

OpenEye
SCIENTIFIC

Bioisostere TK – Java

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Attention

Bioisostere TK is currently only available in C++ and Python.

CHAPTER

ONE

THEORY

1.1 Theory

There is a long history to fragment and bioisosteric replacement (see [Chen-2003]). Most medicinal chemists are well versed in standard sets of bioisosteric fragments. Likewise, there is a long history of computational approaches to fragment replacement (see [Verloop-1987] and [Lauri-1994]). There have been several attempts to examine sets of known active compounds to empirically identify bioisosteric fragments (see [Ujváry-2003] and [Sheridan-2002]). While this is an interesting exercise, it has two drawbacks. First, it can only identify bioisosteric fragment pairs that are already known. While these provide interesting study, they are often already familiar to experienced medicinal chemists and modelers. Second, it identifies many incidental rather than meaningful fragment pairs. These result from the fact that simply because two molecules bind to the same site does not mean they differ only by bioisosteric replacement. For instance, chemists may analog a compound by substituting an N-methyl group with an N-benzyl group in order to identify new binding pockets. However, just because both of these compounds are bioactive does not mean that methyl and benzyl are similar fragments (though they would be identified as such by some methods). While one may apply various heuristics, such as size, to avoid this problem, we hope to explore methods that are more robust.

An alternative approach has been to use an algorithm that would predict whether two fragments are similar in relevant ways. Several groups including Bartlett, Verloop, and Willett (see [Lauri-1994], [Verloop-1987], and [Watson-2001]) have developed methods in this area. Here we seek to capitalize on and extend the ideas developed by these workers.

1.1.1 3D Fragment similarity searching

BROOD allows users to enter a single query fragment and search a very large database of known molecular fragments in order to identify fragments that are similar. Each database fragment is compared to the query fragment in 3D with regard to shape, chemistry, electrostatics, and geometric presentation of attachment vectors. The fragments that are most similar to the query fragment will appear in a hitlist.

All similar fragments in a **BROOD** hitlist are organized into clusters. The clusters are organized so that molecules with the same ring structures and core framework (reduced-graph) are placed in the same cluster. The first cluster in **BROOD** hitlists is always the molecules that are similar to the query, sharing the same core atomic framework. While some of these analogs may be obvious, they often include alternative interesting chemistries. The remaining clusters are each organized around a unique core atomic framework. Each cluster is represented by its best scoring member and the clusters themselves are ranked by the score of their best member.

1.1.2 Clash detection and selectivity

BROOD allows users to specify protein structures for the purpose of testing whether newly constructed analogs fit into the active site. When the **BROOD** query ligand is based upon a crystallographic co-crystal structure, **BROOD** builds the newly created analog molecules in the same shape and orientation as the query. If the crystallographic ligand was originally in an active site and the protein is passed to **BROOD** as the bump protein, the new analogs will be built in poses that are also in the bump protein's active site. When a bump protein is passed, **BROOD** checks for clashes between the bump protein and each analog. By default, if any ligand heavy atom is less than 2.25 Angstroms from a protein heavy atom, the analog is removed from the hitlist.

Users can also specify another protein for selectivity testing (referred to here as the selectivity protein). In order for an analog to remain in the final hitlist, it must clash with the selectivity protein. The bump protein and the selectivity protein should be aligned and the **BROOD** query should be based on a molecule that fits within the bump protein active site. In this case, analogs in the final **BROOD** hitlist will also fit into the bump protein's active site, while they will also have clashes with the selectivity protein. This combination is a simple model for analogs that have a chance to be active against the bump protein, but have a very low chance of being active against the selectivity protein. This model assumes the analog molecules bind to the bump protein in a manner that is similar to the original ligand and that the most favorable pose for the ligand class in the selectivity protein is similar to that in the bump protein.

1.1.3 Strain energy

BROOD's output includes newly constructed analog molecules that are intended to have a similar 3D shape to the query molecule. These new analogs are constructed partially from the original molecule and partially from new fragments. When these new molecules are generated and built into a conformation that has good shape and chemistry overlap with the query molecules, some strain may be introduced. To produce high-quality results, it is essential that the analogs are optimized while maintaining the query shape and that little strain is introduced in the process.

The **BROOD** search process guarantees that each of the molecular fragments alone is in a low energy state. After the fragments are joined, this may no longer be true. For every **BROOD** analog in the final hitlist, two optimizations are carried out to determine the local strain introduced by maintaining a shape similar to the original query. In the first optimization, the ligand is allowed to relax into a local minimum. In the second optimization, the ligand atoms are only allowed to move a fraction of an Angstrom, keeping the same overall shape of the molecule. In both calculations, the OEMMFF [Halgren-I-1996], [Halgren-II-1996], [Halgren-III-1996], [Halgren-IV-1996], [Halgren-V-1996], [Halgren-VI-1999], [Halgren-VII-1999] potential is used with a Sheffield solvation function [Grant-2007]. The local strain energy is the difference in ligand energy between the two calculations. By default, the maximum strain for any successful **BROOD** analog is limited to 6.5 kCal/M.

1.1.4 Fragment joining

One approach to lead identification and development is based on the identification and expansion of physically very small molecule inhibitors that are commonly termed "fragments" (see [Hajduk-2007]). Fragments in this sense are molecules with few atoms and should not be confused with the term fragment used elsewhere in this document that refers to part of a molecule. Nevertheless, the fragment replacement algorithm in **BROOD** can be useful in the modeling of fragment-based design. In fragment-based design, one strategy is to combine two non-overlapping inhibitory fragments to form a single molecule. While this is sometimes empirically done with a series of flexible linear linkers, the linkers can also be modeled.

1.1.5 Cyclization

One of the first applications of **BROOD** many users want to explore is the replacement of a flexible portion of a molecule with a more rigid fragment that fills the same space. **BROOD** excels at this application. This type of exercise can be considered a local cyclization. In some molecules, rather than a local cyclization, some chemists prefer to design a bridge between two portions of a molecule that do not have a local link. This is another task where **BROOD** can be quite useful. Long-distance cyclization, like fragment joining, is about finding a chemical fragment that can bridge to moieties given a particular 3D orientation.

1.1.6 Molecular complexity

In the early 1980's, Bertz first published a measure of the complexity of molecules and asserted that his calculated complexity could be related to synthetic ease ([Bertz-1981], [Bertz-1982]). Bertz built complexity terms that are similar to a Shannon entropy ([Shannon-1949]) but with regard to the elements in a molecule and the diversity of small fragments that make up the structure of the molecule. While the actual synthetic accessibility can be heavily influenced by the availability of complex synthetic building blocks and advances in stereo synthetic methods, molecular complexity remains a useful tool for prioritizing which compounds chemists should look at first when primary modeling methods don't readily distinguish between them.

In 2007, Boda and coworkers extended Bertz's idea and compared it to experimental chemists' predictions of synthetic accessibility ([Boda-2007]).

Boda made the significant advance of adding stereo complexity to Bertz's elemental, graph, and ring complexity. We noted in the paper that nearly all the signal was generated by the molecular complexity and stereo complexity. In fact, each of these measures, without the linear fitting presented in the paper, correlated with chemists' predictions of synthetic accessibility as well as the chemists' predictions correlated with one another. Thus, in **BROOD**, we have implemented a molecular complexity that is a normalized sum of the graph and size complexity, elemental complexity, and stereo complexity. The normalized complexity score starts at zero for the simplest, smallest molecule and grows to values that generally don't exceed 1.0 for medicinally relevant small molecules.

BROOD uses molecular complexity to sort analog molecules in the final hitlist that have very similar shape and color scores.

1.1.7 Aromatic fragment comparison

This is an example of applying **BROOD** as a technology to explore fragment similarity outside the direct context of a specific drug-discovery project. Tu and coworkers at Pfizer explored the chemical space of aromatic ring systems ([Tu-2012]). In their work, they used **BROOD** at the core of the NEAT (Novel and Electronically Equivalent Aromatic Templates) tool. This tool uses a combination of high-level QM-derived partial charges along with **BROOD**'s electrostatic similarity calculation to explore potentially aromatic system replacements. It allows medicinal chemists to explore the large space of complex aromatic ring systems for replacements that are both electronically and sterically analogous. We present this example as an illustration of the more diverse applications of **BROOD**'s fragment-matching technology.

1.1.8 Shape-based belief model

It is a well-known concept in medicinal chemistry that compounds with greater similarity have a higher probability of having shared properties. It is by this premise that project teams seek to explore chemical space around a lead compound in order to discover new active molecules. Based on this concept, Muchmore and colleagues at Abbott attempted to quantify the relationship between various measures of ligand similarity and binding activity ([Muchmore-2008]). A large number of ligands with activities measured across a large number and wide variety of targets were used to generate the probability that two molecules with a given similarity would have activity within one log unit of one another (the p[active]). Several well-regarded ligand similarity techniques showed sigmoidal curves where, at very low similarity, the probability of shared activity was related to the prevalence of inhibitors in the underlying data; whereas, as two molecules approached very high similarity, the probability of similar activity approached something like 35-55%. While perhaps surprising at first, both of these results are sensible. It is well known that while similar molecules are much more likely to have shared activity than two random molecules, similarity is by no means a guarantee of shared activity.

As reported in their paper, one of the similarity techniques with the highest maximum probability was the combo score (shape + color score) from the OpenEye tool ROCS. The critical change from color score to color Tanimoto occurred in ROCS since the publication of Muchmore's paper. The change to color Tanimoto resulted in an even higher maximum probability of 0.512 ([Brown-Muchmore-2008]) for shape + color Tanimoto. The curve that was refit using the Abbott data is used in **BROOD** to convert the overall shape + color Tanimoto similarity of the analog molecule to the query molecule to generate a p(Active) value that indicates the probability, according the Abbott's belief model, that the analog compound will have activity within one log unit of the query compound.

1.1.9 Abbott bioavailability score

In 2005, Martin published a predictive model for the probability that a compound will have bioavailability (f) > 10% in rats ([Martin-2005]). Despite attempts to identify a useful model using straightforward linear combinations of simple parameters, such as logP, logD, donors, acceptors, PSA, or flexibility, Martin noted that different predictive models were required for different ionization states. Anions require a bioavailability model that depends strongly on PSA. By contrast, neutral species, cations, and zwitterions require a model based on the rule-of-five. The combination of these models provides a single model for bioavailability in rats.

1.1.10 Similarity to available compounds

Sometimes it may be desirable to check whether compounds similar to the analogs generated by **BROOD** already exist in commercial or internal databases, allowing a chemist to consider molecules available for purchase before undertaking the synthesis of a given analog.

BROOD uses similarity searching between compounds, based on two-dimensional circular fingerprints, to access compound similarity. The cricular fingerprints encode the presence of molecular substructures based on atom neighborhoods. This similarity is quantified using the Tanimoto coefficient, which measures the ratio of the intersection to the union of the fingerprint bit vectors. A Tanimoto similarity threshold of 0.15 is used as the cutoff to determine whether two compounds are considered structurally similar.

1.1.11 BROOD Database Generation (CHOMP)

BROOD's database generation program, **CHOMP**, fragments molecules by identifying critical bonds that can be broken. **CHOMP** includes three sets of bond-breaking patterns: *RLF (ring, linkers & functional groups)*, RECAP rules [Lewell-1998], and ALL (indicating breaking all non-ring, non-resonance single bonds). By default, **CHOMP** breaks all bonds identified using any of these methods. Users can also specify a SMARTS file of their own bond identifiers. This file should include a series of SMARTS patterns (one per line) that each define two atoms on opposite ends of the bond to be broken. For example, a line with the SMARTS "-" will cause all single bonds to be broken, while a line with the SMARTS "[R]-[!R]" will cause all bonds between ring atoms and non-ring atoms to be broken and "[#6]-!@[!#6!#1]" will cause CHOMP to break every single non-ring bond between a carbon atom and a heteroatom.

The RLF chemical heuristics seek to break compounds into three types of primary fragments; contiguous ring systems, functional groups, and linkers. Contiguous ring systems include any set of atoms that are bonded together by at least one ring bond. Thus, fused rings and spiro rings are included as a single ring system, but biphenyl is broken into two ring systems. Functional groups are defined as any collection of bonded atoms including one or more heteroatoms or unsaturated carbons separated by at most a single fully saturated carbon atom. The linkers are the remaining saturated carbon skeletons. It should be noted that linkers, like functional groups and ring systems, can be terminal (i.e., degree 1).

CHOMP systematically identifies all the molecular fragments that can be generated by breaking one or more of the specified bonds. **CHOMP** first eliminates fragments that have more than 15 heavy atoms or that have more than three attachment points. **CHOMP** also filters the fragments based on commonly used molecular filters, eliminating unstable, reactive, or toxic functional groups. As a final fragment generation step, for every fragment with two attachment points, **CHOMP** generates two single attachment fragments; for every fragment with three attachment points, **CHOMP** generates six fragments with two attachment points and three fragments with single attachment points by capping the open attachment valence with hydrogens. **CHOMP** then eliminates any duplicate fragments.

This first portion of the **CHOMP** algorithm involves only graph processing and can proceed very quickly. Please note, however, that when processing molecular databases of more than a few million compounds, **CHOMP** will use significant amounts of memory. Memory usage is especially aggressive early in the execution, when many new fragments are being identified, and slows somewhat as the algorithm progresses.

The next stage of the **CHOMP** algorithm is to generate 3D conformers using a specialized version of the **OMEGA** algorithm. **CHOMP**'s version of **OMEGA** has a modified TORLIB in order to sample more generously around the attachment points. It also differs from default **OMEGA** parameters in having tighter constraints for removal of RMSD duplicates (as the measure is very sensitive to size) and for having scaled MAXCONFS and EWINDOW parameters based on the size of the fragments. Finally, **CHOMP** writes the fragments into a **BROOD** database. To accomplish this, **CHOMP** carries out several precalculations, including generating physical properties and adding color atoms. CHOMP also segregates the fragment conformers into groups that are likely to match the same types of queries. All these processes help **BROOD** search the databases more quickly.

1.1.12 BROOD Database

BROOD databases are currently in the format of a directory or folder that contains many files. The databases can be easily compressed and uncompressed with standard compression algorithms. They can also be moved, but not easily renamed. To rename the **BROOD** database, you must also rename all the files contained within it. Consistency is required to prevent confusion between the name of the database and the files being searched under that name.

Of the files in the database directory, only one is human-readable. This is the `.info` file. If you open the `.info` file with a text reader, you will see some information about the database, its version, and a manifest of the files that are supposed to be in the database. Whenever a database is read, the manifest is checked to ensure the database has not been corrupted.

CHAPTER

TWO

BIOISOSTERE EXAMPLES

The following table lists the currently available **Bioisostere TK** examples:

2.1 Building Brood Database (CHOMP)

The following code example shows how to build a **Brood** database from a library of molecules.

This example demonstrates end-to-end fragment database construction, including fragment generation, optional filtering, and writing the final Brood database.

