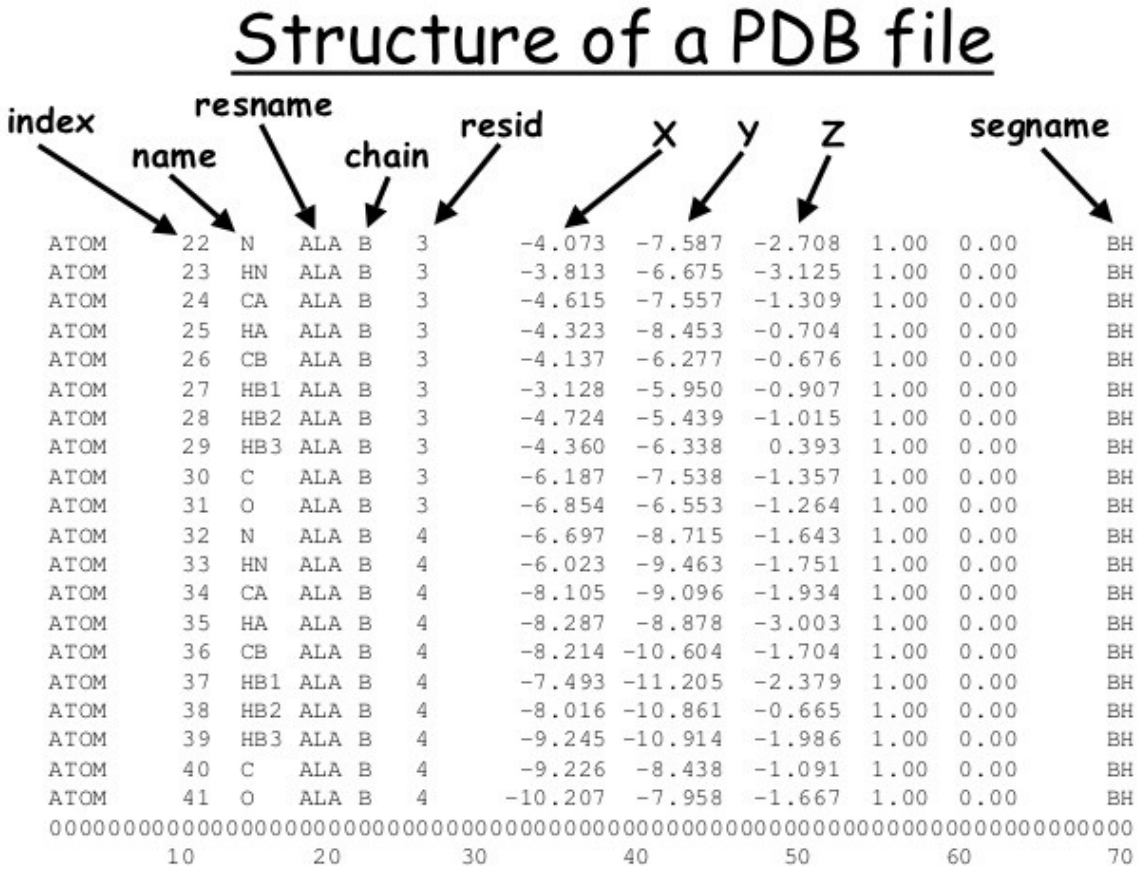
Science-1 Tutorial

Topic: Basics of Visual molecular Dynamics (VMD)

VMD Input – PDB files



- Has 3-D structural data of the molecules
- Does not have connectivity information

Loading the pdb file and interaction modes

- Load pdb file
- Interaction mode: Rotate, translate, scale mouse modes

Drawing styles and coloring methods

- Atoms and molecules can be visualised in various drawing methods

Drawing Methods	Description
Lines	Default
HBonds	Draws Hydrogen Bonds
VDW	Space filling visualization
Ribbons/New Ribbons	Draws backbone of DNA/protein as a ribbon
Cartoon/New Cartoon	Draws secondary structure of proteins

Atom Selection

- Atom Selection in selections tab of the graphical representation window.
  Example: all, protein, resname X, name X, resid X
- Multiple representation
- Loading a trajectory
- Saving an image with file -> render -> start rendering

Scripting in VMD

- Scripting in vmd is in the language called TCL
- TCL/TK console

- Write a tcl script to select the backbone atoms of the 1ubq.pdb protein and write it to a pdb file name backbone.pdb

  [Hint : Use “$selection writepdb output_name” to write the select atoms into a external pdb]

Trajectory file format

- Different file formats like .dcd,.xyz etc
- Format of .xyz file format:

```
<number of atoms>
comment line
atom_symbol11 x-coord11 y-coord11 z-coord11
atom_symbol12 x-coord12 y-coord11 z-coord12
...
atom_symbol1n x-coord1n y-coord1n z-coord1n
<number of atoms>
comment line
atom_symbol21 x-coord21 y-coord21 z-coord21
atom_symbol22 x-coord22 y-coord21 z-coord22
...
atom_symbol2n x-coord2n y-coord2n z-coord2n
.
.
.
<number of atoms>
comment line
atom_symbolm1 x-coordm1 y-coordm1 z-coordm1
atom_symbolm2 x-coordm2 y-coordm1 z-coordm2
...
atom_symbolmn x-coordmn y-coordmn z-coordmn
```

Submission

- Visualise your N random walkers for 10,000 steps and write the coordinates for each of the random walkers after each time step into a .xyz file and visualise it in vmd
- Submit your .xyz file on moodle
- Deadline : 12:00pm tonight (hard deadline)