**CHEM523 PDB Homework Name: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_**

This homework assignment is meant to get you familiar with the resources available to you on the PDBe.org website. You will use your two assigned proteins as the subjects of your investigations. Save all of your work in this document (use Ctrl-Alt-PrintScreen in Windows or the Grab Utility in OSX to make screen captures) and save the final, completed assignment as “LastName\_FirstName\_CHEM523PDB.docx”. Failure to save the document in the Dropbox folder by the start of class on the day the assignment is due will result in no points being awarded. No late assignments will be accepted without extensive medical documentation.

For the first of your assigned proteins, perform the following:

1. Go to the main entry page for your protein. Answer the following:
   1. What organism does your protein come from?
   2. How was the structure determined?
   3. What publication was the work published in?
   4. How many chains are found in the PDB file? How many of those chains are the same molecule? How many unique protein molecules are found in the PDB file? For example, if your PDB file contains 6 chains of the exact same protein, your answer would be “One unique protein molecule”.
   5. How many residues are in each chain? What percentage of those residues were observed by the structural biologists determining the structure?
   6. Are there ligands in your protein? Are they artifacts of crystallization or are they inhibitors/substrate/substrate analogues?
   7. Click on the “Quaternary Structure” Button in the top center of the main page to be taken to the PISA page that will display the quaternary structures possible for your protein.
      1. Look for the “Biomol R350” column and find the entry marked with a “1”. This is likely the biologically relevant multimer for your protein. What is the likely quaternary structure of your protein?
2. Go to the PDBSum entry for your protein and answer the following questions:
   1. On the left side of the PDBSum mainpage for your protein, report the Contents of the PDB file. If there are any ligands, what are their abbreviations?
   2. Click on the Ramachandran plot for your protein found on the right side of the PDBSum mainpage for your protein. How many residues are in Disallowed regions of the Ramachandran plot? If there are any, what are they (eg: Trp313 or Asp199).
   3. Take a screenshot of the Ramachandran plot and draw arrows to the positions of the amino acids that are in the Disallowed Regions.
   4. Click on the “Protein” tab and report the entries of the ProMotif file for the protein.
   5. Click on the “Ligands” tab for your protein (if it has any ligands) and evaluate the LigPlot for your protein. Take a screenshot of the LigPlot image.
   6. Which residues of your protein are in contact with the ligand(s)?
   7. If you have more than one ligand, you can click on its abbreviation on the left side of the screen and a new LigPlot drawing will appear for that ligand. Repeat steps e) and f) for any other novel ligand.

Repeat the previous steps for your second protein. Save the document in the Dropbox folder and refer to your answers when you are examining your protein in Chimera.