Computational Physics

Molecular Simulations Lab

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EXPERIMENT 1: Lysozyme in Water

PROCEDURE:

Commands

VMD TkConsole [removing the crystal waters]

```
set sel [atomselect top all]

set sel1 [atomselect top protein]

set sel2[atomselect top water]

$sel1 writepdb protein.pdb

$sel2 writepdb water.pdb
```

1XEI.pdb

1XEI_clean.pdb

Generate Topology

generate a topology file for the (15: OPLS-AA/L all-atom force field (2001 aminoacid dihedrals) force field together with the SPC/E water model using the gmx pdb2gmx tool:

gmx pdb2gmx -f 1xei_clean.pdb -o 1AKI_processed.gro -water spce

1AKI_processed.gro is a GROMACS-formatted structure file that contains all the atoms defined

within the force field

Box and solvate [Adding Water]

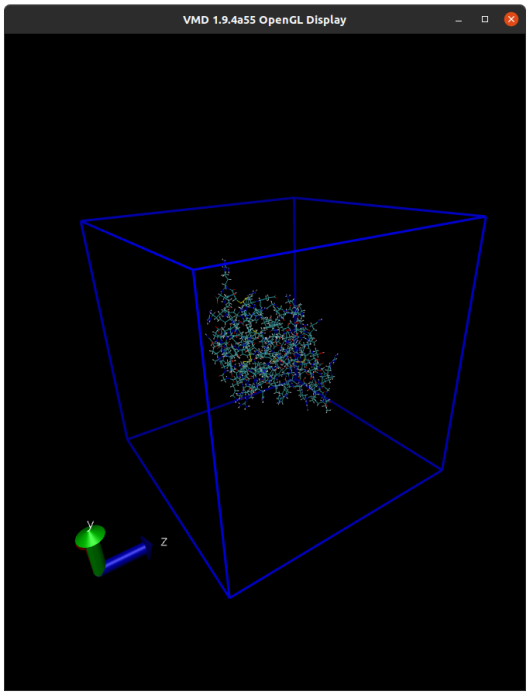
Create a simulation box with gmx editconf and add solvent with gmx solvate

gmx editconf -f 1xei_processed.gro -o 1xei_newbox.gro -c -d 1.0 -bt cubic

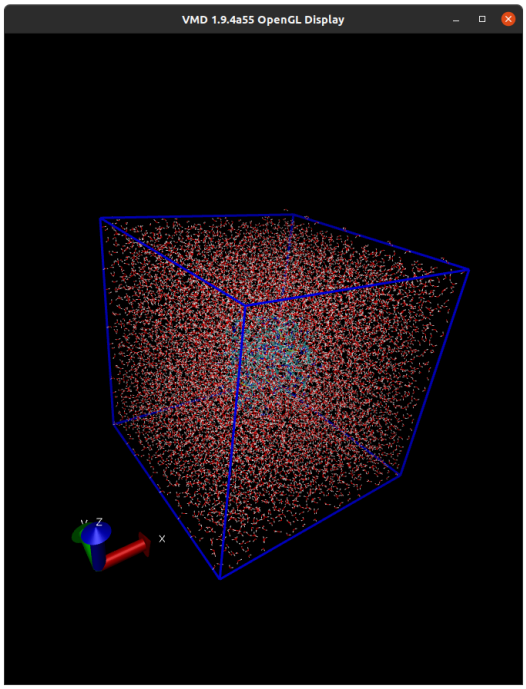
minimum protein-edge distance 1.0 nm, `-d 1.0`); for simulations you want to publish this number should be 1.2…1.5 nm so that the electrostatic interactions between copies of the protein across periodic boundaries are sufficiently screened.

gmx solvate -cp 1xei_newbox.gro -cs spc216.gro -o 1xei_solv.gro -p topol.top

- **-cp input file (protein with box)**
- **-cs water box model**
- **-p topology**
- **-o output file (protein the box and the solvent)**



1xei_newbox.gro



1xei_solv_ions.gro

Adding ions

Ions can be added with the gmx genion

gmx grompp -f ions.mdp -c 1xei_solv.gro -p topol.top -o ions.tpr

gmx genion -s ions.tpr -o 1xei_solv_ions.gro -p topol.top -pname NA -nname CL -neutral

-s Topology Portable Run file

-o Output file, it will be called

-p New topology file

```
; 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      = 50000         ; Maximum number of (minimization) steps to perform
```

