```
#############################################################
## ADJUSTABLE PARAMETERS                                   ##
#############################################################

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


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

# 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


#############################################################
## EXTRA PARAMETERS                                        ##
#############################################################
```

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

# 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 10^2 fs
```