Selecting Stuff:

- To select residues near a ligand, try:
  - $ select ligand :<4
    - This means select all residues less than 4 Angstroms away from the ligand
    - Note that instead of "ligand" you can insert the name of the molecule as it appears on the log pane, like this:
      - $ show :BTN :<4
  - $ show sel
    - This will show them as the sticks. You can also do this by clicking the "show" button on the "atoms" pane of the "Molecule display tab."
- To invert a selection, you can use:
  - $ select ~sel
- To select all water (solvent) molecules within 4A of the ligand, use:
  - $ sel ligand :<4 & solvent

Hiding Unwanted Residue Sticks and atoms:

- Hold CTL and click one part of the residue, then hit the "up" arrow key to select the entire residue. Then, click on the "Hide" button for the atoms. This should make it go away!
- If you know the residue number, you can do this:
  - $ hide :90
    - This gets rid of the sticks on residue 90
- If you want to hide atoms, you can specify by atomic symbol. For example:
  - $ hide H
    - This command hides all explicit hydrogens, leaving you with the classic line-angle structures only (useful for structures that have all the H's added in).

Coloring Stuff:

- To see a list of available colors in the log, use:
  - $ color list
- To color a selection a particularse color, use:
  - $ color sel red
    - Here, we've used "red" as our selection, from the list of available colors in the log.
- To change the color of your labels (like red):
  - $ label color red
- To change the color of a specific residue:
  - $ color :88 red
    - This colors residue #88 red.
- You can color the entire protein silver with:
  - $ color protein silver

Labeling Stuff:

- To label all shown residues and ligands that are currently show, use:
    - $ label @@display
        - This means to label everything currently displayed in stick form
- To label a specific residue:
    - $ label :88
        - This will add a label to residue #88
- To change the label text size, use:
    - $ label height 1.0
        - Here, the 1.0 refers to the size. Different numbers = different sizes
- To delete a specific label, then use:
    - $ label delete a/:90
        - This means delete the label on chain a, residue 90 (for multiple chains)
    - $ label delete :88
        - Gets rid of the label on residue 88, if there is only one chain
    - $ label delete ligand
        - Gets rid of the ligand label
    - $ label delete
        - Gets rid of all labels

<u>H-Bond Stuff:</u>

- To find only H-bond contacts First, clear away any unwanted atoms (or all of them), then use:
    - $ hbonds ligand restrict protein reveal true
- To label the distances for all of the H-bonds to the ligand, use:
    - $ hbonds :BTN showdist true
- To label the distances and color them with the bonds, use:
    - $ hbonds ligand showdist true color magenta

<u>Salt Bridge Stuff:</u>

- If you want to see all salt bridges in the protein, use:
    - $ hbond saltonly true reveal true
- If you want to see the salt bridges between the protein and ligand (if they exist), use:
    - $ hbond ligand saltonly true reveal true

<u>Finding Non-Polar Contacts:</u>

- The easiest way to do this is something like this:
    - $ contacts /a@C* restrict :BTN@C* distance 3.8 reveal true
        - The C* means “carbon wildcard” and :BTN is the ligand here. The 3.8 is the distance in angstroms and can be modified.
- To find all non-polar contacts between a ligand and a specific residue, try this:
    - $ contacts :BTN@C* :108@C* restrict both distance 3.8
        - Here, we asking for all carbon-to-carbon contacts between ligand BTN and residue 108 within a distance of 3.8 Angstroms
- If you need to prune down for clarity, you can delete individual contacts by first selecting them with CTL+SHIFT+Clicking with the mouse, then use the following:

    - $ hide sel
- If you want to make separate collections of contacts that you can independently color, then use the name command like this:
    - $ contacts #1@C* restrict #2@C* distance 3.8 reveal true name vdW
        - Here I'm looking for C-C interactions between 2 models (#1 and #2)

Measuring the Center of Something:

- To measure the center of a ligand, you can use either:
    - $ measure center ligand
        - Where "ligand" is letting it interpret
    - $ measure center :BTN
        - Here, BTN is the explicit ligand of interest

Deleting Stuff:

Warning! Deleting anything is permanent and cannot be undone without reloading the starting file!

- To get rid of the water molecules, you need:
    - $ delete solvent
- You can get rid of the ligand with:
    - $ delete ligand
- Likewise, you can delete the protein, leaving the ligand behind with:
    - $ delete protein
- To remove specific ions like a sulfate, use:
    - $ delete :SO4

Changing Amino Acids (Mutations)

- Easiest way is to select a single residue, then use the following:
    - $ swapaa sel tyr
        - Here, we're changing the selected residue into a tyrosine. Note that by using "sel" you can actually change lots of things at once.
- Alternatively, you can do it by residue number, such as:
    - $ swapaa :146 v
        - Here, we're changing residue 146 to a valine (note you can use one or three-letter codes)

Surface Stuff:

- You can change the surface color with:
    - $ surface color grey
- You can make it partly transparent with:
    - $ trans 50
        - Here, we're indicating 50% transparency
- You can show only the surface around the ligand using something like this:
    - $ surface ligand @<5 visible 1

        - The “5” here indicates 5 Å

Metal Stuff:

- You can get rid of the default purple coordination bonds with
    - $ hide pseudo
        - delete can also be used instead of hide
- To find interactions between a metal and nearby electronegative atoms, the following is an example:
    - $ contacts :ZN restrict #1@N*,O* distance 3.5 reveal true name metalbonds color gold

Saving Images:

- The default option is to hit the “Snapshot” button found on the “Home” tab. This will place a .png image in a default directory.
- You can also save different formats using the following command as an example:
    - $ save image foo format tiff
        - You can replace jpeg/gif/bmp/ppm for tiff to get other formats
        - You can add “transparentbackground true” at the end to add transparency
- To change the image destination, ether specify the default or just enter the directory in the command line like:
    - $ save “C:\path\to\my\directory\image.png” supersample 3
        - The “supersample 3” here is the default for the quality and pixel density. A setting of “3” means it first saves an image 3x the display area, then shrinks it down to the original size, giving a smoother appearance.
- Files can be saved as png, tif(f), jpeg, gif, bmp or ppm format. Just specify the file extension like this (using a tif as an example):
    - $ save “C:\path\to\my\directory\image.tif” supersample 3

Saving PDB Files:

- To save a PDB to the desktop, use the following:
    - $ save 1stp_DOCK.pdb
- To save to a specific directory, you can use this:
    - $ save “C:\path\to\my\directory\1stp_DOCK.pdb”

Calculating RMSD between Docked Ligands:

- To do this, your molecules must have exactly the same number and type of atoms. So, be sure to delete any H's if you are converting from PDBQT to PDB. The command you need is:
    - $ align :BTN toatoms #2 move nothing
        - Here I’m aligning the BTN ligand to #2 which is a loaded PDB file of my docked ligand
            - The “Models” pane will display the # of the loaded ligand in the ID column. You can also hover your mouse over it to see the number.

- The “move nothing” flag stops it from actually aligning (moving) the molecules on top of each other.
- If you’re going from a PDBQT to a PDB, you’ll need to delete the hydrogens (because PDB files have no hydrogens). You can do this with babel using the -d flag:
    - $ babel foo.pdbqt foo.pdb -d
- Some RMSD rules of thumb:
    - < 1.5 = great
    - 1.5-3 = okay
    - 3-5 = bad
    - > 5 = call an ambulance, because this molecule’s not going to make it

<u>Aligning Proteins:</u>

- Easiest way is to use the matchmaker (mm) command:
    - $ mm #2 to #1
        - Here, I’m telling the program to align model #2 on top of model #1