

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

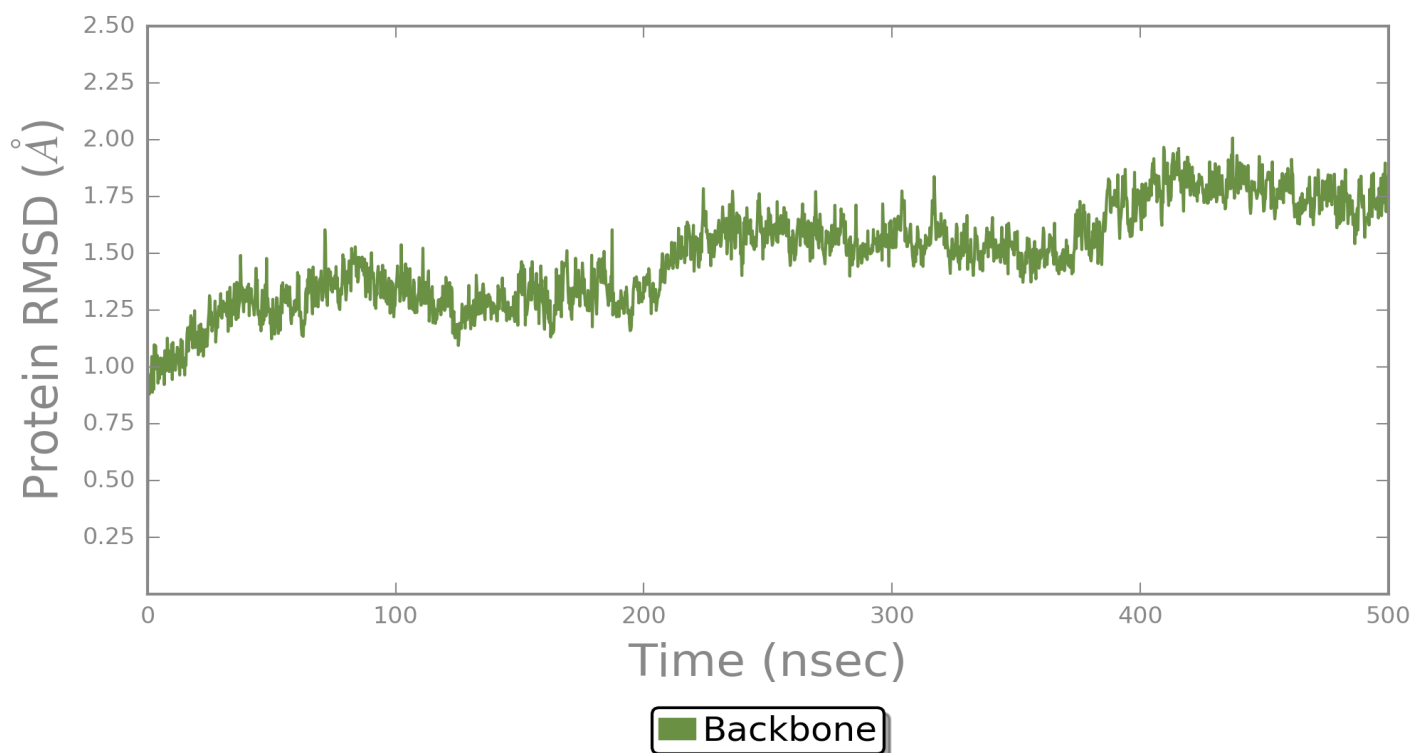
Protein Information

	Tot. Residues	Prot. Chain(s)	Res. in Chain(s)	# Atoms	# Heavy Atoms	Charge
	464	'A'	464	7326	3669	-2
- A SSA	34	35 40 45 50 55 60 65 70 75 80 85 90 95 100	PPGPLPLPGLGNLLHVDQNTPYCFDQLRRRFGDVFSLQLAWTPVVVLNGLAAVREALVTHGEDTADRP	103		
- A SSA	104	105 110 115 120 125 130 135 140 145 150 155 160 165 170	VPITQILGFGPRSQGVFLARYGPAWREQRRFSVSTLRNLGLGKKSLEQWVTEEAACLCAAFANHSGRPFR	173		
- A SSA	174	175 180 185 190 195 200 205 210 215 220 225 230 235 240	PNGLLDKAVSNVIASLTCGRRFEYDDPRFLRLDLAQEGLKEESGFLREVLNAVVPVLLHIPALAGKVLRF	243		
- A SSA	244	245 250 255 260 265 270 275 280 285 290 295 300 305 310	QKAFLLQLDELLTEHRMTWDPAPPRDLTEAFLAEMEKAKGNPESFNDENLRIVVADLFSAGMVTSTT	313		
- A SSA	314	315 320 325 330 335 340 345 350 355 360 365 370 375 380	LAWGLLLMILHPDVQRRVQQEIDDVIGQVRRPEMGDAQHMPYTTAVIHEVQRFGDIVPLGVTHMTSRDIE	383		
- A SSA	384	385 390 395 400 405 410 415 420 425 430 435 440 445 450	VQGFRI PKGTTLITNLSSVLKDEAVWEKPFRRFHPHFDAQGHFVKPEAFLPFSAGRRACLGEP LARMEL	453		
- A SSA	454	455 460 465 470 475 480 485 490	FLFFTSLLQHFSFSVPTGQPRPSHHGVFAFLVSPSPYELCAVPR	497		

