Molecular Modeling Assignment II:

(1) Describe what you see, using terms that indicate the type of secondary structure shown.

The image that appears on the screen is of two alpha helices. Both appear to be right handed. There are not any amino acid sequences connecting the two helices. They seem to be floating in space.

(2) Why is this amino acid found predominantly on the side of the helices that face each other?

Leucine is classified as a hydrophobic amino acid. Therefore, it is often found on the inner side of alpha helices if in a hydrophilic environment because the conditions are favorable for other hydrophobic amino acids (in this case the hydrophobic leucines on the second chain) to have weak interactions with each other to help stabilize the overall structure.

(3) The labels will include the 1-letter designation of the amino acid, followed by a number and letter. What does the number indicate? What does the letter indicate? Is this structure a homodimer or heterodimer?

The number is the specifier and it indicates the number of the amino acid in the sequence assigned by Chimera. The letter that follows the number is either A or B. The A’s indicate one chain while the B’s indicate the other. The structures are homodimers according to the leucine amino acids because both alpha helices have Leucines located in the same place on their respective helix.

(4) What atom is blue? Red?

The red areas indicate that a oxygen atom is present and the blue areas indicate a nitrogen atom is present within an amino acid or in a peptide bond.

(5) Which color corresponds to the most hydrophobic atoms? The most hydrophilic? What can you conclude about the protein’s cellular location from this view of the protein?

The gray corresponds to the hydrophobic regions of the cell which are the carbon chains. The yellow, red, and blue correspond to the hydrophilic portions of the the chain. The yellow (sulfur atoms), blue (nitrogen atoms), and red (oxygen atoms) all have the ability to hydrogen bond. It is hard to tell for sure because with the model you cannot see the inside, but judging from the fact that our leucine atoms are hydrophobic and lie on the inside of the helices that the inside of the protein complex is more hydrophobic than the outside. The outside of the molecule is more hydrophilic because the nitrogen, oxygen, and sulfur atoms can be seen on the outside of the protein complex. I would predict that the protein would be present in the cytosol or another area/organelle with an environment rich in water.

(6) **What leucine atom is participating in the bond? What atom on which neighboring amino acid is at the other end of the bond? The residues involved in the H-bond are separated by how many residues? Add image.
The hydrogen atom attached to the nitrogen of the N-terminus of Leucine is participating in the H-bond. The oxygen atom on the C-terminus of the Glutamate is also participating in the H-bond. The amino acids are 4 residues apart (E 22-L 26).

(7) What is the length of a typical hydrogen bond? What is the length of this hydrogen bond? Why don’t these values agree? (Hint: many of the X-ray crystal structures of proteins don’t include hydrogens)

A typical hydrogen bond is about 1.5-2.5Å. This hydrogen bond spans a distance of 3.012Å. One turn of an alpha helix contains approximately . The physical environment of a crystal analyzed by X-ray diffraction is different from the environment of the protein within a living cell. Therefore, the hydrogen bond angles will be different depending on the environment they are analyzed in.