
UCSF Chimera
QUICK REFERENCE GUIDE
May 2008

Commands

*reverse function ~**command** available

<i>2dlabels</i>	create arbitrary text labels and place them in 2D
<i>ac</i>	enable accelerators (keyboard shortcuts)
<i>addaa</i>	add an amino acid to a peptide C-terminus
<i>addcharge</i>	assign partial charges to atoms
<i>addh</i>	add hydrogens
<i>alias*</i>	create an alias or list aliases
<i>align</i>	align two atoms or sets of atoms along the line of sight
<i>angle</i>	measure a bond angle or torsion angle
<i>bond*</i>	add/delete bonds
<i>bondcolor*</i>	color bonds independently from atoms
<i>bonddisplay</i>	control how bond display depends on atom display
<i>bondrepr</i>	control bond style (wire, stick)
<i>bondzone*</i>	make zoning tools use points along bonds
<i>brotation</i>	make a bond rotatable
<i>cd</i>	change the working directory
<i>center</i>	center the view on specified atoms
<i>chain</i>	chain specified atoms, undisplay the others
<i>chirality</i>	report the R/S configuration of a chiral center
<i>clip*</i>	move clipping planes
<i>close</i>	close a model
<i>cofr*</i>	report or change the center of rotation
<i>color*</i>	color atoms/bonds, ribbons, labels, and surfaces
<i>colordef</i>	define a new color
<i>conic</i>	create a shadowed space-filling image
<i>copy</i>	save an image (Chimera graphics or POV-Ray)
<i>crystalcontacts</i>	identify clashes between PDB symmetry copies
<i>defattr</i>	assign attribute values to atoms, residues, or models
<i>delete</i>	delete atoms and bonds
<i>display*</i>	display specified atoms
<i>distance*</i>	measure the distance between two atoms
<i>echo</i>	send text to the Reply Log
<i>export</i>	save the scene (x3d, vrml, pov-ray, renderman, obj)
<i>findclash*</i>	identify clashes and/or contacts
<i>focus</i>	adjust the view and center of rotation
<i>freeze</i>	stop all motion
<i>getcrd</i>	report untransformed coordinates
<i>hbonds*</i>	(<i>findhbond</i>) identify possible hydrogen bonds
<i>help</i>	display the manual page for a command
<i>hkage</i>	create a hexagon/pentagon mesh that covers an icosahedron
<i>intersurf</i>	generate and display interface surfaces
<i>ksdssp</i>	determine secondary structure from protein coordinates
<i>label*</i>	display atom labels
<i>labelopt</i>	control the information in atom labels
<i>linewidth</i>	control the width of wire bonds

<i>load</i>	restore a saved Chimera session
<i>longbond*</i>	show/hide pseudobonds representing missing segments
<i>mask</i>	extract volume data bounded by surfaces
<i>match</i>	superimpose two models
<i>matrixcopy</i>	apply the transformation matrix of one model to another
<i>matrixget</i>	write the current transformation matrices to a file
<i>matrixset</i>	read and apply transformation matrices from a file
<i>mclip*</i>	control per-model clipping
<i>meshmol</i>	create a "molecule" from surface mesh for stick display
<i>minimize</i>	energy-minimize structures
<i>mmaker</i>	(<i>matchmaker</i>) align models in sequence, then in 3D
<i>modelcolor</i>	set color at the model level
<i>modeldisplay*</i>	set display at the model level
<i>molmap</i>	create a density map from atomic coordinates
<i>move</i>	translate along the X, Y, or Z axis
<i>movie</i>	capture image frames and assemble them into a movie
<i>msc*</i>	color multiscale surfaces to match atoms
<i>namesel</i>	name and save the current selection
<i>neon</i>	create a shadowed stick/tube image (not on Windows)
<i>objdisplay*</i>	display graphical objects
<i>open*</i>	read local files or fetch by ID
<i>pdbrun</i>	send an annotated PDB file to the system shell
<i>perframe*</i>	specify an alias to be executed at each display frame
<i>preset</i>	apply a predefined combination of display settings
<i>push.pop</i>	push or pop images on the picture stack
<i>rainbow</i>	color residues, chains, or models over a range
<i>rangecolor</i>	color over a range according to attribute values
<i>read</i>	execute a command file, updating the display at the end
<i>represent</i>	control atom/bond style (wire, stick, bs, sphere)
<i>reset</i>	restore default or saved orientations
<i>ribbackbone*</i>	allow display of both ribbon and backbone atoms
<i>ribbon*</i>	display ribbon
<i>ribcolor*</i>	set ribbon color
<i>ribrepr</i>	control ribbon style (flat, edged, rounded)
<i>ribscale</i>	control ribbon scaling (Chimera default, licorice)
<i>rlabel*</i>	display residue labels
<i>rmsd</i>	evaluate the RMSD between specified sets of atoms
<i>rock</i>	rock about the X, Y or Z axis
<i>roll</i>	roll about the X, Y, or Z axis
<i>rotation</i>	make a bond rotatable
<i>save</i>	save the current Chimera session
<i>savepos*</i>	save the current orientations
<i>scale*</i>	scale the view
<i>section</i>	move the clipping planes in parallel
<i>select*</i>	activate models for motion or select atoms
<i>set*</i>	set options (see Set/Unset Options)
<i>setattr*</i>	set an attribute to a specified value
<i>shape</i>	create a surface of a specified geometric shape
<i>show*</i>	display specified atoms, undisplay the others
<i>sleep</i>	pause command processing
<i>source</i>	execute a command file, updating the display continually
<i>split</i>	make chains of a molecule model separate submodels
<i>start</i>	start Chimera tools by name

