFactor in the **Spruce TK** manual.

2.6.13 OEReceptor Parameters

-targetMask

Subset of design unit components to be used as target for the receptor. Multiple components can be combined as a comma separated string to create the input

[Default=protein,nucleic,cofactors,metals,lipids,other_proteins,other_nucleics,other_ligands,other_cofactors]

Please see more details at *SPRUCE* and ReceptorInDU.

2.6.14 Special Parameters

-no_prep

Option to skip all preparation steps. This will supersede any other optional flags set.

[Default=false]

2.6.15 Filter Options Parameters

-allow_filter_error

Option to allow running spruce prep even when structure fails spruce filter.

[Default=false]

-fix_res_names

Option to fix incorrect residue names.

[Default=true]

> **See also**
>
> - OESpruce::OESpruceFilterOptions::SetFixNames in the **Spruce TK** manual.

`-fix_res_states`
: Option to fix incorrect residue states.

[Default=true]

> **See also**
>
> - OESpruce::OESpruceFilterOptions::SetFixResStates in the **Spruce TK** manual.

`-fix_bonds_to_metals`
: Option to fix incorrect covalent bonds to metals.

[Default=true]

> **See also**
>
> - OESpruce::OESpruceFilterOptions::SetFixBondsToMetals in the **Spruce TK** manual.

`-fix_bb_atoms`
: Option to fix protein backbone atom states.

[Default=true]

> **See also**
>
> - OESpruce::OESpruceFilterOptions::SetFixBackboneAtoms in the **Spruce TK** manual.

`-fix_float_res`
: Option to delete floating residues

[Default=true]

> **See also**
>
> - OESpruce::OESpruceFilterOptions::SetDeleteFloatingRes in the **Spruce TK** manual.

`-fix_chainID`
: Option to fix missing chain ID

[Default=true]

> **See also**
>
> - OESpruce::OESpruceFilterOptions::SetFixChainIDs in the **Spruce TK** manual.

`-fix_covalent_bond`
: Option to fix incorrect covalent bonds to halogens

[Default=true]

See also

- OESpruce::OESpruceFilterOptions::SetFixInvalidCovalentBonds in the **Spruce TK** manual.

`-allow_validation_error`

Option to allow writing OEDesignUnits even if they fail validation

[Default=true]

CHAPTER

THREE

SUPERPOSITION

3.1 Overview

Superposition is an application that structurally superposes a given biomolecular structure file (oedu, PDB, mmCIF, oeb, etc.) onto a reference structure (oedu, PDB, mmCIF, oeb, etc.).

3.2 Example Commands

The simplest way to run **Superposition** is by passing in both a reference and a fit input biomolecular structure file:

```
prompt> superposition -ref 4obd.pdb -fit 1hhp.pdb
```

Here, **Superposition** will fit the protein in `1hhp.pdb` against the reference protein in `4obd.pdb`. The output will list the RMSD of the superposed result, the order in which the ref and fit chains were superposed, and the sequence alignment score, if the method is sequence based. The command should generate a PDB file called `superposed_1hhp.pdb` that contains the superposed protein and the following message in the log file:

```
Superposition - RMSD: 1.16, Ref: ABCDEF, Fit: A, SeqScore: 492
```

The structural superposition method can be set on the command line with the *-method* option:

For example:

```
prompt> superposition -ref 1a29.pdb -fit 1cll.pdb -method ddm
```

will superpose `1cll.pdb` onto the reference file `1a29.pdb` using the `ddm` (*difference-distance matrix*) method. The command should generate a PDB file called `superposed_1cll.pdb` that contains the superposed protein and the following message in the log file:

```
Superposition - RMSD: 0.60, Ref: A, Fit: A, SeqScore: 642
```

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

```
prompt> superposition -ref 1a29.pdb -fit 1cll.pdb -method sse -prefix FOO
```

will write the output structures into a file named `FOO_1cll.pdb` and following message to the log file:

```
Superposition - Tanimoto: 0.31, Ref: A, Fit: A
```

3.3 Command Line Help

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

```
prompt> superposition --help
```

will generate the following output:

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

3.4 Required Parameters

-fit <filename>

File containing the 3D biomolecules that will be structurally superposed.

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

File type	Extension
OEDesignUnit	.oedu
OEBinary	.oeb .oeb.gz
PDB	.pdb .ent .pdb.gz .ent.gz
mmCIF	.cif .cif.gz

-ref <filename>

File containing the 3D biomolecules that will act as the reference for the structural superposition.

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

File type	Extension
OEDesignUnit	.oedu
OEBinary	.oeb .oeb.gz
PDB	.pdb .ent .pdb.gz .ent.gz
mmCIF	.cif .cif.gz

3.5 Optional Parameters

3.5.1 Input Options

-fit_lig <filename>

A file containing a ligand to use as a constraint during the superposition. Should only be used if the input is not an OEDesignUnit

See also

- OESpruce::OESuperpose::SetupRef and OESpruce::OESuperpose::Superpose in the **Spruce TK** manual.

-ref_lig <filename>

A file containing a reference ligand to use as a constraint during the superposition. Should only be used if the input is not an OEDesignUnit

See also

- OESpruce::OESuperpose::SetupRef and OESpruce::OESuperpose::Superpose in the **Spruce TK** manual.

3.5.2 Output Options

-prefix <prefix>

Prefix used to name output files, default is blank. To avoid overwriting input files, all structure files are automatically using the prefix *superposed_* if no prefix is specified.

-log <logfile>

The argument for this flag specifies the name of the log file. This overrides any specified prefix.

-settings_file <settingsfile>

(Alias: -settings)

The argument for this flag specifies the name of the settings file. This overrides any specified prefix.

-verbose

Triggers copious logging output

3.5.3 Parameters

-method <method>

The method to use for superposition

Method	Description
global	Global Sequence Alignment to identify CA pairs
site	Global Sequence Alignment to identity CA pairs - focusing on the subset in active site
ddm	Superposition using the Distance Difference Matrix method (DDM)
sse	Superposition using an overlap of Secondary Structure Elements (SSE)
weighted	Superposition using Weighted DDM method
sitehopper	Superposition using SiteHopper

See also

- OESpruce::OESuperposeOptions::SetMethod in the **Spruce TK** manual.

-valid_seqscore <value>

Minimum sequence alignment score for the superposition to be considered valid

[Default=200]

See also

- OESpruce::OESuperposeOptions::SetValidSeqScore in the **Spruce TK** manual.

-valid_rmsd <value>

Maximum RMSD threshold for the superposition to be considered valid

[Default=10.0]

See also

- OESpruce::OESuperposeOptions::SetValidRMSD in the **Spruce TK** manual.

-valid_tanimoto <value>

Minimum Tanimoto similarity threshold for the superposition to be considered valid

[Default=0.0]

See also

- OESpruce::OESuperposeOptions::SetValidTanimoto in the **Spruce TK** manual.