Energy Minimization

Before we can begin dynamics, we must ensure that the system has no steric clashes or inappropriate geometry. harmonic force constants of 1000 kJ mol^{-1} nm^{-2}

use the simple *steepest descent* minimizer `integrator = steep` in `minim.mdp`

`The *.mdp file contains the settings that dictate the nature of the simulation.`

gmx grompp -f minim.mdp -c 1AKI_solv_ions.gro -p topol.top -o em.tpr

gmx mdrun -v -deffnm em

; minim.mdp - used as input into grompp to generate em.tpr

; Parameters describing what to do, when to stop and what to save

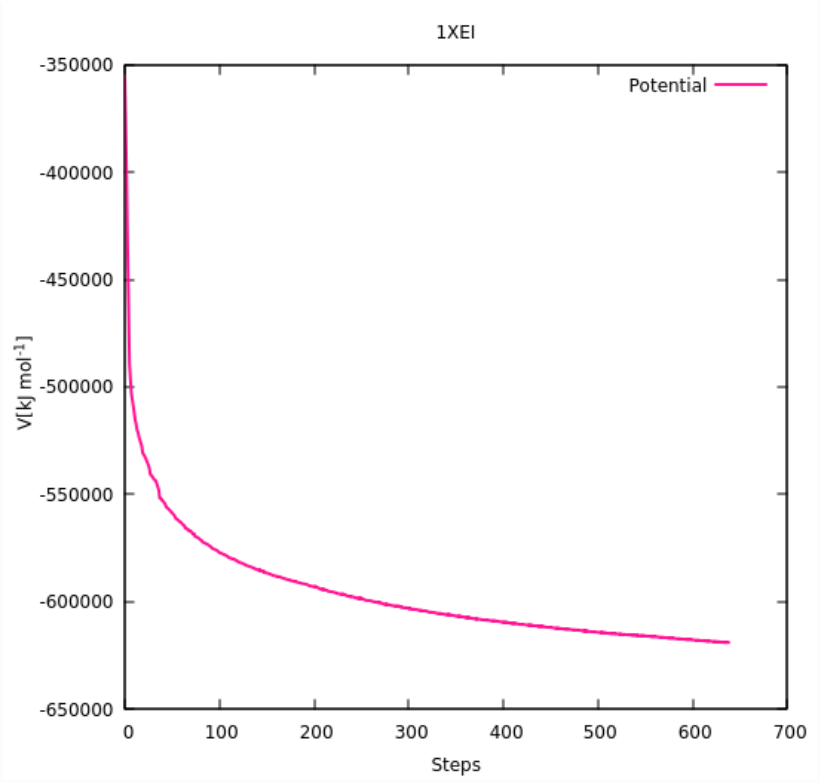
integrator = steep ; Algorithm (steep = steepest descent minimization)

emtol = 1000.0 ; Stop minimization when the maximum force < 1000.0 kJ/mol/nm

emstep = 0.01 ; Minimization step size

nsteps = 50000 ; Maximum number of (minimization) steps to perform

run input file (TPR) from the run parameter file (MDP), coordinate file (the solvated system with ions; PDB), and the topology (TOP)



Equilibration

The purpose of posre.itp is to apply a position restraining force on the heavy atoms of the protein (anything that is not a hydrogen).

NVT

This will help the added water molecules find a stable (equilibrium) distribution around the protein.

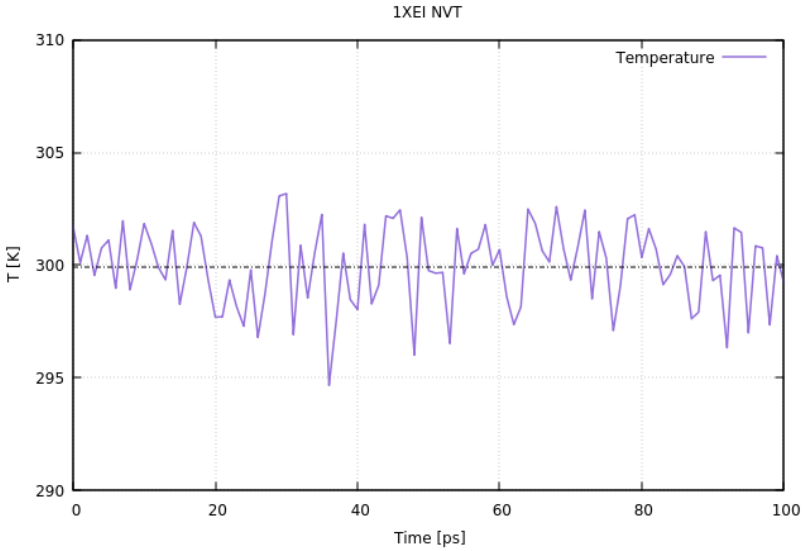
gmx grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -o nvt.tpr

gmx mdrun -deffnm nvt

Temperature

gmx energy -f nvt.edr -o temperature.xvg

$T = 299.937 \pm 1.776\ [K]$



NPT

This will adjust the box size, ensuring that the density of water in the periodic box is correct for the simulation temperature and pressure.

gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr

gmx mdrun -deffnm npt

title = OPLS Lysozyme NPT equilibration

define = -DPOSRES ; position restrain the protein

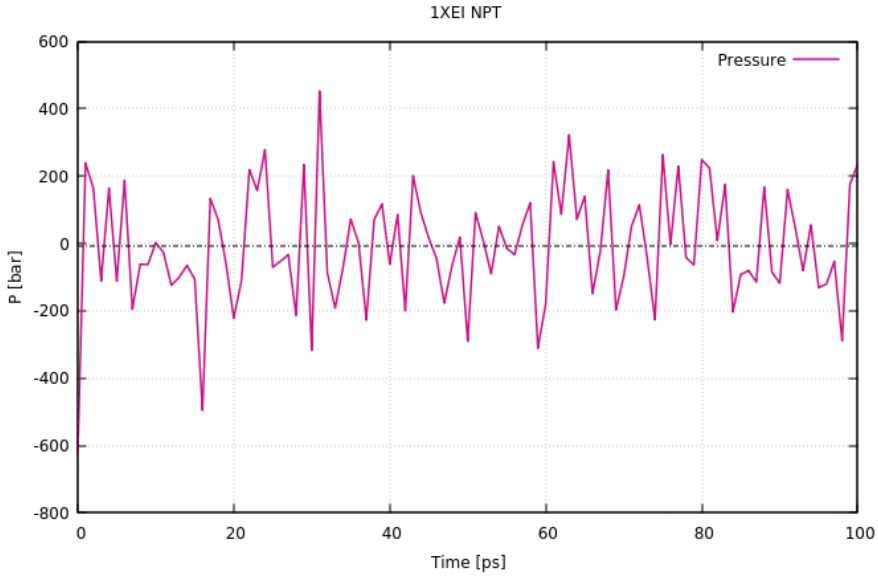
; Run parameters

integrator = md ; leap-frog integrator

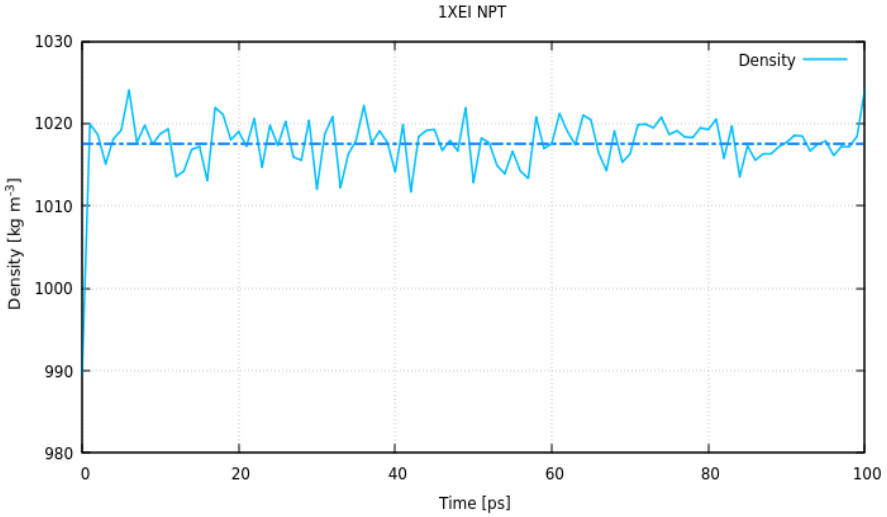
*nsteps = 50000 ; 2 * 50000 = 100 ps*

dt = 0.002 ; 2 fs

gmx energy -f npt.edr -o pressure.xvg $P = -8.8621 \pm 174.157\ [bar]$



gmx energy -f npt.edr -o density.xvg $\rho = 1017.490 \pm 3.754\ [kgm^{-3}]$



MD run

The final step is the actual molecular dynamics simulation.Upon completion of the two equilibration phases, the system is now well-equilibrated at the desired temperature and pressure.

gmx grompp -f md.mdp -c npt.gro -t npt.cpt -p topol.top -o md_0_1.tpr

gmx mdrun -deffnm md_0_1

title = OPLS Lysozyme NPT equilibration

; Run parameters

integrator = md ; leap-frog integrator

*nsteps = 500000 ; 2 * 500000 = 1000 ps (1 ns)*

dt = 0.002 ; 2 fs

ANALYSIS

Generate a centered trajectory in the primary unit cell

gmx trjconv -s md_0_1.tpr -f md_0_1.xtc -o md_0_1_noPBC.xtc -pbc mol -center

Select 1 ("Protein") as the group to be centered and 0 ("System") for output.

