PyMol Tutorial & Summary

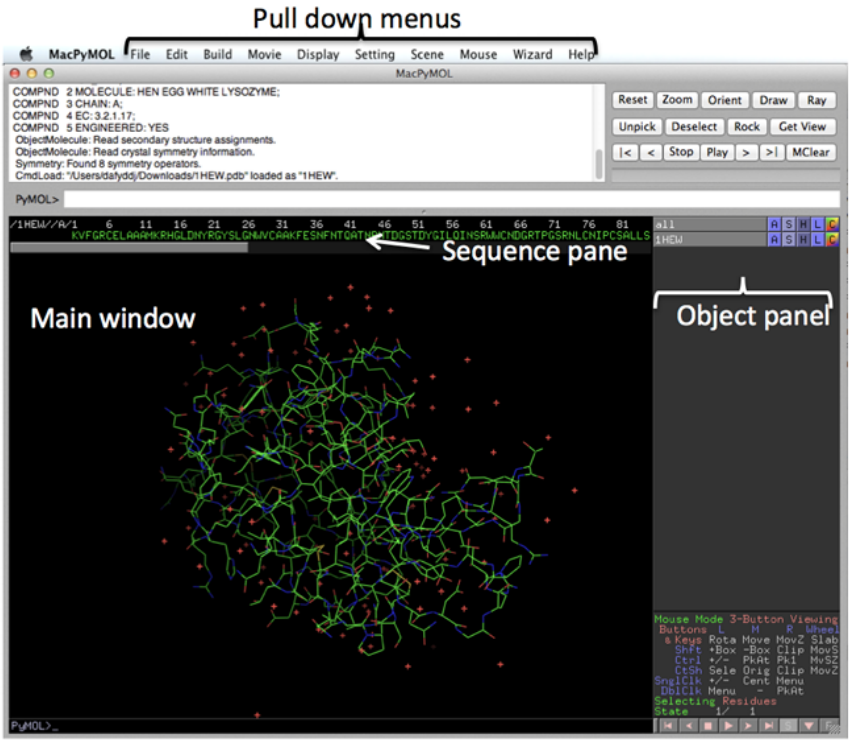
Accessing PyMol:

- Option 1 (recommended): Use the in-person LTS machines, which have PyMOL already downloaded
- Option 2: log in remotely to an LTS machine according to this handout
- Option 3: Download PyMOL from the Robin Li and Melissa Ma Science Library website. The University has a campus-wide license agreement for PyMOL, and can be accessed here (simply scroll down to the Academic and Non-Profit Price List, and click to determine if your institution has a site-wide PyMOL Subscriber. If you are on Stanford wifi, or using a Stanford VPN, you should receive a license file download.)

The Protein Data Bank

- The RCSB Protein Data Bank (RCSB PDB) is an online databank of known protein structures. Each protein has a unique 4 character code that can be used in PyMol to access the protein. Additional data is available about the protein, including its classification, organisms, any mutations, the paper & researchers who determined the structure, and more.

Navigating PyMOL:



3 Ways to load structures into PyMOL (demo each one with the same structure, ubiquitin):

1. Download in PyMOL (PDB format), open the structure from your files
2. >> load Path/to/Structure.pdb
3. >> fetch StructurePDBTag #fetch 1ubq for ubiquitin

Command line arguments

>> reinit #reinitializes PyMOL: useful if you want to clear everything/ start from scratch

Navigating the 3D structure:

- Left click lets you rotate the protein
- Pinching with the mouse lets you zoom in and out
- Opt + right click (on mac, ctrl click on windows) to move left & right
    - Must be clicking within the structure
- Two button viewing by going to the mouse menu: can choose two button viewing and you change the commands (If you have a mouse, it does make it easier, but its doable with a trackpad for sure.)
- Control z is undo

Action menu on the right side:

- As you click on different parts of the structure, your selections are automatically added here — allows you to manipulate them

Other actions (can click in action menu or type in command line):

- Show/Hide ('S', 'H' in action menu):
    - Spheres: spacefilling view
    - Lines: basic representation of atoms & bonds
    - Sticks: bonds are drawn as sticks (thicker than lines)
    - Cartoon: shows alpha helices & beta pleated sheets
- Color ('C' in action menu):
    - By secondary structure: helix sheet loop (in cartoon view)
    - By element (in line view)
    - Chainbows: colors residues in each protein chain as a rainbow that begins with blue and ends with red (line view)
- Label: ('L' in action menu):
    - Residues
    - Chains

Sequence viewer:

- Helpful for selection
- >>set seq_view, on
- >> set seq_view, off

Demo: Taking measurements:

PkAt ('pick at'): depends on mouse mode

- Can only select more than one in 'editing'

Click on two and it shows the distance between them.

>> get_distance pk1, pk2 # gives the exact distance

>>get_angle pk1, pk2, pk3

>> get_dihedral pk1, pk2, pk3, pk4

Demo: Selection

>> select resN phe #selects residue Name phenylalanine

>> select resi 3 # selects residue number id 3

>> select resi 24-27

>> select element O # selects all oxygens

>> select name ca #selects all the c_alphas, or The alpha carbon (α-carbon or Cα)
is what connects the amino group to the acid carboxyl group, giving amino acids their name.

>> select resi 1-10 and (not resi 4)

>> select bb. # selects the backbone. Can hide everything, and then show the backbone as sticks

Adding/removing hydrogens:

>> h_add adds hydrogens (you won't see them in cartoon view.)

Remove with the actions menu (A > hydrogens > remove)

Passing in selections as arguments:

>> show licorice, sele

>> color red, sele

Running scripts in PyMOL

>>reinit

>>cd /Users/lucibresette/Downloads/Assignment 1

>>load pdbs/helices.pdb
>>run analysis.py
>>get_residue_numbers helices #won't do anything on your computer, demo script

Further resources/guidance:

- Get the list of all commands by hitting <TAB>
- Get the list of arguments for one command with a question mark: >> color ?
- Read the online help for a command with 'help': >> help color
- Official PyMOL documentation