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#####
## ADJUSTABLE PARAMETERS ##
#####
structure      stmv.psf
coordinates    stmv.pdb

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

# Input
paraTypeCharmm      on
parameters          par_all127_prot_na.inp
temperature         298

# Force-Field Parameters
exclude            scaled1-4
1-4scaling        1.0
cutoff            12.
switching         on
switchdist       10.
pairlistdist     13.5

# Integrator Parameters
timestep          1.0
nonbondedFreq    1
fullElectFrequency 4
stepspercycle    20

# Constant Temperature Control
langevin          on      ;# do langevin dynamics
langevinDamping  5       ;# damping coefficient (gamma) of 5/ps
langevinTemp     298
langevinHydrogen off    ;# don't couple langevin bath to hydrogens

# Constant Pressure Control (variable volume)
useGroupPressure  yes ;# needed for rigidBonds
useFlexibleCell   no
useConstantArea   no

langevinPiston    on
langevinPistonTarget 1.01325 ;# in bar -> 1 atm
langevinPistonPeriod 100.
langevinPistonDecay 50.
langevinPistonTemp 298

cellBasisVector1  216.832  0.  0.
cellBasisVector2  0.  216.832  0.
cellBasisVector3  0.  0  216.832
cellOrigin        0.  0.  0.

PME               on
PMEGridSizeX     216
PMEGridSizeY     216
PMEGridSizeZ     216

# Output
outputName       /usr/tmp/stmv-output

```

outputEnergies	20
outputTiming	20
numsteps	500