CHAPTER

FOUR

ENUMSITES

4.1 Overview

EnumSites is an application that enumerates biounit OEDesignUnit (oedu) files, and it creates individual oedu files for every active site discovered.

4.2 Example Commands

The simplest way to run **EnumSites** is by passing in an unprepped, biounit OEDesignUnit file (oedu) as the input and a fully prepared OEDesignUnit file as a reference.

```
prompt> enumsites -ref 4OBD_AB__DU__E-2-PGNFFQNRP-10.oedu -in 1HHP_AB__DU__biounit.oedu
```

Here, **EnumSites** will use the biounit OEDesignUnit `1HHP_AB__DU__biounit.oedu` with the *-in* parameter, along with a reference OEDesignUnit file `4OBD_AB__DU__E-2-PGNFFQNRP-10.oedu` with the *-ref* option, in order to create an OEDesignUnit from `1HHP_AB__DU__biounit.oedu` using the site defined in the reference structure. The output is a single OEDesignUnit (.oedu): `1HHP_AB_DU_apo_ASP_B-25.oedu`.

Instead of a fully prepared OEDesignUnit file as a reference, one may simply specify the site residues required to define the new site of interest.

So for example:

```
prompt> enumsites -site_residue "ASP:25: :A" -in 1HHP_AB__DU__biounit.oedu
```

will construct an OEDesignUnit based on enumeration from the same biounit OEDesignUnit file as before (`1HHP_AB__DU__biounit.oedu`), but here the definition of the site comes from the *-site_residue* option instead of another fully-prepared OEDesignUnit.

To calculate the Iridium classification as a metric of structure quality with `enumsites`, one must provide the map file that corresponds to experiment from which the biomolecular structure was derived:

```
prompt> enumsites -site_residue "MET:124: :A" -map 1a29_validation_2fo-fc_map_coef.cif.
↪gz -in 1A29_A__DU__biounit.oedu
```

Here two OEDesignUnit files (`1A29_A__DU__TFP_A-153.oedu` and `1A29_A__DU__TFP_A-154.oedu`) will be produced from `1A29_A__DU__biounit.oedu` and the site defined as `MET:124:  :A`, but the Iridium classification can be made since the structure factor CIF file (`1a29_validation_2fo-fc_map_coef.cif.gz`) was passed in through the *-map* option. The two files are resulting from the two different ligands binding in that site simultaneously.

> **Note**
>
> The *-map* option accepts structure factor CIF files (`.cif`, `.cif.gz`) as provided by *GetStructure* and the RCSB, as well as legacy MTZ files (`.mtz`).

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

```
prompt> enumsites -site_residue "ASP:25: :A" -in 1HHP_AB__DU__biounit.oedu -prefix FOO
```

will write the output structure into a file named `FOO_1HHP_AB__DU__apo_ASP_A-25.oedu`.

4.3 Command Line Help

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

```
prompt> enumsites --help
```

will generate the following output:

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

4.4 Required Parameters

-in <filename>

File containing a biounit OEDesignUnit that whose active site will be enumerated based on the input reference or site residues input.

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

File type	Extension
OEDesignUnit	.oedu

[keyless parameter 1]

-ref <filename>

File containing an OEDesignUnit with a site defined that can be used as a reference structure.

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

File type	Extension
OEDesignUnit	.oedu

NOTE: Either *-ref* or *-site_residue* must be set, but not both.

-site_residue <filename>

String containing one or more comma-separated residue strings that have the following format:

"RESIDUE_NAME:RESIDUE_NUMBER:INSERTION_CODE:CHAIN_ID"

As an example, this is what the string would look like for an asparagine residue, at position 25, with a blank insertion code, on chain A. "ASP:25: :A"

NOTE: Either *-site_residue* or *-ref* must be set, but not both.

4.5 Optional Parameters

4.5.1 Input Options

-map <filename>

Input electron density map from X-ray crystallography, to be used for Iridium score calculation.

Accepted formats are structure factor CIF files (`.cif`, `.cif.gz`) and legacy MTZ files (`.mtz`). See OEReadMTZ in the **OEChem TK** manual for MTZ map and column conventions.

-ref <filename>

Reference OEDesignUnit indicating the proper biological unit and relevant binding site.

-site_residue <residue identifier>

Input option to specify a binding site using a single residue specification if apo (or holo). The format is "name:num:insert code:chainid", e.g. "ASP:25: :A" indicating Aspartic acid 25 in chain A. Note: A blank/whitespace character is used for the insert code, which is a typical use case.

4.5.2 Output Options

-prefix <prefix>

Prefix used to name output files, default is blank

-log <logfile>

The argument for this flag specifies the name of the log file. This overrides any specified prefix. The default will be enumsites_output.log, if no prefix is specified.

-settings_file <settingsfile>

(Alias: -settings)

The argument for this flag specifies the name of the settings file. This overrides any specified prefix. The default will be enumsites_settings.param, if no prefix is specified.

-verbose

Triggers copious logging output

4.5.3 Enumerate Sites Parameters

-add_interactions

Option to add OEInteractionHints to the design unit(s)

[Default=true]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetAddInteractionHints in the **Spruce TK** manual.

`-add_style`

Option to add visualization style to the design unit(s)

[Default=true]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetAddStyle in the **Spruce TK** manual.

`-collapse_nonsite_alts`

Option to deduplicate structures with different alternate locations if those alternate locations are far from the binding site

[Default=true]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetCollapseNonSiteAlts in the **Spruce TK** manual.

`-duplicate_removal`

Option to deduplicate identical structures resulting from symmetry operations

[Default=true]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetDuplicateRemoval in the **Spruce TK** manual.

`-enum_cofactors_sites`

Option to generate design units with sites based on components classified as co-factors

[Default=false]

See also

- OESpruce::OEDesignUnitEnumerateSitesOptions::SetEnumerateCofactorSites in the **Spruce TK** manual.

`-restrict_to_refsite`

Option to skip generating design units for sites identified, that do not match a provided reference design unit

[Default=true]

> **See also**
>
> - OESpruce::OEDesignUnitEnumerateSitesOptions::SetRestrictToRefSite in the **Spruce TK** manual.

`-site_size` <value>

Distance from the ligand used to determine the size of the site

[Default=5.0 (angstroms)]

> **See also**
>
> - OESpruce::OEDesignUnitEnumerateSitesOptions::SetSiteSize in the **Spruce TK** manual.

`-superpose`

Option to superpose generated design units, if multiple. If a reference is provided, the first generated design unit will be superposed onto the reference structure, and subsequent structures onto that one.

[Default=true]

> **See also**
>
> - OESpruce::OEMakeDesignUnitOptions::SetSuperpose in the **Spruce TK** manual.