See also

- *OEFragmentOptions* class
- *OEDBScreenOptions* class
- *OEDBBuilder* class
- *OEDBWriter* class
- *OEGenerateConformers* function

2.2 Creating Brood Query

The following code example shows how to create a **Brood** query from a molecule that could be used for bioisosteric fragment replacements using **Brood**.

See also

- *OEBroodQuery* class
- *OECreateBroodQuery* function

2.3 Generating Brood Hits

The following code example shows how to perform bioisosteric fragment replacements on a **Brood** query and generate a hit list.

See also

- *OEBroodGeneralOptions* class
- *OEBroodScoreOptions* class
- *OEBroodHitlistOptions* class
- *OEBroodOverlay* class
- *OEHitlistBuilder* class

2.4 Generating Brood Matches

The following code example shows how to perform bioisosteric fragment replacements on a **Brood** query and generate all possible matches. This could be a use case when generating all possible design ideas using **BROOD** and postprocessing them with other tools.

See also

- *OEBroodGeneralOptions* class
- *OEBroodScoreOptions* class
- *OEBroodOverlay* class
- *OEBroodMolBuilder* class

2.5 Overlay between Fragments

The following code example shows how to overlay a fragment against a query fragment. This could be a use case when working with synthons and trying to find similar synthons based on 3D similarity.

See also

- *OEBroodGeneralOptions* class
- *OEBroodScoreOptions* class
- *OEFragOverlay* class

2.6 Replacing a Fragment in a Molecule

The following code example shows how to replace a fragment in a molecule defined in the form of a **BROOD** query.

See also

- *OEBroodGeneralOptions* class
- *OEBroodScoreOptions* class
- *OEBroodOverlay* class
- *OEBroodMolBuilder* class

2.7 Building and Using an External Compound Database

The following code example shows how to build and use an external (in-house) compound database to find similar 2D compounds to a generated hit list. It demonstrates optional analog lookup against a user-provided compound database to annotate Brood hits with similar known molecules.

See also

- *OECPDDatabase* class
- *OEBroodGeneralOptions* class
- *OEBroodScoreOptions* class
- *OEBroodOverlay* class
- *OEDBBuilder* class
- *OEDBWriter* class

2.8 Creating Brood Query by Linking Two Molecules (Bridging)

The following code example shows how to create a **Brood** query from two molecules to find a suitable linker between the two using bioisosteric fragment replacements using **Brood**.

See also

- *OEBroodQuery* class
- *OECreateBroodQuery* function

2.9 Clustering Brood Hits

The following code example shows how to cluster a generated **Brood** hit list using *OEBroodClusterBuilder* and *OEBroodCluster*. It demonstrates post-processing of hits into similarity clusters and cluster-level prioritization.

See also

- *OEBroodGeneralOptions* class
- *OEBroodScoreOptions* class
- *OEBroodHitlistOptions* class
- *OEBroodOverlay* class
- *OEHitlistBuilder* class
- *OEBroodClusterBuilder* class
- *OEBroodCluster* class

2.10 Building Combined Hits from Different Queries of the Same Molecule with OEBroodComboBuilder

The following code example shows how to use two **Brood** queries for the same molecule, where the first query is used to select a limited set of primary hits (controlled by `-primaryQueryMaxHits`) and the second query uses *OEBroodComboBuilder* to generate all possible secondary (combo) hits from those selected primary hits. The second stage is bounded by `-secondaryQueryMaxHits`.

This example demonstrates a two-query combo workflow using `-in` and `-in2`: it builds primary hits from the first query, expands secondary combo hits from the second query, then clusters and ranks the resulting combo hits before writing the final output molecules.

See also

- *OEDBReader* class
- *OEBroodOverlay* class
- *OEBroodMolBuilder* class
- *OEBroodComboBuilder* class
- *OEBroodClusterBuilder* class
- *OEBroodCluster* class

2.11 Curating Scored Fragment Hits with OEScoreHitlist

The following code example shows how to collect scored fragment matches for a query and curate them with *OEScoreHitlist*.

This example demonstrates score-level deduplication and ranking prior to full molecule building.

See also

- *OEDBReader* class
- *OEBroodOverlay* class
- *OEScoreHitlist* class

- *OEBroodScore* class

2.12 Comparing Connection and Molecule Building Outcomes

The following code example shows how to compare connection-table construction and full molecule-building outcomes from curated scored fragments.

This example demonstrates use of *OEMolCTBuilder*, *OEBroodMolBuilder*, and *OEBroodBuildResult* for build diagnostics.

See also

- *OEScoreHitlist* class
- *OEMolCTBuilder* class
- *OEBroodMolBuilder* class
- *OEBroodBuildResult* class

CHAPTER

THREE

PRELIMINARY API

3.1 Preliminary OEBioisostere Classes

3.1.1 OEBroodBuildOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodBuildOptions : public OESystem::OEOptions
```

This class provides an interface to setup options required for building molecules with replaced fragments. These options are used both from *OEBroodMolBuilder* and *OEHitlistBuilder*.

The *OEBroodBuildOptions* class defines the following public methods:

- *GetBuildType* and *SetBuildType*
- *GetNeutralPH* and *SetNeutralPH*
- *GetTautomers* and *SetTautomers*
- *GetCheckBond* and *SetCheckBond*
- *GetMaxLocalStrain* and *SetMaxLocalStrain*
- *GetDeltaLocalStrain* and *SetDeltaLocalStrain*

Constructors

```
OEBroodBuildOptions()
OEBroodBuildOptions(const OEBroodBuildOptions &)
```

Default and copy constructors.

operator=

Assignment operator.

GetBuildType

```
unsigned GetBuildType() const
```

See *SetBuildType* method.

GetNeutralPH

```
bool GetNeutralPH() const
```

See *SetNeutralPH* method.

GetTautomers

```
bool GetTautomers() const
```

See *SetTautomers* method.

GetCheckBond

```
bool GetCheckBond() const
```

See *SetCheckBond* method.

GetMaxLocalStrain

```
double GetMaxLocalStrain() const
```

See *SetMaxLocalStrain* method.

SetBuildType

```
bool SetBuildType(const unsigned)
```

Sets if **Build Type** to be applied in constructing the new analogs. Possible choices of methods are described in *OEBroodBuildType*. Default: *Optimize3D*.

SetNeutralPH

```
bool SetNeutralPH(const bool)
```

Sets if **Neutral pH model** to be applied on newly constructed analogs. **Default: True.**

SetTautomers

```
bool SetTautomers(const bool)
```

Sets if **Reasonable tautomer model** to be applied on newly constructed analogs. **Default: False.**

SetCheckBond

```
bool SetCheckBond(const bool)
```

Sets if **Bond stability should be checked** in generating hitlist. **Default: True.**

SetMaxLocalStrain

```
bool SetMaxLocalStrain(const double)
```

Sets the **Number allowable local strain** in the generated hits. **Default: 6.5.**

GetDeltaLocalStrain

```
bool GetDeltaLocalStrain() const
```

See *SetDeltaLocalStrain* method.

SetDeltaLocalStrain

```
bool SetDeltaLocalStrain(const bool)
```

Sets if **relative local strain** between the query fragment and the analog should be used as a measure of strain, rather than the absolute local strain of the analog alone. **Default: False.**

3.1.2 OEBroodBuildResult

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodBuildResult
```

This class stores the outcome of building a candidate molecule from a scored replacement, build status, Tanimoto combo, local strain, and delta local strain etc, used for downstream filtering and analysis. This works as a container of output from *OEBroodMolBuilder*.

The *OEBroodBuildResult* class defines the following public methods:

- *GetBuildStatus*
- *GetDeltaLocalStrain*
- *GetLocalStrain*
- *GetMolTanimotoCombo*

Constructors

```
OEBroodBuildResult()
OEBroodBuildResult(const OEBroodBuildResult&)
OEBroodBuildResult& operator=(const OEBroodBuildResult&)
```

Default constructors.

GetBuildStatus

```
unsigned GetBuildStatus() const
```

This method returns the status code indicating the result of the build operation. See the *OEBroodStatusCode* for possible values.

GetDeltaLocalStrain

```
double GetDeltaLocalStrain() const
```

This method returns the change in local strain energy relative to the query fragment.

GetLocalStrain

```
double GetLocalStrain() const
```

This method returns the local strain value computed for the built molecule.

GetMolTanimotoCombo

```
double GetMolTanimotoCombo() const
```

This method returns the combined Tanimoto score (shape and color) for the built molecule.

3.1.3 OEBroodCluster

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodCluster
```

This class represents a cluster of bioisosteric hits grouped by structural similarity. Each cluster has a head hit and optional member hits that are considered similar to that head under the clustering mode.

The *OEBroodCluster* class defines the following public methods:

- *Count*
- *GetHead*
- *GetInterest*
- *GetMembers*
- *GetRank*
- *operator*

Constructors

```
OEBroodCluster()
OEBroodCluster(const OEBroodCluster&)
OEBroodCluster& operator=(const OEBroodCluster&)
```

Default and copy constructors.

Count

```
unsigned Count() const
```

This method returns the total number of hits in the cluster (head + members).

GetHead

```
const OEBroodHit& GetHead() const
```

This method returns the cluster head hit, which serves as the representative hit for the cluster.

GetInterest

```
double GetInterest() const
```

This method returns the computed interest score used to prioritize this cluster during ranking. Larger values indicate clusters that are more favorable for follow-up inspection.

GetMembers

```
const std::vector<OEBroodHit>& GetMembers() const
```

This method returns a reference to the vector of member hits in the cluster.

GetRank

```
unsigned GetRank() const
```

This method returns the rank assigned by *Rank*.

operator

This is a comparison operator for sorting clusters by interest score (higher interest ranks ahead of lower interest).

3.1.4 OEBroodClusterBuilder

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodClusterBuilder
```

This class builds and organizes bioisosteric hits into clusters based on structural similarity and optionally ranks them by calculated interest scores. See the *cluster* example.

The *OEBroodClusterBuilder* class defines the following public methods:

- *Add*
- *GetClusters*
- *Rank*

Constructors

```
OEBroodClusterBuilder(const OEChem::OEMolBase& molQuery,
                      const bool fragment = false)
OEBroodClusterBuilder(const OEBroodQuery& query)
```

This method constructs an *OEBroodClusterBuilder* from either a query molecule or an *OEBroodQuery*. The `fragment` flag controls clustering mode: fragment-centric (`true`) or full-molecule-centric (`false`).

Add

```
bool Add(const std::vector<OEBroodHit>& vecHits)
```

This method adds one or more hits to the cluster builder. The builder groups similar hits into clusters as they are added.

GetClusters

```
const std::vector<OEBroodCluster>& GetClusters() const
```

This method returns a reference to the vector of clusters created by the builder.

Rank

```
bool Rank()
```

This method computes cluster priority scores and assigns final cluster ranks. Call this method before consuming ranked output from *GetClusters*.

3.1.5 OEBroodComboBuilder

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodComboBuilder
```

This class enables multipoint bioisosteric exploration by combining overlaid fragments from different query replacements of the same molecule into a single composite hit. Given a primary *OEBroodQuery* and its corresponding *OEBroodHit*, a second query can be applied to the same molecule and the builder merges both fragment replacements into a combined result via its *Build* method. See the *combo_builder* example for a complete walkthrough.

The *OEBroodComboBuilder* class defines the following public method:

- *Build*

Constructors

```
OEBroodComboBuilder(const OEBroodQuery& query,
                    const OEBroodHit& hit,
                    const OEBroodGeneralOptions& genOpts = OEBroodGeneralOptions(),
                    const OEBroodBuildOptions& options = OEBroodBuildOptions())
```

This method constructs an *OEBroodComboBuilder* from a secondary query and a previously built primary hit, together with general and build options used for the combination step.

Build

```
unsigned Build(const OEBroodScore& score, OEBroodHit& hit)
```

This method builds a combined hit by applying the replacement encoded in `score` to the current primary hit context and writing the resulting combined hit to `hit`. It returns a status code from *OEBroodStatusCode*.

3.1.6 OEBroodDBFilter

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodDBFilter
```

This class defines objects that can be used to check if a *database packet* contains fragments relevant to a certain *OEBroodQuery*.

The *OEBroodDBFilter* class defines the following public methods:

- *Setup*

Constructors

```
OEBroodDBFilter()
OEBroodDBFilter(const OEBroodDBFilter &)
```

Default and copy constructors.

operator=

Assignment operator.

Setup

```
bool Setup(const OEBroodQuery& query,
           const OEBroodGeneralOptions& scoreOpts = OEBroodGeneralOptions())
bool Setup(OEChem::OEMCMolBase& mol,
           const OEBroodGeneralOptions& opts)
```

This method associates the filter with either a specific *OEBroodQuery* or a prepared OEMCMolBase, along with *OEBroodGeneralOptions*, to initialize packet-level filtering constraints.

3.1.7 OEBroodDBPacket

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodDBPacket
```

This class defines objects that hold a chunk of fragment data from a Brood database. A packet contains additional metadata that can be used to check relevance for bioisosteric replacement of a specific *OEBroodQuery*.

The *OEBroodDBPacket* class defines the following public methods:

- *GetIdx*
- *GetFragCount*
- *GetFrags*
- *IsValid*
- *Load*
- *ToRecord*

Constructors

```
OEBroodDBPacket()
OEBroodDBPacket(const OEBroodDBPacket &)
```

Default and copy constructors.

GetIdx

```
unsigned GetIdx() const
```

Returns the index corresponding to database storage.

GetFragCount

```
unsigned GetFragCount() const
```

Returns the number of fragments contained in the packet.

GetFrags

```
OESystem::OEIterBase<OEChem::OEMCMolBase>* GetFrags() const
```

Returns fragments that are contained in the packet.

IsValid

```
bool IsValid(const OEBroodDBFilter& filter)
```

Returns whether packet contents are relevant for the *OEBroodQuery* associated with the *OEBroodDBFilter*.

Load

```
bool Load(const OEDataFlow::OERecord &)
```

Loads packet contents from an OERecord.

ToRecord

```
bool ToRecord(OEDataFlow::OERecord &) const
```

Saves packet contents into an OERecord.

3.1.8 OEBroodFragPrep

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodFragPrep
```

This class provides facilities to prepare fragments for overlay calculations using *OEBroodOverlay* or *OEFragOverlay*.

The *OEBroodFragPrep* class defines the following public methods:

- *Prep*

Constructors

```
OEBroodFragPrep()
```

Default constructor.

Prep

```
bool Prep(OEChem::OEMCMolBase& fragment)
```

Prepares the specified fragment for overlay optimization.

