Pymol_Basic Cheat Sheet

by leilaP via cheatography.com/36664/cs/11524/

Set up

Set working directory	`cd C:\Users\...`
Load pdb file from pdb website	`fetch 1ubq`
Load pdb file from local disk	`load 1ubq.pdb`

Log files

new log file	`log_open file_name.pml`
save and quit log file	`log_close`
comment	#
record the view coordinate	`get_view`
run a log as a script	`@file_name.pml

resume log file = run then edit at the end
append log file = edit at the end without running

Selection

select selection_name, selection_expression	`select carbon_beta, n. cb`
select selection_name= (selection expression)	`select carbon_beta = (n; cb)`

logical operator: and (/), not, or. !order of precedence --> use ()

Selection - single word

All atoms	all	*
No atoms	none	none
All hydrogen atoms	hydro	h.
All atoms from HETATM record	het	hetatm

Porperty selector identifiers

Atom by chemical symbol ex: Oxygen = O	symbol	e.
Atom/nucleic acid by code ex: Cα = ca, Cβ = cb	name	n
Aa/nucleic acid by code ex: Asparagine = asp / adenosine = a	resn	r
residue identifier (1-9999)	resi	i
PDB chain identifier (check in PDB file if letter or number ID)	chain	c
Secondary structure: α helix = 'H', β strand = "S", Loop = 'L'	ss	ss

carbon α : first carbon bond to the side chain
carbon β : second carbon bond to the side chain

selection macros

/object-name/segi-identifier/chain-identifier/resi-identifier/name-identifier

start by "/": start from the top of the hierarchie (object-name)

end by "/": start from the bottom of the hierarchie (name-id)

// :skip one level of hierarchie

ex: `select lys, /helix_alpha///lys`

select all the residue of lysine from the object "helix_alpha"

Diplay

show the selection as this diplay type	`show_as lines, selection_name` `cmd.show_as("lines", "selection_name")`
add this display type of the selection	`show lines, selection_name` `cmd.show("lines", "selection_name")`
hide this display type of the selection	`hide lines, selection_name` `cmd.hide("lines", "selection_name")`
color the selection	`coloc color_name, selection_name`
zoom on the selection	zoom selection_name

Show (S button) - Hide (H button) - Color (C button)
display type: lines, ribbon, cartoon, stick, label, nonbonded, mainchain, sidechain

Structure modification

adds hydrogens in the appropriate places	h_add

get information

count the number of atome of the selection	`count_atoms selection_name`

selection algebra

Selects atoms that are not included in s1	`not s1`	`! s1`
Selects atoms included in both s1 and s2	`s1 and s2`	`s1 & s2`
Selects atoms included in either s1 or s2	`s1 or s2`	`s1 | s2`

selection algebra (cont)		
Selects atoms in s1 whose identifiers name, resi, resn, chain and segi all match atoms in s2	`s1 in s2`	`s1 in s2`
Selects atoms in s1 whose identifiers name and resi match atoms in s2	`s1 like s2`	`s1 l. s2`
Selects all atoms whose van der Waals radii are separated from the van der Waals radii of s1 by a minimum of X Angstroms.	`s1 gap X`	`s1 gap X`
Selects atoms with centers within X Angstroms of the center of any atom in s1	`s1 around X`	`s1 a. X`
Expands s1 by all atoms within X Angstroms of the center of any atom in s1	`s1 expand X`	`s1 e. X`
Selects atoms in s1 that are within X Angstroms of the s2	`s1 within X of s2`	`s1 w. X of s2`
Expands selection to complete residues	`byres s1`	`br. s1`
Expands selection to complete objects	`byobject s1`	`bo. s1`
Selects atoms directly bonded to s1	`neighbor s1`	`nbr. s1`