`-superpose_method` <method>

The method to use for superposition

Method	Description
global	Global Sequence Alignment to identify CA pairs
site	Global Sequence Alignment to identity CA pairs - focusing on the subset in active site
ddm	Superposition using the Distance Difference Matrix method (DDM)
sse	Superposition using an overlap of Secondary Structure Elements (SSE)
weighted	Superposition weighting residues by B-factor or occupancy
sitehopper	Superposition based on binding site similarities (sitehopper)
GlobalSequence	Alias for global — Global Sequence Alignment to identify CA pairs
DDMatrix	Alias for ddm — Superposition using the Distance Difference Matrix method
SiteSequence	Alias for site — Global Sequence Alignment focusing on the active site

> **See also**
>
> - OESpruce::OEMakeDesignUnitOptions::SetSuperpositionMethod in the **Spruce TK** manual.

CHAPTER

FIVE

GETSTRUCTURE

5.1 Overview

GetStructure is a simple application to download structure files from the RCSB servers for a given PDB code.

Input for the application is the 4-character PDB code identifying the structure. By default, the following files are downloaded if available:

- **MMCIF** (`.cif.gz`): the structure in mmCIF format
- **Structure factor CIF** (`_validation_2fo-fc_map_coef.cif.gz`): 2Fo-Fc map coefficient file for X-ray structures
- **CryoEM map** (`.map.gz`) and **header** (`.xml`): density map and metadata for cryo-EM structures

The legacy PDB format (`.pdb.gz`) can be requested with the `-pdb` flag. The Fo-Fc structure factor file (`_validation_fo-fc_map_coef.cif.gz`) can be requested with the `-fofc` flag.

Note

GetStructure downloads structure factor **CIF** files, not MTZ files.

Note

On macOS and RHEL 8, the user has to install openSSL 1.1 for the application to work. To install openssl on macOS we recommend using HomeBrew (https://brew.sh/), and the command: `brew install openssl@1.1`

Or, if you are using a conda environment, specify the openssl version with:

conda install openssl=1.1 -y

GetStructure is not supported on RedHat 9 and Windows 11 at this time due to an incompatibility with openSSL 1.1

5.2 Example Commands

The **getstructure** utility program is run by passing in a 4-letter PDB code:

```
prompt> getstructure 4OBD
```

Here, **getstructure** will download `4obd.cif.gz` (mmCIF structure) and `4obd_validation_2fo-fc_map_coef.cif.gz` (2Fo-Fc structure factor CIF) for X-ray structures.

To also download the legacy PDB format and the Fo-Fc structure factor file:

```
prompt> getstructure -pdb -fofc 4OBD
```

This additionally downloads `4obd.pdb.gz` and `4obd_validation_fo-fc_map_coef.cif.gz`.

For cryo-EM structures, **getstructure** downloads the mmCIF file along with the associated EMDB density map (`.map.gz`) and header (`.xml`) instead of structure factor CIF files.

CHAPTER

SIX

LOOPDBBUILDER

6.1 Overview

loopdb_builder is an application to build a database of loops in known structures, that can subsequently be used in *Spruce* to modeling missing loops.

Input for the application is a directory of PDB structures. An existing database can be appended to as new structures become available. OpenEye ships a pre-built database, which can be added to with internal/proprietary structures.

Loops are extracted from the structures in a sliding window producing loops of length 4, to the maximum length of a loop specified (default 22). The extracted loops are deduplicated so a loop with an identical sequence, rough distance between the anchor atoms, and similar backbone shape are only included once. The option to exclude "loops" with a regular secondary structure content (helix,strand) of >75% is on by default but can be turned off. The crop length removes N number of residues at the different termini of the protein structure before processing, knowing that the terminal residues are often flexible and poorly resolved in crystal structures, the default value is 1.

6.2 Example Commands

The **loopdb_builder** utility program is run by specifying a directory containing PDB files and a name of the source of the data

```
prompt> loopdb_builder -in PDB_DIR -source_name RCSB -prefix rcsb
```

Here, **loopdb_builder** will build a database of the loops in the structures provided in the directory. The resulting file will be named *rcsb_spruce.loop_db*.

6.3 Command Line Help

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

```
prompt> loopdb_builder --help
```

will generate the following output:

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

6.4 Required Parameters

-in <directory>
: Directory containing PDB files that will be processed for known loops

-source_name <value>
: Source name of the files, e.g. RCSB, EBI, PDBJ, or internal/proprietary sources.

6.5 Optional Parameters

-append <bool>
: Option to append to current loop dictionary with additional structures, otherwise will fail if output DB exists

  [Default=false]

-title <title>
: Title of the added structures, e.g. "Loops of aspartic acid protease structures"

  [Default=LoopTemplateDatabase]

-source_date <value>
: Date the source was updated in the format MM-DD-YYYY. Defaults to today's date.

-ncpu <value>
: Number of processors to run with, 0 means all available.

  [Default=0]

-max_length <value>
: Max length of loops to add to the database. Note to add a buffer for necessary crop back in loop modeling

  [Default=22]

-crop_length <value>
: Crop back this number of residues at the termini/breaks for each structure being evaluated

  [Default=2]

> **See also**
>
> - OESpruce::OELoopBuilderOptions::SetCropLength in the **Spruce TK** manual.

-exclude_reg_ss <value>
: Exclude sections with >75% regular secondary structures like helices and strand/sheets.

  [Default=true]

-prefix <prefix>
: Prefix used to name output files, default is blank

-log <logfile>
: The argument for this flag specifies the name of the log file. This overrides any specified prefix.

-settings_file <settingsfile>
: The argument for this flag specifies the name of the settings file. This overrides any specified prefix. [Aliases=**-settings**]

-skip_file <filename>

File containing PDB codes to skip, one code per line

-verbose

Triggers copious logging output

CHAPTER

SEVEN

DU2PDB

7.1 Overview

du2pdb is a simple utility application to convert DesignUnit OEDU files to PDB files.

7.2 Example Commands

The **du2pdb** utility program is run by specifying a directory containing PDB files and a name of the source of the data

```
prompt> du2pdb -in 5YE9_B__DU__8U6_B-501.oedu
```

Here, **du2pdb** will convert the OEDU file to 5YE9_B__DU__8U6_B-501.pdb, by default it will not include packing residues

7.3 Command Line Help

A description of the commandline interface can be obtained by executing **du2pdb** with the *–help* option.

```
prompt> du2pdb --help
```

will generate the following output:

```
Help functions:
  du2pdb --help simple      : Get a list of simple parameters
  du2pdb --help all         : Get a complete list of parameters
  du2pdb --help defaults    : List the defaults for all parameters
  du2pdb --help <parameter> : Get detailed help on a parameter
  du2pdb --help html        : Create an html help file for this program
  du2pdb --help version     : List the toolkits and versions used in the application
```

7.4 Required Parameters

-in <filename>

Input OEDesignUnit file to be converted

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

File type	Extension
OEDesignUnit	.oedu

[keyless parameter 1]

7.5 Optional Parameters

7.5.1 InputOutput Options

-includePackingResidues

Option to add include packing residues in the conversion

[Default=false]

-prefix <prefix>

Prefix used to name output files, default is blank

-log <logfile>

The argument for this flag specifies the name of the log file. This overrides any specified prefix. The default will be du2pdb_output.log, if no prefix is specified.