3.1.9 OEBroodGeneralOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodGeneralOptions : public OESystem::OEOptions
```

This class provides an interface to setup basic options related to bioisosteric fragment replacement.

The *OEBroodGeneralOptions* class defines the following public methods:

- *GetAttachScale* and *SetAttachScale*
- *GetBumpRadius* and *SetBumpRadius*
- *GetScoreType* and *SetScoreType*
- *GetIgnoreProtein* and *SetIgnoreProtein*
- *GetIgnoreSelectionProtein* and *SetIgnoreSelectionProtein*
- *GetRangeSize* and *SetRangeSize*

- *GetRangeOffset* and *SetRangeOffset*
- *GetRingOnly* and *SetRingOnly*

Constructors

```
OEBroodGeneralOptions()
OEBroodGeneralOptions(const OEBroodGeneralOptions &)
```

Default and copy constructors.

operator=

Assignment operator.

GetAttachScale

```
double GetAttachScale() const
```

See *SetAttachScale* method.

GetBumpRadius

```
double GetBumpRadius() const
```

See *SetBumpRadius* method.

GetScoreType

```
unsigned GetScoreType() const
```

See *SetScoreType* method.

SetAttachScale

```
bool SetAttachScale(const double)
```

Sets the **scaling factor** for attachment point scores. This value determines the balance between the chemical color score and the attachment point scores. Higher values indicate more weighting for the attachment-point alignment. **Default: 1.5.**

SetBumpRadius

```
bool SetBumpRadius(const double)
```

Sets the **minimum distance defining clash** between ligand heavy atoms and protein heavy atoms. New analogs with atoms closer than this cutoff to the active-site protein are marked as clashing, and eventually discarded from the hitlist. **Default: 2.25.**

SetScoreType

```
bool SetScoreType(const unsigned)
```

Sets the **method** to be used for scoring overlap between the query fragment and the replacement fragment. Possible choices of methods are described in *OEBroodScoreType*. Default: *ROCS*.

GetIgnoreProtein

```
bool GetIgnoreProtein() const
```

See *SetIgnoreProtein* method.

GetIgnoreSelectionProtein

```
bool GetIgnoreSelectionProtein() const
```

See *SetIgnoreSelectionProtein* method.

GetRangeSize

```
unsigned GetRangeSize() const
```

See *SetRangeSize* method.

GetRangeOffset

```
unsigned GetRangeOffset() const
```

See *SetRangeOffset* method.

GetRingOnly

```
int GetRingOnly() const
```

See *SetRingOnly* method.

SetIgnoreProtein

```
bool SetIgnoreProtein(const bool)
```

Sets whether the **protein associated with the query** should be ignored during scoring. When true, receptor clash and protein-select checks are skipped even if a protein was provided to *OECreateBroodQuery*. **Default: False.**

SetIgnoreSelectionProtein

```
bool SetIgnoreSelectionProtein(const bool)
```

Sets whether the **selectivity protein associated with the query** should be ignored during scoring. When true, protein-select scoring is skipped even if a selectivity protein was provided to *OECreateBroodQuery*. **Default: False.**

SetRangeSize

```
bool SetRangeSize(const unsigned)
```

Sets the **range of heavy atom counts** around the query fragment heavy atom count to examine from the database. Fragments whose heavy atom count falls outside `[queryHeavy - rangeOffset - rangeSize, queryHeavy - rangeOffset + rangeSize]` are skipped. **Default: 6.**

SetRangeOffset

```
bool SetRangeOffset(const unsigned)
```

Sets a **bias toward smaller or larger fragments** relative to the query. A positive offset shifts the search window toward larger fragments; a negative offset toward smaller fragments. Works together with *SetRangeSize*. **Default: 0.**

SetRingOnly

```
bool SetRingOnly(const int)
```

Sets the **requirement for rings** in selecting a fragment. This flag has to do with a count of the number of ring atoms in the shortest path between attachment points in a fragment. In cases with more than 2 attachment points, all shortest paths are calculated and the number of ring atoms is summed. **Default: -2**

3.1.10 OEBroodHit

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodHit
```

This class defines objects that contain results corresponding to a generated **Brood** hit from bioisosteric replacement.

The *OEBroodHit* class defines the following public methods:

- *GetAbbottBioScore*
- *GetAromaticRingCount*
- *GetAttachScore*
- *GetBeliefScore*
- *GetBuildRes*
- *GetBuildStatus*
- *GetColorScore*
- *GetComboScore*
- *GetComplexity*
- *GetDeltaLocalStrain*
- *GetEgan*
- *GetFragSmiles*
- *GetFrequency*
- *GetHeavyCount*
- *GetIdeaGroup*
- *GetIdeaRank*
- *GetLipinskiAcc*
- *GetLipinskiDon*

- *GetLipinskiFail*
- *GetLocalStrain*
- *GetMol*
- *GetMolTanimotoCombo*
- *GetMolWt*
- *GetRingCount*
- *GetRingRatio*
- *GetRotorCount*
- *GetScores*
- *GetShapeScore*
- *GetSourceMolLabel*
- *GetSourceMolSmiles*
- *GetTPSA*
- *GetVeber*
- *GetXLogP*
- *Getfsp3C*
- *Load*
- *ToRecord*

Constructors

```
OEBroodHit()
OEBroodHit(const OEBroodHit &)
```

Default and copy constructors.

operator=

Assignment operator.

GetAbbottBioScore

```
double GetAbbottBioScore() const
```

This method returns the Abbott bioavailability score of the generated molecule.

GetAromaticRingCount

```
unsigned GetAromaticRingCount() const
```

This method returns the number of aromatic rings in the generated molecule.

GetAttachScore

```
double GetAttachScore() const
```

This method returns the attachment score corresponding to fragment matching.

GetBeliefScore

```
double GetBeliefScore() const
```

This method returns the belief score of the generated molecule.

GetBuildRes

```
const OEBroodBuildResult& GetBuildRes() const
```

This method returns a const reference to the *OEBroodBuildResult* object containing detailed build status and scoring information.

GetBuildStatus

```
unsigned GetBuildStatus() const
```

This method returns the status of the built hit. The method returns *OEBroodStatusCode.Success* if the build was successful, otherwise it returns an error code from the *OEBroodStatusCode* namespace.

GetColorScore

```
double GetColorScore() const
```

This method returns the color score corresponding to fragment matching.

GetComboScore

```
double GetComboScore() const
```

This method returns the combo (shape+color) score corresponding to fragment matching.

GetComplexity

```
double GetComplexity() const
```

This method returns the complexity of the generated molecule.

GetDeltaLocalStrain

```
double GetDeltaLocalStrain() const
```

This method returns the calculated delta local strain (HitStrain - QueryStrain) of the generated molecule.

GetEgan

```
unsigned GetEgan() const
```

This method returns the Egan bioavailability score of the generated molecule.

GetFragSmiles

```
std::string GetFragSmiles() const
```

This method returns the SMILES string corresponding to the replacement fragment.

GetFrequency

```
unsigned GetFrequency() const
```

This method returns the frequency of the replacement fragment in the database.

GetHeavyCount

```
unsigned GetHeavyCount() const
```

This method returns the number of heavy atoms in the generated molecule.

GetIdeaGroup

```
unsigned GetIdeaGroup() const
```

This method returns the index of the idea group the generated molecule belongs to.

GetIdeaRank

```
unsigned GetIdeaRank() const
```

This method returns the rank of the generated molecule within the idea group it belongs to.

GetLipinskiAcc

```
unsigned GetLipinskiAcc() const
```

This method returns the number of Lipinski donors in the generated molecule.

GetLipinskiDon

```
unsigned GetLipinskiDon() const
```

This method returns the number of Lipinski acceptors in the generated molecule.

GetLipinskiFail

```
unsigned GetLipinskiFail() const
```

This method returns the number of Lipinski rule-of-five failures in the generated molecule.

GetLocalStrain

```
double GetLocalStrain() const
```

This method returns the calculated local strain in the generated molecule.

GetMol

```
const OEChem::OEGraphMol& GetMol() const
```

This method returns the generated hit molecule.

GetMolTanimotoCombo

```
double GetMolTanimotoCombo() const
```

This method returns the Tanimoto combo (shape+color) score of the molecule against the query molecule.

GetMolWt

```
double GetMolWt() const
```

This method returns the molecular weight of the generated molecule.

GetRingCount

```
unsigned GetRingCount() const
```

This method returns the number of rings in the generated molecule.

GetRingRatio

```
double GetRingRatio() const
```

This method returns the ratio of ring atoms to heavy atoms in the generated molecule.

GetRotorCount

```
unsigned GetRotorCount() const
```

This method returns the number of rotors in the generated molecule.

GetScores

```
const OEBroodScore& GetScores() const
```

This method returns a const reference to the *OEBroodScore* object containing detailed scoring information for the hit.

GetShapeScore

```
double GetShapeScore() const
```

This method returns the shape score corresponding to fragment matching.

GetSourceMolLabel

```
std::string GetSourceMolLabel() const
```

This method returns the labels of the source molecules associated with the replacement fragment.

GetSourceMolSmiles

```
std::string GetSourceMolSmiles() const
```

This method returns the SMILES of the source molecules associated with the replacement fragment.

GetTPSA

```
double GetTPSA() const
```

This method returns the calculated topological polar surface area of the generated molecule.

GetVeber

```
unsigned GetVeber() const
```

This method returns the Veber bioavailability score of the generated molecule.

GetXLogP

```
double GetXLogP() const
```

This method returns the calculated LogP of the generated molecule.

Getfsp3C

```
double Getfsp3C() const
```

This method returns the fraction of sp^3 hybridized carbon atoms in the generated molecule.

Load

```
bool Load(const OEDataFlow::OERecord&)
```

This method loads *OEBroodHit* from the specified OERecord. It returns `true` if successful.

ToRecord

```
bool ToRecord(OEDataFlow::OERecord&) const
```

This method saves *OEBroodHit* into the specified OERecord. It returns `true` if successful.

3.1.11 OEBroodHitlist

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodHitlist: public OEHitlistBase
```

This class manages curated, built *OEBroodHit* objects and provides final hit list filtering behavior for molecule-level results.

The *OEBroodHitlist* class defines the following public methods:

- *AddHits*
- *Build*
- *GetHits*

Constructors

```
OEBroodHitlist()
OEBroodHitlist(const OEChem::OEMolBase& mol,
               const OEBroodHitlistOptions& options = OEBroodHitlistOptions())
OEBroodHitlist(const OEBroodQuery& query,
               const OEBroodHitlistOptions& options = OEBroodHitlistOptions())
```

This method constructs an *OEBroodHitlist* either with no arguments (default), with a query molecule and options, or with an *OEBroodQuery* and options.

AddHits

```
bool AddHits(const std::vector<OEBroodHit>&)
```

This method adds a batch of *OEBroodHit* objects to the hit list.

Build

```
bool Build(const bool final = true) override
```

This method builds the final hit list from all added hits, filtering duplicates and applying scored-based filtering if configured.

GetHits

```
const std::vector<OEBroodHit>& GetHits() const
```

This method returns a reference to the vector of final *OEBroodHit* objects after building and filtering.

3.1.12 OEBroodHitlistOptions

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodHitlistOptions : public OESystem::OEOptions
```

This class provides an interface to set up options used when generating a hitlist in *OEHitlistBuilder* from a set of *Brood scores*.

The *OEBroodHitlistOptions* class defines the following public methods:

- *GetGenerateIdea* and *SetGenerateIdea*
- *GetMaxHits* and *SetMaxHits*

Constructors

```
OEBroodHitlistOptions()
OEBroodHitlistOptions(const OEBroodHitlistOptions &)
```

Default and copy constructors.

GetGenerateIdea

```
bool GetGenerateIdea() const
```

See *SetGenerateIdea* method.

GetMaxHits

```
unsigned GetMaxHits() const
```

See *SetMaxHits* method.

SetGenerateIdea

```
bool SetGenerateIdea(const bool)
```

Sets whether **cluster information** is generated for the created hitlist. **Default: True.**

SetMaxHits

```
bool SetMaxHits(const unsigned)
```

Sets the **maximum number of hits** to generate. **Default: 1000.**

3.1.13 OEBroodMolBuilder

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodMolBuilder
```

This class defines the interface for building a fragment-replaced molecule with 3D coordinates from an *OEBroodScore*.

The *OEBroodMolBuilder* class defines the following public method:

- *Build*

Constructors

```
OEBroodMolBuilder(const OEBroodQuery& query,
                  const OEBroodGeneralOptions& genOpts = OEBroodGeneralOptions(),
                  const OEBroodBuildOptions& options = OEBroodBuildOptions())
```

Default and copy constructor.

Build

```
unsigned Build(const OEBroodScore& score, OEBroodHit& hit)
unsigned Build(OEChem::OEMolBase& mol)
```

This method builds a fragment replaced 3D Molecule. The first overload generates corresponding hit data from the specified *OEBroodScore*. The second overload works directly with a fragment-replaced molecule.

3.1.14 OEBroodOverlay

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodOverlay: public OEBroodOverlayBase
```

This class defines an interface for fragment overlay optimization against a *Brood query*.

The *OEBroodOverlay* class defines the following public methods:

- *Overlay*
- *SetupRef*
- *Transform*

Constructors

```
OEBroodOverlay(const OEBroodGeneralOptions& genOpts = OEBroodGeneralOptions(),
               const OEBroodScoreOptions& scoreOpts = OEBroodScoreOptions())
```

Default constructor.

Overlay

```
std::vector<OEBroodScore> Overlay(const OEBroodDBPacket&)
unsigned Overlay(std::vector<OEBroodScore>&, const OEBroodDBPacket&)
unsigned Overlay(OEChem::OEMCMolBase& fragment, OEBroodScore& score)
```

Performs overlay optimization against the specified fragments. The first two overloads optimize against all fragments in the provided *OEBroodDBPacket*, and return a vector of *OEBroodScore* values. The third overload performs optimization against the specified fragment and populates the specified *OEBroodScore* with optimization results. Both the second and third overloads return an optimization status from *OEBroodStatusCode*.

SetupRef

```
unsigned SetupRef(const OEBroodQuery& query)
```

Sets up the overlay optimization with the desired *OEBroodQuery*. Method returns *OEBroodStatusCode.Success* if the initialization is successful, otherwise returns an error code from the *OEBroodStatusCode* namespace.

Transform

```
bool Transform(OEChem::OEMolBase& mol) const
```

Transforms the specified molecule to the optimized overlay position determined by a prior call to *Overlay*.

3.1.15 OEBroodOverlayBase

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodOverlayBase
```

This is a base class for fragment overlay optimization.

The *OEBroodOverlayBase* class defines the following public methods:

- *Overlay*

Overlay

```
unsigned Overlay(OEChem::OEMCMolBase& fragment, OEBroodScore& score)
```

Performs overlay optimization of the specified fragment. Populates the provided *OEBroodScore* with optimization results. Returns the status of the optimization; see *OEBroodStatusCode* for possible values.

3.1.16 OEBroodQuery

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodQuery
```

This class defines objects that represent a **Brood** query.

The *OEBroodQuery* class defines the following public methods:

- *GetAttachCount*
- *GetHeavyCount*
- *GetQueryID*
- *SetQueryID*
- *HasProtein*
- *HasProteinSelect*
- *Init*

Constructors

```
OEBroodQuery()
OEBroodQuery(const OEBroodQuery &)
```

Default and copy constructors.

