

OpenEye
SCIENTIFIC

Zap TK – Java

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Cadence Design Systems, Inc.

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CHAPTER

ONE

THEORY AND EXAMPLES

1.1 The What of Zap

"A Smooth Permittivity Function for Poisson-Boltzmann Solvation Methods," J. Andrew Grant, Barry T. Pickup and Anthony Nicholls, J. Comp. Chem, Vol 22, No.6, pgs 608-640, April 2001.

ZAP is, at its heart, a Poisson-Boltzmann (PB) solver. The Poisson equation describes how electrostatic fields change in a medium of varying dielectric, such as an organic molecule in water. The Boltzmann bit adds in the effect of mobile charge, e.g. salt. PB is an effective way to simulate the effects of water in biological systems. It relies on a charge description of a molecule, the designation of low (molecular) and high (solvent) dielectric regions and a description of an ion-accessible volume and produces a grid of electrostatic potentials. From this, transfer energies between different solvents, binding energies, pKa shifts, pI's, solvent forces, electrostatic descriptors, solvent dipole moments, surface potentials and dielectric focusing can all be calculated. As electrostatics is one of the two principal components of molecular interaction (the other, of course, being shape), ZAP is OpenEye's attempt to get it right.

1.2 The Why of Zap

ZAP happened by surprise. It had always been at the back of my mind that Something Should Be Done About DelPhi, the program written at Columbia University in the lab of Barry Honig by Barry, Kim Sharp, Mike Gilson, Shridhara Shridharan and me. While a very useful program, it was getting harder and harder to develop, partly because it was written in FORTRAN (not that there's anything wrong with that), partly because that's just the way academic code is. We don't know how to program but we want answers and we want them now.

ZAP really came about because of Andrew Grant. Andy was in the Scheraga lab struggling, as most of us do, with the nonlinear PB equation. He left to join AstraZeneca in 1993 but we kept in contact. In '95, he and Barry Pickup at the University of Sheffield published a remarkable paper (J. Comp. Chem.). They reported the hard-sphere volume of a molecule could be calculated to 0.1% accuracy by using atom-centered Gaussians. The correspondence between a discrete and a smooth, continuous function was nothing short of remarkable. Since the dielectric approach of PB is essentially volumetric because molecules are low-dielectric and solvent high, it occurred to us that this was the bedrock on which to build a new PB approach. That approach became ZAP.

There were several reasons to be excited about the Gaussian based approach. A smooth-function dielectric mapped onto a grid has few of the numerical problems plaguing DelPhi - instability with respect to grid placement, sensitivity to grid spacing. Also it is an interesting alternative physical model to most PB implementations. Typically it is assumed that the dielectric changes from molecular to solvent "discretely," or infinitely fast. Why? As there was no experimental information on the variation of dielectric it was the simplest assumption and also the simplest to implement. As is often the way with a successful scientific approach, these early decisions become ossified over time.

Another ossification is the choice of molecular surface as the dielectric threshold, as first proposed by BH (J. Phys. Chem). It is not a bad choice. If a water molecule is excluded from some crevice of a molecule that ought to be reflected in a lower dielectric in the crevice: a molecular surface-delimited volume reflects this where an atomic surface does not. There was also a numerical issue. When Mike Gilson first applied DelPhi to proteins (PROTEINS: Vol 17..), the atomic approach would place grid points randomly in tiny solvent crevices. Moving the protein relative to the grid

shuffled the grid representation of the protein interior leading to large, unphysical changes in energy. The molecular surface removed these crevices unless they were large enough to fit a whole water molecule, in which case a high dielectric assignment was not unreasonable.

In retrospect, however, the molecular surface is a terrible choice! It's difficult to calculate and unstable with respect to small displacements of atoms or to the choice of a radius for water. And there is always the question of what dielectric should be assigned to the volume that lies between the molecular and the atomic surfaces.

The Gaussian approach answers several of the physical objections. First and foremost, the dielectric varies smoothly from interior to exterior. Although we made no attempt to correlate this variation with empirical evidence, choosing instead to match our method to DelPhi energies, the variation of polarizability over a span of about one Angstrom is physically appealing. Secondly, we achieve much of the crevice exclusion that the molecular surface produces. Because the Gaussian functions spread out beyond the hard sphere radius of each atom, a crevice receives density contributions from all neighboring atoms, lowering its dielectric to molecular levels. Thirdly, we do not see water "pops", those large changes in dielectric from small atomic displacements (or, worse, small changes of the protein placement on the grid) that occur in active sites. The Gaussian effectively interpolates between water absence and presence.

An advantage to this approach that we did not anticipate was its correspondence to DelPhi when applied to proteins. We parameterized the dielectric variation in ZAP so that it agrees with DelPhi for small molecules ("we" meaning Christine Kitchen's heroic work for her Ph.D. thesis). Given that the difference between the molecular surface and Gaussian model will be much larger for proteins with concavities, crevices and internal water pockets, we wondered how well the two would agree. The remarkable finding was that ZAP applied to proteins looks like DelPhi with twice the polarizability: ZAP with internal dielectric set to 2.0 looks like DelPhi set to 4.0. Why is this useful? Because there is circumstantial and theoretical evidence that 4.0 is a good dielectric to use with DelPhi for proteins, but that always left a loose thread in applying the method to protein-drug interactions - small molecules should have a dielectric of 2.0, proteins 4.0, but DelPhi only allows you to choose one internal dielectric. With ZAP it appears you get the best of both worlds. Protein and drug are set to internal dielectrics of 2.0 and because the protein is a little more "hydrated" in ZAP, it acts like the dielectric is set to 4.0. Please note that while 2.0 is the historic value for the inner dielectric, the current recommended value for the inner dielectric while using ZAP is 1.0.

On the numerical side, every advantage we had hoped for in ZAP came to pass. As mentioned in the previous section, we saw faster convergence, remarkable stability with respect to grid placement and much improved asymptotic behavior with decreasing grid spacing. We also, for the first time, had gradients that could be applied in dynamics or minimization.

1.3 The Way of Zap

There follow a dozen or so examples of using ZAP. The list is always growing because the toolkit philosophy really does work. Most of the examples use OEInterface to provide consistent command-line argument handling.

1.3.1 Partial Charges and Atomic Radii

There are three essential quantities for any PB calculation: coordinates, dielectric model (including radii), and charge. Coordinates will come from the atomic coordinates of the input molecule, but partial charges and the dielectric model deserve some extra attention.

Charges and radii can be calculated at run-time using functions provided by OEChem or other OpenEye toolkits (AM1-BCC charges from **Quacpac TK** for example). The dielectric model consists of both the value of the inner and outer dielectric, as well as how the dielectric adjusts from one to the other. ZAP uses atomic radii as the basis for its dielectric algorithm. By default, we recommend using Bondi VdW radii which can be set on a molecule using the function OEAssignBondiVdWRadii Or you can set specific radii on an atom-by-atom basis using the OEAtomBase::SetRadius function.

The current recommended value for the inner and outer dielectrics for a molecule in an aqueous solution are 1.0 and 80.0. Therefore, these are the default values for the OEZap and OEBind implementations. The historic value for the

inner dielectric is 2.0, and this value may be set using the SetInnerDielectric method. Additionally, the default value for the inner dielectric of the OEET implementation remains at 2.0 for the time being.

Accurate PB calculations also depend on quality atomic charges. In OEChem, we provide MMFF94 partial charges as the lowest level of charges that we consider usable in PB. The examples that follow will use these charges, so that they don't depend on any toolkits beside ZAP and OEChem. But for production use, we recommend AM1-BCC charges

If your input file format can store partial charges and/or radii, you can use those values instead of calculating them at run time. OEB files can store radii and partial charges, so they serve as a useful intermediate file between many OpenEye programs. Note that charges and radii will only be written to an OEB file if they are present on the molecule when written.

Atomic charges can come in a PDB file, along with atomic radii, in the form of the extra fields added after the coordinates. This style originated with DelPhi. Note that to get OEChem to read charges and radii from these fields in a PDB file, you need to set a specific flavor on the input oemolistream before reading any molecules from the stream.

Example of using OEChem to read charges and radii from PDB

```
oemolistream ifs = new oemolistream();
ifs.SetFlavor(OEFormat.PDB, OEIFlavor.PDB.Default | OEIFlavor.PDB.DELPHI);
```

1.3.2 Grids

ZAP uses regular cubic lattices, or grids, to solve the PB equation. The examples here illustrate how to retrieve such from the calculation and to manipulate and store the information held by each. Typically, grids are not used per se but information is extracted, such as the potential at particular points in space, as is illustrated in the next section. However, some programs, such as VIDA, can read grids and display their properties. Also, having direct access to grids allows for manipulations of the potential map that may not have been anticipated.

This first example shows the simplest method of generating a grid of potentials using ZAP. We save the grid in OpenEye GRD (*.grd) format which is a compact, binary format that can be visualized in VIDA. Alternatively, the grid can be written into GRASP format (*.phi), which means that the grid stored will be 65 cubed regardless of the size of the grid used in the calculation. A 65^3 grid is obtained by interpolation to a grid with that many points that fits over the largest dimension of the grid calculated.

Listing 1: Calculating a potential grid

```
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```
package openeye.examples.oezap;

import openeye.oechem.*;
import openeye.oegrid.*;
import openeye.oezap.*;

public class ZapGrid1 {

    public static void main(String argv[]) {
        if (argv.length != 1) {
            System.err.println("usage: ZapGrid1 <molfile>");
            System.exit(1);
        }

        OEGraphMol mol = new OEGraphMol();
        oemolistream ifs = new oemolistream();
        if (!ifs.open(argv[0])) {
            System.err.println("Unable to open for reading: " + argv[0]);
            System.exit(1);
        }
        oechem.OEReadMolecule(ifs, mol);
        oechem.OEAssignBondiVdWRadii(mol);
        oechem.OEMMFFAtomTypes(mol);
        oechem.OEMMFF94PartialCharges(mol);
        ifs.close();

        OEZap zap = new OEZap();
        zap.SetInnerDielectric(1.0f);
        zap.SetGridSpacing(0.5f);
        zap.SetMolecule(mol);

        OEScalarGrid grid = new OEScalarGrid();
        if (zap.CalcPotentialGrid(grid))
            oegrid.OEWriteGrid("zap.grd", grid);
        zap.delete();
    }
}
```

The next example is an elaboration of the previous simple version where we add in control of the parameters of the calculation. Options are provided to set the internal and external (solute and solvent) dielectric constants, the distance between the molecule and the edges of the grid (boundary spacing or buffer) and the grid spacing. A smaller grid spacing implies a more dense and accurate grid, but it does come with a larger memory footprint.

