

OpenEye
SCIENTIFIC

Omega TK – C#

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Cadence Design Systems, Inc.

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CHAPTER

ONE

THEORY

1.1 Torsion Driving (TD) in OMEGA

The torsion driving (TD) algorithm of **OMEGA** is composed of two main components; building the molecular scaffold (model) from non-rotor fragments and sampling the torsional degrees of freedom. Model generation may be bypassed by importing fragment structures from external sources ([Hawkins-2010]; [Hawkins-2012]).

OMEGA builds initial structures for the molecule by assembling fragment templates along sigma bonds. Input molecules' graphs are fragmented at exocyclic sigma, and carbon to heteroatom acyclic (but not exocyclic) sigma bonds. Conformations for the fragments are either retrieved from pregenerated libraries built with MakeFraglib or constructed on-the-fly using the same approach that MakeFraglib uses. Molecule assembly is accomplished by simple vector alignment since all interfragment joints are along sigma bonds.

Once an initial structure is constructed or given as input, **OMEGA** generates additional ones enumerating ring conformations and invertible nitrogen atoms. Ring conformations are taken from the same fragment library used to build the initial model. **OMEGA** detaches all exocyclic substituents from a ring system, then aligns and attaches them relative to the new ring conformation. **OMEGA** attempts to generate every possible combination of ring conformations possible for a given structure.

The next step in model generation is to detect and enumerate invertible nitrogens. Nitrogens that have pyramidal geometry, no specified stereochemistry, no more than one hydrogen, are three valent, and have no more than three ring bonds are considered by **OMEGA** to be invertible. Invertible in this context simply means that at room temperature a pyramidal nitrogen is likely to be able to rapidly (on an NMR timescale) interconvert between two puckered forms. All multiconformer ring models are further expanded by enumerating all possible nitrogen puckers. The resulting model set is the starting point for conformer search by torsion driving.

OMEGA begins the torsion search process by examining the molecular graph and determining the bonds that may freely rotate. By default, **OMEGA** selects acyclic sigma bonds that have at least one non-hydrogen atom attached to each end of the bond. By default, hydrogen rotors (e.g., hydroxyl groups) are not altered during the torsion search; however, this can be enabled. The final ensemble selection is based on RMS distance of heavy atoms and sampled hydrogen atoms; unsampled hydrogen atoms do not affect this RMS distance. A list of possible dihedral angles are then assigned to each rotatable bond. The current mechanism for assignment is based on SMARTS matching, although alternate strategies for assigning angles based on experimental (i.e., X-ray) or theoretical (i.e., fragment optimization studies) are possible. The molecular graph is then subjected to pattern and geometric symmetry detection. Common patterns such as para-disubstituted benzene are used to reduce the number of symmetry equivalent dihedral angles that need to be searched. All torsions are altered by 120 and 180 degrees, and an RMS calculation is performed, taking into account symmetry-equivalent atoms in order to detect two- and three-fold symmetries. Once a set of nonredundant dihedral angles is assigned to each rotatable bond, **OMEGA** samples the torsion space through a systematic enumeration of combinations of these angles. Depending on the flexibility of the molecule, the maximum number of conformers to be generated, and the mode in which **OMEGA** is run, the algorithm to sample the torsion space is decided. By default, Thompson sampling, a Bayesian reinforcement learning algorithm, is used. The best conformers identified in the torsion search are rank-ordered by energy. A final ensemble is selected by sequentially testing the conformers using the RMS distance cutoff. To be accepted into the final ensemble, a conformer must have an RMS distance to every

other member of the ensemble that exceeds the user-defined cutoff value. The final ensemble is populated up to the user-defined maximum ensemble size limit, or until the list of low energy conformers is exhausted.

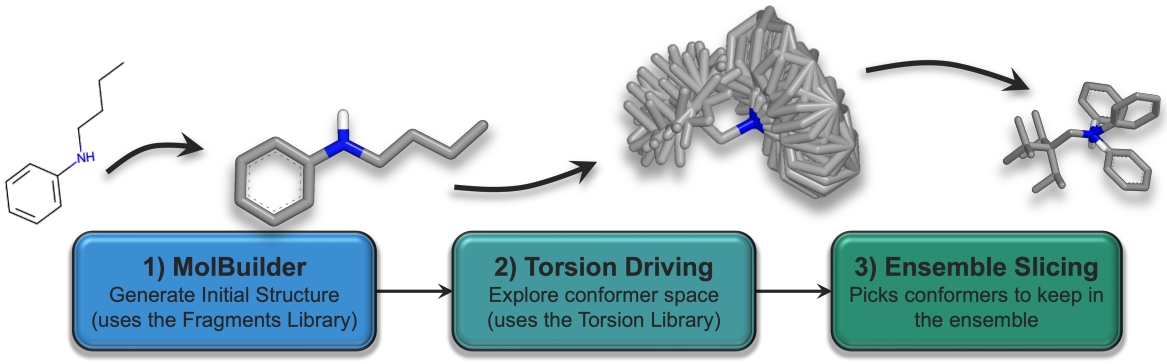


Fig. 1: **Figure 1.** Illustration of steps in torsion driving **OMEGA**.

1.2 Thompson Sampling in OMEGA

The torsion library provides a set of likely dihedral angles for each rotatable bond. In Thompson sampling for torsion driving, we use these angles from the torsion rules as priors for a Bayesian process. Instead of enumerating every possible combination of angles and searching the combinatorially expanding space of conformers, conformers are instead generated based on these priors. For every angle for a given rotatable bond, a distribution of beliefs is maintained for modeling the likelihood of that angle to be part of a new low strain conformer. We sample these distributions to pick an angle for a given rotor. This process is repeated for every rotatable bond to pick a combination of angles that defines a conformer. After a conformer is generated, its energy is evaluated and the beliefs are updated based on the result. As we generate more conformers while continuously updating the beliefs, the sampling process is steered toward the low-strain structures of interest.

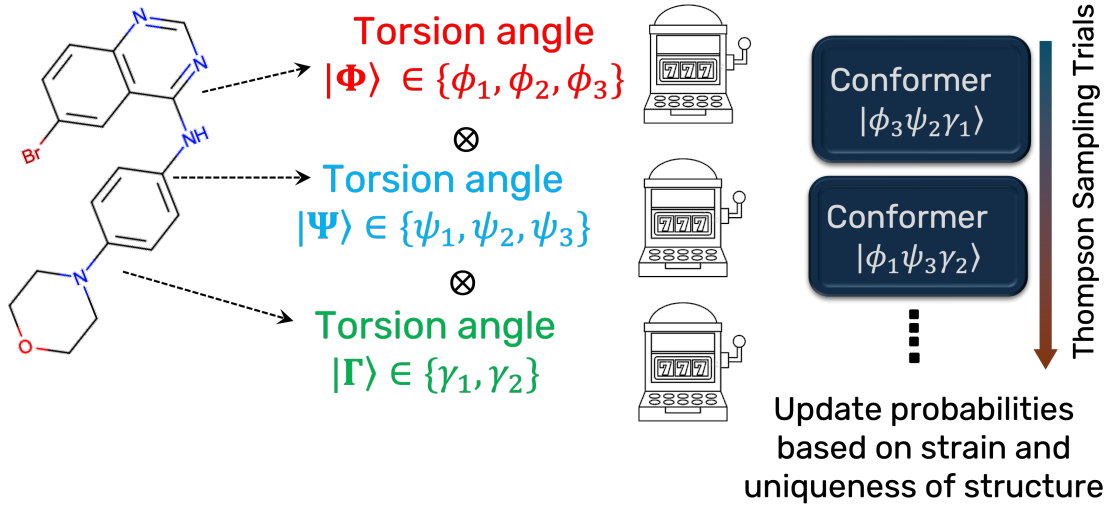


Fig. 2: **Figure 2.** Illustration of Thompson sampling algorithm in torsion driving **OMEGA**.

> **Note**
>
> Conformers generated from **OMEGA** with default options do not maintain input relative stereochemistry, that is, cis/trans configurations for cyclohexane or other cyclic molecules.

1.3 Macrocycle Conformations

Torsion driving conformational sampling methods such as described in the *Torsion Driving (TD) in OMEGA* section often perform poorly for macrocyclic molecules due to the problem of ring closure after the torsion driving step. Conformational sampling of macrocycles therefore requires a different approach; we address this issue with **OMEGA** using distance geometry (DG) [Hawkins-2020]. Other methods have been applied to this problem, such as distance geometry (DG) [Crippen-1988], molecular dynamics (MD/LLMOD) [Watts-2014], MD with perturbation along low energy eigenvectors [Labute-2010], and inverse kinematics [Coutsias-2016]. It is important to note that **OMEGA** DG also works well for very flexible linear molecules which have such a large conformational space that torsion driving may not be able to adequately sample it.

OMEGA's method of conformational sampling of macrocycles is an adaptation of the distance geometry method of Spellmeyer et al. [Spellmeyer-1997]. In this method, a traditional embedding DG algorithm is replaced with a direct error function minimization of the random atomic coordinates, followed by force field refinement. Each initial Cartesian atomic coordinate *x* is assigned by choosing a random number *r* between *-1* and *1*, multiplied by a factor $f\sqrt{N}$ which determines the box of maximum extent for a molecule with *N* atoms:

$$x = f\sqrt{N}r \tag{1.1}$$

Alternatively, instead of randomly placing atoms in Cartesian space, the method allows for random placement of rigid fragments such as aromatic rings, nitro groups, and so on. After randomly placing molecules, atoms, or rigid fragments, an error function of the form:

$$F = \sum_{i,j}(d_{ij} - c_{i,j})^2 + \sum_k V_k \tag{1.2}$$

is optimized. In the above equation, the first sum runs over all pairs of atoms in the molecule, where d_{ij} are the interatomic distances and c_{ij} are elements of the constraint matrix; they are obtained from the MMFF94 force field parameters. When atoms *(i,j)* are bonded or are the first and last atoms in a bond angle, the upper and lower bounds are the same and are taken as the corresponding equilibrium force field distances. When atoms *(i,j)* are the first and last atoms of a torsion angle, the lower bound corresponds to the cis configuration and the upper bound to the trans configuration of those atoms. Finally, when atoms *(i,j)* are separated by more than three bonds, the lower bound is taken as the sum of the vdW radii and the upper bound as the sum of bond lengths which separate the pair. The second summation in equation (1.2) is over the tetrahedral constraints which result from:

1. planarity
2. chirality
3. cis-trans isomerism

Optimization of the error function (1.2) leads to a rough conformation. No hydrogen atoms except those which are bonded to chiral atoms are included in the error function minimization. Each rough conformation is checked for chirality correctness before refinement. If the rough conformation passes the chirality checks, it is refined against a forcefield, MMFF94 ([Halgren-I-1996], [Halgren-II-1996], [Halgren-III-1996], [Halgren-IV-1996], [Halgren-V-1996]). Solvent forces can be included in the refinement step using a simple continuum solvation model (the Sheffield model [Grant-2007]). When the sequence of random placement followed by error function minimization and force field refinement is repeated for a large enough number of times for a given macrocycle, its conformational space is reasonably well covered.

Special measures are taken for zwitterionic molecules (containing both positively and negatively charged groups, such as CO_2^- and NH_3^+). In order to prevent possible Coulombic collapse in the absence of a stabilizing receptor, zwitterionic molecules are neutralized before performing the distance geometry calculation and the refined structures are recharged before writing them out. This approach meaningfully improves **OMEGA**'s ability to reproduce solid-state conformations of zwitterionic ligands.

This method of conformation sampling is completely general and can be used to generate conformations for any molecule, whether or not it contains a large ring. However the `macrocycle` mode in **OMEGA** has been specifically developed and parameterized to perform well on macrocycles, therefore its performance on linear and small ring molecules is worse than with `classic` **OMEGA**.

CHAPTER

TWO

GPU-OMEGA

GPU-Omega refers to the CUDA-enabled GPU implementation of **Omega TK**. **GPU-Omega** takes advantage of a GPU during torsion driving for accelerated conformer generation. To make use of **GPU-Omega** conformer generation, please follow the guidelines below.

> **Attention**
>
> **GPU-Omega** is not available in the C# version of the toolkit.

2.1 GPU-Related Requirements

The following features are required in order to use GPU-accelerated OpenEye toolkits and applications.

2.1.1 Supported Platforms

CUDA-enabled OpenEye software is only available on supported Linux platforms. For supported Linux platforms see the Platform Support Page.

2.1.2 Supported GPUs

An NVIDIA Tesla, Quadro, or GeForce GPU with a **compute capability of 3.5 or higher** is required on your system. For a comprehensive table of compute capability categories for each GPU, please refer to the CUDA Wikipedia page.

2.1.3 NVIDIA Drivers

- **Minimum NVIDIA Driver version: 450.x**.
- CUDA is **not** required to be installed.

We recommend driver 450.80.02, and we strongly advise manually downloading and installing the appropriate NVIDIA driver for your system as opposed to using a package manager.

To install, root privilege is required. Follow these steps:

1. Download the driver to the machine you are installing it on.
2. `chmod +x` the driver package to make it executable.
3. Ensure you have disabled X-server by killing any running sessions. Reboot may be required if X-server is still running after this step.

> **Warning**
>
> Disabling X-server requires different processes to be killed depending on your Linux distribution. See the NVIDIA installation guide for more details.

> **Warning**
>
> The NVIDIA kernel module can often conflict with the open source Nouveau display drivers, depending on your specific Linux distribution. The NVIDIA documentation is a much more complete and up-to-date source for information on how to work around this issue. See Disabling Nouveau on the NVIDIA website.

4. Install the driver by `sudo ./NVIDIA-Linux-x86_64-450.80.02.run` and follow the step-by-step installation instructions.

For more details on driver installations, see the CUDA Installation Guide

> **Note**
>
> The output of the `nvidia-smi` command is extremely useful when debugging GPU issues. Please include the output from `nvidia-smi` in any request to support@eyesopen.com.

2.1.4 Performance Tuning

To get the most performance out of an NVIDIA graphics card, use the persistence daemon to switch persistence mode across all cards on the system (root privilege required):

```
sudo nvidia-persistenced --user foo
```

This will automatically enable persistence mode after reboot.

For full instructions on the persistence daemon, see the Persistence daemon section of the NVIDIA docs.

2.2 Usage

- **GPU-Omega** accelerates the torsion driving component of conformer generation in **Omega TK** and is available through the *OEOmega* and *OETorDriver* classes.
- For all torsion driving sampling modes except `dense` modes, if a GPU is detected at runtime, torsion driving will be carried out on the GPU by default. To turn this feature off, use *OETorDriveOptions.SetUseGPU*.
- The following code shows how to turn off **GPU-Omega** prior to conformer generation using the `sparse` mode.
- **GPU-Omega** uses the default `OEMMFFSheffieldFFType.MMFF94Smod_NOESTAT` force field. If attempting to use an alternative force field, conformer generation will fall back to the CPU. **GPU-Omega** is also incompatible with `hydrogen sampling`, which is turned off in the default sampling mode. As a result, **GPU-Omega** is not compatible with the default settings of *OEOmegaSampling.Dense* sampling mode. To take advantage of a GPU with `dense` sampling mode, set *OETorDriveOptions.SetForceField* to `OEMMFFSheffieldFFType.MMFF94Smod_NOESTAT`, and set *OEMolBuilderOptions.SetSampleHydrogens* to *false*.
- The *OEOmegaIsGPUReady* utility function is provided for detecting available GPUs on a system.
- The following code demonstrates how to query the system for an available GPU and then set the force field to default in order to use the GPU for `dense` mode conformer generation.

- **GPU-Omega** does **not** support the distance geometry method of torsion driving, and therefore is incompatible with *OEMacrocycleOmega*.

Caution

To use **GPU-Omega** with child processes, a new *OEOmega* object must be created for each child. If attempting to use the same instance of an *OEOmega* object in child processes, conformer generation will fall back to the CPU.

CHAPTER

THREE

OMEGA EXAMPLES

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

Program	Description
SimpleOmega	Generating conformers
SingleConformer	Generating a single conformer
DensOmega	Generating densely sampled conformers
StereoAndTorsion	Generating stereoisomers
TorsionDrive	Generating conformer ensembles using torsion driving
MakeFraglib	Making fragment library
Macrocycle	Generating macrocycle conformers
SingleConformerMacrocycle	Generating single macrocycle conformer

Note

If the input molecule has SD tag data, the data will be copied to every conformer in the results molecule.

3.1 Classic OEOmega Examples

3.1.1 Generating Conformers

The following code example is a simple illustration of how to generate conformers using the *OEOmega* object.

See also

- *OEOmegaOptions* class
- *OEOmega* class
- OESimpleAppOptions class

Listing 1: Generating Conformers

```
/*
(C) 2022 Cadence Design Systems, Inc. (Cadence)
All rights reserved.
TERMS FOR USE OF SAMPLE CODE The software below ("Sample Code") is
```

(continues on next page)

(continued from previous page)

```
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NOT LIMITED TO, WARRANTIES OF MERCHANTABILITY, FITNESS FOR A
PARTICULAR PURPOSE AND NONINFRINGEMENT. In no event shall Cadence be
liable for any damages or liability in connection with the Sample Code
or its use.
*/
using System;
using OpenEye.OEChem;
using OpenEye.OEOmega;

public class SimpleOmega
{
    static void Main(string[] args)
    {
        OEOmegaOptions omegaOpts = new OEOmegaOptions(OEOmegaSampling.Dense);
        omegaOpts.SetParameterVisibility(OEParamVisibility.Hidden);
        omegaOpts.SetParameterVisibility("-rms", OEParamVisibility.Simple);
        omegaOpts.SetParameterVisibility("-ewindow", OEParamVisibility.Simple);
        omegaOpts.SetParameterVisibility("-maxconfs", OEParamVisibility.Simple);

        OESimpleAppOptions opts = new OESimpleAppOptions(omegaOpts, "SimpleOmega",␣
↪OEFileStringType.Mol, OEFileStringType.Mol3D);
        if(OEChem.OEConfigureOpts(opts, args, false) == OEOptsConfigureStatus.Help)
            Environment.Exit(1);

        omegaOpts.UpdateValues(opts);
        OEOmega omega = new OEOmega(omegaOpts);

        oemolistream ifs = new oemolistream();
        if(!ifs.open(opts.GetInFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetInFile() + " for reading");
        oemolostream ofs = new oemolostream();
        if(!ofs.open(opts.GetOutFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetOutFile() + " for writing");

        OEMol mol = new OEMol();
        while (OEChem.OEReadMolecule(ifs, mol))
        {
            OEChem.OEThrow.Info(mol.GetTitle());
            bool success = omega.Call(mol);
            if (success)
                OEChem.OEWriteMolecule(ofs, mol);
            else
                OEChem.OEThrow.Warning(mol.GetTitle() + ": failed");
```

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```
        }
    }
}
```

3.1.2 Generating a Single Conformer

The following code example is a simple illustration of how to generate a single conformer.

See also

- *OEConformerBuilder* class

Listing 2: Generating a Single Conformer

```
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*/
using System;

using OpenEye.OEChem;
using OpenEye.OEOmega;

public class SingleConformer
{
    public static int Main(String[] args)
    {
        if (args.Length!=2)
        {
            OEChem.OEThrow.Usage("SingleConformer <infile> <outfile>");
        }

        oemolistream ifs = new oemolistream();
        if(!ifs.open(args[0]))
            OEChem.OEThrow.Fatal("Unable to open " + args[0] + " for reading");
        oemolostream ofs = new oemolostream();
```

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```
        if(!ofs.open(args[1]))
            OEChem.OEThrow.Fatal("Unable to open " + args[1] + " for writing");

        OEConformerBuilder builder = new OEConformerBuilder();

        OEMol mol = new OEMol();
        while (OEChem.OEReadMolecule(ifs, mol))
        {
            OEChem.OEThrow.Info("Title: " + mol.GetTitle());
            uint retCode = builder.Build(mol);
            if(retCode == OEOmegaReturnCode.Success)
                OEChem.OEWriteMolecule(ofs, mol);
            else
                OEChem.OEThrow.Warning(mol.GetTitle() + ": failed with error " +␣
↪retCode);
        }
        return 0;
    }
}
```

3.1.3 Generating Densely Sampled Conformers

The following code example is a simple illustration of how to generate densely sampled conformers, as used in OEFreeFormConf calculations, using the *OEOmega* object.

See also

- *OEOmegaOptions* class
- *OEOmega* class
- *OEOmegaSampling* namespace
- OESimpleAppOptions class

Listing 3: Generating Densely Sampled Conformers

```
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```

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```
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*/
using System;
using OpenEye.OEChem;
using OpenEye.OEOmega;

public class DenseOmega
{
    static void Main(string[] args)
    {
        OEOmegaOptions omegaOpts = new OEOmegaOptions(OEOmegaSampling.Dense);
        omegaOpts.SetParameterVisibility(OEParamVisibility.Hidden);
        omegaOpts.SetParameterVisibility("-rms", OEParamVisibility.Simple);
        omegaOpts.SetParameterVisibility("-ewindow", OEParamVisibility.Simple);
        omegaOpts.SetParameterVisibility("-maxconfs", OEParamVisibility.Simple);

        OESimpleAppOptions opts = new OESimpleAppOptions(omegaOpts, "DenseOmega",␣
↪OEFileStringType.Mol, OEFileStringType.Mol3D);
        if(OEChem.OEConfigureOpts(opts, args, false) == OEOptsConfigureStatus.Help)
            Environment.Exit(1);

        omegaOpts.UpdateValues(opts);
        OEOmega omega = new OEOmega(omegaOpts);


        oemolistream ifs = new oemolistream();
        if(!ifs.open(opts.GetInFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetInFile() + " for reading");
        oemolostream ofs = new oemolostream();
        if(!ofs.open(opts.GetOutFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetOutFile() + " for writing");

        OEMol mol = new OEMol();
        while (OEChem.OEReadMolecule(ifs, mol))
        {
            OEChem.OEThrow.Info(mol.GetTitle());
            bool success = omega.Call(mol);
            if (success)
                OEChem.OEWriteMolecule(ofs, mol);
            else
                OEChem.OEThrow.Warning(mol.GetTitle() + ": failed");
        }
    }
}
```

3.2 Flipper Examples

3.2.1 Generating Stereoisomers

The following code example is a simple illustration of how to use the *OEFlipper* function to generate stereoisomers. The code example also demonstrates that stereoisomers should be generated before generating conformers.