GetAttachCount

```
unsigned GetAttachCount() const
```

This method returns the number of attachment points in the query fragment.

GetHeavyCount

```
unsigned GetHeavyCount() const
```

This method returns the number of heavy atoms in the query fragment.

GetQueryID

```
std::string GetQueryID() const
```

This method returns the identifier associated with the query. If no identifier has been assigned with *SetQueryID*, it returns the query's isomeric SMILES (the fragment representation) as a sensible default, so every query always has a non-empty, meaningful identifier.

SetQueryID

```
void SetQueryID(const std::string& id)
```

This method assigns a user-defined identifier to the query. The identifier is stored as string data on the query molecule, so it persists when the query is written and read with *OEWriteBroodQuery* and *OEReadBroodQuery*, and it is carried onto every *OEBroodScore* produced from the query (see *GetQueryIDs*). When no identifier is assigned, *GetQueryID* falls back to the query's isomeric SMILES.

Note

Assigning an identifier is optional: by default the identifier is the query's SMILES, which keeps queries apart during hit-list de-duplication. Assign a **unique** identifier when two *distinct* queries can share the same SMILES, so that their hits are not merged during de-duplication. In the combo-building process the identifier is also used to map each hit back to its originating query, so a unique identifier is recommended there. Two queries that share an identifier (for example, two distinct queries that share a SMILES and neither overrides the default) are treated as the same query.

HasProtein

```
bool HasProtein() const
```

This method returns *true* if the query contains an associated protein.

HasProteinSelect

```
bool HasProteinSelect() const
```

This method returns *true* if the query contains an associated selectivity protein.

Init

```
unsigned Init(const OEChem::OEMCMolBase& queryMol)
```

This method initializes the query from contents in the specified *query molecule*. A *query molecule* is an OEMol containing a set of specific data tags. The method returns *OEBroodStatusCode.Success* if the initialization is successful, otherwise it returns an error code from the *OEBroodStatusCode* namespace.

3.1.17 OEBroodScore

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodScore
```

This class defines objects that contains results corresponding to a bioisosteric fragment overlap.

The *OEBroodScore* class defines the following public methods:

- *Add*
- *GetAttachCount*

- *GetAttachScore*
- *GetColorScore*
- *GetComboScore*
- *GetEnergy*
- *GetFrag*
- *GetFragMol*
- *GetQueryIDs*
- *GetScoreType*
- *GetShapeScore*
- *GetStatus*
- *Load*
- *ToRecord*

Constructors

```
OEBroodScore()
OEBroodScore(const OEBroodScore &)
```

Default and copy constructors. The scoring type is determined by the *SetScoreType* option and defaults to *OEBroodScoreType.ROCS*.

operator=

Assignment operator.

Add

```
bool Add(const OEBroodScore& score)
```

This method merges another *OEBroodScore* into this score by appending query provenance and combining similarity components (attachment, shape, and color). The method returns `true` only when both score objects have successful status.

GetAttachCount

```
unsigned GetAttachCount() const
```

This method returns the number of attachment points in the fragment overlay.

GetAttachScore

```
double GetAttachScore() const
```

This method returns the attachment score corresponding to fragment overlay.

GetColorScore

```
double GetColorScore() const
```

This method returns the color score corresponding to fragment overlay.

GetComboScore

```
double GetComboScore() const
```

This method returns the combo (shape+color) score corresponding to fragment overlay.

GetEnergy

```
double GetEnergy() const
```

This method returns the *energy* associated with the fragment. *Energy* refers to the entity that is used for ranking fragments in building the hit list using *OEScoreHitlist*.

GetFrag

```
const OEChem::OEMol& GetFrag() const
```

This method returns a const reference to the generated molecule with fragment replacement.

GetFragMol

```
bool GetFragMol(OEChem::OEMolBase& mol) const
```

This method copies the generated molecule with fragment replacement into the provided molecule parameter. It returns `true` if successful and `false` otherwise.

GetQueryIDs

```
const std::vector<std::string>& GetQueryIDs() const
```

This method returns the query identifiers of the originating *OEBroodQuery* objects. Each identifier is the one assigned with *SetQueryID*, or the originating query's isomeric SMILES when no identifier was assigned. In single-query workflows this is typically one entry; in combined (combo-built) workflows it can contain multiple entries, one per contributing query.

> **Note**
>
> A score can be associated with multiple query identifiers when multiple queries are used to build it. Assign a **unique** identifier to each distinct query with *SetQueryID* when distinct queries could otherwise share the same default (SMILES) identifier; this is what disambiguates scores from different queries during hit list deduplication and combo building. See the *combo_builder* example for more details.

GetScoreType

```
unsigned GetScoreType() const
```

This method returns the scoring mode associated with this result. The value is one of the constants from the *OEBroodScoreType* namespace:

- *OEBroodScoreType.ROCS* - shape and color based scoring.
- *OEBroodScoreType.ET* - shape and electrostatics based scoring.
- *OEBroodScoreType.LinkOnly* - attachment-only based scoring.

The scoring type is set via *SetScoreType* before running the overlay. The default is *OEBroodScoreType.ROCS*.

GetShapeScore

```
double GetShapeScore() const
```

This method returns the shape score corresponding to fragment overlay.

GetStatus

```
unsigned GetStatus() const
```

This method returns the status of fragment overlay. The method returns *OEBroodStatusCode.Success* if the overlay was successful, otherwise it returns an error code from the *OEBroodStatusCode* namespace.

Load

```
bool Load(const OEDataFlow::OERecord&)
```

This method loads contents of *OEBroodScore* from OERecord. It returns `true` if successful and `false` otherwise.

ToRecord

```
bool ToRecord(OEDataFlow::OERecord&) const
```

This method saves the contents of *OEBroodScore* into an OERecord. It returns `true` if successful and `false` otherwise.

3.1.18 OEScoreHitlist

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEScoreHitlist: public OEHitlistBase
```

This class collects and manages scores from overlay operations, filtering duplicates and creating a hit list of unique, high-scoring fragment matches.

The *OEScoreHitlist* class defines the following public methods:

- *AddScores*
- *Build*
- *GetHits*

- *GetMatchCount*

Constructors

```
OEScoreHitlist(const unsigned maxHits = 1000)
```

This method constructs an *OEScoreHitlist* with a specified maximum number of hits to retain.

AddScores

```
bool AddScores(const std::vector<OEBroodScore>&)
```

This method adds a batch of *OEBroodScore* objects for score-stage hit list curation.

Build

```
bool Build(const bool final = true) override
```

This method builds the final hit list from all added scores, filtering duplicates and retaining the top-scoring unique fragments.

GetHits

```
const std::vector<OEBroodScore>& GetHits() const
```

This method returns curated score-level hits as *OEBroodScore* objects.

GetMatchCount

```
unsigned GetMatchCount() const
```

This method returns the number of unique score matches retained in the hit list.

3.1.19 OEBroodScoreOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEBroodScoreOptions : public OESystem::OEOptions
```

This class provides an interface to setup options required for finding bioisosteric fragment replacement matches, used with scoring fragments while performing overlay optimization with *OEBroodOverlay*.

The *OEBroodScoreOptions* class defines the following public methods:

- *GetUseBondOrder* and *SetUseBondOrder*
- *GetUseProperty* and *SetUseProperty*
- *GetCheckGeometry* and *SetCheckGeometry*
- *GetAttachCutoff* and *SetAttachCutoff*
- *GetShapeCutoff* and *SetShapeCutoff*

- *GetChargeType* and *SetChargeType*
- *GetPropertyOptions* and *SetPropertyOptions*

Constructors

```
OEBroodScoreOptions()
OEBroodScoreOptions(const OEBroodScoreOptions &)
```

Default and copy constructors.

operator=

Assignment operator.

GetUseBondOrder

```
bool GetUseBondOrder() const
```

See *SetUseBondOrder* method.

GetUseProperty

```
bool GetUseProperty() const
```

See *SetUseProperty* method.

GetCheckGeometry

```
bool GetCheckGeometry() const
```

See *SetCheckGeometry* method.

GetAttachCutoff

```
double GetAttachCutoff() const
```

See *SetAttachCutoff* method.

GetShapeCutoff

```
double GetShapeCutoff() const
```

See *SetShapeCutoff* method.

GetChargeType

```
unsigned GetChargeType() const
```

See *SetChargeType* method.

GetPropertyOptions

```
OEMolPropertyOptions& GetPropertyOptions()
const OEMolPropertyOptions& GetPropertyOptions() const
```

See *SetPropertyOptions* method.

SetUseBondOrder

```
bool SetUseBondOrder(const bool)
```

Sets if **Same attachment bond order** should be required for a possible match. **Default: True.**

SetUseProperty

```
bool SetUseProperty(const bool)
```

Sets if **Fragment property should be checked** for a possible match. **Default: False.**

SetCheckGeometry

```
bool SetCheckGeometry(const bool)
```

Sets if **Minimal geometric difference should be required** for a possible match. **Default: True.**

SetAttachCutoff

```
bool SetAttachCutoff(const double)
```

Sets the **Minimum acceptable attachment tanimoto** for a possible match. **Default: 0.78.**

SetShapeCutoff

```
bool SetShapeCutoff(const double)
```

Sets the **Minimum acceptable shape tanimoto** for a possible match. **Default: 0.6.**

SetPropertyOptions

```
void SetPropertyOptions(const OEMolPropertyOptions&)
```

Sets *options* related to required molecular property values.

SetChargeType

```
bool SetChargeType(const unsigned)
```

Sets the **partial charge model** to use for electrostatic Tanimoto calculations when scoring with the *ET* score type. Legal values: MMFF94 and NoOp. (NoOp means to use charges already on the molecule, as with the BROOD option fileChrg.) **Default:** MMFF94.

3.1.20 OECPDDatabase

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OECPDDatabase
```

This class provides an interface to use an external compound database to identify similar compounds to a **Brood**-generated hitlist, as described in *Similarity to available compounds*.

The *OECPDDatabase* class defines the following public methods:

- *GetNumMolecules*
- *GetSimilarMolecules*
- *HasNewFingerPrints*
- *IsPrepared*
- *Prep*
- *Write*

Constructor

```
OECPDDatabase()
```

Default constructor.

GetNumMolecules

```
unsigned GetNumMolecules()
```

Returns the number of molecules in the prepared external compound database that are ready for hitlist comparison.

See also *IsPrepared* method.

GetSimilarMolecules

```
bool GetSimilarMolecules(const OEChem::OEMolBase& hitMol,
                         std::vector<std::string>& vecCpddbInfo)
std::vector<std::string> GetSimilarMolecules(const OEChem::OEMolBase& hitMol)
```

Retrieves information (SMILES and labels) for molecules similar to the provided hit molecule from the external compound database. The `bool` overload returns `true` when similar molecules are found. This method should be used after the compound database has been prepared using the *Prep* method.

HasNewFingerPrints

```
bool HasNewFingerPrints()
```

Returns `true` if new fingerprints were generated during preparation.

See also *Prep* method.

IsPrepared

```
bool IsPrepared()
```

Returns whether the external compound database has been prepared.

Prep

```
unsigned Prep(OEChem::oemolistream& cpddbifs,
              OESystem::OETracerBase& tracer = OESystem::OENoTracer)
```

Prepares the input stream molecules by generating 2D fingerprints for each, if they do not already have one. The method returns an unsigned. The unsigned code number can be extracted using *OEGetBroodStatus*.

Write

```
bool Write(OEChem::oemolistream& cpddbifs,
           OEChem::oemolostream& cpddbofs)
```

Writes newly generated fingerprints from `cpddbifs` into `cpddbofs` for more efficient reuse in future runs.

See also *HasNewFingerPrints* method.

3.1.21 OEDBBuffer

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEDBBuffer
```

This class defines objects representing a Brood database held in memory. This is suitable for generating a database from a small set of molecules, to be used on-the-fly, without storing it on disk.

The *OEDBBuffer* class defines the following public methods:

- *Add*
- *Finalize*
- *GetPackets*

Constructors

```
OEDBBuffer()
```

Default constructor.

Add

```
bool Add(OEChem::OEMCMolBase& mol)
```

Adds the specified fragment into the database.

Finalize

```
bool Finalize()
```

Finalizes the database. This method must be called before packets can be retrieved from the database.

GetPackets

```
const std::vector<OEBroodDBPacket>& GetPackets() const
```

Returns the data packets from the database.

3.1.22 OEDBBuilder

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEDBBuilder
```

This class defines an interface for building a two-dimensional Brood fragment database.

The *OEDBBuilder* class defines the following public methods:

- *Add*
- *AddCSV*
- *Expand*
- *Filter*
- *Generate*
- *GetFrag*
- *GetFragSmiles*
- *GetFragSmilesCSV*
- *GetFrags*
- *NumFrags*
- *Screen*

Constructors

```
OEDBBuilder(const OEFragmentOptions& opts = OEFragmentOptions())
```

Default constructor.

Add

```
bool Add(OEChem::OEMCMolBase& frag)
bool Add(OESystem::OEIter<OEChem::OEMCMolBase>& frag)
bool Add(const std::string& smiles)
bool Add(const std::vector<std::string>& vecSmiles)
```

Adds the specified fragment(s) to the database. In the SMILES-based overloads, fragment SMILES in the format obtained from *GetFragSmiles* are expected.

AddCSV

```
bool AddCSV(const std::vector<std::string>& vecSmiles)
```

Adds fragments from the specified CSV SMILES strings. SMILES as obtained from *GetFragSmilesCSV* are expected.

Expand

```
bool Expand(const OEConfGen::OEFlipperOptions& opts)
```

Expands the database by stereo-enumerating currently contained fragments.

Filter

```
bool Filter(OEMolProp::OEFilter& filter)
```

Filters currently contained database fragments.

Generate

```
bool Generate(const OEChem::OEMolBase& mol)
```

Generates fragments from the specified molecule and adds the generated fragment(s) to the database.

GetFrag

```
bool GetFrag(OEChem::OEMCMolBase& mol, const std::string& smiles) const
```

Obtains the fragment defined by the specified SMILES string. Returns `false` if a fragment with the specified SMILES does not exist. SMILES in the format obtained from *GetFragSmiles* is expected.

GetFragSmiles

```
std::vector<std::string> GetFragSmiles() const
bool GetFragSmiles(std::vector<std::string>&) const
```

Returns SMILES strings corresponding to the current database.

GetFragSmilesCSV

```
std::vector<std::string> GetFragSmilesCSV() const
bool GetFragSmilesCSV(std::vector<std::string>&) const
```

Returns CSV SMILES strings corresponding to the current database. CSV SMILES contains fragment SMILES in a special comma-separated string format.

GetFrags

```
OESystem::OEIterBase<OEChem::OEMCMolBase>* GetFrags() const
```

Returns two-dimensional fragments corresponding to the current database.

