Few PyMol commands
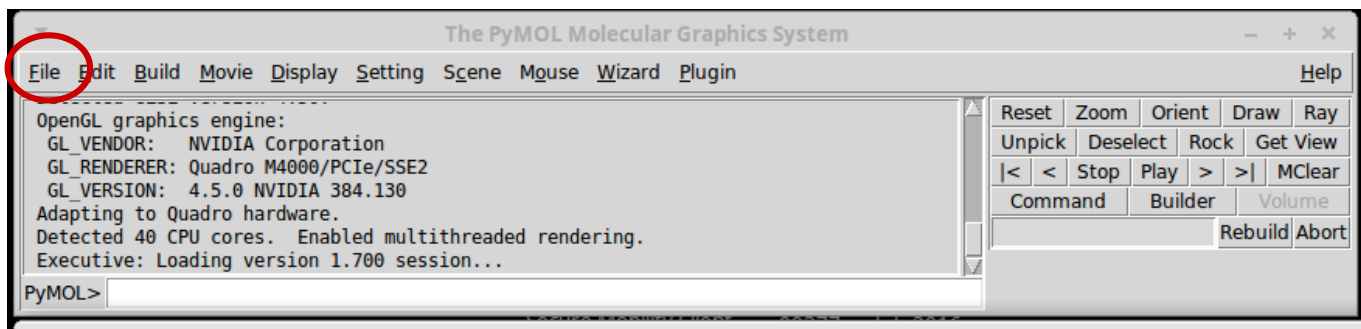
For more, make a search on the PyMol wiki https://pymolwiki.org/index.php/Main_Page

You can open several pdb in command-line: % pymol file1.pdb file2.pdb file?.pdb

When pymol is open, you can add a pdb file in the menu of the small gray window: *file > open*
You can save a session / molecule / image by *file > save*

Navigate in the visualization window
Left click :   rotate
Right click :   go forth/back
Middle click : translate
Mouse wheel: cut trough the molecules

!!! If you get lost in space, use *[A] > center* to be back at the center of your system

Change representations

In the visualization window, use the right panel to change the viewing parameters.

[A] = action (center molecule, fit two molecules, find polar contacts…)
[S] = show (represent atoms as lines, sticks, spheres ...)
[H] = hide (specifically hide cartoons, water, hydrogens…)
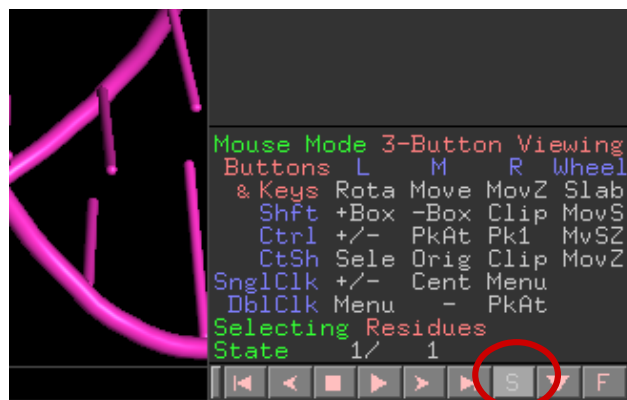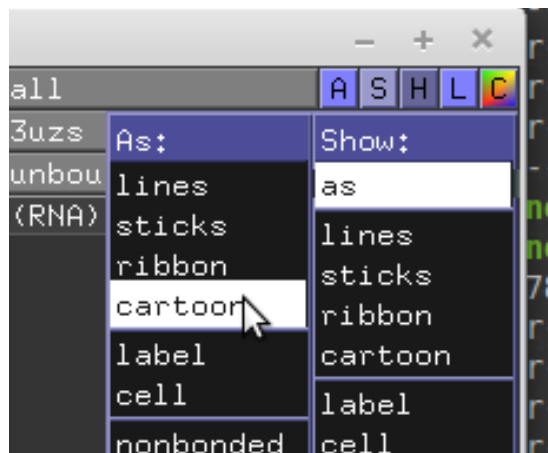[L] = label (charge, atom name …)
[C] = color