RMSD

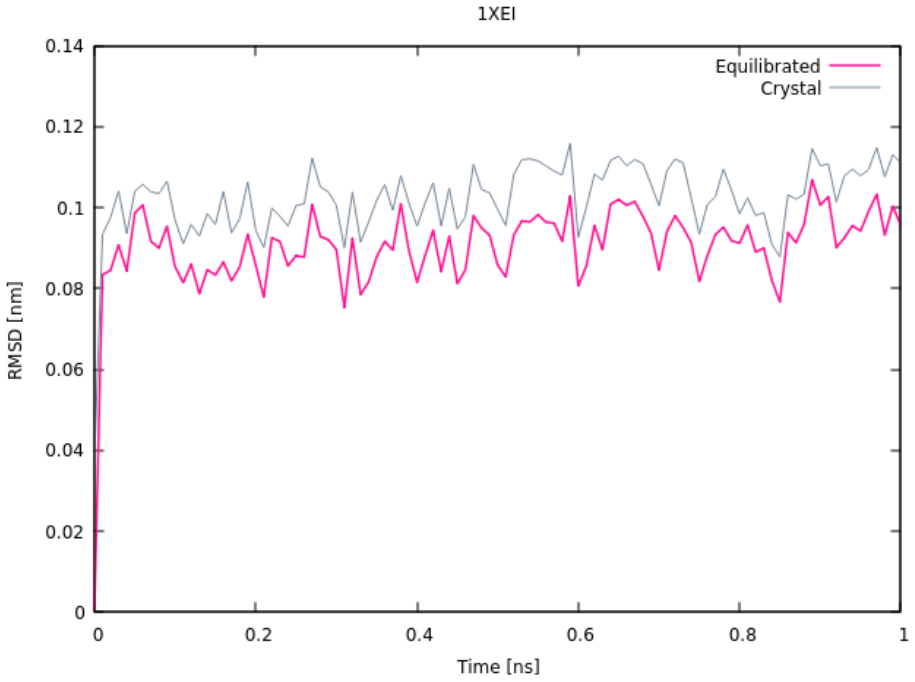
gmx rms -s md_0_1.tpr -f md_0_1_noPBC.xtc -o rmsd.xvg -tu ns

Select 4 ("Backbone") as the group to be centered and 4 ("Backbone") for output.

RMSD relative to the crystal structure

gmx rms -s em.tpr -f md_0_1_noPBC.xtc -o rmsd_xtal.xvg -tu ns

$$\rho^{\mathrm{RMSD}}(t) = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\mathbf{r}_i(t) - \mathbf{r}_i^{\mathrm{ref}}\right)^2}$$



$$\rho^{RMSD} = 0.0902 \pm 0.011\ [nm]$$

Radius of Gyration

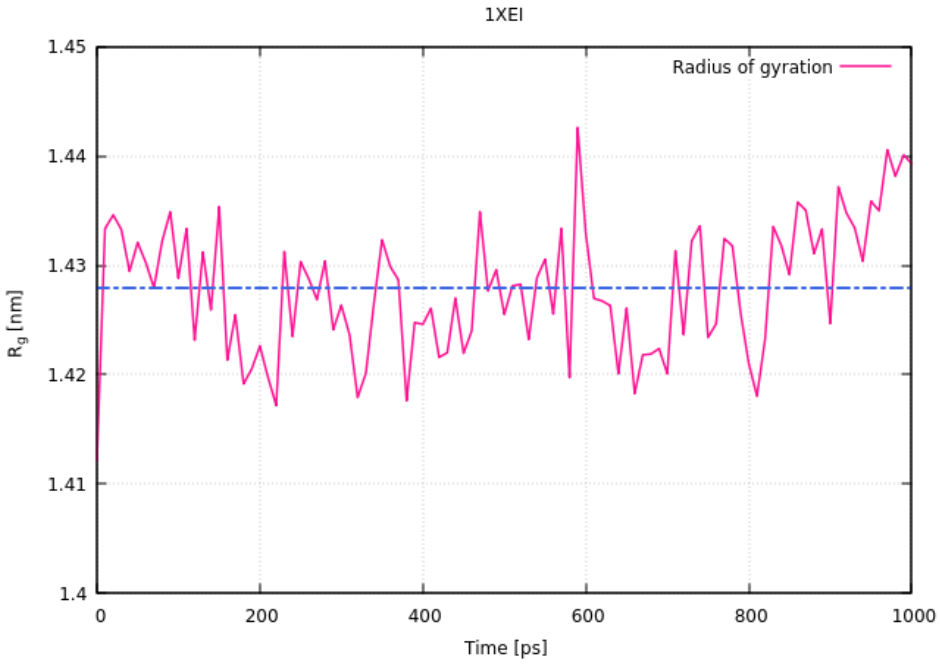
gmx gyrate -s md_0_1.tpr -f md_0_1_noPBC.xtc -o gyrate.xvg

