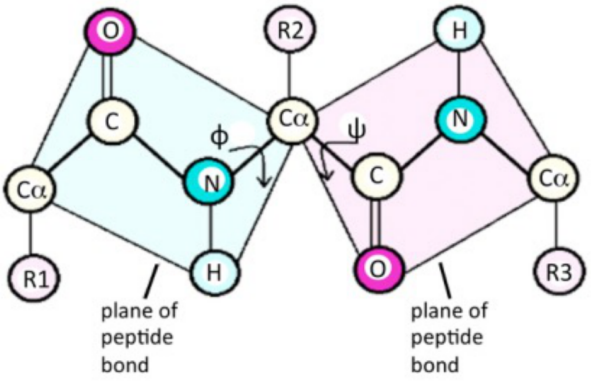
(45 points total) You are not required to upload your PyMOL measurement results.

1. (12 pts, 20 min) Open up the alpha helix.pse file in the PS03 folder. This shows a short idealized, all alanine α-helix.

   i) Select the third alanine of the helix and find the amide hydrogen to which the carbonyl oxygen is H-bonded (use the command button: Action->find->polar contacts->any atoms). Which alanine residue is it H-bonded to? (2 pts) Repeat for the fourth alanine residue. (2 pts)

   ii) What is the distance ***between the 2 electronegative atoms*** in the hydrogen bond? (3 pts)

   iii) This next problem is meant to illustrate the ϕ,ψ dihedral angles of the helical backbone. Here is how to measure these in PyMOL: It may be easier if you select the residue of interest (A5) and color it by element using yellow instead of green for carbon.



To measure the ϕ and ψ angles, go to Wizard->Measurement as you would to measure a distance, but change distances to dihedrals. To measure the ϕ angle at a residue (R2), select the 4 backbone atoms C,N,Cα,C. To measure the ψ angle, select the 4 backbone atoms N,Cα,C,N.

What are the ϕ,ψ dihedral angles about A5 (the fifth Alanine)? (5 pts)

2. (12 pts, 20min) Next open up the beta sheet.pse file in the PS03 folder. This shows a 2-stranded β-sheet.

   i) Pick any residue and find its H-bonding partner within the structure. How many ***total*** H-bonds are there ***per residue***? (2 pts)

   ii) What is the distance ***between the 2 electronegative atoms*** in the hydrogen bond? (3 pts)

iii) How is the H-bond pattern in this β-sheet different from that in the α-helix? (2 pts)

iv) Now measure the ϕ,ψ dihedral angles about the A5 residue just as instructed above. What are they? (5 pts)

3. (21 pts, 30min) Now open the pse file 5HBS in the PS03 folder (or you can fetch it using the pdb code 5HBS). Change the view to cartoon and display the amino acid sequence of the protein. As you can see, this protein is mostly β sheet with two short α helices.

i) How many amino acids are in the protein structure? (2 pts)

ii) What is the N-terminal residue in this structure? (2 pts)

iii) In cartoon mode, the center of the protein appears to have a lot of empty space. Is this the case? How did you determine this? (3 pts)

iv) Are the β strands in this protein parallel or anti-parallel? (2 pts)

v) Take a look at the side chains emanating from the beta sheet formed by the 3 beta strands (D39-Q65). The easiest way to do this is: First, select all other residues and under the selection menu, hide everything; second, select D39-Q65 and under selection menu show sticks, third, select D39-Q65 and hide main chain. This should prominently reveal the side chains. Is one face more polar or nonpolar than the other? (2 pts) Can you provide a reasonable explanation for why that might be? (2 pts)

vi) Return to the cartoon view of the whole protein and highlight the bound ligand (RTL) found at the end of the amino acid sequence. How would you describe the ligand? (2 pts)

vii) What predominant type of interaction or force would you predict to drive the interaction between protein and ligand? (2 pts)

viii) Indicate one polar interaction between the ligand and protein by naming the type of bond (2 pts) and the residues participating in the bond. (2 pts)