---
ions.mdp

```
; ions.mdp - used as input into grompp to generate ions.tpr
; Parameters describing what to do, when to stop and what to save
integrator  = steep         ; Algorithm (steep = steepest descent minimization)
emtol       = 1000.0        ; Stop minimization when the maximum force < 1000.0 kJ/mol/nm
emstep      = 0.01          ; Minimization step size
nsteps      = 5000000       ; Maximum number of (minimization) steps to perform

; Parameters describing how to find the neighbors of each atom and how to calculate the interactions only for CHAR
MM27
constraints = h-bonds
cutoff-scheme = Verlet
vdwtype = cutoff
vdw-modifier = force-switch
rlist = 1.2
rvdw = 1.2
rvdw-switch = 1.0
coulombtype = PME
rcoulomb = 1.2
DispCorr = no
```

___md.mdp_____

```
title                = CHARMM36 RNA MD
; Run parameters
integrator           = md       ; leap-frog integrator
nsteps               = 1000000000    ; 0.002 * 500000000 = 10^6 ps (1 us)
dt                   = 0.001   ; 0.002 ps
; Output control
nstxout              = 0        ; suppress bulky .trr file by specifying
nstvout              = 0        ; 0 for output frequency of nstxout,
nstfout              = 0        ; nstvout, and nstfout
nstenergy            = 50000      ; save energies every 10.0 ps
nstlog               = 50000      ; update log file every 10.0 ps
nstxout-compressed   = 50000      ; save compressed coordinates every 10.0 ps
compressed-x-grps    = System    ; save the whole system
; Bond parameters
continuation         = yes       ; Restarting after NPT
constraint_algorithm = lincs     ; holonomic constraints
constraints          = h-bonds   ; bonds involving H are constrained
lincs_iter           = 1         ; accuracy of LINCS
lincs_order          = 4         ; also related to accuracy
; Neighborsearching
cutoff-scheme        = Verlet    ; Buffered neighbor searching
ns_type              = grid      ; search neighboring grid cells
nstlist              = 10        ; 20 fs, largely irrelevant with Verlet scheme
rcoulomb             = 1.2       ; short-range electrostatic cutoff (in nm)
rvdw                 = 1.2       ; short-range van der Waals cutoff (in nm)
; Electrostatics
coulombtype          = PME       ; Particle Mesh Ewald for long-range electrostatics
pme_order            = 4         ; cubic interpolation
fourierspacing       = 0.16      ; grid spacing for FFT
```

```
; Temperature coupling is on
tcoupl               = V-rescale            ; modified Berendsen thermostat
tc-grps              = RNA SOD_SOL   ; 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 is on
pcoupl               = Parrinello-Rahman     ; Pressure coupling on in 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
; Dispersion correction
DispCorr             = no  ; account for cut-off vdW scheme
; Velocity generation
gen_vel              = no       ; Velocity generation is off
; Simulated Annealing
; Type of annealing for each temperature group (no/single/periodic) annealing
;annealing   = single single
; Number of time points to use for specifying annealing in each group
;annealing_npoints = 7 7
; List of times at the annealing points for each group
;annealing_time = 0 50 100 150 200 250 300 0 50 100 150 200 250 300
; Temp at each annealing point, for each group
;annealing_temp = 273 278 282 287 292 297 300 273 278 282 287 292 297 300
```

---

minim.mdp

```
; ions.mdp - used as input into grompp to generate ions.tpr
; Parameters describing what to do, when to stop and what to save
integrator  = steep         ; Algorithm (steep = steepest descent minimization)
emtol       = 100.0        ; Stop minimization when the maximum force < 1000.0 kJ/mol/nm
emstep      = 0.001          ; Minimization step size
nsteps      = 50000        ; Maximum number of (minimization) steps to perform


; Parameters describing how to find the neighbors of each atom and how to calculate the interactions only for CHAR
MM27
;nstlist = 10
;cutoff-scheme = Verlet
;ns_type = grid
;coulombtype = PME
;rcoulomb = 1.2
;rvdw = 1.2
;pbc = xyz
;define = -DFLEXIBLE


;constraints = h-bonds
cutoff-scheme = Verlet
vdwtype = cutoff
```

```
vdw-modifier = force-switch
;rlist = 1.0
rvdw = 1.2
rvdw-switch = 1.0
coulombtype = PME
rcoulomb = 1.2
DispCorr = no
;define = -DFLEXIBLE


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npt.mdp
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title                = CHARMM RNA NPT equilibration
define               = -DPOSRES  ; position restrain the rna
; Run parameters
integrator           = md        ; leap-frog integrator
nsteps               = 500000    ; 2 * 50000 = 100 ps
dt                   = 0.001     ; 2 fs
; Output control
nstxout              = 500       ; save coordinates every 1.0 ps
nstvout              = 500       ; save velocities every 1.0 ps
nstenergy            = 500       ; save energies every 1.0 ps
nstlog               = 500       ; update log file every 1.0 ps
; Bond parameters
continuation         = yes     ; after NVT
constraint_algorithm    = lincs     ; holonomic constraints
constraints          = h-bonds   ; bonds involving H are constrained
lincs_iter           = 1         ; accuracy of LINCS
lincs_order          = 4         ; also related to accuracy
; Nonbonded settings
cutoff-scheme        = Verlet    ; Buffered neighbor searching
ns_type              = grid      ; search neighboring grid cells
nstlist              = 10        ; 20 fs, largely irrelevant with Verlet
rcoulomb             = 1.2       ; short-range electrostatic cutoff (in nm)
rvdw                 = 1.2       ; short-range van der Waals cutoff (in nm)
DispCorr             = no  ; account for cut-off vdW scheme ; Note that dispersion correction should be applied in the
case of lipid monolayers, but not bilayers.
; Electrostatics
coulombtype          = PME       ; Particle Mesh Ewald for long-range electrostatics
pme_order            = 4         ; cubic interpolation
fourierspacing       = 0.16      ; grid spacing for FFT
; Temperature coupling is on
tcoupl               = V-rescale             ; modified Berendsen thermostat
tc-grps              = RNA SOD_SOL   ; 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 is on
pcoupl               = Berendsen     ; Pressure coupling on in 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
refcoord_scaling     = com
```

```
; Periodic boundary conditions
pbc                 = xyz       ; 3-D PBC
; Velocity generation
gen_vel             = no        ; velocity generation is off;
```

