MD SIMULATIONS

GROMACS TOOL

pdb2gmx

-f [<.gro/.g96/…>] (protein.pdb)
Structure file: gro g96 pdb brk ent esp tpr

Options to specify output files:

-o [<.gro/.g96/…>] (conf.gro)
Structure file: gro g96 pdb brk ent esp

-p [<.top>] (topol.top)
Topology file

-i [<.itp>] (posre.itp)
Include file for topology

-n [<.ndx>] (index.ndx) (Optional)
Index file

-q [<.gro/.g96/…>] (clean.pdb) (Optional)
Structure file: gro g96 pdb brk ent esp

gmx editconf

-f [<.gro/.g96/…>] (conf.gro)
Structure file: gro g96 pdb brk ent esp tpr

-n [<.ndx>] (index.ndx) (Optional)
Index file

-bf [<.dat>] (bfact.dat) (Optional)
Generic data file

Options to specify output files:

-o [<.gro/.g96/…>] (out.gro) (Optional)
Structure file: gro g96 pdb brk ent esp

-mead [<.pqr>] (mead.pqr) (Optional)
Coordinate file for MEAD

-bt <enum> (triclinic)
Box type for -box and -d: triclinic, cubic, dodecahedron, octahedron

-box <vector> (0 0 0)
Box vector lengths (a,b,c)

-angles <vector> (90 90 90)
Angles between the box vectors (bc,ac,ab)

-d <real> (0)
Distance between the solute and the box

-[no]c (no)
Center molecule in box (implied by -box and -d)

gmx solvate

-cp [<.gro/.g96/…>] (protein.gro) (Optional)
Structure file: gro g96 pdb brk ent esp tpr

-cs [<.gro/.g96/…>] (spc216.gro) (Library)
Structure file: gro g96 pdb brk ent esp tpr

Options to specify input/output files:

-p [<.top>] (topol.top) (Optional)
Topology file

Options to specify output files:

-o [<.gro/.g96/…>] (out.gro)
Structure file: gro g96 pdb brk ent esp

gmx grompp

-f [<.mdp>] (grompp.mdp)
grompp input file with MD parameters

-c [<.gro/.g96/…>] (conf.gro)
Structure file: gro g96 pdb brk ent esp tpr

-p [<.top>] (topol.top)
Topology file

Options to specify output files:

-o [<.tpr>] (topol.tpr)
Portable xdr run input file

gmx mdrun

-s [<.tpr>] (topol.tpr)
Portable xdr run input file

Options to specify output files:

-o [<.trr/.cpt/…>] (traj.trr)
Full precision trajectory: trr cpt tng

-x [<.xtc/.tng>] (traj_comp.xtc) (Optional)
Compressed trajectory (tng format or portable xdr format)

-c [<.gro/.g96/…>] (confout.gro)
Structure file: gro g96 pdb brk ent esp

-e [<.edr>] (ener.edr)
Energy file

-g [<.log>] (md.log)

Energy Minimization MD Paramater files

```
integrator  = steep
emtol       = 1000.0
emstep      = 0.001
nsteps      = 500
nstlist         = 1
cutoff-scheme           = Verlet
ns_type         = grid
rlist                   = 1.2
coulombtype             = PME
rcoulomb= 1.2
vdwtype         = cutoff
vdw-modifier    = force-switch
rvdw-switch     = 1.0
rvdw                    = 1.2
pbc             = xyz
DispCorr        = no
```

```
integrator              = md        ; leap-frog integrator
nsteps                  = 50000
dt                      = 0.002     ; 2 fs
; Output control
nstenergy               = 500       ; save energies every 10.0 ps
nstlog                  = 500       ; update log file every 10.0 ps
nstxout-compressed      = 500       ; save coordinates every 10.0
ps
; Bond parameters
continuation            = yes       ; continuing from NPT
constraint_algorithm    = lincs     ; holonomic constraints
constraints             = all-bonds ; Convert all bonds to constraints
lincs_iter              = 1         ; accuracy of LINCS
lincs_order             = 4         ; also related to accuracy
```

```
; Electrostatics
coulombtype             = PME      ; Particle Mesh Ewald for long-
range electrostatics
rcoulomb                = 1.2
pme_order               = 4        ; cubic interpolation
fourierspacing          = 0.16     ; grid spacing for FFT
; Temperature coupling
tcoupl                  = V-rescale                ; modified Berendsen
thermostat
tc-grps                 = Protein Non-Protein    ; two coupling groups -
more accurate
tau_t                   = 0.1   0.1                ; time constant, in ps
ref_t                   = 300   300                ; reference temperature,
one for each group, in K
```

```
; Pressure coupling
pcoupl              = Parrinello-Rahman          ; pressure coupling
is on for NPT
pcoupltype          = isotropic                  ; uniform scaling of
box vectors
tau_p               = 2.0                        ; time constant, in ps
ref_p               = 1.0                        ; reference pressure, in bar
compressibility     = 4.5e-5                     ; isothermal
compressibility of water, bar^-1
; Periodic boundary conditions
pbc                 = xyz       ; 3-D PBC
DispCorr            = EnerPres  ; account for cut-off vdW scheme
; Velocity generation
gen_vel             = no        ; continuing from NPT equilibration
```