

# Simulation Interactions Diagram Report

## Simulation Details

Jobname: 2D6-POR2\_MD\_MD  
Entry title: 2D6-POR2\_SystemSetup\_3-out

CPU #	Job Type	Ensemble	Temp. [K]	Sim. Time [ns]	# Atoms	# Waters	Charge
1	mdsim	NPT	310.1	500.254	207789	49215	0

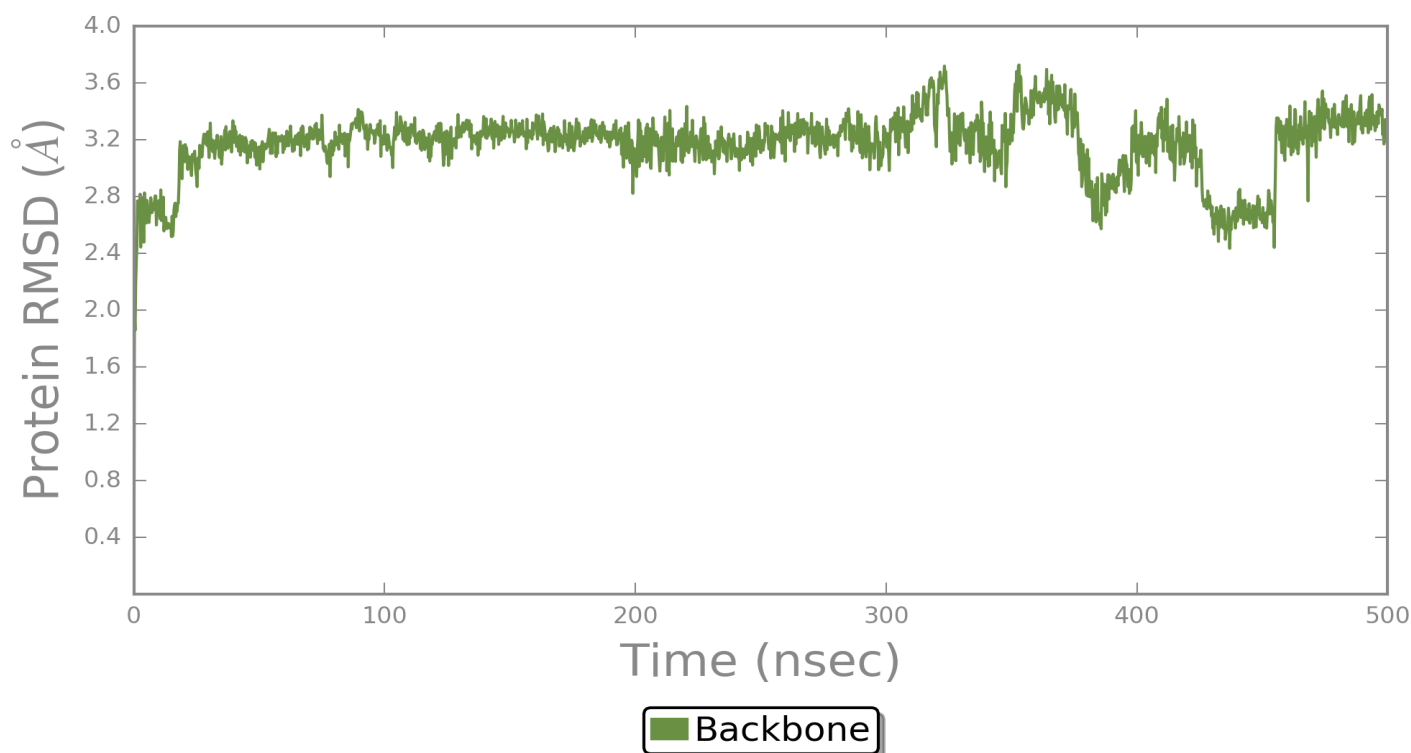
## Protein Information

	Tot. Residues	Prot. Chain(s)	Res. in Chain(s)	# Atoms	# Heavy Atoms	Charge
	169	'B'	169	2593	1346	-17
- B SSA	67	70 75 80 85 90 95 100 105 110 115 120 125 130	SSFVEKMKKTGRNIIVFYGSQTGTAEFFANRLSKDAHRYGMRGMSADPEEYDLADLSSLPEIDNALVVFC	136		
- B SSA	137	140 145 150 155 160 165 170 175 180 185 190 195 200	MATYGEEDPTDQAQDFYDWLQETDVLDSGVKFAVFGNGKTYEHFNAMGKYVDKRLEQLGAQRIFELGLG	206		
- B SSA	207	210 215 220 225 230	DDGNLEEDFITWREQFWPAVCEHFGVEA	235		