See also

- *OEOmegaOptions* class
- *OEOmega* class
- *OEFlipper* function
- OESimpleAppOptions class

Listing 4: Generating Stereoisomers

```
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*/
using System;

using OpenEye.OEChem;
using OpenEye.OEOmega;

public class StereoAndTorsion
{
    public static int Main(String[] args)
    {
        OEFlipperOptions flipperOpts = new OEFlipperOptions();

        OESimpleAppOptions opts = new OESimpleAppOptions(flipperOpts, "StereoAndTorsion",
↪ OEFileStringType.Mol, OEFileStringType.Mol);
        if(OEChem.OEConfigureOpts(opts, args, false) == OEOptsConfigureStatus.Help)
            Environment.Exit(1);

        flipperOpts.UpdateValues(opts);
        OEOmega omega = new OEOmega();

        oemolistream ifs = new oemolistream();
        if(!ifs.open(opts.GetInFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetInFile() + " for reading");
        oemolostream ofs = new oemolostream();
```

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```
        if(!ofs.open(opts.GetOutFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetOutFile() + " for writing");

        OEMol mol = new OEMol();
        while (OEChem.OEReadMolecule(ifs, mol))
        {
            OEChem.OEThrow.Info(mol.GetTitle());
            foreach (OEMolBase enantiomer in OEOmegalib.OEFlipper(mol.GetActive(),␣
↪flipperOpts))
            {
                OEMol fmol = new OEMol(enantiomer);
                bool success = omega.Call(fmol);
                if(success)
                    OEChem.OEWriteMolecule(ofs, fmol);
                else
                    OEChem.OEThrow.Warning(fmol.GetTitle() + ": failed");
            }
        }
        return 0;
    }
}
```

3.3 Generating Torsion Driven Conformation Examples

3.3.1 Generating Conformer Ensembles Using Torsion Driving

The following code example is a simple illustration of how torsion driving from a given 3D structure can be used to generate a conformer ensemble.

See also

- *OETorDriveOptions* class
- *OETorDriver* class
- OESimpleAppOptions class

Listing 5: Generating Conformer Ensembles Using Torsion Driving

```
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*/
using System;
using OpenEye.OEChem;
using OpenEye.OEOmega;

public class TorsionDrive
{
    static void Main(string[] args)
    {
        OETorDriveOptions torOpts = new OETorDriveOptions();
        torOpts.SetParameterVisibility(OEParamVisibility.Hidden);
        torOpts.SetParameterVisibility("-rms", OEParamVisibility.Simple);
        torOpts.SetParameterVisibility("-ewindow", OEParamVisibility.Simple);
        torOpts.SetParameterVisibility("-maxconfs", OEParamVisibility.Simple);

        OESimpleAppOptions opts = new OESimpleAppOptions(torOpts, "TorsionDrive",␣
↪OEFileStringType.Mol, OEFileStringType.Mol3D);
        if(OEChem.OEConfigureOpts(opts, args, false) == OEOptsConfigureStatus.Help)
            Environment.Exit(1);

        torOpts.UpdateValues(opts);
        OETorDriver tordriver = new OETorDriver(torOpts);

        oemolistream ifs = new oemolistream();
        if(!ifs.open(opts.GetInFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetInFile() + " for reading");
        oemolostream ofs = new oemolostream();
        if(!ofs.open(opts.GetOutFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetOutFile() + " for writing");

        OEMol mol = new OEMol();
        while (OEChem.OEReadMolecule(ifs, mol))
        {
            OEChem.OEThrow.Info(mol.GetTitle());
            uint retCode = tordriver.GenerateConfs(mol);
            if(retCode == OEOmegaReturnCode.Success)
                OEChem.OEWriteMolecule(ofs, mol);
            else
                OEChem.OEThrow.Warning(mol.GetTitle() + ": failed with error " +␣
↪retCode);
        }
    }
}
```

3.4 Fragment Library Generation Examples

3.4.1 Making a Fragment Library

The following code example is a simple illustration of how to generate a fragment library.

See also

- *OEFragBuilderOptions* class
- *OEMakeFragLib* class
- OESimpleAppOptions class

Listing 6: Making a Fragment Library

```
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*/
using System;

using OpenEye.OEChem;
using OpenEye.OEOmega;

public class MakeFraglib
{
    public static int Main(String[] args)
    {
        OEFragBuilderOptions libOpts = new OEFragBuilderOptions();
        libOpts.SetParameterVisibility(OEParamVisibility.Hidden);
        libOpts.SetParameterVisibility("-buildFF", OEParamVisibility.Simple);

        OESimpleAppOptions opts = new OESimpleAppOptions(libOpts, "MakeFraglib",␣
↪OEFileStringType.Mol, OEFileStringType.Mol3D);
        if(OEChem.OEConfigureOpts(opts, args, false) == OEOptsConfigureStatus.Help)
           Environment.Exit(1);

        libOpts.UpdateValues(opts);
```

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```
        OEMakeFragLib makefraglib = new OEMakeFragLib(libOpts);

        oemolistream ifs = new oemolistream();
        if(!ifs.open(opts.GetInFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetInFile() + " for reading");
        oemolostream ofs = new oemolostream();
        if(!ofs.open(opts.GetOutFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetOutFile() + " for writing");

        if(ofs.GetFormat() != OEFormat.OEB)
            OEChem.OEThrow.Fatal("Output file has to have OEB format!");

        makefraglib.ClearFragLibs();
        makefraglib.GenerateMissingFrags(ifs, ofs);
        return 0;
    }
}
```

3.5 Macrocycle Examples

3.5.1 Generating Macrocycle Conformers

The following code example is a simple illustration of how to generate conformers using the OEMacrocycleOmega object.

See also

- *OEMacrocycleOmegaOptions* class
- *OEMacrocycleOmega* class
- OESimpleAppOptions class

Listing 7: Generating Macrocycle Conformers

```
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```

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```
or its use.
*/
using System;
using OpenEye.OEChem;
using OpenEye.OEOmega;

public class Macrocycle
{
    static void Main(string[] args)
    {
        OEMacrocycleOmegaOptions omegaOpts = new OEMacrocycleOmegaOptions();
        omegaOpts.SetParameterVisibility(OEParamVisibility.Hidden);
        omegaOpts.SetParameterVisibility("-rms", OEParamVisibility.Simple);
        omegaOpts.SetParameterVisibility("-ewindow", OEParamVisibility.Simple);
        omegaOpts.SetParameterVisibility("-maxconfs", OEParamVisibility.Simple);

        OESimpleAppOptions opts = new OESimpleAppOptions(omegaOpts, "Macrocycle",␣
↪OEFileStringType.Mol, OEFileStringType.Mol3D);
        if(OEChem.OEConfigureOpts(opts, args, false) == OEOptsConfigureStatus.Help)
            Environment.Exit(1);

        omegaOpts.UpdateValues(opts);
        OEMacrocycleOmega mcomega = new OEMacrocycleOmega(omegaOpts);

        oemolistream ifs = new oemolistream();
        if(!ifs.open(opts.GetInFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetInFile() + " for reading");
        oemolostream ofs = new oemolostream();
        if(!ofs.open(opts.GetOutFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetOutFile() + " for writing");

        OEMol mol = new OEMol();
        while (OEChem.OEReadMolecule(ifs, mol))
        {
            OEChem.OEThrow.Info(mol.GetTitle());
            uint retCode = mcomega.Build(mol);
            if(retCode == OEOmegaReturnCode.Success)
                OEChem.OEWriteMolecule(ofs, mol);
            else
                OEChem.OEThrow.Warning(mol.GetTitle() + ": failed with error " +␣
↪retCode);
        }
    }
}
```

3.5.2 Generating a Single Macrocycle Conformer

The following code example is a simple illustration of how to generate a single macrocycle conformer using the OEMacrocycleBuilder object.

See also

- *OEMacrocycleBuilderOptions* class
- *OEMacrocycleBuilder* class
- OESimpleAppOptions class

Listing 8: Generating a Single Macrocycle Conformer

```
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or its use.
*/
using System;
using OpenEye.OEChem;
using OpenEye.OEOmega;

public class SingleConformerMacrocycle
{
    static void Main(string[] args)
    {
        OEMacrocycleBuilderOptions buildOpts = new OEMacrocycleBuilderOptions();
        buildOpts.SetParameterVisibility(OEParamVisibility.Hidden);
        buildOpts.SetParameterVisibility("-seed", OEParamVisibility.Simple);
        buildOpts.SetParameterVisibility("-dielectric_constant", OEParamVisibility.
↪Simple);

        OESimpleAppOptions opts = new OESimpleAppOptions(buildOpts,
↪"SingleConformerMacrocycle", OEFileStringType.Mol, OEFileStringType.Mol3D);
        if(OEChem.OEConfigureOpts(opts, args, false) == OEOptsConfigureStatus.Help)
            Environment.Exit(1);

        buildOpts.UpdateValues(opts);

        oemolistream ifs = new oemolistream();
        if(!ifs.open(opts.GetInFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetInFile() + " for reading");
        oemolostream ofs = new oemolostream();
```

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```
        if(!ofs.open(opts.GetOutFile()))
            OEChem.OEThrow.Fatal("Unable to open " + opts.GetOutFile() + " for writing");

        OEMol mol = new OEMol();
        while (OEChem.OEReadMolecule(ifs, mol))
        {
            OEChem.OEThrow.Info(mol.GetTitle());
            uint retCode = OEOmegaReturnCode.Failed;
            uint itlimit = 1000;
            uint itnum = 0;
            while(itnum <= itlimit)
            {
                OEMacrocycleBuilder builder = new OEMacrocycleBuilder(buildOpts);
                retCode = builder.Build(mol);
                if(retCode == OEOmegaReturnCode.Success)
                {
                    OEChem.OEWriteMolecule(ofs, mol);
                    break;
                }
                else
                {
                   buildOpts.SetRandomSeed(buildOpts.GetRandomSeed()+1);
                }
                ++itnum;
            }
            if(retCode != OEOmegaReturnCode.Success)
                OEChem.OEThrow.Warning(mol.GetTitle() + ": failed with error " +␣
↪retCode);
        }
    }
}
```

CHAPTER

FOUR

API

4.1 OEConfGen Classes

4.1.1 OEBuilderBase

```
class OEBuilderBase
```

This is an abstract base class for structure builder classes that use a fragment library.

The *OEBuilderBase* class defines the following public methods:

- *AddFragLib*
- *ClearFragLibs*

The following classes derive from this class:

- *OEMakeFragLib*
- *OEMolBuilder*

AddFragLib

```
bool AddFragLib()
bool AddFragLib(const std::string &)
bool AddFragLib(OEPlatform::oeistream &)
```

Adds a **fragment library** to be used for pregenerated fragment coordinates. When the *OEBuilderBase.AddFragLib* is called without a parameter, the *built-in* fragment library is loaded immediately. By default, the *built-in* fragment library does not load until it is required in use for the first time.

The `string` and oeistream versions of *OEBuilderBase.AddFragLib* can be used to add external fragments libraries. These external libraries are used in addition to the built-in one. Returns *true* if the fragment library is added successfully.

See also

- *OEBuilderBase.ClearFragLibs* method

ClearFragLibs

```
void ClearFragLibs()
```

Clears all fragment libraries from the builder.

See also

- *OEBuilderBase.AddFragLib* method

4.1.2 OEConfFixOptions

```
class OEConfFixOptions : public OESystem::OEOptions
```

This class provides an interface to set up options required for constraining a fragment of the molecule during conformational search.

There are multiple ways to define the substructure for defining the constraints.

- The first is to provide a substructure query using the command *SetFixSubSearch*. If the input query pattern is in 3D, the corresponding substructure of the target is fixed to the query coordinates. For a non-3D query, the mapped substructure of an input 3D target is fixed, provided that *SetIncludeInput* is set to *true*.
- The second method is to pass in a 3D structure using the command *SetFixMol*. The *SetFixDeleteH* command can be used to control whether hydrogens should be retained or discarded from the *FixMol*. The corresponding substructure of the target has the atom coordinates fixed to those from the *FixMol*.
- The third method is to provide a SMARTS pattern using the command *SetFixSmarts*. The SMARTS pattern is matched against the input molecule to identify a substructure, provided that the input molecule is in 3D and that *SetIncludeInput* is set to *true*. The corresponding substructure of the target is fixed during the conformer generation.
- The fourth method is to provide both a *FixMol* using the command *SetFixMol*, and a SMARTS string using the command *SetFixSmarts*. In this case, the SMARTS pattern is matched against the *FixMol* structure to identify a substructure of the *FixMol*. The corresponding substructure of the target is fixed to the coordinates of the *FixMol* substructure during conformer generation.
- The fifth method is to provide both a *FixMol* using the command *SetFixMol* and to turn on MCS-based fix using the command *SetFixMCS*. In this case, the maximum common substructure is matched against the *FixMol* structure to identify a substructure of the *FixMol*. The corresponding substructure of the target is fixed to the coordinates of the *FixMol* substructure during conformer generation.
- The final method is to provide an atom predicate using the command *SetFixPredicate*, which is used to identify target atoms to be fixed.

For all of the above methods, the initialization of the substructure, when applicable, can be controlled using *SetAtomExpr* and *SetBondExpr*.

The *unique match* flag defined using *SetFixUniqueMatch* applies to all substructure matches performed, either during creation of molecule fragments or when applying the actual constraints.

The *MaxMatch* defines how many of the matches found during constraint application should be applied and can be set using the command *SetFixMaxMatch*. If the constraining fragment substructure appears twice in the target molecule and the *MaxMatch* is set to two or more, the molecule would be constrained to the substructure coordinates twice for each of the generated conformers and could result in twice the number of conformers compared to setting this value to 1.

In all cases, the constraints are evaluated by the proximity between the initial generated structure of the molecule and the coordinates of the constraining substructure. The precision of the proximity evaluation can be controlled by an *RMS* value set using *SetFixRMS*.

See also

- *OEMolBuilder* class
- *OETorDriver* class

The *OEConfFixOptions* class defines the following public methods:

- *GetAtomExpr* and *SetAtomExpr*
- *GetBondExpr* and *SetBondExpr*
- *GetFixDeleteH* and *SetFixDeleteH*
- *GetFixMaxMatch* and *SetFixMaxMatch*
- *GetFixMCS* and *SetFixMCS*
- *GetFixMol* and *SetFixMol*
- *GetFixPredicate* and *SetFixPredicate*
- *GetFixRMS* and *SetFixRMS*
- *GetFixSmarts* and *SetFixSmarts*
- *GetFixSubSearch* and *SetFixSubSearch*
- *GetFixUniqueMatch* and *SetFixUniqueMatch*
- *HasFixPattern*
- *GetMCSMinAtoms* and *SetMCSMinAtoms*
- *GetMCSFunc* and *SetMCSFunc*
- *GetMCSType* and *SetMCSType*

Constructors

```
OEConfFixOptions()
OEConfFixOptions(const OEConfFixOptions &)
```

Default and copy constructors.

GetAtomExpr

```
unsigned GetAtomExpr() const
```

See the *SetAtomExpr* method.

GetBondExpr

```
unsigned GetBondExpr() const
```

See the *SetBondExpr* method.

GetFixDeleteH

```
bool GetFixDeleteH() const
```

See the *SetFixDeleteH* method.

GetFixMaxMatch

```
unsigned int GetFixMaxMatch() const
```

See the *SetFixMaxMatch* method.

GetFixMCS

```
bool GetFixMCS() const
```

See the *SetFixMCS* method.

GetFixMol

```
const OEChem::OEMolBase& GetFixMol() const
```

See the *SetFixMol* method.

GetFixPredicate

```
const OESystem::OEUnaryPredicate<OEChem::OEAtomBase>* GetFixPredicate() const
```

See the *SetFixPredicate* method.

GetFixRMS

```
double GetFixRMS() const
```

See the *SetFixRMS* method.

GetFixSmarts

```
std::string GetFixSmarts() const
```

See the *SetFixSmarts* method.

GetFixSubSearch

```
OEChem::OESubSearch GetFixSubSearch() const
```

Returns the substructure search (OESubSearch) for fixed fragments.

GetFixUniqueMatch

```
bool GetFixUniqueMatch() const
```

See the *SetFixUniqueMatch* method.

GetMCSMinAtoms

```
unsigned GetMCSMinAtoms() const
```

See the *SetMCSMinAtoms* method.

GetMCSFunc

```
const OEChem::OEMCSFunc* GetMCSFunc() const
```

See the *SetMCSFunc* method.

GetMCSType

```
unsigned GetMCSType() const
```

See the *SetMCSType* method.

HasFixPattern

```
bool HasFixPattern() const
```

Method checks if a criterion for fixing a portion of the molecule during conformation search is currently set.

SetAtomExpr

```
bool SetAtomExpr(const unsigned)
```

Sets the **atom expression** to be used for substructure initialization from a molecule fragment. Default: `OEExprOpts.DefaultAtoms`

See also

- `OEExprOpts` namespace

SetBondExpr

```
bool SetBondExpr(const unsigned)
```

Sets the **bond expression** to be used for substructure initialization from a molecule fragment. Default: `OEExprOpts.DefaultBonds`

See also

- `OEExprOpts` namespace

SetFixDeleteH

```
bool SetFixDeleteH(const bool)
```

Sets whether **hydrogens should be stripped** from the fix molecule before it is used to match structures. Default: True

SetFixMaxMatch

```
bool SetFixMaxMatch(const unsigned int)
```

Sets the **maximum number of substructure search matches** to be used for constraining molecule fragments. Default: 1

SetFixMol

```
bool SetFixMol(const OEChem::OEMolBase&)
bool SetFixMol(OEChem::oemolistream& fstream)
```

Uses the 3D coordinates of the provided molecule to fix the corresponding substructure in the target molecule during conformer generation. For the second overload, only the first molecule from the input oemolistream is used.

SetFixMCS

```
bool SetFixMCS(const bool)
```

Sets flag to use **MCS** to fix a portion of the molecule during conformation search. If set to *true*, the maximum common substructure against the *FixMol* is used to define the portion of the molecule to be kept fixed. Default: False

SetFixPredicate

```
bool SetFixPredicate(const OESystem::OEUnaryPredicate<OEChem::OEAtomBase>&)
```

Uses the **atom predicate** to define which atoms should be kept fixed during conformation search.

SetFixRMS

```
bool SetFixRMS(const double)
```

Sets the **RMS distance** (Root Mean Square (RMS) Cartesian) below which two atom positions are treated as identical. Default: 0.15

SetFixSmarts

```
void SetFixSmarts(const std::string&)
```

Uses the SMARTS pattern to define which portion of the molecule should be kept fixed during conformational search.

SetFixSubSearch

```
bool SetFixSubSearch(const OEChem::OESubSearch value)
```

Uses the substructure search (OESubSearch) to define which portion of the molecule should be kept fixed during conformation search.

SetFixUniqueMatch

```
bool SetFixUniqueMatch(const bool)
```

Sets whether only the **unique** substructure matches should be used for coordinate replacement. Default: True

SetMCSMinAtoms

```
bool SetMCSMinAtoms(const unsigned)
```

Sets the **minimum number of atoms** required of a subgraph match to be used for MCS-based fixes. Default: 1

SetMCSFunc

```
bool SetMCSFunc(const OEChem::OEMCSFunc&)
```

Sets the **scoring function** to be used for subgraph matching for MCS-based fixes. Default: `OEMCSMaxBondsCompleteCycles`

SetMCSType

```
bool SetMCSType(const unsigned)
```

Sets the **MCS search type** to be used for subgraph matching for MCS-based fixes, defined in the `OEMCSType` namespace. Default: `OEMCSType.Exhaustive`

4.1.3 OEConformerBuilder

```
class OEConformerBuilder
```

This class defines an interface for generating 3D structures of small molecules. This class differs from *OEMolBuilder* in that it makes an effort to ensure that the generated conformer is clash free. However, this is faster than *OEOmega* for generating a single conformer, as this method does not search for the lowest energy conformer.

Code Examples

- *Generating a Single Conformer* example

The *OEConformerBuilder* class defines the following public methods:

- *Build*

Constructors

```
OEConformerBuilder()
OEConformerBuilder(const OEConformerBuilder&)
```

Default and copy constructors.

Build

```
unsigned Build(OEChem::OEMolBase&) const
unsigned Build(OEChem::OEMCMolBase&) const
```

Generates a 3D structure of a small molecule. Returns *OEOmegaReturnCode.Success* if the process succeeds, otherwise returns an error code from the *OEOmegaReturnCode* namespace.

4.1.4 OEConfSlicer

```
class OEConfSlicer
```

This class defines an interface for reducing the number of conformers in a molecule by detecting duplicates. This allows for *OEOmega* to generate a very large ensemble with much looser deduplication parameters and then to "slice" that ensemble of conformations by various different parameters after the fact.

See also

- *OESliceEnsembleOptions* class
- *OESliceEnsemble* method

The *OEConfSlicer* class defines the following public methods:

- *Slice*

Constructors

```
OEConfSlicer(const OESliceEnsembleOptions& opts = OESliceEnsembleOptions())
```

Constructor.

Slice

```
bool Slice(OEChem::OEMCMolBase&)
```

Slices the input molecule to remove duplicates.

4.1.5 OEFlipperClassicOptions

```
class OEFlipperClassicOptions : public OEFlipperOptions
```

Caution

This is a deprecated API.

This class was introduced to allow validation of previous **Flipper** results against the preferred updated flag options. It will be removed in a subsequent release.

See also

- *OEFlipperOptions* class
- *OEFlipper* function

The *OEFlipperClassicOptions* class defines the following public methods:

- *GetAtomPredicate* and *SetAtomPredicate*
- *GetBondPredicate* and *SetBondPredicate*
- *GetEnhancedStereo* and *SetEnhancedStereo*

- *GetEnumBridgehead* and *SetEnumBridgehead*
- *GetEnumEZ* and *SetEnumEZ*
- *GetEnumNitrogen* and *SetEnumNitrogen*
- *GetEnumRS* and *SetEnumRS*
- *GetEnumSpecifiedStereo* and *SetEnumSpecifiedStereo*
- *GetMaxCenters* and *SetMaxCenters*
- *GetWarts* and *SetWarts*

Constructors

```
OEFlipperClassicOptions()
OEFlipperClassicOptions(const OEFlipperClassicOptions &)
```

Default and copy constructors.

GetAtomPredicate

```
const OESystem::OEUnaryPredicate<OEChem::OEAtomBase>* GetAtomPredicate() const
```

See the *SetAtomPredicate* method.

GetBondPredicate

```
const OESystem::OEUnaryPredicate<OEChem::OEBondBase>* GetBondPredicate() const
```

See the *SetBondPredicate* method.

GetEnhancedStereo

```
bool GetEnhancedStereo() const
```

See the *SetEnhancedStereo* method.

GetEnumBridgehead

```
bool GetEnumBridgehead() const
```

See the *SetEnumBridgehead* method.

GetEnumEZ

```
bool GetEnumEZ() const
```

See the *SetEnumEZ* method.

GetEnumNitrogen

```
bool GetEnumNitrogen() const
```

See the *SetEnumNitrogen* method.

GetEnumRS

```
bool GetEnumRS() const
```

See the *SetEnumRS* method.

GetEnumSpecifiedStereo

```
bool GetEnumSpecifiedStereo() const
```

See the *SetEnumSpecifiedStereo* method.

GetMaxCenters

```
unsigned GetMaxCenters() const
```

See the *SetMaxCenters* method.

GetWarts

```
bool GetWarts() const
```

See the *SetWarts* method.

SetAtomPredicate

```
bool SetAtomPredicate(const OESystem::OEUnaryPredicate<OEChem::OEAtomBase>&)
```

Provides an input atom predicate to define the selection of the atom stereocenters which should be enumerated. For explicit user predicates, the bond predicate must also be provided explicitly. See the *SetBondPredicate* method.

SetBondPredicate

```
bool SetBondPredicate(const OESystem::OEUnaryPredicate<OEChem::OEBondBase>&)
```

Provides an input bond predicate to define the selection of the bond stereocenters which should be enumerated. For explicit user predicates, the atom predicate must also be provided explicitly. See the *SetAtomPredicate* method.

SetEnhancedStereo

```
bool SetEnhancedStereo(const bool)
```

Sets whether to consider explicit MDL enhanced stereogroups during flipping or not. Enhanced stereogroups generally contain a collection of stereocenters which should be considered as a collective unit, where a "flip" implies that all centers in the group should be flipped, thus retaining the relative stereo parity between the grouped stereocenters. With this flag enabled, far fewer enantiomers will be generated than for individual stereocenter flipping activities, and relative stereo configurations will be retained. When enabled, explicitly marked absolute stereocenters are excluded from the flipping activities. Default: False

Note

The membership and type of existing enhanced stereogroups are not modified as a result of the flipping operation. That is, the explicit stereogroups of `and` and `or` are not promoted to `abs` groups as a result of stereocenter parity

flips. This retains the source of original stereogroup(s) in the generated isomer(s) for post-flipping validations and processing. This behavior is true regardless of the setting of *GetEnhancedStereo*. Stereocenters can be explicitly promoted to `abs` centers by deletion of all stereogroups, or by deleting all stereogroups and adding marked stereocenters to a single new `abs` stereogroup.

See also

- `GetGroups` method
- `OEIsMDLStereoGroup` class

SetEnumBridgehead

```
bool SetEnumBridgehead(const bool)
```

Sets whether to enumerate bridgehead stereocenters or not. Default: False

SetEnumEZ

```
bool SetEnumEZ(const bool)
```

Sets whether to enumerate *only* E/Z stereocenters or not. If *true*, no atoms are enumerated. Default: False

SetEnumNitrogen

```
bool SetEnumNitrogen(const bool)
```

Controls the behavior with respect to enumeration of nonterminal nitrogens. Any nitrogen with pyramidal geometry in the initial model of the input molecule, and having no more than two ring bonds is considered to be *invertible*. This will enumerate all possible puckers if set to *true*. Default: False

SetEnumRS

```
bool SetEnumRS(const bool)
```

Sets whether to enumerate *only* R/S stereocenters or not. If *true*, no bonds are enumerated. Default: False

SetEnumSpecifiedStereo