-settings_file <settingsfile>

(Alias: -settings)

The argument for this flag specifies the name of the settings file. This overrides any specified prefix. The default will be du2pdb_settings.param, if no prefix is specified.

-verbose

Triggers copious logging output

[Default=false]

CHAPTER

EIGHT

DU2MMCIF

8.1 Overview

du2mmcif is a simple utility application to convert DesignUnit OEDU files to MMCIF files.

8.2 Example Commands

The **du2mmcif** utility program is run by specifying a directory containing MMCIF files and a name of the source of the data

```
prompt> du2mmcif -in 5YE9_B__DU__8U6_B-501.oedu
```

Here, **du2mmcif** will convert the OEDU file to 5YE9_B__DU__8U6_B-501.cif, by default it will not include packing residues

8.3 Command Line Help

A description of the commandline interface can be obtained by executing **du2mmcif** with the *–help* option.

```
prompt> du2mmcif --help
```

will generate the following output:

```
Help functions:
  du2mmcif --help simple      : Get a list of simple parameters
  du2mmcif --help all         : Get a complete list of parameters
  du2mmcif --help defaults    : List the defaults for all parameters
  du2mmcif --help <parameter> : Get detailed help on a parameter
  du2mmcif --help html        : Create an html help file for this program
  du2mmcif --help version     : List the toolkits and versions used in the application
```

8.4 Required Parameters

-in <filename>

Input OEDesignUnit file to be converted

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

File type	Extension
OEDesignUnit	.oedu

[keyless parameter 1]

8.5 Optional Parameters

8.5.1 InputOutput Options

-includePackingResidues

Option to add include packing residues in the conversion

[Default=false]

-prefix <prefix>

Prefix used to name output files, default is blank

-log <logfile>

The argument for this flag specifies the name of the log file. This overrides any specified prefix. The default will be du2mmcif_output.log, if no prefix is specified.

-settings_file <settingsfile>

(Alias: -settings)

The argument for this flag specifies the name of the settings file. This overrides any specified prefix. The default will be du2mmcif_settings.param, if no prefix is specified.

-verbose

Triggers copious logging output

[Default=false]

CHAPTER

NINE

RELEASE HISTORY

9.1 SPRUCE 1.9.0

9.1.1 Related Toolkit Information

Spruce TK 1.9.0

New Features

- The maximum cluster size for partial residues built using OEBuildSidechains can now be set in OESidechainBuilderOptions using SetMaxClusterSize.
- The chemical component dictionary has been updated. However, if using mmCIF, the metadata will be used as primary information and the dictionary only engages if metadata is unavailable.

Minor Bug Fixes

- An issue has been fixed in the routine to reassign ambiguous water and metals from packing residues to the protein chain of interest. The issue caused HEME analogs and connected amino acids to be soaked into a given chain ID.
- An issue has been fixed to allow `OEHeterogenMetadata` to inform the component splitter during design unit generation and preparation. This also fixes an issue where the splitter would not allow reclassification of a metal ion to an excipient.
- An issue has been fixed that caused the option to collapse redundant alternate locations to improperly engage if there were multiple binding sites in a protein.
- An issue has been fixed that caused the option to collapse redundant alternate locations to improperly engage for different ligands in the same binding site.
- An issue has been fixed that caused `OEMutateResidues` to incorrectly leave the backbone nitrogen of a residue in a bad valence state when mutating from Proline.
- An issue has been fixed in `OEBuildSidechains` with the shell mutation option turned on that would leave side chains clashing with water molecules. The water molecules are now removed if the option to allow for removal of clashing waters is set to `True`.

9.2 SPRUCE 1.8.0

9.2.1 New Features

- The **SPRUCE** application can now read structure factor CIF files for electron density maps.

- The **GetStructure** utility application now downloads structure factor CIF files in place of MTZ files, which were deprecated by the wwPDB/RCSB.
- The **GetStructure** utility application can now download cryoEM maps and the related XML file, which stores the author-recommended contour value.

9.2.2 Minor Bug Fixes

- An issue has been fixed where some parameters were shown as required that were not required.

9.2.3 Related Toolkit Information

Spruce TK 1.8.0

New Features

- The function OEBuildSingleLoop now checks for loop clashes after minimization. The option can be set using SetRejectClashingLoopsPostMinimization.
- The function OEBuildSingleLoop can now delete residues already present at sites where a new loop needs to be built. The option can be set using SetDeleteExistingResidues.
- The function OEBuildSidechains can now partially build target residues in the event that some targets fail.
- Improved loop modeling has been added involving disulfide bridge creation by adding a bond length check.
- When running with SetFixResStates set to True, if the input molecule contains CIF header data, the filter will utilize the chemical component header section to inform a residue's bond order and subsequent formal charge.
- A new method, SetUseSeqScoreChainMatching, has been added to OESuperposeOptions which, when enabled, optimizes the sequence score over the overall RMSD when matching on multiple protein chains.

Major Bug Fixes

- An issue has been fixed where gaps in the protein structure were misidentified due to unconventional insert code usage.

Minor Bug Fixes

- Loop modeling results have been improved by setting OELoopBuilderOptions StrictProlineMatch to `False` by default. The updated default is due to an improved side chain building routine in a prior toolkit release.
- An issue has been fixed to ensure loops extracted from the loop database had the desired structural properties.
- When truncating a residue or converting a residue to a capping group, if that residue had a crosslink bond, the residue opposite would retain an atom in a bad valence state. That issue has been fixed.
- An issue has been fixed in the routine to reassign ambiguous water and metals from packing residues to the protein chain of interest. The issue caused HEME-analogs and connected amino acids to be soaked into a given chain ID.
- An issue has been fixed causing loop-relevant information with insert codes in an mmCIF header to be incorrectly read.
- The OECapCTermini, OECapNTermini, and OECapTermini functions address an issue that could result in an incorrectly labeled cap residue SequenceID.
- Several improvements were made to address performance issues in the OESpruceFilter.

Documentation Changes

- Several examples have been added, and the advanced protein preparation tutorial has been expanded.

9.3 SPRUCE 1.7.0

Minor internal improvements have been made.