Listing 2: Calculating potential grid with optional parameters

```
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*/
package openeye.examples.oezap;

import java.net.URL;
import openeye.oechem.*;
import openeye.oegrid.*;
import openeye.oezap.*;

public class ZapGrid2 {
    static {
        oechem.OEThrow.SetStrict(true);
    }

    private void createGrid(OEInterface itf) {
        OEGraphMol mol = new OEGraphMol();
        oemolistream ifs = new oemolistream();
        if (!ifs.open(itf.GetString("-in"))) {
            System.err.println("Unable to open for reading: " + itf.GetString("-in"));
            System.exit(1);
        }
        oechem.OEReadMolecule(ifs, mol);
        oechem.OEAssignBondiVdWRadii(mol);
        oechem.OEMMFFAtomTypes(mol);
        oechem.OEMMFF94PartialCharges(mol);
        ifs.close();

        OEZap zap = new OEZap();
        zap.SetInnerDielectric(itf.GetFloat("-epsin"));
        zap.SetOuterDielectric(itf.GetFloat("-epsout"));
        zap.SetGridSpacing(itf.GetFloat("-grid_spacing"));
        zap.SetBoundarySpacing(itf.GetFloat("-buffer"));
        zap.SetMolecule(mol);

        OEScalarGrid grid = new OEScalarGrid();
        if (zap.CalcPotentialGrid(grid)) {
            if (itf.GetBool("-mask")) {
                oegrid.OEMaskGridByMolecule(grid, mol);
            }
        }
        oegrid.OEWriteGrid(itf.GetString("-out"), grid);
        zap.delete();
    }
```

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```
    public static void main(String argv[]) {
        ZapGrid2 app = new ZapGrid2();
        OEInterface itf = new OEInterface();
        URL fileURL = app.getClass().getResource("ZapGrid2.txt");
        try {
            oechem.OEConfigureFromURL(itf, fileURL);
            if (oechem.OECheckHelp(itf, argv)) {
                return;
            }
            oechem.OEParseCommandLine(itf, argv);
            app.createGrid(itf);
        } catch (java.io.IOException e) {
            System.err.println("Unable to open interface file");
        }
    }
}
```

Here we show how to calculate a difference-map, that is to say the potential difference between a standard, two dielectric, calculation and a single dielectric calculation (approximating pure Coulombic potentials). These difference potentials represent the electrostatic response of the solvent to the charges within the solute molecule. If we mask away everything outside the molecule, we can see the contributions from the charges inside the molecule.

Listing 3: Calculating potential grid with optional parameters

```
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*/
package openeye.examples.oezap;

import openeye.oechem.*;
import openeye.oegrid.*;
import openeye.oezap.*;

public class ZapGrid3 {

    public static void main(String argv[]) {
```

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```
        if (argv.length != 1) {
            System.err.println("usage: ZapGrid3 <molfile>");
            System.exit(1);
        }

        OEGraphMol mol = new OEGraphMol();
        oemolistream ifs = new oemolistream();
        if (!ifs.open(argv[0])) {
            System.err.println("Unable to open for reading: " + argv[0]);
            System.exit(1);
        }
        oechem.OEReadMolecule(ifs, mol);
        ifs.close();

        oechem.OEAssignBondiVdWRadii(mol);
        oechem.OEMMFFAtomTypes(mol);
        oechem.OEMMFF94PartialCharges(mol);

        OEZap zap = new OEZap();
        zap.SetInnerDielectric(1.0f);
        zap.SetGridSpacing(0.5f);
        zap.SetMolecule(mol);

        // calculate standard 2-dielectric grid
        OEScalarGrid grid1 = new OEScalarGrid();
        zap.CalcPotentialGrid(grid1);

        // calculate grid with single dielectric
        OEScalarGrid grid2 = new OEScalarGrid();
        zap.SetOuterDielectric(zap.GetInnerDielectric());
        zap.CalcPotentialGrid(grid2);

        // take the difference
        oegrid.OESubtractScalarGrid(grid1, grid2);

        // mask out everything outside the molecule
        oegrid.OEMaskGridByMolecule(grid1, mol, OEGridMaskType.GaussianMinus);

        oegrid.OEWriteGrid("zap_diff.grd", grid1);

        // explicit clean ups
        grid1.delete();
        grid2.delete();
        zap.delete();
    }
}
```

1.3.3 Atom Potentials

The potentials at any charge, as calculated by PB, can be decomposed into three forms

1. Induced solvent potential: the potential produced by the polarization of the solvent.

2. Inter-charge Coulombic energy: the potential that would be produced if the solvent had the same dielectric as the solute molecule from all other charges.
3. Self potential: the potential produced by a charge at itself. Of course, as mentioned above, this is infinite analytically, but PB will produce an "approximation" to this infinity because the grid spacing is finite.

This example program shows how to calculate each of these quantities. In addition to command line flags to control dielectric, grid spacing, etc., there are three flags that affect the type of potentials calculated:

- -calc_type solvent_only
- -calc_type remove_self
- -calc_type coulombic

With none of these flags, the code executes a single PB calculation, interpolates the potentials from the grid produced, reports the sum of these potentials multiplied by the charge on the respective atoms and outputs these potentials and charges in a table. This potential corresponds to (a)+(b)+(b) above.

Using the -calc_type solvent_only option executes two PB calculations, the standard calculation plus a second calculation where the external dielectric has been set to the solute dielectric. The atom potentials are then formed from the difference of these two calculations such that the remaining potential is that produced by the solvent alone. The sum of this set of atomic potentials multiplied by atomic charges all multiplied by 0.5 is the electrostatic component of transferring from a media of the same dielectric as the solute to water. These potentials correspond to (a) above.

The -calc_type remove_self flag for the example program below executes an internal algorithm in the ZAP toolkit that extracts from each atom potential that potential produced by that atom, if it is charged. This it removes the artifactual energy from the grid, i.e. energy that is not actually physical but a manifestation of the finite resolution of the grids used. The remaining potential is then that from the solvent and that from all the other charges, that is (a)+(b) above.

The -calc_type coulombic flag actually prevents any PB calculation. It merely uses Coulomb's Law to calculate the potential (b), the inner-atomic Coulombic potential.

Listing 4: Calculating atom potentials

```
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or its use.
*/
package openeye.examples.oezap;

import java.net.URL;
import openeye.oechem.*;
import openeye.oezap.*;
```

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```
public class ZapAtoms1 {
    static {
        oechem.OEThrow.SetStrict(true);
    }

    private static void Output(OEMolBase mol, OEFloatArray apot, boolean atomtable) {
        System.out.println("Title: " + mol.GetTitle());
        if (atomtable) {
            System.out.println("Atom potentials");
            System.out.println("Index Elem Charge Potential");
        }
        double energy = 0.0f;
        OEAtomBaseIter aiter = mol.GetAtoms();
        while (aiter.hasNext()) {
            OEAtomBase atom = aiter.next();
            energy += atom.GetPartialCharge() * apot.getItem(atom.GetIdx());
            if (atomtable) {
                System.out.println(String.format("%4d   %2s   %4.1f  %8.3f",
                        atom.GetIdx(),
                        oechem.OEGetAtomicSymbol(atom.GetAtomicNum()),
                        atom.GetPartialCharge(),
                        apot.getItem(atom.GetIdx())));
            }
        }
        System.out.println("Sum of (Potential * Charge * 0.5) in kT = " + energy * 0.5f);
    }

    private void Calc(OEInterface itf) {
        OEGraphMol mol = new OEGraphMol();
        oemolistream ifs = new oemolistream();
        String infile = itf.GetString("-in");

        if (!ifs.open(infile)) {
            System.err.println("Unable to open for reading: " + infile);
            System.exit(1);
        }
        oechem.OEReadMolecule(ifs, mol);
        oechem.OEAssignBondiVdWRadii(mol);

        if (!itf.GetBool("-file_charges")) {
            oechem.OEMMFFAtomTypes(mol);
            oechem.OEMMFF94PartialCharges(mol);
        }
        ifs.close();

        OEZap zap = new OEZap();
        zap.SetMolecule(mol);
        zap.SetInnerDielectric(itf.GetFloat("-epsin"));
        zap.SetBoundarySpacing(itf.GetFloat("-boundary"));
        zap.SetGridSpacing(itf.GetFloat("-grid_spacing"));
```

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```
        String calcType = itf.GetString("-calc_type");
        if (calcType.equals("default")) {
            OEFloatArray apot = new OEFloatArray(mol.GetMaxAtomIdx());
            zap.CalcAtomPotentials(apot);
            System.out.println("Before Output");
            Output(mol, apot, itf.GetBool("-atomtable"));
        } else if (calcType.equals("solvent_only")) {
            OEFloatArray apot = new OEFloatArray(mol.GetMaxAtomIdx());
            zap.CalcAtomPotentials(apot);
            OEFloatArray apot2 = new OEFloatArray(mol.GetMaxAtomIdx());
            zap.SetOuterDielectric(zap.GetInnerDielectric());
            zap.CalcAtomPotentials(apot2);
            OEAtomBaseIter aiter = mol.GetAtoms();
            float potdiff;
            while (aiter.hasNext()) {
                OEAtomBase atom = aiter.next();
                potdiff = apot.getItem(atom.GetIdx()) - apot2.getItem(atom.GetIdx());
                apot.setItem(atom.GetIdx(), potdiff);
            }
            Output(mol, apot, itf.GetBool("-atomtable"));
        } else if (calcType.equals("remove_self")) {
            OEFloatArray apot = new OEFloatArray(mol.GetMaxAtomIdx());
            zap.CalcAtomPotentials(apot);
            Output(mol, apot, itf.GetBool("-atomtable"));
        } else if (calcType.equals("coulombic")) {
            float x = oezaplib.OECoulombicSelfEnergy(mol, itf.GetFloat("-epsin"));
            System.out.println("Coulombic Assembly Energy ");
            System.out.println("Sum of {Potential * Charge over all atoms * 0.5} in kT =
↪" + x);
        }
        zap.delete();
    }

    public static void main(String argv[]) {
        ZapAtoms1 app = new ZapAtoms1();
        OEInterface itf = new OEInterface();

        URL fileURL = app.getClass().getResource("ZapAtoms1.txt");
        try {
            oechem.OEConfigureFromURL(itf, fileURL);
            if (oechem.OECheckHelp(itf, argv)) {
                return;
            }
            oechem.OEParseCommandLine(itf, argv);
            app.Calc(itf);
        } catch (java.io.IOException e) {
            System.err.println("Unable to open interface file");
        }
    }
}
```

