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Supporting Information 2

Validating Molecular Dynamics Simulations Against Experimental Observables in Light of Underlying Conformational Ensembles

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AMBER Input Files

Minimization

```
Minimization Stage 1
 &cntrl
  imin=1,
  ntmin=1,
  maxcyc=1000,
  ncyc=500,
  ntx=1,
  ntf=1,
  ntp=1,
  ntt=1,
  cut=10,
  ntr=1,
  restraint_wt=100,
  restraintmask=':1-56',
  iwrap=1,
  ntxo=2,
  ntpr=50,
  ntwr=50,
 /
```

```
Minimization Stage 2
 &cntrl
  imin=1,
  ntmin=1,
  maxcyc=1000,
  ncyc=500,
  ntx=1,
  irest=0,
  ntpr=50,
  ntwr=50,
  iwrap=1,
  ntf=1,
  ntp=1,
  ntt=1,
  cut=10,
  ntr=1,
  ntxo=2,
  restraint_wt=100,
  restraintmask=':1-56 & !@H',
 /
```

```
Minimization Stage 3
 &cntrl
  imin=1,
  ntmin=1,
  maxcyc=1000,
  ncyc=500,
  ntx=1,
  ntpr=50,
  ntwr=50,
  iwrap=1,
  ntf=1,
  ntp=1,
  ntt=1,
  ntxo=2,
  cut=10,
  ntr=1,
  restraint_wt=25,
  restraintmask=':1-56@CA',
 /
```

Heating

```
Heating Stage 1
 &cntrl
  imin = 0,
  irest = 0,
  ntx = 1,
  ntc = 2,
  ntf = 2,
  ntp = 1,
  cut = 10.0,
  tempi = 0.0,
  temp0 = 50.0,
  ntt = 1,
  tautp=1.0,
  nstlim = 25000,
  dt = 0.002,
  iwrap = 1,
  ntpr = 50,
  ntwx = 50,
  ntwr = 500,
  nscm = 1000,
  ntr=1,
  restraint_wt=25,
  restraintmask=':1-56@CA',
  ig=-1,
  ioutfm=1,
  ntxo=2,
 /
```

```
Heating Stage 2
 &cntrl
  imin = 0,
  irest = 1,
  ntx = 5,
  ntc = 2,
  ntf = 2,
  ntp = 1,
  cut = 10.0,
  temp0 = 100.0,
  ntt = 1,
  tautp=1.0,
  nstlim = 25000,
  dt = 0.002,
  iwrap = 1,
  ntpr = 50,
  ntwx = 50,
  ntwr = 500,
  nscm = 1000,
  ntr=1,
  restraint_wt=25,
  restraintmask=':1-56@CA',
  ig=-1,
  ioutfm=1,
  ntxo=2,
 /
```

```
Heating Stage 3
 &cntrl
  imin = 0,
  irest = 1,
  ntx = 5,
  ntc = 2,
  ntf = 2,
  ntp = 1,
  cut = 10.0,
  temp0 = 150.0,
  ntt = 1,
  tautp=1.0,
  nstlim = 25000,
  dt = 0.002,
  iwrap = 1,
  ntpr = 50,
  ntwx = 50,
  ntwr = 500,
  nscm = 1000,
  ntr=1,
  restraint_wt=25,
  restraintmask=':1-56@CA',
  ig=-1,
  ioutfm=1,
  ntxo=2,
 /
```

```
Heating Stage 4
 &cntrl
  imin = 0,
  irest = 1,
  ntx = 5,
  ntc = 2,
  ntf = 2,
  ntp = 1,
  cut = 10.0,
  temp0 = 200.0,
  ntt = 1,
  tautp=1.0,
  nstlim = 25000,
  dt = 0.002,
  iwrap = 1,
  ntpr = 50,
  ntwx = 50,
  ntwr = 500,
  nscm = 1000,
  ntr=1,
  restraint_wt=25,
  restraintmask=':1-56@CA',
  ig=-1,
  ioutfm=1,
  ntxo=2,
 /
```

```
Heating Stage 5
 &cntrl
  imin = 0,
  irest = 1,
  ntx = 5,
  ntc = 2,
  ntf = 2,
  ntp = 0,
  cut = 10.0,
  temp0 = 250.0,
  ntt = 1,
  tautp=1.0,
  nstlim = 25000,
  dt = 0.002,
  iwrap = 1,
  ntpr = 50,
  ntwx = 50,
  ntwr = 500,
  nscm = 1000,
  ntr=1,
  restraint_wt=25,
  restraintmask=':1-56@CA',
  ig=-1,
  ioutfm=1,
  ntxo=2,
 /
```

```
Heating Stage 6
 &cntrl
  imin = 0,
  irest = 1,
  ntx = 5,
  ntc = 2,
  ntf = 2,
  ntp = 1,
  cut = 10.0,
  temp0 = 298.0,
  ntt = 1,
  tautp=1.0,
  nstlim = 25000,
  dt = 0.002,
  iwrap = 1,
  ntpr = 50,
  ntwx = 50,
  ntwr = 500,
  nscm = 1000,
  ntr=1,
  restraint_wt=25,
  restraintmask=':1-56@CA',
  ig=-1,
  ioutfm=1,
  ntxo=2,
 /
```

