Biophysical Chemistry I, Fall 2010

Homework Assignment #4, due Oct. 21

1. Go to *http://w3dna.rutgers.edu*. Ask to analyze PDB code 1BNA, which is the crystal structure of the "Drew-Dickerson dodecamer", which was the first atomic level resolution crystal structure of DNA to be reported. What is the nucleic acid sequence of this short piece of DNA? Compare the sequences of the two strands; why do think this relation was important? (Save the files here, or bookmark this page, since you will need to return to it below.)

2. At the same web site, go back to the home page and click on "reconstruction". This provides a facility to build a structure (given its sequence) from a fiber-diffraction model. (X-ray analysis of fibers of DNA was the principal method used from the 1950's to the 1970's to explore the structure of DNA; it is an averaged process, which does not provide structures that are sequence-specific.) Choose a "B-DNA generic" fiber model and reconstruct the model using the sequence from part 1 above. Download the resulting PDB file, go back to the "analyze" tab, and upload your pdb file. Download the resulting base-pair and base-pair step parameter file, and copy this into your answer for this question.

3. Now compare the base-pair and base-pair step parameters for the 1BNA crystal structure with those you obtained from the fiber diffraction model. In three to four sentences, *qualitatively* discuss the similarities and differences.

4. Now analyze the DNA in a protein-DNA complex, PDB code 2LEF; (only consider model 1). This complex has a bent DNA. Again, in a few sentences, point out the most important differences in base-pair and base-pair-step parameters between the straight DNA in pdb code 1BNA and the bent DNA in 2LEF. (The sequences are different, so you will have to look for general trends.)

5. Look at the original paper describing the 2LEF structure. Describe, again in just a few sentences, what the authors of that paper thought was the mechanism for DNA bending by the protein. (Note: there is a lot of information in this paper; please concentrate on the analysis of DNA bending.)