Step	Ensemble[1]	Timesteps	Equilibration Time	Force Constants for Harmonic Restraint[2]				
				Protein Backbone[3]	Protein Sidechain[3]	Water[4]	Lipid[5]	Ion[3]
1	NVT	1 fs	25 ps	10.0	5.0	2.5	2.5	10.0
2	NVT	1 fs	25 ps	5.0	2.5	2.5	2.5	0.0
3	NPAT	1 fs	25 ps	2.5	1.0	1.0	1.0	0.0
4	NPAT	2 fs	100 ps	1.0	0.5	0.5	0.5	0.0
5	NPAT	2 fs	100 ps	0.5	0.1	0.1	0.1	0.0
6	NPAT	2 fs	100 ps	0.1	0.0	0.0	0.0	0.0

[1.] NVT stands for constant volume and temperature, and NPAT for constant pressure, area, and temperature.
[2.] Force constants are in kcal/(mol·Å^2).
[3.] Positional harmonic restraints.
[4.] Harmonic restraints to keep water molecules away from the membrane hydrophobic region.
[5.] Harmonic restraints to keep the lipid tail in -5 Å$<Z<5$ Å, and lipid head groups close to the membrane surface ($Z=\pm17$ Å for DMPC and $Z=\pm19$ Å for DPPC and POPC).

doi:10.1371/journal.pone.0000880.t001