

## UCSF Chimera: Molecular Graphics for Research and Analysis

**Abstract:** UCSF Chimera is a program for interactive molecular graphics and modeling. Chimera can be used to study molecular structure and how structure relates to function, interactions with other molecules, and evolution. Chimera provides many standard features of molecular graphics programs as well as more unique tools for analysis and domain-specific visualization.

Molecules can be shown as stick, ball-and-stick, space-filling, and ribbon representations, with or without surfaces; all can be moved interactively. There are many options for coloring, including transparency, and the background color, lighting, and shininess can be controlled by the user. Special VRML representations of nucleic acid bases and sugars can be generated. Images of arbitrarily high resolution can be saved in a number of common formats, including TIFF and PNG.

Menu and command-line interfaces provide a rich and overlapping set of functionality. Structures can be opened from local files or, with internet connectivity, retrieved from the Protein DataBank (PDB) or the ASTRAL Compendium when specified by PDB or SCOP ID, respectively.

Hydrogen bonds can be identified from the geometric relationships between potential donor and acceptor atoms. The criteria are based on high-quality crystallographic data, but the stringency can be adjusted by the user. Hydrogens can be added to structures, but this is not required for hydrogen bond identification. Distances, angles and torsions can be measured, and bonds (torsions) can be rotated interactively. Atom types are known for standard amino acid and nucleic acid residues, and for nonstandard residues, are determined automatically from the coordinates.

The sequences of peptides/proteins and nucleic acids can be viewed in a separate window. Residues selected in the sequence are highlighted on the structure, and vice versa. Besides sequences generated directly from the structures being viewed, users can read in and display sequence alignments that have been generated externally. Many common sequence alignment formats can be read (and written out), including GCG MSF, Clustal, aligned FASTA, and Stockholm. Sequences in an alignment will automatically associate with structures being viewed if they match well enough, and pairs that do not associate automatically can be associated manually. Association of a sequence in an alignment with a structure enables several operations: selection in the sequences will select the corresponding structure regions and vice versa; protein helix/sheet assignments can be viewed on the sequences; structures can be superimposed according to the sequence alignment. Conversely, if structures are already superimposed in Chimera, the Match -> Align tool can be used to generate a corresponding structure-based multiple sequence alignment.

Properties of atoms and residues (such as crystallographic B-factor and Kyte-Doolittle hydrophobicity values, respectively) can be visualized with colors, scaling of atomic radii, and/or scaling of "worm" radii. Various properties are automatically present, but users can define their own arbitrary properties, assign values, and then use the same methods to visualize the properties on the structures.

More domain-specific features include:

- (1) display of volume data (anything with numerical values on a 3D grid, such as electron density, light microscope data, and electrostatic potential) as contour surfaces or transparent solids, with interactively adjustable thresholds
- (2) a tool for facilitating screening of docked compounds from DOCK
- (3) a tool for playing back and analyzing molecular dynamics trajectories (many formats supported, including AMBER, GRO-MOS, X-PLOR, and multi-PDB)
- (4) a Multiscale Models tool for generating higher-order structures from symmetry matrices, navigating structural hierarchies, and showing structures as low-resolution surfaces
- (5) a Demos feature for creating and replaying presentations in Chimera
- (6) a Collaboratory feature that allows researchers in separate locations to share a modeling session

There are many additional features not described here. Tools interoperate transparently; for example, hydrogen bonds can be identified and sequence(s) shown for structures within a molecular dynamics trajectory.

Chimera was designed to be highly extensible. It is largely implemented in Python, with certain features coded in C++ for efficiency. All of Chimera's functionality is accessible through Python; users can implement their own extensions without changing Chimera.

Chimera includes full user documentation and is available for Windows, Linux, Mac OS X (with X11), IRIX, and Tru64 Unix. Development is funded by the NIH National Center for Research Resources (grant P41-RR01081). Chimera is free for academic, government, and non-profit use and can be downloaded from <http://www.cgl.ucsf.edu/chimera>. One must consent to a licensing agreement prior to download. Registration is optional, however. Information on commercial licensing can be obtained by contacting [chimera@cgl.ucsf.edu](mailto:chimera@cgl.ucsf.edu).

**Reference:** "UCSF Chimera - A Visualization System for Exploratory Research and Analysis." E.F. Pettersen, T.D. Goddard, C.C. Huang, G.S. Couch, D.M. Greenblatt, E.C. Meng, and T.E. Ferrin, *J. Comput. Chem.* 25:1605-1612 (2004).