

## Resources

- Programmer's Examples ([www.cgl.ucsf.edu/chimera/docs/ProgrammersGuide](http://www.cgl.ucsf.edu/chimera/docs/ProgrammersGuide))
  - Example scripts: [socrates2.cgl.ucsf.edu/trac/chimera/wiki/Scripts](http://socrates2.cgl.ucsf.edu/trac/chimera/wiki/Scripts)
- IDLE (Tools→General Controls): `help(object)`, `dir(object)`
- Python language/modules: [www.python.org/doc/current/](http://www.python.org/doc/current/)
- Numpy examples: [www.scipy.org/Numpy\\_Example\\_List\\_With\\_Doc](http://www.scipy.org/Numpy_Example_List_With_Doc)
- Chimera developer mailing list: [chimera-dev@cgl.ucsf.edu](mailto:chimera-dev@cgl.ucsf.edu)
- C++ source code: browse SVN [socrates2.cgl.ucsf.edu/trac/chimera/browser](http://socrates2.cgl.ucsf.edu/trac/chimera/browser) or download from [www.cgl.ucsf.edu/chimera/sourcecode.html](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)
  - direct Python equivalent usually in Midas module

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