```
bool SetEnumSpecifiedStereo(const bool)
```

Sets whether to force the modification of all stereocenters in a molecule. If *false*, it will only enumerate stereocenters which do not already have a specified stereochemistry. Default: False

SetMaxCenters

```
bool SetMaxCenters(const unsigned)
```

Sets the maximum number of stereocenters or groups of stereocenters which will be fully enumerated. Default: 12

SetWarts

```
bool SetWarts(const bool)
```

Sets whether to generate unique titles for molecules. Default: False

4.1.6 OEFlipperOptions

```
class OEFlipperOptions : public OESystem::OEOptions
```

See also

- *OEFlipper* function

Code Examples

- *Generating Stereoisomers* example

The *OEFlipperOptions* class defines the following public methods:

- *GetAtomPredicate* and *SetAtomPredicate*
- *GetBondPredicate* and *SetBondPredicate*
- *GetEnhancedStereo* and *SetEnhancedStereo*
- *GetEnumAtoms* and *SetEnumAtoms*
- *GetEnumAtomSpecifiedStereo* and *SetEnumAtomSpecifiedStereo*
- *GetEnumBonds* and *SetEnumBonds*
- *GetEnumBondSpecifiedStereo* and *SetEnumBondSpecifiedStereo*
- *GetEnumBridgehead* and *SetEnumBridgehead*
- *GetEnumEZ* and *SetEnumEZ*
- *GetEnumNitrogen* and *SetEnumNitrogen*
- *GetEnumRS* and *SetEnumRS*
- *GetEnumSpecifiedStereo* and *SetEnumSpecifiedStereo*
- *GetEnumRelativeAtomStereo* and *SetEnumRelativeAtomStereo*
- *GetMaxCenters* and *SetMaxCenters*
- *GetWarts* and *SetWarts*

Constructors

```
OEFlipperOptions()
OEFlipperOptions(const OEFlipperOptions &)
```

Default and copy constructors.

GetAtomPredicate

```
const OESystem::OEUnaryPredicate<OEChem::OEAtomBase>* GetAtomPredicate() const
```

See the *SetAtomPredicate* method.

GetBondPredicate

```
const OESystem::OEUnaryPredicate<OEChem::OEBondBase>* GetBondPredicate() const
```

See the *SetBondPredicate* method.

GetEnhancedStereo

```
bool GetEnhancedStereo() const
```

See the *SetEnhancedStereo* method.

GetEnumAtoms

```
bool GetEnumAtoms() const
```

See the *SetEnumAtoms* method.

GetEnumAtomSpecifiedStereo

```
bool GetEnumAtomSpecifiedStereo() const
```

See the *SetEnumAtomSpecifiedStereo* method.

GetEnumBonds

```
bool GetEnumBonds() const
```

See the *SetEnumBonds* method.

GetEnumBondSpecifiedStereo

```
bool GetEnumBondSpecifiedStereo() const
```

See the *SetEnumBondSpecifiedStereo* method.

GetEnumBridgehead

```
bool GetEnumBridgehead() const
```

See the *SetEnumBridgehead* method.

GetEnumEZ

```
bool GetEnumEZ() const
```

See the *SetEnumEZ* method.

GetEnumNitrogen

```
bool GetEnumNitrogen() const
```

See the *SetEnumNitrogen* method.

GetEnumRS

```
bool GetEnumRS() const
```

See the *SetEnumRS* method.

GetEnumRelativeAtomStereo

```
bool GetEnumRelativeAtomStereo() const
```

See the *SetEnumRelativeAtomStereo* method.

GetEnumSpecifiedStereo

```
bool GetEnumSpecifiedStereo() const
```

See the *SetEnumSpecifiedStereo* method.

GetMaxCenters

```
unsigned GetMaxCenters() const
```

See the *SetMaxCenters* method.

GetWarts

```
bool GetWarts() const
```

See the *SetWarts* method.

SetAtomPredicate

```
bool SetAtomPredicate(const OESystem::OEUnaryPredicate<OEChem::OEAtomBase>&)
```

Provides an input atom predicate to define the selection of the atom stereocenters which should be enumerated.

SetBondPredicate

```
bool SetBondPredicate(const OESystem::OEUnaryPredicate<OEChem::OEBondBase>&)
```

Provides an input bond predicate to define the selection of the bond stereocenters which should be enumerated.

SetEnhancedStereo

```
bool SetEnhancedStereo(const bool)
```

Sets whether to consider explicit MDL enhanced stereogroups during flipping. Enhanced stereogroups generally contain a collection of stereocenters which should be considered as a collective unit, where a "flip" implies that all centers in the group should be flipped, thus retaining the relative stereo parity between the grouped stereocenters. With this flag enabled, far fewer enantiomers will be generated than for individual stereocenter flipping activities, and relative stereo configurations will be retained. When enabled, explicitly marked absolute stereocenters are excluded from the flipping activities. Care should be taken to ensure that any custom atom predicate returns all atoms involved in enhanced stereogroups. Default: False

Note

The membership and type of existing enhanced stereogroups are not modified as a result of the flipping operation. That is, the explicit stereogroups of `and` and `or` are not promoted to `abs` groups as a result of stereocenter parity flips. This retains the source of original stereogroup(s) in the generated isomer(s) for post-flipping validations and processing. This behavior is *true* regardless of the setting of *GetEnhancedStereo*. Stereocenters can be explicitly promoted to `abs` centers by deletion of all stereogroups, or by deleting all stereogroups and adding marked stereocenters to a single new `abs` stereogroup.

See also

- `GetGroups` method
- `OEIsMDLStereoGroup` class

SetEnumAtoms

```
bool SetEnumAtoms(const bool)
```

Sets whether to include R/S stereocenters in the enumeration or not. If *false*, disregards atom enumerations. Default: True

SetEnumAtomSpecifiedStereo

```
bool SetEnumAtomSpecifiedStereo(const bool)
```

Sets whether to force the modification of all R/S stereocenters in a molecule. If *false*, it will only enumerate stereocenters which do not already have a specified stereochemistry. Default: False

SetEnumBonds

```
bool SetEnumBonds(const bool)
```

Sets whether to include E/Z bonds in the enumeration. If *false*, disregards bond enumerations. Default: True

SetEnumBondSpecifiedStereo

```
bool SetEnumBondSpecifiedStereo(const bool)
```

Sets whether to force the modification of all E/Z stereocenters in a molecule. If *false*, it will only enumerate bonds which do not already have a specified stereochemistry. Default: False

SetEnumBridgehead

```
bool SetEnumBridgehead(const bool)
```

Sets whether to enumerate bridgehead stereocenters. Default: False

SetEnumEZ

```
bool SetEnumEZ(const bool)
```

Sets whether to enumerate E/Z stereocenters. Default: True

SetEnumNitrogen

```
bool SetEnumNitrogen(const bool)
```

Controls the behavior with respect to the enumeration of nonterminal nitrogens. Any nitrogen with pyramidal geometry in the initial model of the input molecule, and having no more than two ring bonds, is considered to be *invertible*. This will enumerate all possible puckers if set to *true*. Default: False

SetEnumRS

```
bool SetEnumRS(const bool)
```

Sets whether to enumerate R/S stereocenters. Default: True

SetEnumRelativeAtomStereo

```
bool SetEnumRelativeAtomStereo(const bool)
```

Sets whether to include enumeration of internally perceived relative atom stereocenters (e.g., 1,4-disubstituted cyclohexanes) in a molecule. If *true*, consider relative stereocenters during stereo enumeration. Default: False

SetEnumSpecifiedStereo

```
bool SetEnumSpecifiedStereo(const bool)
```

Sets whether to force the modification of all of the atom and bond stereocenters in a molecule. If *false*, it will only enumerate stereocenters which do not already have a specified stereochemistry. Default: False

SetMaxCenters

```
bool SetMaxCenters(const unsigned)
```

Sets the maximum number of stereocenters or groups of stereocenters which will be fully enumerated. Default: 12

SetWarts

```
bool SetWarts(const bool)
```

Sets whether to generate unique titles for molecules. Default: False

4.1.7 OEFragBuilder

```
class OEFragBuilder
```

This class defines an interface for generating 3D structures of molecule fragments using a distance geometry based algorithm. A fragment is a building block that is used for initial 3D structure generation of molecules.

See also

- *OEFragBuilderOptions* class

The *OEFragBuilder* class defines the following public methods:

- *Build*
- *GetOptions* and *SetOptions*

Constructors

```
OEFragBuilder(const OEFragBuilderOptions& argOpts = OEFragBuilderOptions())
OEFragBuilder(const OEFragBuilder&)
```

Default and copy constructors.

Build

```
unsigned Build(OEChem::OEMCMolBase&) const
```

Generates 3D structures for a molecule fragment. Returns *OEOmegaReturnCode.Success* if the process succeeds, otherwise returns an error code from the *OEOmegaReturnCode* namespace.

GetOptions

```
const OEFragBuilderOptions& GetOptions() const
```

See the *SetOptions* method.

SetOptions

```
void SetOptions(OEFragBuilderOptions& argOpts)
```

Sets *options* for building the fragment structures. Default: *OEFragBuilderOptions* with *OEFragBuilderMode.Default* mode.

See also

- *OEFragBuilderOptions* class

4.1.8 OEFragBuilderOptions

```
class OEFragBuilderOptions : public OESystem::OEOptions
```

This class provides an interface to set up options required for generating fragment coordinates for different types of fragments. A fragment is a building block that is used for initial 3D structure generation of molecules.

See also

- *OEMolBuilderOptions* class
- *OEFragOptions* class
- *OERingFragOptions* class

Code Examples

- *Making a Fragment Library* example

The *OEFragBuilderOptions* class defines the following public methods:

- *GetForceField* and *SetForceField*
- *GetMacroCycOptions* and *SetMacroCycOptions*
- *GetNonRingOptions* and *SetNonRingOptions*
- *GetRingOptions* and *SetRingOptions*

Constructors

```
OEFragBuilderOptions(const unsigned int mode = OEFragBuilderMode::Default)
```

The *mode* parameter defines the fragment build modes from the *OEFragBuilderMode* namespace. Default: *OEFragBuilderMode.Default*

See also

- *OEFragBuilderMode* namespace

```
OEFragBuilderOptions(const OEFragBuilderOptions &)
```

Copy constructor.

GetForceField

```
unsigned GetForceFieldType() const
```

See the *SetForceField* method.

GetMacroCycOptions

```
OEFragOptions& GetMacroCycOptions()
const OEFragOptions& GetMacroCycOptions() const
```

See the *SetMacroCycOptions* method.

GetNonRingOptions

```
OEFragOptions& GetNonRingOptions()
const OEFragOptions& GetNonRingOptions() const
```

See the *SetNonRingOptions* method.

GetRingOptions

```
OERingFragOptions& GetRingOptions()
const OERingFragOptions& GetRingOptions() const
```

See the *SetRingOptions* method.

SetForceField

```
bool SetForceField(const unsigned)
bool SetForceField(const std::string&)
```

Sets the **force field** used for torsion driving. The first overload takes an *unsigned* from the `OEMMFFSheffieldFFType` namespace, and the second overload takes corresponding string values. Method returns *false* when the invalid selection is chosen, *true* otherwise. Default: `OEMMFFSheffieldFFType.MMFF_NOESTAT`

SetMacroCycOptions

```
void SetMacroCycOptions(const OEFragOptions&)
```

Sets *options* related to building macrocycle fragments.

See also

- *OEFragOptions* class

SetNonRingOptions

```
void SetNonRingOptions(const OEFragOptions&)
```

Sets *options* related to building general fragments that are not rings.

See also

- *OEFragOptions* class

SetRingOptions

```
void SetRingOptions(const OERingFragOptions&)
```

Sets *options* related to building ring fragments.

See also

- *OERingFragOptions* class

4.1.9 OEFragOptions

```
class OEFragOptions
```

This class provides an interface to setup options required for generating fragment coordinates for a specific type of fragment. A fragment is a building block that is used for initial 3D structure generation of molecules.

See also

- *OEFragBuilderOptions* class

The *OEFragOptions* class defines the following public methods:

- *GetEnergyWindow* and *SetEnergyWindow*
- *GetFragGen* and *SetFragGen*
- *GetFragKeep* and *SetFragKeep*
- *GetRMS* and *SetRMS*
- *GetTimeLimit* and *SetTimeLimit*

Constructors

```
OEFragOptions()
OEFragOptions(const OEFragOptions &)
```

Default and copy constructors.

GetEnergyWindow

```
double GetEnergyWindow() const
```

See the *SetEnergyWindow* method.

GetFragGen

```
unsigned int GetFragGen() const
```

See the *SetFragGen* method.

GetFragKeep

```
unsigned int GetFragKeep() const
```

See the *SetFragKeep* method.

GetRMS

```
double GetRMS() const
```

See the *SetRMS* method.

GetTimeLimit

```
double GetTimeLimit() const
```

See the *SetTimeLimit* method.

SetEnergyWindow

```
bool SetEnergyWindow(const double)
```

Sets the **maximum allowable energy difference** between the lowest and the highest energy fragment conformers, in units of kcal/mol. Default: 8.0 kcal/mol

SetFragGen

```
bool SetFragGen(const unsigned int)
```

Sets the **maximum number of fragment conformers** to generate in obtaining the ensemble of fragment conformers. Default: 40

SetFragKeep

```
bool SetFragKeep(const unsigned int)
```

Sets the **maximum number of fragments** to keep from the generated ensemble. Default: 1

SetRMS

```
bool SetRMS(const double)
```

Sets the **RMS distance** (Root Mean Square Cartesian distance) below which two conformers are treated as duplicates. Default: 0.1

SetTimeLimit

```
bool SetTimeLimit(const double)
```

Sets the **maximum allowable time** for generating conformers of a fragment, in units of seconds. Default: 300.0 s

4.1.10 OEMacrocycleBuilder

```
class OEMacrocycleBuilder
```

This class defines an interface for generating 3D structures of macrocyclic molecules. Macrocycle structures are generated by first creating an initial structure using distance geometry, followed by a force field based refinement of the structure.

See also

- *OEMacrocycleBuilderOptions* class

Code Examples

- *Generating a Single Macrocycle Conformer* example

The *OEMacrocycleBuilder* class defines the following public methods:

- *Build*
- *GetOptions* and *SetOptions*

Constructors

```
OEMacrocycleBuilder(const OEMacrocycleBuilderOptions& argOpts =␣
↪OEMacrocycleBuilderOptions())
OEMacrocycleBuilder(const OEMacrocycleBuilder&)
```

Default and copy constructors.

Build

```
unsigned Build(OEChem::OEMolBase&) const
unsigned Build(OEChem::OEMCMolBase&) const
```

Generates a 3D structure for a macrocycle molecule. Returns *OEOmegaReturnCode.Success* if the process succeeds, otherwise returns an error code from the *OEOmegaReturnCode* namespace.

GetOptions

```
const OEMacrocycleBuilderOptions& GetOptions() const
```

See the *SetOptions* method.

SetOptions

```
void SetOptions(OEMacrocycleBuilderOptions& argOpts)
```

Sets *options* for building the molecule 3D structures.

See also

- *OEMacrocycleBuilderOptions* class

4.1.11 OEMacrocycleBuilderOptions

```
class OEMacrocycleBuilderOptions : public OESystem::OEOptions
```

This class provides an interface to set up options required for generating 3D structures of macrocycle molecules.

See also

- *OEMacrocycleOmegaOptions* class
- *OEMacrocycleBuilder* class

Code Examples

- *Generating a Single Macrocycle Conformer* example

The *OEMacrocycleBuilderOptions* class defines the following public methods:

- *GetDielectricConst* and *SetDielectricConst*
- *GetRandomSeed* and *SetRandomSeed*
- *GetRefTolerance* and *SetRefTolerance*
- *GetSkipRefinement* and *SetSkipRefinement*

Constructors

```
OEMacrocycleBuilderOptions()
OEMacrocycleBuilderOptions(const OEMacrocycleBuilderOptions &)
```

Default and copy constructors.

GetDielectricConst

```
double GetDielectricConst() const
```

See the *SetDielectricConst* method.

GetRandomSeed

```
unsigned GetRandomSeed() const
```

See the *SetRandomSeed* method.

GetRefTolerance

```
double GetRefTolerance() const
```

See the *SetRefTolerance* method.

GetSkipRefinement

```
bool GetSkipRefinement() const
```

See the *SetSkipRefinement* method.

SetDielectricConst

```
bool SetDielectricConst(const double)
```

Sets the **dielectric constant of the solvent** to be used in the refinement stage. Default: 80.0

SetRandomSeed

```
bool SetRandomSeed(const unsigned)
```

Sets the **random seed** for initial structure generation. Default: 0

SetRefTolerance

```
bool SetRefTolerance(const double)
```

Sets the **tolerance criteria** for the optimizer during refinement. Default: 0.001

SetSkipRefinement

```
bool SetSkipRefinement(const bool)
```

Sets whether **refinement** of the generated initial structure should be **performed or skipped**. If true, refinement is skipped. Default: False

4.1.12 OEMacrocycleOmega

```
class OEMacrocycleOmega
```

This class defines an interface for generating ensembles of conformers of macrocycle molecules.

See also

- *OEMacrocycleOmegaOptions* class
- *OEMacrocycleBuilder* class

Code Examples

- *Generating Macrocycle Conformers* example

The *OEMacrocycleOmega* class defines the following public methods:

- *Build*
- *GetOptions* and *SetOptions*

Constructors

```
OEMacrocycleOmega(const OEMacrocycleOmegaOptions& argOpts = OEMacrocycleOmegaOptions())
OEMacrocycleOmega(const OEMacrocycleOmega&)
```

Default and copy constructors.

Build

```
unsigned Build(OEChem::OEMCMolBase&) const
```

Generates conformer ensemble for a macrocyclic molecule. Returns *OEOmegaReturnCode.Success* if the process succeeds, otherwise returns an error code from the *OEOmegaReturnCode* namespace.

GetOptions

```
const OEMacrocycleOmegaOptions& GetOptions() const
```

See the *SetOptions* method.

SetOptions

```
void SetOptions(OEMacrocycleOmegaOptions& argOpts)
```

Sets the *options* for generating a conformer ensemble.

See also

- *OEMacrocycleOmegaOptions* class

4.1.13 OEMacrocycleOmegaOptions

```
class OEMacrocycleOmegaOptions : public OESystem::OEOptions
```

This class provides an interface to set up options required for generating an ensemble of macrocycle molecule conformers.

See also

- *OEMacrocycleOmega* class
- *OESliceEnsembleOptions* class
- *OEMacrocycleBuilderOptions* class

Code Examples

- *Generating Macrocycle Conformers* example

The *OEMacrocycleOmegaOptions* class defines the following public methods:

- *GetEnergyWindow* and *SetEnergyWindow*
- *GetIterCycleSize* and *SetIterCycleSize*
- *GetMacrocycleBuilderOptions* and *SetMacrocycleBuilderOptions*
- *GetMaxConfs* and *SetMaxConfs*
- *GetMaxIter* and *SetMaxIter*
- *GetSliceEnsembleOptions* and *SetSliceEnsembleOptions*

Constructors

```
OEMacrocycleOmegaOptions()
OEMacrocycleOmegaOptions(const OEMacrocycleOmegaOptions &)
```

Default and copy constructors.

GetEnergyWindow

```
double GetEnergyWindow() const
```

See the *SetEnergyWindow* method.

GetIterCycleSize

```
unsigned int GetIterCycleSize() const
```

See the *SetIterCycleSize* method.

GetMacrocycleBuilderOptions

```
OEMacrocycleBuilderOptions& GetMacrocycleBuilderOptions()
const OEMacrocycleBuilderOptions& GetMacrocycleBuilderOptions() const
```

See the *SetMacrocycleBuilderOptions* method.

GetMaxConfs

```
unsigned GetMaxConfs() const
```

See the *SetMaxConfs* method.

GetMaxIter

```
unsigned int GetMaxIter() const
```

See the *SetMaxIter* method.

GetSliceEnsembleOptions

```
OESliceEnsembleOptions& GetSliceEnsembleOptions()
const OESliceEnsembleOptions& GetSliceEnsembleOptions() const
```

See *SetSliceEnsembleOptions* method.

SetEnergyWindow

```
bool SetEnergyWindow(const double)
```

See the *SetEnergyWindow* method. Default: 20

SetIterCycleSize

```
bool SetIterCycleSize(const unsigned int)
```

Sets the **number of new conformers** that are to be attempted before checking if a new minimum was found. Conformer generation finishes if no new minimum is found during an iteration cycle. Default: 100

SetMacrocycleBuilderOptions

```
void SetMacrocycleBuilderOptions(const OEMacrocycleBuilderOptions&)
```

Sets the *options* that are to be used for generating new conformers.

See also

- *OEMacrocycleBuilderOptions* class

SetMaxConfs

```
bool SetMaxConfs(const unsigned)
```

See the *SetMaxConfs* method. Default: 400

SetMaxIter

```
bool SetMaxIter(const unsigned int)
```

Sets the **maximum number of iteration cycles** are to be attempted. If the desired number of unique conformers are already generated in the ensemble, conformer generation will terminate before reaching this number. Default: 2000

SetSliceEnsembleOptions

```
void SetSliceEnsembleOptions(const OESliceEnsembleOptions&)
```

Sets the *options* that are to be used for removing duplicate conformers during macrocycle conformer ensemble generation.

See also

- *OESliceEnsembleOptions* class

4.1.14 OEMakeFragLib

```
class OEMakeFragLib : public OEBuilderBase
```

This class defines an interface for generating a fragment library. The builder allows building either a partial or a complete fragment library by controlling the content of the fragment library currently loaded in the builder.

Code Examples

- *Making a Fragment Library* example

The following methods are publicly inherited from *OEBuilderBase*:

- *AddFragLib*
- *ClearFragLibs*

The *OEMakeFragLib* class defines the following public methods:

- *AddFrag*
- *GenerateMissingFrags*
- *GetMissingFrags*

Constructors

```
OEMakeFragLib(const OEFragBuilderOptions& argOpts =␣
↪OEFragBuilderOptions(OEFragBuilderMode::Strict))
OEMakeFragLib(const OEMakeFragLib&)
```

Default and copy constructors. The default constructor instantiates the class with *OEFragBuilderOptions* with the *OEFragBuilderMode.Strict* mode.

AddFrag

```
void AddFrag(const OEChem::OEMCMolBase&)
```

Adds the specified **fragment** to the currently loaded fragment library.

See also

- *AddFragLib* method.

GenerateMissingFrags

```
void GenerateMissingFrags(OEChem::oemolistream& ,
                          OEChem::oemolostream&) const
void GenerateMissingFrags(const OEChem::OEMolBase&,
                          OEChem::oemolostream&) const
```

Finds the missing fragments corresponding to the given input file stream or molecule, generates 3D structures of the fragments, and adds those to the output file stream.

GetMissingFrags

```
OESystem::OEIterBase<OEChem::OEMCMolBase>* GetMissingFrags(OEChem::oemolistream&) const
OESystem::OEIterBase<OEChem::OEMCMolBase>* GetMissingFrags(const OEChem::OEMolBase&)␣
↪const
```

Finds the missing fragments corresponding to the given input file stream or molecule and returns a collection of the fragments. This method does not generate 3D structures of the fragments.

4.1.15 OEMolBuilder

```
class OEMolBuilder : public OEBuilderBase
```

This class defines an interface for generating an initial 3D structure of a molecule by connecting pregenerated fragment coordinates that constitute the molecule. Building the 3D structure of a molecule with this builder is fast when all the fragments constituting a molecule are available in the fragment library associated with the builder. This builder makes no effort to obtain a low energy conformer of the molecule.

See also

- *OEMolBuilderOptions* class
- *OEConfFixOptions* class

The following methods are publicly inherited from *OEBuilderBase*:

- *AddFragLib*
- *ClearFragLibs*

The *OEMolBuilder* class defines the following public methods:

- *Build*
- *GetOptions* and *SetOptions*
- *Prep*

Constructors

```
OEMolBuilder(const OEMolBuilderOptions& argOpts = OEMolBuilderOptions())
OEMolBuilder(const OEMolBuilder&)
```

Default and copy constructors.

Build

