

Using 3DNA: A Mini-Tutorial

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In the following guide we'll show a step by step introduction to 3DNA from installation of the software to practical examples.

1 Installation

To install 3DNA you will first have to download the software from:

<http://forum.x3dna.org/downloads/3dna-download>

The webpage will ask you to register before allowing you to download the program.

Once registered you'll be able to download the file which corresponds to your operating system. If you download the Linux 64-bit version your file will be named **x3dna-v2.1beta-linux-64bit-2012may02.tar.gz**

To uncompress, issue the following command in a terminal:

```
tar -xvzf x3dna-v2.1beta-linux-64bit-2012may02.tar.gz
```

This will create a new folder named **X3DNA** which you will have to include in your environment variables by changing your shell environment configuration file named ".bashrc" in bash, and ".chsrc" in csh and tcsh.

If you are using .bashrc the following lines will need to be added:

```
export X3DNA=/home/yourusername/X3DNA
export PATH=$PATH:$X3DNA/bin
```

A detailed explanation of how to configure X3DNA can be found in the pdf file **x3dna_v1.5.pdf** found in the X3DNA/doc folder. If you're stuck in the installation process feel free to drop me a line at mauricio.esguerra@gmail.com

2 fiber

The **fiber** program included in the 3DNA package allows you to easily generate protein data bank (pdb) files of fiber models corresponding to common nucleic acid conformations, for example A-DNA, B-DNA, and Z-DNA. To get a list of all possible fiber models which you can reconstruct using **fiber**, type:

```
fiber -l
```

If you type **fiber** alone in the terminal you will get a usage message.

Stop and read the usage message carefully.

Now, you know that the crystal structures of A-RNA and B-DNA must have a total of 11 and 10 residues per turn respectively, so, go ahead and use **fiber** to make an A-RNA with 12 residues and a B-DNA with 11 residues. Using a molecular visualization program such as pymol, vmd, or chimera check the generated structure to corroborate that you have the correct number of residues per turn.

3 find_pair

The **find_pair** program of 3DNA allows you to find pairs in a given pdb file. To read the usage message open a terminal and type:

```
find_pair
```

Now go to the protein data bank website at <http://www.pdb.org> and download the structure with PDB_ID: 1ehz. This is the structure for yeast phenylalanine tRNA. Run it through `find_pair`:

```
find_pair 1ehz.pdb 1ehz.inp
```

The output will be a file named *1ehz.inp*. Go ahead and open the resulting file in a text editor and you will see that the `find_pair` program has found the canonical Watson-Crick base-pairs G·C and A·U, as well as non-canonical base-pairs such as G·U and A·G.

4 analyze

The `analyze` program of the 3DNA software package allows you to compute the base-pair, and base-pair step parameters associated with a given nucleic acid structure. `Analyze` provides additional analysis features such as computing the overlap areas between stacked nucleic acid bases, sugar conformations, and sugar-phosphate backbone torsion angles.

A requirement of the `analyze` program is that you have to run the `find_pair` program beforehand. Go ahead and read the usage message of the `analyze` program by typing:

```
analyze --help
```

in your terminal.

Now run the `analyze` program on the previously produced file using the `find_pair` program:

```
analyze 1ehz.inp
```

Notice that you can run the `find_pair` and `analyze` programs in one line by issuing the command:

```
find_pair 1ehz.pdb stdout | analyze
```

This command will produce a wealth of files with derived structural information, but the main one will just have the name of the input file followed by the `.out` extension. That is, you should now have a *1ehz.out* file in your folder. Go ahead and take a look at the *1ehz.out* file in your favorite text editor.

5 rebuild

The very useful 3DNA program called `rebuild` can do just that, rebuild nucleic acid structures. It uses as input either a set of base step, or base-pair step parameters, or a set of helical parameters to create a `pdb` file. To test the `rebuild` program first run `find_pair` and `analyze` on the A-RNA structure you previously created:

```
find_pair A-RNA.pdb stdout | analyze
```

Issuing the previous command must have created a file called *bp_step.par*. Open this file in a text editor and change the Twist values from 31.5 degrees to a smaller value, say 25.0 degrees, and save the new file with the name *undertwisted.par*.

Rebuild the undertwisted RNA by typing the following command in your good-ole terminal:

```
rebuild -atomic undertwisted.par undertwisted.pdb
```

This will generate a `pdb` structure with no sugar-phosphate backbone. To add a sugar-phosphate backbone you will need to issue the `cp_std` command before you perform the `rebuild` command, in the following way:

```
cp_std RNA
rebuild -atomic undertwisted.par undertwisted.pdb
```

Now rebuild a pdb file using the unmodified base-pair step parameters, that is, using the original *bp_step.par* file. Open both structures in a molecular visualization program and confirm that one helix is undertwisted with respect to the original.

6 blocview

Blocview is a perl script which calls various 3DNA functionalities as well as raster3D, molscript, and pymol to generate an automated picture. Since blocview is just a script it can be easily modified, for example, following row 83 which invokes `get_part -c` (an undocumented command that creates a molscript header) one can add a line to change the inner color of protein ribbons:

```
# change inner color of ribbons from default 0.8
system("sed 's/grey 0.8/grey 0.5/g' temp2a > temp2");
```

7 Exercises

1. Run `find_pair` and `analyze` on your A-RNA structure and modify the resulting *bp_step.par* file so that the sequence is AAAGGGUUUCCC instead of AAAAAAAAAAAAAA. Use `rebuild` to generate a pdb file with the AAAGGGUUUCCC sequence.
2. Download the file with PDB_ID: 1aoi, that is, chromatin's nucleosome core particle, from the protein data bank website. Run it through `find_pair` and `analyze`.
3. Produce a "publication quality" plot of Slide vs. base-pair step number for the chromatin parameters you've computed in the previous exercise. Ask around (e.g. drop me a line) for which solutions are good for such a task.
I recommend `xmgrace`, the `matplotlib` library of python, and `igor-pro`.
4. Repeat the recipe for Twist vs. base-pair step number (bpsn), and Roll vs. bpsn.
5. Compare your graphs to Figure 2 of the journal article "DNA Sequence-Directed Organization of Chromatin: Structure-Based Computational Analysis of Nucleosome-Binding Sequences" *Biophysical Journal*, **2009**, 96, 2245-2260.
What regularities do you see?
How would you describe the DNA wrapping around the nucleosome in terms of Sliding, Twisting, and Rolling?
6. Go to the website: <http://w3dna.rutgers.edu> and analyze the structure of your choice, for example the large subunit of the ribosome.

8 Config

In the config folder one can find most of the files for configuration of 3DNA internals. The following are descriptions of what they do.

8.1 col_chain.dat

This file specifies color defaults for the molscript files which 3DNA produces. I don't like to have purple proteins, so the first thing I do in this file is to change the default protein color from purple to blue. I also dislike having a wide tube to represent the nucleic acid backbone so I change the value from 0.8 (default) to 0.5

8.2 my_header_hres.r3d

The header file for the raster3d objects.

8.3 my_raster3d.par

The name is self-explanatory.