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 altlocs
- *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