UCSF Chimera Quick Reference Guide

November 2014

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
adjust	change bond angle or bond length
*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 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 graphical scene
*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 coordinates
help	display the manual page for a command
hkcage	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	perform least-squares fitting of 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**	save and 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
ramachandran	show Ramachandran plot of protein residues
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)
ribspline	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	partition a molecule model into 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
vseries	display, process, and save volume series
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	**#** *model* (integer)
#.	submodel number	**#.** *submodel* (integer)
:	residue	**:** *residue* (name or number)
::	residue name	**::** *residue*
:.	chain ID	**:.** *chain*
@	atom name	**@***atom*
@.	alternate location ID	**@.** *alt_loc*
–	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 *zone* 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

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*	*mode* can be 0 (dot), 1 (sphere), 2 (endcap, as in stick), or 3 (ball)
@/element=*atno*	atomic # or element symbol
@/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@n,ca,c,o
- atoms named N, CA, C, and O 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

:.A & protein
- chain A residues classified as protein

:26-28.a,33.a & side chain/base.with CA/C1'
- or -

:26-28.a,33.a & with CA/C1'
- sidechain + CA of residues 26-28 and 33 in chain A

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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