```
unsigned Build(OEChem::OEMCMolBase&,
               const OEConfFixOptions& fixOpts = OEConfFixOptions()) const
```

Generates a 3D structure for a molecule. Returns *OEOmegaReturnCode.Success* if the process succeeds, otherwise returns an error code from the *OEOmegaReturnCode* namespace. The second argument provided with appropriate options can be used to fix part of a molecule structure to predefined coordinates.

See also

- *OEConfFixOptions* class

GetOptions

```
const OEMolBuilderOptions& GetOptions() const
```

See the *SetOptions* method.

Prep

```
unsigned Prep(OEChem::OEMCMolBase& mol) const
```

Prepares molecules for 3D structure generation. Returns *OEOmegaReturnCode.Success* if the process succeeds, otherwise returns an error code from the *OEOmegaReturnCode* namespace.

A call to the *OEMolBuilder.Prep* is not required before calling *OEMolBuilder.Build*; however, it is useful in determining if some of the pre-conditions are met for building.

SetOptions

```
void SetOptions(const OEMolBuilderOptions&)
```

Sets *options* for building the molecule's 3D structures.

See also

- *OEMolBuilderOptions* class

4.1.16 OEMolBuilderOptions

```
class OEMolBuilderOptions : public OESystem::OEOptions
```

This class provides an interface to set up options required for generating an initial 3D structure of a molecule by connecting pregenerated fragment coordinates that constitute the molecule.

See also

- *OEMolBuilder* class
- *OEFragBuilderOptions* class

The *OEMolBuilderOptions* class defines the following public methods:

- *GetCanonOrder* and *SetCanonOrder*
- *GetEnumNitrogen* and *SetEnumNitrogen*
- *GetEnumRing* and *SetEnumRing*
- *SetFragBuilderMode*
- *GetFragBuilderOptions* and *SetFragBuilderOptions*
- *GetFromCT* and *SetFromCT*
- *GetIgnoreStereo* and *SetIgnoreStereo*
- *GetMaxEnumConfs* and *SetMaxEnumConfs*
- *GetSampleHydrogens* and *SetSampleHydrogens*
- *GetStrictAtomTypes* and *SetStrictAtomTypes*

Constructors

```
OEMolBuilderOptions()
OEMolBuilderOptions(const OEMolBuilderOptions &)
```

Default and copy constructors.

GetCanonOrder

```
bool GetCanonOrder() const
```

See the *SetCanonOrder* method.

GetEnumNitrogen

```
unsigned int GetEnumNitrogen() const
```

See the *SetEnumNitrogen* method.

GetEnumRing

```
bool GetEnumRing() const
```

See the *SetEnumRing* method.

GetFragBuilderOptions

```
OEFragBuilderOptions& GetFragBuilderOptions()
const OEFragBuilderOptions& GetFragBuilderOptions() const
```

See the *SetFragBuilderOptions* method.

GetFromCT

```
bool GetFromCT() const
```

See the *SetFromCT* method.

GetIgnoreStereo

```
bool GetIgnoreStereo() const
```

See the *SetIgnoreStereo* method.

GetMaxEnumConfs

```
unsigned GetMaxEnumConfs() const
```

See the *SetMaxEnumConfs* method.

GetSampleHydrogens

```
bool GetSampleHydrogens() const
```

See the *SetSampleHydrogens* method.

GetStrictAtomTypes

```
bool GetStrictAtomTypes() const
```

See the *SetStrictAtomTypes* method.

SetCanonOrder

```
bool SetCanonOrder(const bool)
```

This method can be used to enable/disable the automatic reordering of input molecules to a canonical atom and bond order. In order to obtain consistent results from different file formats and different connection table orders, **OMEGA** reorders the input connection table. If *true*, the atoms of the molecule are indexed in canonical order before building the molecule structure. Default: True

SetEnumNitrogen

```
bool SetEnumNitrogen(const unsigned int)
```

Sets whether the generated initial conformation should be **enumerated for invertible nitrogens**. Default: *OENitrogenEnumeration.Unspecified*

See also

- *OENitrogenEnumeration* namespace

SetEnumRing

```
bool SetEnumRing(const bool)
```

Sets whether the generated initial conformation should be **enumerated for ring stereo**. If *true*, the builder will enumerate alternate ring conformations and generate multiple conformations, if available. Default: True

SetFragBuilderMode

```
bool SetFragBuilderMode(const unsigned mode)
```

Sets the *OEFragBuilderOptions* parameter defaults corresponding to the specified `mode`.

SetFragBuilderOptions

```
void SetFragBuilderOptions(const OEFragBuilderOptions&)
```

Sets *OEFragBuilderOptions* related to building fragment coordinates.

See also

- *OEFragBuilderOptions* class

SetFromCT

```
bool SetFromCT(const bool)
```

Sets whether the initial 3D coordinates should be generated from the **connection table of the input molecule**. If *true*, the initial 3D coordinates are generated from the connection table. Default: True

SetIgnoreStereo

```
bool SetIgnoreStereo(const bool)
```

Sets whether **conformer generation should continue** even when specified stereo signatures in a molecule could not be honored. Default: False

SetMaxEnumConfs

```
bool SetMaxEnumConfs(const unsigned)
```

Sets the **maximum number of conformers** to be generated during enumeration. Default: 1024

SetSampleHydrogens

```
bool SetSampleHydrogens(const bool)
```

Sets whether **hydrogen sampling** should be performed on generated structures. If *true*, hydrogen sampling is performed. Default: False

SetStrictAtomTypes

```
bool SetStrictAtomTypes(const bool)
```

Sets whether **strict definition of atom typing** should be used. If *true*, a molecule will fail if any atom does not have a valid atom type. Calling this method with *false* will allow the atom typer to look for a different atom type of the same element and replace the failing atom type with a valid one that is "close enough." Default: True

4.1.17 OEOmega

```
class OEOmega
```

This class defines an interface for generating ensembles of conformers of small molecules.

See also

- *OEOmegaOptions* class

Code Examples

- *Generating Conformers* example
- *Generating Densely Sampled Conformers* example
- *Generating Stereoisomers* example

Constructors

```
OEOmega( OEPlatform::oeistream* torlib = 0 );
OEOmega(const OEOmegaOptions&)
OEOmega(const OEOmega&)
```

Default and copy constructors.

AddFragLib

```
void AddFragLib()
void AddFragLib(const std::string &)
void AddFragLib(OEPlatform::oeistream &)
```

The parameterless version will load the built-in fragment library immediately. By default, the built-in fragment library does not load until *OEOmega.Build* is called for the first time.

The *string* and *oeistream* versions will add an external fragment library. This will be used in addition to the built-in fragment library. To use only this fragment library, call *OEOmega.ClearFragLibs* first.

Note

An enhanced fragment library, `omega_fragment_lib_2020.oeb.gz`, that improves the performance of conformer generation is available on request from the database downloads page.

Build

```
unsigned Build(OEChem::OEMCMolBase&) const
```

Generates conformers for a molecule. Returns *OEOmegaReturnCode.Success* if the process succeeds, otherwise returns an error code from the *OEOmegaReturnCode* namespace.

ClearFragLibs

```
void ClearFragLibs()
```

Clears all fragment libraries from the *OEOmega* object.

GetOptions

```
const OEOmegaOptions& GetOptions() const
```

Retrieves a constant reference to the *OEOmegaOptions* instance as currently set.

SetOptions

```
void SetOptions(const OEOmegaOptions&)
```

Sets the structure generation options by passing in an *OEOmegaOptions* instance.

4.1.18 OEOmegaOptions

```
class OEOmegaOptions : public OESystem::OEOptions
```

See also

- *OEOmega* class

Code Examples

- *Generating Conformers* example
- *Generating Densely Sampled Conformers* example
- *Generating Stereoisomers* example

There is a *list of suboption default values* later in this section.

The *OEOmegaOptions* class defines the following public methods:

- *GetConfFixOptions* and *SetConfFixOptions*
- *GetEnergyWindow* and *SetEnergyWindow*
- *GetIncludeInput* and *SetIncludeInput*
- *GetMaxConfs* and *SetMaxConfs*
- *GetMolBuilderOptions* and *SetMolBuilderOptions*
- *GetSliceEnsembleOptions* and *SetSliceEnsembleOptions*
- *GetStrictStereo* and *SetStrictStereo*
- *GetTorDriveOptions* and *SetTorDriveOptions*
- *GetTorsionDrive* and *SetTorsionDrive*
- *GetWarts* and *SetWarts*

Constructors

```
OEOmegaOptions(const unsigned int sampling = OEOmegaSampling::Classic)
OEOmegaOptions(const OEOmegaOptions &)
```

Default and copy constructors.

GetConfFixOptions

```
OEConfFixOptions& GetConfFixOptions()
const OEConfFixOptions& GetConfFixOptions() const
```

See the *SetConfFixOptions* method.

GetEnergyWindow

```
double GetEnergyWindow() const
```

See the *SetEnergyWindow* method.

GetIncludeInput

```
bool GetIncludeInput() const
```

See the *SetIncludeInput* method.

GetMaxConfs

```
unsigned GetMaxConfs() const
```

See the *SetMaxConfs* method.

GetMolBuilderOptions

```
OEMolBuilderOptions& GetMolBuilderOptions()
const OEMolBuilderOptions& GetMolBuilderOptions() const
```

See the *SetMolBuilderOptions* method.

GetSliceEnsembleOptions

```
OESliceEnsembleOptions& GetSliceEnsembleOptions()
const OESliceEnsembleOptions& GetSliceEnsembleOptions() const
```

See the *SetSliceEnsembleOptions* method.

GetStrictStereo

```
bool GetStrictStereo() const
```

See the *SetStrictStereo* method.

GetTorDriveOptions

```
OETorDriveOptions& GetTorDriveOptions()
const OETorDriveOptions& GetTorDriveOptions() const
```

See the *SetTorDriveOptions* method.

GetTorsionDrive

```
bool GetTorsionDrive() const
```

See the *SetTorsionDrive* method.

GetWarts

```
bool GetWarts() const
```

See the *SetWarts* method.

SetConfFixOptions

```
void SetConfFixOptions(const OEConfFixOptions&)
```

Sets *options* related to partially fixing conformers.

See also

- *OEConfFixOptions* class

SetEnergyWindow

```
bool SetEnergyWindow(const double)
```

See the *SetEnergyWindow* method. Default: 10

SetIncludeInput

```
bool SetIncludeInput(const bool)
```

Sets whether to pass the unmodified input structure into output conformer ensembles. If *true*, the input conformers are appended at the beginning of the generated conformer ensemble. Default: False

SetMaxConfs

```
bool SetMaxConfs(const unsigned)
```

See the *SetMaxConfs* method. Default: 200

SetMolBuilderOptions

```
void SetMolBuilderOptions(const OEMolBuilderOptions&)
```

Sets *options* related to generating initial conformers.

See also

- *OEMolBuilderOptions* class

SetSliceEnsembleOptions

```
void SetSliceEnsembleOptions(const OESliceEnsembleOptions&)
```

Sets *options* related to deduplicating generated ensembles.

See also

- *OESliceEnsembleOptions* class

SetStrictStereo

```
bool SetStrictStereo(const bool)
```

Sets whether conformer generation should fail if **stereo is not specified** on the input molecules. Default: True

SetTorDriveOptions

```
void SetTorDriveOptions(const OETorDriveOptions&)
```

Sets *options* related to torsion driving for conformer generation.

See also

- *OETorDriveOptions* class

SetTorsionDrive

```
bool SetTorsionDrive(const bool)
```

Sets whether to perform torsion driving. Default: True

SetWarts

```
bool SetWarts(const bool)
```

Sets whether to generate unique titles for conformers. Default: False

4.1.19 Suboption Parameter Defaults

Default values of the parameters from the suboption classes are compiled below.

parameter	Default
CanonOrder	True
EnumNitrogen	*OENitrogenEnumeration.Unspecified*
EnumRing	True
FromCT	True
IgnoreStereo	False
MaxEnumConfs	1024
SampleHydrogens	False
StrictAtomTypes	True
MaxTerminalHeavy	0
RangeIncrement	5
RMSThreshold	0.5
CommentEnergy	False
ForceField	OEMMFFSheffieldFFType.MMFF94Smod_NOESTAT
MaxRotors	9999
MaxSearchTime	120.0 sec
RotorOffset	False
SDEnergy	False
UseGPU	True

4.1.20 OERingFragOptions

```
class OERingFragOptions : public OEFragOptions
```

This class provides an interface to set up options required for generating coordinates for ring fragments. A fragment is a building block that is used for initial 3D structure generation of molecules.

See also

- *OEFragBuilderOptions* class

The following methods are publicly inherited from *OEFragOptions*:

- *GetEnergyWindow* and *SetEnergyWindow*
- *GetFragGen* and *SetFragGen*
- *GetFragKeep* and *SetFragKeep*
- *GetRMS* and *SetRMS*
- *GetTimeLimit* and *SetTimeLimit*

The *OERingFragOptions* class defines the following public methods:

- *GetStartFactor* and *SetStartFactor*

Constructors

```
OERingFragOptions()
OERingFragOptions(const OERingFragOptions &)
```

Default and copy constructors.

GetStartFactor

```
unsigned GetStartFactor() const
```

See the *SetStartFactor* method.

SetStartFactor

```
bool SetStartFactor(const unsigned)
```

Sets a **multiplicative factor** that determines how many starts are to be used for generating ring fragment coordinates. Default: 2

4.1.21 OESliceEnsembleOptions

```
class OESliceEnsembleOptions : public OESystem::OEOptions
```

This class provides an interface to set up options required for reducing a molecule conformer ensemble by removing duplicates and high energy conformers.

The *OESliceEnsembleOptions* allows multiple ways to set up the desired settings for each parameter for slicing an ensemble. There are three main control parameters: *EnergyWindow*, *RMSThreshold*, and *MaxConfs*. The default usage is to use the same control settings for slicing all molecule ensembles. However, for each of the three parameters, the parameter settings can be made a variable based on the number of rotatable bonds in the molecule. The variable settings can be applied by using the *range* based API points.

This describes how to use the range based settings for *MaxConfs*, however, the same applies to *EnergyWindow* and *RMSThreshold*. A *MaxConfs* setting of *100,200,300* for *SetMaxConfRange* along with a value of *5* for the *RangeIncrement* set with *SetRangeIncrement* would use a *MaxConfs* value of *100* for a molecule with a number of rotatable bonds between 0 and 4, that of *200* for a molecule with a number of rotatable bonds between 5 and 9, and *300* for a molecule with a number of rotatable bonds of 10 or higher.

See also

- *OETorDriver* class

The *OESliceEnsembleOptions* class defines the following public methods:

- *GetEnergyWindow* and *SetEnergyWindow*
- *GetEnergyRange* and *SetEnergyRange*
- *GetMaxConfs* and *SetMaxConfs*
- *GetMaxConfRange* and *SetMaxConfRange*
- *GetMaxTerminalHeavy* and *SetMaxTerminalHeavy*
- *GetOverlayRMS* and *SetOverlayRMS*
- *GetRangeIncrement* and *SetRangeIncrement*
- *GetRMSThreshold* and *SetRMSThreshold*
- *GetRMSRange* and *SetRMSRange*

Constructors

```
OESliceEnsembleOptions()
OESliceEnsembleOptions(const OESliceEnsembleOptions &)
```

Default and copy constructors.

GetEnergyWindow

```
double GetEnergyWindow() const
double GetEneWindow(const unsigned numRotors) const
```

See the *SetEnergyWindow* method. The second variation of the method returns the value of the energy window that is in effect for a given molecule with a specified number of rotors.

GetEnergyRange

```
std::vector<double> GetEnergyRange() const
```

See the *SetEnergyRange* method.

GetMaxConfs

```
unsigned GetMaxConfs() const
unsigned GetMaxConfs(const unsigned numRotors) const
```

See the *SetMaxConfs* method. The second variation of the method returns the value of the maximum conformers that is in effect for a given molecule with a specified number of rotors.

GetMaxConfRange

```
std::vector<unsigned int> GetMaxConfRange() const
```

See the *SetMaxConfRange* method.

GetMaxTerminalHeavy

```
unsigned GetMaxTerminalHeavy() const
```

See the *SetMaxConfRange* method.

GetOverlayRMS

```
bool GetOverlayRMS() const
```

See the *SetOverlayRMS* method.

GetRangeIncrement

```
unsigned int GetRangeIncrement() const
```

See the *SetRangeIncrement* method.

GetRMSThreshold

```
double GetRMSThreshold() const
double GetRMSCutoff(const unsigned numRotors) const
```

See the *SetRMSThreshold* method. The second variation of the method returns the value of RMS threshold that is in effect for a given molecule with the specified number of rotors.

GetRMSRange

```
std::vector<double> GetRMSRange() const
```

See the *SetRMSRange* method.

SetEnergyWindow

```
void SetEnergyWindow(const double)
```

Sets the **maximum allowable energy** difference between the lowest and the highest energy conformers, in units of kcal/mol. Default: 10.0 kcal/mol

SetEnergyRange

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

Sets the **energy range** defines a varying *EnergyWindow* energy window in conjunction with the *RangeIncrement*. Defining the range overrides the singly defined energy window value. The string version of the overload expects a comma-separated string.

SetMaxConfs

```
void SetMaxConfs(const unsigned int)
```

Sets the **maximum number of conformers** to be included in the output ensemble for each molecule. For molecules with few conformational degrees of freedom, the number of output conformers might be lower than the value set for this flag but will never exceed it. Default: 200

SetMaxConfRange

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

Sets the **maximum number of conformers range** that defines a varying number of *MaxConfs* in conjunction with the *RangeIncrement*. Defining the range overrides the singly defined *MaxConfs* value. The string version of the overload expects a comma-separated string.

SetMaxTerminalHeavy

```
bool SetMaxTerminalHeavy(const unsigned int)
```

Sets the **maximum number of terminal heavy atoms** that should be allowed in calculating *RMSD* between conformers. If the number of terminal heavy atoms in the molecule exceeds the specified limit, all terminal heavy atoms are ignored in the *RMSD* calculation. If the number is set to *0*, this value is treated as not set. Default: 0

SetOverlayRMS

```
bool SetOverlayRMS(const bool)
```

Sets flag indicating if **overlay should be performed for RMSD calculation** between conformers. Default: True

SetRangeIncrement

```
bool SetRangeIncrement(const unsigned)
```

Sets the **number of rotatable bonds range** to be used when the *OESliceEnsembleOptions.SetEnergyRange*, *OESliceEnsembleOptions.SetRMSRange*, and *OESliceEnsembleOptions.SetMaxConfRange* are defined in terms of ranges. Default: 5

SetRMSRange

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

Sets the **RMS range** that allows to define a varying *RMSThreshold* in conjunction with the *RangeIncrement*. Defining the range overrides the singly defined RMS threshold value. The string version of the overload expects a comma-separated string.

SetRMSThreshold

```
bool SetRMSThreshold(const double)
```

Sets the **RMS threshold** (Root Mean Square Cartesian distance) below which two conformers are treated as duplicates. Default: 0.5

4.1.22 OETorDriveOptions

```
class OETorDriveOptions : public OESystem::OEOptions
```

This class provides an interface to set up options required for generating an ensemble of molecule conformers by torsion driving from an initial 3D structure of a molecule.

See also

- *OETorDriver* class
- *OETorLib* class

Code Examples

- *Generating Conformer Ensembles Using Torsion Driving* example

The *OETorDriveOptions* class defines the following public methods:

- *ExceedsMaxRotors*
- *GetCommentEnergy* and *SetCommentEnergy*
- *GetForceField* and *SetForceField*

- *GetMaxRotors* and *SetMaxRotors*
- *GetMaxSearchTime* and *SetMaxSearchTime*
- *GetRotorOffset* and *SetRotorOffset*
- *GetRotorPredicate* and *SetRotorPredicate*
- *GetSDEnergy* and *SetSDEnergy*
- GetThompsonOptions and SetThompsonOptions
- *GetTorLib* and *SetTorLib*
- *GetUseGPU* and *SetUseGPU*
- *GetUseThompson* and *SetUseThompson*

Constructors

```
OETorDriveOptions()
OETorDriveOptions(const OETorDriveOptions &)
```

Default and copy constructors.

ExceedsMaxRotors

```
bool ExceedsMaxRotors(const OEChem::OEMolBase&) const
```

This method checks if the number of rotors in the molecule is within the currently specified limit. See the *SetMaxRotors* method.

GetCommentEnergy

```
bool GetCommentEnergy() const
```

See the *SetCommentEnergy* method.

GetForceField

```
unsigned GetForceFieldType() const
```

See the *SetForceField* method.

GetMaxRotors

```
unsigned int GetMaxRotors() const
```

See the *SetMaxRotors* method.

GetMaxSearchTime

```
double GetMaxSearchTime() const
```

See the *SetMaxSearchTime* method.

GetRotorOffset

```
bool GetRotorOffset() const
```

See the *SetRotorOffset* method.

GetRotorPredicate

```
const OESystem::OEUnaryPredicate<OEChem::OEBondBase>* GetRotorPredicate() const
```

See the *SetRotorPredicate* method.

GetSDEnergy

```
bool GetSDEnergy() const
```

See the *SetSDEnergy* method.

GetTorLib

```
const OETorLib* GetTorLib() const
```

See the *SetTorLib* method.

GetUseGPU

```
bool GetUseGPU() const
```

See the *SetUseGPU* method.

GetUseThompson

```
bool GetUseThompson() const
```

See the *SetUseThompson* method.

SetCommentEnergy

```
bool SetCommentEnergy(const bool)
```

Sets whether to add **conformer energy** in kcal/mol into the comments that appear if the output is written to a MOL2 file. If *true*, the comment energy is written. Default: False

SetForceField

```
bool SetForceField(const unsigned)
bool SetForceField(const std::string&)
```

Sets the **force field** used for torsion driving. The first overload takes an *unsigned* from the OEMMFFSheffieldFFType constant namespace, and the second overload takes corresponding string values. The method returns *false* when the invalid selection is chosen and *true* otherwise. Default: MMFF94Smod_NOESTAT

SetMaxRotors

```
bool SetMaxRotors(const unsigned int)
```

Sets the **limit of molecules with maximum number of rotors** that would be handled by torsion driving. If a value of 9999 or higher is defined, this limit is ignored. Default: 9999

SetMaxSearchTime

```
bool SetMaxSearchTime(const double)
```

Sets the **maximum time** that should be spent for the torsion driving of a molecule, in units of seconds. Default: 120.0 sec

SetRotorOffset

```
bool SetRotorOffset(const bool)
```

Sets whether the **rotor offset compression** should be turned on. Turning on the rotor offset compression reduces the space required when saved in an OEB file. Default: False

SetRotorPredicate

```
bool SetRotorPredicate(const OESystem::OEUnaryPredicate<OEChem::OEBondBase>&)
```

Sets the **predicate** that is used to decide whether a bond is *rotatable*.

SetSDEnergy

```
bool SetSDEnergy(const bool)
```

Sets whether the **conformer energy** in kcal/mol should be stored as SD data. Default: False

SetTorLib

```
bool SetTorLib(const unsigned)
bool SetTorLib(const std::string&)
bool SetTorLib(const OETorLib&)
```

Sets the **torsion library** that is used for torsion driving. The first overload takes an *unsigned* from the *OETorLibType* constant namespace, and the second overload takes the corresponding string values. Default: *Original*

See also

- *OETorLib* class.
- *OETorLibType* constant namespace.

SetUseGPU

```
bool SetUseGPU(const bool)
```

Sets whether to use the GPU implementation for torsion driving (**GPU-Omega**). The default is *true*, however, if no GPU is detected on your system, **Omega** will fall back to the CPU implementation. **GPU-Omega** is only available with the default force field MMFF94Smod_NOESTAT.

SetUseThompson

```
bool SetUseThompson(const bool)
```

Sets whether to use Thompson sampling for exploring the conformer space. The default is *false*, that is, **Omega** will use exhaustive sampling by default. If switched Thompson sampling is used, the parameters can be controlled by the Thompson Options class.

4.1.23 OETorDriver

```
class OETorDriver
```

This class defines an interface for generating conformer ensembles of molecules by torsion driving on the provided 3D structures of the molecules.

See also

- *OETorDriveOptions* class
- *OESliceEnsembleOptions* class
- *OEConfFixOptions* class

Code Examples

- *Generating Conformer Ensembles Using Torsion Driving* example

The *OETorDriver* class defines the following public methods:

- *GenerateConfs*
- *GetForceField* and *SetForceField*
- *GetSliceEnsembleOptions* and *SetSliceEnsembleOptions*
- *GetTorDriveOptions* and *SetTorDriveOptions*

Constructors

