Exercise 04

GROMACS simulation setup and MD data analysis

Deadline: Please hand in Exercise 04 by **Friday, 5 June, 10.15 a.m.** to saleksic@zedat.fu-berlin.de

1.1 Gromacs Set Up - Equilibration in NPT ensemble (25)

Modify given npt.mdp file so that, integration step is 2 fs, NPT equlibration lasts for 100 ps, trajectory is updated every 1 ps, Parrinello-Rahman barostat is used, and velocity generation is switched off. Include **modified npt.mdp** file into your report. (10)

Run NPT equilibration, detect the time needed for NPT equilibration, and check total, potential, and kinetic energy, as well as pressure, of the system by using g_energy command. (10)

Generated *.gro file after NPT equilibration convert to new *.gro file without water molecules and with fixed pbc conditions (hint: use trjconv command). Newly generated *.gro file upload in VMD together with *.gro file generated with pdb2gmx command. Align both structures and color them differently (New Cartoon as view style). Background color is set to white. Include the snapshot in your report. (5)

1.2 Gromacs Set Up - MD run (10)

Modify given md.mdp file so that, integration step is 2 fs, MD run lasts for 100 ns, compressed trajectory is updated every 1 ps, while full trajectory, log,velocity, and energy files every 50 ns. Include **modified md.mdp** file into your report and compare it with **modified nvt.mdp**. (10)

Since MD simulation of a protein is computationally quite expensive, we will not run it now.

1.3 Gromacs Tools for analysis of MD data (50)

Calculate RMSF values for every residue of Langerin monomer from the given trajectory. How many residues are in Langerin monomer? Visualize the RMSF plot in xmgrace program. Which five amino acids have the greates RMSF values (name them by using one letter code)? Include RMSF plot into your report. (15)

Calculate RMSD values for the whole trajectory by taking into account every 100th frame. Visualize the RMSD plot via xmgrace program. Include RMSD plot into your report and discuss the range of RMSD values observed in plot. (5)

By using g_rama command plot the backbone torsion angle distribution for the first 70 ns of the simulation. Are values for GLY-198 and PRO-325 avaiable in the output file? Plot in xmgrace Ramachandran plots for ALA-258, PRO-283, GLY-284 and ALA-289. How many populations (minima) are in respective Ramachandran plots ? Name visited regions of Ramachandran plain and include plots in your report. (15)

Using g_chi command plot χ-1 sidechain torsion angle distribution by considering the first 70 ns of the simulation. Are there output files for all 20 proteogenic amino acids? For K257 plot χ-1 angle distribution in xmgrace (output file of choice is called chi1LYS60.xvg). (10)

2 Files

Trajectory files can be downloaded under:

$https://www.dropbox.com/s/dk3ljfwa7tu68ff/files_Ex04.zip?dl=0$