1.3.4 Solvation Energies: PBSA

A principle use of PB is to calculate the energy stored in the exterior dielectric, for example the partial alignment of water dipoles. This corresponds to the difference between a calculation with uniform dielectric and one with a different external dielectric. In the examples for atom potentials this would be the sum of the solvent potentials at each atom, multiplied by the charges on that atom all multiplied by 0.5.

However, we know water also has an energy component due to hydrophobicity, which is typically estimated as a constant (approximately 10-25 calories per square Angstrom) multiplied by the accessible area of the molecule. This value is an open scientific question. We recommend using 10 for vacuum-water transfer energies and 25 for protein calculations, but ultimately your own scientific judgment should be used. These examples include an area calculation. Taken together these numbers are an approximation of the transfer energy from a low dielectric medium (alkane solvent, protein interior) into water.

The following examples use the OEArea object to calculate the accessible surface area of the molecule. The area is calculated using the same grid based Gaussians that ZAP uses. Therefore, it will not give the same results as triangle summation methods for calculating surface area, which are used in OESpicoli.

Listing 5: Calculating solvation energies

```
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*/
package openeye.examples.oezap;

import openeye.oechem.*;
import openeye.oezap.*;

public class ZapSolv1 {

    private static float epsin = 1.0f;

    public static void main(String argv[]) {
        if (argv.length != 1) {
            System.err.println("usage: ZapSolv1 <molfile>");
            System.exit(1);
        }

        OEZap zap = new OEZap();
        zap.SetInnerDielectric(epsin);
```

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```
        zap.SetGridSpacing(0.5f);

        OEArea area = new OEArea();

        oemolistream ifs = new oemolistream();
        if (!ifs.open(argv[0])) {
            System.err.println("Unable to open for reading: " + argv[0]);
            System.exit(1);
        }
        OEGraphMol mol = new OEGraphMol();
        while (oechem.OEReadMolecule(ifs, mol)) {
            oechem.OEAssignBondiVdWRadii(mol);
            oechem.OEMMFFAtomTypes(mol);
            oechem.OEMMFF94PartialCharges(mol);
            zap.SetMolecule(mol);
            float solv = zap.CalcSolvationEnergy();
            float aval = area.GetArea(mol);
            float coul = oezaplib.OECoulombicSelfEnergy(mol, epsin);
            float total = 0.59f * solv + 0.025f * aval;
            System.out.println("Title: " + mol.GetTitle());
            System.out.println("  Solv (kcal)          : " + 0.59 * solv);
            System.out.println("  Area (Ang^2)         : " + aval);
            System.out.println("  Total (kcal)         : " + total);
            System.out.println("  Int.Coulombic (kcal): " + 0.59 * coul);
            System.out.println();
        }
        ifs.close();
        area.delete();
        zap.delete();
    }
}
```

This next solvation example calculates the transfer energy from vacuum to water.

Listing 6: Calculating vacuum-water transfer energies

```
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```

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```
or its use.
*/
package openeye.examples.oezap;

import openeye.oechem.*;
import openeye.oezap.*;

public class ZapTransfer {

    private static float epsin = 1.0f;

    public static void main(String argv[]) {
        if (argv.length != 1) {
            System.err.println("usage: ZapTransfer <molfile>");
            System.exit(1);
        }

        OEZap zap = new OEZap();
        zap.SetInnerDielectric(epsin);
        zap.SetGridSpacing(0.5f);

        OEArea area = new OEArea();

        oemolistream ifs = new oemolistream();
        if (!ifs.open(argv[0])) {
            System.err.println("Unable to open for reading: " + argv[0]);
            System.exit(1);
        }
        OEGraphMol mol = new OEGraphMol();
        while (oechem.OEReadMolecule(ifs, mol)) {
            oechem.OEAssignBondiVdWRadii(mol);
            oechem.OEMMFFAtomTypes(mol);
            oechem.OEMMFF94PartialCharges(mol);
            zap.SetMolecule(mol);
            float solv = zap.CalcSolvationEnergy();
            float aval = area.GetArea(mol);
            float total = 0.59f * solv + 0.010f * aval;
            System.out.println("Title: " + mol.GetTitle());
            System.out.println("Vacuum->Water(kcal)        : " + total);
            System.out.println();
        }
        ifs.close();
        area.delete();
        zap.delete();
    }
}
```

1.3.5 Binding Energies

Binding energies and other binding related properties can be calculated using the *OEBind* class. The OEBind class serves two primary purposes: 1) to have a class in place for users to easily calculate binding related data, and 2) to show how binding related data may be calculated. OEBind is not particularly well-suited for extremely efficient calculations

required by simulations. This is because some of the data available from OEBind may be considered uninteresting for the project and there is no need to spend time calculating it, or because OEBind calculates the unbound protein and ligand properties every time, which is unnecessary if the same protein and ligand appear in multiple calculations. The API section for OEBind is detailed with regard to implementation, so the user can see how to create their own class or set of function calls if needed.

There are two classes that store the results of a binding calculation, *OEBindResults* and *OESimpleBindResults*. OEBindResults is a superset of OESimpleBindResults. For an in-depth understanding of what is calculated, the electrostatics portion of the algorithm for the SimpleBind function is shown in the API section.

The following is a sample program for using the OEBind class that is provided in the distribution.

Listing 7: Bind example

```
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or its use.
*/
package openeye.examples.oezap;

import openeye.oechem.*;
import openeye.oezap.*;

public class ZapBind {

    public static void main(String argv[]) {
        if (argv.length != 2) {
            System.err.println("usage: ZapBind <protein> <ligands>");
            System.exit(1);
        }

        OEMol protein = new OEMol();
        oemolistream ifs = new oemolistream();
        if (!ifs.open(argv[0])) {
            System.err.println("Unable to open for reading: " + argv[0]);
            System.exit(1);
        }
        oechem.OEReadMolecule(ifs, protein);
        oechem.OEAssignBondiVdWRadii(protein);
        oechem.OEMMFFAtomTypes(protein);
```

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```
        oechem.OEMMFF94PartialCharges(protein);
        System.err.println("protein: " + protein.GetTitle());
        ifs.close();

        OEBind bind = new OEBind();
        bind.SetProtein(protein);
        OEBindResults results = new OEBindResults();

        OEMol ligand = new OEMol();
        if (!ifs.open(argv[1])) {
            System.err.println("Unable to open for reading: " + argv[1]);
            System.exit(1);
        }
        ifs.SetConfTest(new OEIsomericConfTest());
        while (oechem.OEReadMolecule(ifs, ligand)) {
            oechem.OEAssignBondiVdWRadii(ligand);
            oechem.OEMMFFAtomTypes(ligand);
            oechem.OEMMFF94PartialCharges(ligand);
            System.err.println("ligand: " + ligand.GetTitle());

            for (OEConfBase conf : ligand.GetConfs()) {
                bind.Bind(conf, results);
                System.err.println(" conf# " + conf.GetIdx() + " be = "
                        + results.GetBindingEnergy());
            }
            System.err.println();
        }
        results.delete();
        bind.delete();
    }
}
```

1.3.6 Focusing

Focusing is a way to achieve the desired precision around a target (such as a ligand) while maintaining reasonable time and memory limits for the calculation. The target for focusing is set using the *OEZap.SetFocusTarget* method.

For a typical ZAP electrostatics calculation, a consistent grid spacing is used for the entire system, where the default value is 0.5 Angstroms but it may be set to a custom value using *OEZap.SetGridSpacing*. This method is entirely appropriate for certain calculations, such as solvation energy calculations for small molecules. For other types of calculations, such as a binding energy calculation for a protein and ligand, a consistent grid spacing may cause the calculation to be either prohibitively expensive or insufficiently precise around the binding area.

Focusing alleviates this problem by using a fine grid for the target volume, and coarser grids away from the target. The grid spacing setting for ZAP is applied to the target volume, and the grid spacing is doubled for each addition coarse grid surrounding the target. A quadratic interpolation is used for the grid intersections. The implementation of the bind uses the SetFocusTarget() method to set the ligand as the target for focusing.

The following example program computes the binding energy of a protein and ligand twice, once without focusing and once with the ligand as the focusing target. The values of the binding energy and the time it took to calculate them are displayed. For a focused atom potential calculation, the full electrostatics for the protein and complex would each be computed with multiple electrostatics calculations. The first calculation would create the potential grid for the target volume with a grid spacing of 0.5 (assuming the default spacing is being used). An additional calculation with a grid spacing of 1.0 would be done on a larger volume volume, and then additional calculations with grid spacings of 2.0,

4.0, and so on would be done until the grid is large enough to contain the entire volume of the system.