NumFrags

```
unsigned NumFrags() const
```

Returns the number of fragments corresponding to the current database.

Screen

```
bool Screen(const OEDBScreenOptions& opts)
```

Screens the fragments in the current database.

3.1.23 OEDBReader

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEDBReader
```

This class defines an interface for accessing a **Brood** fragment database from disk.

The *OEDBReader* class defines the following public methods:

- *GetFragCount*
- *GetIndices*
- *GetNextPacket*
- *Init*

Constructors

```
OEDBReader()
```

Default constructor.

GetFragCount

```
unsigned GetFragCount() const
```

Returns the number of fragments in the database currently associated with this reader.

GetIndices

```
const std::vector<unsigned>& GetIndices() const
```

Returns the database indices currently associated with this reader.

GetNextPacket

```
bool GetNextPacket(OEBroodDBPacket&)
```

Retrieves the next available database packet.

Init

```
unsigned Init(const std::string& prefix, OEBroodQuery& query,
              const OEBroodGeneralOptions& generalOpts = OEBroodGeneralOptions())
unsigned Init(const std::string& prefix,
              const std::vector<unsigned>& vecIdx = std::vector<unsigned>());
```

Initializes the reader using the database specified by `prefix`. The first overload configures loading for packets from the specified database indices. The second overload determines relevant indices from the provided `query` and general options, then configures loading for those packets. Returns *OEBroodStatusCode.Success* if initialization is successful, otherwise an error code from *OEBroodStatusCode*.

3.1.24 OEDBScreenOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEDBScreenOptions : public OESystem::OEOptions
```

This class provides an interface to setup options related to screening two-dimensional Brood databases in *OEDBBuilder*.

The *OEDBScreenOptions* class defines the following public methods:

- *GetMinFreqHeavy* and *SetMinFreqHeavy*
- *GetMinFrequency* and *SetMinFrequency*

Constructors

```
OEDBScreenOptions()
OEDBScreenOptions(const OEDBScreenOptions&)
```

Default and copy constructors.

operator=

Assignment operator.

GetMinFreqHeavy

```
unsigned GetMinFreqHeavy() const
```

See *SetMinFreqHeavy* method.

GetMinFrequency

```
unsigned GetMinFrequency() const
```

See *SetMinFrequency* method.

SetMinFreqHeavy

```
bool SetMinFreqHeavy(const unsigned)
```

Sets the **fragment size defined by the number of heavy atoms** affecting minimum frequency. The *minimum frequency* is only applicable to fragments larger this size defined here. **Default: 1.**

SetMinFrequency

```
bool SetMinFrequency(const unsigned)
```

Sets the **Minimum frequency** required for a fragment to be kept. The `Minimum frequency` is only applicable to fragments larger than size defined in *SetMinFreqHeavy*. The `frequency` is the number of parent molecule a specific fragment belongs to, in a database. A value of zero indicates that all fragments should be kept. **Default: 0.**

3.1.25 OEDBWriter

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEDBWriter
```

This class defines an interface for writing a Brood database to disk.

The *OEDBWriter* class defines the following public methods:

- *Finish*
- *Init*
- *Write*

Constructors

```
OEDBWriter()
```

Default constructor.

Finish

```
bool Finish()
```

Closes database files and finalizes the database. This method must be called to produce a valid database.

Init

```
bool Init(const std::string& prefix, unsigned max = 1000)
```

Initializes the database for writing. The `prefix` parameter specifies the database folder and file prefix, and `maxBufferSize` specifies the maximum in-memory buffer size before flushing to disk.

Write

```
bool Write(OEChem::OEMCMolBase& mol)
Writes the specified fragment to the database.
```

3.1.26 OEExtrinsicPropOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEExtrinsicPropOptions : public OESystem::OEOptions
```

This class provides an interface to setup options related to medicinal chemistry property limits during fragment replacement scoring.

The *OEExtrinsicPropOptions* class defines the following public methods:

- *GetComplexity* and *SetComplexity*
- *GetFrequency* and *SetFrequency*
- *GetLipinski* and *SetLipinski*
- *GetLipinskiAcc* and *SetLipinskiAcc*
- *GetLipinskiDon* and *SetLipinskiDon*
- *GetLogP* and *SetLogP*
- *GetMartin* and *SetMartin*

Constructors

```
OEExtrinsicPropOptions(const unsigned type = OEBroodMolPropertyType::MIN)
OEExtrinsicPropOptions(const OEExtrinsicPropOptions&)
```

Default and copy constructors.

operator=

Assignment operator.

GetComplexity

```
double GetComplexity() const
```

See *SetComplexity* method.

GetFrequency

```
unsigned GetFrequency() const
```

See *SetFrequency* method.

GetLipinski

```
unsigned GetLipinski() const
```

See *SetLipinski* method.

GetLipinskiAcc

```
unsigned GetLipinskiAcc() const
```

See *SetLipinskiAcc* method.

GetLipinskiDon

```
unsigned GetLipinskiDon() const
```

See *SetLipinskiDon* method.

GetLogP

```
double GetLogP() const
```

See *SetLogP* method.

GetMartin

```
double GetMartin() const
```

See *SetMartin* method.

SetComplexity

```
bool SetComplexity(const double)
```

Sets the molecular complexity range for any selected analog. **Default: [Min: 0.0, Max: 1.0]**

SetFrequency

```
bool SetFrequency(const unsigned)
```

Sets the fragment frequency in the database for any selected analog. The frequency is a percentile number indicating the frequency of each fragment normalized relative to the frequency of fragments in the database. Frequency as assessed here is a measure of how common each fragment is among the source molecules. The most commonly occurring fragment would be in the 99th percentile, while the least commonly occurring fragments would be in the 1st percentile. **Default: [Min: 0, Max: 100]**

SetLipinski

```
bool SetLipinski(const unsigned)
```

Sets the allowed Lipinski violations for any selected analog. In order to segregate molecules that progressed through clinical trials, Lipinski determined that one violation was acceptable, but two were not [Lipinski-1997]. **Default: [Min: 0 Max: 1]**

SetLipinskiAcc

```
bool SetLipinskiAcc(const unsigned)
```

Sets the required number of Lipinski hydrogen bond acceptors for any selected analog. For the purpose of this measure, H-bond acceptors are determined by the method of Lipinski [Lipinski-1997]. **Default: [Min: 2, Max: 11]**

SetLipinskiDon

```
bool SetLipinskiDon(const unsigned)
```

Sets the required number of Lipinski hydrogen bond donors for any selected analog. For the purpose of this measure, H-bond donors are determined by the method of Lipinski [Lipinski-1997]. **Default: [Min: 1, Max: 8]**

SetLogP

```
bool SetLogP(const double)
```

Sets the required calculated LogP for any selected analog. **Default: [Min: -1.0, Max: 5.0]**

SetMartin

```
bool SetMartin(const double)
```

Sets the required Abbott Bioavailability Score (ABS) for any selected analog. This floating point ABS parameter (range 0.0-1.0) indicates the minimum allowable probability that F will be >10% in rats according the QSAR model developed and published by Yvonne Martin [Martin-2005]. A value of 0.0 will allow all compounds to pass. **Default: [Min: 0.2, Max: 1.0]**

3.1.27 OEFragConfReader

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEFragConfReader
```

This class defines an interface to perform fragment conformer sampling from provided 3D molecular structures.

The *OEFragConfReader* class defines the following public methods:

- *Init*
- *NumMols*
- *ReadConformers*

Constructors

```
OEFragConfReader()
```

Default constructor.

Init

```
bool Init(OEChem::oemolistream& ifs)
```

Initializes the reader with 3D molecules from which to sample fragment conformers.

NumMols

```
unsigned NumMols() const
```

Returns the number of molecules obtained during initialization.

ReadConformers

```
bool ReadConformers(OEChem::OEMCMolBase& mol) const
```

Reads fragment conformers from initialized molecule structures and outputs conformers into the provided molecule.

3.1.28 OEFragmentOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEFragmentOptions : public OESystem::OEOptions
```

This class provides an interface to set up options for fragmenting molecules when building a bioisosteric fragment database. These options control fragment generation, size constraints, and structural properties.

The *OEFragmentOptions* class defines the following public methods:

- *GetMaxChiral* and *SetMaxChiral*
- *GetMaxDegree* and *SetMaxDegree*
- *GetMaxHeavy* and *SetMaxHeavy*
- *GetMaxMolWt* and *SetMaxMolWt*
- *GetMinDegree* and *SetMinDegree*
- *GetMinHeavy* and *SetMinHeavy*
- *GetSingleSourceMol* and *SetSingleSourceMol*
- *GetSmarts* and *SetSmarts*
- *SetSmartsFile*

Constructors

```
OEFragmentOptions()
OEFragmentOptions(const OEFragmentOptions &)
```

Default and copy constructors.

operator=

Assignment operator.

GetMaxChiral

```
unsigned GetMaxChiral() const
```

See *SetMaxChiral* method.

GetMaxDegree

```
unsigned GetMaxDegree() const
```

See *SetMaxDegree* method.

GetMaxHeavy

```
unsigned GetMaxHeavy() const
```

See *SetMaxHeavy* method.

GetMaxMolWt

```
double GetMaxMolWt() const
```

See *SetMaxMolWt* method.

GetMinDegree

```
unsigned GetMinDegree() const
```

See *SetMinDegree* method.

GetMinHeavy

```
unsigned GetMinHeavy() const
```

See *SetMinHeavy* method.

GetSingleSourceMol

```
bool GetSingleSourceMol() const
```

See *SetSingleSourceMol* method.

GetSmarts

```
std::string GetSmarts() const
```

See *SetSmarts* method.

SetMaxChiral

```
bool SetMaxChiral(const unsigned)
```

Sets the maximum allowable number of chiral centers (atom and bond) in generated fragments. **Default: 3.**

SetMaxDegree

```
bool SetMaxDegree(const unsigned)
```

Sets the maximum allowed attachment points in generated fragments. **Default: 3.**

SetMaxHeavy

```
bool SetMaxHeavy(const unsigned)
```

Sets the maximum allowed heavy atoms in generated fragments. **Default: 15.**

SetMaxMolWt

```
bool SetMaxMolWt(const double)
```

Sets the maximum allowed molecular weight for generated fragments. **Default: 350.**

SetMinDegree

```
bool SetMinDegree(const unsigned)
```

Sets the minimum required attachment points in generated fragments. **Default: 1.**

SetMinHeavy

```
bool SetMinHeavy(const unsigned)
```

Sets the minimum required heavy atoms in generated fragments. **Default: 1.**

SetSingleSourceMol

```
bool SetSingleSourceMol(bool)
```

Sets whether to store only a *single source molecule* per fragment. When disabled (default), stores information for up to five source molecules. **Default: false**

SetSmarts

```
bool SetSmarts(const std::string value)
```

Sets the SMARTS pattern for bonds to break during fragmentation. Built-in options are `recap`, `rlf`, `both` (both rlf and recap), and `all`. **Default: all**

SetSmartsFile

```
bool SetSmartsFile(const std::string&)
bool SetSmartsFile(const OEPlatform::oeisstream value)
```

Sets SMARTS patterns for bonds to break from a file. The first overload accepts a `filename` and the second accepts an oeisstream. This method takes precedence over the *SetSmarts* method.

3.1.29 OEFragOverlay

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEFragOverlay: public OEBroodOverlayBase
```

This class defines an interface for fragment overlay optimization against another fragment.

The *OEFragOverlay* class defines the following public methods:

- *GetRefFrag*
- *SetupRef*
- *Transform*

The following methods are publicly inherited from *OEBroodOverlayBase*:

- *Overlay*

Constructors

```
OEFragOverlay(const OEBroodGeneralOptions& genOpts = OEBroodGeneralOptions(),
              const OEBroodScoreOptions& scoreOpts = OEBroodScoreOptions())
```

Default constructor.

GetRefFrag

```
bool GetRefFrag(OEChem::OEMolBase& mol) const
```

Gets the reference fragment currently set to perform overlay. Method returns `true` if successful, `false` otherwise.

SetupRef

```
unsigned SetupRef(const OEChem::OEMolBase& fragment)
```

Sets up the overlay optimization with the desired fragment molecule. Method returns *OEBroodStatusCode.Success* if the initialization is successful, otherwise returns an error code from the *OEBroodStatusCode* namespace.

Transform

```
bool Transform(OEChem::OEMolBase& mol) const
```

Transforms the specified molecule to the optimized overlay position determined by a prior call to *Overlay*.

3.1.30 OEHitlistBase

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEHitlistBase
```

This is an abstract base class for hit list management that defines the common interface for collecting and filtering bioisosteric hits.

The following classes have been derived from this class:

- *OEScoreHitlist*
- *OEBroodHitlist*

The *OEHitlistBase* class defines the following public methods:

- *Build*
- *GetAddCount*
- *GetDuplicateCount*
- *GetHitCount*

Build

```
virtual bool Build(const bool final = true) = 0
```

This method builds and finalizes the hit list, performing duplicate filtering and hit list creation. The `final` parameter controls whether this is the final build (`true`) or an intermediate build (`false`).

GetAddCount

```
unsigned GetAddCount() const
```

This method returns the total number of entries submitted to the hit list.

GetDuplicateCount

```
unsigned GetDuplicateCount() const
```

This method returns the number of entries recognized as duplicates.

GetHitCount

```
unsigned GetHitCount() const
```

This method returns the number of retained hits currently in the hit list.

