

Resources

- Programmer's Examples (<http://www.cgl.ucsf.edu/chimera/docs/ProgrammersGuide/Examples/index.html>)
- IDLE (Tools→General Controls): `help(object)`, `dir(object)`
- Python language/modules: <http://www.python.org/doc/current/>
- Numpy examples: http://www.scipy.org/Numpy_Example_List_With_Doc
- Chimera developer mailing list: chimera-dev@cgl.ucsf.edu
- C++ source code: <http://www.cgl.ucsf.edu/chimera/sourcecode.html>
 - Python source code included with distribution

Chimera Molecular Data

- `chimera.openModels.list()`: list of open models
 - `modeltypes=[chimera.Molecule]`: restrict list to Molecules
- `m.residues` / `m.atoms` / `m.bonds`: a Molecule's residues / atoms / bonds

Residues

- `type`: LYS, HEM, etc.
- `id.position` / `id.chainId` / `id.insertionCode`: number / chain ID / insertion code
- `molecule`: parent Molecule
- `atoms`: list of atoms
- `atomsMap`: dict of atom-name → list of atoms
- `isHelix` / `isStrand`: in helix / strand

Atoms

- `name`: name
- `coord()` / `xformCoord()`: untransformed / transformed coordinates
- `residue` / `molecule`: parent Residue / Molecule
- `bonds`: list of bonds
- `neighbors`: list of bonded atoms
- `primaryBonds()` / `primaryNeighbors()`: same as above but only primary atlocs
- `bondsMap`: dict of bonded-atom → bond
- `color`: Color
- `display`: True if shown
- `drawMode`: one of chimera.Atom.X with X being Dot, Sphere, EndCap, or Ball
- `element`: chemical element (type chimera.Element, settable with string or number)
- `label`: label shown in graphics window
- `radius`: VdW radius

Bonds

- `atoms`: 2-tuple of atoms
- `otherAtom(a)`: [*a* is one of the bond's atoms] other atom in bond
- `drawMode`: one of chimera.Bond.Y with Y being Wire or Stick
- `label`: label shown in graphics window
- `molecule`: parent Molecule
- `length()`: length

Useful Chimera modules/functions

Molecular Measurements

chimera module

functions use Points, which are returned by Atom's *coord()* or *xformCoord()* methods

- *distance / sqdistance*
 - also: *a1.coord().[sq]distance(a2.coord())* [similar for *xformCoord*]
- *angle* — in degrees
- *dihedral* — in degrees

Molecular Editing

chimera.molEdit module

- *addAtom*
 - if adding in bulk, make sure to specify optional *serialNumber* keyword
 - *addBond*
 - *addDihedralAtom* — add atom given a bond length / angle / dihedral
- look in *BuildStructure/___init___*.py for examples of creating new Molecules and Residues

Setting/Querying The Selection

chimera.selection module

- *currentAtoms / currentBonds / currentResidues / currentMolecules*: currently selected Atoms / Bonds / Residues / Molecules
- *setCurrent*: set current selection to given items
- *addCurrent / addImpliedCurrent*: add given items to current selection
 - the "implied" version also selects endpoint Atoms of added Bonds and connecting Bonds of added Atoms
- *removeCurrent*: remove items from current selection, if present

Miscellaneous

chimera module

- *runCommand*: execute any command-line command (arg is a string)

chimera.colorTable module

- *getColorByName*: get a Color by name

OpenSave module

- *osOpen*: open a file or HTTP URL, with or without compression

chimera.extension module

- *manager.instances*: running dialogs listed at end of Tools menu