```
OETorDriver(const OETorDriveOptions& argTorOpts = OETorDriveOptions(),
            const OESliceEnsembleOptions& argSlicerOpts = OESliceEnsembleOptions())
OETorDriver(const OETorDriver&)
```

Default and copy constructors.

GenerateConfs

```
unsigned GenerateConfs(OEChem::OEMCMolBase&,
                       const OEConfFixOptions& = OEConfFixOptions()) const
```

Generates a conformer ensemble for a molecule. Returns *OEOmegaReturnCode.Success* if the process succeeds, otherwise returns an error code from the *OEOmegaReturnCode* namespace. The second argument provided with appropriate options can be used to fix part of a molecule structure to predefined coordinates.

See also

- *OEConfFixOptions* class

GetForceField

```
const OEMolPotential::OEForceField& GetForceField() const
```

See the *SetForceField* method.

GetSliceEnsembleOptions

```
const OESliceEnsembleOptions& GetSliceEnsembleOptions() const
```

See the *SetSliceEnsembleOptions* method.

GetTorDriveOptions

```
const OETorDriveOptions& GetTorDriveOptions() const
```

See the *SetTorDriveOptions*.

SetForceField

```
void SetForceField(OEMolPotential::OEForceField&)
```

Sets the **force field** for torsion driving. Default: OEMMFFSheffield with `OEMMFFSheffieldFFType.MMFF94Smod_NOESTAT`

See also

- OEForceField class
- OEMMFFSheffield

SetSliceEnsembleOptions

```
void SetSliceEnsembleOptions(const OESliceEnsembleOptions&)
```

Sets *options* for slicing ensemble to remove duplicates.

See also

- *OESliceEnsembleOptions* class

SetTorDriveOptions

```
void SetTorDriveOptions(const OETorDriveOptions&)
```

Sets *options* for torsion driving.

See also

- *OETorDriveOptions* class

4.1.24 OETorLib

```
class OETorLib
```

Stores and manages torsion libraries used during conformer generation. Torsion rules can be loaded from files or added as SMARTS-based rule strings, and are consulted by *OETorDriver* when sampling rotatable-bond dihedral angles.

See also

- *OETorDriveOptions* class

Constructors

```
OETorLib(const unsigned type = OETorLibType::Default)
```

Default and copy constructors. The constructor with the type parameter allows the user to set the torsion library type from values in the *OETorLibType* namespace.

operator bool

```
operator bool() const
```

Returns *false* if the *OETorLib* object is empty, otherwise returns *true*.

AddTorsionLibrary

```
bool AddTorsionLibrary(const std::string &)
bool AddTorsionLibrary(OEPlatform::oeistream &)
```

Takes a `string` or an oeistream object to add a torsion library. This will put the new torsion library above the current torsion library, which means that they will be checked first for a match. To replace the torsion library, call *OETorLib.SetTorsionLibrary*. The method returns *true* if the library is added successfully.

AddTorsionRule

```
bool AddTorsionRule(const std::string &)
```

Adds a single torsion rule as a string. The format for rules is a SMARTS pattern followed by the torsion angles. The method returns *true* if the rule is added successfully. The following is an example of a general rule:

```
[*:1][CH2:2][a:3][a:4] 0 180 90 -90 45 -45 135 -135
```

The following code demonstrates how to add a new torsion rule to an existing *OEOmega* object named `omega`.

See the appendix for a full listing.

Example of adding a new torsion rule

```
// Adding the torsion rule "[O:1]=[C:2]-[O:3][CH3:4] 90" as a string
// This takes precedent over previous rule
string rule = "[O:1]=[C:2]-[O:3][CH3:4] 90";
if(!torlib.AddTorsionRule(rule))
    OEChem.OEThrow.Fatal("Failed to add torsion rule: " + rule);

omegaOpts.SetTorLib(torlib);
omega.SetOptions(omegaOpts);
if(omega.Call(mol))
    OEChem.OEWriteMolecule(ofs, mol);
```

The new rule will take precedence over all rules previously added to this object either from a file or from calling this method.

```
bool AddTorsionRule(OEChem::OEQMolBase &qmol,
                    std::vector<int> &degrees)
```

The next signature of `AddTorsionRule` takes a generic OEQMolBase with a corresponding `std::vector<int>` containing the angles. The pattern represented by OEQMolBase should have map indices set on the atoms considered in the torsion. In SMARTS, this means the atoms should have map indices numbered from 1 to 4. This can theoretically allow torsion rules to be written in other query file formats provided there is a method for setting the appropriate map indices. The following code demonstrates how to initialize an OEQMolBase and use it to define a new torsion rule.

See the appendix for a full listing.

Example of adding a new torsion rule from a query molecule

```
// Adding torsion rule "[O:1]=[C:2]-[O:3][CH3:4] 45" as a query
// molecule. This takes precedent over default rule
OEQMol qmol = new OEQMol();
OEChem.OEParseSmarts(qmol, "[O:1]=[C:2]-[O:3][CH3:4]");
OEIntVector degrees = new OEIntVector();
degrees.Add(45);

if (!torlib.AddTorsionRule(qmol, degrees))
    OEChem.OEThrow.Fatal("Failed to add torsion rule");

omegaOpts.SetTorLib(torlib);
omega.SetOptions(omegaOpts);
```

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```
if (omega.Call(mol))
    OEChem.OEWriteMolecule(ofs, mol);
```

ClearTorsionLibrary

```
void ClearTorsionLibrary()
```

Clears the current torsion library. **Omega** cannot operate with an empty torsion library, so a new torsion library must be set before running **Omega**.

GetTorRule

```
const OEChem::OESubSearch* GetTorRule(const OEChem::OEMolBase&,
                                      const OEChem::OEBondBase&) const
```

Returns the torsion rule associated with the specified bond of the specified molecule. The method returns a null pointer if a torsion rule is not found. The rules are stored as OESubSearch objects.

See also

- *OEGetTorValues* function.

GetTorRules

```
OESystem::OEIterBase<OEChem::OESubSearch>* GetTorRules()
```

Returns an iterator over the torsion rules. The rules are stored as OESubSearch objects.

HasTorRule

```
bool HasTorRule(const OEChem::OEMolBase&, const OEChem::OEBondBase&) const
```

Checks if a torsion rule exists with the specified bond of the specified molecule. Returns *true* if a rule exists.

ResetTorsionLibrary

```
bool ResetTorsionLibrary()
```

Resets the torsion library stored internally by **Omega**. The method returns *true* if the library is reset successfully.

SetTorsionLibrary

```
bool SetTorsionLibrary(const std::string &)
bool SetTorsionLibrary(OEPlatform::oeistream &)
bool SetTorsionLibrary(unsigned int type)
```

Replaces the current torsion library with the one passed in as an argument. If the argument is a type, it is expected to be a value in the *OETorLibType* namespace. The method returns *true* if the library is set successfully.

4.1.25 OETorLibParameter

```
class OETorLibParameter : public OESystem::OEMultiParameter<OEConfGen::OETorLib>
```

The *OETorLibParameter* represents a parameter that has a value of type *OETorLib*.

The following methods are publicly inherited from OEParameter:

- `AddAlias` and `GetAliases`
- `AddDetail` and `GetDetail`
- `AddIllegalRange` and `GetIllegalRanges`
- `AddIllegalValue` and `GetIllegalValues`
- `AddLegalRange` and `GetLegalRanges`
- `AddStringDefault` , `GetStringDefault` and `GetStringDefaults`
- `AddStringValue` , `GetStringValue` and `GetStringValues`
- `ClearDefaults`
- `ClearValues`
- `CreateCopy`
- `GetBrief` and `SetBrief`
- `GetHasDefault`
- `GetHasValue`
- `GetIsList` and `SetIsList`
- `GetKeyless` and `SetKeyless`
- `GetName` and `SetName`
- `GetOrderPriority` and `SetOrderPriority`
- `GetVisibility` and `SetVisibility`
- `IsLegalString`
- `IsSet` and `IsSetToString`

The following methods are publicly inherited from OEMultiParameter:

- `AddLegalEntry`
- `GetDefault` and `SetDefault`
- `GetSetting`
- `GetValue` and `SetValue`

Constructors

```
OETorLibParameter()
OETorLibParameter(const OETorLibParameter&)
```

Default and copy constructors.

Constructs an *OETorLibParameter* instance using the specified set of parameters.

4.2 OEConfGen Constants

4.2.1 OEFragBuilderMode

This namespace contains constants that are used with *OEFragBuilderOptions* to control the defaults to be set for fragment building options. Different sets of default options prepare the FragBuilder to generate structures that are suitable for different uses.

Default

Same as *OEFragBuilderMode.Fast*.

Dense

Options suitable for building fragments with the *OEMolBuilder* in the *OEOmegaSampling.Dense* mode.

Option	Non-Ring	Ring	Macrocycle
EnergyWindow	15.0	15.0	25.0
FragGen	40	1024	2000
FragKeep	1	1024	1024
RMS	0.05	0.05	0.1
TimeLimit	3600	3600	1800
StartFactor	X	100	X

Fast

Options suitable for fast, on-the-fly building of fragments during molecule building with the *OEMolBuilder*.

Option	Non-Ring	Ring	Macrocycle
EnergyWindow	8.0	8.0	25.0
FragGen	40	1024	2000
FragKeep	1	1024	1024
RMS	0.1	0.1	0.1
TimeLimit	400	400	1800
StartFactor	X	2	X

Strict

Options suitable for rigorous fragment structure generation, suitable for building a fragment library with the *OEMakeFragLib*.

Option	Non-Ring	Ring	Macrocycle
EnergyWindow	4.0	4.0	25.0
FragGen	40	50000	2000
FragKeep	1	1024	1024
RMS	0.1	0.1	0.1
TimeLimit	400	400	1800
StartFactor	X	20	X

4.2.2 OENitrogenEnumeration

This namespace contains constants that are used with *OEMolBuilderOptions.SetEnumNitrogen* to control the behavior of *OEOmega* with respect to enumeration of nonterminal nitrogens. Any nitrogen with pyramidal geometry in the initial model of the input molecule, and having no more than two ring bonds, is considered by *OEOmega* to be *invertible*.

Default

Equivalent to *OENitrogenEnumeration.Unspecified*.

Off

Nitrogens are not enumerated.

All

All invertible nitrogens will be enumerated.

Unspecified

Only invertible nitrogens with unspecified stereochemistry will be enumerated.

4.2.3 OEOmegaForceFieldType

This namespace contains constants that refer to force fields that are available in *OEOmega*.

SAGE

The Sage force field from the Open Force Field Initiative. Name: sage

SAGE_NOESTAT

The Sage force field without electrostatics. Name: sage_NoEstat

SAGE_SHEFF

The Sage force field with Sheffield solvation. Name: sage_Sheff

MMFF

The Merck Molecular Force Field (MMFF). Name: mmff

MMFF_NOESTAT

The MMFF force field without electrostatics. Name: mmff_NoEstat

MMFF_TRUNC

The MMFF force field truncated at potential minimum. Name: mmff_Trunc

MMFF_SHEFF

The MMFF force field with Sheffield solvation. Name: mmff_Sheff

MMFF94S

The 94s variation of the Merck molecular force field (MMFF). Name: mmff94s

MMFF94S_NOESTAT

The MMFF94S force field without electrostatics. Name: mmff94s_NoEstat

MMFF94S_TRUNC

The MMFF94S force field truncated at potential minimum. Name: mmff94s_Trunc

MMFF94S_SHEFF

The MMFF94S force field with Sheffield solvation. Name: mmff94s_Sheff

MMFF94Smod

The modified 94s variation of the Merck molecular force field (MMFF). Name: mmff94smod

MMFF94Smod_NOESTAT

The modified MMFF94S force field without electrostatics. Name: mmff94smod_NoEstat

MMFF94Smod_TRUNC

The modified MMFF94S force field truncated at potential minimum. Name: mmff94smod_Trunc

MMFF94Smod_SHEFF

The modified MMFF94S force field with Sheffield solvation. Name: mmff94smod_Sheff

Invalid

Invalid force field type.

4.2.4 OEOmegaReturnCode

This namespace contains constants that are returned by various methods in **Omega TK** to indicate the outcome.

Success

Method returned successfully.

MissingFFParams

Force field setup failed due to missing parameters.

ExplicitHydrogens

Failed to add explicit hydrogens.

InvalidOptions

Failed due to invalid options.

No3DFromCT

Molecule must be three-dimensional when fromCT is set to *false*.

TooManyRotors

Maximum number of rotors exceeded.

UnspecifiedStereo

Failed due to unspecified stereochemistry.

FailedCTBuild

Failed to build structure from connection table (CT).

FailedTorDrive

Failed to complete torsion driving.

ExceedsAtomDegree4

Contains atom with degree greater than 4.

FailedDupSetup

Duplicate removal setup failed.

FailedDGConfGen

Unable to generate 3D conformer.

FailedTorAssign

Torsion assignment failed.

FailedSmartMatch

Unable to match SMARTS.

FailedFixMatch

Fixfile match failed.

NoFixedFragment

No fixed fragment found.

NoValidConfs

No valid conformers generated.

No3DTorDrive

Input must be three-dimensional for torsion driving.

FailedCharges

Failed to assign partial charges.

Failed

Method failed.

4.2.5 OEOmegaSampling

This namespace contains constants that are used with *OEOmegaOptions* to control the defaults to be set for **Omega** options. Different sets of default options prepare **Omega** to generate structures that are optimal for different uses.

Code Examples

- *Generating Densely Sampled Conformers* example

Classic

Options to generate a set of conformers representing a gas phase ensemble.

Dense

Options to generate a dense set of conformers optimal for FreeFormConf usage.

Caution

GPU-Omega is not compatible with the dense mode default force field. To enable **GPU-Omega** and utilize a GPU, set *OETorDriveOptions.SetForceField* to `OEMMFFSheffieldFFType.MMFF94Smod_NOESTAT`.

Pose

Options to generate a set of conformers suitable for molecular alignment and pose prediction by docking.

ROCS

Options to generate a set of conformers suitable for **ROCS** usage.

FastROCS

Options to generate a sparse set of conformers suitable for **FastROCS** usage.

The following options are overridden by various modes from the default *OEOmegaSampling.Classic* mode.

Option	Classic	Dense	Pose	ROCS	FastROCS
RangeIncrement	4		4		
MaxConfs	200	20000	200, 800	50	10
UseThompson	True	False	True	True	True
StrictStereo	True	False			
MaxSearchTim	120.0	3600.0			
EnergyWindow	[10.0, 15.0, 15.0, 20.0]	15.0	[10.0, 15.0, 25.0, 30.0]	10	10
RMSThreshold	0.5	0.3			
EnumNitrogen	OENitrogenEnumeration_Unspecified	OENitrogenEnumeration_All			
SampleHydrogens	False	True			
SearchForceField	mmff94smod_NoEstat	mmff94s_Sheff			
FragBuilderOptions	Fast	Dense			

4.2.6 OESliceEnsembleDefaults

This namespace contains constants that are used for defaults of *OESliceEnsemble*.

RMS

RMS value for duplicate removal. Set to 0.5.

MaxConfs

Maximum number of conformers in the ensemble. Set to 200.

EnergyRange

Energy windows range is set to [10.0, 15.0, 15.0, 20.0]. With the default range increment of 4, this means that the energy window is 10.0 for the molecules with 0–3 rotors, 15 for ones with 4–11 rotors and 20 for 12 or more rotors.

RangeIncrement

RangeIncrement is set to 4.

4.2.7 OETorLibType

This namespace contains constants that are used to construct an *OETorLib* object.

See also

- *OETorDriveOptions.SetTorLib* method to control the torsion library used for conformation generation.

Default

The default torsion library is *OETorLibType.Original*.

Original

The default **Omega TK** torsion library.

GubaV21

Torsion library (version 2.1) based on the work of Wolfgang Guba.

See also

- [Guba-2016]

4.3 OEConfGen Functions

4.3.1 OEAddGlobalFragLib

```
bool OEAddGlobalFragLib(const std::string& fraglib_filename,
                        bool replace = true)
```

Adds a fragment library located at *fraglib_filename* to **Omega**'s global fragment library. If *replace* is true, previously existing fragments in the current global fragment library are replaced with the ones from *fraglib_filename*.

Unlike the fragment libraries loaded by *OEOmega.AddFragLib*, the global fragment library is accessible to all **Omega** instances. It is most useful in the Java programming language to minimize memory usage when running multiple *OEOmega* instances in threads. Other languages have the default fragment library preloaded.

If you use *OEAddGlobalFragLib* to load your fragment library, do not use *OEOmega.AddFragLib*, as this will load the fragment library only into that particular *OEOmega* instance.

Note

This function is not thread-safe and must be called before starting any threads.

See also

- *OEClearGlobalFragLib* function

4.3.2 OEClearGlobalFragLib

```
void OEClearGlobalFragLib()
```

Clears the global fragment library. This function can be used to remove the default fragment library in order to load a new one or to ensure that any force field parameter change will be used during the subsequent runs in favor of the preloaded default fragment library.

Note

This function is not thread-safe and must be called before starting any threads.

See also

- *OEAddGlobalFragLib* function

4.3.3 OEGetOmegaError

```
std::string OEGetOmegaError(const unsigned)
```

Returns error messages corresponding to return codes defined in the *OEOmegaReturnCode* namespace.

4.3.4 OEGetTorValues

```
bool OEGetTorValues(const OEChem::OESubSearch& torrule,
                    std::vector<double>& values)
```

Provides the torsion values corresponding to the specified torsion rule. The method returns *false* if the specified OESubSearch object does not contain torsion rules.

See also

- *OETorLib.GetTorRule* method.

4.3.5 OEIsMacrocycle

```
bool OEIsMacrocycle(const OEChem::OEMolBase& mol,
                    const unsigned int minSize = 10)
```

Checks if the specified molecule is a macrocycle. The second argument refers to the minimum number of atoms required to be in a ring for the molecule to be treated as a macrocycle molecule. By default, a molecule is defined as macrocycle when it contains a 10-membered or larger ring, regardless of aromaticity and heteroatom content. For example, large cyclic alkanes, annulenes, crown ethers, and porphyrins are all macrocycles.

See also

- *OEMacrocycleOmega* class
- *OEMacrocycleBuilder* class

4.3.6 OEFlipper

```
OESystem::OEIterBase<OEChem::OEMolBase>* OEFlipper(const OEChem::OEMolBase& mol,
                                                   const OEFlipperOptions& options)
OESystem::OEIterBase<OEChem::OEMolBase>* OEFlipper(const OEChem::OEMCMolBase& mol,
                                                   const OEFlipperOptions& options)
```

Enumerates the stereocenters of `mol` and returns them as a series of new molecules.

Parameters:

mol
The molecule to enumerate. The input molecule will always be returned even if there are no stereocenters to enumerate.

options
The *options* for enumerating stereocenters of molecules.

Deprecated

```
OESystem::OEIterBase<OEChem::OEMolBase>* OEFlipper(const OEChem::OEMolBase& mol,
                                                   unsigned int maxcenters = 12,
                                                   bool forceFlip = false,
                                                   bool enumNitrogen = false,
                                                   bool warts = false)
OESystem::OEIterBase<OEChem::OEMolBase>* OEFlipper(const OEChem::OEMCMolBase& mol,
                                                   unsigned int maxcenters = 12,
                                                   bool forceFlip = false,
                                                   bool enumNitrogen = false,
                                                   bool warts = false)
```

Enumerates the stereocenters of `mol` and returns them as a series of new molecules.

Parameters:

mol
The molecule to enumerate. The input molecule will always be returned even if there are no stereocenters to enumerate.

maxcenters
The number of molecules generated by enumerating the stereocenters is 2^N, where N is the number of stereocenters. In some instances, this may be larger than is desired. This parameter indicates the maximum number of stereocenters which will be fully enumerated. If a molecule has more than `maxcenters` stereocenters, this function will randomly enumerate $2^{maxcenters}$ instances from the full set of potential isomers.

forceFlip
This parameter forces the modification of all of the stereocenters in a molecule. If *false* (the default), it will only enumerate stereocenters which do not already have a specified stereochemistry.

enumNitrogen
Controls the behavior with respect to the enumeration of nonterminal nitrogens. Any nitrogen with pyramidal

geometry in the initial model of the input molecule, and having no more than two ring bonds is considered to be *invertible*. It will enumerate all possible puckers if set to *true*.

warts
Adds wart to the title of each stereoisomer. A "wart" is a systematic naming scheme for the output titles.

Caution

This function will remove the molecule coordinates.

Code Examples

- *Generating Stereoisomers* example

4.3.7 OEFlipperStereoCenters

```
unsigned OEFlipperStereoCenters(const OEChem::OEMolBase& mol,
                                const OEFlipperOptions& options)
```

Computes the number of the stereocenters of `mol`.

Parameters:

mol
The input molecule.

options
The *options* for enumerating the stereocenters of a molecule.

4.3.8 OEOmegaGetArch

```
const char* OEOmegaGetArch()
```

Returns the internal build string used by OpenEye, Cadence Molecular Sciences to identify the hardware architecture. The format of these strings may change over time.

4.3.9 OEOmegaGetLibraryRelease

```
const char* OEOmegaGetLibraryRelease()
```

Caution

Deprecated, please use *OEOmegaGetRelease* instead.

4.3.10 OEOmegaGetLibraryVersion

```
unsigned int OEOmegaGetLibraryVersion()
```

Caution

Deprecated, please use *OEOmegaGetVersion* instead.

4.3.11 OEOmegaGetLicensee

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

Returns the licensee name from the license file.

4.3.12 OEOmegaGetPlatform

```
const char* OEOmegaGetPlatform()
```

Returns the internal build string used by OpenEye, Cadence Molecular Sciences to identify a platform. The format of these strings may change over time, and future distributions may contain different values even when using the same operating system, compiler, and processor. For example, on a `x86_64` Red Hat Enterprise Linux box, this would return `redhat-RHEL5-g++4.1-x64`.

4.3.13 OEOmegaGetRelease

```
const char* OEOmegaGetRelease()
```

Returns the release name of the **Omega TK** library being used. This returns a value similar to *0.10.0* for production versions of the library, and *0.10.0 debug* for the checking version of the library.

4.3.14 OEOmegaGetSite

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

Returns the physical site location of the licensee as registered in the license file.

4.3.15 OEOmegaGetVersion

```
unsigned int OEOmegaGetVersion()
```

Returns the version number of the library being used. This is an unsigned integer value indicating the date on which the library was built, for example, *20141001* refers to October 1, 2014. This value should be used when reporting problems; unlike the release string, it may be used in comparisons if needed.

4.3.16 OEOmegaIsGPUReady

```
bool OEOmegaIsGPUReady()
```

Determines whether a GPU is present and available for use on the current system.

This can be used to determine if conformer generation using the torsion driving method will be accelerated by a GPU.

Caution

This function causes GPU context creation and so is only safe to use from within a process when using a multithreaded environment such as Python's multiprocessing.

See also

- *GPU-Omega* chapter in the *OEOmega TK* documentation.