Equilibration

```
Equilibration Stage 1
 &cntrl
  imin=1,
  ntmin=1,
  maxcyc=1000,
  ncyc=500,
  ntx=5,
  irest=1,
  ntt=1,
  tautp=1.0,
  ntpr=50,
  ntwr=50,
  iwrap=1,
  ntf=1,
  cut=10.0,
  ntr=1,
  restraint_wt=5,
  restraintmask=':1-56@CA',
 /
```

```
Equilibration Stage 2
 &cntrl
  imin=1,
  ntmin=1,
  maxcyc=1000,
  ncyc=500,
  ntx=1,
  irest=0,
  ntt=1,
  tautp=1.0,
  ntpr=50,
  ntwr=50,
  iwrap=1,
  ntf=1,
  cut=10.0,
  ntr=1,
  restraint_wt=4,
  restraintmask=':1-56@CA',
 /
```

```
Equilibration Stage 3
 &cntrl
  imin=1,
  ntmin=1,
  maxcyc=1000,
  ncyc=500,
  ntx=1,
  irest=0,
  ntt=1,
  tautp=1.0,
  ntpr=50,
  ntwr=50,
  iwrap=1,
  ntf=1,
  cut=10.0,
  ntr=1,
  restraint_wt=3,
  restraintmask=':1-56@CA',
 /
```

```
Equilibration Stage 4
 &cntrl
  imin=1,
  ntmin=1,
  maxcyc=1000,
  ncyc=500,
  ntx=1,
  irest=0,
  ntt=1,
  tautp=1.0,
  ntpr=50,
  ntwr=50,
  iwrap=1,
  ntf=1,
  cut=10.0,
  ntr=1,
  restraint_wt=2,
  restraintmask=':1-56@CA',
 /
```

```
Equilibration Stage 5
 &cntrl
  imin=1,
  ntmin=1,
  maxcyc=1000,
  ncyc=500,
  ntx=1,
  irest=0,
  ntt=1,
  tautp=1.0,
  ntpr=50,
  ntwr=50,
  iwrap=1,
  ntf=1,
  cut=10.0,
  ntr=1,
  restraint_wt=1,
  restraintmask=':1-56@CA',
 /
```

```
Equilibration Stage 6
 &cntrl
  imin=0,
  ntpr=50,
  ntwx=500,
  ntwr=500,
  iwrap=1,
  ntx=1,
  irest=0,
  ntf=2,
  ntc=2,
  cut=10.0,
  nstlim=500000,
  dt=0.002,
  nscm=1000,
  temp0=298.0,
  tempi=298.0,
  ntt=1,
  ntp=0,
  ntb=1,
  ntr=1,
  restraint_wt=0.5,
  restraintmask=':1-56@CA',
  ig=-1,
  ioutfm=1,
  ntxo=2,
 /
```

```
Equilibration Stage 7
 &cntrl
  imin=0,
  ntpr=50,
  ntwx=500,
  ntwr=500,
  iwrap=1,
  ntx=1,
  irest=0,
  ntf=2,
  ntc=2,
  cut=10.0,
  nstlim=500000,
  dt=0.002,
  nscm=1000,
  temp0=298.0,
  tempi=298.0,
  ntt=1,
  ntp=1,
  tautp=0.2,
  ntr=1,
  restraint_wt=0.5,
  restraintmask=':1-56@CA',
  ig=-1,
  ioutfm=1,
  ntxo=2,
 /
```