group 1 (Protein) for analysis

$$R^2_{\mathrm{gyr}} = \frac{1}{M}\sum_{i=1}^{N} m_i(\mathbf{r}_i - \mathbf{R})^2 \qquad \text{where} \qquad \mathbf{R} = N^{-1}\sum_{i=1}^{N}\mathbf{r}_i$$

is the center of mass of the protein

$$R_g = 1.4279 \pm 0.006\ [nm]$$



EXPERIMENT 2 : Biphasic System **15 Nov 2022**

PROCEDURE:

chx.gro Cyclohexane coordinate file chx.top Cyclohexane topology file

```
PRODRG COORDS
    6
    1CHX  CAA      1  -0.086   0.815  -0.018
    1CHX  CAB      2   0.009   0.913   0.051
    1CHX  CAD      3  -0.066   1.039   0.094
    1CHX  CAF      4  -0.181   1.002   0.188
    1CHX  CAE      5  -0.277   0.905   0.120
    1CHX  CAC      6  -0.201   0.779   0.076
  0.43600   0.43600   0.43600
```

Commands

gmx insert-molecules -ci chx.gro -nmol 1200 -box 5 5 5 -o chx_box.gro

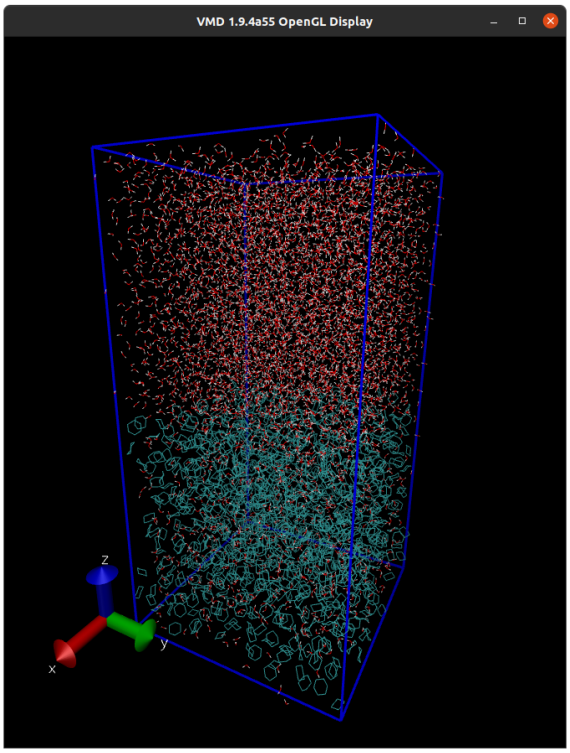
Expand the box:

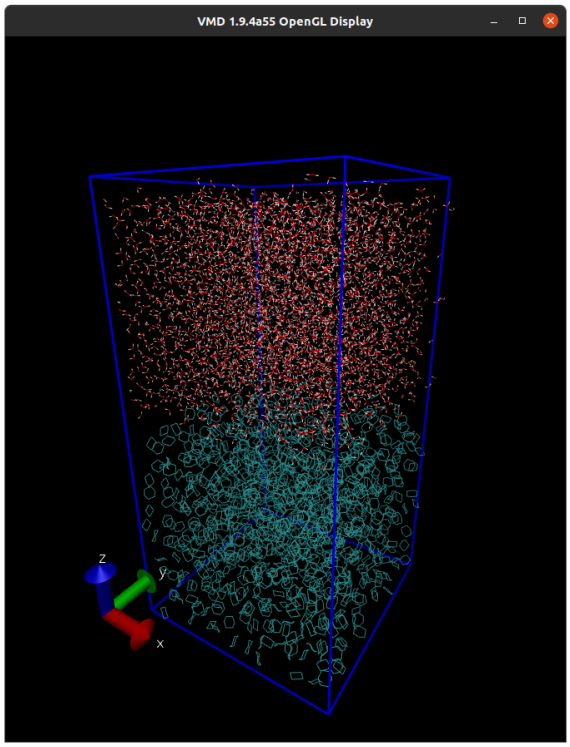
gmx editconf -f chx_10ns.gro -o chx_newbox.gro -box 5 5 10 -center 2.5 2.5 2.5