Listing 8: Focusing example

```
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*/
package openeye.examples.oezap;

import openeye.oechem.*;
import openeye.oezap.*;

public class ZapFocussing {
    static {
        oechem.OEThrow.SetStrict(true);
    }

    public static void CalcBindingEnergy(OEZap zap, OEGraphMol protein,
            OEGraphMol ligand, OEGraphMol cmplx) {
        OEStopwatch stopwatch = new OEStopwatch();
        stopwatch.Start();

        OEFloatArray ppot = new OEFloatArray(protein.GetMaxAtomIdx());
        zap.SetMolecule(protein);
        zap.CalcAtomPotentials(ppot);
        double proteinEnergy = 0.0;
        for (OEAtomBase atom : protein.GetAtoms()) {
            proteinEnergy += ppot.getItem(atom.GetIdx()) * atom.GetPartialCharge();
        }
        proteinEnergy *= 0.5;

        OEFloatArray lpot = new OEFloatArray(ligand.GetMaxAtomIdx());
        zap.SetMolecule(ligand);
        zap.CalcAtomPotentials(lpot);
        double ligandEnergy = 0.0;
        for (OEAtomBase atom : ligand.GetAtoms()) {
            ligandEnergy += lpot.getItem(atom.GetIdx()) * atom.GetPartialCharge();
        }
```

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```
        ligandEnergy *= 0.5;

        OEFloatArray cpot = new OEFloatArray(cmplx.GetMaxAtomIdx());
        zap.SetMolecule(cmplx);
        zap.CalcAtomPotentials(cpot);
        double cmplxEnergy = 0.0;
        for (OEAtomBase atom : cmplx.GetAtoms()) {
            cmplxEnergy += cpot.getItem(atom.GetIdx()) * atom.GetPartialCharge();
        }
        cmplxEnergy *= 0.5;

        double energy = cmplxEnergy - ligandEnergy - proteinEnergy;
        float time = stopwatch.Elapsed();

        if (zap.IsFocusTargetSet()) {
            System.out.println("Yes\t\t" + (float) energy + "\t" + time);
        } else {
            System.out.println("No\t\t" + (float) energy + "\t" + time);
        }

    }

    public static void main(String argv[]) {
        if (argv.length != 2) {
            System.err.println("usage: ZapFocussing <protein> <ligand>");
            System.exit(1);
        }

        oemolistream ifs = new oemolistream();
        if (!ifs.open(argv[0])) {
            System.err.println("Unable to open file for reading: " + argv[0]);
            System.exit(1);
        }
        OEGraphMol protein = new OEGraphMol();
        oechem.OEReadMolecule(ifs, protein);

        oechem.OEAssignBondiVdWRadii(protein);
        oechem.OEMMFFAtomTypes(protein);
        oechem.OEMMFF94PartialCharges(protein);

        if (!ifs.open(argv[1])) {
            System.err.println("Unable to open file for reading: " + argv[1]);
            System.exit(1);
        }
        OEGraphMol ligand = new OEGraphMol();
        oechem.OEReadMolecule(ifs, ligand);

        oechem.OEAssignBondiVdWRadii(ligand);
        oechem.OEMMFFAtomTypes(ligand);
        oechem.OEMMFF94PartialCharges(ligand);

        OEGraphMol cmplx = new OEGraphMol(protein);
```

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```
        oechem.OEAddMols(cmplx, ligand);

        float epsin = 1.0f;
        float spacing = 0.5f;
        OEZap zap = new OEZap();
        zap.SetInnerDielectric(epsin);
        zap.SetGridSpacing(spacing);

        System.out.println("\nBinding Energy and Wall Clock Time for " + protein.
↪GetTitle() + " and " + ligand.GetTitle());
        System.out.println("\nFocussed?\tEnergy(kT)\tTime(s)");

        CalcBindingEnergy(zap, protein, ligand, cmplx);
        zap.SetFocusTarget(ligand);
        CalcBindingEnergy(zap, protein, ligand, cmplx);
        zap.delete();
        ifs.close();
    }
}
```

1.3.7 Gradients/Forces

The solvent forces acting on the atoms in a molecule may be calculated using the *OEZap.CalcForces* method. The components of the forces are set to a float array of length 3N, where N is the number of atoms. The components of the gradient are equal in magnitude to the force, but have the opposite sign.

Listing 9: Calculating solvation forces

```
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*/
package openeye.examples.oezap;

import openeye.oechem.*;
import openeye.oezap.*;

public class ZapForces {
```

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```
    static {
        oechem.OEThrow.SetStrict(true);
    }

    public static void main(String argv[]) {
        if (argv.length != 1) {
            System.err.println("usage: ZapForces <molfile>");
            System.exit(1);
        }

        OEZap zap = new OEZap();
        zap.SetInnerDielectric(1.0f);
        zap.SetGridSpacing(0.5f);

        oemolistream ifs = new oemolistream();
        if (!ifs.open(argv[0])) {
            System.err.println("Unable to open file for reading: " + argv[0]);
            System.exit(1);
        }
        OEGraphMol mol = new OEGraphMol();
        while (oechem.OEReadMolecule(ifs, mol)) {
            System.out.println(String.format("\nForce Components for %s, in kT/Angstrom",
                    mol.GetTitle()));
            System.out.println("Index   Element   -dE/dx    -dE/dy    -dE/dz");

            OEFloatArray forces = new OEFloatArray(mol.GetMaxAtomIdx() * 3);
            oechem.OEAssignBondiVdWRadii(mol);
            oechem.OEMMFFAtomTypes(mol);
            oechem.OEMMFF94PartialCharges(mol);
            zap.SetMolecule(mol);
            zap.CalcForces(forces);
            for (OEAtomBase atom : mol.GetAtoms()) {
                System.out.println(String.format(" %4d     %2s     %7.3f   %7.3f   %7.3f
↪",
                        atom.GetIdx(),
                        oechem.OEGetAtomicSymbol(atom.GetAtomicNum()),
                        forces.getItem(atom.GetIdx()),
                        forces.getItem(atom.GetIdx() + 1),
                        forces.getItem(atom.GetIdx() + 2)));
            }
        }
        zap.delete();
        ifs.close();
    }
}
```

1.3.8 Electrostatic Similarity

Electrostatic similarity may be calculated using the *OEET* class. The following example program shows how to obtain the electrostatic Tanimoto between a reference molecule and a trial molecule. The electrostatic Tanimoto is affected by the partial charges of the molecules as well as the three-dimensional structure, including the tautomer state, spacial orientation, and conformation. In the example program shown below, MMFF charges are assigned to the molecules,

but it is assumed that they have already been spatially aligned.

Listing 10: Calculating electrostatic tanimoto

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*/
package openeye.examples.oezap;

import openeye.oechem.*;
import openeye.oezap.*;

public class CalcET {

    public static void main(String argv[]) {
        if (argv.length != 2) {
            System.err.println("usage: CalcET <reference> <fitfile>");
            System.exit(1);
        }

        OEGraphMol refmol = new OEGraphMol();
        oemolistream ifs = new oemolistream();
        if (!ifs.open(argv[0])) {
            System.err.println("Unable to open for reading: " + argv[0]);
            System.exit(1);
        }
        oechem.OEReadMolecule(ifs, refmol);
        oechem.OEAssignBondiVdWRadii(refmol);
        oechem.OEMMFFAtomTypes(refmol);
        oechem.OEMMFF94PartialCharges(refmol);
        ifs.close();

        OEET et = new OEET();
        et.SetRefMol(refmol);

        System.err.println("dielectric: " + et.GetDielectric());
        System.err.println("inner mask: " + et.GetInnerMask());
        System.err.println("outer mask: " + et.GetOuterMask());
```

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```
        System.err.println("salt conc : " + et.GetSaltConcentration());
        System.err.println("join      : " + et.GetJoin());

        OEGraphMol fitmol = new OEGraphMol();
        if (!ifs.open(argv[1])) {
            System.err.println("Unable to open for reading: " + argv[1]);
            System.exit(1);
        }
        while (oechem.OEReadMolecule(ifs, fitmol)) {
            oechem.OEAssignBondiVdWRadii(fitmol);
            oechem.OEMMFFAtomTypes(fitmol);
            oechem.OEMMFF94PartialCharges(fitmol);
            System.err.println("Title: " + fitmol.GetTitle() + " ET "
                    + et.Tanimoto(fitmol));
        }
        ifs.close();
        et.delete();
    }
}
```

Note

Units of all energies reported from **ZapTK** are in `kcal/mol`.

CHAPTER

TWO

APPENDIX: ADDITIONAL EXAMPLES IN PYTHON

Zap programming examples are dispersed among the descriptions of parts of the toolkits and in the overall chapter *The Way of Zap*. Full listings are provided here for examples that are presented as incomplete snippets in the Zap chapter.

CHAPTER

THREE

API

3.1 OEPB Classes

3.1.1 OEArea

```
class OEArea
```

Calculates surface area using the same grid-based Gaussians that Zap uses. Mostly used for calculating the area term in solvation calculations or the buried area term in bind calculations.

Constructors

```
OEArea()
OEArea(const OEArea &)
```

Default and copy constructors.

3.1.2 GetArea

```
float GetArea(const OEChem::OEMolBase& mol)
bool GetArea(const OEChem::OEMolBase& mol, float* atomArea)
float GetArea(const OEChem::OEMolBase& mol,
              const OEChem::OEResidue& res)
float GetArea(const OEChem::OEMolBase& mol, const float* atomArea,
              const OEChem::OEResidue& res)
```

Calculate the surface area of the passed-in molecule. The first version calculates the surface area of the entire molecule. The second version takes an array sized by `OEMolBase::GetMaxAtomIdx` to return the contribution of each atom to the total surface area. The third and fourth versions calculates and returns the surface area of the residue passed into the function. The fourth version differs from the third version by taking a already calculated atom area array, which avoids calculating atom area repeatedly.

Note that whether or not hydrogens are included in these calculations is controlled by *OEArea.SetUseHydrogens* which is set to `false` by default.

The following demonstrates how to calculate the area of a molecule:

Example of calculating the surface area of a molecule

