Name (s):
_____

Swiss PDB viewer assignment chapter 4.

If you wish to have extra practice with swiss pdb viewer or to familiarize yourself with how to use the program here is a tutorial:

http://spdbv.vital-it.ch/TheMolecularLevel/SPVTut/index.html

Open pdb file for triose phosphate isomerase (8TIM).
Menu wind > control panel
Shift click on the window to make all residues not visible.
Select residues LYS18 through GLY30
Make the residues visible with the selection
What is the name of this secondary structure type?

Looking at the sequence of the structure are their any residues that you would expect not to be in this type of structure? Which are they?

Make sidechains and the van der waals visible with the selection.
Make sure menu > display > render in solid 3D is checked
Menu color > act on backbone and sidechains
Menu color > type

Rotate the helix and look the pattern of hydrophobic, polar, acidic, and basic residues. What would you expect of the orientation of the helix with respect to the protein from this pattern?

Select residues PHE6 through ALA43
Make the ribbon visible
Make the residues and sidechains visible.

Remove the van der waals visibility
Menu color > act on ribbon
Menu color > by secondary structure
What is the name of this motif?

Does your prediction about the orientation of the helix fit with the new elements of the structure that are visible?

Identify the sequence from the beta strands, would you predict that the strands are on the surface or interior of the protein? Are their any residues that would not fit with this prediction?

Select the 38^{th} residue, which aa is this? If this is on the interior of the protein what interaction would you expect it to have?

Identify the amino acid it is interacting with by finding nearby residues:

Menu > select > neighbors of selected residues sidechains …

Select residues that are within 3.00 A of the selected atom.

Which residue is now selected? Is that what you predicted?

Make the residue visible by clicking on the plus sign above both show and side

Measure the distance between the two residues by using the distance measuring tool. What is the distance? (it is in angstroms) (In order to see the label you may have to change the background to white, select Menu prefs > color… > background then change it to white)

Select all and make the ribbon visible.
Menu color > secondary structure
Menu window > ramachandran plot
In this plot the most likely place to find amino acids are is in the yellow and blue areas. Of the amino acids outside of either what types do you find? (you can identify them by placing the pointer over the dots) Is there one type that you would expect to find predominantly? Do you find that one predominantly?

Which section are the helix residues in? Which one has the majority of the beta sheet residues? (note the dots will still have the colors you selected for the residues)

Menu select > group kind > Pro (P)
Where do you find the proline residues in the ramachandran plot? Does proline have psy or phi conserved?

Close 8TIM
Open 1CAG

What does the molecule look like?

Notice the sequence of the protein, does it fit into a pattern? Does anything not fit?

Make the sidechains and backbone not visible and make the ribbon visible.
Is there any part of the structure that does not fit with the rest? Which part? Why do you suppose that is?

Make the ribbon not visible and make the sidechains and backbone visible again.

Menu tools > Compute H bonds

Are the hydrogen bonds within the individual chains or between the chains?

Close 1CAG
Open 3TNU

Hide backbone and show ribbon.
Menu display > Show sidechains when backbone is hidden

What do you think this protein is?

What are the interactions between the strands? (It might be helpful to color by type)

Menu select > group kind > Cys (C)
Color > selection
Are there any disulfide bonds? Could these strands disulfide bond with other strands?

Close 3TNU
Open 5RSA

Using the knowledge you have learned identify the number of disulfide bonds in this protein.