9.3.1 Related Toolkit Information

Spruce TK 1.7.0

New Features

- The functions OEMakeDesignUnit and OEMakeBioDesignUnits will now use provided *OEHeterogenMetadata* in *OEStructureMetadata* as information for the splitting of a structure into a design unit, including such details as which parts should be considered cofactors.

Major Bug Fixes

- An issue has been fixed that caused charge and radii assignment to not happen, in paths where **Spruce** was also not allowed to protonate the structure.
- An issue has been fixed that caused radii to not be properly assigned to all atoms in the design unit.

Minor Bug Fixes

- An issue has been fixed which caused some mmCIF files to not be able to be prepared due to lack of missing metadata.
- An issue has been fixed where OEMutateResidues would crash if the structure contained the N-terminal capping group *NME*.

9.4 SPRUCE 1.6.1

9.4.1 New features

- Command line arguments have been added to control the gap and extend penalties for the sequence alignment used for loop building.

9.5 Spruce TK 1.6.1.1

9.5.1 Major bug fixes

- An issue has been fixed where OEExtractBioUnits function would fail if there was a mismatch in author assigned chain names and PDB assigned chain names in the case where a molecule was extracted from an mmCIF file.
- An issue was fixed in OEProtonateDesignUnit where a rule to flip clashing in-plane hydrogens on double bonded nitrogens was triggering incorrectly in specific instances.

9.6 Spruce TK 1.6.1

9.6.1 New features

- OEBuildSidechains now minimizes target side chains by default. Minimization can be controlled by setting minimizeSidechains and minimizeSidechainsShell options in the OESidechainBuilderOptions class.
- A feature has been added to support a next generation mmCIF feature, such that when an mmCIF file provides a connectivity record for the heterogens, **Spruce** will no longer look up the heterogen in the Chemical Component Dictionary but trust the input provided.
- A feature has been added that allows in-plane flipping of a single hydrogen on a double bonded nitrogen, when a clash is detected as part of hydrogen bond network optimization.

9.6.2 Major bug fixes

- An issue has been fixed related to using the OEHeterogenMetadata class, where the provided SMILES string was not respected for tautomer generation; when tautomers were not provided; and when the title (residue name) collided with existing residue names in the stored Chemical Component Dictionary.
- An issue has been fixed related to covalently bound ligands, where the pre-reaction input SMILES and related tautomers were not adjusted properly when accounting for the formed covalent bond.
- An issue has been fixed where the **Spruce** filter deleted single (disconnected) amino acid residues when they were marked HETATMs and were not real "floating" residues in part of the regular protein sequence.

9.6.3 Minor bug fixes

- OEMutateResidues, OEMutateResidue, and OEBuildSidechains now reduce failures arising from clashes by using shell minimization by default.
- An issue has been fixed that caused HEME-like molecules to be excluded from the stored chemical component database.

9.6.4 Documentation changes

- Information has been added about setting and getting minimizeSidechains and minimizeSidechainsShell options in the OESidechainBuilderOptions class.

9.7 SPRUCE 1.6.0

Minor internal improvements have been made.

9.8 Spruce TK 1.6.0

9.8.1 New features

- The chemical components dictionary has been updated with latest structures from the wwPDB.
- A feature has been added to OEProtonateDesignUnit to detect acceptor–acceptor clashes, modify the protonation state of one of the moieties, and reoptimize the hydrogen bond network.
- The following preliminary API classes have been made permanent.
  - OECapBuilderOptions
  - OELoopBuilderOptions

  - OEPocket
  - OEPocketOptions
  - OESidechainBuilderOptions
  - OESpruceFilter
  - OESpruceFilterOptions
  - OEValidateDesignUnit
- The following preliminary API functions have been made permanent.
  - OEBuildLoops
  - OEBuildSingleLoop
  - OEFindPockets
  - OEMakeDesignUnitFromPocket

9.8.2 Major bug fixes

- A crash in OESpruceFilter has been fixed in relation to atoms that were cleaned up during the standardization process.

9.8.3 Minor bug fixes

- An issue has been fixed that ensures radii are assigned to all atoms in a design unit.

9.8.4 Documentation changes

- An example has been added showing how to convert FASTA files to structure metadata for structures missing the SEQRES information in the PDB metadata and MMCIF equivalent.

9.9 SPRUCE 1.5.3

Minor internal improvements have been made.

9.10 Spruce TK 1.5.3

9.10.1 New features

- The chemical components dictionary was updated with latest data from the RCSB.

9.10.2 Major bug fixes

- An issue that caused OESpruceFilter to segfault has been fixed and safeguarded.

9.10.3 Minor bug fixes

- An issue has been fixed that caused incorrectly built loops when the protein structure contains nonstandard amino acids, particularly in the gap needing to be built or anchoring to it.
- An issue with sequence mutation for cysteine residues, where an explicit hydrogen was left over after the mutation, has been fixed.

9.11 SPRUCE 1.5.2.1

- Legal values for the *targetMask* flag have been added to docs and command-line help.

9.12 SPRUCE 1.5.2.0

Minor internal improvements have been made.

9.13 Spruce TK 1.5.2

9.13.1 New features

- OESpruceFilterOptions has an option to automatically assign chain IDs (default is true) when they are missing either completely or partially in the structure for a structure processed by OESpruceFilter.
- The built-in heterogen database has been updated with the latest structures from the ligand-expo at the RCSB.

9.13.2 Major bug fixes

- An issue where tautomers passed using metadata were not respected has been fixed.
- An issue has been fixed where, in a small fraction of cases, an OXT atom was not correctly built out when needed at the protein C-terminals.
- An issue has been fixed where the option to fix the state of backbone atoms and bonds in OESpruceFilterOptions was sometimes not respected in OESpruceFilter, which led to issues such as OXT atoms being built even if the option was disabled.

9.13.3 Minor bug fixes

- An issue was fixed in filter options to not accept the disallowed residue names UNL and UNK. Instead, they are renamed to LIG, which is a change filter that applies in the structure upon standardization.
- An issue where the maximum number of atoms in the biological unit was not being respected has been fixed.

9.13.4 Documentation changes

- Minor documentation and example improvements have been fixed.

9.14 SPRUCE 1.5.1

Fall 2022

9.14.1 New features

- When providing a site-residue to Spruce, the output title and output filenames of apo design units will now use that site residue in the name. Previously, the residue closest to the center of the binding site was used.

9.15 Spruce TK 1.5.1

9.15.1 New features

- If a site residue is provided to OEMakeDesignUnits, the output design unit title now includes the site residue in the title for apo structures. Previously, the residue in the title was the residue closest to the center of the binding site.

- Standardization using Spruce Filter now checks for metal chelation before forming disulfide bridges.

9.15.2 Major bug fixes

- An issue causing accumulation of generic data on the molecule components stored in the design unit object during prep has been fixed. This accumulation led to large memory consumption, slow preparation, and larger file size.

