BT4110 COMPUTATIONAL BIOLOGY LABORATORY

MOLECULAR DYNAMICS MODULE

ASSIGNMENT 1 - VMD

Instructions:

- Please provide answers as screenshots for the VMD questions
- Your submission should be in PDF format with the file name "Roll no_Assignment 1"
- Each question carries one mark (1*10 questions = 10 marks for this assignment)
- Submission deadline: Tuesday, 3rd September 2024, 1 pm

Answer the following:

1. Read the remarks sections of the PDB file and describe your protein.
2. Is your PDB structure determined by NMR or X-RAY? What is the resolution?
3. In VMD, represent the protein in New Cartoon and ligand/DNA/sugar (non-protein) in CPK.
4. Represent the protein using different colours for different residue types. Change the background to grey and hide the axes.
5. Show all heteroatoms lying within 3.0 Angstrom of your protein in CPK form. List them.
6. Label the first five amino acid residues of your protein. List them.
7. Write a line about the different molecule status flags [T A D F].
8. Display the Ramachandran plot for your protein using in-built function. Name any two residues that lie in the disallowed region of the plot.
9. Find out from the sequence viewer about the secondary structure of your protein. Is there any occurrence of H (helix) in the secondary structure? If yes, mention which residues contribute towards those structures.
10. Load the same PDB twice and place them next to each other in different colour.