

	Gromacs 4.0.7	Gromacs 4.6.5	Difference
G96Angle	12952.15137	12952.1543	0.00293
Proper Dih.	9579.225586	9579.223633	-0.001953
Improper Dih.	497.637329	497.637115	-0.000214
LJ-14	-1381.257324	-1381.257202	0.000122
Coulomb-14	15079.12988	15079.12988	0
LJ (SR)	12735.0166	12735	-0.016602
LJ (LR)	-7496.064453	-7496.074219	-0.009766
Coulomb (SR)	-378489.1875	-378489.3125	-0.125
Coulomb (LR)	-897.365112	-897.363892	0.00122
RF excl.	-52541.38672	-52541.41016	-0.023437
Potential	-389962.0938	-389962.2813	-0.1875
Kinetic En.	65052.72266	65058.27734	5.554688
Total Energy	-324909.375	-324904	5.375
Temperature	326.217407	326.24527	0.027863
Pressure (bar)	1.636197	10.578368	8.942171
Cons. rmsd ()	0.000006	0.000006	0
Box-X	6.12229	6.12229	0
Box-Y	6.12229	6.12229	0
Box-Z	9.01159	9.01159	0
Volume	337.776367	337.776367	0
Density (SI)	979.22229	979.22229	0
pV	33.282459	20.341356	-12.941103
Vir-XX	20135.96875	20069.85156	-66.117188
Vir-XY	-201.496094	-289.907196	-88.411102
Vir-XZ	61.570404	37.36554	-24.204864
Vir-YX	-238.727905	-278.357849	-39.629944
Vir-YY	23495.5	23435.21875	-60.28125
Vir-YZ	1492.471069	1484.944092	-7.526977
Vir-ZX	0.251434	51.632324	51.38089
Vir-ZY	1535.411377	1472.929565	-62.481812
Vir-ZZ	21371.32813	21230.4375	-140.890625
Pres-XX (bar)	180.828094	189.103271	8.275177
Pres-XY (bar)	24.003698	32.851803	8.848105
Pres-XZ (bar)	17.420185	18.472696	1.052511
Pres-YX (bar)	27.664396	31.716249	4.051853
Pres-YY (bar)	-149.124878	-142.105621	7.019257
Pres-YZ (bar)	-144.909485	-145.304153	-0.394668
Pres-ZX (bar)	23.449183	17.069954	-6.379229
Pres-ZY (bar)	-149.131454	-144.122864	5.00859
Pres-ZZ (bar)	-26.794626	-15.262547	11.532079
#Surf*SurfTen	-384.310394	-349.301605	35.008789
Box-Vel-XX	0	0	0
Box-Vel-YY	0	0	0
Box-Vel-ZZ	0	0	0
Mu-X	177.912521		
Mu-Y	-691.331116		
Mu-Z	1798.444824		
T-DPPC	333.500824	333.382996	-0.117828
T-SOL	323.531036	323.61264	0.081604
Xi-DPPC	0.001939		
Xi-SOL	-0.000514		
Enthalpy		-324883.6563	