

Table 3: Thermodynamic quantities for each of the trajectories

Quantities	Trajectory				
	[RC]	[P1]	[P2]	[DU]	[RCS]
Box size, Å					
L_X	41.81	42.88	43.01	41.73	41.09
L_Y	41.84	43.03	42.98	41.76	41.12
L_Z	41.84	42.96	43.00	41.79	41.12
Water molecules	2,542	2,544	2,544	2,540	2,399
No. of atoms	7,754	7,760	7,760	7,749	7,375
Total mass, amu	46,764.1	46,800.1	46,800.1	46,705.1	45,648.9
Volume, Å ³	73,185.2	79,263.0	79,497.7	72,820.8	69,495.1
Density, amu/Å ³	0.63898	0.59044	0.58870	0.64137	0.65686
Density, g/cm ³	1.06091	0.98031	0.97742	1.06487	1.09059
Temperature, K	283.2 ± 2.6	283.2 ± 2.6	283.2 ± 2.6	283.2 ± 2.6	283.2 ± 2.7
Pressure, bar	-2.1 ± 220.4	-1,420.7 ± 198.4	-1,458.5 ± 198.2	111.6 ± 249.8	76.5 ± 230.2