```
OEArea area = new OEArea();
float a = area.GetArea(mol);
System.out.println("Molecule area = " + a );
```

The following demonstrates how to retrieve the individual atom contributions to the surface area:

Example of calculating the surface area contribution of individual atoms

```
OEFloatArray atomArea = new OEFloatArray(mol.GetMaxAtomIdx());
OEArea area = new OEArea();
area.GetArea(mol, atomArea);
for (OEAtomBase atom: mol.GetAtoms()) {
    int index = atom.GetIdx();
    System.out.println(index + " " + atomArea.getItem(index));
}
```

The following demonstrates how to retrieve the per residue contributions to the surface area:

Example of calculating the surface area contribution of indivdual residues

```
OEArea area = new OEArea();
for (OEResidue res: oebio.OEGetResidues(mol)) {
    System.out.println(oechem.OEResidueToString(res) + " " + area.GetArea(mol,␣
↪res));
}
```

The following demonstrates how to retrieve the per residue contributions to the surface area, in an optimized way where the per atom contributions are pre-calculated and used for the residue based calculation. This is particularly important if this calculation is done on a large set of residues:

Example of calculating the surface area contribution of indivdual residues

```
OEFloatArray atomArea = new OEFloatArray(mol.GetMaxAtomIdx());
OEArea area = new OEArea();
area.GetArea(mol, atomArea);
for (OEResidue res: oebio.OEGetResidues(mol)) {
    System.out.println(oechem.OEResidueToString(res) + " " + area.GetArea(mol,␣
↪res));
}
```

3.1.3 GetMethod

```
unsigned int GetMethod() const
```

Returns an `int` indicating the method that is used to model the area of the molecule. The two possible return values are *OEAreaMethod.Gaussian* and *OEAreaMethod.Discrete*.

3.1.4 GetUseHydrogens

```
bool GetUseHydrogens() const
```

Returns a `bool` where `true` means explicit hydrogens are turned on and `false` means they are turned off for the area calculation.

3.1.5 SetMethod

```
bool SetMethod(const unsigned int method)
```

Takes an `int` with the value of *OEAreaMethod.Gaussian* of *OEAreaMethod.Discrete*

3.1.6 SetUseHydrogens

```
bool SetUseHydrogens(bool state)
```

This method takes a `bool` where `true` turns on explicit hydrogens for calculating area and `false` turn them off.

3.1.7 OEBind

```
class OEBind
```

Calculates protein-ligand binding properties. The protein may either be passed in as an argument during construction or set with *OEBind.SetProtein*. The ligand is passed in as an argument to *OEBind.Bind* as well as an *OEBindResults* instance.

Constructors

```
OEBind()
OEBind(const OEBind& rhs)
OEBind(const OEChem::OEMolBase& protein)
```

Default and copy constructors. Besides the default and copy constructors, OEBind includes a constructor that takes the protein to be used in binding calculations. Constructing an OEBind object with the protein is identical to using the default constructor and then calling *OEBind.SetProtein*.

Bind

```
bool Bind(const OEChem::OEMolBase& ligand, OEBindResults& results)
OESystem::OEIterBase<OEBindResults>* Bind(const OEChem::OEMCMolBase& ligand)
```

Calculate full binding results, including Coulombic terms. For a single molecule, pass in the molecule and the *OEBindResults* class will be filled in. The following is a simple example of how *Bind* is used.

Example of using the OEBind object

```
openeye.oezap.OEBind bind = new openeye.oezap.OEBind();
bind.SetProtein(protein);
OEBindResults results = new OEBindResults();
bind.Bind(ligand, results);
results.Print(oechem.OEThrow);
```

GetZap

```
OEZap& GetZap()
const OEZap& GetZap() const
```

Get a reference to the internal *OEZap* object contained in an OEBind instance. With the non-const version, you can adjust *OEZap* parameters that affect the *OEBind* calculation. For example, to use an *OEBind* instance with a specific grid spacing:

Example of setting the grid spacing of a OEBind object

```
openeye.oezap.OEBind bind = new openeye.oezap.OEBind();
bind.GetZap().SetGridSpacing(0.6f);
```

Note that some properties of the *OEZap* object are not controllable via this mechanism.

SetProtein

```
bool SetProtein(const OEChem::OEMolBase& protein)
```

Set the protein molecule to be used by the *OEBind* object. Note that the protein should have radii and partial charges pre-calculated before passing to *OEBind.SetProtein*.

SetZap

```
bool SetZap(const OEZap& zap)
```

Update the internal OEZap object. Note that some properties of the OEZap object are not controllable via this mechanism.

SimpleBind

```
bool SimpleBind(const OEChem::OEMolBase& ligand,
                OESimpleBindResults& results)
OESystem::OEIterBase<OESimpleBindResults>* SimpleBind(const OEChem::OEMCMolBase& ligand)
```

Calculate simple binding results, without the Coulombic terms. See the discussion in *Binding Energies* about the differences between *OEBind.Bind* and *OEBind.SimpleBind*. See *OESimpleBindResults* to see all the values available.

Additionally, both the *SimpleBind* and *OEBind.Bind* methods calculate area contributions.

3.1.8 OEBindResults

```
class OEBindResults : public OESimpleBindResults
```

All energy results are in units of kT.

The following methods are publicly inherited from *OESimpleBindResults*:

operator=	*GetBuriedArea*	*GetUnboundLigandZapEnergy*
GetBindingEnergy	*GetBuriedAreaEnergy*	*GetUnboundProteinArea*
GetBoundLigandArea	*GetComplexArea*	*GetUnboundProteinAreaEnergy*
GetBoundLigandAreaEnergy	*GetComplexAreaEnergy*	*GetUnboundProteinZapEnergy*
GetBoundLigandZapEnergy	*GetComplexZapEnergy*	*GetZapEnergy*
GetBoundProteinArea	*GetConf*	*Print*
GetBoundProteinAreaEnergy	*GetUnboundLigandArea*	
GetBoundProteinZapEnergy	*GetUnboundLigandAreaEnergy*	

Constructors

```
OEBindResults()
OEBindResults(const OEBindResults &)
```

Default and copy constructors.

GetAnalyticCoulombicBindingEnergy

```
float GetAnalyticCoulombicBindingEnergy() const
```

This returns the value of the analytic binding energy for the ligand and protein that have been set to the OEBind object. This is equivalent to calling *OECalculateCoulombicBinding* where the same ligand and protein and inner dielectric are the arguments.

GetBoundLigandCoulombEnergy

```
float GetBoundLigandCoulombEnergy() const
```

Returns the grid-based coulomb energy for the ligand in the bound state, including self-interaction. Specially, it returns the boundLigandCoulombEnergy variable shown in the *OEBind.Bind* API section.

GetBoundProteinCoulombEnergy

```
float GetBoundProteinCoulombEnergy() const
```

Returns the grid-based coulomb energy for the protein in the bound state, including self-interaction. Specially, it returns the boundProteinCoulombEnergy variable shown in the *OEBind.Bind* API section.

GetComplexCoulombEnergy

```
float GetComplexCoulombEnergy() const
```

Returns the grid-based coulomb energy for the complex, including self-interaction. Specially, it returns the complexCoulombEnergy variable shown in the *OEBind.Bind* API section. This is equivalent to the sum of the results returned by *OEBindResults.GetBoundLigandCoulombEnergy* and *OEBindResults.GetBoundProteinCoulombEnergy*.

GetCoulombEnergy

```
float GetCoulombEnergy() const
```

Returns the difference in Coulomb energy between the complex and the unbound ligand and protein. This is equivalent to *OEBindResults.GetComplexCoulombEnergy* - *OEBindResults.GetUnboundProteinCoulombEnergy* - *OEBindResults.GetUnboundLigandCoulombEnergy*.

GetDesolvationEnergy

```
float GetDesolvationEnergy() const
```

This is equivalent to *OESimpleBindResults.GetZapEnergy* - *OEBindResults.GetCoulombEnergy*.

GetLigandDesolvationEnergy

```
float GetLigandDesolvationEnergy() const
```

This is equivalent to *OESimpleBindResults.GetBoundLigandZapEnergy* - *OEBindResults.GetBoundLigandCoulombEnergy* - *OESimpleBindResults.GetUnboundLigandZapEnergy* + *OEBindResults.GetUnboundLigandCoulombEnergy*.

GetProteinDesolvationEnergy

```
float GetProteinDesolvationEnergy() const
```

This is equivalent to *OESimpleBindResults.GetBoundProteinZapEnergy* - *OEBindResults.GetBoundProteinCoulombEnergy* - *OESimpleBindResults.GetUnboundProteinZapEnergy* + *OEBindResults.GetUnboundProteinCoulombEnergy*.

GetUnboundLigandCoulombEnergy

```
float GetUnboundLigandCoulombEnergy() const
```

Returns the grid-based coulomb energy for the ligand in the unbound state, including self-interaction. Specially, it returns the unboundLigandCoulombEnergy variable shown in the *OEBind.Bind* API section.

GetUnboundProteinCoulombEnergy

```
float GetUnboundProteinCoulombEnergy() const
```

Returns the grid-based coulomb energy for the protein in the unbound state, including self-interaction. Specially, it returns the unboundProteinCoulombEnergy variable shown in the *OEBind.Bind* API section.

Print

```
void Print(OEPlatform::oeostream& ofs) const
void Print(OESystem::OEErrorHandler& log) const
```

Prints out all of the available data to the oeostream of the OEErrorHandle passed in.

3.1.9 OEET

```
class OEET
```

Used to calculate electrostatic similarity between molecules using Poisson-Boltzmann electrostatic potentials.

Constructors

```
OEET(const OEET& rhs)
OEET(float dielectric = 80.0f)
```

Default and copy constructors.

GetDielectric

```
float GetDielectric() const
```

Returns the setting for the outer dielectric constant.

GetGridBuffer

```
float GetGridBuffer() const
```

Returns the setting for the amount of space between the molecule and the edge of the grid.

GetGridSpacing