9.16 SPRUCE 1.5.0

Spring 2022

9.16.1 New Features

- **Spruce** has been enhanced to perform standardization and a filter checks before Spruce preparation.

  The following are detected and fixed:

  - invalid component names
  - invalid residue states
  - invalid metal bonds

  The following are detected and fail the structure:

  - invalid CRYST1 from header file
  - low overlap between the electron density map and the structure
  - invalid sequence alignment
  - blank Chain IDs
  - invalid alternate locations

- **Spruce** has been enhanced to perform checks on the generated design unit after running Spruce preparation.

  Issues detected and reported include:

  - partial side chains
  - missing loops
  - implicit hydrogens
  - incorrect partial charges
  - termini that are not capped properly
  - heavy atoms overlapping with each other
  - broken chains

- A new command line option `-enum_pockets` has been added. When enabled it automatically detects pockets and generates design units from them.

9.16.2 Minor Bug Fixes

- An issue with the value of the parameter `-min_align_score` not being properly respected has been fixed.

9.17 Spruce TK 1.5.0

9.17.1 New features

- The new OESpruceFilter class has been added to provide checks and corrections on input to **Spruce**. For input it can take an OEMolBase, OEStructureMetadata, or an options class, OESpruceFilterOptions, that holds the options to turn on each of the fixing options.
- The new OEValidateDesignUnit class has been added for validation of **Spruce** produced design units. For input it can take an OEDesignUnit or OEStructureMetadata.

9.17.2 Major bug fixes

- A bug that caused memory leaks in **OEBio TK** has been fixed.

9.17.3 Minor bug fixes

- An issue was fixed in OEBuildLoops to allow better sequence alignment for peptides.
- An issue was fixed in OEBuildLoops where free amino acids, as co-factors or ligands, were incorrectly included in sequence alignments and causing mismatched alignments to the SEQRES.
- An issue was fixed in OEExtractBioUnits to be able to lower the minimum sequence alignment score threshold.

9.18 SPRUCE 1.4.0

Fall 2021

9.18.1 New Features

- The application *loopdb_builder* now reads `MMCIF` files. If the same structure is available in both `PDB` and `MMCIF` format in the provided directory, the `PDB` file is used.

9.18.2 Minor Bug Fixes

- A minor bugfix affecting stability of the *loopdb_builder* has been fixed.

9.19 Spruce TK 1.4.0

Fall 2021

9.19.1 New features

- A new method, SetForceCapping, has been added to enable capping even if it will result in a clash.
- Two new methods, SetBuildTails and GetBuildTails, have been added to set and get an option that controls whether to build tails when there is missing residues at the N- and C- termini.
- SiteHopper is now a supported superposition method in OESuperpose, and can be set using the SetMethod method of OESuperpose.
- All Options classes have been modified to derive from OEOptions. This affects classes:
  - OEDesignUnitEnumerateSitesOptions
  - OEProtonateDesignUnitOptions
  - OEDesignUnitBuildOptions

  - OEDesignUnitPrepOptions
  - OEDesignUnitSplitOptions
  - OEBioUnitExtractionOptions
  - OEMakeDesignUnitOptions
  - OEPlaceHydrogensOptions

9.19.2 Major bug fixes

- An issue causing capping a nonstandard residue to fail has been fixed.
- An issue causing covalent ligands to have their covalent bond broken when there were alternate locations in the structure, has been fixed.
- An issue causing side-chains to either not be built or being built in non-optimal configurations has been fixed.
- An issue with pockets identifying liganded sites in OEMakeDesignUnitFromPocket not generating a proper design unit with a ligand bound in the identified site has been fixed.

9.19.3 Minor bug fixes

- An issue causing the warning message 'Truncated cap due to clash' to appear when SetAllowTruncate is *False* has been fixed.
- An issue caused by Heuristic score offset being added before comparing to original structure therefore unable to pick the more energy favorable conformation has been fixed.
- An issue causing the gap finding code to mis-identify gaps in the protein structure due to residues with missing backbone atoms has been fixed. The function now removes these residues prior to gap detection inside OEBuildLoops.
- An issue caused by malformed `PDB` Header data, specifically with regards to REMARK 300 sections, has been fixed.

9.20 SPRUCE 1.3.0

July 2021

9.20.1 New Features

- *getstructure* now retrieves structures using a secure HTTPS connection using openSSL.
- A no-prep option has been added to **SPRUCE** to enable conversion of prepared structures into the OEDesignUnit format. This option supersedes all other options.
- An optional `-out` parameter has been added to **SPRUCE**, for specifying the output filename. **SPRUCE** can write multiple design units per PDB file, and the default option is to write all of them to the single specified file. An additional option `-warts` has been added that will postfix a #n (n being an incrementing number) to the output filename.
- An `OEReceptor` is now added by default when using **SPRUCE**. The feature can be turned off using the *-add_receptors false* flag. A *-targetMask* can be specified to augment the receptor content. Furthermore, these OEDesignUnits with receptors can be further edited in the Make Receptor GUI application.
- Options for setting the RMSD, sequence alignment score, and Tanimoto thresholds for validating the superposition result have been added to *superposition*.
- The names of the available superposition methods for *SPRUCE*, *enumsites*, and *superposition* have been unified.

9.21 Spruce TK 1.3.0

July 2021

9.21.1 New features

- A molecule-based API for OEMakeDesignUnitFromPocket has been added.
- New high-level superposition APIs were added that unify the sequence-based (OEStructuralSuperposition) and shape-based (OESecondaryStructureSuperposition) APIs. This includes a new OESuperpose class that can calculate different types of structural superposition, a new OESuperposeOptions class that allows the users to control various behaviors of the superposition calculation, such as the superposition method, and a new OESuperposeResults class that holds the transformation and scores of the superposition. More detailed changes are as follows:
  - The new OESuperpose class can take either OEMol or OEDesignUnit as the reference for the fit molecule. The reference molecule can be set by using the SetupRef method, and the superposition can be calculated via OESuperpose with the fit molecule supplied as one of its arguments.
  - A new OESuperposeMethod namespace was added that contains the constants for different superposition methods. Functions OEGetSuperposeMethodName and OEGetSuperposeMethodFromName were added to obtain the superposition method's name (as a string literal) from its designated constant and vice versa.
  - Methods OESuperposeOptions, OESuperposeOptions, and OESuperposeOptions have been added. These methods can be used to set score thresholds for validating superposition results in the new OESuperposeOptions class. The validity of the superposition result can be obtained by OESuperposeResults from the new OESuperposeResults class.
  - The new OESuperpose API returns an OESuperposeResults object that can be used to transform the fit molecule to its superposed position with its Transform method. Alternatively, the users can use GetRotMatrix and GetTranslation to obtain the rotation matrix and translation vector, respectively, for their analyses. The RMSD and sequence alignment score after the superposition can be obtained using OESuperposeResults's GetRMSD and GetSeqScore methods for sequence-based superpositions, and the Tanimoto score can be obtained using GetTanimoto.

