Homework 3 (parts 1 and 3 are due next Tuesday, April 9)

1. Calculate the average coordination number of each residue using a cutoff distance $R_c$ of 6.5 Å using (i) the $C^{\alpha}$-atom as the residue interaction site, and (ii) the side chain centroid as the residue interaction site. Give the number of bonded and non-bonded neighbors in both cases. (Results will be combined by Zerrin to find the average values for each residue type, as well as the distributions of coordination numbers. Compare with the values tabulated in Table IV.6.1)
2. Consider the virtual bond representation. Calculate the torsional angles $\varphi_i$ and $\varphi_{i+1}$ preceding and succeeding the ith $\alpha$-carbon. The torsional angles may be classified into three groups, associated with $\alpha$-helical, $\beta$-stranded and coiled conformations. See "Short-range conformational energies, secondary structure propensities, and recognition of correct sequence-structure matches" I. Bahar, M. Kaplan, & R. L. Jernigan *Proteins* **29**, 292-308, 1997. Calculate the probability of occurrence of each region for each amino acid, and the corresponding energies. (Results to be combined by Alpay and compared with those in the above reference).
3. Calculate the solvent-mediated inter-residue effective contact potentials using (i) the $\alpha$-carbon and (ii) the side chain centroid representation as in part 1, with eq IV.6.2, 12-14, Table IV.6.1 and $R_c$ = 6.5 Å). Display the results in the form of a 20x20 table. (Results to be combined by Lucy, using raw data as the number of occurrences of different pairs, versus the total number of pairs)
4. Estimate the solvation energies for different residue types using eq IV.6.19 (results to be combined by Zhongren. Compare with the results in Figure IV.6.6.)