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 and the viewer

- **Show:**
- 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

Wizard

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

Examples of commands to type in Control Panel command line:

Load protein coordinates:

- fetch 1ubq (ubiquitin X-ray structure)
- fetch 1d3z (ubiquitin NMR structure)
- fetch 1aar (di-Ub structure)
- fetch 1ndd (ubiquitin-like protein Nedd8)

Select an object or part of it

- select ubiq, 1ubq (or shorter: sele ubiq, 1ubq)
- select chA, 1ubq and chain A
- select posit, 1ubq and resname lys+arg (or shorter: sele posit, 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 commends but with create):

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

Overlay two structures or objects or selections:

- align 1ubq, 1d3z moves first object 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

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

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 helix, 1ubq and resid 23-34
- helix, 1d3z_mod1 and resid 23-34
- Select pos, 1ubq and chain a and resname lys+arg

- Align 1ubq, 1d3z

move/align first object onto the second based on sequence

- super 1ubq, 1d3z

move/superimpose first object onto the second based on the structure (alpha and beta) instead of the sequence to

Create 1ubq_hel, 1ubq and resid 23-34