Solvate your system

gmx solvate -cp chx_newbox.gro -cs spc216.gro -p chx.top -o chx_solv.gro

vdwradii.dat change C atom radius





$R_{Carbon} = 0.17$ $R_{Carbon} = 0.60$

Energy Minimization

Before we can begin dynamics, we must ensure that the system has no steric clashes or inappropriate geometry. harmonic force constants of 1000 kJ mol^{-1} nm^{-2}

use the simple *steepest descent* minimizer `integrator = steep` in `minim.mdp`

`The *.mdp file contains the settings that dictate the nature of the simulation.`

gmx grompp -f minim.mdp -c chx_solv.gro -p chx.top -o em.tpr

gmx mdrun -v -deffnm em

; minim.mdp - used as input into grompp to generate em.tpr

; Parameters describing what to do, when to stop and what to save

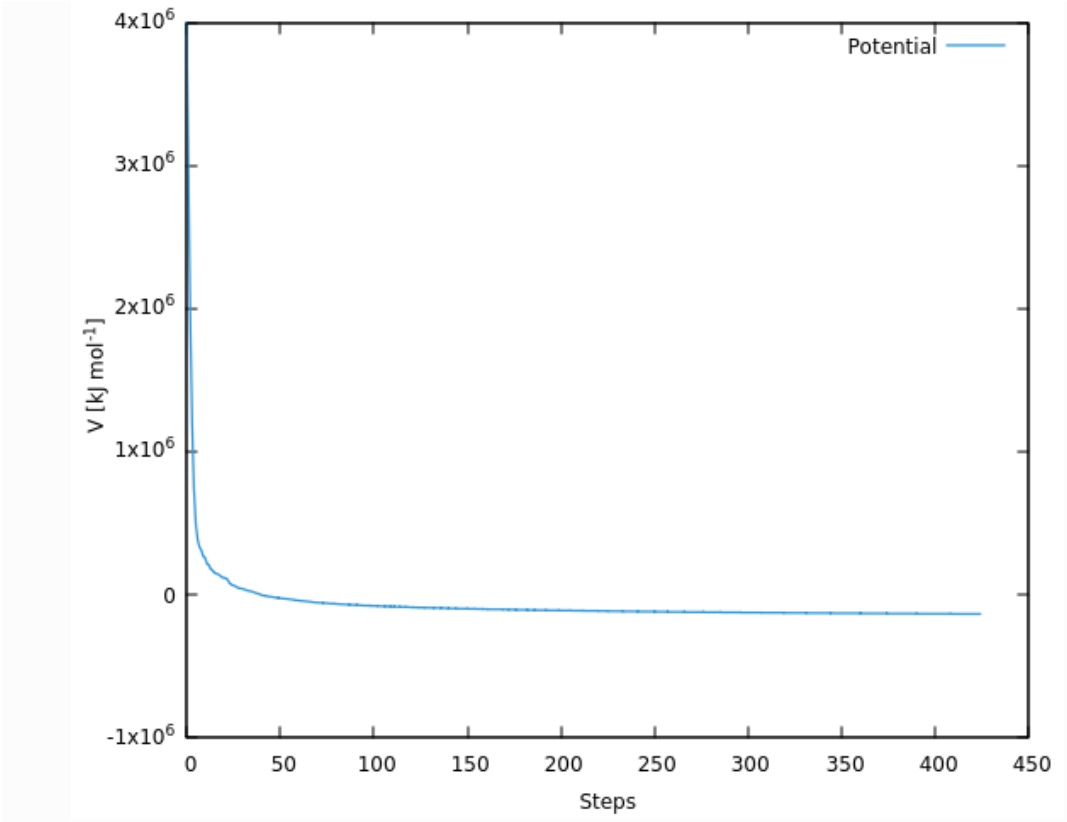
integrator = steep ; Algorithm (steep = steepest descent minimization)

emtol = 1000.0 ; Stop minimization when the maximum force < 1000.0 kJ/mol/nm

emstep = 0.01 ; Minimization step size

nsteps = 50000 ; Maximum number of (minimization) steps to perform

run input file (TPR) from the run parameter file (MDP), coordinate file (the solvated system with ions; PDB), and the topology (TOP)



Equilibration

NVT

This will help the added water molecules find a stable (equilibrium) distribution around the cyclohexane molecules.

