Forcefield = charmm36 constraint tolerance = 1.00e-12 9.3 ×10⁴ -3.6 ×10⁵ 9.2 -3.8 9.1 -4 Potential energy (kJ/mol) 9 Kinetic energy (kJ/mol)

8 8 8

2 8 6

6 8 8.6 -5 8.5 8.4 8000 2000 4000 6000 14000 16000 2000 4000 16000 8000 10000 12000 6000 10000 12000 14000 0 number of steps number of steps