  Please refer to the documentation for more information on these new superposition APIs.

9.21.2 Minor bug fixes

- A bug that caused the loop modeling algorithm to crash in rare instances has been fixed.
- Examples have been modified to use appropriate command-line arguments.
- An issue that caused style on OEDesignUnit objects to disappear when calling OEProtonateDesignUnit has been fixed.
- An issue with the return value of superposition when two structures cannot be superposed has been fixed. It now properly returns a -1.00 RMSD.
- An issue in OEMakeDesignUnitFromPocket that caused style to remain on both the previous binding site and the one defined from the pocket has been fixed.
- A bug in superposition that resulted in a crash when using site residues that were not present on a design unit has been fixed.
- A bug that kept the insert code from its anchor residue when there was an N-terminal cap has been fixed.

9.21.3 Documentation changes

- Documentation has been added for the Iridium classification. Iridium.
- Documentation has been added for the new superposition APIs. Superposition related APIs are now fully supported. Superposition.

9.22 SPRUCE 1.2.0.2

March 2021

- An issue with modeled loops having incorrect fragment numbers in their residue information has been fixed.

9.23 SPRUCE 1.2.0.0

Fall 2020

- Minor internal improvements have been made.

9.24 Spruce TK 1.2.0

Fall 2020

9.24.1 New features

- New methods have been added to OEDesignUnitSplitOptions (AddLipidCode, SetLipidCodes, ClearLipidCodes, and GetLipidCodes). They allow users to specify the names of molecules to be considered as lipids.
- Support has been added for HEME and related cofactors in OEMakeDesignUnits. The state of HEME, contains two negatively charged nitrogens to balance the +2 Fe formal charge. The nitrogens coordinating the iron atom are indicated by zero-order bonds.
- A new function, OEFindPockets, has been added that finds cavities in protein or nucleic acid complexes. The parameters for the search can be tuned with OEPocketOptions. The pockets are output as OEPocket objects in an iterator. The function can take a predicate that will control only outputting pockets with a given set of residues or atoms in it. This function is also used in OEMakeDesignUnits when a site residue is provided.
- A new function, OEMakeDesignUnitFromPocket, has been added that takes a prepared biological unit from an OEMakeDesignUnit and an OEPocket and coverts it into an OEDesignUnit does with a reference structure.
- New methods have been added in OELoopBuilderOptions, SetSeqAlignMethod, SetSeqAlignGapPenalty, SetSeqAlignExtendPenalty, GetSeqAlignMethod, GetSeqAlignGapPenalty, and GetSeqAlignExtendPenalty that allow users to control the sequence alignment done to find gaps in protein structures related to loop modeling.

9.24.2 Major bug fixes

- A bug that caused some modeled loops to be missing the backbone NH hydrogen where the modeled loops were attached has been fixed.
- Fragment numbers for build loops have been fixed to be consistent with the anchor residues where the loops are inserted.
- A bug in OEFixBackbone has been fixed to ensure that OXT atoms are always built on C-terminal residues.
- An issue with atom order for built pieces like loops or caps has been fixed to ensure that these are sequential with the location they are built.

- A bug in OEBuildLoops that in specific situations caused incorrect detection of gaps in protein structures has been fixed. Additionally, options have been exposed in OELoopBuilderOptions to allows users to control the underlying sequence alignment in the event of a failure.

9.24.3 Minor bug fixes

- Improvements have been made to standard amino acid residue perception when preparing structures.
- Site residues in OEMakeDesignUnits are now being checked against all the biological units so one can serve as a reference for the rest.
- A bug in loop modeling that caused the function to create residues with identical residue numbers has been fixed. The function now properly builds using insertion codes.
- A bug in loop modeling that caused problems for the underlying sequence alignment code and incorrect loops when a single residue was floating in space between two gaps has been fixed.
- The chemical component dictionary used internally in OEMakeDesignUnits has been updated with the latest changes from the RCSB, including some fixes for incorrect entries in the source data based on rules and literature searches.

9.25 SPRUCE 1.1.0

Spring 2020.1

- An issue resulting in a floating point exception on MacOS has been fixed.
- Minor errors in the help text have been fixed.

9.26 SPRUCE 1.1.0

Spring 2020.0

This version of **SPRUCE** has been built using **OEToolkits 2020.0**.

9.26.1 New Features

This release contains two new applications:

- **LoopDB_Builder** uses existing structures to build a dictionary of known loops that can be used in loop modeling of unresolved gaps in protein structures.
- **du2pdb** converts the entire content of an `OEDesignUnit` to a PDB file.

9.26.2 Major bug fixes

- The **GetStructure** application has been enhanced to prevent partial downloads. Retries and timeouts have been improved.

9.26.3 Minor bug fixes

- The prefix input behavior has been standardized across all **SPRUCE** applications.
- The input option `--restrict_to_refsite` is now being respected for both **SPRUCE** and **EnumSites**.
- The `-site_residue` input option to **EnumSites** now performs correctly.
- The **GetStructure** application now checks that the input PDB code contains 4 characters.
- **SPRUCE** now fails if an MTZ file is specified but is not present or is unreadable.

- The documentation around the `-site_residue` option used for APO structures has been simplified.

9.27 SPRUCE 1.0.0

Nov 2019

This version of **SPRUCE** has been built using **OEToolkits 2019.Oct**.

This is first release of the **SPRUCE** application suite. **SPRUCE** takes experimental biomolecular structure data in either `PDB` or `mmCIF` formats, and prepares the structures for use with downstream modeling applications. The **SPRUCE** application suite consists of the following applications and utilities:

- **SPRUCE** prepares biomolecular structure files (`PDB`, `mmCIF`, `OEB`, etc.) for downstream modeling applications such as docking a ligand with **FRED** or **HYBRID**, predicting poses with **POSIT**, or for running **SZMAP** to analyze active-site hydration thermodynamics.
- **Superposition** structurally superposes a given biomolecular structure onto a reference structure.
- **EnumSites** enumerates biounit OEDesignUnit (`OEDU`) files, and creates individual `OEDU` files for every active site discovered.
- **GetStructure** downloads `PDB`, `mmCIF`, and `MTZ` files if available for a given PDB code. The downloads are from the RCSB website.

CHAPTER

TEN

CITATION

Note

To cite Spruce please use the following:

Spruce 1.9.0.0. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.eyesopen.com.

CHAPTER

ELEVEN

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TWELVE

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13.2 Orion Floes

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OpenEye Large-Scale Floes 4.2.3. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
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- OEFF TK
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- FastROCS TK
- Grapheme TK
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- OEMedChem TK
- MolProp TK
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```
SZYBKI Application 2.8.0.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://
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```

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.

