UCSF MidasPlus

QUICK REFERENCE GUIDE

February 1990

Programs in the MidasPlus package

cartoon	generate ribbon representation of proteins
conic	generate CPK-style molecular models with shadows
esp	calculate electrostatic potential
fixatname	correct AMBER pseudo-PDB files so they are in standard PDB format
gentpl	generate a MIDAS template from a Protein Data Bank coordinate file
ilabel	label an IRIS image with arbitrary text
irs	interior atom removal and site selection
makesurf	convert ‘‘ms’’ format surface files to MIDAS surface databases
maketpl	create MIDAS residue templates
midas	MidasPlus molecular interactive display program
midas.dump	print information about MIDAS databases
midas.in	convert Protein Data Bank format to MIDAS format
midas.bond,midas.link	miscellaneous MIDAS database maintenance utilities
midas.out	convert a MIDAS database to Protein Data Bank format
midas.tty	terminal based version of MidasPlus display program
ms	calculate a solvent accessible molecular surface

MidasPlus Commands

addaa	add an amino acid to the end of a molecule
addgrp	add a new group to a residue
alias	set command aliases
align	align two atoms along the z-axis
angle	calculate the angle between three atoms
assign	assign functions to pseudo-sliders
bond	make a bond between two atoms
brotation	initiate a ‘‘backwards’’ bond rotation
cd	change current working directory
chain	chain specified atoms together
clip	move clipping planes
cofr	change center of rotation
color	color bonds, labels and surfaces
conic	display shadowed, space-filling image
copy	send display image to a printer or file
delete	delete a group from a residue
display	display specified molecules, residues, atoms
distance	display atom distances
fix	make bond rotations permanent
fixreverse	fix bond rotations and reverse rotation
freeze	stop rock or roll motion
getcrd	return <x,y,z> coordinates for an atom
help	show information about MidasPlus commands
intensity	set depth cue intensity at hither and yon clipping planes
label	label atoms and residues
link	join two residue chains
match	superimpose two models
midaspop	pop MIDAS window to front of other screen windows
midaspush	push MIDAS window behind other screen windows
move	translate selected models
open	open a MIDAS database or PDB file for display
pdbrun	pipe PDB file describing current models to arbitrary command
push,pop	push or pop images on the picture stack
read	read a command file
record	record all executed MidasPlus commands in a file
reset	reset all models to original orientations
reverse	reverse the direction of a rotation
rlabel	enable residue labeling
rock	rock a structure about the x, y or z axis
roll	roll a structure or bond rotation about the x, y, or z axis
rotation	activate a bond rotation
run	execute a shell command and send output to MIDAS
save	save a MIDAS session
savepos	save a model’s current orientation
scale	apply a scaling factor to all models
section	change sectioning of the display
select	select models for move, rock, roll, or turn commands
set,unset	set options (see ‘‘set/unset options" below)
setcom	set molecule’s center of mass
show	display specified atoms and no others
sleep	temporarily suspend all display activity
source	read and execute a command file
speed	set the control speed of pseudo-sliders and spaceball
stop	terminate the current MidasPlus session
surface	display a model’s ‘‘ms’’ surface
swapaa	exchange one amino acid for another
swapna	exchange a nucleotide for another
system	execute a UNIX shell command
thickness	change thickness of the displayed image cross section
turn	turn a structure about the x, y, or z axis
vdw	display van der Waals surface
vdwopt	set van der Waals surface options
wait	interrupt processing until model has stopped moving
window	display the entire molecule on the screen
write	output a model as a MIDAS database or PDB file
zone	display only those atoms within specified distance

Reverse Command Functions

~assign	deactivate pseudo-sliders
~bond	remove a bond between two atoms
~brotation	remove a ‘‘backwards’’ rotation
~chain	break chaining for all atoms listed
~display	delete atoms from the display
~distance	remove a distance calculation
~link	break a residue chain into two parts
~label	remove atom and residue labels
~open	close a model
~pop	equivalent to *push* command
~push	equivalent to *pop* command
~rock	terminate *rock* motion
~roll	terminate *roll* motion
~rotation	remove a rotation
~select	deselect a model
~set	unset an option (see ‘‘set/unset options’’ below)
~show	delete atoms from the display
~surface	remove a ‘‘ms’’ surface display
~turn	terminate *turn* motion
~vdw	remove a van der Waals surface display

Set/Unset Toggle Options

cofg Puts a '+' at the center of rotation for the selected models. The '+' corresponds to the center of gravity if there is only one molecule or if the rotations are independent (center of mass of selected molecules).

control
If set, display the control panel.

halfbond
If set, atoms are colored by halfbond connections to other atoms instead of each atom having one whole bond associated with it. Note that using halfbond mode may degrade response time.

independent
If set, models rotate about their independent centers of mass, otherwise models rotate about the common center of mass.

labels Turns on distance, rotation, and angle monitoring labels.