4.3.17 OEOmegaIsLicensed

```
bool OEOmegaIsLicensed(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 **Omega TK** functionality.

The feature argument can be used to check for a valid license to **Omega TK** along with the following features: 'python', 'java', or 'clr' (for CSharp).

The expdate argument can be used to obtain the expiration date of the current **Omega TK** license.

See also

- `OEChemIsLicensed` function

4.3.18 OEOmegaSystemHasGPU

```
bool OEOmegaSystemHasGPU()
```

Determines whether a GPU is present on the current system. This will check that the system is a Linux platform and the */dev/nvidiaN* file exits, where N can be between 0 and 100. It will not try to create a context on the GPU, so there is still the possibility that the GPU will not be available, either due to the driver being uninstalled or the GPU being used by another system user.

4.3.19 OESliceEnsemble

```
bool OESliceEnsemble(OEChem::OEMCMolBase& mol,
                     double rms = OESliceEnsembleDefaults::RMS,
                     double ewindow = OESliceEnsembleDefaults::EWindow,
                     unsigned maxconfs = OESliceEnsembleDefaults::MaxConfs)
bool OESliceEnsemble(OEChem::OEMCMolBase& mol,
                     const OESliceEnsembleOptions& options)
```

Reduces the number of conformers in the input `mol` using the **OMEGA** deduplication algorithm. This allows for *OEOmega* to generate a very large ensemble with much looser deduplication parameters and then to "slice" that ensemble of conformations by various different parameters after the fact.

The default values for the first overload of the function are picked from the *OESliceEnsembleDefaults* namespace.

Conformer slicing proceeds in the following order:

1. Slice by energy window. Decreasing this value will result in fewer conformers. For slicing by energy, the algorithm assumes that the energy for each conformer has been precalculated and set as the energy property of the conformer using the `OEMolBase.SetEnergy` method. Conformer generation using *OEOmega*, sets this property by default.
2. Slice by RMS. Increasing this value will result in fewer conformers.
3. Slice by maximum number of conformers. Decreasing this value will result in fewer conformers.

Note

If the same energy window and RMS values are being chosen as the defaults being used in the previous *OEOmega* calculation, it will be faster to delete conformers directly with `OEMCMolBase.DeleteConf`. This function is really intended to be run whenever the RMS has changed, or when the conformer geometries themselves have changed.

CHAPTER

FIVE

RELEASE HISTORY

5.1 Omega TK 7.0.0

5.1.1 New Features

- The following changes have been made to extend Thompson sampling usage for torsion driving in *OEOmega*:
  - The *Thompson sampling* algorithm for torsion driving has been improved for robustness and speed.
  - The default value for *SetUseThompson* in *OETorDriveOptions* has been changed to `True`.
  - The *SetUseThompson* is honored even when *SetUseGPU* is set to `True`.
  - The preliminary API class `OEThompsonOptions` has been removed, as it is no longer relevant.
- The default energy window for torsion driving in *Classic* mode has been changed to a range-based value to better suit **OMEGA** with Thompson sampling. Similarly, the energy range for the *Pose* mode has also been adjusted.

5.1.2 Minor Bug Fixes

- *OEMolBuilder* now respects the *MaxEnumConfs* provided in the *OEMolBuilderOptions* even when an input molecule has more conformers than specified.
- Certain edge cases where the torsion driving algorithm would fail with a FailedTorDrive error message have been addressed.

5.2 Omega TK 6.1.1

5.2.1 Minor Bug Fixes

- The default value and the lower range for MaxTrials in OEThompsonOptions have been changed from `0` to `1`.

5.3 Omega TK 6.1.0

5.3.1 New Features

- The new methods *SetOverlayRMS* and *GetOverlayRMS* have been added to *OESliceEnsembleOptions*, enabling conformer slicing with in-place RMSD calculation between conformers, with *OEConfSlicer* and *OESliceEnsemble*.

5.3.2 Minor Bug Fixes

- *OEOmega* now properly places carboxylic acids in cis configuration when hydrogen sampling is not performed.
- All conformers generated with *OEMacrocycleOmega* now properly set the dimensionality of the conformers to 3.

5.4 Omega TK 6.0.0

5.4.1 New features

- The following new methods have been added to *OETorDriveOptions* to enable use of Thompson sampling, instead of exhaustive sampling, of torsion angles during torsion driving. Use of Thompson sampling is especially useful, being significantly faster without losing quality, in generating smaller ensembles as obtained with the *FastROCS* or *ROCS* modes.
  - *GetUseThompson*
  - *SetUseThompson*
  - GetThompsonOptions
  - SetThompsonOptions
- A new class, OEThompsonOptions, has been added that enables controlling Thompson sampling during torsion driving.
- Generation of a single conformer with *OEConformerBuilder* has been modified to use Thompson sampling.

5.4.2 Minor bug fixes

- User-defined values passed through *SetEnergyWindow*, *SetMaxConfs*, and *SetRMSThreshold* are now properly accounted for, even when the corresponding defaults are range-based.
- Molecule titles are retained when *Build* fails in *OEOmega* with `fails to build structure from CT`.
- A verbose log is provided for fragments that fail when *Build* fails in *OEOmega* with `fails to build structure from CT`.
- The *OEOmegaIsGPUReady* function has been safeguarded from a rare crash. The function has also been updated to check not only for device 0, but for devices from 0 to 100.

5.5 Omega TK 5.1.0

5.5.1 New features

- A new **Flipper** option has been added to enumerate internally perceived relative stereocenters (e.g., 1,4-disubstituted cyclohexanes). See *SetEnumRelativeAtomStereo*.

5.5.2 Minor bug fixes

- Stereochemistry of input molecules is now respected more consistently in *OEMacrocycleBuilder*.
- For *SetMacroCycOptions* in *OEFragBuilderOptions*, defaults for *SetFragGen*, *SetFragKeep*, and *SetStartFactor* have been changed to more appropriate values of 50000, 1024, and 20, respectively.
- An issue with the order of loading rules to an existing torsion library with *AddTorsionLibrary* has been fixed.
- A duplicate entry from the `GUBA` torsion library has been removed.

5.6 Omega TK 5.0.0

5.6.1 New features

- The default fragment library for *OEOmega* and *OEMolBuilder* has been updated. The new fragment library consists of over 580 K fragments, replacing the previous library with ~80 K fragments.
- Three new force fields have been added and can be used with *OEMolBuilder* and *OETorDriver* in *OEOmega*:
  - *SAGE*
  - *SAGE_NOESTAT*
  - *SAGE_SHEFF*
- The behavior of *OEFlipperOptions* has changed. New flags have been added to *OEFlipperOptions*, facilitating more complete decoupling of individual flags and more selective enumeration of specific stereocenter classes and environments than was previously possible.
- A new option class, *OEFlipperClassicOptions*, has been added to allow a detailed comparison of the new flag behaviors with the previous OEFlipper enumeration behavior. This class will be deprecated in a future toolkit release.
- The internal algorithm for storage and usage of torsion rules in *OETorLib* has been modified to improve performance when working with a library containing a large set of rules.
- A new return code *FailedCharges* has been added to *OEOmegaReturnCode* to indicate failures due to partial charge assignment.

5.6.2 Minor bug fixes

- The order of torsion rules in the default *OETorLib* has been changed to ensure that a specific rule is not ignored due to the presence of a more generic rule.

5.7 Omega TK 4.2.2

5.7.1 Minor bug fixes

- The OEOmega method *Build* will now fail when `MCS matching` is requested but a corresponding `FixMol` has not been set.

5.8 Omega TK 4.2.1

5.8.1 New features

- The ability to fix a part of a molecule during conformer generation based on maximum common substructure (MCS) has been added. The following new methods have been added to the *OEConfFixOptions* to enable this functionality:
  - *SetFixMCS*
  - *GetFixMCS*
  - *SetMCSFunc*
  - *GetMCSFunc*
  - *SetMCSType*
  - *GetMCSType*

  - *SetMCSMinAtoms*
  - *GetMCSMinAtoms*

- New methods *SetIgnoreStereo* and *GetIgnoreStereo* have been added to *OEMolBuilderOptions* to allow continuation of conformer generation when specified stereo signatures in a molecule could not be honored.
- New methods *SetMaxEnumConfs* and *GetMaxEnumConfs* have been added to *OEMolBuilderOptions* to allow specifying the maximum number of conformers to be generated from ring enumeration, nitrogen enumeration, and/or hydrogen sampling.
- Verbose mode logging now reports torsion angles sampled, along with the rules, during torsion driving.

5.8.2 Minor bug fixes

- Conformer generation with *OEOmega.Build* or *OEMolBuilder.Build* now fails correctly when specified stereo signatures on a molecule cannot be honored. The existing behavior, to carry on even if stereo signatures could not be honored, can be obtained by setting *IgnoreStereo* to `true`.
- Ring fragment building during *OEOmega.Build*, *OEFragBuilder.Build*, *OEMolBuilder.Build*, or *GenerateMissingFrags* now properly honors the *SetFragKeep* parameter regarding the maximum number of generated fragment conformers to be kept.

5.9 Omega TK 4.2.0

5.9.1 New features

- Support for consideration of MDL enhanced stereo collection information during isomer generation has been added. *The OEFlipperOptions class* adds a new `SetEnhancedStereo` option to control consideration of explicit enhanced stereo groups defined by OEGroupBase information that may have been read from `V3000` the OEFormat values indicating `SDF` structures or `CXSMILES` files.
- A new method, *SetFragBuilderMode*, has been added that allows setting fragment building mode in the corresponding *OEFragBuilderOptions*.

5.9.2 Minor bug fixes

- Internal generic data tags applied to the `flip-ee` used for performance during the flipping activity are now stripped from the structures returned by *OEFlipper* as this information is no longer relevant.

5.10 Omega TK 4.1.2

Fall 2021

5.10.1 Minor bug fixes

- An issue with overwriting partial charges of atoms in input molecules has been fixed.
- The *Generating Stereoisomers* example has been modified to use *OEFlipperOptions*.
- An issue running *OEOmega* when both SetUseGPU and *SetSampleHydrogens* are set to *True* was fixed by disabling SetUseGPU in these cases.

5.11 Omega TK 4.1.1

July 2021

5.11.1 New features

- Function *OEOmegaSystemHasGPU* has been added to test for availability of a GPU.

5.11.2 Major bug fixes

- A bug that caused a segmentation fault when zero was passed to the *SetMaxConfs* method has been fixed.
- And issue that prevented oeomega from using the GPU in child threads when *OEOmegaIsGPUReady* was called from the main thread has been fixed.

5.11.3 Minor bug fixes

- An issue with stereo specificity of the imino group (=NH) not being retained in a macrocycle has been fixed.
- An issue with loss of relative stereo marked atoms in macrocycle mode has been fixed.

5.12 Omega TK 4.1.0

Fall 2020

5.12.1 New features

- **GPU-Omega** now requires a minimum NVIDIA Driver version of 450.x and a minimum GPU compute capability of 3.5. See NVIDIA Drivers and Supported GPUs for more details.
- Conformer generation using `dense` mode now defaults to running on the CPU instead of the GPU. The other torsion-driving sampling modes (`sparse`, `rocs`, `fastrocs`, and `pose`) will still run on a GPU by default if one is available on a Linux platform. For details on how to run with `dense` mode sampling on a GPU, see the *Usage* section of the **GPU-Omega** docs.
- A new class, *OEFlipperOptions*, has been added that defines parameters for specifying stereo centers and other options.
- *OEFlipper* has been updated to take a molecule and an *OEFlipperOptions* value. The old version of *OEFlipper* that takes five parameters has been deprecated.
- A new function, *OEFlipperStereoCenters*, has been added that returns a number of undefined stereo centers in a molecule as interpreted by *OEFlipper*.

5.12.2 Major bug fixes

- A memory leak in **GPU-Omega** has been fixed.
- An issue with generating conformers on the CPU using child processes with the same *OEOmega* object has been fixed.
- **GPU-Omega** no longer throws an error when attempting to generate conformers with the same *OEOmega* object in child processes. Instead, it falls back to the CPU. To use **GPU-Omega** with child processes, each child must construct a new *OEOmega* object.

5.12.3 Minor bug fixes

- *OEConfGen* now clears **all** fragment libraries. Previous releases did not clear the internal shared fragment library (a shared memory library of fragments accrued while generating conformers with the same OEOmega object).

5.12.4 Documentation changes

- *OEOmegaReturnCode* has been updated to reflect the current possible values.

5.13 Omega TK 4.0.0.6

- *OEMolBuilder.Build* no longer enumerates specified nitrogen when *OEMolBuilderOptions.GetEnumNitrogen* is *OENitrogenEnumeration.Unspecified*.

5.14 Omega TK 4.0.0

As part of the integration of **OEToolkits** and **OEApplications** into a single release, the version number of **Omega TK** has been upgraded to 4.0.0 to make it consistent with that of the **OMEGA** application.

5.14.1 New features

- **GPU-Omega**, a GPU-accelerated implementation of the torsion driving algorithm, is now available. This will make use of any suitable Nvidia GPU on supported Linux platforms by default for `classic` mode runs. It is advised to read the *GPU-Omega* section of the documentation to ensure that your system meets all the prerequisites and that availability is understood for the different sampling modes. On systems that do not meet the requirements, **GPU-Omega** will be disabled and fall back to the CPU.

  GPU-Omega introduces the following new APIs:

  - *OETorDriveOptions.GetUseGPU*
  - *OETorDriveOptions.SetUseGPU*
  - *OEOmegaIsGPUReady*

- The following APIs have been promoted from preliminary API to stable API status:

  - *OEMacrocycleOmega*
  - *OEMacrocycleOmegaOptions*
  - *OEMacrocycleBuilder*
  - *OEMacrocycleBuilderOptions*
  - *OEMolBuilder*
  - *OEMolBuilderOptions*
  - *OEConformerBuilder*
  - *OEFragBuilder*
  - *OEFragBuilderOptions*
  - *OEFragBuilderOptions*
  - *OETorDriver*
  - *OETorDriveOptions*
  - *OEFragOptions*

  - *OERingFragOptions*
  - *OEConfFixOptions*
  - *OEConfSlicer*
  - *OESliceEnsembleOptions*
  - *OEFragBuilderMode*
  - *OEOmegaReturnCode*
  - *OEGetOmegaError*
  - *OEIsMacrocycle*
- The *OEOmegaOptions* class has been simplified and now consists of multiple sub-options: *OEMolBuilderOptions*, *OETorDriveOptions*, *OESliceEnsembleOptions*, and *OEConfFixOptions*. The specific methods to set or get option values are now provided through these sub-option classes.
- A new abstract base class, *OEBuilderBase*, has been added that contains the basic functionality of the builders that use a fragment library.
- The following new methods have been added to *OEConfFixOptions*:
  - *OEConfFixOptions.GetAtomExpr*
  - *OEConfFixOptions.SetAtomExpr*
  - *OEConfFixOptions.GetBondExpr*
  - *OEConfFixOptions.SetBondExpr*
- Two new methods, *OEFragBuilderOptions.SetForceField* and *OEFragBuilderOptions.GetForceField*, have been added to the *OEFragBuilderOptions* class.
- Two new methods, *OEMacrocycleBuilderOptions.SetRandomSeed* and *OEMacrocycleBuilderOptions.GetRandomSeed*, have been added to the *OEMacrocycleBuilderOptions* class.
- The following new methods have been added to *OEMacrocycleOmegaOptions*:
  - *OEMacrocycleOmegaOptions.GetEnergyWindow*
  - *OEMacrocycleOmegaOptions.SetEnergyWindow*
  - *OEMacrocycleOmegaOptions.GetMaxConfs*
  - *OEMacrocycleOmegaOptions.SetMaxConfs*
- A new method, *OEMolBuilder.Prep*, has been added to the *OEMolBuilder* class to prepare molecules for building.

5.14.2 Minor bug fixes

- The following methods now return `bool`, instead of a `void`:
  - *OEConfFixOptions.SetFixDeleteH*
  - *OEConfFixOptions.SetFixMaxMatch*
  - *OEConfFixOptions.SetFixMol*
  - *OEConfFixOptions.SetFixPredicate*
  - *OEConfFixOptions.SetFixRMS*
  - *OEConfFixOptions.SetFixSmarts*

  - *OEConfFixOptions.SetFixSubSearch*
  - *OEConfFixOptions.SetFixUniqueMatch*
  - *OEFragOptions.SetEnergyWindow*
  - *OEFragOptions.SetFragGen*
  - *OEFragOptions.SetFragKeep*
  - *OEFragOptions.SetRMS*
  - *OEFragOptions.SetTimeLimit*
  - *OEMacrocycleBuilderOptions.SetDielectricConst*
  - *OEMacrocycleBuilderOptions.SetRefTolerance*
  - *OEMacrocycleBuilderOptions.SetSkipRefinement*
  - *OEMacrocycleOmegaOptions.SetIterCycleSize*
  - *OEMacrocycleOmegaOptions.SetMaxIter*
  - *OEMolBuilderOptions.SetCanonOrder*
  - *OEMolBuilderOptions.SetEnumNitrogen*
  - *OEMolBuilderOptions.SetEnumRing*
  - *OEMolBuilderOptions.SetFromCT*
  - *OEMolBuilderOptions.SetSampleHydrogens*
  - *OEMolBuilderOptions.SetStrictAtomTypes*
  - *OERingFragOptions.SetStartFactor*
  - *OESliceEnsembleOptions.SetEnergyWindow*
  - *OESliceEnsembleOptions.SetEnergyRange*
  - *OESliceEnsembleOptions.SetMaxConfs*
  - *OESliceEnsembleOptions.SetMaxConfRange*
  - *OESliceEnsembleOptions.SetMaxTerminalHeavy*
  - *OESliceEnsembleOptions.SetRangeIncrement*
  - *OESliceEnsembleOptions.SetRMSThreshold*
  - *OESliceEnsembleOptions.SetRMSRange*
  - *OETorDriveOptions.SetCommentEnergy*
  - *OETorDriveOptions.SetMaxRotors*
  - *OETorDriveOptions.SetMaxSearchTime*
  - *OETorDriveOptions.SetRotorOffset*
  - *OETorDriveOptions.SetRotorPredicate*
  - *OETorDriveOptions.SetSDEnergy*
  - *OETorDriveOptions.SetTorLib*

- New arguments have been added to the *OEMacrocycleBuilder.Build* method for consistency with the other classes in **OMEGA**.

- The following preliminary APIs have been removed from the *OESliceEnsembleOptions* class:
  - `OESliceEnsembleOptions::SetEnergyThreshold`
  - `OESliceEnsembleOptions::GetEnergyThreshold`
  - `OESliceEnsembleOptions::SetSliceByEnergy`
  - `OESliceEnsembleOptions::GetSliceByEnergy`
- Two methods, `OETorDriver::SetForceField` and `OETorDriver::GetForceField`, that were preliminary APIs, have been removed from the *OETorDriver* class.
- Two methods, `OEMolBuilder::SetForceField` and `OEMolBuilder::GetForceField`, that were preliminary APIs, have been removed from the *OEMolBuilder* class.
- Two methods, `OEFragBuilder::SetForceField` and `OEFragBuilder::GetForceField`, that were preliminary APIs, have been removed from the *OEFragBuilder* class.
- Two methods, `OEMakeFragLib::SetForceField` and `OEMakeFragLib::GetForceField`, that were preliminary APIs, have been removed from the *OEMakeFragLib* class.
- Two methods, `OEConfFixOptions::ClearFixFile` and `OEConfFixOptions::SetFixFile`, that were preliminary APIs, have been removed from the *OEConfFixOptions* class. Accordingly, *OEConfFixOptions.SetFixMol* has an overload that takes a molecule file as input.
- *OETorDriver.GenerateConfs* now errors out properly if the input molecule is not 3D.
- *OEOmega.Build* now properly de-duplicates the generated conformers in the case when *MaxConfs* is set to 0.
- *OEOmega.Build* no longer copies the molecule title to every conformer.
- *OEGetOmegaError* now returns a value for each entry in the *OEOmegaReturnCode* namespace.
- *OEMakeFragLib.GenerateMissingFrags* and *OEFragBuilder.Build* now perform a de-duplication on the generated fragment conformers.
- *OEFragBuilder.Build* now returns an appropriate failure code if it fails due to lack of atom types.
- *SampleHydrogens* is now robust when the potential number of conformers is too high due to hydrogen sampling.
- Default values for the parameters in *OEMacrocycleOmegaOptions* are now consistent with their respective counterparts in the **OMEGA** command line application.
- *OEIsMacrocycle* has been improved to better identify macrocycles when hetero atoms are involved.

5.14.3 Documentation changes

- A *GPU-Omega* chapter has been added to the documentation.
- **OMEGA** examples have been updated to reflect the latest changes for all supported languages.

5.14.4 General Notices

- In the C++ toolkit, **GPU-Omega** is not available on RHEL8 or Ubuntu18 in this release.

5.15 Omega TK 2.9.1

5.15.1 New features

- The following new methods have been added to the *OESliceEnsembleOptions* class to make it more efficient with large macrocycles and energy-optimized structures:
  - SetEnergyThreshold

  - GetEnergyThreshold
  - *OESliceEnsembleOptions.SetMaxTerminalHeavy*
  - *OESliceEnsembleOptions.GetMaxTerminalHeavy*
  - SetSliceByEnergy
  - GetSliceByEnergy

- A new class, *OEConfSlicer*, has been added that complements the *OESliceEnsemble* method. In addition, a new overload has been added to *OESliceEnsemble* that provides broader functionality by working with an *OESliceEnsembleOptions* object.
- Deduplication of conformer ensembles in *OEMacrocycleOmega* has been improved by replacing two preliminary API methods, `OEConfGen::OEMacrocycleOmegaOptions::SetDeduplicateScanOptions` and `OEConfGen::OEMacrocycleOmegaOptions::GetDeduplicateScanOptions`, with *OEMacrocycleOmegaOptions.SetSliceEnsembleOptions* and *OEMacrocycleOmegaOptions.GetSliceEnsembleOptions*, respectively.

5.15.2 Major bug fixes

- *OEMacrocycleOmega.Build* now generates conformer ensembles that are centered and aligned to each other, and with better deduplication.
- An issue that occasionally caused knotted conformations of some complex molecules generated with *OEOmega.Build* has been fixed.

5.15.3 Minor bug fixes

- *OEOmega.Build* now properly adds hydrogens to single heavy atom molecules.
- Two preliminary API classes, `OEConfGen::OEDuplicateScanner` and `OEConfGen::OEDuplicateScanOptions`, have been removed.
- Two preliminary API methods, `OEConfGen::OETorDriveOptions::SetIncludeInput` and `OEConfGen::OETorDriveOptions::GetIncludeInput`, have been removed.
- Defaults for *OEMolBuilderOptions.SetEnumNitrogen* and *SetSampleHydrogens* in the *OEOmegaSampling.Dense* mode have been changed from *OENitrogenEnumeration.Unspecified* and `false` to *OENitrogenEnumeration.All* and `true`, respectively.
- An issue regarding the *OEOmegaOptions.SetEnergyWindow* not being properly honored for some molecules with *OEOmega.Build* has been fixed.
- Fragment conformations for `CCN` and `CN` have been updated in the built-in fragments library to properly reflect the tetrahedral geometry.
- Occasional failure to generate conformations for molecules containing chiral N=N or C=N bonds has been fixed.

5.16 Omega TK 2.9.0

5.16.1 New features

- A new method, *OEOmega.Build*, has been introduced that provides a proper return code on failure, unlike the operator(). Operator() was then deprecated.
- A new namespace, *OEOmegaReturnCode*, has been introduced that defines return codes for various API methods.
- A new function, *OEGetOmegaError*, has been introduced that returns error descriptions corresponding to various **Omega** return codes.

- A new method, *OETorLib.GetTorRule*, has been introduced that returns the torsion rule corresponding to a rotatable bond.
- A new method, *OETorLib.HasTorRule*, has been introduced that determines whether a torsion rule is defined for a rotatable bond.
- A new function, *OEGetTorValues*, has been introduced that provides torsion values from a torsion rule-defined OESubSearch object.
- The following preliminary APIs, which were introduced in **Omega TK 2.8.0**, have been modified to return an `unsigned` return code instead of a `bool`:
  - *OEConformerBuilder.Build*
  - *OEFragBuilder.Build*
  - *OEMacrocycleBuilder.Build*
  - *OEMacrocycleOmega.Build*
  - *OEMolBuilder.Build*
  - *OETorDriver.GenerateConfs*

> **Note**
>
> The change in the preliminary APIs mentioned above is a breaking change and needs to be addressed properly by scripts and code that use these APIs. Since `bool` and `unsigned` are mutually compatible, any scripts or code using these API methods may continue to function without a proper fix and may not give any runtime or compile-time error. However, the end results obtained from such scripts or codes could be incorrect.

- The following APIs have been modified to be `const` and some of their arguments have been modified to be `const`:
  - *OEConformerBuilder.Build*
  - *OEFragBuilder.Build*
  - *OEMacrocycleBuilder.Build*
  - *OEMacrocycleOmega.Build*
  - *OEMakeFragLib.GenerateMissingFrags*
  - *OEMakeFragLib.GetMissingFrags*
  - *OEMolBuilder.Build*
  - operator()
  - *OEIsMacrocycle*
  - *OETorDriveOptions.ExceedsMaxRotors*
  - *OETorDriver.GenerateConfs*
- The following APIs have been modified to return a `bool` instead of a `void`:
  - *OEBuilderBase.AddFragLib*
  - *OETorLib.AddTorsionLibrary*
  - *OETorLib.SetTorsionLibrary*
  - *OETorLib.ResetTorsionLibrary*

5.16.2 Major bug fixes

- An issue that caused an occasional Coulombic collapse for conformations of zwitterionic molecules generated with the *Macrocycle algorithm* has been fixed.
- An issue that caused *Omega** to fail to produce conformations for molecules containing chiral nitrogen atom using macrocycle mode has been fixed.

5.16.3 Minor bug fixes

- *OEConformerBuilder.Build* no longer fails due to unspecified stereo in the input molecule.
- *OEConformerBuilder.Build* no longer generates more than one conformer in the output molecule.
- *OEConformerBuilder.Build* no longer writes anything in standard output.
- The default for *EnumNitrogen* in *OEMolBuilderOptions* has been changed from *OENitrogenEnumeration.All* to *OENitrogenEnumeration.Unspecified* so that any user-specified stereo information is not lost by default.
- *OEMacrocycleOmega.Build* has been fixed to generate conformers in cases when a `MaxConfs` of 1 is requested.
- operator() now generates a title in the output even when the input molecule has no OEMCMolBase title.
- operator() now produces a title in output conformers when *OEOmegaOptions.GetWarts* is `false`.
- operator() now produces correct conformer coordinates when both *OEOmegaOptions.SetIncludeInput* and *OEMolBuilderOptions.SetCanonOrder* are set to be `true`.
- **Omega** calculations no longer repeat an error message.
- *OEMakeFragLib.GenerateMissingFrags* no longer crashes with extreme energy window value.
- The torsion rule for `[CH3:1][CX4H:2]([CH3])[CX4H2:3][!#1:4]` in the `default` torsion library has been improved.

5.17 Omega TK 2.8.0

5.17.1 New features (Preliminary API)

The following new preliminary APIs have been added for macrocycle functionality in the **Omega TK**:

- *OEMacrocycleOmega* and *OEMacrocycleOmegaOptions* classes to generate a macrocycle molecule conformer ensemble
- *OEMacrocycleBuilder* and *OEMacrocycleBuilderOptions* classes to generate a single conformer structure of a macrocycle molecule
- `OEConfGen::OEDuplicateScanner` and `OEConfGen::OEDuplicateScanOptions` classes to enable fast scanning and removal of duplicate conformers from a conformer ensemble
- *OEIsMacrocycle* function to detect if a molecule contains a macrocycle

The following new preliminary APIs have been added to enhance small molecule conformer generation functionality in the **Omega TK**:

- *OEMakeFragLib* class to generate a fragment library
- *OEMolBuilder* and *OEMolBuilderOptions* classes to generate small molecule conformers using a fragment library
- *OEConformerBuilder* class to generate a single conformer structure of a small molecule

- *OEFragBuilder* and *OEFragBuilderOptions* classes to generate fragment conformers using distance geometry. The *OEFragBuilderOptions* class combines multiple options related to building a fragment library for both *OEMakeFragLib* and *OEMolBuilder*.
- *OETorDriver* and *OETorDriveOptions* classes to generate small molecule conformer ensembles from torsion driving
- *OEFragOptions* class to store options related to generating a single fragment structure
- *OERingFragOptions* class to store options related to generating a single ring fragment structure
- *OEConfFixOptions* class to store options related to fixing part of the structure of small molecules during a conformational search
- *OESliceEnsembleOptions* class to store options for ensemble pruning during a small molecule conformational search
- `OEFragBuilderMode` namespace to set up *OEFragBuilderOptions* for specific uses

5.17.2 New features

New additions and modifications have been made to existing APIs to enhance small molecule conformer generation functionality in **Omega TK**:

- Three new modes, `OEOmegaSampling.Pose`, `OEOmegaSampling.ROCS`, and `OEOmegaSampling.FastROCS`, have been added to the `OEOmegaSampling` namespace.
- A new torsion library based on the work of Wolfgang Guba has been added. A new namespace, `OETorLibType`, has been introduced to provide options for the choice of torsion library. Additionally, the *OETorLib* constructor now takes a torsion type value from the `OETorLibType` namespace. Also, a new overload of the `OETorLib.SetTorsionLibrary` method has been added to allow setting the desired torsion library from the above-mentioned namespace.
