PROJ 102 Fall 2013

Modeling and Simulations of Molecules

Assignment 2, due beginning of meeting on **Thursday**, **October 31**, or **Friday**, **November 1**, 2013

1. What's in a `.pdb` file?

Open one of the files `ap-rna_lbl.pdb` (group 1), `a-dna-rna_lbl.pdb` (group 2), and `a-rna_lbl.pdb` (group 3) with a text editor (e.g., wordpad, emacs, etc.). Choose a font which assigns equal width to each character (e.g., Courier). If necessary, reduce the font size until you no longer see lines that are half filled.

The first two lines of the file contain `REMARK`s which are not read by VMD. The lines starting with the word `ATOM` contain information about the atoms that are visualized by VMD.

The `name` of the atom is in the *third* column. The first letter of the name determines the `type` of the atom (e.g., oxygen, nitrogen, carbon, hydrogen, etc.). VMD looks at this letter to decide whether an atom should be red, blue, cyan or white.

The *fourth* column indicates whether the atom belongs to Adenine, Guanine, etc. These are called `residues`.

The last (*eleventh*) column shows the name of the `segment` to which this atom belongs. In our case each chain of the RNA double helix is a segment.

The *second* column gives the number of the atom from the beginning of the file, while the *fifth* column gives the residue number from the beginning of the segment.

Columns *six*, *seven*, and *eight* contain the x, y, and z coordinates of the atoms. VMD uses these numbers when placing the atoms on the screen. For example, the coordinates of atom `N7` on the first `GUA`nine of the segment `RNA1` are 3.516, 3.480, and -1.579.

Using this information answer the following questions:

(a) How many atoms does the first `GUA`nine contain?

(b) How many residues does the segment `RNA1` contain?

(c) How many atoms does the segment `RNA1` contain?

(d) What is the name of the first residue of the segment `RNA2`?

(e) What is the name of the *third* segment contained in the `.pdb` file?

(f) How many residues does this third segment contain?

(g) What are the names of these residues?

2. Making figures with VMD

Go to `http://www.ks.uiuc.edu/Training/Tutorials/`. Download the pdf file and required tutorial files of the tutorial *Using VMD*.

(a) Work over the exercises in the first section *Working with a Single Molecule*. (Skip part 1.4 *Sequence Viewer Extension*.)

(b) After completing your work on the first section *Working with a Single Molecule* load the molecular structure contained in one of the files `ap-rna_lbl.pdb` (group 1), `a-dna-rna_lbl.pdb` (group 2), and `a-rna_lbl.pdb` (group 3) and prepare a figure clearly showing the RNA double helix as well as the spin labels attached to it.
Print the figure and bring it to our next meeting.

3. Tcl scripting in VMD

(a) Work over the exercises in the third section *Scripting in VMD*. (Skip part 3.3 *Drawing Shapes*.)

(b) After completing your work on the third section *Scripting in VMD* load the molecular structure contained in one of the files `ap-rna_lbl.pdb` (group 1), `a-dna-rna_lbl.pdb` (group 2), and `a-rna_lbl.pdb` (group 3).

Show the two spin labels and the two `CYT` bases to which they are attached as big balls (i.e., `VDW`). (The spin labels are attached to residues 6 and 16 on the segment RNA1.)

On the `VMD Main` panel, select `Extensions` and `Tk Console`. In the window that appears, source the file `chi1.tcl` and visually examine how it changes the conformation of one of the spin labels.

Describe the changes that you see with one or two sentences and bring your description to our next meeting.