```
title = energy minimization of the environment with positional restraints
on the biomolecule
define = -DFLEXIBLE -DPOSRES

; Leap-frog integrator stuff
integrator = steep

emtol = 500
emstep = 0.01

tinit = 0
dt = 0.002
nsteps = 250000

; Nonbonded interactions calculation parameters
pbc = xyz

cutoff-scheme = verlet
coulombtype = PME

rcoulomb = 1.2
rcoulomb_switch = 1.0
fourierspacing = 0.12

pme_order = 4
optimize_fft = yes

vdwtype = Cut-off
vdw_modifier = Force-switch

rvdw = 1.2
rvdw_switch = 1.0

DispCorr = no

; Neighbourlist searching algorithms
nstlist = 10
rlist = 1.2
ns_type = grid

; Output parameters
nstxout = 10
nstlog = 10 ;5000
nstenergy = 10

; Temperature and pressure coupling
gen_vel = no
tcoupl = no
pcoupl = no
annealing = no

; Constraints parameters
constraints = none
```