Forcefield = charmm36 constraint tolerance = 1.00e-04 9 ×10⁴ -4.7×10^{5} 8.9 -4.8 8.8 Potential energy (kJ/mol) Kinetic energy (kJ/mol) 8 8 8 2 8 2 -5 -5.2 8.4 -5.3 8.3 2000 16000 4000 6000 8000 10000 12000 14000 16000 2000 4000 6000 8000 10000 12000 14000 0 number of steps number of steps