3.1.31 OEHitlistBuilder

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEHitlistBuilder
```

This class defines an interface for generating a hit list from calculated *Brood scores*.

The *OEHitlistBuilder* class defines the following public methods:

- *AddScores*
- *Build*
- *GetAddCount*
- *GetBumpCount*
- *GetDeleteCount*
- *GetDuplicateCount*
- *GetFailedCount*
- *GetHitCount*
- *GetHits*
- *GetInitHitCount*
- *GetMatchCount*
- *GetSelectCount*
- *GetSecDuplicateCount*
- *GetStrainCount*
- *GetUnstableCount*

Constructors

```
OEHitlistBuilder(const OEBroodQuery& query,
                 const OEHitlistBuilderOptions& options)
OEHitlistBuilder(const OEBroodQuery& query,
                 const OEBroodGeneralOptions& genOpts = OEBroodGeneralOptions(),
                 const OEBroodHitlistOptions& options = OEBroodHitlistOptions())
```

Default and copy constructors.

AddScores

```
bool AddScores(const std::vector<OEBroodScore> &)
```

This method adds the specified scores for building the hit list.

Build

```
bool Build(OESystem::OETracerBase& tracer = OESystem::OENoTracer)
```

This method builds the hit list. This method should be called after all scores have been added via *AddScores*.

GetAddCount

```
unsigned GetAddCount() const
```

This method returns the total number of scores added.

GetBumpCount

```
unsigned GetBumpCount() const
```

This method returns the total number of matches that were rejected due to bumping with protein.

GetDeleteCount

```
unsigned GetDeleteCount() const
```

This method returns the total number of matches that were deleted.

GetDuplicateCount

```
unsigned GetDuplicateCount() const
```

This method returns the total number of matches that were marked as duplicates.

GetFailedCount

```
unsigned GetFailedCount() const
```

This method returns the total number of matches that were failed due to reasons other than being duplicated or having excessive strain, an unstable bond, or a protein clash. These are failed whether due to unsuccessful protonation, elongated bond, or the inability to calculate or attach the medicinal chemistry data.

GetHitCount

```
unsigned GetHitCount() const
```

This method returns the total number of generated hits in the hit list.

GetHits

```
const std::vector<OEBroodHit>& GetHits() const
```

This method returns the generated hits.

GetInitHitCount

```
unsigned GetInitHitCount() const
```

This method returns the initial size of the hit list.

GetMatchCount

```
unsigned GetMatchCount() const
```

This method returns the total number of matches found.

GetSelectCount

```
unsigned GetSelectCount() const
```

This method returns the number of matches rejected with *OEBroodStatusCode.SelectFail* during build.

GetSecDuplicateCount

```
unsigned GetSecDuplicateCount() const
```

This method returns the number of secondary duplicates.

GetStrainCount

```
unsigned GetStrainCount() const
```

This method returns the number of matches rejected due to strain.

GetUnstableCount

```
unsigned GetUnstableCount() const
```

This method returns the number of matches rejected due to unstable bonds.

3.1.32 OEHitlistBuilderOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEHitlistBuilderOptions : public OESystem::OEOptions
```

This class defines configuration options for the *OEHitlistBuilder* and consolidates options from general, hit list, and build option groups.

The *OEHitlistBuilderOptions* class defines the following public methods:

- *GetBuildOptions* and *SetBuildOptions*
- *GetGeneralOptions* and *SetGeneralOptions*
- *GetHitlistOptions* and *SetHitlistOptions*

Constructors

```
OEHitlistBuilderOptions()
OEHitlistBuilderOptions(const OEHitlistBuilderOptions&)
OEHitlistBuilderOptions& operator=(const OEHitlistBuilderOptions&)
```

Default and copy constructors.

GetBuildOptions

```
const OEBroodBuildOptions& GetBuildOptions() const
```

This method returns the *OEBroodBuildOptions* contained in this object.

See the *SetBuildOptions* method.

GetGeneralOptions

```
const OEBroodGeneralOptions& GetGeneralOptions() const
```

This method returns the *OEBroodGeneralOptions* contained in this object.

See the *SetGeneralOptions* method.

GetHitlistOptions

```
const OEBroodHitlistOptions& GetHitlistOptions() const
```

This method returns the *OEBroodHitlistOptions* contained in this object.

See the *SetHitlistOptions* method.

SetBuildOptions

```
void SetBuildOptions(const OEBroodBuildOptions&)
```

This method sets the *OEBroodBuildOptions* to be used.

SetGeneralOptions

```
void SetGeneralOptions(const OEBroodGeneralOptions&)
```

This method sets the *OEBroodGeneralOptions* to be used.

SetHitlistOptions

```
void SetHitlistOptions(const OEBroodHitlistOptions&)
```

This method sets the *OEBroodHitlistOptions* to be used.

3.1.33 OEIntrinsicPropOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEIntrinsicPropOptions : public OESystem::OEOptions
```

This class provides an interface to set up options related to medicinal chemistry property limits during fragment replacement scoring.

The *OEIntrinsicPropOptions* class defines the following public methods:

- *GetAromaticJCT* and *SetAromaticJCT*
- *GetHeavyAtomCount* and *SetHeavyAtomCount*
- *GetMolWt* and *SetMolWt*
- *GetRotorCount* and *SetRotorCount*
- *GetSp3CFrac* and *SetSp3CFrac*
- *GetTPSA* and *SetTPSA*

Constructors

```
OEIntrinsicPropOptions(const unsigned type = OEBroodMolPropertyType::MIN)
OEIntrinsicPropOptions(const OEIntrinsicPropOptions&)
```

Default and copy constructors.

operator=

Assignment operator.

GetAromaticJCT

```
unsigned GetAromaticJCT() const
```

See *SetAromaticJCT* method.

GetHeavyAtomCount

```
unsigned GetHeavyAtomCount() const
```

See *SetHeavyAtomCount* method.

GetMolWt

```
double GetMolWt() const
```

See *SetMolWt* method.

GetRotorCount

```
unsigned GetRotorCount() const
```

See *SetRotorCount* method.

GetSp3CFrac

```
double GetSp3CFrac() const
```

See *SetSp3CFrac* method.

GetTPSA

```
unsigned GetTPSA() const
```

See *SetTPSA* method.

SetAromaticJCT

```
bool SetAromaticJCT(const unsigned)
```

Sets the aromatic ring count for any selected analog. The number of aromatic rings is defined as the number of aromatic rings is #aromatic bonds - #aromatic atoms + 1 **Default: [Min: 0, Max: 5]**

SetHeavyAtomCount

```
bool SetHeavyAtomCount(const unsigned)
```

Sets the number of heavy atoms for any selected analog. **Default: [Min: 7, Max: 35]**

SetMolWt

```
bool SetMolWt(const double)
```

Sets the required molecular weight for any selected analog. **Default: [Min: 100, Max: 500]**

SetRotorCount

```
bool SetRotorCount(const unsigned)
```

Sets the required number of rotatable bonds for any selected analog. **Default: [Min: 0, Max: 13]**

SetSp3CFrac

```
bool SetSp3CFrac(const double)
```

Sets the required fraction of carbons that are sp^3 for any selected analog. There is some evidence that increasing the fraction of carbons in a series that are sp^3 (escaping from "Flatland") improved success in clinical trials [Lovering-2009]. **Default: [Min: 0.3, Max: 1.0]**

SetTPSA

```
bool SetTPSA(const unsigned)
```

Sets the required topological polar surface area (TPSA) for any selected analog. **Default: [Min: 60, Max: 150]**

3.1.34 OEMolCTBuilder

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEMolCTBuilder
```

This class builds molecule from structural connection table during bioisosteric fragment replacements, including validation of required chemical constraints.

The *OEMolCTBuilder* class defines the following public method:

- *Build*

Constructors

```
OEMolCTBuilder(const OEBroodQuery& query,
               const OEBroodGeneralOptions& genOpts = OEBroodGeneralOptions(),
               const OEBroodBuildOptions& options = OEBroodBuildOptions())
```

This method constructs an *OEMolCTBuilder* with query and option settings that define the connection-table validation context.

Build

```
bool Build(OEChem::OEMolBase& mol)
```

This method validates the connection table of the given molecule based on query constraints. It returns `true` if the molecule connection table is valid and `false` otherwise.

3.1.35 OEMolPropertyOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OEMolPropertyOptions : public OESystem::OEOptions
```

This class provides an interface to set up options related to medicinal chemistry property limits during fragment replacement scoring.

The *OEMolPropertyOptions* class defines the following public methods:

- *GetEganEgg* and *SetEganEgg*
- *GetExtrinsicMaxOptions* and *SetExtrinsicMaxOptions*

- *GetExtrinsicMinOptions* and *SetExtrinsicMinOptions*
- *GetIntrinsicMaxOptions* and *SetIntrinsicMaxOptions*
- *GetIntrinsicMinOptions* and *SetIntrinsicMinOptions*
- *GetVeber* and *SetVeber*

Constructors

```
OEMolPropertyOptions()
OEMolPropertyOptions(const OEMolPropertyOptions&)
```

Default and copy constructors.

operator=

Assignment operator.

GetEganEgg

```
bool GetEganEgg() const
```

See *SetEganEgg* method.

GetExtrinsicMaxOptions

```
OEExtrinsicPropOptions& GetExtrinsicMaxOptions()
const OEExtrinsicPropOptions& GetExtrinsicMaxOptions() const
```

See *SetExtrinsicMaxOptions* method.

GetExtrinsicMinOptions

```
OEExtrinsicPropOptions& GetExtrinsicMinOptions()
const OEExtrinsicPropOptions& GetExtrinsicMinOptions() const
```

See *SetExtrinsicMinOptions* method.

GetIntrinsicMaxOptions

```
OEIntrinsicPropOptions& GetIntrinsicMaxOptions()
const OEIntrinsicPropOptions& GetIntrinsicMaxOptions() const
```

See *SetIntrinsicMaxOptions* method.

GetIntrinsicMinOptions

```
OEIntrinsicPropOptions& GetIntrinsicMinOptions()
const OEIntrinsicPropOptions& GetIntrinsicMinOptions() const
```

See *SetIntrinsicMinOptions* method.

GetVeber

```
bool GetVeber() const
```

See *SetVeber* method.

SetEganEgg

```
bool SetEganEgg(const bool)
```

Sets the requirement to fulfill the "Egan egg" measure of bioavailability for any selected analog. This measure was published by Bill Egan while at Pharmacopia [Egan-2000] and rejects compounds with a LogP > 5.88 or a PSA > 131.6. **Default: true**

SetExtrinsicMaxOptions

```
void SetExtrinsicMaxOptions(const OEExtrinsicPropOptions&)
```

Sets *options* related to maximum values of the extrinsic molecule properties.

SetExtrinsicMinOptions

```
void SetExtrinsicMinOptions(const OEExtrinsicPropOptions&)
```

Sets *options* related to minimum values of the extrinsic molecule properties.

SetIntrinsicMaxOptions

```
void SetIntrinsicMaxOptions(const OEIntrinsicPropOptions&)
```

Sets *options* related to maximum values of the intrinsic molecule properties.

SetIntrinsicMinOptions

```
void SetIntrinsicMinOptions(const OEIntrinsicPropOptions&)
```

Sets *options* related to minimum values of the intrinsic molecule properties.

SetVeber

```
bool SetVeber(const bool)
```

Sets the requirement to fulfill the measure of Veber bioavailability for any selected analog. This eliminates compounds with a PSA > 140 or more than 10 rotatable bonds. Veber measured bioavailability during his time at GSK [Veber-2002]. **Default: False**

3.1.36 OESimilarity

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
class OESimilarity
```

This class is a container for overlap-derived similarity components and derivative metrics. *OEBroodScore* consists of multiple instances of *OESimilarity* of various types.

The *OESimilarity* class defines the following public methods:

- *Add*
- *GetFitScore*
- *GetOverlap*
- *GetRefScore*
- *GetScaledScore*
- *GetTanimoto*
- *Load*
- *ToRecord*

Constructors

```
OESimilarity(const double refScore = 0.0,
             const double fitScore = 0.0,
             const double ovScore = 0.0,
             const unsigned type = OEBroodScoreType::ROCS)
OESimilarity(const OESimilarity&)
```

Default and copy constructors.

The `type` argument selects the scoring mode used when deriving the Tanimoto and scaled metrics. It accepts one of the following values from the *OEBroodScoreType* namespace:

- *OEBroodScoreType.ROCS* - shape and color based scoring.
- *OEBroodScoreType.ET* - shape and electrostatics based scoring.

The default value is *OEBroodScoreType.ROCS*.

operator=

Assignment operator.

Add

```
bool Add(const OESimilarity&)
```

This method adds the scores from another *OESimilarity* object to this object and recalculates the combined Tanimoto score.

GetFitScore

```
double GetFitScore() const
```

This method returns the fit score component of the similarity calculation.

GetOverlap

```
double GetOverlap() const
```

This method returns the overlap score component of the similarity calculation.

GetRefScore

```
double GetRefScore() const
```

This method returns the reference score component of the similarity calculation.

GetScaledScore

```
double GetScaledScore() const
```

This method returns the scaled score, calculated as the ratio of overlap to reference score.

GetTanimoto

```
double GetTanimoto() const
```

This method returns the calculated Tanimoto coefficient based on the similarity scores.

Load

```
bool Load(const OEDataFlow::OERecord&)
```

This method loads the similarity scores from an OERecord.

ToRecord

```
bool ToRecord(OEDataFlow::OERecord&) const
```

This method stores the similarity scores onto an OERecord.

3.2 Preliminary OEBioisostere Constants

3.2.1 OEBroodBuildType

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

This namespace contains constants.

Optimize3D

Build 3D molecule with replaced fragment, and optimize

NoOpt3D

Build 3D molecule with replaced fragment, but skip optimization

TwoD

Build 2D molecule with replaced fragment

3.2.2 OEBroodMolPropertyType

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

This namespace defines constants used to specify property comparison types when filtering molecules during bioisosteric replacement.

MIN

Specifies minimum value comparison for molecular properties.

MAX

Specifies maximum value comparison for molecular properties.

3.2.3 OEBroodScoreType

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

This namespace contains constants.

ET

Scoring based on shape and electrostatics

LinkOnly

Scoring based on attachments only

ROCS

Scoring based on shape and color

3.2.4 OEBroodStatusCode

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

This namespace contains constants. The error code number can be extracted using *OEGetBroodStatus*.

BondOrderMismatch

Mismatch attachment bond orders

DBSetupFailed

Failed to setup database reader with query molecule

EmptyDatabase

Database is empty of fragments

ExcessStrain

Excess strain

Failed

Failed

Failed2DConstr

Failed to pass 2D constraint

FailedAttachCut

Failed to pass attachment cutoff

FailedConstraints

Failed to pass 3D constraints & receptor clash

FailedETAttach

ET attach failure

FailedFragFilter

Failed to initialize fragment filtering

FailedInit

Failed to initialize database fragment

FailedInitAttach

Failed to initialize attachment geometries

FailedPropFilter

Failed to pass property filter

FailedProteinSelect

Protein receptor/selection failure

FailedQueryInit

Failed query initialization

FailedQueryMolRead

Failed to read query molecule

FailedRMSCut

Failed to pass rms Cutoff

FailedSetupOpt

Failed to setup optimization

FailedShapeCut

Failed to pass shape Cutoff

HasRingAtoms

Has ring atoms

InsuffRingAtoms

Insufficient ring atoms

InvalidOptions

Invalid Options

InvalidScore

Invalid Score

InvalidQuery3D

Query molecule must have 3D coordinates

InvalidQueryAttach

Query selection contains none or more than 3 attachments

InvalidQueryMol

Invalid query molecule

InvalidQueryNoHeavyAtoms

Query selection contains no heavy atoms

InvalidQueryProtein

Invalid query protein

InvalidQueryRing

Query selection contains invalid partial ring

InvalidQuerySel

Query selection does not match molecule

InvalidQuerySelProt

Invalid query selectivity protein

ManifestCheckFailed

Manifest check failed to find a complete brood database

MissingQueryFrag

Missing query fragment

NewFPGenerated

New fingerprints generated

NoAttachPt

No attachment points in database fragment

NoConformers

No conformers available in DB fragment

NoCPDDBGenerated

Unable to generate similarity database from cpddb

NoRingAtoms

No ring atoms

NoSelectionClash

No selection clash

PreGeneratedFPDetected

Identified and using pre-generated fingerprints for cpddb similarity

ProteinBump

Molecule clashes with protein

ReceptorClash

Receptor clash

SelectFail

Molecule not clashing with selection protein

Success

Success

UnableToFindDatabase

Unable to find brood database directory

UnableToOpenDatabase

Unable to open database (corrupt or nonexistent file)

UnequalAttachPt

Different number of attachments

UnstableBonds

Unstable bonds

3.3 Preliminary OEBioisostere Functions

3.3.1 OEBioisostereGetArch

```
const char* OEBioisostereGetArch()
```

Returns the architecture of the current version of Bioisostere TK. Examples include:

- microsoft-win32-x86
- redhat-RHEL9-x86_64

3.3.2 OEBioisostereGetLicensee

```
std::string OEBioisostereGetLicensee()
bool OEBioisostereGetLicensee(std::string& licensee)
```

Returns the LICENSEE from the current valid Bioisostere TK license.