<i>stereo</i>	switch amongst stereo options and mono viewing
<i>stop</i>	exit from Chimera
<i>surface*</i>	calculate and display molecular surfaces
<i>surfcut</i>	(<i>msms cat</i>) group atoms for surface calculations
<i>surfcolor</i>	set surface color source
<i>surfrepr</i>	(<i>msms repr</i>) control surface style (solid, mesh, dot)
<i>surftransparency*</i>	adjust molecular surface transparency
<i>swapaa</i>	mutate amino acids or swap rotamers
<i>swapna</i>	mutate nucleic acid residues
<i>sym*</i>	generate symmetry copies that update automatically
<i>system</i>	send a command to the system shell
<i>thickness</i>	move the clipping planes in opposite directions
<i>topography</i>	plot values in a volume data plane as surface heights
<i>turn</i>	rotate about the X, Y, or Z axis
<i>vdw*</i>	display van der Waals (VDW) surface
<i>vdwdefine*</i>	set VDW radii
<i>vdwdensity</i>	set VDW surface dot density
<i>version</i>	show copyright information and Chimera version
<i>viewdock</i>	start ViewDock and load docking results
<i>volume</i>	visualize volume data such as electron density
<i>vop</i>	edit volume data to create a new volume data set
<i>wait</i>	suspend command processing until motion has stopped
<i>window</i>	adjust the view to contain the specified atoms
<i>windowsize</i>	adjust the dimensions of the graphics window
<i>write</i>	save atomic coordinates (pdb, mol2)
<i>writesel</i>	write a list of the currently selected (or unselected) items

Set/Unset Toggle Options

<i>autocolor</i>	make each newly opened model a unique color
<i>independent</i>	make each model rotate about its own center of mass instead of the combined center of mass

Set/Unset Value Options

<i>bg_color</i>	set background color; <i>value</i> can be any color name
<i>dc_color</i>	set depth cue color; <i>value</i> can be any color name

Miscellaneous Operations (Default Settings)

Action	Procedure
<i>selection from screen</i>	Ctrl-left mouse button
<i>add/toggle selection</i>	Shift-Ctrl-left mouse button
<i>XY-rotation</i>	left mouse button inside "spaceball"
<i>Z-rotation</i>	left mouse button outside "spaceball"
<i>XY-translation</i>	middle mouse button
<i>Z-translation</i>	Ctrl-middle mouse button
<i>scaling</i>	right mouse button or the Side View
<i>Preferences</i>	Favorites...Preferences
<i>searching help</i>	Help... Search Documentation...

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, <i>e.g.</i> , : G?? @ CA specifies the alpha carbons of all residues
=	partial wildcard	matches partial atom or residue names, <i>e.g.</i> , @ C= specifies all atoms with names beginning with C
?	single-char wildcard	used for atom and residue names only, <i>e.g.</i> , : G?? selects all residues with three-letter names beginning with G
;	command separator	separates multiple commands on a single line
z<	zone specifier	z<zone or zr<zone specifies all residues within <i>zone</i> angstroms, za<zone 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 (when space-delimited)

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 the atomic display bit is "on"
@/drawMode=mode	<i>mode</i> can be 0 (dot, as in wireframe), 1 (sphere, as in CPK), 2 (endcap, as in stick), or 3 (ball, as in ball-and-stick)
@/element=atno	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, <i>etc.</i>)
@/surfaceDisplay	per-atom surface display bit (can be true for buried atoms with no surface)

Selected Residue Attributes

Usage	Description
:/areaSAS=sasa	solvent-accessible surface area
:/areaSES=sesa	solvent-excluded surface area
:/isHelix	whether the residue is in an alpha helix
:/isHet	whether the residue is in PDB HETATM records (or the mmCIF equivalent)
:/isStrand or /isSheet	whether the residue is in a beta strand
:/isTurn	whether the residue is assigned to a turn in the input file
:/kdHydrophobicity=value	Kyte-Doolittle amino acid hydrophobicity
:/ribbonColor=ribcolor	color of the residue's ribbon segment
:/ribbonDisplay	per-residue ribbon display bit (can be true for residues such as water that cannot be shown with ribbon)
:/type=resname	residue name

Selected Molecule Model Attributes

Usage	Description
#/ballScale=factor	ball size relative to VDW radius
#/color=color	model-level color assignment
#/display	model display bit
#/explicitHydrogens	whether the model has hydrogen atoms
#/lineWidth=width	linewidth of wire representation

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
element.S
- all sulfur atoms
@ca!/label and color!=green and color!=red
- atoms named CA which are not labeled, and are not green or red
@/color=yellow or color=blue and label
- atoms that are yellow and atoms that are both blue and labeled
:asn/isHelix
- asparagine residues in alpha 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 sp ³ -hybridized, formally positive nitrogens
@/bfactor>50 & ~ solvent & ~ ions
- atoms with B-factor values over 50, excluding solvent and ions

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