<How to visualize protein structures using PyMol>

A. Retrieving Pdb (protein data base) files:

1. Go to http://www.rcsb.org.
2. Search and download the pdb files: 1NYM.pdb (Structure of the complex between β-lactamase and a boronic ester inhibitor (CXB))

B. Using Pymol

1. Download and install Pymol (http://pymol.sourceforge.net/)
2. Start Pymol.
3. Open the β-lactamase (1NYM) file.
4. Show a ribbon diagram (called "cartoon" in Pymol) and hide the lines and waters.
5. Change the color of the α-helices and β-sheets in different ways (try "chainbows"). Try to change the background color. Leave the molecule colored in green.
6. Turn the sequence (in Display menu) on and click on CXB at position 300 (inhibitor)
7. Display the CXB in a space-filling model (called "spheres") and highlight it in red.
8. Generate the "Ray" image and save the session and image (as PNG file).

9. On the top of the ribbon diagram, show a surface model.
10. Change the transparency of the surface from 0 to 100% to (partially) expose the ribbons.
11. Select CXB and show a stick or space-filling model and highlight it in red.
12. Again generate the "Ray" image and save the image (as PNG file).

13. Zoom in on the inhibitor.
14. Select Ser-70, Lys-73, Glu-166, and Lys-234 and display them as sticks.
15. Again generate the "Ray" image and save the image (as PNG file).
16. Hyde CXB
17. Measure (in Wizard menu) the distances between
      i) Ser-70-O and Lys-73-N
      ii) Ser-70-O and Glu-166-COO

C. Assignment

Combine all three PNG files generated above and the distance information in a Word file and send the file to your TA as email attachment by next Thursday 6 PM.

<How to make protein structure movies using PyMol>

Example 1: Simple rocking

1. Load a protein onto PyMOL
2. Create a view that is interesting to you
3. Save the view created for future use
4. Now we will create frames for a movie based this view
5. Before you create frames, you need to create a directory to save all the frames that will be created
6. Type the following commands on the PyMOL command line:

mset 1 x120	# This will create 120 frames
util.mrock(1, 120, 10, 1,1)	# This command will rock the view +/- 10degree upto 120 frames
mplay	# This will play the 120 frames and the frames created will be saved on a cache. You will be able to see your molecule rocking on PyMOL viewer.

7. Now you need to save the frames.
   File→Save Movie→Select the directory created in step 5→enter the name of the prefix of the frames→Save
8. Now if you go the directory created in step 5, you will see 120 images in PNG format. To complete the movie-making process, you need to stack the 120 image sequences in AVI format or in MPEG format etc. We will do it using ImageJ that is freely available from NIH website (http://rsb.info.nih.gov/ij/) (Or you can make a movie with QuickTime Pro.)
9. Go to ImageJ webiste and download the latest version. If you are using Windows OS, I suggest that you download a precompiled version bundled with Java.
10. Once you have downloaded and installed ImageJ, start ImageJ.
11. File→Import→Image Sequence…→Go to the directory in which you installed the 120 frames in step 7→Select the first frame (for example, *001.png)
12. You will see "Sequence Options" window pop up. Accept all the default setting. Then click "OK"
13. Once ImageJ has finished importing all the frames into a image stack, you need to save the image stack in a movie format.
14. File→Save As→AVI…
15. This will bring up "Save as AVI…" popup window. Enter maximum JPEG Quality. You can also change the speed for the movie. Accept the default speed. Click "OK". Select a directory to save the movie. If the movie plays too fast/slow, you can come back and change the speed. (Usually 30 frames per second should work find.)

    (**Before you type any PyMOL commands, you can also use viewport command to adjust frame size. For example to create a frame of 640x480 pixels, issue the following command before any other commands:

    viewport 640 480

But this command is only optional.)

Example 2: Simple rolling

1. Just follow the same procedure as in Example 1 except the following command
2. In step 6, instead of util.mrock, use util.mroll
3. Type the following commands on the PyMOL command line:

mset 1 x120   # we will create 120 frames
util.mroll(1, 120, 1)   # this command will create full rotation over 120 frames
mplay   # this will play the 120 frames and the frames created will be saved on a
    cache. You will be able to see your molecule rocking on PyMOL viewer.

4. Now you need to save the frames.
    File→Save Movie→Select a directory →enter the name of the prefix of the frames→Save

Note: Before you make movies, practise and get familiar with the following key PyMOL commands:
 mset
 mdo
 mplay
 util.mrock
 util.mroll
 rock
 rotate
 turn
 translate etc.

They can be all found in PyMOL Wiki (http://www.pymolwiki.org/index.php/Main_Page) commands
part.