- The `OEOmegaForceFieldType` namespace has been replaced by the `OEMMFFSheffieldFFType` namespace. The new namespace adds 4 new options for the force field used in the *OEOmega* class. These new options are based on a modified variation of the OEMMFF94sParams parameters that prefers the appropriate axial/equatorial conformers for many molecules in *OEOmega*.

5.17.3 Major bug fixes

- The SMILES string hash in the internal fragment library in the *OEOmega* class has been updated to reflect the proper canonicalization of the fragments. This ensures that *OEOmega* will always find the fragment in the library if it exists.
- The default search force field in the *OEOmega* class has been changed to the newly introduced `OEMMFFSheffieldFFType.MMFF94Smod_NOESTAT` type to generate more appropriate axial/equatorial conformers.
- An issue that caused the *OEOmega* class to not honor the parity bits on relative stereo marked rings has been fixed.

5.17.4 Minor bug fixes

- An issue that caused the *OEOmega* class to report the same warning about atoms multiple times has been fixed.

5.17.5 Documentation changes

The following C++ and Python examples have been added to demonstrate using the new preliminary APIs:

- New examples have been added to the *Macrocycle Examples* section that generate a macrocycle conformer ensemble or a single macrocycle conformer.
- A new example has been added to the *Fragment Library Generation Examples* section that generates fragment libraries.
- A new example has been added to the *Generating Torsion Driven Conformation Examples* section that generates a conformer ensemble by torsion driving from a given 3D structure.

5.18 Omega TK 2.7.0

- Minor internal improvements have been made.

5.19 Omega TK 2.6.7

5.19.1 New features

- A new torsion library, based on the work of Guba et al. [Guba-2016], has been added. The *OETorLib* constructor now includes an optional parameter in the `OETorLibType` namespace to select either the original or new `OETorLibType.GubaV21` torsion library. A new overload of the OEConfGen_SetTorsionLibrary method can also be used to change the torsion library.

5.19.2 Documentation changes

- The function *OEFlipper* now removes molecule coordinates during its processing. This behavior change was introduced in the 2017.Feb release.

5.20 Omega TK 2.6.6

5.20.1 Major bug fixes

- The *OEFlipper* function with `forceFlip=false` no longer flips 3D molecules if stereo is defined.

5.20.2 Minor bug fixes

- Molecule titles have been added to some emitted warnings to aid in identifying problematic molecules.

5.21 Omega TK 2.6.5

5.21.1 New features

- New functionality has been added for generating a densely sampled set of conformers, as required during conformer free energy calculations using OEFreeFormConf.
- Omega has used random coordinate embedding with distance-geometry refinement to generate initial 3D fragment and ring conformers for more than a decade. The pseudo-random number generator used has been upgraded to an implementation of the Mersenne Twister adapted from the work of Kohei Takeda.
- Omega now recognizes and adjusts ring sampling for macrocycles. This improves reproduction of small and medium-sized macrocycle structures without increasing maximum ensemble sizes.

- A new class, *OEOmegaOptions*, has been added that sets all options of the *OEOmega* object during its construction. All the *OEOmega* methods with the same name as their *OEOmegaOptions* counterparts are now deprecated except for the options for `fraglib`, which are still maintained through the *OEOmega* interface.

  The following table shows the older, deprecated functions and their new option replacements:

Deprecated Method	New option Method
OEConfGen::OEOmega::SetCommentEnergy	OEConfGen::OEOmegaOptions::SetCommentEnergy
OEConfGen::OEOmega::GetCommentEnergy	OEConfGen::OEOmegaOptions::GetCommentEnergy
OEConfGen::OEOmega::SetIncludeInput	OEConfGen::OEOmegaOptions::SetIncludeInput
OEConfGen::OEOmega::GetIncludeInput	OEConfGen::OEOmegaOptions::GetIncludeInput
OEConfGen::OEOmega::SetRotorOffset	OEConfGen::OEOmegaOptions::SetRotorOffset
OEConfGen::OEOmega::GetRotorOffset	OEConfGen::OEOmegaOptions::GetRotorOffset
OEConfGen::OEOmega::SetSDEnergy	OEConfGen::OEOmegaOptions::SetSDEnergy
OEConfGen::OEOmega::GetSDEnergy	OEConfGen::OEOmegaOptions::GetSDEnergy
OEConfGen::OEOmega::SetWarts	OEConfGen::OEOmegaOptions::SetWarts
OEConfGen::OEOmega::GetWarts	OEConfGen::OEOmegaOptions::GetWarts
OEConfGen::OEOmega::SetBuildForceField	OEConfGen::OEOmegaOptions::SetBuildForceField
OEConfGen::OEOmega::GetBuildForceField	OEConfGen::OEOmegaOptions::GetBuildForceField
OEConfGen::OEOmega::SetCanonOrder	OEConfGen::OEOmegaOptions::SetCanonOrder
OEConfGen::OEOmega::GetCanonOrder	OEConfGen::OEOmegaOptions::GetCanonOrder
OEConfGen::OEOmega::SetFromCT	OEConfGen::OEOmegaOptions::SetFromCT
OEConfGen::OEOmega::GetFromCT	OEConfGen::OEOmegaOptions::GetFromCT
OEConfGen::OEOmega::SetFixRMS	OEConfGen::OEOmegaOptions::SetFixRMS
OEConfGen::OEOmega::GetFixRMS	OEConfGen::OEOmegaOptions::GetFixRMS
OEConfGen::OEOmega::SetFixDeleteH	OEConfGen::OEOmegaOptions::SetFixDeleteH
OEConfGen::OEOmega::GetFixDeleteH	OEConfGen::OEOmegaOptions::GetFixDeleteH
OEConfGen::OEOmega::SetFixUniqueMatch	OEConfGen::OEOmegaOptions::SetFixUniqueMatch
OEConfGen::OEOmega::GetFixUniqueMatch	OEConfGen::OEOmegaOptions::GetFixUniqueMatch
OEConfGen::OEOmega::SetFixMaxMatch	OEConfGen::OEOmegaOptions::SetFixMaxMatch
OEConfGen::OEOmega::GetFixMaxMatch	OEConfGen::OEOmegaOptions::GetFixMaxMatch
OEConfGen::OEOmega::SetStrictAtomTypes	OEConfGen::OEOmegaOptions::SetStrictAtomTypes
OEConfGen::OEOmega::GetStrictAtomTypes	OEConfGen::OEOmegaOptions::GetStrictAtomTypes
OEConfGen::OEOmega::SetStrictStereo	OEConfGen::OEOmegaOptions::SetStrictStereo
OEConfGen::OEOmega::GetStrictStereo	OEConfGen::OEOmegaOptions::GetStrictStereo
OEConfGen::OEOmega::SetEnumNitrogen	OEConfGen::OEOmegaOptions::SetEnumNitrogen
OEConfGen::OEOmega::GetEnumNitrogen	OEConfGen::OEOmegaOptions::GetEnumNitrogen
OEConfGen::OEOmega::SetEnumRing	OEConfGen::OEOmegaOptions::SetEnumRing
OEConfGen::OEOmega::GetEnumRing	OEConfGen::OEOmegaOptions::GetEnumRing
OEConfGen::OEOmega::SetSampleHydrogens	OEConfGen::OEOmegaOptions::SetSampleHydrogens
OEConfGen::OEOmega::GetSampleHydrogens	OEConfGen::OEOmegaOptions::GetSampleHydrogens
OEConfGen::OEOmega::SetEnergyWindow	OEConfGen::OEOmegaOptions::SetEnergyWindow
OEConfGen::OEOmega::GetEnergyWindow	OEConfGen::OEOmegaOptions::GetEnergyWindow
OEConfGen::OEOmega::SetEnergyRange	OEConfGen::OEOmegaOptions::SetEnergyRange
OEConfGen::OEOmega::GetEnergyRange	OEConfGen::OEOmegaOptions::GetEnergyRange
OEConfGen::OEOmega::SetMaxConfs	OEConfGen::OEOmegaOptions::SetMaxConfs
OEConfGen::OEOmega::GetMaxConfs	OEConfGen::OEOmegaOptions::GetMaxConfs
OEConfGen::OEOmega::SetMaxConfRange	OEConfGen::OEOmegaOptions::SetMaxConfRange
OEConfGen::OEOmega::GetMaxConfRange	OEConfGen::OEOmegaOptions::GetMaxConfRange
OEConfGen::OEOmega::SetMaxRotors	OEConfGen::OEOmegaOptions::SetMaxRotors
OEConfGen::OEOmega::GetMaxRotors	OEConfGen::OEOmegaOptions::GetMaxRotors
OEConfGen::OEOmega::SetMaxSearchTime	OEConfGen::OEOmegaOptions::SetMaxSearchTime
OEConfGen::OEOmega::GetMaxSearchTime	OEConfGen::OEOmegaOptions::GetMaxSearchTime

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Table 1 – continued from previous page

OEConfGen::OEOmega::SetRangeIncrement	OEConfGen::OEOmegaOptions::SetRangeIncrement
OEConfGen::OEOmega::GetRangeIncrement	OEConfGen::OEOmegaOptions::GetRangeIncrement
OEConfGen::OEOmega::SetRMSRange	OEConfGen::OEOmegaOptions::SetRMSRange
OEConfGen::OEOmega::GetRMSRange	OEConfGen::OEOmegaOptions::GetRMSRange
OEConfGen::OEOmega::SetRMSThreshold	OEConfGen::OEOmegaOptions::SetRMSThreshold
OEConfGen::OEOmega::GetRMSThreshold	OEConfGen::OEOmegaOptions::GetRMSThreshold
OEConfGen::OEOmega::SetSearchForceField	OEConfGen::OEOmegaOptions::SetSearchForceField
OEConfGen::OEOmega::GetSearchForceField	OEConfGen::OEOmegaOptions::GetSearchForceField
OEConfGen::OEOmega::SetTorsionDrive	OEConfGen::OEOmegaOptions::SetTorsionDrive
OEConfGen::OEOmega::GetTorsionDrive	OEConfGen::OEOmegaOptions::GetTorsionDrive
OEConfGen::OEOmega::SetDielectric	OEConfGen::OEOmegaOptions::SetDielectric
OEConfGen::OEOmega::GetDielectric	OEConfGen::OEOmegaOptions::GetDielectric
OEConfGen::OEOmega::SetExponent	OEConfGen::OEOmegaOptions::SetExponent
OEConfGen::OEOmega::GetExponent	OEConfGen::OEOmegaOptions::GetExponent
OEConfGen::OEOmega::SetFixMol	OEConfGen::OEOmegaOptions::SetFixMol
OEConfGen::OEOmega::GetFixMol	OEConfGen::OEOmegaOptions::GetFixMol
OEConfGen::OEOmega::SetFixFile	OEConfGen::OEOmegaOptions::SetFixFile
OEConfGen::OEOmega::ClearFixFile	OEConfGen::OEOmegaOptions::ClearFixFile
OEConfGen::OEOmega::SetFixQuery	OEConfGen::OEOmegaOptions::SetFixQuery
OEConfGen::OEOmega::SetFixSmarts	OEConfGen::OEOmegaOptions::SetFixSmarts
OEConfGen::OEOmega::GetFixSubSearch	OEConfGen::OEOmegaOptions::GetFixSubSearch
OEConfGen::OEOmega::SetTorLib	OEConfGen::OEOmegaOptions::SetTorLib
OEConfGen::OEOmega::GetTorLib	OEConfGen::OEOmegaOptions::GetTorLib

5.22 Omega TK 2.6.4

5.22.1 Minor bug fixes

- Memory allocation for limited stack memory usage has been improved.

5.23 Omega TK 2.6.3

5.23.1 Major bug fixes

- The problem of stripping off all SD data from a multi-conformer molecule has been fixed by introducing an overloaded version of the *OEFlipper* function that takes an OEMCMolBase object.

5.23.2 Minor bug fixes

- operator() no longer returns `true` when it fails due to a timeout.

5.23.3 Documentation changes

- Method operator() is now documented.

5.24 Omega TK 2.6.2

5.24.1 Major bug fixes

- *SetSearchForceField* and *SetBuildForceField* no longer accept illegal inputs and throw a warning for incorrect force field types.

5.24.2 Documentation changes

- *SetSearchForceField* and *SetBuildForceField* are now documented in more detail.

5.25 Omega TK 2.6.1

5.25.1 Minor bug fixes

- *OEOmegaGetLibraryRelease* and *OEOmegaGetLibraryVersion* will now throw deprecation warnings and will be removed in a future release. We recommend using *OEOmegaGetRelease* and *OEOmegaGetVersion* instead.

5.26 Omega TK 2.6.0

5.26.1 Major bug fixes

- *OEOmega* will no longer cause non-deterministic amounts of superfluous messages to be thrown to `OEThrow` when running in multiple threads. This had been happening because *OEOmega* calls `OEErrorHandler.SetLevel` to selectively silence warning messages it knows to be benign. This was fixed by only allowing the `OEErrorHandler.SetLevel` method to change the error level for the current thread, using an OEThreadLocal object to control message visibility.

> **See also**
>
> The **OpenEye** GitHub account contains an example of a multi-threaded OMEGA implementation.

5.26.2 Documentation changes

- *OEOmegaGetLibraryRelease* and *OEOmegaGetLibraryVersion* have been marked deprecated and will be removed in a future release. Please use *OEOmegaGetRelease* and *OEOmegaGetVersion* instead.

5.27 Omega TK 2.5.7

5.27.1 Minor bug fixes

- The *OEOmega* constructor will now initialize all data members appropriately to avoid subtle unreproducible errors based on random values in memory.
- Calling *SetWarts* with true had been broken until the 2014.Oct release. The output conformers would have the numeric index(wart) in the `.oeb` format but not the `.sdf` format. This is now fixed. The default behavior of OETautomerOptions has been changed from `true` to `false` when applying a numeric index(wart) to titles.

5.27.2 C#-specific changes

- *OETorLib.AddTorsionRule* is now usable from C#.

5.28 Omega TK 2.5.6

5.28.1 New features

- **Omega TK** conformers can be produced in `double` precision and round-tripped through rotor-offset-compress OEB files.

5.28.2 Minor bug fixes

- Rare possible race condition prevented.

5.28.3 Documentation fixes

- Examples will now check the return value of the omega process before writing out the molecule.

5.29 Omega TK 2.5.5

5.29.1 Minor bug fixes

- Removed unbounded stack allocations.

5.29.2 Documentation fixes

- **Omega TK** examples for Java, C#, and Python will now check to see whether *OEOmega* failed and not write the molecule in those cases.
- **Omega TK** examples for Java, C# and Python were renamed to more accurately reflect their function.
- `OETorLib.AddTorsionRule` more thoroughly documented.

5.30 Omega TK 2.5.4

5.30.1 New features

- The namespace `OESliceEnsembleDefaults` has been created with defaults for `OESliceEnsemble`. These defaults have been updated in order to match the defaults that OMEGA uses during conformer generation.

5.30.2 Major bug fixes

- Fixed possible crash caused when reading empty lines in torsion library files.
- Fixed a bug where `OENitrogenEnumeration.All` was equivalent to `OENitrogenEnumeration.Unspecified`. Now `OENitrogenEnumeration.All` will properly enumerate nitrogen atoms with specified stereochemistry.

5.30.3 Minor bug fixes

- A bug has been fixed where OESubSearch warnings could appear due to unset bond stereochemistry. Bond stereochemistry is now always set properly.

5.31 Omega TK 2.5.3

5.31.1 New features

- `OEAddGlobalFragLib` added to allow a given fragment library to be preloaded into the global fragment library where it can be shared among all *OEOmega* instances.

5.31.2 Minor bug fixes

- The wart symbol has been changed from @ to _ in order to help with parsing SMILES formatting.
- Bond stereochemistry is now properly perceived when strictstereo is set to *false*. Previously, there could be an *OESubSearch* warning due to unperceived bond stereochemistry.

- The *OENitrogenEnumeration* namespace has been created. The namespace constants should be used in place of magic numbers.

5.32 Omega TK 2.5.2

5.32.1 New features

- The fragment library is now shared across multiple instances of the *OEOmega* objects in a thread-safe manner. This can greatly reduce the amount of memory needed to run a multi-threaded version of Omega TK. For example, the memory consumption of Omega TK running across 8-cores dropped from 715MB to 258MB for 14,000 lead-like compounds from MDDR. This can also lead to a performance improvement since expensive fragment generation can sometimes be avoided if it has already been completed by another thread.

5.32.2 Minor bug fixes

- Now operator() will fail nicely and return false for non-3D input if *SetFromCT* is set to false.
- All ring bonds will be left unset by *OEFlipper* unless forceFlip=true.

5.33 Omega TK 2.5.1

5.33.1 New features

- An option has been added to allow hydrogen atoms in -OH, -SH, and amines to take part in conformational sampling. New methods have been added for accessing this option: *GetSampleHydrogens* and *SetSampleHydrogens*. By default, hydrogen atoms are not sampled.
- A warts option has been added to *OEFlipper*. Enabling this option will number the output molecules with an @ symbol.
- The parameterless version of *OEOmega.AddFragLib* will now load the built-in fraglib immediately. By default, the built-in fraglib does not load until operator() is called for the first time.

5.33.2 Major bug fixes

- Now using *SetFixSmarts* without *SetFixMol* will rematch for every input structure. Previously, this would only match the first input structure and reuse that match for the rest of the calculation. Using both *SetFixSmarts* and *SetFixMol* will continue to match against the fixmol and use that match for the entire calculation.
- Partial ring matching with *SetFixSmarts* or *SetFixMol* could cause a crash. Now only full ring systems may be specified and any attempt at matching a partial ring system will fail gracefully.
- The default value for max matches with *SetFixSmarts* or *SetFixMol* has been changed from 10 to 1. This value can be adjusted with *SetFixMaxMatch*.
- A bug has been fixed where multiple threads using OEOmega could cause a license failure.
- Planar molecules could have problems sprouting hydrogens when disabling *SetFromCT* because OMEGA was treating them as 2D. Now OMEGA will assume that planar molecules are properly defined 3D coordinates in this situation.
- Stereochemistry at the attachment points of rings with four or less atoms could be lost. Now stereochemistry is saved for rings of all sizes.
- A bug has been fixed where exceptionally long torsion rules could get cutoff early.

5.33.3 Minor bug fixes

- Only 3D coordinates were being cleared in FLIPPER. Now 2D coordinates are cleared as well.
- Fragment generation during an OMEGA calculation with *SetStrictFrags* enabled could yield slightly different fragments than the MakeFraglib app. This has been corrected for consistency.

5.33.4 Documentation fixes

- The *Omega TK* documentation was showing the incorrect version number.

5.34 Omega TK 2.5.0

5.34.1 New features

- The *Omega TK* library is now thread safe. Note, different *OEOmega* objects are still required per thread.

5.34.2 Major bug fixes

- *OEOmega* class would cause a crash on destruction whenever a copy was made. This has been fixed by specifying a proper copy constructor.

5.34.3 Minor bug fixes

- Tags for rotor compression are no longer attached to the output molecules when rotoroffsetcompress is false. It was discovered that these tags confuse VIDA when they are attached but not used.
- The torsion library has been updated with better angles for a biphenyl torsion. The entry for 90 degrees has been removed and +/-30 degrees has been added.

5.35 Omega TK 2.4.6

5.35.1 Minor bug fixes

- The treatment of single-atom systems has been changed to explicitly set the dimension to 3D so that they are not labeled 2D when writing to SDF format.

5.36 Omega TK 2.4.5

5.36.1 New features

- Now uses an extension of the MMFF94 force field for tricoordinate boron compounds. Most compounds containing B-X bonds where X=C,N,O,S, and H are covered with the following exceptions: X=N(imine),N(sulfonamide), N(pyridinium) and N(quaternary). Also not supported are compounds in which boron is bonded to X=F,Cl,Br,I,B and Si, or makes a bond angle BYX. Compounds in which boron is a part of four-membered rings of B1CCC1 type are also not available in the current parameterization because their existence is questionable: Ab initio calculations at the MP2/6-31G** level failed to identify stable structures for them (highly polar structures in which boron is four-coordinated are formed).

5.37 Omega TK 2.4.4

5.37.1 Bug fixes

- Fixed a bug where OMEGA wasn't checking if 3D construction of fragment generation was successful.

- Fixed a bug where output from flipper could still fail in OMEGA for missing stereo chemistry. Now the rules for required stereo chemistry are consistent.
- Fixed a bug where setting stereo chemistry in too small of a ring could cause a crash. Now only rings greater than 7 members and only one double bond will be set with flipper.

5.38 Omega TK 2.4.1

5.38.1 New features

- OMEGA and MakeFraglib may now be run with MPI using the *oempirun* script. (May not available on all platforms)
- The default for OMEGA has been changed to require all stereocenters to be specified. Molecules with any unspecified stereo will fail. The previous behavior was for OMEGA to choose a random stereoisomer. This default can be changed back to the previous behavior by setting *-strictstereo* to `false`.
- The default for OMEGA has been changed to no longer use 'close enough' atom typing. If a proper MMFF atom type cannot be found for an atom then the molecule will fail. Previous versions would use a different atom type of the same element if it was available. The previous behavior for atom type substitution can be enabled by setting *-strictatomtyping* to `false`.
- OMEGA now has the option to require on-the-fly generation of fragments to be the same as the MakeFraglib utility by setting *-strictfrags* to `true`. This fragment generation is more rigorous but also more time consuming.
- The convenience flag *-strict* has been added to turn on or off all of the strict options. These include *-strictstereo*, *-strictatomtyping* and *-strictfrags*.
- On-screen progress has been enabled for OMEGA and MakeFraglib using the *-progress* flag. The options are *none*, *dots*, *log*, and *percent*.
- The *-maxconfgen* and *-maxpoolsize* flags have been removed. These options are set internally and adjusted automatically subject to the user defined variable of *-maxconfs*. Additionally, hard limits have been removed from these variables and they are now only limited by available memory.
- The flag *-fixsmarts* has been created to allow a smarts pattern to be used to fix a portion of the molecule. This requires 3D coordinates to be available from either a 3D input file with *-fromCT* set to `false` or from a molecule set using *-fixfile*.

5.38.2 Bug fixes

- Crashes have been fixed that could occur when the *-fixfile* could not find a valid match or did not have enough atoms to match against in a ring system.
- Program no longer crashes if there is not enough memory for duplicate removal. If there is not enough memory available for allocation then the application will exit immediately.

5.39 Omega TK 2.4.0

5.39.1 New features

- The MaxConfGen and MaxPoolSize variables are now set internally and adjusted automatically subject to the user defined variable of MaxConfs. Additionally, hard limits have been removed from these variables and they are now only limited by available memory. The following methods are deprecated: *SetMaxConfGen*, *GetMaxConfGen*, *SetMaxPoolSize*, *GetMaxPoolSize*.

- The method *SetMaxConfs* has been changed from *void* to *bool*. The method will return `true` if the parameter has been set properly and will return `false` if the number is too high and would cause the memory required for duplicate removal to exceed the maximum theoretical memory for the platform.
- The method *SetFixSmarts* has been created to allow a smarts pattern to be used to fix a portion of the molecule. This requires 3D coordinates to be available from either a 3D input file with *SetFromCT* set to `false` or from a molecule set using *SetFixMol*.
- Fragment generation for *OEOmega* is now the same as the MakeFraglib application. Previous versions used a faster but more approximate version of fragment generation.
- The *OEOmega* default has been changed to no longer use "close enough" atom typing. If a proper MMFF atom type cannot be found for an atom then the molecule will fail. Previous versions would use a different atom type of the same element if it was available. The previous behavior of atom type substitution can be enabled by calling *SetStrictAtomTypes* with the argument `false`.
- The error level for most messages coming from the Omega library has been lowered to *Verbose*. The library can be run in a much quieter manner if the error level is set to *Info* by the user.

5.39.2 Bug fixes

- Crashes have been fixed that could occur when the FixFile could not find a valid match or did not have enough atoms to match against in a ring system.
- Program no longer crash if there is not enough memory for duplicate removal. If there is not enough memory available for allocation then duplicate removal will be skipped for the molecule and operator() will return `true`.

5.40 Omega TK 2.3.3

5.40.1 New features

- New API points have been added: *OETorLib.ResetTorsionLibrary*, *OETorLib.ClearTorsionLibrary*, and *OETorLib.AddTorsionRule*. The torsion rules may be created by passing in a `OEQMolBase` and `vector<int>` of angles, or by passing in a string with the standard rule format.
- The corresponding atom symbols, bond symbols, and torsion angles are now printed on a line under the matching smarts pattern.

5.40.2 Bug fixes

- Rotor offset compression is now set to `false` by default. Coordinate changes made in the toolkits after an Omega calculation are lost if rotor offset compression is set to `true`. If molecules are sent to `OEWriteMolecule` directly after an Omega run then rotor offset compression may safely be set to `true`, which will significantly reduce the filesize of the output.
- The energy window set by *SetEnergyRange* and *SetRangeIncrement* is now used consistently. Previous versions of Omega did not use this value properly for all aspects of an Omega calculation.

5.41 Omega TK 2.3.2

5.41.1 Bug fixes

- Fixed a bug where molecules containing boron or selenium could cause a crash. These molecules now are written to the *'.fail'* file due to missing force field parameters and the program will proceed to the next molecule.

5.42 Omega TK 2.3.1

5.42.1 New features

- The OMEGA application now includes a utility named oeb2sdconf that allows OMEGA generated conformers to be used with the MOE program. Please contact Chemical Computing Group support if you require assistance with this utility.

5.42.2 Bug fixes

- Fixed a bug where the omega2 PVM features would not work on some platforms.
- Fixed a bug where the omega2 script would not function properly with filenames that had spaces in them.

5.43 Omega TK 2.3.0

5.43.1 New features

- The distribution and installation of OMEGA has been modified. The Windows distribution is now a standard .exe installer, and the OS X distribution is a dmg containing a standard pkg installer. The executables are now scripts that chose the correct version of the program at runtime. Please see the Installation and Platform Notes for details.
- The defaults for MaxConfs and RMSThreshold are changed in this version. The default for MaxConfs is reduced from 400 to 200, while the value for RMSThreshold goes from 0.8 down to 0.5. These changes are based on maintaining good reproduction of the crystal structure test set, virtual screening tests with ROCS and FRED, and pose prediction tests with FRED.
- The method `OEConfGen::OEOmega::ClearFixFile` is added to the OMEGA library. This allows an `OEConfGen::OEOmega` instance to be reused for an unrestrained search after it has previously been used for a fixed search.
- Untitled molecules are given unique titles of omega_1, omega_2, and so on. Titles allow molecules to be located in the log files.

5.43.2 Bug fixes

- Fixed a major bug where molecules that have missing torsion rules caused OMEGA to crash. Molecules with missing torsion rules are now sent to the *omega2.fail* file and are not processed. Missing torsion rules are typically caused by highly unusual molecules for which OEChem cannot properly assign valence to all atoms.
- Fixed a bug in duplicate conformer removal that caused some conformers that should have been removed to pass through as unique. This bug also caused occurrences where a reduction in maxconfs led to an increase in the number of conformers returned.
- Fixed a bug that caused SD data on single conformer molecules to be removed.
- Fixed a bug in the *flipper* library that left 3D coordinates intact, which caused stereo chemistry to be ambiguous. The *flipper* library now replaces 3D coordinates with zeros.
- Fixed a bug where the `SyM` tag from previous OMEGA calculations caused problems when those molecules where passed back in. Also, the `O2MolId` tag is now removed from molecules before they are sent to the output.
- When the number of stereo centers exceeds the number of -maxcenters M, *flipper* now generates 2^M random non-repeating flips. Previous versions generated 2^M random flips, leading to molecules with the same stereochemistry being returned multiple times.

5.44 Omega TK 2.2.2

5.44.1 Bug fixes

- Fixed a major bug that would cause highly-symmetric, highly-fluorinated compounds to crash the program or hang a slave in PVM mode.
- Fixed a bug in atom typing when building fragments from scratch that, in some rare cases, could result in differing fragment geometries depending on the order of input of the molecules.
- Added more places that check for time exceeding max time. This is more just to prevent overly large molecules from appearing to hang.
- If OMEGA is called with a fixed predicate, this now implies that FromCT is false. In other words, if you want to use a predicate to fix atoms, you need to use a 3D structure as input.

5.45 Omega TK 2.2.1

5.45.1 Bug fixes

- The new build algorithm introduced in v2.2.0 could, on rare occasions, generate a structure with heavy atom clashes. This release is mainly a bug fix for this problem.

CHAPTER

SIX

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CHAPTER

SEVEN

SAMPLE CODE

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CHAPTER

EIGHT

CITATION

Please follow the guidelines in this document to cite use of our products in research publications and other documents.

For more information, please contact OpenEye Support.

8.1 Orion®

To cite use of Orion, please use the following:

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

For example:

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

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

8.2 Orion Floes

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

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

For example:

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

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

8.3 Toolkits and Applications

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

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

For example:

