```
title                    = bilayer from 162 DPPC
define                   =

; RUN CONTROL PARAMETERS
integrator               = md ; Leap-frog integrator

; start time and timestep in ps
tinit                    = 0.0
dt                       = 0.002
nsteps                   = 150000

; number of steps for center of mass motion removal
comm_mode                = Linear
nstcomm                  = 1
comm_grps                = System

; OUTPUT CONTROL OPTIONS =
; 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

; Output frequency and precision for xtc file
;nstxtcout               = 500
xtc_precision            = 50

; NEIGHBORSEARCHING PARAMETERS
nstlist                  = 10

; ns algorithm (simple or grid)
ns_type                  = grid

; Periodic boundary conditions: xyz or none
pbc                      = xyz
rlist                    = 1.2

; 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                  = Switch
rvdw                     = 1.2   ; cut-off lengths
rvdw_switch              = 1.0

; Apply long range dispersion corrections for Energy and Pressure
```

```
DispCorr                 = no

; Temperature coupling
tcoupl                   = V-rescale
tc_grps                  = SURF SOL Cal NA CL
tau_t                    = 0.1 0.1 0.1 0.1 0.1 ; Time constant (ps)
ref_t                    = 298 298 298 298 298  ; reference temperature
(K)


; 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           = 0 300 0 300 0 300 0 300 0 300
annealing_temp           = 2 298 2 298 2 298 2 298 2 298

; 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
; rotates over more degrees than
lincs_warnangle          = 30

cutoff-scheme          = verlet
```