Modeling and Simulations of Molecules

Assignment 1, due beginning of meeting on **Thursday**, **October 24**, or **Friday**, **October 25**, 2013

1. Visualization of a DNA double helix using VMD

(a) Visualize the structure in the file `b-dna.pdb` using the program VMD.
How many base <u>pairs</u> is the helix comprised of?

(b) Make VMD show the hydrogen bonds in this structure. (You do this by creating a new representation by hitting the button `Create Rep`, and choosing `Hbonds` for `Drawing Method`. To see the hydrogen bonds better you may need to increase the `Line Thickness` to 5. It could be helpful to color the hydrogen bonds green by changing the `Coloring Method` to `ColorID` and selecting color number `7`.)
How many hydrogen bonds are there?

(c) Zoom into a hydrogen bond that has an *oxygen* atom on one side and a *hydrogen* (white) atom attached to a *nitorogen* on the other. (It may be helpful to change the action of the mouse from 'rotation' (press the `R` key on the keyboard), to 'translation' (the `T` key) and to 'scaling' (the `S` key).)
For the hydrogen bond that you selected, measure the distance between the *oxygen* and *nitrogen* atoms involved in that bond and report its value. Make sure the distance you report has the correct units. In addition, report information about the two atoms, including the `name`, `resname`, `resid`, and `segname`. (To do so, press `2` on the keyboard and click with the mouse first on one of the atoms and then on the other. The information about the atoms that you need to report and the distance between the two selected atoms will appear in the third (MS-DOS) window of the screen. After your selection of atoms is over you can go back to 'rotation' mode by pressing `R`.)