

Commands

*reverse function ~**command** available

<i>ac</i>	enable accelerators (keyboard shortcuts)
<i>addaa</i>	add an amino acid to a peptide C-terminus
<i>addh</i>	add hydrogens
<i>alias*</i>	create an alias or list aliases
<i>align</i>	align two 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 the representation of bonds (wire, stick)
<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, labels and surfaces
<i>colordef</i>	define a new color
<i>conic</i>	create a shadowed space-filling image (static; UNIX only)
<i>copy</i>	save or print the displayed image
<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>focus</i>	adjust the view and center of rotation to the specified atoms
<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>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 lines in the wireframe representation
<i>load</i>	restore a saved Chimera session
<i>longbond</i>	find and remove excessively long bonds
<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>mmaker</i>	(<i>matchmaker</i>) align models in sequence and then superimpose them accordingly

<i>modelcolor</i>	set color at the model level
<i>modeldisplay*</i>	set display at the model level
<i>move</i>	translate along the X, Y, or Z axis
<i>neon</i>	create a shadowed solid stick image (static; UNIX only)
<i>objdisplay*</i>	display graphical objects
<i>open*</i>	open structures or data for display or execute a command file
<i>pdbrun</i>	send an annotated PDB file of the current display to the system shell (UNIX only)
<i>push,pop</i>	push or pop images on the picture stack
<i>rainbow</i>	color residues, chains, models over a range (default blue to red)
<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 the representation of atoms and bonds (wire, stick, bs or b+s, sphere or cpk)
<i>reset</i>	restore default or saved orientations
<i>ribbackbone*</i>	allow residue ribbon and backbone atoms to be displayed simultaneously
<i>ribbon*</i>	display a secondary structure ribbon
<i>ribbonjr</i>	create a ribbon image (static; UNIX only)
<i>ribcolor*</i>	set ribbon color
<i>ribrepr</i>	control the ribbon representation (flat, edged, round)
<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 for further operations
<i>set*</i>	set options (see Set/Unset Options)
<i>show*</i>	display specified atoms, undisplay the others
<i>sleep</i>	suspend command processing for a specified length of time
<i>source</i>	execute a command file, updating the display continually
<i>stereo</i>	switch amongst stereo options and mono viewing
<i>stop</i>	exit from Chimera
<i>surface*</i>	calculate and display molecular surface
<i>surfcat</i>	(<i>msms cat</i>) group atoms for subsequent surface calculations
<i>surfcolor</i>	set whether surface color is determined at the atom or model level
<i>surfrepr</i>	(<i>msms repr</i>) control surface representation (solid, mesh, dot)
<i>swapaa</i>	mutate amino acid residues
<i>swapna</i>	mutate nucleic acid residues
<i>system</i>	send a command to the system shell
<i>tcolor</i>	color using texture map colors
<i>texture</i>	define texture maps and associated colors
<i>thickness</i>	move the clipping planes in opposite directions
<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 which version of Chimera is being used
<i>wait</i>	suspend command processing until motion has stopped
<i>window</i>	adjust the view to contain the specified atoms
<i>write</i>	save a molecule model as a PDB file
<i>x3dsave</i>	save the graphical scene as an X3D file

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>picking from the screen</i>	Ctrl-left mouse button
<i>adding to a selection</i>	Shift-Ctrl-left mouse button
<i>XY-rotation</i>	left mouse button when inside the "spaceball"
<i>Z-rotation</i>	left mouse button when outside the "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 (below)
<i>Side View</i>	Tools...Viewing Parameters...Side View
<i>Command Line</i>	Tools...Keyboard...Command Line
<i>Reply Log</i>	Tools...Utilities...Reply Log
<i>Preferences</i>	Favorites...Preferences
<i>listing of tools/extensions</i>	Tools category of Preferences (above); also specify which tools start when Chimera starts, which appear in the Favorites menu, and which icons appear in the tool bar

Atom 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., :*@CA specifies the alpha carbons of all residues
=	partial wildcard	matches partial atom or residue names, e.g., @C= specifies all atoms with names beginning with C
?	single-char wildcard	used for atom and residue names only, e.g., :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 of the indicated atoms, and za<zone specifies all atoms (rather than entire residues) within <i>zone</i> angstroms of the indicated atoms. Using > instead of < gives the complement.
&	intersection	intersection of specified sets
	union	union of specified sets
~	negation	negation of specified set (when space-delimited)

Atom Attributes

Usage	Description
@/altLoc=altloc	altloc is the alternate location ID
@/bfactor=bfactor	bfactor is the B-factor
@/color=color	color is the color assigned on a per-atom basis
@/drawMode=mode	mode 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)

@/defaultRadius=rad	rad is the default VDW radius
@/display	whether display is enabled at the atom level
@/element=atno	atno is the atomic number
@/idatmType=type	type is the atom type
@/label	whether the atom is labeled
@/label=label	label is the text of the atom label
@/labelColor=labcolor	labcolor is the color of the atom label
@/name=name	name is the atom name
@/occupancy=occupancy	occupancy is the occupancy
@/radius=radius	radius is the current radius (may have been changed from the default VDW radius)
@/serialNumber=n	n is the atom serial number in the input file
@/surfaceCategory=catname	catname is the category the atom belongs to for surface calculation purposes (main, ligand, etc.)
@/surfaceColor=surfcolor	surfcolor is the color of the atom's molecular surface
@/surfaceDisplay	whether molecular surface display is turned on for the atom
@/vdw	whether VDW surface display is turned on for the atom

Residue Attributes

Usage	Description
:/isHelix	whether the residue is in an alpha helix
:/isStrand or /isSheet	whether the residue is in a beta strand
:/isTurn	whether the residue is in a turn according to PDB TURN records
:/kdHydrophobicity=value	value is the Kyte-Doolittle hydrophobicity
:/ribbonColor=ribcolor	ribcolor is the color of the residue's ribbon segment
:/ribbonDisplay	whether ribbon display is turned on for the residue (can be true for residues such as water that cannot be shown with ribbon)
:/type=resname	resname is the residue name

Molecule Model Attributes

Usage	Description
#/color=color	color is the color assigned on a per-model basis
#/display	whether display is enabled at the model level

#/explicitHydrogens	whether the model has hydrogen atoms
#/lineWidth=width	width is the wireframe linewidth
#/pointSize=size	size is the font size of labels
#/vdwDensity=density	density is the dot density used for VDW surfaces

Atom Specification Examples

#0
- all atoms in model 0

#3:45-83,90-98
- residues 45 through 83 and 90 through 98 in model 3

:lys,arg
- lysine and arginine residues

:12,14@ca
- alpha carbons in residue 12 and residue 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

:12-15,16-18.a,15.b@ca
- CA atoms within the following residues: 12 through 15 (with no chain ID), 16 through 18 in chain A, and 15 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 sp³-hybridized, formally positive nitrogens

@/bfactor>50 & ~ solvent & ~ ions
- atoms with B-factor values over 50, excluding solvent and ions

UCSF Chimera was developed by the Computer Graphics Laboratory at the University of California, San Francisco, under support of NIH grant P41-RR01081. The software is copyrighted and licensed by the Regents of the University of California.