Production Dynamics

```
Production Dynamics
  imin=0,
  irest=1,
  ntx=5,
  nstlim=500000,
  dt=0.002,
  ntc=2,
  ntf=2,
  ntt=3,
  gamma_ln=1.0,
  temp0=298.0,
  ntpr=50000,
  ntwx=500,
  ntwr=50000,
  ntp=1,
  iwrap=1,
  cut=10.0,
  ntr=0,
  ntxo=2,
  ioutfm=1,
  ig=-1
 /
```

GROMACS Input Files

Minimization

```
integrator          = steep
emtol               = 1000.0
emstep              = 0.005
nsteps              = 50000
nstlist             = 1
cutoff-scheme       = Verlet
ns_type             = grid
coulombtype         = PME
rcoulomb            = 1.0
rvdw                = 1.0
pbc                 = xyz
```

Equilibration

NPT Equilibration

```
define                  = -DPOSRES
integrator              = md
nsteps                  = 50000
dt                      = 0.002
nstxout                 = 500
nstvout                 = 50000
nstenergy               = 50000
nstlog                  = 50000
continuation            = yes
constraint_algorithm    = lincs
constraints             = all-bonds
lincs_iter              = 1
lincs_order             = 4
cutoff-scheme           = Verlet
ns_type                 = grid
nstlist                 = 10
rcoulomb                = 1.0
rvdw                    = 1.0
coulombtype             = PME
pme_order               = 4
fourierspacing          = 0.16
tcoupl                  = V-rescale
tc-grps                 = Protein Non-Protein
tau_t                   = 0.5   0.5
ref_t                   = 298   298
pcoupl                  = Parrinello-Rahman
pcoupltype              = isotropic
tau_p                   = 2.0
ref_p                   = 1.0
compressibility         = 4.5e-5
refcoord_scaling        = com
pbc                     = xyz
DispCorr                = EnerPres
gen_vel                 = no
```

NVT Equilibration

```
define                  = -DPOSRES
integrator              = md
nsteps                  = 50000
dt                      = 0.002
nstxout                 = 500
nstvout                 = 500
nstenergy               = 500
nstlog                  = 500
continuation            = no
constraint_algorithm    = lincs
constraints             = all-bonds
lincs_iter              = 1
lincs_order             = 4
cutoff-scheme           = Verlet
ns_type                 = grid
nstlist                 = 10
rcoulomb                = 1.0
rvdw                    = 1.0
coulombtype             = PME
pme_order               = 4
fourierspacing          = 0.16
tcoupl                  = V-rescale
tc-grps                 = Protein Non-Protein
tau_t                   = 0.5   0.5
ref_t                   = 298         298
pcoupl                  = no
pbc                     = xyz
DispCorr                = EnerPres
gen_vel                 = yes
gen_temp                = 298
gen_seed                = -1
```