```
float GetGridSpacing() const
```

Returns the setting for the grid spacing.

GetInnerDielectric

```
float GetInnerDielectric() const
```

Returns the value for the inner dielectric.

GetInnerMask

```
float GetInnerMask() const
```

Returns the value for the inner mask.

GetJoin

```
bool GetJoin() const
```

Returns the setting for whether or not to join the molecules for masking.

GetOuterMask

```
float GetOuterMask() const
```

Returns the value for the outer mask.

GetSaltConcentration

```
float GetSaltConcentration() const
Returns the setting for the salt concentration
```

SetDielectric

```
void SetDielectric(float d)
```

Sets the outer dielectric constant

SetGridBuffer

```
void SetGridBuffer(float f)
```

Sets the grid buffer, or boundary spacing, which is the amount of distance between the molecule and the edge of the grid. The default value is 6.0.

SetGridSpacing

```
void SetGridSpacing(float f)
```

Sets the grid spacing. The default value is 0.75.

SetInnerDielectric

```
void SetInnerDielectric(float d)
```

Sets the inner dielectric constant

SetInnerMask

```
void SetInnerMask(float f)
```

Sets the inner mask for electrostatic comparison. The default value is set to 0.05. The inner mask is used to mask out the inner part of a molecule. The inner part of the molecule is masked out so that the important regions surrounding the molecule dominate the electrostatic comparison.

SetJoin

```
void SetJoin(bool j)
```

Turns molecular joining on(`true`) or off(`false`). The default value is `true`, which uses the combine reference molecule and trial molecule when applying the inner and outer mask.

SetOuterMask

```
void SetOuterMask(float f)
```

Sets the outer mask for electrostatic comparison. The default value is set to 0.0005. The outer mask is used to mask out regions far from the molecule.

SetRefMol

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

Sets the reference molecule.

SetSaltConcentration

```
void SetSaltConcentration(float conc)
```

Sets the salt concentration. The default value is 0.04.

Tanimoto

```
float Tanimoto(const OEChem::OEMolBase& mol)
```

Returns the electrostatic Tanimoto between the reference molecule that has been set and the trial molecule that is passed in as an argument.

3.1.10 OESimpleBindResults

```
class OESimpleBindResults
```

This class represents *OESimpleBindResults*. The Zap calculations used for the SimpleBindResults are performed with the 2 separate dielectric constants, the internal for the molecule and the external for the solvent. All energy results are in units of kT.

The following classes derive from this class:

- *OEBindResults*

Constructors

```
OESimpleBindResults()
OESimpleBindResults(const OESimpleBindResults &)
```

Default and copy constructors.

GetBindingEnergy

```
float GetBindingEnergy() const
```

Returns the binding energy of the ligand and protein. Equivalent to *OESimpleBindResults.GetBuriedAreaEnergy* + *OESimpleBindResults.GetZapEnergy*.

GetBoundLigandArea

```
float GetBoundLigandArea() const
```

Returns the `boundLigandArea` variable shown in the *OEBind.SimpleBind* API section. The bound ligand area is the area of the ligand exposed to the solvent while in the bound state.

GetBoundLigandAreaEnergy

```
float GetBoundLigandAreaEnergy() const
```

Returns the `boundLigandAreaEnergy` variable shown in the *OEBind.SimpleBind* API section. This is the energy associated with the bound ligand area.

GetBoundLigandZapEnergy

```
float GetBoundLigandZapEnergy() const
```

Returns the `boundLigandZapEnergy` variable shown in the *OEBind.SimpleBind* API section. This is the ligand grid energy obtained from a Zap calculation of the complex.

GetBoundProteinArea

```
float GetBoundProteinArea() const
```

Returns the boundProteinArea variable shown in the *OEBind.SimpleBind* API section. This is the area of the protein exposed to the solvent while in the bound state.

GetBoundProteinAreaEnergy

```
float GetBoundProteinAreaEnergy() const
```

Returns the boundProteinAreaEnergy variable shown in the *OEBind.SimpleBind* API section. This is the energy associated with the bound protein area.

GetBoundProteinZapEnergy

```
float GetBoundProteinZapEnergy() const
```

Returns the boundProteinZapEnergy variable shown in the *OEBind.SimpleBind* API section. This is the protein grid energy obtained from a Zap calculation of the complex.

GetBuriedArea

```
float GetBuriedArea() const
```

Returns the amount of area that has become buried as a result of binding. Equivalent to *OESimpleBindResults.GetUnboundProteinArea* + *OESimpleBindResults.GetUnboundLigandArea* - *OESimpleBindResults.GetComplexArea*.

GetBuriedAreaEnergy

```
float GetBuriedAreaEnergy() const
```

Returns the energy penalty associated with the buried area of the complex. Equivalent to *OESimpleBindResults.GetComplexAreaEnergy* - *OESimpleBindResults.GetUnboundProteinAreaEnergy* - *OESimpleBindResults.GetUnboundLigandAreaEnergy*.

GetComplexArea

```
float GetComplexArea() const
```

Returns the complexArea variable shown in the *OEBind.SimpleBind* API section. This is the solvent accessible surface area of the complex.

GetComplexAreaEnergy

```
float GetComplexAreaEnergy() const
```

Returns the complexAreaEnergy variable shown in the *OEBind.SimpleBind* API section. This is the energy of the solvent accessible surface area of the complex.

GetComplexZapEnergy

```
float GetComplexZapEnergy() const
```

Returns the grid energy of the complex. This is equivalent to *OESimpleBindResults.GetBoundProteinZapEnergy* + *OESimpleBindResults.GetBoundLigandZapEnergy*.

GetConf

```
OEChem::OEConfBase* GetConf()
const OEChem::OEConfBase* GetConf() const
```

Returns a pointer to the active conformer.

GetUnboundLigandArea

```
float GetUnboundLigandArea() const
```

Returns the unboundLigandArea variable shown in the *OEBind.SimpleBind* API section. This is the solvent accessible surface area of the unbound ligand.

GetUnboundLigandAreaEnergy

```
float GetUnboundLigandAreaEnergy() const
```

Returns the unboundLigandAreaEnergy variable shown in the *OEBind.SimpleBind* API section. This is the energy of the solvent accessible surface area of the unbound ligand.

GetUnboundLigandZapEnergy

```
float GetUnboundLigandZapEnergy() const
```

Returns the unboundLigandZapEnergy variable shown in the *OEBind.SimpleBind* API section. This is the grid energy of the unbound ligand obtained from a Zap calculation.

GetUnboundProteinArea

```
float GetUnboundProteinArea() const
```

Returns the unboundProteinArea variable shown in the *OEBind.SimpleBind* API section. This is the solvent accessible surface area of the unbound protein.

GetUnboundProteinAreaEnergy

```
float GetUnboundProteinAreaEnergy() const
```

Returns the unboundProteinAreaEnergy variable shown in the *OEBind.SimpleBind* API section. This is the energy of the solvent accessible surface area of the unbound protein.

GetUnboundProteinZapEnergy

```
float GetUnboundProteinZapEnergy() const
```

Returns the unboundProteinZapEnergy variable shown in the *OEBind.SimpleBind* API section. This is the grid energy of the unbound protein obtained from a Zap calculation.

GetZapEnergy

```
float GetZapEnergy() const
```

Returns the difference in grid energy between the complex and the unbound ligand and protein. This is equivalent to *OESimpleBindResults.GetComplexZapEnergy* - *OESimpleBindResults.GetUnboundProteinZapEnergy* - *OESimpleBindResults.GetUnboundLigandZapEnergy*.

Print

```
void Print(OEPlatform::oeostream& ofs) const
void Print(OESystem::OEErrorHandler& log) const
```

Prints out all of the available data to the oeostream of the OEErrorHandle passed in.

3.1.11 OEZap

```
class OEZap
```

The principal interface for Poisson-Boltzmann electrostatics calculations. Stores a molecule and computes solvation energies, potential grids, and atomic potentials using an implicit solvent model. See *OEZap.SetMolecule* for molecule preparation requirements.

Constructors

```
OEZap()
OEZap(const OEZap& rhs)
```

Default and copy constructors.

CalcAtomPotentials

```
bool CalcAtomPotentials(float* pot, bool no_grid = false)
```

Calculates the atom potentials and fills the `float` array with their values. The `float` array should be of length `N`, where `N` is the number of atoms.

CalcForces

```
bool CalcForces(float* forces)
```

Calculates the forces on the atoms and fills the `float` array with the values of their x, y, and z components. The `float` array should be of length `3N`, where `N` is the number of atoms.

CalcPotentialGrid

```
bool CalcPotentialGrid(OESystem::OEScalarGrid& grid)
```

Calculates the potential grid and updates the `OEScalarGrid` with the values. The calculated electrostatic potential is a dimensionless value defined as eV/kT where eV is the electric work, in kcal/mol, of bringing an electron charge to the point with potential V, and kT = 0.59 kcal/mol (value of kT at room temperature).

CalcSolvationEnergy

```
float CalcSolvationEnergy()
```

Returns the solvation energy in kT of the molecule that has been set. This result does not include an area term.

ClearFocusTarget

```
void ClearFocusTarget()
```

Clears the target setting for focusing.

GetBoundarySpacing

```
float GetBoundarySpacing() const
```

Returns the boundary spacing setting, which is the amount of distance between the molecule and the edge of the grid. The default setting is 4.0.

GetDielectricModel

```
unsigned int GetDielectricModel() const
```

Returns an `int` representing the dielectric model being used. The two available models are *OEZapDielectricModel.Gaussian* and *OEZapDielectricModel.Molecular*.

GetError

```
float GetError() const
```

Returns the error setting. See *OEZap.SetError*.

GetFocusTarget

```
const OEChem::OEMolBase* GetFocusTarget() const
```

Returns a pointer to the molecule that has been set as the focus target.

GetGridSpacing

```
float GetGridSpacing() const
```

Returns the setting for the grid spacing. The default value is 0.5.

GetInnerDielectric

