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## ADJUSTABLE PARAMETERS ##

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structure Example.psf # load system PSF file

coordinates Example.pdb # load system PDB file

set temperature 500.0 # set temperature 500 K

set outputname Example\_eq # base name of output files

firsttimestep 0 # start simulation at t=0

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## SIMULATION PARAMETERS ##

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# Input

paraTypeCharmm on ;# use CHARMM forcefield parameters

parameters cg\_ Example.inp ;# load parameter file

#temperature $temperature ;# set temperature

# Force-Field Parameters

exclude 1-2

1-4scaling 1.0

**# User specified settings**

**#(cutoff local interaction distance common to both electrostatic and van der #Waals calculations (Å))**

cutoff 25.0 **#(switching on smoothing functions are applied to both the electrostatics and #van der Waals forces)**

switching on

**# Distance at which the switching function should begin to take effect.**

switchdist 10.

**# distance between pairs for inclusion in pair lists**

pairlistdist 45.5

# margin 2.5

# Integrator Parameters

timestep 6.0 ;# 6fs/step

**# if “all” all water made rigid**

# rigidBonds all ;# needed for 2fs steps;

nonbondedFreq 1 ;# non-bonded forces calc every steps

**#(fullElectFreq number of timesteps btwn full electrostatic evaluations)**

fullElectFrequency 2 ;# use PME only every other step

stepspercycle 20 ;# redo pairlists every ten steps

# Constant Temperature Control

langevin on ;# do langevin dynamics

langevinDamping 5 ;# damping coefficient (gamma) of 5/ps

langevinTemp $temperature

langevinHydrogen on ;# Not couple langevin bath to Hdrogens

# Periodic Boundary Conditions

**# lengths of the sides of the unit cell**

cellBasisVector1 80. 0. 0.

cellBasisVector2 0. 80. 0.

cellBasisVector3 0. 0. 80.

cellOrigin 40 42 40

wrapAll on

# PME (for full-system periodic electrostatics)

PME yes ;# Particle Mesh Ewald

**#(full electrostatic method used w/ periodic boundary conditions)**

#PMEGridSizeX 80 ;# number of grid points in x dimension

**#grid size partially determines the accuracy and efficiency of PME**

#PMEGridSizeY 80

#PMEGridSizeZ 80

# Constant Pressure Control (variable volume)

useGroupPressure no ;# needed for rigidBonds

useFlexibleCell no

useConstantArea no

**# langevin Piston pressure control method**

langevinPiston on

langevinPistonTarget 1.000 ;# in bar -> 1 atm

langevinPistonPeriod 100. ;# oscillation period (fs)

**#Larger value results in underdamped dynamics(decaying ringing in cell vol)**

**#Smaller value then langevinPistonPeriod approaches exponential decay.**

**#Also corresponds to larger random forces with increased coupling.**

langevinPistonDecay 50. ;# damping time scale (fs)

langevinPistonTemp $temperature ;# Set equal to the target temperature

# Output

outputName $outputname

restartfreq 5000;# 5000steps = every 1ps

dcdfreq 5000;# output coord in DCD trajectory file ever 5000 steps

xstFreq 5000

outputEnergies 5000;# output energies/temperature, etc every 5000 steps

outputPressure 5000;# output pressure every 5000 steps

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## EXTRA PARAMETERS ##

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## EXECUTION SCRIPT ##

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# Minimization

#minimize 1000;# run structure minimization for 1000 steps

#reinitvels $temperature ;# reinitialize velocities corresponding to 500K

run 1000000 ;# run MD simulation (equilibration) for 10ps

;# recall: timeStep = 60 x 102 fs