PyMol Quick Reference

Top Menu Options:

File:
Open – opens a .pdb file
Save session – saves the current session as a .pml file
Save molecule – saves the current molecule as a .pdb file
Save Image - saves the current viewscreen as an image (.png file)
Reinitialize – restarts the Pymol application
Quit - exits the program

Display:
Background – changes the color of the background

Mouse:
Selection mode – allows user to select by atom, residue, chain etc. with mouse
Editing/view modes – allows user to change mouse settings

Wizard:
Measurement – Allows the user to calculate measurements such as **distances**, bond **angles**, **dihedral** angles, etc.. Select measurement mode by clicking on blue box under 'Measurement' in the right hand menu.
Mutagenesis – Allows the user to change a selected residue for a different residue

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Right Menu Options: These actions are carried out on a user-defined *selection*. A selection can be a subset of all residues in the pdb file (i.e. chain A), or the entire pdb file. A selection can be made using **Selection mode** (see above) or with using script commands (see script commands).

[A]ctions
Allows the user to **zoom** on a selection, **orient** the selection appropriately on the screen and **center** it on the screen as well. The user can also

[S]how
Displays the selection in the form of **line, stick, ribbon, cartoon, sphere** and **surface** form. It can be applied exclusively to **main chain** or **side chain** atoms within the selection.

[H]ide
Hides that specific displayed form of the selection (i.e. **lines, sticks, cartoon, sphere** and **surface**) or hides every display form of the selection (**everything**) or all atoms not in the selection (**unselected**).

[L]abel
Labels the selection by a number of characteristics from residue name to chain id.

[C]olor
Colors the selection according to **element**, **chain**, or **ss**.

Online resources for Pymol:

Protein Data Bank	www.rcsb.org.
PyMol On-Line Manual	pymol.sourceforge.net/html/index.html
PyMol Wiki	www.pymolwiki.org

Script commands: These commands are typed into the *terminal* which is the small text window which usually opens on the top of the screen, or by pressing `Esc` on the keyboard in the main window.

`select [selection_name], [selection commands]` – creates a selection with a user-defined name that is a subset of the atoms based on the selections below.

Command	Subset	Example
`name`	Atom names	`name n+ca+cb+co+o`
`symbol`	Elements	`symbol o+n`
`resn`	Residue types	`resn asp+glu`
`chain`	Chain	`chain a+b`
`resi`	Residue numbers	`resi 101-110`
`ss`	Secondary structure	`ss h+s+l`
`hydro`	Waters	`hydro`
`hetatm`	Non-protein atoms	`hetatm`
`within`	Nearby atoms	`1FSS within 10 of res 14`

Example (creates a selection called '`A_Calphas`' that consists of all C_α atoms in chain A):

```
select A_Calphas, chain a and name ca
```

Help commands:

```
help select
help selections
help [command]
```

Miscellaneous useful commands:

`show cartoon`	show the cartoon representation
`hide everything`	clears the display window
`disable [selection]`	equivalent to 'unselecting' the object in the right menu bar
`run [script]`	runs a pymol script (.py file)
`color red, [sel1]`	colors selection sel1 red
`zoom [sel]`	zoom to fit the window to the selection
`orient`	zoom the window and alter the rotation center on the selection
`get_view`	returns the point-of-view settings
`ray`	produces a ray-traced image that can be saved as a png file.
`h_add [selection]`	adds hydrogen atoms to the selection
`align [sel1],[sel2]`	aligns selection sel1 to sel2