3.3.3 OEBioisostereGetPlatform

```
const char* OEBioisostereGetPlatform()
```

Returns the platform, including compiler version, of the current version of Bioisostere TK. Examples include:

- microsoft-win32-msvc9-MD-x86
- redhat-RHEL9-g++11.11-x86_64

3.3.4 OEBioisostereGetRelease

```
const char* OEBioisostereGetRelease()
```

Returns the version of this toolkit release. For example: `4.0.0`.

3.3.5 OEBioisostereGetSite

```
std::string OEBioisostereGetSite()
bool OEBioisostereGetSite(std::string& site)
```

Returns the SITE from the current valid Bioisostere TK license.

3.3.6 OEBioisostereGetVersion

```
unsigned int OEBioisostereGetVersion()
```

Returns the build date of the toolkit as an unsigned int. For example: `20240227`.

3.3.7 OEBioisostereIsLicensed

```
bool OEBioisostereIsLicensed(const char* feature = 0,
                             unsigned int* expdate = 0)
```

Determines whether a valid license file is present. This function may be called without a legitimate run-time license to determine whether it is safe to call any **Bioisostere TK** functionality.

The 'feature' argument can be used to check for a valid license to **Bioisostere TK** along with the following features: 'python'. Pass `nullptr` (or `0`) to check the default **Bioisostere TK** feature.

The 'expdate' argument can be used to obtain the expiration date of the current **Bioisostere TK** license. If non-null, the expiration date is written as a `YYYYMMDD` integer. Pass `nullptr` to ignore.

See also

- `OEChemIsLicensed` function

3.3.8 OECreateBroodQuery

Query Creation without Protein

Attention

This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
unsigned OECreateBroodQuery(OEBroodQuery& query,
                            const OEChem::OEMCMolBase& mol,
                            const OEChem::OEMatchBase& selection)
unsigned OECreateBroodQuery(OEBroodQuery& query,
                            const OEChem::OEMCMolBase& mol,
                            const OEChem::OEAtomBondSet& selection)
```

Creates a **BROOD** query. The function returns a status code from *OEBroodStatusCode*.

query

The *OEBroodQuery* to be created.

mol

The input molecule from which a query is to be created by replacing a fragment of the molecule.

selection

Criteria for selecting atoms and bonds of the molecule that becomes the fragment to be replaced. The atoms and bonds must collectively become a single fragment.

Query Creation with Associated Protein

```
unsigned OECreateBroodQuery(OEBroodQuery& query,
                            const OEChem::OEMCMolBase& mol,
                            const OEChem::OEMatchBase& selection,
                            const OEBio::OEDesignUnit& du,
                            const unsigned proteinMask,
```

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```
                            const bool passingProteinSelect = false)
unsigned OECreateBroodQuery(OEBroodQuery& query,
                            const OEChem::OEMCMolBase& mol,
                            const OEChem::OEAtomBondSet& selection,
                            const OEBio::OEDesignUnit& du,
                            const unsigned proteinMask,
                            const bool passingProteinSelect = false)
```

Creates a **BROOD** query. The function returns a status code from *OEBroodStatusCode*.

du

The OEDesignUnit corresponding to the protein target.

proteinMask

Mask to be applied with the OEDesignUnit to determine the protein target.

passingProteinSelect

To create a **BROOD** query with a protein select, this boolean needs to be true.

Query Creation with Associated Protein and Protein Select

```
unsigned OECreateBroodQuery(OEBroodQuery& query,
                            const OEChem::OEMCMolBase& mol,
                            const OEChem::OEMatchBase& selection,
                            const OEBio::OEDesignUnit& du,
                            const unsigned proteinMask,
                            const OEBio::OEDesignUnit& protSelectDu,
                            const unsigned proteinSelectMask)
unsigned OECreateBroodQuery(OEBroodQuery& query,
                            const OEChem::OEMCMolBase& mol,
                            const OEChem::OEAtomBondSet& selection,
                            const OEBio::OEDesignUnit& du,
                            const unsigned proteinMask,
                            const OEBio::OEDesignUnit& protSelectDu,
                            const unsigned proteinSelectMask)
```

Creates a **BROOD** query. The function returns a status code from *OEBroodStatusCode*.

protSelectDu

The OEDesignUnit corresponding to the protein select target.

proteinSelectMask

Mask to be applied with the OEDesignUnit to determine the protein select target.

Linker Query Creation with Two Molecules (Bridging) without Protein

```
unsigned OECreateBroodQuery(OEBroodQuery& query,
                            const OEChem::OEMCMolBase& firstMol,
                            const OEChem::OEMCMolBase& secondMol,
                            const OEChem::OEMatchBase& firstMolSelection,
                            const OEChem::OEMatchBase& secondMolSelection)
unsigned OECreateBroodQuery(OEBroodQuery& query,
                            const OEChem::OEMCMolBase& firstMol,
```

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```
                              const OEChem::OEMCMolBase& secondMol,
                              const OEChem::OEAtomBondSet& firstMolSelection,
                              const OEChem::OEAtomBondSet& secondMolSelection)
```

Creates a **BROOD** query. The function returns a status code from *OEBroodStatusCode*.

firstMol & secondMol

Input molecules from which a query is to be created by bridging a fragment between them. Molecules need to prepared in proper relative coordinates and should not be clashing for optimum results.

firstMolSelection and secondMolSelection

Criteria for selecting atoms and bonds of each molecule that becomes part of the bridge fragment to be replaced. The atoms and bonds must collectively become a single fragment for each molecule.

Linker Query Creation with Two Molecules (Bridging) with Protein

```
unsigned OECreateBroodQuery(OEBroodQuery& query,
                              const OEChem::OEMCMolBase& firstMol,
                              const OEChem::OEMCMolBase& secondMol,
                              const OEChem::OEMatchBase& firstMolSelection,
                              const OEChem::OEMatchBase& secondMolSelection,
                              const OEBio::OEDesignUnit& du,
                              const unsigned proteinMask,
                              const bool passingProteinSelect = false)
unsigned OECreateBroodQuery(OEBroodQuery& query,
                              const OEChem::OEMCMolBase& firstMol,
                              const OEChem::OEMCMolBase& secondMol,
                              const OEChem::OEAtomBondSet& firstMolSelection,
                              const OEChem::OEAtomBondSet& secondMolSelection,
                              const OEBio::OEDesignUnit& du,
                              const unsigned proteinMask,
                              const bool passingProteinSelect = false)
```

Creates a **BROOD** query. The function returns a status code from *OEBroodStatusCode*.

Linker Query Creation with Two Molecules (Bridging) with Protein and Protein Select

```
unsigned OECreateBroodQuery(OEBroodQuery& query,
                              const OEChem::OEMCMolBase& firstMol,
                              const OEChem::OEMCMolBase& secondMol,
                              const OEChem::OEMatchBase& firstMolSelection,
                              const OEChem::OEMatchBase& secondMolSelection,
                              const OEBio::OEDesignUnit& du,
                              const unsigned proteinMask,
                              const OEBio::OEDesignUnit& protSelectDu,
                              const unsigned proteinSelectMask)
unsigned OECreateBroodQuery(OEBroodQuery& query,
                              const OEChem::OEMCMolBase& firstMol,
                              const OEChem::OEMCMolBase& secondMol,
                              const OEChem::OEAtomBondSet& firstMolSelection,
                              const OEChem::OEAtomBondSet& secondMolSelection,
                              const OEBio::OEDesignUnit& du,
                              const unsigned proteinMask,
```

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```
                                const OEBio::OEDesignUnit& protSelectDu,
                                const unsigned proteinSelectMask)
```

Creates a **BROOD** query. The function returns a status code from *OEBroodStatusCode*.

3.3.9 OECreateFragFilter

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
OEMolProp::OEFilter* OECreateFragFilter()
```

This function creates and returns a configured OEFilter object for use in filtering fragments by molecular properties during database construction. The returned object should be deleted by the caller.

This function is typically used in conjunction with *OEDBBuilder::Filter* to apply property-based constraints to fragments during bioisosteric database building.

3.3.10 OECreateFlipperOptions

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
OEConfGen::OEFlipperOptions* OECreateFlipperOptions()
```

This function creates and returns a configured OEFlipperOptions object for use with conformer expansion during bioisosteric database building. The returned object should be deleted by the caller.

This function is typically used in conjunction with *OEDBBuilder::Expand* to configure conditional conformer generation for rotatable bonds in fragments.

3.3.11 OEGenerateConformers

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
bool OEGenerateConformers(OEChem::OEMCMolBase& mol,
                          bool rotorOffset = false)
```

Generates conformers for the specified fragment molecule. Method returns *true* if conformer generation was successful.

The overload with the `rotorOffset` enables rotor offset compression during conformer generation, as described in SetRotorOffset. For fragment conformer generation, this can only be turned on when generating conformers specifically for use with *OEDBWriter*. Due to subtleties with fragment conformer generation, rotor offset compression may otherwise lead to undesired behavior. `rotorOffset` is *false* by default.

3.3.12 OEGetBroodStatus

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
std::string OEGetBroodStatus(const unsigned code)
```

Returns the description string for the status *code* corresponding to constants defined in *OEBroodStatusCode*.

3.3.13 OEGetDBIndices

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
std::vector<unsigned> OEGetDBIndices(OEBroodQuery& query,
                                     const OEBroodGeneralOptions& opts =␣
↪OEBroodGeneralOptions())
```

Method returns Brood database indices corresponding to the specified *OEBroodQuery*.

3.3.14 OEIsFragment

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
bool OEIsFragment(const OEChem::OEMolBase& mol)
```

This function determines whether the given molecule satisfies the structural criteria to be considered a valid fragment for bioisosteric replacement. It returns `true` if the molecule is a valid fragment and `false` otherwise.

3.3.15 OEReadBroodQuery

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
unsigned OEReadBroodQuery(OEChem::oemolistream& ifs,
                          OEBroodQuery& query)
```

Reads a *OEBroodQuery* from the specified stream. Method returns a status code from *OEBroodStatusCode*.

3.3.16 OEWriteBroodQuery

> **Attention**
>
> This is a preliminary API and may be improved based on user feedback. It is currently available in C++ and Python.

```
unsigned OEWriteBroodQuery(OEChem::oemolostream& ofs,
                           const OEBroodQuery& query)
```

Writes a *OEBroodQuery* to the specified stream. Method returns a status code from *OEBroodStatusCode*.

CHAPTER

FOUR

RELEASE HISTORY

4.1 Bioisostere TK 5.0.0

4.1.1 New Features

- The following new classes have been added as preliminary API:
  - *OEBroodBuildResult*
  - *OEBroodCluster*
  - *OEBroodClusterBuilder*
  - *OEBroodComboBuilder*
  - *OEHitlistBuilderOptions*
  - *OEHitlistBase*
  - *OEScoreHitlist*
  - *OEBroodHitlist*
  - *OEMolCTBuilder*
  - *OESimilarity*
- The following new methods have been added to *OEBroodQuery*:
  - *GetQueryID*
  - *SetQueryID*
- A new constructor overload has been added to *OEHitlistBuilder* that takes a *OEHitlistBuilderOptions* as an argument.
- A new overload of *Setup* has been added to *OEBroodDBFilter* that takes a molecule as argument.
- The following new methods have been added to *OEBroodQuery*:
  - *GetBuildRes*
  - *GetScores*
- The following new methods have been added to *OEBroodScore*:
  - *Add*
  - *GetQueryIDs*
- The following new functions have been added:
  - *OECreateFlipperOptions*

  - *OECreateFragFilter*
  - *OEIsFragment*

- The following methods have been removed from the *OEHitlistBuilder*, as they are no longer relevant:
  - GetTrimmedCount
  - TrimHitlist
  - An overload of GetHits that took a vector of *OEBroodHit* as an argument.
  - GetRemovedHits

4.1.2 Minor Bug Fixes

- The *OECreateBroodQuery* method now keeps any incoming color atoms associated with the query selection, when available, and does not add any additional color atoms to the query. The behavior is unchanged when no color atoms are present with the incoming selection.
- A bug in fragment property filtering has been resolved. Now by setting the *SetUseProperty* option in *OEBroodScoreOptions* to true, you can activate the fragment filtering based on the properties defined by *OEExtrinsicPropOptions* and *OEIntrinsicPropOptions*. Previously, the filter was not being applied correctly, which could lead to unexpected fragments being included in the results.
- An issue has been fixed related to proper usage of *SetRangeSize* and *SetRangeOffset* so that fragment retrieval from the database during the overlay step now properly respects the specified range boundaries.
- A bug has been fixed where the color score reported by *GetColorScore* could exceed its valid range in ROCS mode, causing the combined score to exceed its range as well. The color Tanimoto is now computed consistently from the scored conformer.

4.2 OEBioisostere TK 4.2.1

4.2.1 New Features

- A new overload has been added to the *SetSmartsFile* method in *OEFragmentOptions*, enabling the ability to pass in a file name directly.
- A new overload has been added to the *OEGenerateConformers*, enabling the option for `rotorOffset` compression during conformer generation. The existing overload no longer performs `rotorOffset` compression.
- A new method, *HasProteinSelect*, has been added to the *OEBroodQuery* class that can be called on a query to check whether it has a selectivity protein.

4.2.2 Minor Bug Fixes

- Both *OEBroodOverlay* and *OEFragOverlay* now transfer any residue information of query fragments into the overlaid fragments within the *Overlay* method.
- The *Build* method in *OEHitlistBuilder* now properly updates the tracer when provided.
- The *Init* method in *OEBroodQuery* now properly adds the protein structures for a selectivity check to the query when provided.

4.3 Bioisostere TK 4.2.0

4.3.1 New Features

- The new class *OECPDDatabase* has been added as a preliminary API, which can be used to perform 2D similarity comparisons between a **Brood** hit list and an external compound database.
- Eight new overloads have been added to the existing *OECreateBroodQuery* function. The new overloads extend the API for query generation in the presence of an active site protein and/or a selectivity protein. Additionally, there are new overloads to create a bridging query between two molecules.
- The following new methods have been added to *OEHitlistBuilder*:
  - GetRemovedHits
  - *GetFailedCount*
  - TrimHitlist
  - GetTrimmedCount
- The *Build* method in the *OEHitlistBuilder* has been expanded to accept an OETracerBase as an optional argument.
- The following new methods have been added to *OEBroodHit*:
  - *GetBuildStatus*
  - *GetDeltaLocalStrain*

4.3.2 Minor Bug Fixes

- Some memory management issues have been fixed in *AddScores* of the *OEHitlistBuilder* class.
- The *OEBroodScore* returned from the *Overlay* calculation now always contains the fragment, irrespective of whether the overlay was a success.
- The *GetFrags* method in the *OEBroodDBPacket* now properly returns an empty iterator if there are no fragments in a packet.
- The *SetupRef* method in *OEFragOverlay* is now substantially faster for subsequently initializing it with new reference fragments.
- The *Init* method in *OEDBReader* is now returning an unsigned int (instead of bool), reflecting the *OEBioisostere OEBroodStatusCode Success* or other error codes for database initialization.

4.4 Bioisostere TK 4.1.0

4.4.1 New features

- A new algorithm, based on OEFlexiOverlay, has been adapted in *Build* for optimization of generated poses for molecules obtained from fragment replacement. The new algorithm is more robust for optimization of poses for all geometries, including cyclic peptides.

4.4.2 Major bug fixes

- Query building algorithms in *OECreateBroodQuery* have been improved for robustness. The improved API automatically includes any associated hydrogen atoms as part of the query fragment. Behavior has also been improved to provide better error behavior against invalid selections.

- The new methods *SetSingleSourceMol* and *GetSingleSourceMol* have been added to *OEFragmentOptions* to provide flexibility regarding source molecule storage during database building.

4.4.3 Minor bug fixes

- Some memory management issues have been fixed in *Build* and *Generate*.

4.5 Bioisostere TK 4.0.0

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

4.5.1 New features

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

- *OEBroodBuildOptions*
- *OEBroodDBFilter*
- *OEBroodDBPacket*
- *OEBroodFragPrep*
- *OEBroodGeneralOptions*
- *OEBroodHit*
- *OEBroodHitlistOptions*
- *OEBroodOverlay*
- *OEBroodOverlayBase*
- *OEBroodQuery*
- *OEBroodScore*
- *OEBroodScoreOptions*
- *OEDBBuffer*
- *OEDBBuilder*
- *OEDBReader*
- *OEDBScreenOptions*
- *OEDBWriter*
- *OEFragConfReader*
- *OEFragmentOptions*
- *OEFragOverlay*
- *OEHitlistBuilder*
- *OEMolPropertyOptions*
- *OEIntrinsicPropOptions*
- *OEExtrinsicPropOptions*

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

- *OEBioisostereGetArch*

- *OEBioisostereGetLicensee*
- *OEBioisostereGetPlatform*
- *OEBioisostereGetRelease*
- *OEBioisostereGetSite*
- *OEBioisostereGetVersion*
- *OEBioisostereIsLicensed*
- *OECreateBroodQuery*
- *OEGenerateConformers*
- *OEGetBroodStatus*
- *OEGetDBIndices*
- *OEReadBroodQuery*
- *OEWriteBroodQuery*

CHAPTER

FIVE

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CHAPTER

SIX

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CHAPTER

SEVEN

CITATION

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7.1 Orion®

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```

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```
Orion 2025.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM. http://www.eyesopen.com.
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The version number for Orion appears in the product's release notes, for example, https://docs.eyesopen.com/orion-user-interface/releasenotes/index.html.

7.2 Orion Floes

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

