

# UCSF Chimera Quick Reference Guide

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Commands (\*reverse function ~**command** available)

*2dlabels* create labels with text, symbols, and arrows in 2D  
*ac* enable accelerators (keyboard shortcuts)  
*addaa* add an amino acid to a peptide N- or C-terminus  
*addcharge* assign partial charges to atoms  
*addh* add hydrogens  
*alias\** create an alias or list the existing aliases  
*align* align two atoms or sets of atoms along the line of sight  
*angle* measure angles formed by atoms or by axes and planes  
*aniso\** show thermal ellipsoids  
*aromatic\** show ring aromaticity  
*background* set background color, gradient, or image  
*bond\** add/delete bonds  
*bondzone\** make zoning tools use points along bonds  
*cd* change the working directory  
*center* center the view on specified atoms  
*changechains* reassign chain identifiers  
*chirality* report the R/S configuration of a chiral center  
*clip\** move global clipping planes  
*close* close a model  
*cofr\** report or change the center of rotation  
*color\** color atoms/bonds, ribbons, labels, surfaces  
*colordef* define a new color  
*combine* combine molecule models into a single model  
*coordset* play through frames of a trajectory  
*copy* save image files  
*coulombic* color molecular surfaces by Coulombic electrostatics  
*crystalcontacts* identify clashes between PDB symmetry copies  
*defattr* assign attribute values to atoms, residues, or models  
*define\** calculate and display axes, planes, centroids  
*delete* delete atoms and bonds  
*display\** display specified atoms  
*distance\** measure distances between atoms, axes, planes, centroids  
*echo* send text to the status line and Reply Log  
*export* save the scene (x3d, vrml, povray, renderman, stl, obj)  
*fillring\** show rings as filled  
*findclash\** identify clashes and contacts  
*findhbond\** (*hbonds*) identify hydrogen bonds  
*fitmap* fit atoms or map into map  
*fly* smoothly traverse a series of saved positions  
*focus\** adjust the view and center of rotation  
*freeze* stop all motion  
*getcrd* report untransformed coordinates  
*help* display the manual page for a command  
*hkcgage* create icosahedron as hexagon/pentagon mesh  
*intersurf* generate and display interface surfaces  
*invert* swap substituents of an atom  
*ksdssp* determine secondary structure from protein coordinates  
*label\** display atom labels  
*labelopt* control the information in atom labels

*lighting* adjust lighting and shininess  
*linewidth* control the width of wire bonds  
*longbond\** show/hide pseudobonds representing missing segments  
*mask* extract volume data bounded by surfaces  
*match* superimpose two models using specified atoms  
*matchmaker* (*mmaker*) align models in sequence, then in 3D  
*matrixcopy* apply the transformation of one model to another  
*matrixget* write the current transformation matrices to a file  
*matrixset* read and apply transformation matrices from a file  
*mclip\** control per-model clipping  
*mcopy* copy settings from one molecule model to another  
*measure* perform calculations on structures, surfaces, maps  
*meshmol* create a "molecule" to show surface mesh as sticks  
*minimize* energy-minimize structures  
*modelcolor* set color at the model level  
*modeldisplay\** set display at the model level  
*molmap* create a density map from atomic coordinates  
*morph* morph (interpolate) between different structures  
*move* translate models  
*movie* capture image frames and assemble them into a movie  
*msc\** color multiscale surfaces to match atoms  
*namesel* name the current selection  
*nucleotides\** create special nucleotide representations  
*objdisplay\** display graphical objects  
*open\** read local files or fetch by ID  
*pause* pause script execution until the user presses a key  
*perframe\** specify commands to be executed at each display frame  
*play* script various complex motions  
*preset* apply a predefined combination of display settings  
*rainbow* color residues, chains, or models over a range  
*rangecolor* color over a range according to attribute values  
*read* execute a command file, updating display at the end  
*represent* control atom/bond style (wire, stick, bs, sphere)  
*reset* restore default or saved orientations  
*resrenumber* reassign residue numbers  
*ribbackbone\** allow display of both ribbon and backbone atoms  
*ribbon\** display ribbon  
*ribclass* set ribbon residue class  
*ribinsidecolor\** set a separate color for inside protein helix ribbons  
*ribrepr* control ribbon style (flat, edged, rounded)  
*ribscale* control ribbon scaling (Chimera default, licorice)  
*rib spline* control ribbon path (B-spline or cardinal spline)  
*rlabel\** display residue labels  
*rmsd* evaluate the RMSD between specified sets of atoms  
*rock* rock (rotate back and forth)  
*roll* roll (rotate continuously)  
*rotation\** make a bond rotatable  
*runscript* run Python script with command-line arguments  
*save* save the current Chimera session  
*savepos\** save model positions  
*scale\** scale the view  
*scene\** save/restore scenes (positions, styles, colors, labels, etc.)  
*scolor* color surfaces by volume data or geometry  
*section* move global clipping planes in parallel