```
float GetInnerDielectric() const
```

Returns the setting for the internal dielectric constant. The default value is 1.0.

GetIterations

```
unsigned int GetIterations() const
```

Returns the maximum number of iterations allowed for the zap calculation. The default value is 10.

GetMolecule

```
const OEChem::OEMolBase* GetMolecule() const
```

Returns a pointer to the molecule that has been set to Zap.

GetOuterDielectric

```
float GetOuterDielectric() const
```

Returns the setting for the outer dielectric constant. The default value is 80.0.

GetProbeRadius

```
float GetProbeRadius() const
```

Returns the setting for the probe radius. The default value is 1.4.

GetVerbose

```
bool GetVerbose() const
```

Returns the setting for very low-level verbosity. The default value is false.

GetSaltConcentration

```
float GetSaltConcentration() const
```

Returns the setting for the salt concentration. The default value is 0.0.

IsFocusTargetSet

```
bool IsFocusTargetSet()
```

Returns a `bool` for whether the focus target is currently set. See the section of focusing for more information.

SetBoundarySpacing

```
bool SetBoundarySpacing(float spacing)
```

Sets the boundary spacing, which is the amount of distance between the molecule and the edge of the grid. The default setting is 4.0.

SetDielectricModel

```
bool SetDielectricModel(unsigned int model)
```

Sets the dielectric model. The two available models are *OEZapDielectricModel.Gaussian* and *OEZapDielectricModel.Molecular*. The default is the Gaussian model.

SetError

```
bool SetError(float zaperr)
```

Rather than setting the grid spacing, the acceptable error may be set instead using this method. The default value is set to 0.0, which means that the grid spacing is set explicitly.

SetFocusTarget

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

Sets the focus target. See the section of *Focusing* for more information.

SetGridSpacing

```
bool SetGridSpacing(float spacing)
```

Sets the grid spacing. The default value is 0.5.

SetInnerDielectric

```
bool SetInnerDielectric(float epsin)
```

Sets the internal dielectric constant. The default value is 1.0.

SetIterations

```
bool SetIterations(unsigned int iters)
```

Sets the maximum number of iterations allowed for the zap calculation. The default value is 10

SetMolecule

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

Sets the molecule to Zap. Partial charges, 3-D coordinates, and radii need to be set to the molecule before the molecule is set to Zap.

SetOuterDielectric

```
bool SetOuterDielectric(float epsout)
```

Sets the external dielectric constant. The default value is 80.0.

SetProbeRadius

```
bool SetProbeRadius(float radius)
```

Sets the probe radius, the default value is 1.4.

SetSaltConcentration

```
bool SetSaltConcentration(float conc)
```

Sets the salt concentration. The default value is 0.0.

SetVerbose

```
bool SetVerbose(bool verbose)
```

Sets very low-level verbosity. The default value is false.

3.2 OEPB Constants

3.2.1 OEAreaMethod

This namespace contains constants.

Undefined

This value represents an unset OEAreaMethod.

Gaussian

This method uses Gaussians to compute area and is faster and less sensitive to rotation and translation on the grid.

Discrete

This method uses a hard sphere model to compute area.

Default

The default is set to Gaussian.

3.2.2 OEZapDielectricModel

This namespace contains constants.

Gaussian

This model uses Gaussians to represent atoms and is faster and less sensitive to rotation and translation on the grid.

Molecular

This model uses hard spheres to represent atoms.

Default

The default model is Gaussian.

3.3 OEPB Functions

3.3.1 OECalculateCoulombicBinding

```
float OECalculateCoulombicBinding(const OEChem::OEMolBase& protein,
                                  const OEChem::OEMolBase& ligand,
                                  float dielectric)
```

Returns the analytic binding energy in kT for the ligand and protein in the specified dielectric using Coulomb's Law. Both `protein` and `ligand` must have 3D coordinates and partial charges assigned.

3.3.2 OECoulombicAtomPotentials

```
bool OECoulombicAtomPotentials(const OEChem::OEMolBase& mol, float D,
                               float* apot)
```

Calculates the Coulombic atom potentials with the dielectric constant `D` and fills the float array `apot` with the values. `apot` should be of length `N`, where `N` is the number of atoms. The molecule must have 3D coordinates and partial charges assigned.

3.3.3 OECoulombicSelfEnergy

```
float OECoulombicSelfEnergy(const OEChem::OEMolBase& mol, float D)
```

Returns the integral energy in kT of a molecule from its partial charges in universal dielectric `D` using Coulomb's Law. The molecule must have partial charges assigned.

3.3.4 OEMakeETGrid

```
bool OEMakeETGrid(OESystem::OEScalarGrid& grid,
                  const OEChem::OEMolBase& mol, const OEET& et)
```

Calculates the electrostatic Tanimoto grid for the `mol` passed in and the reference molecule that needs to be already set to the *OEET* instance. Both `mol` and the reference molecule set via *OEET.SetRefMol* must have 3D coordinates and partial charges assigned.

3.3.5 OEZapBind

```
bool OEZapBind(const OEChem::OEMolBase& protein,
               const OEChem::OEMolBase& ligand, OEBindResults& results)
bool OEZapBind(const OEChem::OEMolBase& protein,
               const OEChem::OEMolBase& ligand,
               OESimpleBindResults& results)
```

Convenience functions for obtaining *OEBindResults* or *OESimpleBindResults* of a `ligand` and `protein`. Both `protein` and `ligand` must have 3D coordinates, partial charges, and VDW radii assigned.

3.3.6 OEZapGetArch

```
const char* OEZapGetArch()
```

Returns the architecture on which the release was built

3.3.7 OEZapGetLicensee

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

Fills the parameter `string &licensee` with the licensee of the license file being used

3.3.8 OEZapGetPlatform

```
const char* OEZapGetPlatform()
```

Returns the platform on which the release was built

3.3.9 OEZapGetRelease

```
const char* OEZapGetRelease()
```

Returns the version number as a `const char*` in major.minor.bugfix form

3.3.10 OEZapGetSite

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

Fills the parameter `string &licensee` with the site on the license file being used

3.3.11 OEZapGetVersion