## Counter Ion/Salt Information

Type	Num.	Concentration [mM]	Total Charge
Na	33	12.191	+33

## Protein-Ligand RMSD



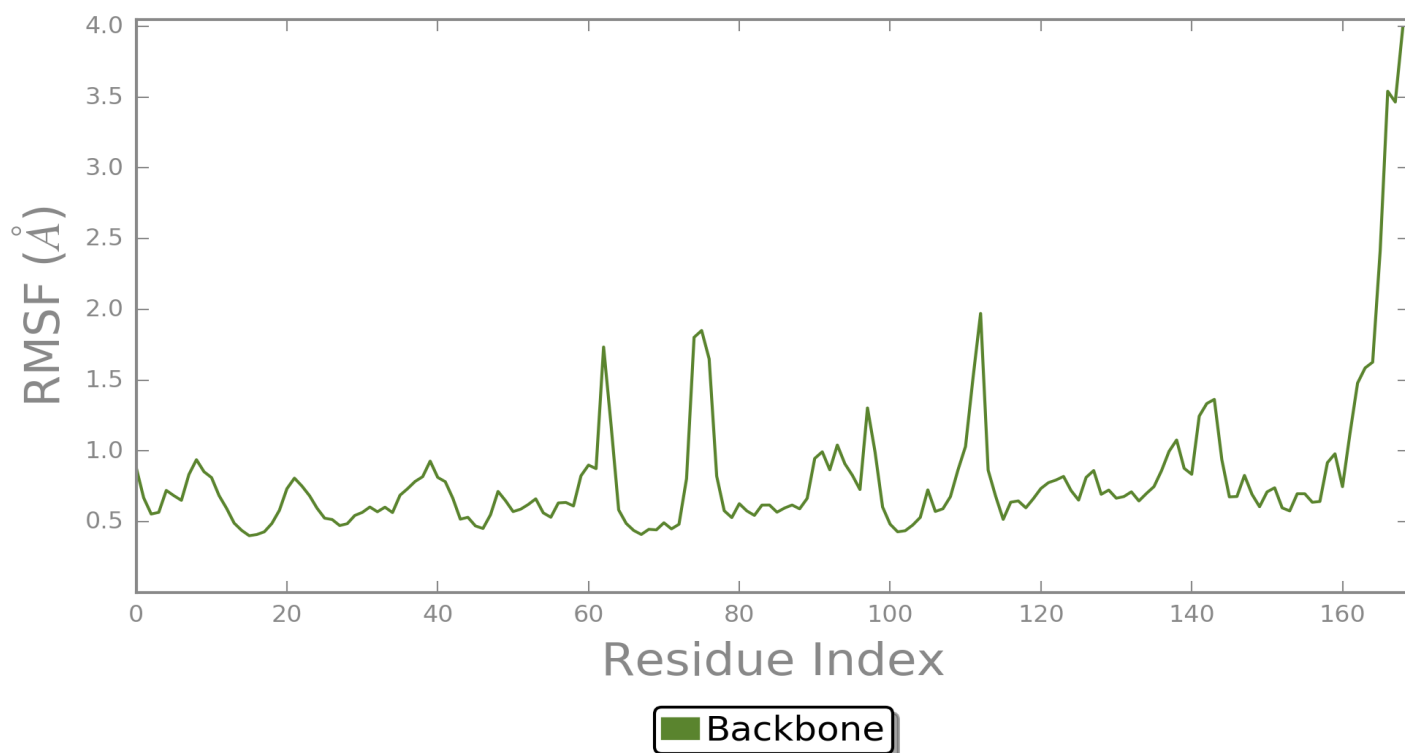
The Root Mean Square Deviation (RMSD) is used to measure the average change in displacement of a selection of atoms for a particular frame with respect to a reference frame. It is calculated for all frames in the trajectory. The RMSD for frame  $x$  is:

$$RMSD_x = \sqrt{\frac{1}{N} \sum_{i=1}^N (r'_i(t_x) - r_i(t_{ref}))^2}$$

where  $N$  is the number of atoms in the atom selection;  $t_{ref}$  is the reference time, (typically the first frame is used as the reference and it is regarded as time  $t=0$ ); and  $r'$  is the position of the selected atoms in frame  $x$  after superimposing on the reference frame, where frame  $x$  is recorded at time  $t_x$ . The procedure is repeated for every frame in the simulation trajectory.

