

Part A: Recommended questions from Campbell: Chapter 4: 6, 7, 18

Part B: Problems for grading. Assume $T=300^{\circ}\text{K}$ unless stated otherwise.

Questions 1-3 will require viewing the Retinol Binding Protein chime page

http://www.bio.cmu.edu/Courses/03231/psetF05/PSET03/RBP_prob/RBP.html also accessed through problem sets link on course home page.

1. (5 points, 10 min) Identify the α -helix in Retinol Binding protein (RBP). Determine the following parameters associated with this helix:
 - i) Starting and ending residue
 - ii) Number of residues in the helix
 - iii) Length of the helix
 - iv) Number of turns of the helix
 - v) The pitch of the helix (rise/turn)
2. (4 points, 5 min) Select one residue in the α -helix that forms an intra-chain hydrogen bond within the helix. State the residue that donates to the hydrogen bond, the residue that accepts the hydrogen bond, and the distance between the amide nitrogen and the carbonyl oxygen.
3. (5 points, 10 min) Identify the β -sheet in Retinol Binding Protein.
 - i) Is the β -sheet parallel or anti-parallel?
 - ii) How many strands make up the β -sheet?
 - iii) Are the hydrogen bonds *within* a strand or *between* strands?
 - iv) The β -sheet in Retinol Binding Protein forms a barrel, with side chains facing both inward and outward. What general statement can be made about the amino acid residues that face the inside of the barrel?
 - v) The function of RBP is to transport the visual pigment precursor retinol (vitamin A) in the bloodstream. View the retinol molecule in the structure using the Select_Hetero_Ligand command. Give a reasonable explanation for why the structure of RBP is well suited for its function.
4. (9 points, 20 min)
 - i) Calculate the configurational entropy change, ΔS° , that occurs when a stable α -helix consisting of 22 residues unfolds. Does the entropy change for the unfolding depend on whether the peptide started out in an α -helical or β -sheet configuration? Why?
 - ii) Assume that the enthalpy associated with the unfolding of this peptide is due entirely to the breaking of H-bonds. (Ignore 'end effects' and assume that 22 H-bonds are broken on unfolding and that each H-bond contributes 5 kJ/mol). What is the fraction of unfolded molecules at 300K?
 - iii) What is the T_m of this peptide?

5. (10 points, 25 min) The melting curve for an hypothetical protein is shown below. Determine the enthalpy and entropy for denaturation of the protein.
- Use a van't Hoff analysis to determine the enthalpy. Feel free to use Excel to determine the slope of the van't Hoff plot. If you do use Excel, include a printout of your spread sheet.
 - Once you have determined ΔH° , calculate ΔS° .

Melting Curve for a Hypothetical Protein