```
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.␣
↪http://www.eyesopen.com.
```

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.

8.4 Publications for Bibliographies

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

8.4.1 Orion

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

8.4.2 AFITT and FLYNN Applications

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

8.4.3 OEDocking Application and Toolkit

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

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

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

8.4.4 OMEGA Application and Toolkit

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

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

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

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

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

8.4.5 ROCS Application

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

8.5 OpenEye MMDS Web Service

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

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

For example:

```
Macromolecular Data Service 1.1. OpenEye, Cadence Molecular Sciences, Santa Fe, NM.␣
↪http://www.eyesopen.com.
```

The MMDS version number appears on the web service's release notes.

CHAPTER

NINE

TECHNOLOGY LICENSING

OpenEye products use the following technology under license.

Some of the open source technologies we use are licensed under the GNU Public License (GPL) version 2 or 3. In all instances, these technologies are communicated with using the "at arms length" principle, using pipes and command line arguments.

While the software is in some instances assembled into a container, that assembly does not invoke the GPL copyleft scope. For each Floe package where these are used, the environment log clearly details the installed programs and their version numbers. With the links below for each technology, the source for each of those programs is available.

Table 1: Licensed Technology

Name of Project	Website	License URL
_libgcc_mutex	https://github.com/conda-forge/_libgcc_mutex-feedstock	https://github.com/conda-forge/_libgcc_mutex-feedstock/blob/master/LICENSE.txt
_openmp_mutex	https://github.com/conda-forge/_openmp_mutex-feedstock	https://github.com/conda-forge/_openmp_mutex-feedstock/blob/main/LICENSE.txt
ablang2	https://github.com/TobiasHeOl/AbLang2	https://github.com/TobiasHeOl/AbLang2/blob/main/LICENSE
abseil-cpp	https://github.com/abseil/abseil-cpp	https://github.com/abseil/abseil-cpp/blob/master/LICENSE
absl-py	https://github.com/abseil/abseil-py	https://github.com/abseil/abseil-py/blob/main/LICENSE

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Table 1 – continued from previous page

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

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Table 1 – continued from previous page

Name of Project	Website	License URL
angular-loggly-logger	https://github.com/ajbrown/angular-loggly-logger	https://github.com/ajbrown/angular-loggly-logger/raw/master/LICENSE.md
angular-mocks	https://github.com/angular/angular.js	https://raw.githubusercontent.com/angular/angular.js/master/LICENSE
angular-resource	https://github.com/angular/angular.js	https://raw.githubusercontent.com/angular/angular.js/master/LICENSE
angular-toggle-switch	https://github.com/cgarvis/angular-toggle-switch	https://github.com/cgarvis/angular-toggle-switch/blob/master/LICENSE
angular-ui-grid	https://github.com/angular-ui/ui-grid	https://github.com/angular-ui/ui-grid
angular-ui-router	https://github.com/angular-ui/ui-router	https://github.com/angular-ui/ui-router/raw/master/LICENSE
angular-ui-tree	https://github.com/angular-ui-tree/angular-ui-tree	https://github.com/angular-ui-tree/angular-ui-tree/raw/master/LICENSE
angular-vs-repeat	https://github.com/kamilkp/angular-vs-repeat	https://raw.githubusercontent.com/kamilkp/angular-vs-repeat/master/LICENSE
aniso8601	https://bitbucket.org/nielsenb/aniso8601	https://bitbucket.org/nielsenb/aniso8601/src/master/LICENSE
annotated-types	https://github.com/annotated-types/annotated-types	https://github.com/annotated-types/annotated-types/blob/main/LICENSE
antlr4-python3-runtime	http://www.antlr.org OR https://pypi.org/project/antlr4-python3-runtin	https://github.com/conda-forge/antlr4-python3-runtin/blob/master/LICENSE.txt

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Table 1 – continued from previous page

Name of Project	Website	License URL
anyio	https://github.com/agronholm/anyio	https://github.com/agronholm/anyio/blob/master/LICENSE
appdirs	http://github.com/ActiveState/appdirs	http://github.com/ActiveState/appdirs/blob/master/LICENSE.txt
appengine	https://google.golang.org/appengine	https://github.com/golang/appengine/blob/master/LICENSE
arabic-reshaper	https://github.com/mpcabd/python-arabic-reshape	https://github.com/mpcabd/python-arabic-reshape/blob/master/LICENSE
archspec	https://github.com/archspec/archspec/blob/master/README.md	https://github.com/archspec/archspec/blob/master/COPYRIGHT
argon2-cffi	https://github.com/hynek/argon2-cffi	https://github.com/hynek/argon2-cffi/blob/master/LICENSE
argon2-cffi-bindings	https://github.com/hynek/argon2-cffi-bindings	https://github.com/hynek/argon2-cffi-bindings/blob/master/LICENSE
arpack	https://www.caam.rice.edu/software/ARPACK/	https://www.caam.rice.edu/software/ARPACK/
arrow	https://github.com/arrow-py/arrow	https://github.com/arrow-py/arrow?tab=Apache-2.0-1-ov-file#readme
ascii85	https://github.com/huandu/node-ascii85	https://github.com/huandu/node-ascii85/raw/master/LICENSE
ase	https://wiki.fysik.dtu.dk/ase/	https://wiki.fysik.dtu.dk/ase/development/licenseinfo.html#license-info
asgiref	https://github.com/django/asgiref/	https://github.com/django/asgiref/blob/main/LICENSE

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Table 1 – continued from previous page

Name of Project	Website	License URL
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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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

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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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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Table 1 – continued from previous page

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

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

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

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Name of Project	Website	License URL		
urllib3	https://urllib3.readthedocs.io/	https://github.com/urllib3/urllib3/blob/main/LICENSE.txt		
vine	https://github.com/celery/vine	https://github.com/celery/vine/blob/master/LICENSE		
vue	https://github.com/vuejs/vue	https://github.com/vuejs/vue/raw/master/LICENSE		
wadler_lindig	https://github.com/patrick-kidger/wadler_lindig	https://github.com/patrick-kidger/wadler_lindig?tab=Apache-2.0-1-ov-file#readme		
wadler_lindig	https://github.com/patrick-kidger/wadler_lindig	https://github.com/patrick-kidger/wadler_lindig?tab=Apache-2.0-1-ov-file#readmewcwidth	https://github.com/jquast/wcwidth	https://github.com/jquast/wcwidth/blob/master/LICENSE
wandb	https://github.com/wandb/wandb	https://github.com/wandb/wandb/blob/main/LICENSE		
webcolors	https://github.com/ubernostrum/webcolors	https://github.com/ubernostrum/webcolors?tab=BSD-3-Clause-1-ov-file#readme		
webencodings	https://github.com/gsnedders/python-webencodings	https://github.com/gsnedders/python-webencodings/blob/master/LICENSE		
websocket-client	https://github.com/websocket-client/websocket-client.git	https://github.com/websocket-client/websocket-client/blob/master/LICENSE		
Werkzeug	https://palletsprojects.com/p/werkzeug/	https://werkzeug.palletsprojects.com/en/2.1.x/license/		
westpa	http://github.com/westpa/westpa	https://github.com/westpa/westpa/blob/westpa2/LICENSE		
wheel	https://github.com/pypa/wheel	https://github.com/pypa/wheel/blob/main/LICENSE.txt		

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Name of Project	Website	License URL
widgetsnbextension	https://github.com/jupyter-widgets/ipywidgets#readme	https://github.com/jupyter-widgets/ipywidgets/blob/main/LICENSE
wrapt	https://github.com/GrahamDumpleton/wrapt	https://github.com/GrahamDumpleton/wrapt/blob/develop/LICENSE
wsutil	https://github.com/yhat/wsutil	https://github.com/yhat/wsutil/blob/master/LICENSE
x/lint	https://golang.org/x/lint	https://github.com/golang/lint/blob/master/LICENSE
x/mod	https://golang.org/x/mod/semver	https://cs.opensource.google/go/x/mod/+/master:LICENSE
x/net	https://golang.org/x/net	https://cs.opensource.google/go/x/net/+/master:LICENSE
x/oauth2	https://golang.org/x/oauth2	https://cs.opensource.google/go/x/oauth2/+/master:LICENSE
x/sys	https://golang.org/x/sys	https://cs.opensource.google/go/x/sys/+/master:LICENSE
x/text	https://golang.org/x/text	https://cs.opensource.google/go/x/text/+/master:LICENSE
x/tools	https://golang.org/x/tools	https://cs.opensource.google/go/x/tools/+/master:LICENSE
x/xerrors	https://golang.org/x/xerrors	https://cs.opensource.google/go/x/xerrors/+/master:LICENSE
xgboost	https://github.com/dmlc/xgboost	https://github.com/dmlc/xgboost/blob/master/LICENSE
xhtml2pdf	http://github.com/xhtml2pdf/xhtml2pdf	https://github.com/xhtml2pdf/xhtml2pdf/blob/master/LICENSE.txt

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Name of Project	Website	License URL
xlrd	https://github.com/python-excel/xlrd	https://github.com/python-excel/xlrd/blob/master/LICENSE
xlsxwriter	https://github.com/jmcnamara/XlsxWriter	https://github.com/jmcnamara/XlsxWriter/blob/main/LICENSE.txt
xmlsec	https://github.com/mehcode/python-xmlsec	https://github.com/mehcode/python-xmlsec/blob/master/LICENSE
xmltodict	https://github.com/martinblech/xmltodict	https://github.com/martinblech/xmltodict/blob/master/LICENSE
xorg-kbproto	https://gitlab.freedesktop.org/xorg/proto/kbproto	https://gitlab.freedesktop.org/xorg/proto/kbproto/-/blob/master/COPYING
xorg-libice	https://gitlab.freedesktop.org/xorg/lib/libice	https://gitlab.freedesktop.org/xorg/lib/libice/-/blob/master/COPYING
xorg-libsm	https://gitlab.freedesktop.org/xorg/lib/libsm	https://gitlab.freedesktop.org/xorg/lib/libsm/-/blob/master/COPYING
xorg-libx11	https://gitlab.freedesktop.org/xorg/lib/libx11	https://gitlab.freedesktop.org/xorg/lib/libx11/-/blob/master/COPYING
xorg-libxau	https://gitlab.freedesktop.org/xorg/lib/libxau	https://gitlab.freedesktop.org/xorg/lib/libxau/-/blob/master/COPYING
xorg-libxdmcp	https://gitlab.freedesktop.org/xorg/lib/libxdmcp	https://gitlab.freedesktop.org/xorg/lib/libxdmcp/-/blob/master/COPYING

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Name of Project	Website	License URL
xorg-libxext	https://gitlab.freedesktop.org/xorg/lib/libxext	https://gitlab.freedesktop.org/xorg/lib/libxext/-/blob/master/COPYING
xorg-libxrender	https://gitlab.freedesktop.org/xorg/lib/libxrender	https://gitlab.freedesktop.org/xorg/lib/libxrender/-/blob/master/COPYING
xorg-libxt	https://gitlab.freedesktop.org/xorg/lib/libxt	https://gitlab.freedesktop.org/xorg/lib/libxt/-/blob/master/COPYING
xorg-renderproto	https://gitlab.freedesktop.org/xorg/proto/renderproto	https://gitlab.freedesktop.org/xorg/proto/renderproto/-/blob/master/COPYING
xorg-xextproto	https://gitlab.freedesktop.org/xorg/proto/xextproto	https://gitlab.freedesktop.org/xorg/proto/xextproto/-/blob/master/COPYING
xorg-xproto	https://gitlab.freedesktop.org/xorg/proto/xproto	https://gitlab.freedesktop.org/xorg/proto/xproto/-/blob/master/COPYING
xxhash	https://github.com/cespare/xxhash/v2	https://github.com/cespare/xxhash/blob/main/LICENSE.txt
xz	https://github.com/ulikunitz/xz	https://github.com/ulikunitz/xz/blob/master/LICENSE
yaml	https://pyyaml.org/	https://github.com/yaml/pyyaml/blob/master/LICENSE
yaml-cpp	https://github.com/jbeder/yaml-cpp	https://github.com/jbeder/yaml-cpp/blob/master/LICENSE
yaml.v2	https://gopkg.in/yaml.v2	https://github.com/go-yaml/yaml/blob/v2.4.0/LICENSE
yaml.v3	https://gopkg.in/yaml.v3	https://github.com/go-yaml/yaml/blob/v3/LICENSE

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Name of Project	Website	License URL
yarl	https://github.com/aio-libs/yarl/	https://github.com/aio-libs/yarl/blob/master/LICENSE
yaspin	https://github.com/pavdmyt/yaspin	https://github.com/pavdmyt/yaspin/blob/master/LICENSE
yfiles	https://www.yworks.com/products/yfiles	commercial license
yml	https://pypi.org/project/yml/	N/A
zap	https://go.uber.org/zap	https://github.com/uber-go/zap/blob/master/LICENSE.txt
zipp	https://github.com/jaraco/zipp	https://github.com/jaraco/zipp/blob/main/LICENSE
zlib	https://zlib.net/	https://zlib.net/zlib_license.html
zstandard	https://github.com/indygreg/python-zstandard	https://github.com/indygreg/python-zstandard/blob/main/LICENSE
zstd	https://facebook.github.io/zstd/	https://github.com/facebook/zstd/blob/dev/LICENSE
click-option-group	https://github.com/click-contrib/click-option-group	https://github.com/click-contrib/click-option-group/blob/master/LICENSE

9.1 GCC

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

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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.

9.1.1 GCC RUNTIME LIBRARY EXCEPTION

```
Version 3.1, 31 March 2009

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This GCC Runtime Library Exception ("Exception") is an additional permission under␣
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When you use GCC to compile a program, GCC may combine portions of certain GCC header␣
↪files and runtime libraries with
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↪(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.

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You have permission to propagate a work of Target Code formed by combining the Runtime␣
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licensing of the Independent Modules.

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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

9.1.2 GNU GENERAL PUBLIC LICENSE

```
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                       Version 3, 29 June 2007

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pattern of such abuse occurs in the area of products for individuals to
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stand ready to extend this provision to those domains in future versions
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  Finally, every program is threatened constantly by software patents.
States should not allow patents to restrict development and use of
software on general-purpose computers, but in those that do, we wish to
avoid the special danger that patents applied to a free program could
make it effectively proprietary.  To prevent this, the GPL assures that
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  The precise terms and conditions for copying, distribution and
modification follow.

                    TERMS AND CONDITIONS

  0. Definitions.

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  To "modify" a work means to copy from or adapt all or part of the work
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  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
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Major Component, or to implement a Standard Interface for which an
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"Major Component", in this context, means a major essential component
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produce the work, or an object code interpreter used to run it.

  The "Corresponding Source" for a work in object code form means all
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work) run the object code and to modify the work, including scripts to
control those activities.  However, it does not include the work's
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
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   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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  customarily used for software interchange.

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

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

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

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

  A separable portion of the object code, whose source code is excluded
from the Corresponding Source as a System Library, need not be
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of the particular user or of the way in which the particular user
actually uses, or expects or is expected to use, the product.  A product
is a consumer product regardless of whether the product has substantial
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the only significant mode of use of the product.

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

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

  The requirement to provide Installation Information does not include a
requirement to continue to provide support service, warranty, or updates
for a work that has been modified or installed by the recipient, or for
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  Corresponding Source conveyed, and Installation Information provided,
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