Homework for Protein Bioinformatics 260.841 class on 31 March 2005:

1. Consider the Ramachandran plots that we discussed on 31 March.

   1a. Why are amino acids not typically found with Psi (ψ) dihedral angles near 0° (what atoms are clashing)?

   1b. Would Glycine be more likely to adopt a conformation of Psi = 0°?

   1c. Why are amino acids not typically found with Psi dihedral angles near -120° (what atoms are clashing)?

   1d. Would Glycine be more likely to adopt a conformation of Psi = -120°?

   Now consider D-amino acids instead of L-amino acids.

   1e. Would D-amino acids typically be found with Psi angles near 0°?
      Near -120°?
      Near +120°?

2. The following peptide folds up into a small protein.

   MRGPAERLHQAMSELAPDMVTWHITYRDGQFTISVQYSGGQLMEHFSKQMDAS

   2a. A biophysical technique called circular dichroism indicates that this protein is composed of 43% alpha-helix and 27% beta-strand. Based on the secondary structure preferences of amino acids, where would you assign helix, strand and turns?

   2b. Using the following website to draw a helical wheel for a helix that you predicted (http://cti.itc.virginia.edu/~cmg/Demo/wheel/wheelApp.html). What residues of the helix are likely to face inwards towards the core of the folded protein?

   2c. For a beta strand that you predicted, write the amino acid sequence and indicate which residues are likely to face inwards towards the core of the folded protein and which will face outwards towards solvent.