PyMOL

A very sketchy and completely unsystematic list of PyMOL operations and commands

that might turn useful

Help:

https://pymolwiki.org/
https://www.pymol.org/

Intro for beginners:

https://pymolwiki.org/index.php/Practical_Pymol_for_Beginners

Control panel and the viewer

- For full use of all functions it is important to have a 3-button mouse (or two button + wheel).

- **Object Controls panel**:
- All – applies to all
- A- action
- S –show
- H for hide
- L for label
- C for color

Control panel and the viewer

- Default **mouse controls** in the view port window
- Left mouse button and hold: rotation around central point
- Middle – moving and changing the central atom
- Right mouse; zooming up and down
- Wheel – slab: where you are present in the slab you are viewing
- Wheel -Single click button – will move that atom to the center of the screen
- Holding the left mouse button while the pointer inside the molecule will rotate around the X and Y axes. However, if the pointer is outside the molecule, the rotation will be around the Z axis. (if the virtual trackball is turned on in the mouse menu)

Control panel and the viewer

- In PyMOL, the default orientation of the axes is with the X-axis pointing roughly to the right, the Y-axis pointing upwards, and the Z-axis pointing towards the viewer, essentially aligning with a standard Cartesian coordinate system when viewing a molecule in the center of the screen.
- **"Orient" command:**
- To explicitly align a molecule's principal components with the axes, use the "orient" command, which will position the longest axis along the X-axis.
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Control panel and the viewer

- **Change the viewing**
- Default coloring scheme by atom names in the last column
- Use color to change: by element; …
- By ss: sec. structure
- Spectrum: Rainbow from N to C :blue to red
- Spectrum: Color by b-factors: low =blue, high=red =
- **Labels**

- **By objects or by selection…**

Control panel commands examples

Examples of commands in Control Panel command line:

Load protein coordinates from PDB:

- fetch 1ubq
- fetch 1d3z
- fetch 1aar (di-Ub structure)
- fetch 1ndd (Nedd8)

Load protein coordinates from your computer:

If you have the coordinates stored on your computer, use the File/Open… tab and navigate to the folder where the coordinates file is stored. Click on the file.

Control panel and the viewer

Show menu:

- When you show one representation it doesn't get rid of the previous one
- To step back from the current structure drawing – simplify the view (if you chose ball-and-stick, but then want to show VdW spheres, go back to Preset/simple)
- Ribbon just traces the a-carbons
- Surface – will calculate and show the surface, you can see holes or pockets
- Spheres – good sense how they all are packed together. Same with dots

Control panel and the viewer

Action menu

- Orient – if you lost your molecule or will center. Will align the molecule such that the longest axis is approximately along the X axis
- Hydrogens – add or remove hydrogens
- **Preset representations**:
- ball and stick
- Technical– colors from N to C and shows all polar contacts
- Pretty
- B-factor putty: more motion in the fatter parts less in skinnier parts
- Publication view
- **Find** : find polar contacts etc
- **Align:** align two objects (first object onto the second: rotation and shift)
- **Compute** MW (be careful not to include waters), surface area
- **Delete** object
- **Generate**:
- Generate symmetry mates
- Vacuum electrostatics (colors and color bar show V in units of kT/e)

Control panel and the viewer

- **Objects and selections**
- Single left button click
- Can change the selection with respect to the rest of the molecule
- Rename selection in action
- Sequence view
- Clicking the middle button while on sequence will center it
- Change selection

Control panel and the viewer

- **How to save your work**

All your work on disk: use File/Save Session As

Store (in memory) a scene and retrieve it if needed:

- store scene with function buttons, say F1
  CTRL/F1 or scene F1, store
- F1 scene F1 Retrieve scene

- Or under Scene tab: Scene/Append under 001 then type command: scene 001 and it will restore

Wizard functions

Will discuss in class

- **Measurement**
- **Mutagenesis**
- **dss**

To determine the total molecular weight of the protein:
simply click on the Action button, select “remove waters”,
then select “compute” on the bottom, choose “molecular weight” and then “with missing hydrogens”. Read the output on the screen

Control panel and the viewer

- **Distance (outside the Wizard)**
- Select atoms: ctrl/middle button
  shows pk1 and pk2 (pick 1 and 2)
- Distance
- Color red, dist01

- Delete all
- Generate symmetry mates
- Surface of protein in protein/DNA: need to split them up:
  create protein, chain a
  create dna, chain b
- Pymol.sourceforge.net

More functions

Select an object or part of it

- select ubiq, 1ubq (or shorter: sele ubiq, 1ubq)
- select chA, 1ubq and chain A
- select positive, 1ubq and resname lys+arg
- (or shorter: sele positive, 1ubq and resn lys+arg)
- select helix, 1ubq and resid 23-34

Take a piece of an object and make it a new object (similar to selection commands but with create):

- create 1ubq_helix,1ubq and resid 23-34
- create 1ubq_str,1ubq and resid 64-71

Superimpose/align two structures or objects or selections:

align 1ubq, 1d3z moves first onto second based on sequence similarity

super 1ubq, 1d3z uses the structure (alpha and beta) instead of the sequence

align 1ubq_str, 1ubq_hel

super 1ubq_str, 1ubq_hel