```
; VARIOUS PREPROCESSING OPTIONS =
title                    = heating to body temperature

; Leap-frog integrator stuff
integrator               = md
tinit                    = 0.0
dt                       = 0.002
nsteps                   = 200000

; number of steps for center of mass motion removal =
comm_mode                = Linear
nstcomm                  = 10
comm_grps                = System

; Output frequency for coords (x), velocities (v) and forces (f) =
nstxout                  = 500
nstvout                  = 1000
nstfout                  = 0
; Output frequency for energies to log file and energy file =
nstlog                   = 500
nstenergy                = 500

; NEIGHBORSEARCHING PARAMETERS =
nstlist                  = 10
nstcalcenergy            = 10
rlist                    = 1.2
ns_type                  = grid

; Periodic boundary conditions: xyz or none =
pbc                      = xyz
cutoff-scheme            = verlet


; Method for doing electrostatics =
coulombtype              = PME
rcoulomb                 = 1.2
rcoulomb_switch          = 1.0
fourierspacing           = 0.12
pme_order                = 4
optimize_fft             = yes

; Method for doing Van der Waals =
vdwtype                  = Cut-off
vdw_modifier             = Force-switch
rvdw                     = 1.2
rvdw_switch              = 1.0
DispCorr                 = no

; Temperature coupling
tcoupl                   = V-rescale
tc_grps                  = NA CL SOL MEM Protein
tau_t                    = 0.1 0.1 0.1 0.1 0.1
ref_t                    = 310 310 310 310 310
```

```
; Pressure coupling
pcoupl                  = no

; GENERATE VELOCITIES FOR STARTUP RUN =
gen_vel                 = yes
gen_temp                = 2
gen_seed                = 473529


; ANNEALING PROTOCOL
annealing               = single single single single single
annealing_npoints       = 2 2 2 2 2
annealing_time          = 0 310 0 310 0 310 0 310 0 310
annealing_temp          = 2 310 2 310 2 310 2 310 2 310

; OPTIONS FOR BONDS     =
constraints             = hbonds

; Type of constraint algorithm =
constraint_algorithm    = lincs

; Highest order in the expansion of the constraint coupling matrix =
lincs_order             = 4
lincs_iter              = 4

; Lincs will write a warning to the stderr if in one step a bond =
lincs_warnangle         = 30
```