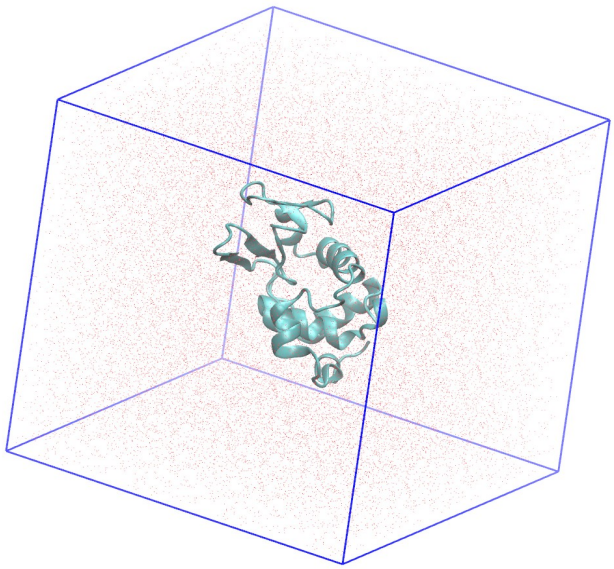
BT5420: Computer Simulation of Biomolecular Systems
Assignment-2 (20 Marks)
Use the PDB ID: 1AKI to answer the following

1. How to build the missing hydrogen atom co-ordinates in GROMACS? Give the syntax and the flag indicating its usage. **(1 Mark)**

2. What is the difference between the input PDB file and the output GRO file generated from step 1 using *gmx pdb2gmx*. Is there any change in the co-ordinates (mention the units wherever necessary)? **(1 Mark)**

3. Solvate your system using *gmx solvate*. **(2 Marks)**

a) Report the box length along X, Y, Z needed for solvating your system.
b) Can we visualize the PBC box in vmd. If yes, state the command.



4. What is the resname identifier for the added ions in your system during neutralization step *gmx genion*? Show using topol.top screenshot. **(1 Mark)**

5. Perform energy minimization of the **neutralized** system using minim.mdp **(3 Marks)**

a) Report the number of steps required to converge potential energy
b) Plot the potential energy curve using plotting tool
c) Load both the input and output .gro files used in minimization step in VMD. Represent in New Cartoon in different colors. Comment on the difference observed in their structure.

6. State the syntax and purpose of a checkpoint file. **(1 Marks)**

7. Why is it necessary to use atleast 1 nm padding for water during solvation? What do you think would happen if we use 0.5 nm and 2 nm padding? **(2 Marks)**

8. What is pbc and why is it necesary to remove pbc before analysis? **(2 Marks)**

9. Plot the temperature graph from 100 ps of NVT simulation. Provide screenshot of the syntax used and the average temperature printed in the terminal. **(2 Marks)**

10. Perform NPT for 150 ps using force constant of 1000 kJ/(mol nm^2). Provide screenshot of the mdp file highlighting the change in run parameters. **(2 Marks)**

11. Perform MD run for 1 ns. **(3 Marks)**

a) Remove PBC from the trajectory. State the command used.
b) Report the distance between N and C terminal atoms of the trajectory (without PBC) as a time vs distance plot (*gmx distance)*
c) How did you generate the index file? Discuss your observation on the distance plot.