Use the "cartoon" representation, for an overview of the structure : *all > [S] > as > cartoon*
Color the system by chain (= by monomeric molecule) : *all > [C] > by chain > by chain*
Test also, on one molecule: *<molecule name> > [C] > spectrum > rainbow*
Display the sequence by [S] in the bottom right of the visualization panel.
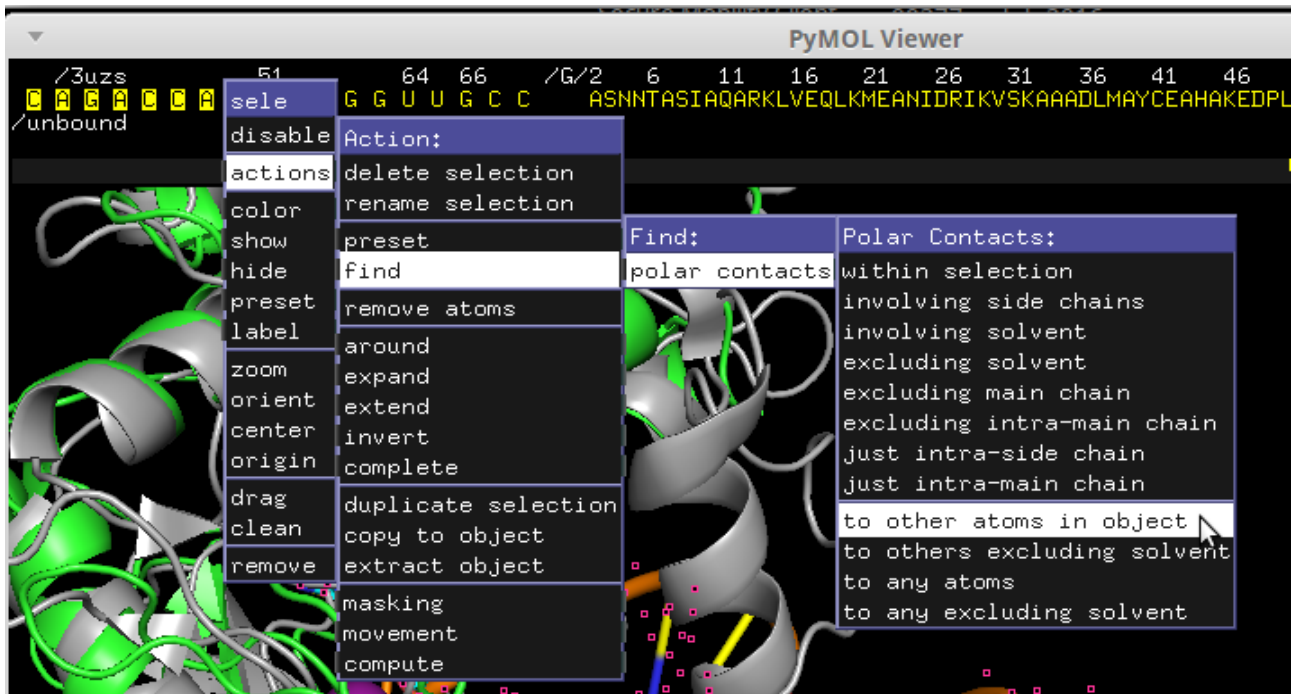
Multiple Models

To see docking results sequentially, use the > button in the bottom-right panel.
To see all results together, use the menu in the gray window: *Movie > Show all state* (last entry)

Selections

To **select nucleotides / amino-acids**, click on the sequence (see next page). The selected atoms are displayed with pink squares.
You can then use the selection to apply action, by right-click on the highlighted residues in the sequence or in the structure. In the above example, you will find the polar contacts (electrostatics) between your selection and the rest of the same pdb file.

To **select an entire chain** (ex the RNA of a structure), you can click on one residue in the sequence, then *right click > action > complete > chain*

Your selection will also appear as a new entry in the right panel, named *(sele)* per defaults. Use *[A] > rename* to avoid erasing it by a new selection.