*segment* act on segmentation models  
*select\** select atoms, (de)activate models for motion  
*set\** set visual effects, individual model rotation  
*setattr\** set an attribute to a specified value  
*shape* create a surface of a specified geometric shape  
*show\** display specified atoms, undisplay the others  
*sleep* pause script execution for a specified time  
*solvate* add solvent using AmberTools  
*sop* adjust capping, edit surface models  
*split* make chains of a molecule model separate submodels  
*start* start Chimera tools by name  
*stereo\** switch amongst stereo options and mono viewing  
*stop* exit from Chimera  
*surface\** calculate and display molecular surfaces  
*surfcat* (*msms cat*) group atoms for surface calculations  
*surfrepr* (*msms repr*) control surface style (solid, mesh, dot)  
*swapaa* mutate amino acids or swap rotamers  
*swapna* mutate nucleic acid residues  
*sym\** generate symmetry-related copies of a structure  
*system* send a command to the system shell  
*thickness* move global clipping planes in opposite directions  
*tile\** arrange models in a plane  
*topography* plot values in a volume data plane as surface heights  
*transparency\** make atoms/bonds, ribbons, and surfaces transparent  
*turn* rotate models  
*vdw\** display van der Waals (VDW) dot surface  
*vdwdefine\** set VDW radii  
*vdwdensity* set VDW surface dot density  
*version* show copyright information and Chimera version  
*viewdock* start ViewDock and load docking results  
*volume* display volume data such as electron density  
*vop* edit volume data  
*wait* suspend command processing until motion has stopped  
*window* adjust the view to contain the specified atoms  
*windoworigin* set graphics window location  
*windowsize\** adjust the dimensions of the graphics window  
*write* save atomic coordinates (pdb, mol2)  
*writesel* write a list of the currently selected (or unselected) items  
*zonesel* select atoms/surfs within cutoff of specified atoms/surfs

## Miscellaneous Operations (Default Settings)

selection from screen	Ctrl-left mouse button
add/toggle selection	Shift-Ctrl-left mouse button
rotation	left mouse button
XY-translation	middle mouse button
scaling	right mouse button or Side View
preferences	Favorites... Preferences...
searching help	Help... Search Documentation...
reporting a problem	Help... Report a Bug...
mailing list	chimera-users@cgl.ucsf.edu

Specification Symbols		
Symbol	Function	Usage
#	model number	# <i>model</i> (integer)
##	submodel number	## <i>submodel</i> (integer)
:	residue	: <i>residue</i> (name or number)
::	residue name	:: <i>residue</i>
..	chain ID	.. <i>chain</i>
@	atom name	@ <i>atom</i>
@.	alternate location ID	@. <i>alt_loc</i>
-	range	specifies a range of models, submodels, or residues
,	name separator	separates models or residues, ranges of models or residues, or names of atoms
*	whole wildcard	matches whole atom or residue names, e.g., <b>*@CA</b> specifies the alpha carbons of all residues
=	partial wildcard	matches partial atom or residue names, e.g., <b>@C=</b> specifies all atoms with names beginning with C
?	single-char wildcard	used for atom and residue names only, e.g., <b>:G??</b> selects all residues with three-letter names beginning with G
;	command separator	separates multiple commands on a single line
z<	zone specifier	<b>z&lt;zone</b> or <b>zr&lt;zone</b> specifies all residues within <i>zone</i> angstroms, <b>za&lt;zone</b> specifies all atoms (rather than entire residues) within that distance. Using > instead of < gives the complement.
&	intersection	intersection of specified sets
	union	union of specified sets
~	negation	negation of specified set