Production Dynamics

```
integrator              = md
nsteps                  = 500000
dt                      = 0.002
nstxout                 = 1000
nstvout                 = 5000
nstenergy               = 5000
nstlog                  = 5000
nstxout-compressed      = 5000
compressed-x-grps       = System
continuation            = yes
constraint_algorithm    = lincs
constraints             = all-bonds
lincs_iter              = 1
lincs_order             = 4
cutoff-scheme           = Verlet
ns_type                 = grid
nstlist                 = 10
rcoulomb                = 1.0
rvdw                    = 1.0
coulombtype             = PME
pme_order               = 4
fourierspacing          = 0.16
tcoupl                  = V-rescale
tc-grps                 = Protein Non-Protein
tau_t                   = 0.5     0.5
ref_t                   = 298     298
pcoupl                  = Parrinello-Rahman
pcoupltype              = isotropic
tau_p                   = 2.0
ref_p                   = 1.0
compressibility         = 4.5e-5
pbc                     = xyz
DispCorr                = EnerPres
gen_vel                 = no
```

*il*mm Input Files

Minimization

```
<?xml version='1.0'?>
<workbook xmlns="http://inlucemmolecularmechanics/workbook" mmpl_uri="file://1enh.xml">
        <add count="1" molecule="1enh">
                <chain id="A"/>
        </add>

        <pdb_read filename="1enh_preH.pdb"/>

        <hydrogen operation="add" select="1enh"/>

        <go steps="500">
                <sdmin select="@H="/>
                <log granularity="100"/>
        </go>

        <pdb_write filename="1enh_Hmin.pdb"/>

        <set name="mechanics" value="bond_pbadi angle_pbadi torsion_pbadi nonbonded_plus_pbadi" type="string"/>
        <set name="pbadi_count" value="10" type="integer"/>
        <go steps="1000">
                <sdmin/>
                <log granularity="100"/>
        </go>

        <chirality/>

        <pdb_write filename="min.pdb"/>

</workbook>
```

Equilibration

```
<?xml version='1.0'?>
<workbook xmlns="http://inlucemmolecularmechanics/workbook" mmpl_uri="file://../1enh.xml">

        <set name="mechanics" value="bond_pbadi angle_pbadi torsion_pbadi nonbonded_plus_pbadi" type="string"/>
        <set name="pbadi_count" value="10" type="integer"/>

        <add count="1" molecule="1enh">
                <chain id="A"/>
        </add>

        <pdb_read filename="../min.pdb"/>

        <solvate water_pdb="/net/programs/ilmm/lib/h2o/298K.pdb" depth="10.0" density="0.997075"
radius_of_exclusion="1.8"/>

        <go steps="1000">
                <sdmin select="WAT"/>
                <log granularity="100"/>
        </go>
        <reset/>

        <go steps="500">
                <dynamics select="WAT"/>
                <thermostat temperature="298" heating_degrees="0.1" random_seed="1"/>
                <log granularity="100"/>
        </go>
        <reset/>

        <go steps="500">
                <sdmin select="WAT"/>
                <log granularity="100"/>
```

```
        </go>
        <reset/>

        <go steps="500">
                <sdmin select="~WAT"/>
                <log granularity="100"/>
        </go>
        <reset/>

        <pdb_write filename="start.pdb" write_solvent="true"/>
        <mdr_write filename="start.mdr"/>

</workbook>
```

Production_Dynamics

```
<?xml version='1.0'?>
<workbook xmlns="http://inlucemmolecularmechanics/workbook" mmpl_uri="file://1enh.xml">

        <add count="1" molecule="1enh">
                <chain id="A"/>
        </add>
        <add count="2912" molecule="WAT"/>

        <mdr_read filename="checkpoint.mdr"/>

        <go steps="50000000" hours="8">
                <dynamics/>
                <thermostat temperature="298" heating_degrees="0.1000" random_seed="1"/>
                <log granularity="500"/>
                <mdc_writer_multi_file steps_per_file="500000" granularity="500" error_maximum="0.0005"/>
                <mdr_writer granularity="500000" checkpoint_granularity="50000" checkpoint_filename="checkpoint.mdr"/>
        </go>

        <mdr_write filename="checkpoint.mdr"/>

</workbook>
```

