which may indicate an unstable simulation (cite: http://manual.gromacs.org/documentation/2018/user-guide/run-time-errors.html) [45]. We arrive at a FMax arrived at the following credentials.

Steepest Descents converged to Fmax <1000 in 4207 steps	
Potential Energy =	-5.3137540e+06
Maximum force =	9.7119373e+02 on atom 67859
Norm of force =	9.4712064e+00

TABLE 1.8: Minimization energy

Potential energy minimization

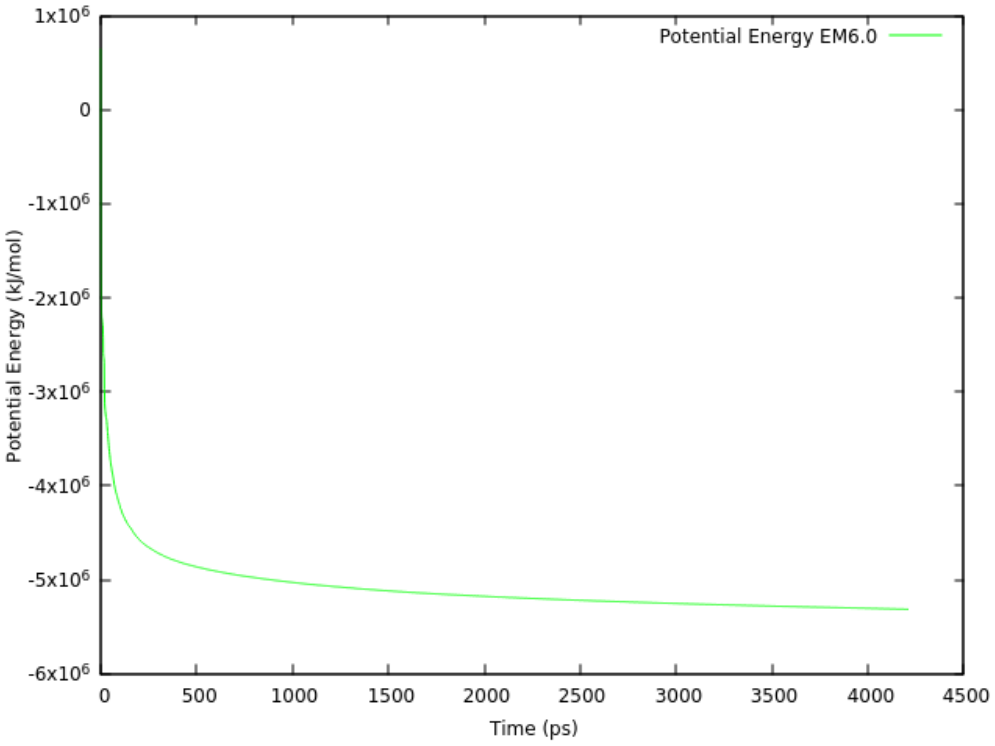

FIGURE 1.6: Energy Minimization - Potential Energy

Average	Err. Est	RMSD	Tot-Drift	
-5.08357e+06	12000	354478	-800318	kJ/mol

TABLE 1.9: Equilibration - RMSD

To do: typo: Density Equilibration this needs to be reproduced (as here yaxis is named as pressure) or check folder in dzl

