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title                = production phase of a biosimulation

integrator           = md ; Leap-frog integrator
tinit                = 0.0
dt                   = 0.002
nsteps               = 25000000

; 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              = 5000
nstvout              = 10000
nstfout              = 0
; Output frequency for energies to log file and energy file
nstlog               = 5000
nstenergy            = 500

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

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

; 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

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; Pressure coupling
pcoupl          = Berendsen
pcoupltype     = surface-tension
tau_p          = 1.0
ref_p          = 220 1.0
compressibility = 4.5e-05 4.5e-5

; GENERATE VELOCITIES FOR STARTUP RUN
gen_vel        = no

; 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
```