Counter Ion/Salt Information

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

Protein-Ligand RMSD



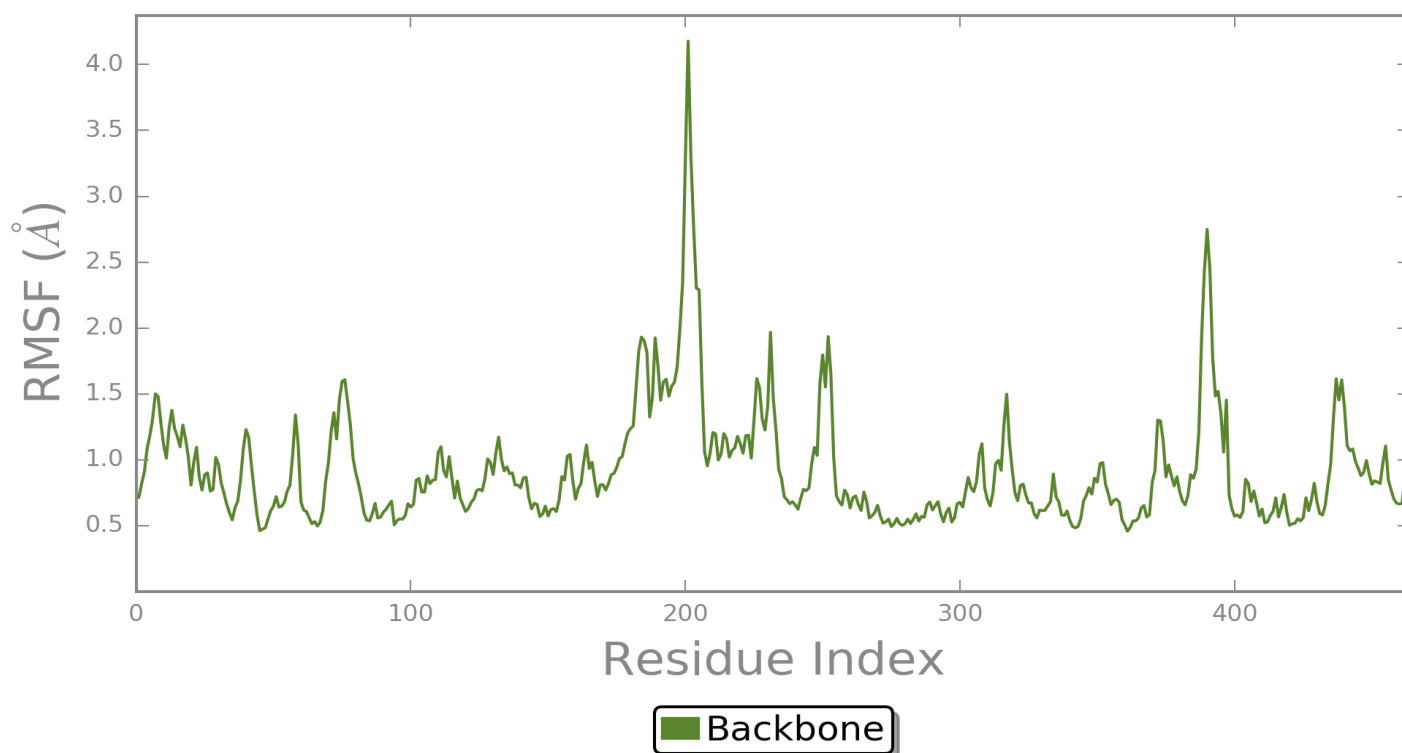
The Root Mean Square Deviation (RMSD) is used to measure the average change in displacement of a selection of atoms for a particular frame with respect to a reference frame. It is calculated for all frames in the trajectory. The RMSD for frame x is:

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

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



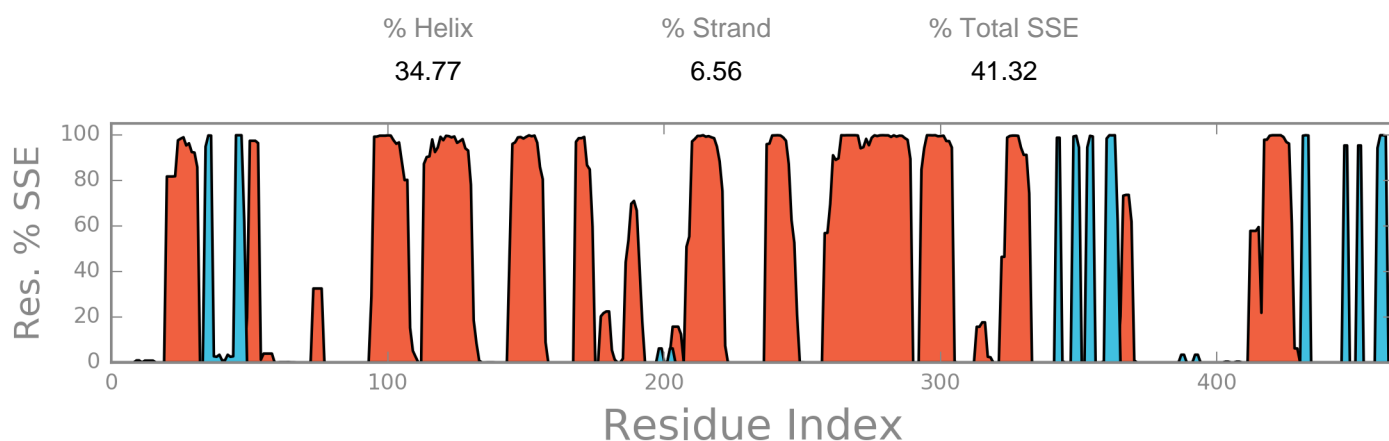
The Root Mean Square Fluctuation (RMSF) is useful for characterizing local changes along the protein chain. The RMSF for residue i is:

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

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.