---

nvt.mdp

```
title               = CHARMM PROTEIN NVT equilibration
define              = -DPOSRES  ; position restrain the rna
; Run parameters
integrator          = md        ; leap-frog integrator
nsteps              = 500000    ; 0.2 * 50000 = 10 ps
dt                  = 0.001     ;0. 2 fs
; Output control
nstxout             = 500       ; save coordinates every 1.0 ps
nstvout             = 500       ; save velocities every 1.0 ps
nstenergy           = 500       ; save energies every 1.0 ps
nstlog              = 500       ; update log file every 1.0 ps
; Bond parameters
continuation        = no        ; first dynamics run
constraint_algorithm    = lincs     ; holonomic constraints
constraints         = h-bonds   ; bonds involving H are constrained
lincs_iter          = 1         ; accuracy of LINCS
lincs_order         = 4         ; also related to accuracy
; Nonbonded settings
cutoff-scheme       = Verlet    ; Buffered neighbor searching
ns_type             = grid      ; search neighboring grid cells
nstlist             = 10        ; 20 fs, largely irrelevant with Verlet
rcoulomb            = 1.2       ; short-range electrostatic cutoff (in nm)
rvdw                = 1.2       ; short-range van der Waals cutoff (in nm)
DispCorr            = no  ; account for cut-off vdW scheme
; Electrostatics
coulombtype         = PME       ; Particle Mesh Ewald for long-range electrostatics
pme_order           = 4         ; cubic interpolation
fourierspacing      = 0.16      ; grid spacing for FFT
; Temperature coupling is on
tcoupl              = V-rescale             ; modified Berendsen thermostat
tc-grps             = RNA SOD_SOL   ; 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 is off
pcoupl              = no        ; no pressure coupling in NVT
; Periodic boundary conditions
pbc                 = xyz       ; 3-D PBC
; Velocity generation
gen_vel             = yes       ; assign velocities from Maxwell distribution
gen_temp            = 300       ; temperature for Maxwell distribution
gen_seed            = -1        ; generate a random seed
```

---

sa.mdp

```
----------------
title       = gromacs
;define       = -DPOSRES    ; position restrain the protein
nstcomm       = 1
comm-mode    = Linear; Run parameters
integrator    = md       ; leap-frog integrator
nsteps       = 300000       ; 2 * 50000 = 100 ps
dt       = 0.001       ; 2 fs
; Output control
nstxout       = 1000       ; save coordinates every 0.2 ps
nstvout       = 1000       ; save velocities every 0.2 ps
nstenergy    = 1000       ; save energies every 0.2 ps
nstlog       = 1000       ; update log file every 0.2 ps
; Bond parameters
continuation    = yes       ; Restarting after NVT
constraint_algorithm = lincs    ; holonomic constraints
constraints    = h-bonds    ; all bonds (even heavy atom-H bonds) constrained
lincs_iter    = 1       ; accuracy of LINCS
lincs_order    = 4       ; also related to accuracy
; Neighborsearching
ns_type       = grid       ; search neighboring grid cells
nstlist       = 5       ; 10 fs
rlist       = 0.9       ; short-range neighborlist cutoff (in nm)
rcoulomb    = 1.2       ; short-range electrostatic cutoff (in nm)
vdw-type       = Cut-off
rvdw       = 1.2       ; short-range van der Waals cutoff (in nm)
; Electrostatics
coulombtype    = PME       ; Particle Mesh Ewald for long-range electrostatics
pme_order    = 4       ; cubic interpolation
fourierspacing    = 0.16       ; grid spacing for FFT
; Temperature coupling is on
tcoupl       = V-rescale    ; modified Berendsen thermostat
tc-grps       = RNA SOD_SOL    ; 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 is on
pcoupl       = Parrinello-Rahman    ; Pressure coupling on in 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
; Dispersion correction
DispCorr    = EnerPres    ; account for cut-off vdW scheme
; Velocity generation
gen_vel       = no       ; Velocity generation is off
; Simulated annealing
annealing             = single single
annealing_npoints       =  8  8
annealing_time         =  0  45 85 125 165 205 245 300 0 45 85 125 165 205 245 300
annealing_temp         = 273 280 287 293 300 310 307 300 273 280 287 293 300 310 307 300
```