NAMD Input Files

Minimization

Minimization Phase 1

```
#############################################################
## MAIN MD CONFIGURATION DESCRIPTION                       ##
#############################################################

# Protein in a 10A Water Box TIP3P

set temperature   298

#############################################################
## SIMULATION PARAMETERS                                   ##
#############################################################

# Input
paraTypeCharmm     on
parameters         ./par_all27_prot_lipid.inp
temperature        $temperature

# Force-Field Parameters
exclude             scaled1-4
1-4scaling          1.0
cutoff              10.0
switching           on
switchdist          9.0
pairlistdist        14.0

# Integrator Parameters
timestep            2.0
rigidBonds          all
nonbondedFreq       1
fullElectFrequency  2
stepspercycle       10

# Constant Temperature Control
langevin            on
langevinDamping     5
langevinTemp        $temperature
langevinHydrogen    off

# Output
restartsave         yes
binaryrestart       yes
restartfreq         500
```

```
dcdfreq             500
outputEnergies      100
outputPressure      100
outputMomenta       100
outputTiming       1000


###############################################################
## EXTRA PARAMETERS                                          ##
###############################################################
cellBasisVector1    47.0    0.0   0.0
cellBasisVector2     0.0   50.5   0.0
cellBasisVector3     0.0    0.0  47.8
cellOrigin           0.0    0.0   0.0

wrapAll              on
wrapNearest          on
PME                  yes
PMEGridSpacing       1
useGroupPressure     yes
useFlexibleCell      no
useConstantArea      no
langevinPiston       on
langevinPistonTarget 1.01325
langevinPistonPeriod 100.
langevinPistonDecay  50.
langevinPistonTemp   $temperature
binaryoutput         no

###############################################################
## ADJUSTABLE PARAMETERS                                     ##
###############################################################

set pdbfilename     1enh_wb
set inputname       min1
set outputname      min1
structure           $pdbfilename.psf
coordinates         $pdbfilename.pdb
outputname          min/$outputname
restartName         res/$outputname.res

firsttimestep       0
numsteps            20000
```

```
#############################################################
## EXECUTION SCRIPT                                        ##
#############################################################

# Minimization with all protein fixed to allow solvent to relax
fixedAtoms          on
fixedAtomsFile      $pdbfilename\_fixprotein.pdb
fixedAtomsCol       B
output              min/$outputname
minimize            20000

puts [format "STATUS: Completed Minimization with protein fixed:
%s" ALL]
```

Minimization Phase 2

```
#############################################################
## MAIN MD CONFIGURATION DESCRIPTION                       ##
#############################################################

# Protein in a 10A water box TIP3P

set temperature   298

#############################################################
## SIMULATION PARAMETERS                                   ##
#############################################################

# Input
paraTypeCharmm      on
parameters          ./par_all27_prot_lipid.inp
temperature         $temperature

# Force-Field Parameters
exclude             scaled1-4
1-4scaling          1.0
cutoff              10.0
switching           on
switchdist          9.0
pairlistdist        14.0

# Integrator Parameters
timestep            2.0
rigidBonds          all
nonbondedFreq       1
fullElectFrequency  2
stepspercycle       10


# Constant Temperature Control
langevin            on
langevinDamping     5
langevinTemp        $temperature
langevinHydrogen    off

# Output
restartsave         yes
binaryrestart       yes
restartfreq         5000
dcdfreq             500
outputEnergies      100
outputPressure      100
```

```
outputMomenta       100
outputTiming        1000


#############################################################
## EXTRA PARAMETERS                                        ##
#############################################################
cellBasisVector1    47.0    0.0   0.0
cellBasisVector2     0.0   50.5   0.0
cellBasisVector3     0.0    0.0  47.8
cellOrigin           0.0    0.0   0.0

wrapAll               on
wrapNearest           on
PME                   yes
PMEGridSpacing        1
useGroupPressure      yes
useFlexibleCell       no
useConstantArea       no
langevinPiston        on
langevinPistonTarget  1.01325
langevinPistonPeriod  100.
langevinPistonDecay   50.
langevinPistonTemp    $temperature
binaryoutput          no



#############################################################
## ADJUSTABLE PARAMETERS                                   ##
#############################################################

set pdbfilename    1enh_wb
set inputname      min1
set outputname     min2
set outputname2    min3
structure          $pdbfilename.psf
coordinates        min/$inputname.coor
outputname         min/$outputname
restartName        res/$outputname.res

firsttimestep      0
numsteps           1000

#############################################################
## EXECUTION SCRIPT                                        ##
#############################################################
```

```
fixedAtomsForces yes
fixedAtoms       on
fixedAtomsfile   $pdbfilename\_fixbb.pdb
fixedAtomsCol    B
minimize         1000

puts [format "STATUS: Completed Minimization with protein fixed:
%s" BACKBONE]

# Minimization with nothing fixed and start to calculate forces
between all atoms
outputname     min/$outputname2
fixedAtoms     no
minimize       1000

puts [format "STATUS: Completed Minimization with protein fixed:
%s" NONE]
```