13.4 Publications for Bibliographies

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

13.4.1 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

13.4.2 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

13.4.3 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

13.4.4 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

13.4.5 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

13.5 OpenEye MMDS Web Service

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

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

CHAPTER

FOURTEEN

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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
click-didyoumean	https://github.com/click-contrib/click-didyoumean	https://github.com/click-contrib/click-didyoumean/blob/master/LICENSE
click-plugins	https://github.com/click-contrib/click-plugins	https://github.com/click-contrib/click-plugins/blob/master/LICENSE.txt

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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

14.1 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).

The OpenEye toolkits are NOT open source software and are NOT governed by GPL or other open source licenses. Your right to use the toolkits are governed by the OpenEye license which is binding to You.

For certain Linux distributions, GCC library components are included as object files. Your rights to use GCC library components (libstdc++, libgcc, and libgomp) included with these distributions are governed by the GPLv3 license as follows:

The components libstdc++, libgcc, and libgomp are part of GCC.

- GCC is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.
- GCC is distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY; without even the

implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the GNU General Public License for more details.

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.

14.1.1 GCC RUNTIME LIBRARY EXCEPTION

```
Version 3.1, 31 March 2009

Copyright © 2009 Free Software Foundation, Inc. http://fsf.org/

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␣
↪section 7 of the GNU General Public License,
version 3 ("GPLv3"). It applies to a given file (the "Runtime Library") that bears a␣
↪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.

1. Grant of Additional Permission.

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

14.1.2 GNU GENERAL PUBLIC LICENSE

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

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

                            Preamble

 The GNU General Public License is a free, copyleft license for
 software and other kinds of works.

   The licenses for most software and other practical works are designed
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to take away your freedom to share and change the works.  By contrast,
the GNU General Public License is intended to guarantee your freedom to
share and change all versions of a program--to make sure it remains free
software for all its users.  We, the Free Software Foundation, use the
GNU General Public License for most of our software; it applies also to
any other work released this way by its authors.  You can apply it to
your programs, too.

  When we speak of free software, we are referring to freedom, not
price.  Our General Public Licenses are designed to make sure that you
have the freedom to distribute copies of free software (and charge for
them if you wish), that you receive source code or can get it if you
want it, that you can change the software or use pieces of it in new
free programs, and that you know you can do these things.

  To protect your rights, we need to prevent others from denying you
these rights or asking you to surrender the rights.  Therefore, you have
certain responsibilities if you distribute copies of the software, or if
you modify it: responsibilities to respect the freedom of others.

  For example, if you distribute copies of such a program, whether
gratis or for a fee, you must pass on to the recipients the same
freedoms that you received.  You must make sure that they, too, receive
or can get the source code.  And you must show them these terms so they
know their rights.

  Developers that use the GNU GPL protect your rights with two steps:
(1) assert copyright on the software, and (2) offer you this License
giving you legal permission to copy, distribute and/or modify it.

  For the developers' and authors' protection, the GPL clearly explains
that there is no warranty for this free software.  For both users' and
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.

  An interactive user interface displays "Appropriate Legal Notices"
to the extent that it includes a convenient and prominently visible
feature that (1) displays an appropriate copyright notice, and (2)
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.

  The Corresponding Source need not include anything that users
can regenerate automatically from other parts of the Corresponding
Source.

  The Corresponding Source for a work in source code form is that
same work.

  2. Basic Permissions.

  All rights granted under this License are granted for the term of
copyright on the Program, and are irrevocable provided the stated
conditions are met.  This License explicitly affirms your unlimited
permission to run the unmodified Program.  The output from running a
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  You may make, run and propagate covered works that you do not
convey, without conditions so long as your license otherwise remains
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of having them make modifications exclusively for you, or provide you
with facilities for running those works, provided that you comply with
the terms of this License in conveying all material for which you do
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not control copyright.  Those thus making or running the covered works
for you must do so exclusively on your behalf, under your direction
and control, on terms that prohibit them from making any copies of
your copyrighted material outside their relationship with you.

  Conveying under any other circumstances is permitted solely under
the conditions stated below.  Sublicensing is not allowed; section 10
makes it unnecessary.

  3. Protecting Users' Legal Rights From Anti-Circumvention Law.

  No covered work shall be deemed part of an effective technological
measure under any applicable law fulfilling obligations under article
11 of the WIPO copyright treaty adopted on 20 December 1996, or
similar laws prohibiting or restricting circumvention of such
measures.

  When you convey a covered work, you waive any legal power to forbid
circumvention of technological measures to the extent such circumvention
is effected by exercising rights under this License with respect to
the covered work, and you disclaim any intention to limit operation or
modification of the work as a means of enforcing, against the work's
users, your or third parties' legal rights to forbid circumvention of
technological measures.

  4. Conveying Verbatim Copies.

  You may convey verbatim copies of the Program's source code as you
receive it, in any medium, provided that you conspicuously and
appropriately publish on each copy an appropriate copyright notice;
keep intact all notices stating that this License and any
non-permissive terms added in accord with section 7 apply to the code;
keep intact all notices of the absence of any warranty; and give all
recipients a copy of this License along with the Program.


  You may charge any price or no price for each copy that you convey,
and you may offer support or warranty protection for a fee.

  5. Conveying Modified Source Versions.

  You may convey a work based on the Program, or the modifications to
produce it from the Program, in the form of source code under the
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,
in or on a volume of a storage or distribution medium, is called an
"aggregate" if the compilation and its resulting copyright are not
used to limit the access or legal rights of the compilation's users
beyond what the individual works permit.  Inclusion of a covered work
in an aggregate does not cause this License to apply to the other
parts of the aggregate.

  6. Conveying Non-Source Forms.

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

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

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

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

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

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

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

  A "User Product" is either (1) a "consumer product", which means any
tangible personal property which is normally used for personal, family,
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
documented (and with an implementation available to the public in
source code form), and must require no special password or key for
unpacking, reading or copying.

  7. Additional Terms.

  "Additional permissions" are terms that supplement the terms of this
License by making exceptions from one or more of its conditions.
Additional permissions that are applicable to the entire Program shall
be treated as though they were included in this License, to the extent
that they are valid under applicable law.  If additional permissions
apply only to part of the Program, that part may be used separately
under those permissions, but the entire Program remains governed by
this License without regard to the additional permissions.

  When you convey a copy of a covered work, you may at your option
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removal in certain cases when you modify the work.)  You may place
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    author attributions in that material or in the Appropriate Legal
    Notices displayed by works containing it; or

    c) Prohibiting misrepresentation of the origin of that material, or
    requiring that modified versions of such material be marked in
    reasonable ways as different from the original version; or

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