#### Selected Atom Attributes

Usage	Description
@/altLoc=altloc	alternate location ID
@/areaSAS=sasa	solvent-accessible surface area
@/areaSES=sesa	solvent-excluded surface area
@/bfactor=bfactor	B-factor
@/color=color	atom-level color assignment
@/defaultRadius=rad	default VDW radius
@/display	whether atom display bit is "on"
@/drawMode=mode	<i>mode</i> can be 0 (dot), 1 (sphere), 2 (endcap, as in stick), or 3 (ball)

@/element=atmo	atomic number
@/idatmType=type	Chimera atom type
@/label	whether the atom is labeled
@/label=label	text of the atom label
@/labelColor=labcolor	color of the atom label
@/name=name	atom name
@/occupancy=occupancy	crystallographic occupancy
@/radius=radius	current VDW radius
@/serialNumber=n	serial number in the input file
@/surfaceCategory=category	surface calculation category (main, ligand, etc.)
@/surfaceDisplay	per-atom surface display bit (can be true for buried atoms without surface)

#### Selected Residue Attributes

Usage	Description
:/areaSAS=sasa	solvent-accessible surface area
:/areaSES=sesa	solvent-excluded surface area
:/isHet	residues in PDB HETATM records (or the mmCIF equivalent)
:/isHelix	amino acid residues in helices
:/isStrand or /isSheet	amino acid residues in strands
:/kdHydrophobicity=value	Kyte-Doolittle amino acid hydrophobicity
:/phi=angle	protein/peptide backbone phi angle
:/psi=angle	protein/peptide backbone psi angle
:/ssId=N	secondary structure element identifier (1 for first helix and first strand, etc.)
:/uniprotIndex=N	residue number in corresponding UniProt sequence, if any

#### Selected Molecule Model Attributes

Usage	Description
#/ballScale=factor	ball radius relative to VDW radius
#/color=color	model-level color assignment
#/display	model display bit
#/lineWidth=width	linewidth of wire representation
#/numAtoms=N	total number of atoms
#/numResidues=M	total number of residues
#/stickScale=factor	stick radius relative to bond radius

#### Specification Examples

```
#
- all models
#0
- model 0
#3:45-83,90-98
- residues 45-83 and 90-98 in model 3
:lys,arg
- lysine and arginine residues
:12,14@ca
- alpha carbons in residues 12 and 14
:12:14@ca
- all atoms in residue 12 and the alpha carbon in residue 14
:A@ca,c,n,o
- peptide backbone atoms in chain A
:50.B,.D
- residue 50 in chain B and all residues in chain D
:12-15,26-28.a,45.b
- residues 12-15 in all chains (except het/water), 26-28 in chain A, and 45 in chain B
#0.1-3,5
- submodels 1-3 of model 0 and all of model 5
#0.1-3,.5
- submodels 1-3 of model 0 and submodel 5 of all models
ligand
- any/all residues automatically classified as ligand
S | Fe
- all sulfur and iron atoms
@ca!/label and color!=green and color!=red
- atoms named CA which are not labeled, and are not green or red
@/bfactor>=20 and bfactor<=40
- atoms with B-factor values ranging from 20 to 40
:asn & helix
- asparagine residues in helices
#1:asp,glu & #0 z<10
- aspartate and glutamate residues in model 1 within 10 angstroms of model 0
solvent & Ng+ z<3 | solvent & N3+ z<3
- solvent residues within 3 angstroms of guanidinium nitrogens or sp3-hybridized, formally positive nitrogens
@/bfactor>50 & ~ solvent & ~ ions
- atoms with B-factor values over 50, excluding solvent and ions
```

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