title = OPLS Lysozyme NPT equilibration

define = -DPOSRES ;-DPOSRES\_LIG ;position restrain the protein

;Run parameters

integrator = md ; leap-frog integrator

nsteps = 50000 ; 2 \* 50000 = 100 ps

dt = 0.002 ; 2 fs

; Output control

nstxout = 500 ; save coordinates every 1.0 ps

nstvout = 500 ; save velocities every 1.0 ps

nstenergy = 500 ; save energies every 1.0 ps

nstlog = 500 ; update log file every 1.0 ps

; Bond parameters

continuation = yes ; Restarting after NVT

constraint\_algorithm = lincs ; holonomic constraints

constraints = ; all bonds (even heavy atom-H bonds) constrained

lincs\_iter = 1 ; accuracy of LINCS

lincs\_order = 4 ; also related to accuracy

; Neighborsearching

cutoff-scheme = Verlet

ns\_type = grid ; search neighboring grid cells

nstlist = 10 ; 20 fs, largely irrelevant with Verlet scheme

rcoulomb = ; short-range electrostatic cutoff (in nm)

rvdw = ; short-range van der Waals cutoff (in nm)

; Electrostatics

coulombtype = PME ; Particle Mesh Ewald for long-range electrostatics

pme\_order = 4 ; cubic interpolation

fourierspacing = 0.16 ; grid spacing for FFT

; Temperature coupling is on

tcoupl = V-rescale ; modified Berendsen thermostat

tc-grps = ;Protein Non-Protein ;Protein Non-Protein ; two coupling groups - more accurate

tau\_t = ; time constant, in ps

ref\_t = ; reference temperature, one for each group, in K

; Pressure coupling is on

pcoupl = Parrinello-Rahman ; Pressure coupling on in NPT

pcoupltype = isotropic ; uniform scaling of box vectors

tau\_p = 2.0 ; time constant, in ps

ref\_p = 1.0 ; reference pressure, in bar

compressibility = 4.5e-5 ; isothermal compressibility of water, bar^-1

refcoord\_scaling = com

; Periodic boundary conditions

pbc = xyz ; 3-D PBC

; Dispersion correction

DispCorr = EnerPres ; account for cut-off vdW scheme

; Velocity generation

gen\_vel = no ; Velocity generation is off