Heating

```
#############################################################
## MAIN MD CONFIGURATION DESCRIPTION                       ##
#############################################################

# Protein in a Truncated Octahedron TIP3P


set temperature     298

#############################################################
## SIMULATION PARAMETERS                                   ##
#############################################################

# Input
paraTypeCharmm      on
parameters          ./par_all27_prot_lipid.inp
temperature         $temperature


# Force-Field Parameters
exclude             scaled1-4
1-4scaling          1.0
cutoff              10.0
switching           on
switchdist          9.0
pairlistdist        14.0


# Integrator Parameters
timestep            2.0
rigidBonds          all
nonbondedFreq       1
fullElectFrequency  2
stepspercycle       10


# Constant Temperature Control
langevin            on
langevinDamping     5
langevinTemp        $temperature
langevinHydrogen    off


# Output saving frequencies
restartsave        yes
```

```
binaryrestart      yes
restartfreq        500
dcdfreq            500
outputEnergies     100
outputPressure     100
outputMomenta      100
outputTiming       1000


###################################################################
## EXTRA PARAMETERS                                              ##
###################################################################
cellBasisVector1    47.0    0.0   0.0
cellBasisVector2     0.0   50.5   0.0
cellBasisVector3     0.0    0.0  47.8
cellOrigin           0.0    0.0   0.0

wrapAll             on
wrapNearest         on

PME                 yes
PMEGridSpacing      1

useGroupPressure    yes
useFlexibleCell     no
useConstantArea     no

langevinPiston           on
langevinPistonTarget     1.01325
langevinPistonPeriod     100.
langevinPistonDecay      50.
langevinPistonTemp       $temperature
binaryoutput             no



###################################################################
## ADJUSTABLE PARAMETERS                                         ##
###################################################################

set pdbfilename    1enh_wb
set inputname      min3
set outputname     heat
set temperature    298

structure          $pdbfilename.psf
coordinates        min/$inputname.coor
outputName         heat/$outputname
```

```
restartName        res/$outputname.res

firsttimestep      0

#############################################################
## EXECUTION SCRIPT                                        ##
#############################################################
puts [format "STATUS: Heating with restraints gradually
decreased: %s" NONE]

reassignFreq        100
reassignTemp        0
reassignIncr        30
reassignHold        $temperature

#Harmonic restraints on protein backbone
constraints         on
consRef             $pdbfilename\_fixbb.pdb
consKFile           $pdbfilename\_fixbb.pdb
consKcol            B

set k_init 5.0
for {set i 0} {$i<=10} {incr i 1} {
set ck [expr {$k_init - $i*0.5}]
constraintScaling $ck
run 1000
}

puts [format "STATUS: Heating stage complete"]
```

