Handout 3
Pymol tips

Pymol resources
A wiki for the Pymol program, with descriptions of commands and tutorials, is available at:

http://pymolwiki.org/index.php/Main_Page

For some Pymol-rendered examples for inspiration, visit:

http://pymolwiki.org/index.php/Gallery

http://pymolwiki.org/index.php/Covers

Manipulating the view
The following mouse commands in the display window are available:

- rotation – click and drag with the right mouse button
- zoom in/out – click and drag with the left mouse button
- translation – click and drag with the center mouse button, or with the scroll button

The "Reset" button will refocus the view to fit all objects in it.

Selection
You can select amino acid residues by clicking on them directly. You can also select residues by going to Display > Sequence, followed by Display > Sequence Mode > Residue Codes. This will show a clickable 1-letter amino acid sequence at the top of the display window. Alternatively, you can select entire protein or ligand chains at a time by changing the sequence mode, Display > Sequence Mode > Chains. Selections create a "(sele)" group in the selection menu of the display that can be manipulated separately from other objects.

Hiding and unhiding objects
Objects can be hidden or unhidden by clicking on their names in the selection menu.

Automatic coloring
A protein can be colored from blue to red as one moves from the N- to the C-terminus. To do so, click the C button > Spectrum > Rainbow. Alternatively, if a protein complex consists of a number of different protein chains, these can each be given a different color. To do so, click the C button > By chain > By chain. To return colors to the usual atomic elements scheme (red=oxygen, blue=nitrogen, white=hydrogen), you can click the C button > By element and then choose an appropriate scheme (with different options for the color of carbon).

Removing waters
Many structure files have crystallographic waters included. If you want to omit these to display a cleaner structure, simply click the A button > Remove waters.

Representations
There are many ways of drawing chemical and protein structures. These can be accessed by the S ("Show") button. Some of the more common ways of representing a structure, with different advantages each, are Sticks, Cartoon, Spheres, Mesh, and Surface. Disulfide bonds can be explicitly shown from the S menu as well, in various forms (usually Sticks is helpful for these). Moreover, different kinds of representations can be overlaid by multiple uses of the S button, or certain representations can be removed by using the H ("Hide") button. In addition, you can give each representation a degree of transparency by going to Setting > Transparency.

Electrostatic surfaces
You can show approximately where positively and negatively charged regions exist on the surface of a protein by choosing the A button > Generate > Vacuum electrostatics > Protein contact potential. Blue regions are positively charged while red are negatively charged.

Split pdb files into individual objects for separate manipulation
It's best to decouple ligands from a protein in Pymol by putting each in a separate "object" that can be accessed from the selection menu as its own row. This makes it easier to manipulate the display of these separately, and in particular, enables the "Surface" representation to work correctly. To do so, use the Sequence menu to select different elements that you want to split off into a new object. Then, next to (sele), click the A button > Create object.

Background settings
You will want to export your images with a transparent background. First go to Display > Background > White. Then go to Display and uncheck Depth Cue. Then go to display and uncheck Opaque. Finally, change the setting for ray tracing by entering the following command at the command line at the bottom of the display screen that starts with PyMOL>: "set ray_opaque_background, off". These commands only need to be run once per Pymol session.

Ray-tracing Pymol images
Ray-tracing will greatly improve the quality of your images. First, manipulate the display to a viewing perspective and representation of your choice. Then maximize the size of the display on your screen (for maximum resolution). Click the "Ray" button in the upper Pymol menu window. It may take a few seconds to complete, after which you can save your image to a file (File > Save image). Note that changing the display in any way will require ray-tracing again.

Assembling images and annotations in Powerpoint
Pymol images can be saved in .png format and then imported into Powerpoint. In Powerpoint, you can resize and arrange them, and add textual annotations, arrows, circles, etc. You can also add a background gradient, color, or pattern to your image (right click on the background > Format Background). You can also add shadows to Pymol images and text to add additional dimension to your piece (Drawing Tools > Format > Shape Effects or Text Effects).

Saving a session
Save your entire Pymol session, with all of your edits, by going to File > Save Session.