BT4110 COMPUTATIONAL BIOLOGY LABORATORY
MOLECULAR DYNAMICS MODULE
ASSIGNMENT 3 – ANALYSIS OF MD TRAJECTORY USING GROMACS

Instructions:

- Each question carries two marks (2*5= 10 marks)
- Please use the production MD trajectories from the previous assignment and answer the questions.
- Your submission should be a single pdf containing your answers along with all the plots. Please name your pdf in this format: "Roll number_Assignment3"
- **Deadline for submission: 17th September 2024, 2 pm**

Q1. a) What is RMSD? Why is it useful to measure RMSD?

b) Calculate the RMSD of the protein backbone after the production run with reference to the backbone of the crystal structure (em.tpr). Provide a plot in grace.

Q2. a) What is Rg? If the Rg of a protein increases with time, what does it indicate?

b) What is the Rg of the protein at the end of production MD? Plot Rg vs time.

Q3. a) How does the distance between the first and last atoms of your protein vary over the course of the simulation? Provide a plot for the same.

b) Calculate the Angle between any three atoms of different residues of your protein that vary over the course of the simulation. Provide a plot for the same.

Q4. a) Expand RMSF. Why is it useful to measure RMSF?

b) Calculate the RMSF of the protein after the production run and provide the plot for the same. Which atom fluctuates the most in your simulation? Name the residue this atom belongs to.

Q5. Report the average number of hydrogen bonds per timeframe and provide plots for the number of hydrogen bonds versus time for the following groups of molecules:

a) Protein-water b) Water-water