Equilibration

```
#############################################################
## MAIN MD CONFIGURATION DESCRIPTION                       ##
#############################################################

# Protein in a 10A water box TIP3P


set temperature     298

#############################################################
## SIMULATION PARAMETERS                                   ##
#############################################################

# Input
paraTypeCharmm     on
parameters          ./par_all27_prot_lipid.inp

# Force-Field Parameters
exclude             scaled1-4
1-4scaling          1.0
cutoff              10.0
switching           on
switchdist          9.0
pairlistdist        14.0


# Integrator Parameters
timestep            2.0
rigidBonds          all
nonbondedFreq       1
fullElectFrequency  2
stepspercycle       10


# Constant Temperature Control
langevin            on
langevinDamping     5
langevinTemp        $temperature
langevinHydrogen    off


# Output saving frequencies
restartsave         yes
binaryrestart       yes
restartfreq         500
dcdfreq             500
```

```
outputEnergies      100
outputPressure      100
outputMomenta       100
outputTiming        1000
binaryoutput        no

#####################################################################
## EXTRA PARAMETERS                                                ##
#####################################################################
cellBasisVector1    47.0    0.0   0.0
cellBasisVector2     0.0   50.5   0.0
cellBasisVector3     0.0    0.0  47.8
cellOrigin           0.0    0.0   0.0

wrapAll              on
wrapNearest          on
PME                  yes
PMEGridSpacing       1
useGroupPressure     yes
useFlexibleCell      no
useConstantArea      no
langevinPiston       on
langevinPistonTarget 1.01325
langevinPistonPeriod 100.
langevinPistonDecay  50.
langevinPistonTemp   $temperature



#####################################################################
## ADJUSTABLE PARAMETERS                                           ##
#####################################################################

set pdbfilename    1enh_wb
set inputname      heat
set outputname     eqm

structure          $pdbfilename.psf
coordinates        heat/$inputname.coor
outputName         eqm/$outputname
restartName        res/$outputname.res
velocities         heat/$inputname.vel
extendedSystem     heat/$inputname.xsc

firsttimestep      0
```

```
#############################################################
## EXECUTION SCRIPT                                        ##
#############################################################
constraints off

run 100000
puts [format "STATUS: NPT equilibration stage complete"]
```

Production Dynamics

```
#############################################################
## MAIN MD CONFIGURATION DESCRIPTION                       ##
#############################################################
set temperature    298

#############################################################
## SIMULATION PARAMETERS                                   ##
#############################################################
# Input
paraTypeCharmm     on
parameters         ./par_all27_prot_lipid.inp


# Force-Field Parameters
exclude              scaled1-4
1-4scaling           1.0
cutoff               10.0
switching            on
switchdist           9.0
pairlistdist         14.0


# Integrator Parameters
timestep             2.0
rigidBonds           all
nonbondedFreq        1
fullElectFrequency   2
stepspercycle        10


# Constant Temperature Control
langevin             on
langevinDamping      5
langevinTemp         $temperature
langevinHydrogen     off


# Output saving frequencies
restartsave        yes
binaryrestart      yes
restartfreq        500
dcdfreq            500
outputEnergies     100
outputPressure     100
outputMomenta      100
outputTiming       1000
```

```
#############################################################
## EXTRA PARAMETERS                                        ##
#############################################################
cellBasisVector1    47.0    0.0   0.0
cellBasisVector2     0.0   50.5   0.0
cellBasisVector3     0.0    0.0  47.8
cellOrigin           0.0    0.0   0.0

wrapAll             on
wrapNearest         on
PME                 yes
PMEGridSpacing      1
useGroupPressure    yes
useFlexibleCell     no
useConstantArea     no
binaryoutput        yes


#############################################################
## ADJUSTABLE PARAMETERS                                   ##
#############################################################

set pdbfilename     1enh_wb
set inputname       eqm
set outputname      prod


structure           $pdbfilename.psf
coordinates         eqm/$inputname.coor
velocities          eqm/$inputname.vel
extendedSystem      eqm/$inputname.xsc
outputName          prod/$outputname\_0
restartName         res/$outputname.res

firsttimestep       0

#############################################################
## EXECUTION SCRIPT                                        ##
#############################################################

constraints off
run 500000
```