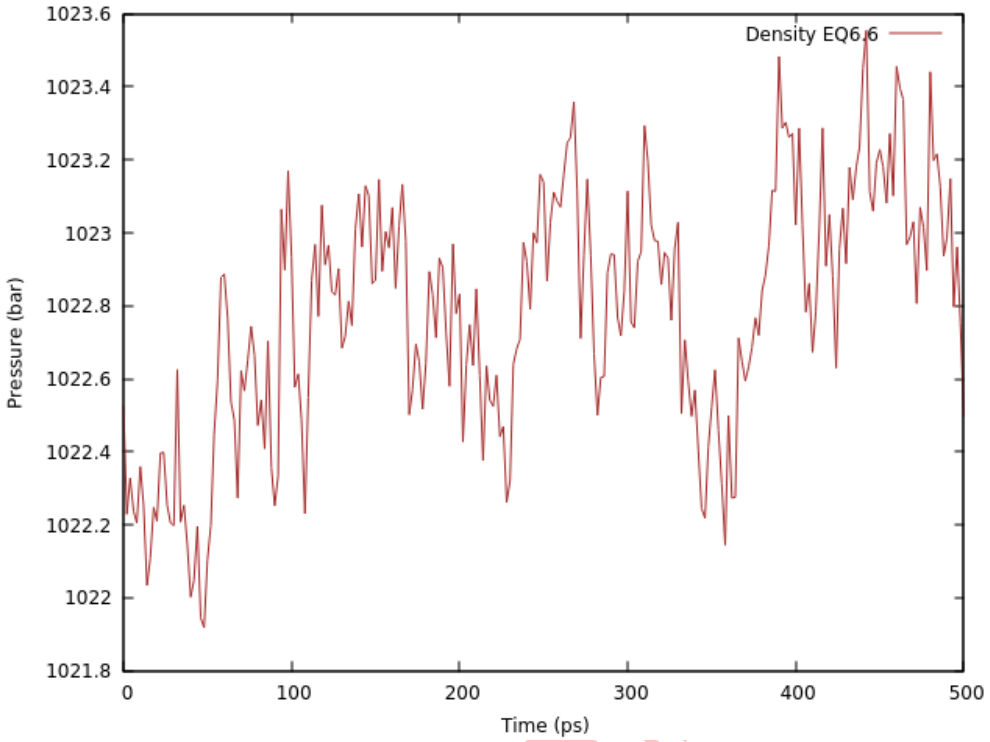

FIGURE 1.7: Equilibration - Density

Temperature Equilibration

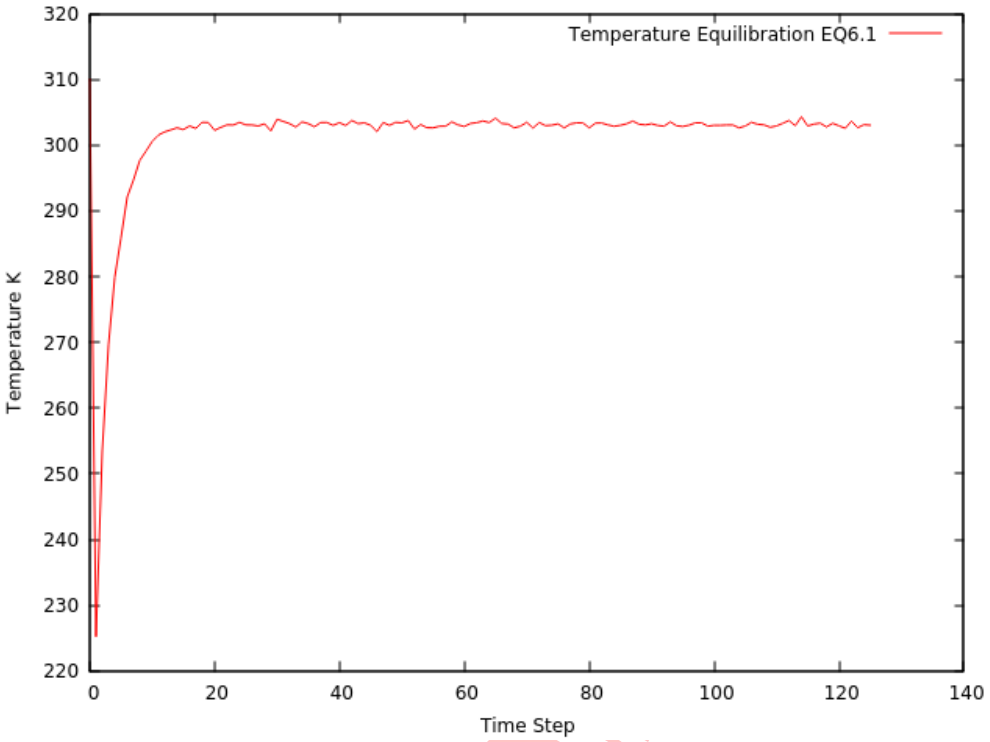

FIGURE 1.8: Equilibration - Temperature

Average	Err. Est	RMSD	Tot-Drift	
300.808	2.3	11.726	13.4605	K

TABLE 1.10: Equilibration 6.1- Temperature (seems like 303∼K), indeed it was 303.15K following Jiang ([2]) method, subsequent temp was reset to 310K per Khoa ([6])

Pressure Equilibration

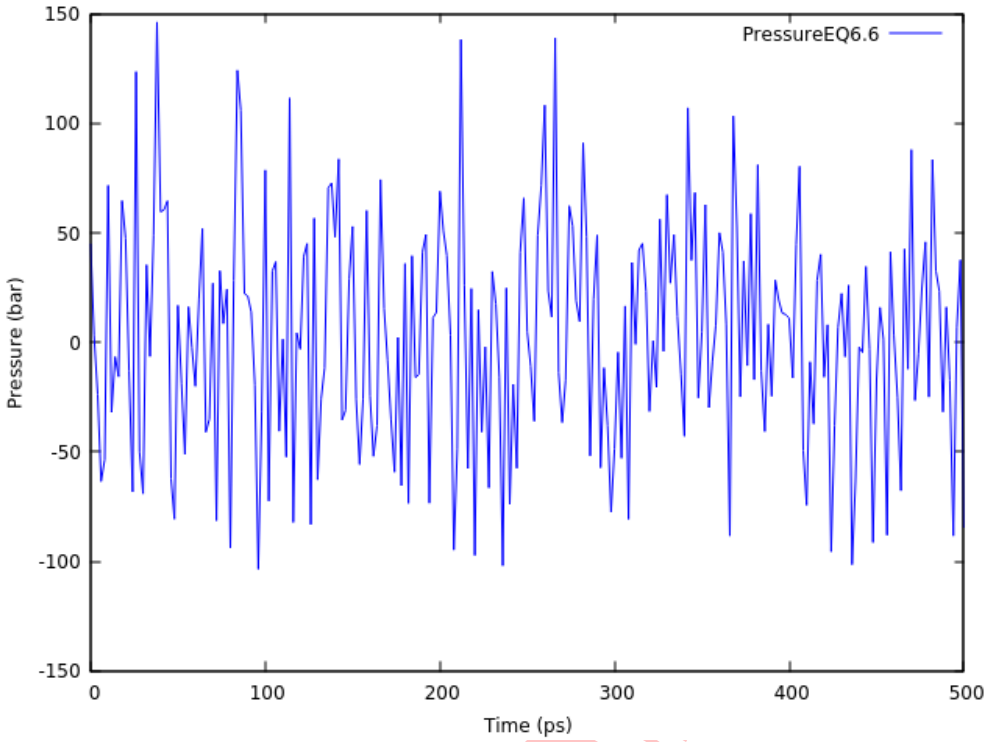

FIGURE 1.9: Equilibration - Pressure

Therefore the pre-production plots that are presented here, were first analysed in order to prepare the MD simulation in right conditions. The following plots are based on the data from 100ns simulation of enzyme with lipids composition of native environment (refer to methods section 2:7x).

RMSD calculates how much a molecule deviates from its initial structure over the course of the simulation. Therefore, it is used as an indicator of convergence and is generally plotted as a function of time. When the RMSD curve becomes flat the system is not changing significantly anymore and it can be considered equilibrated for pre-production runs as discussed above.

FIGURE 1.10: RMSD equilibrtion

1.5.9 MD trajectory analysis - methods

It's important to note this MD chapter was written as if a tutorial.

Next sections present the 3D structural coordination environment of the protein residues and bilayer membrane and their atomic level interactions that were characterised using a range of analysis, distribution functions over a trajectory of 100ns.