

```
title =minimizaciq
define = -DFLEXIBLE
cpp = /usr/bin/cpp
; Leap-frog integrator stuff
integrator = l-bfgs
nstcgsteep = 20
emtol = 50
emstep = 0.25
tinit = 0
dt = 0.002
nsteps = 150000
comm_mode = Linear
nstcomm = 1
comm_grps = System
; Nonbonded interactions calculation parameters
pbc = xyz
coulombtype = PME
rcoulomb = 1.2
rcoulomb_switch = 1.0
fourierspacing = 0.12
pme_order = 4
optimize_fft = yes
vdwtype = 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
nstvout = 1000
nstlog = 1
nstenergy = 1
; Temperature and pressure coupling
gen_vel = no
tcoupl = no
pcoupl = no
annealing = no
; Constraints parameters
constraints = none
constraint_algorithm = lincs
lincs_order = 4
lincs_iter = 4
```