```
unsigned int OEZapGetVersion()
```

Returns the build date of the release

CHAPTER

FOUR

RELEASE HISTORY

4.1 Zap TK 2.5.3

4.1.1 Major Bug Fixes

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

4.2 Zap TK 2.5.2

Minor internal improvements have been made.

4.3 Zap TK 2.5.1

Minor internal improvements have been made.

4.4 Zap TK 2.5.0

Minor internal improvements have been made.

4.5 Zap TK 2.4.7

Minor internal improvements have been made.

4.6 Zap TK 2.4.6

4.6.1 New features

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

4.7 Zap TK 2.4.5

Minor internal improvements have been made.

4.8 Zap TK 2.4.4

Minor internal improvements have been made.

4.9 Zap TK 2.4.3

- Minor internal improvements have been made.

4.10 Zap TK 2.4.2

Fall 2021

- Minor internal improvements have been made.

4.11 Zap TK 2.4.1

July 2021

Minor internal improvements have been made.

4.12 Zap TK 2.4.0

- Minor internal improvements have been made.

4.13 Zap TK 2.3.7

- Minor internal improvements have been made.

4.14 Zap TK 2.3.6

4.14.1 Python-specific changes

- The runtime error that occurred when using *OEMakeETGrid* in Python has been fixed.

4.15 Zap TK 2.3.5

- Minor internal improvements have been made.

4.16 Zap TK 2.3.4

- Minor internal improvements have been made.

4.17 Zap TK 2.3.3

- Minor internal improvements have been made.

4.18 Zap TK 2.3.2

- Minor internal improvements have been made.

4.19 Zap TK 2.3.1

- Minor internal improvements have been made.

4.20 Zap TK 2.3.0

- Minor internal improvements have been made.

4.21 Zap TK 2.2.7

4.21.1 Minor bug fixes

- A bug that resulted in a crash when attempting to use the *OEZapDielectricModel.Molecular* model on Windows has been fixed.

4.22 Zap TK 2.2.6

4.22.1 Minor bug fixes

- A single atom identified as 3D but centered at the origin previously returned an incorrect warning about 3D coordinates being required. The internal coordinate checking has been overhauled to validate the input coordinates more systematically. Accordingly, the dimensionality of the input molecule must now be explicitly set to 3D.

4.22.2 Documentation changes

- The example *Calculating potential grid with optional parameters* is now synchronized for all supported languages.

4.23 Zap TK 2.2.5

4.23.1 Major bug fixes

- A serious memory leak in **Zap TK** was discovered and has been fixed. The leak was introduced in the 2015.Jun toolkit release and affected **Zap TK** and its dependent toolkits (e.g., **Szmap TK**).

4.24 Zap TK 2.2.4

- Minor internal improvements have been made.

4.25 Zap TK 2.2.3

4.25.1 Documentation fixes

- New Java and C# snippets have been added to the documentation.

4.26 Zap TK 2.2.2

4.26.1 Minor bug fixes

- Internal refactoring has been performed to improve stability.

4.26.2 Documentation fixes

- Cross-references have been fixed.

4.27 Zap TK 2.2.1

4.27.1 Major Bug Fixes

- Potential buffer overrun that could cause crashes fixed.

4.27.2 Documentation fixes

- The Java documentation no longer contains C++ code.

4.28 Zap TK 2.2.0

4.28.1 Minor bug fixes

- Removed unbounded stack allocations.
- *OEZap.SetIterations* and *OEZap.GetIterations* now deal with `unsigned int` instead of `int`.

4.29 Zap TK 2.1.7

- Minor internal improvements.

4.30 Zap TK 2.1.6

4.30.1 New features

- *OEET.GetInnerDielectric* and *OEET.SetInnerDielectric* have been added to allow custom inner dielectric settings.

4.30.2 Minor bug fixes

- Warnings for missing coordinates and missing charges has been separated for better warning messages.

4.30.3 Documentation fixes

- Documentation has been updated to specify units of kT.

4.31 Zap TK 2.1.5

4.31.1 Documentation fixes

- The documentation has been updated to clarify that energies are reported in units of kT unless otherwise specified.

- A documentation mistake in *OESimpleBindResults.GetUnboundLigandZapEnergy* has been fixed.

4.32 Zap TK 2.1.4

- Internal build system improvements.

4.33 Zap TK 2.1.3

- Internal build system improvements.

4.34 Zap TK 2.1.2

4.34.1 New features

- Added new methods *OEZap.GetVerbose* and *OEZap.SetVerbose* to enable Zap to print out an abundance of low-level information.

4.34.2 Bug fixes

- Fixed memory leak that occurred with multiple calls to *OEArea.GetArea*
- *OEMakeETGrid* now properly wrapped in Java.

4.35 Zap TK 2.1.1

4.35.1 Bug fixes

- *OEZap.GetMolecule* and *OEZap.GetFocusTarget* now return a pointer instead of a reference. This is a breaking change and any code that calls these methods will have to be updated. These methods will return a null pointer if an acceptable molecule has not been set for them.
- A warning has been added for molecules passed into Zap TK that do not return 3 when `GetDimension` is called. The dimension must be 3 for all molecules passed into Zap TK. The dimension is set automatically when using `OEReadMolecule` but a warning will be thrown and the molecule will not be accepted by Zap TK if the molecule has been made from scratch in the toolkits and `SetDimension(3)` has not been called on it.

4.35.2 Minor bug fixes

- Fixed a memory bug related to extremely large files on Windows.

4.36 Zap TK 2.1.0

4.36.1 New features

- Internal defaults have been changed for the *OEZap* object. The internal dielectric now has a default of 1.0, the boundary spacing now has a default of 4.0, and the default number of iterations has been set to 10. The change from 2.0 to 1.0 for the internal dielectric led to dramatically improved results when we performed tests with the Rizzo set, with the RMS error for vacuum-water transfer energy decreasing by more than half.
- Large manual update with complete examples and API documentation.
- *OEZap.IsFocusTargetSet* has been added, which returns a `bool` which indicates whether the focus target has been set.

- New examples for focusing and forces have been added
- All examples have been ported across all three languages (C++, Java, Python)
- Examples assign MMFF94 charges by default

4.36.2 Bug fixes

- Internal and external dielectrics are now properly reset each time the *OEBind* instance is used.
- Internal error checking has been added so that no internal calculations will be attempted if `OEZap.SetMolecule` fails. (`OEZap.SetMolecule` most often fails because all charges are equal to zero.) Calls to methods that would attempt to run internal calculations (e.g. `OEZap.CalcSolvationEnergy`) will return zero or false.
- Internal summations in *OEBind* use doubles now instead of floats for appropriate precision
- Charges are properly assigned to both the refmol and fitmol in the calc_et.cpp example.
- Examples perform error checking when opening files

4.37 Zap TK 2.0.0

4.37.1 New features

- This is the first official release of the C++ version of Zap TK. Note that this is a significant change in the API as we migrate from the C API to the new C++ API built on top of OEChem.

CHAPTER

FIVE

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CHAPTER

SIX

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CHAPTER

SEVEN

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7.2 Orion Floes

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

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

7.4 Publications for Bibliographies

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

7.4.1 Orion

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

7.4.2 AFITT and FLYNN Applications

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

7.4.3 OEDocking Application and Toolkit

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

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

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

7.4.4 OMEGA Application and Toolkit

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

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

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

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

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

7.4.5 ROCS Application

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

7.5 OpenEye MMDS Web Service

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

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CHAPTER

EIGHT

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asgiref	https://github.com/django/asgiref/	https://github.com/django/asgiref/blob/main/LICENSE

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

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

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

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

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Name of Project	Website	License URL
click-repl	https://github.com/untitaker/click-repl	https://github.com/click-contrib/click-repl/blob/master/LICENSE
cloudpickle	https://github.com/cloudpipe/cloudpickle	https://github.com/cloudpipe/cloudpickle/blob/master/LICENSE
cmake	https://cmake.org/	https://cmake.org/licensing/
colorama	https://github.com/tartley/colorama	https://github.com/tartley/colorama/blob/master/LICENSE.txt
comm	https://github.com/ipython/comm	https://github.com/ipython/comm/blob/master/LICENSE
compose	https://github.com/docker/compose	https://github.com/docker/compose/blob/v2/LICENSE
conda-content-trust	https://github.com/conda/conda-content-trust	https://github.com/conda/conda-content-trust/blob/main/LICENSE
conda-libmamba-solver	https://github.com/conda/conda-libmamba-solv	https://github.com/conda/conda-libmamba-solv blob/main/LICENSE
conda-pack	https://conda.github.io/conda-pack/	https://github.com/conda/conda-pack/blob/main/LICENSE.txt
conda-package-handling	https://github.com/conda/conda-package-handli	https://github.com/conda/conda-package-handli blob/main/LICENSE
conda-package-streaming	https://anaconda.org/conda-forge/conda-package-strean	https://github.com/conda/conda-package-strean 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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Table 1 – continued from previous page

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

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Table 1 – continued from previous page

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

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Table 1 – continued from previous page

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

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Table 1 – continued from previous page

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

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Table 1 – continued from previous page

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

8.1 GCC

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

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

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

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

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

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

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

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

8.1.1 GCC RUNTIME LIBRARY EXCEPTION

```
Version 3.1, 31 March 2009

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

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

This GCC Runtime Library Exception ("Exception") is an additional permission under␣
↪section 7 of the GNU General Public License,
version 3 ("GPLv3"). It applies to a given file (the "Runtime Library") that bears a␣
↪notice placed by the copyright holder
of the file stating that the file is governed by GPLv3 along with this Exception.

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

0. Definitions.

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

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

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

"Target Code" refers to output from any compiler for a real or virtual target processor␣
↪architecture, in executable
form or suitable for input to an assembler, loader, linker and/or execution phase.␣
↪Notwithstanding that, Target Code
does not include data in any format that is used as a compiler intermediate␣
↪representation, or used for producing a
compiler intermediate representation.
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The "Compilation Process" transforms code entirely represented in non-intermediate␣
↪languages designed for human-written
code, and/or in Java Virtual Machine byte code, into Target Code. Thus, for example, use␣
↪of source code generators and
preprocessors need not be considered part of the Compilation Process, since the␣
↪Compilation Process can be understood
as starting with the output of the generators or preprocessors.

A Compilation Process is "Eligible" if it is done using GCC, alone or with other GPL-
↪compatible software, or if it is
done without using any work based on GCC. For example, using non-GPL-compatible Software␣
↪to optimize any GCC intermediate
representations would not qualify as an Eligible Compilation Process.

1. Grant of Additional Permission.

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

2. No Weakening of GCC Copyleft.

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

See also

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

8.1.2 GNU GENERAL PUBLIC LICENSE

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

 Copyright (C) 2007 Free Software Foundation, Inc. <http://fsf.org/>
 Everyone is permitted to copy and distribute verbatim copies
 of this license document, but changing it is not allowed.

                            Preamble

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

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

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

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

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

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

  For the developers' and authors' protection, the GPL clearly explains
that there is no warranty for this free software.  For both users' and
authors' sake, the GPL requires that modified versions be marked as
changed, so that their problems will not be attributed erroneously to
authors of previous versions.

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

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

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

                    TERMS AND CONDITIONS

  0. Definitions.

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

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

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

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

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

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

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

  An interactive user interface displays "Appropriate Legal Notices"
to the extent that it includes a convenient and prominently visible
feature that (1) displays an appropriate copyright notice, and (2)
tells the user that there is no warranty for the work (except to the
extent that warranties are provided), that licensees may convey the
work under this License, and how to view a copy of this License.  If
the interface presents a list of user commands or options, such as a
menu, a prominent item in the list meets this criterion.

  1. Source Code.

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

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

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

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

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

  2. Basic Permissions.

  All rights granted under this License are granted for the term of
copyright on the Program, and are irrevocable provided the stated
conditions are met.  This License explicitly affirms your unlimited
permission to run the unmodified Program.  The output from running a
covered work is covered by this License only if the output, given its
content, constitutes a covered work.  This License acknowledges your
rights of fair use or other equivalent, as provided by copyright law.

  You may make, run and propagate covered works that you do not
convey, without conditions so long as your license otherwise remains
in force.  You may convey covered works to others for the sole purpose
of having them make modifications exclusively for you, or provide you
with facilities for running those works, provided that you comply with
the terms of this License in conveying all material for which you do
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not control copyright.  Those thus making or running the covered works
for you must do so exclusively on your behalf, under your direction
and control, on terms that prohibit them from making any copies of
your copyrighted material outside their relationship with you.

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

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

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

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

  4. Conveying Verbatim Copies.

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


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

  5. Conveying Modified Source Versions.

  You may convey a work based on the Program, or the modifications to
produce it from the Program, in the form of source code under the
terms of section 4, provided that you also meet all of these conditions:

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

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

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

  A compilation of a covered work with other separate and independent
works, which are not by their nature extensions of the covered work,
and which are not combined with it such as to form a larger program,
in or on a volume of a storage or distribution medium, is called an
"aggregate" if the compilation and its resulting copyright are not
used to limit the access or legal rights of the compilation's users
beyond what the individual works permit.  Inclusion of a covered work
in an aggregate does not cause this License to apply to the other
parts of the aggregate.

  6. Conveying Non-Source Forms.

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

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

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

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

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

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

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

  A "User Product" is either (1) a "consumer product", which means any
tangible personal property which is normally used for personal, family,
or household purposes, or (2) anything designed or sold for incorporation
into a dwelling.  In determining whether a product is a consumer product,
doubtful cases shall be resolved in favor of coverage.  For a particular
product received by a particular user, "normally used" refers to a
typical or common use of that class of product, regardless of the status
of the particular user or of the way in which the particular user
actually uses, or expects or is expected to use, the product.  A product
is a consumer product regardless of whether the product has substantial
commercial, industrial or non-consumer uses, unless such uses represent
the only significant mode of use of the product.

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

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