reassign
Allows assignment of multiple functions to the same slider, *i.e.* multiple *assign* commands for the same slider give the slider simultaneous functions. If reassign is set, existing or previous assignments are removed before a new device assignment is completed.

ortho Use orthographic instead of perspective projection.

showsphere
Controls whether a circle defining the transition between ***x,y*** versus ***z*** rotation is shown when MidasPlus is in ''virtual trackball'' manipulation mode.

smooth
If set, bonds in wire-frame models are drawn using anti-aliased vectors (no staircasing).

sphere
If set, MidasPlus uses a ''virtual trackball'' method for model manipulation. Otherwise, model interaction is controlled via various combinations of mouse buttons.

stereo Display image for appropriate for stereo viewing.

text Activates the COMMAND and REPLY text lines on the bottom of the display screen. This option can be turned off using **unset text** when taking photographs.

verbose
MIDAS prints confirmation messages after each successful command. If verbose is **unset** these messages will not appear.

Set/Unset Value Options

bg_color
Sets the MIDAS background color. *Value* can be either a color keyword or color index as described in detail under **color**.

bg_intensity
Controls the brightness of the background color. *Value* can vary from 0 (black) to 1 (full intensity). For purposes of backwards compatibility, *value* can be in the range 0-255, in which case it will be interpolated into the range 0-1 and handled appropriately.

eyesep
The separation between the centers of the viewer's eyes, in inches. (Necessary to compute projections for stereo viewing.)

linewidth
This controls the thickness with which bonds are drawn. The default is 1, and larger values produce thicker lines (and slower interaction).

nameplate
This controls the placement of the MidasPlus logo on the bottom of the screen. A *value* of 0.0 puts it to the extreme left; 1.0 puts it to the right.

viewdist
The distance from the viewer to the screen, in inches. (Needed to correctly compute stereo projections.)

vpsep Amount of vertical separation between left and right eye images in stereo mode, in scan lines. (Needs to be set only once for each workstation with stereo.)

Special Symbols

Symbol	Function	Usage
#	model number	**#** *model_number*, where *model_number* is an integer.
:	residue	**:** *residue*, where *residue* is a residue name, residue sequence number, or range of residues.
@	atom name	**@** *atom_name*, where *atom_name* is an atom name or range of atoms.
–	range	specifies a range of atoms such as @CB-* (beta carbon to the last atom in model), a range of residues such as :35-66 (residues 35 through 66) or a range of colors such as red-blue (shades of red, magenta, and blue).
*****	wildcard match	matches whole atom or residue names. *e.g.* #0:*****@CA selects the alpha carbon atoms of all residues.
?	single char wildcard	used for atom and residue names only. *e.g.* :G**??** selects all three letter residue names beginning with ''G''.
%	*nth* residue or atom	*e.g.* :**%**5 selects every fifth residue in the sequence.
b>	temperature factor	**b>** *temp_factor* selects all atoms with temperature factors greater than *temp_factor*. **b<** *temp_factor* selects all atoms with temperature factors less than *temp_factor*. (May be used together to select a range.)
e>	electrostatic potential	**e>** *potential* selects all atoms with electrostatic potentials greater than *potential*. **e<** *potential* selects all atoms with electrostatic potentials less than *potential*. (May be used together to select a range.)
+	atom picking	enables use of the mouse to select atoms whose names are substituted for the leftmost appearance of '+' symbol in the MIDAS command line.

Keyboard Editing Characters

(same as *EMACS* text editor)

Character	Function	Usage
RETURN	return	accept the line.
LINEFEED	linefeed	accept the line.
RUBOUT	backspace	erase the character before the cursor.
CTRL-H	backspace	erase the character before the cursor.
CTRL-U	line kill	erase the whole line.
CTRL-W	word kill	erase the word before the cursor.
CTRL-D	delete	erase the character under the cursor.
CTRL-K		erase to end of line.
CTRL-P	history	retrieve previous command(s).
CTRL-N	history	retrieve next command(s).
CTRL-A		go to beginning of line.
CTRL-E		go to the end of line.
CTRL-B		move back a single character.
CTRL-F		move forward a single character.
CTRL-L		move cursor one word left.
CTRL-R		move cursor one word right.
CTRL-G		insert next character without interpretation.
ESC	break	break after the completion of the current command. (See **source** command.)

MidasPlus was developed by the Computer Graphics Laboratory at the University of California, San Francisco under support of the National Institutes of Health grant RR-01081. The software is copyrighted and licensed by the Regents of the University of California.

Additional copies of the MidasPlus User's Manual, including this Quick Reference Guide, are available for $10 each postage paid by writing to MIDAS Software Distribution, Computer Graphics Laboratory, School of Pharmacy, University of California, San Francisco, CA 94143-0446. Please include a check or money order payable to The Regents of the University of California with your request. Sorry, but purchase orders cannot be accepted. Orders received without payment enclosed will be returned unprocessed.