```
OpenEye <package-name> <version-number>. OpenEye, Cadence Molecular Sciences, Santa Fe,␣
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```
OpenEye Large-Scale Floes 4.2.3. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
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```

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

7.3 Toolkits and Applications

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

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

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

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

where <*product name*> is:

- Bioisostere TK
- OEChem TK
- OEDepict TK
- OEDocking TK
- OEFF TK
- Eon TK
- FastROCS TK
- Grapheme TK
- GraphSim TK
- Lexichem TK
- OEMedChem TK
- MolProp TK
- Omega TK
- Quacpac TK
- Shape TK
- Spicoli TK
- Spruce TK
- Szmap TK
- Szybki TK
- Zap TK
- AFITT Application
- BROOD Application
- OEDocking Application
- EON Application
- OMEGA Application
- PICTO Application
- pKa-Prospector Application
- QUACPAC Application

- ROCS Application
- SiteHopper Application
- SPRUCE Application
- SZMAP Application
- SZYBKI Application
- VIDA Application

You can use the version number of the individual Application or Toolkit. For example:

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

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

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

7.4 Publications for Bibliographies

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

7.4.1 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

7.4.2 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

7.4.3 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

7.4.4 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

7.4.5 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

7.5 OpenEye MMDS Web Service

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

```
Macromolecular Data Service <version-number>. OpenEye, Cadence Molecular Sciences, Santa␣
↪Fe, NM. http://www.eyesopen.com.
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For example:

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

CHAPTER

EIGHT

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Table 1: Licensed Technology

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abseil-cpp	https://github.com/abseil/abseil-cpp	https://github.com/abseil/abseil-cpp/blob/master/LICENSE
absl-py	https://github.com/abseil/abseil-py	https://github.com/abseil/abseil-py/blob/main/LICENSE

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aiohttp	https://docs.aiohttp.org/en/stable/	https://github.com/aio-libs/aiohttp/blob/master/LICENSE.txt
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angular-mocks	https://github.com/angular/angular.js	https://raw.githubusercontent.com/angular/angular.js/master/LICENSE
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angular-ui-grid	https://github.com/angular-ui/ui-grid	https://github.com/angular-ui/ui-grid
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appengine	https://google.golang.org/appengine	https://github.com/golang/appengine/blob/master/LICENSE
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asn1crypto	https://github.com/wbond/asn1crypto	https://github.com/wbond/asn1crypto/blob/master/LICENSE
assertions go-render	https://github.com/smartystreets/assertions/internal/go-render/render	https://github.com/smartystreets/assertions/blob/master/internal/go-render/LICENSE
assertions oglmatchers	https://github.com/smartystreets/assertions/internal/oglematchers	https://github.com/smartystreets/assertions/blob/master/internal/oglematchers/LICENSE
assertions	https://github.com/smartystreets/assertions	https://github.com/smartystreets/assertions/blob/master/LICENSE.md
asttokens	https://github.com/gristlabs/asttokens	https://github.com/gristlabs/asttokens/blob/master/LICENSE
astunparse	https://github.com/simonpercivall/astunparse	https://github.com/simonpercivall/astunparse/blob/master/LICENSE
async-lru	https://github.com/aio-libs/async-lru	https://github.com/aio-libs/async-lru/blob/master/LICENSE
async-timeout	https://github.com/aio-libs/async-timeout	https://github.com/aio-libs/async-timeout/blob/master/LICENSE
atk-1.0	https://docs.gtk.org/atk/	https://gitlab.gnome.org/GNOME/atk/-/blob/master/COPYING
atomic	https://github.com/uber-go/atomic	https://github.com/uber-go/atomic/blob/master/LICENSE.txt

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Name of Project	Website	License URL
atomicwrites	https://github.com/untitaker/python-atomicwrites	https://github.com/untitaker/python-atomicwrites/blob/master/LICENSE
attrs	https://www.attrs.org/	https://github.com/python-attrs/attrs/blob/main/LICENSE
aws-sdk-go	https://github.com/aws/aws-sdk-go	https://github.com/aws/aws-sdk-go/blob/master/LICENSE.txt
babel	https://babel.pocoo.org/ OR https://github.com/python-babel/babel	https://github.com/python-babel/babel/blob/master/LICENSE OR https://babel.pocoo.org/en/latest/license.html#babel-license
Babel	https://github.com/python-babel/babel	https://github.com/python-babel/babel/blob/master/LICENSE
backcall	https://github.com/takluyver/backcall	https://github.com/takluyver/backcall/blob/master/LICENSE
backports	https://github.com/brandon-rhodes/backports	https://github.com/brandon-rhodes/backports/blob/master/LICENSE.TXT
backports.functools-lru-cache	https://github.com/jaraco/backports.functools_lru_cache	https://github.com/jaraco/backports.functools_lru_cache/blob/main/LICENSE
backports.zstd	https://github.com/rogdham/backports.zstd	https://github.com/rogdham/backports.zstd?tab=License-1-ov-file#readme
base62	https://github.com/kare/base62	https://github.com/kare/base62/blob/main/LICENSE
beautifulsoup4	https://www.crummy.com/software/BeautifulSoup/	https://www.crummy.com/software/BeautifulSoup/

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

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Name of Project	Website	License URL
boltons	https://github.com/mahmoud/boltons	https://github.com/mahmoud/boltons/blob/master/LICENSE
Boltz	https://boltz.bio	https://github.com/jwohlwend/boltz/blob/main/LICENSE
boost	https://www.boost.org/doc/libs/1_71_0/libs/python/doc/html/index.html	https://www.boost.org/LICENSE_1_0.txt
boost-cpp	https://www.boost.org/doc/libs/1_71_0/libs/python/doc/html/index.html	https://www.boost.org/LICENSE_1_0.txt
bootstrap-vue	https://github.com/bootstrap-vue/bootstrap-vue	https://github.com/bootstrap-vue/bootstrap-vue/raw/master/LICENSE
boto3	https://github.com/boto/boto3	https://github.com/boto/boto3/blob/develop/LICENSE
botocore	https://github.com/boto/botocore	https://github.com/boto/botocore/blob/develop/LICENSE.txt
Bottleneck	https://bottleneck.readthedocs.io/en/latest/index.html	https://bottleneck.readthedocs.io/en/latest/license.html
Brotli	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
brotli-bin	https://github.com/google/brotli	https://github.com/google/brotli/blob/master/LICENSE
brotli-python	http://python-hyper.org/projects/brotlipy/en/latest/	https://github.com/python-hyper/brotlicffi/blob/main/LICENSE
brotlicffi	https://github.com/python-hyper/brotlicffi	https://github.com/python-hyper/brotlicffi?tab=MIT-1-ov-file#readme
brotlipy	https://github.com/python-hyper/brotlicffi	https://github.com/python-hyper/brotlicffi/blob/main/LICENSE

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Name of Project	Website	License URL
bson	http://github.com/py-bson/bson	https://github.com/py-bson/bson/blob/master/LICENSE_APACHE
bytefmt	https://code.cloudfoundry.org/bytefmt	https://github.com/cloudfoundry/bytefmt/blob/master/LICENSE
bzip2	https://www.bzip.org	https://spdx.org/licenses/bzip2-1.0.6.html
c-ares	https://github.com/c-ares/c-ares	https://github.com/c-ares/c-ares/blob/main/LICENSE.md
ca-certificates	https://github.com/conda-forge/ca-certificates-feedsto	https://wiki.mozilla.org/CA/Included_Certificates
cached-property	https://github.com/pydanny/cached-property	https://github.com/pydanny/cached-property/blob/master/LICENSE
cachetools	https://github.com/tkem/cachetools/	https://github.com/tkem/cachetools/blob/master/LICENSE
cairo	https://pycairo.readthedocs.io/en/latest/	https://github.com/pygobject/pycairo/blob/master/COPYING
canvas	https://github.com/Automattic/node-canvas	https://github.com/Automattic/node-canvas
cctbx	https://github.com/cctbx/cctbx_project	https://github.com/cctbx/cctbx_project/blob/master/cctbx/LICENSE_2_0.txt
celery	https://github.com/celery/celery	https://github.com/celery/celery/blob/master/LICENSE
Cerberus	https://docs.python-cerberus.org/en/stable/	https://docs.python-cerberus.org/en/stable/license.html
certifi	https://certifiio.readthedocs.io/en/latest/	https://wiki.mozilla.org/index.php?title=CA/IncludedCertificates&redirect=no

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Name of Project	Website	License URL
cffi	https://github.com/python-cffi	https://github.com/cffi/cffi/blob/master/COPYRIGHT
cftime	https://pypi.org/project/cftime/	https://github.com/Unidata/cftime/blob/master/LICENSE
chardet	https://github.com/chardet/chardet	https://github.com/chardet/chardet/blob/master/LICENSE
charset-normalizer	https://github.com/ousret/charset_normalizer	https://github.com/Ousret/charset_normalizer/blob/master/LICENSE
ChEMBL Structure Pipeline	https://github.com/chembl/ChEMBL_Structure_Pipeline/tree/master	https://github.com/chembl/ChEMBL_Structure_Pipeline/blob/master/LICENSE
choreographer	https://github.com/mazpie/choreographer	https://github.com/mazpie/choreographer/blob/main/LICENSE
chunkreader	https://github.com/jackc/chunkreader/v2	https://github.com/jackc/chunkreader/blob/master/LICENSE
click	https://palletsprojects.com/p/click/	https://github.com/pallets/click/blob/main/LICENSE.rst
click-completion	https://github.com/click-contrib/click-completion	https://github.com/click-contrib/click-completion/blob/master/LICENSE
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-file#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
tifffile	https://github.com/cgohlke/tifffile/	https://github.com/cgohlke/tifffile/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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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

8.1 GCC

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

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

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

8.1.1 GCC RUNTIME LIBRARY EXCEPTION

```
Version 3.1, 31 March 2009

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

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

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

0. Definitions.

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

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

"GPL-compatible Software" is software whose conditions of propagation, modification and␣
↪use would permit combination with
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"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

8.1.2 GNU GENERAL PUBLIC LICENSE

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

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                            Preamble

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   The licenses for most software and other practical works are designed
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  Developers that use the GNU GPL protect your rights with two steps:
(1) assert copyright on the software, and (2) offer you this License
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  For the developers' and authors' protection, the GPL clearly explains
that there is no warranty for this free software.  For both users' and
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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
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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
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"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
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earlier work or a work "based on" the earlier work.

  A "covered work" means either the unmodified Program or a work based
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  To "propagate" a work means to do anything with it that, without
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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)
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extent that warranties are provided), that licensees may convey the
work under this License, and how to view a copy of this License.  If
the interface presents a list of user commands or options, such as a
menu, a prominent item in the list meets this criterion.

  1. Source Code.

  The "source code" for a work means the preferred form of the work
for making modifications to it.  "Object code" means any non-source
form of a work.
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  A "Standard Interface" means an interface that either is an official
standard defined by a recognized standards body, or, in the case of
interfaces specified for a particular programming language, one that
is widely used among developers working in that language.

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

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

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and you may offer support or warranty protection for a fee.

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   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
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    Appropriate Legal Notices; however, if the Program has interactive
    interfaces that do not display Appropriate Legal Notices, your
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works, which are not by their nature extensions of the covered work,
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in one of these ways:

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  (including a physical distribution medium), accompanied by the
  Corresponding Source fixed on a durable physical medium
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  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
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  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
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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
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