**Protein RMSD:** The above plot shows the RMSD evolution of a protein (left Y-axis). All protein frames are first aligned on the reference frame backbone, and then the RMSD is calculated based on the atom selection. Monitoring the RMSD of the protein can give insights into its structural conformation throughout the simulation. RMSD analysis can indicate if the simulation has equilibrated — its fluctuations towards the end of the simulation are around some thermal average structure. Changes of the order of 1-3 Å are perfectly acceptable for small, globular proteins. Changes much larger than that, however, indicate that the protein is undergoing a large conformational change during the simulation. It is also important that your simulation converges — the RMSD values stabilize around a fixed value. If the RMSD of the protein is still increasing or decreasing on average at the end of the simulation, then your system has not equilibrated, and your simulation may not be long enough for rigorous analysis.

## Protein RMSF



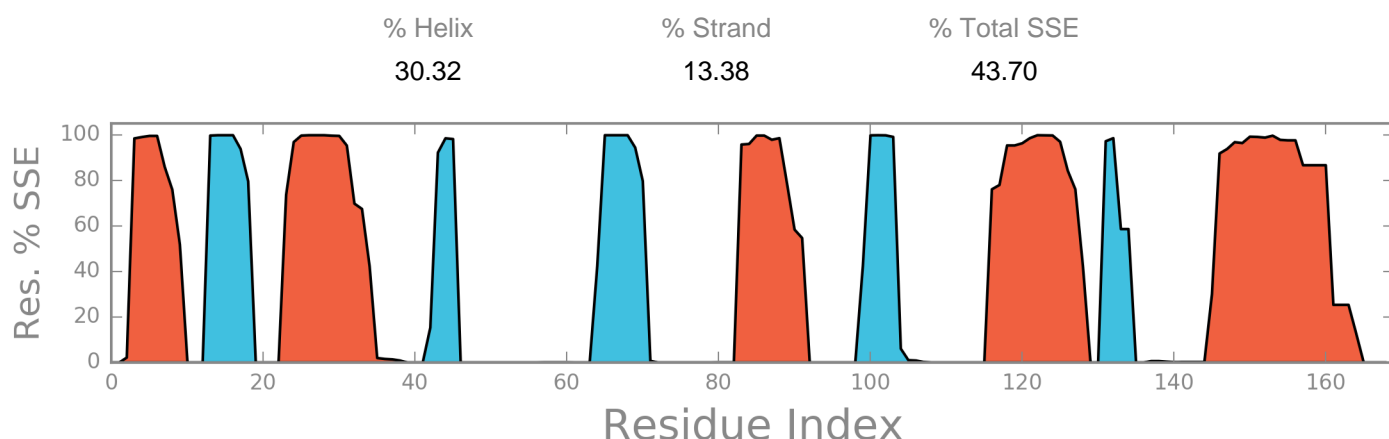
The Root Mean Square Fluctuation (RMSF) is useful for characterizing local changes along the protein chain. The RMSF for residue  $i$  is:

$$RMSF_i = \sqrt{\frac{1}{T} \sum_{t=1}^T \langle (r'_i(t)) - r_i(t_{ref})^2 \rangle}$$

where  $T$  is the trajectory time over which the RMSF is calculated,  $t_{ref}$  is the reference time,  $r_i$  is the position of residue  $i$ ;  $r'$  is the position of atoms in residue  $i$  after superposition on the reference, and the angle brackets indicate that the average of the square distance is taken over the selection of atoms in the residue.

On this plot, peaks indicate areas of the protein that fluctuate the most during the simulation. Typically you will observe that the tails ( $N$ - and  $C$ -terminal) fluctuate more than any other part of the protein. Secondary structure elements like alpha helices and beta strands are usually more rigid than the unstructured part of the protein, and thus fluctuate less than the loop regions.

## Protein Secondary Structure



Protein secondary structure elements (SSE) like **alpha-helices** and **beta-strands** are monitored throughout the simulation. The plot above reports SSE distribution by residue index throughout the protein structure. The plot below summarizes the SSE composition for each trajectory frame over the course of the simulation, and the plot at the bottom monitors each residue and its SSE assignment over time.

