

PYMOL REFERENCE SHEET

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
-

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.

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

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:

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