gmx grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -o nvt.tpr

gmx mdrun -deffnm nvt

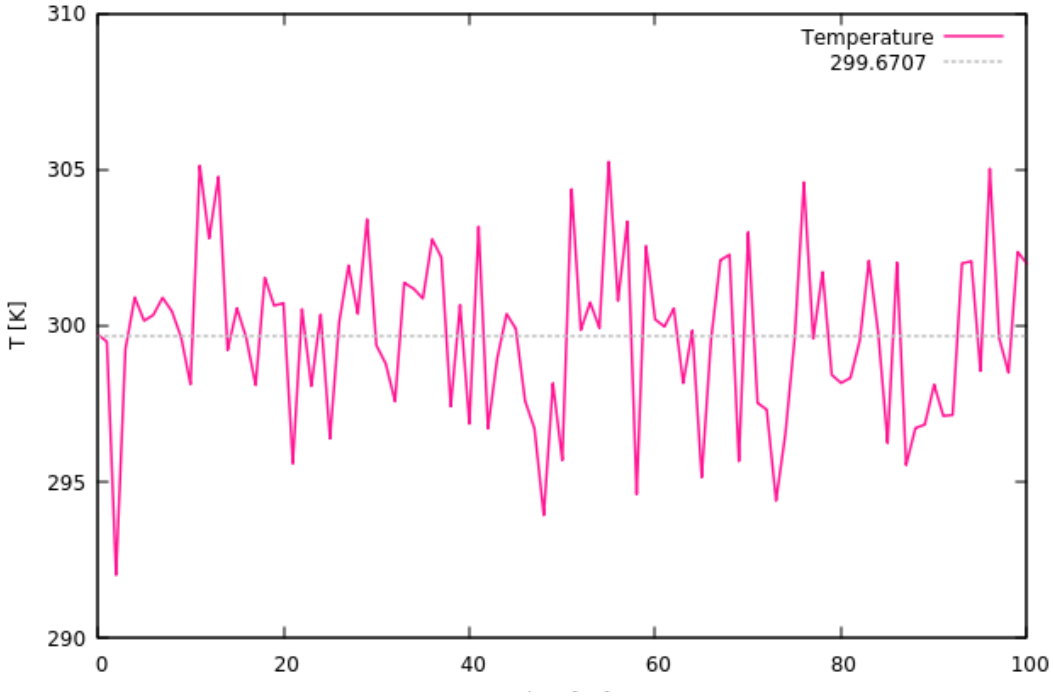
Temperature

gmx energy -f nvt.edr -o temperature.xvg

$$T = 299.670 \pm 2.667\,[K]$$

; Temperature coupling is on

tcoupl	= V-rescale		; modified Berendsen thermostat
tc-grps	= CHX	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



NPT

This will adjust the box size, ensuring that the density of water in the periodic box is correct for the simulation temperature and pressure.

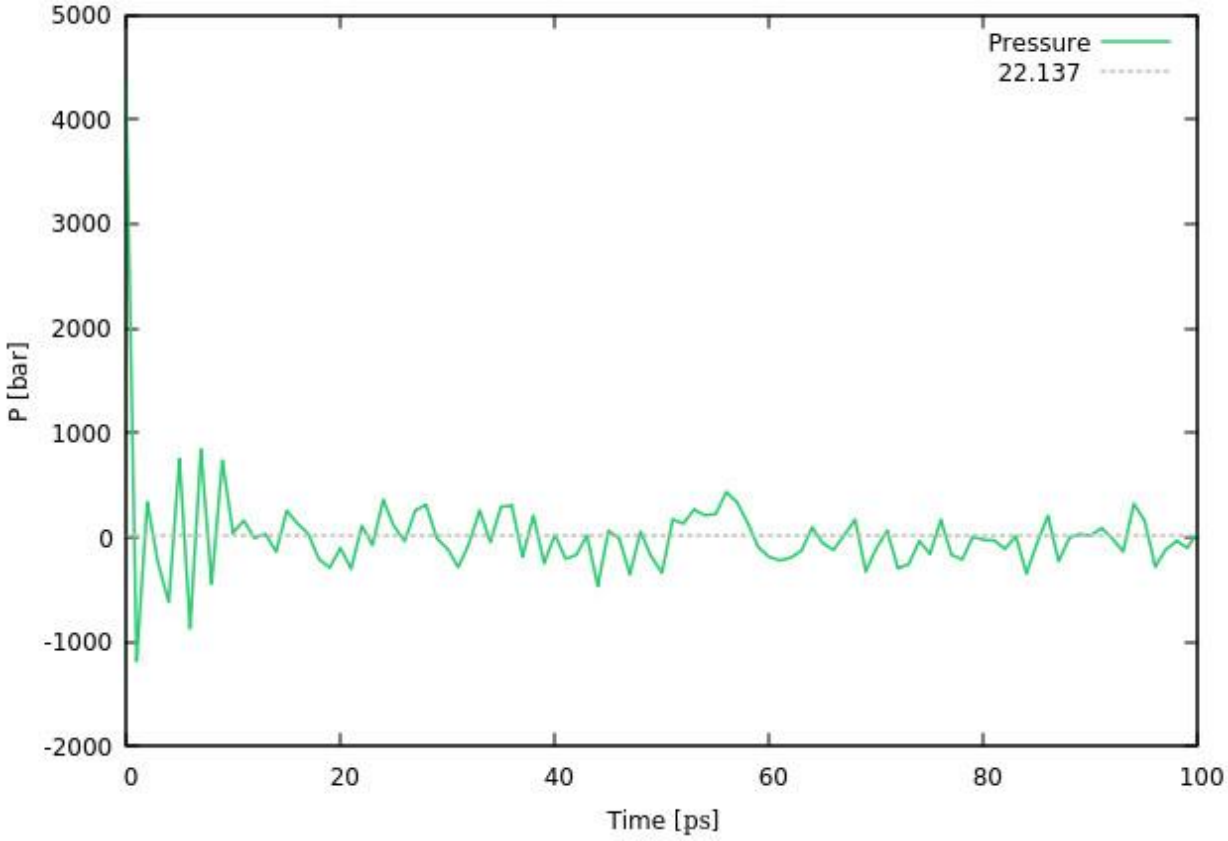
gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr

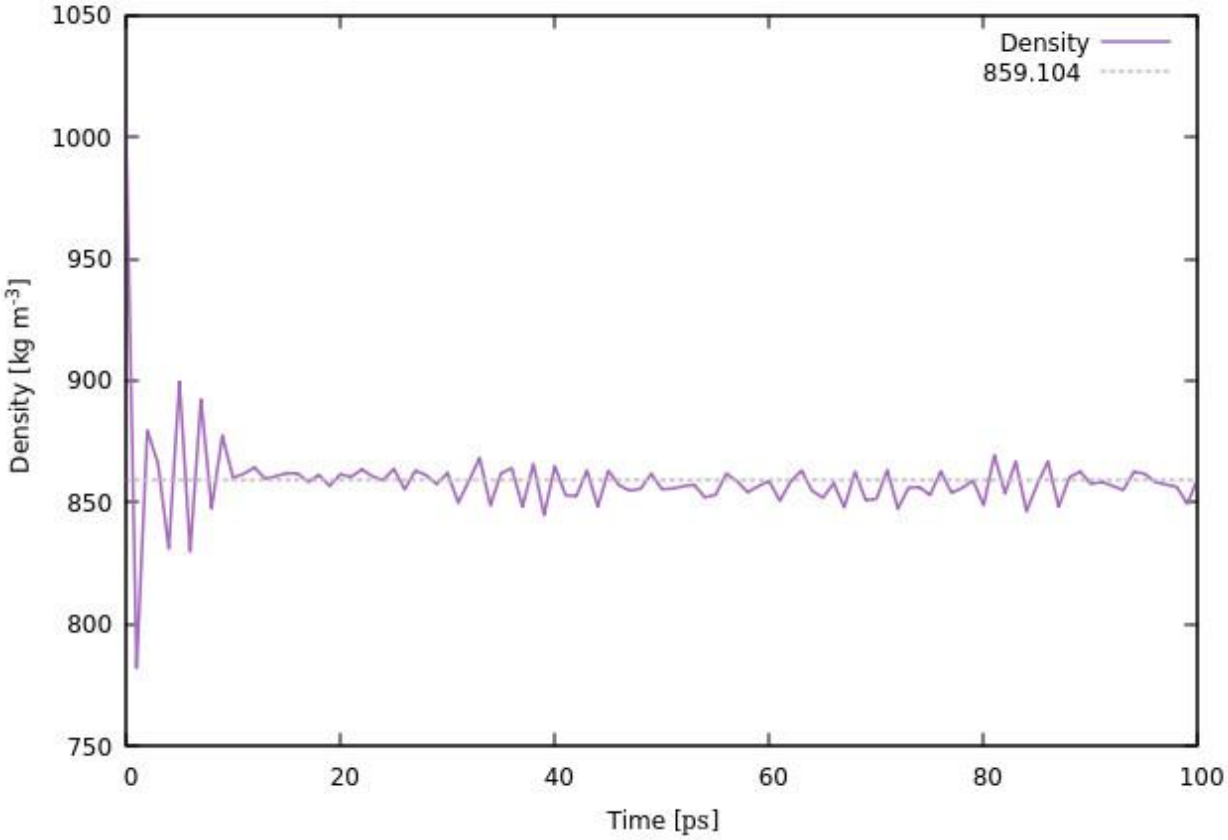
gmx mdrun -deffnm npt

; Temperature coupling is on

tcoupl	= V-rescale		; modified Berendsen thermostat
tc-grps	= CHX	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

$$P = 22.137 \pm 515.776[bar]$$





gmx energy -f npt.edr -o density.xvg $\rho = 859.104 \pm 18.67\ [kgm^{-3}]$

MD run

The final step is the actual molecular dynamics simulation.Upon completion of the two equilibration phases, the system is now well-equilibrated at the desired temperature and pressure.

gmx grompp -f md.mdp -c npt.gro -t npt.cpt -p topol.top -o md_0_1.tpr

gmx mdrun -deffnm md_0_1

title = OPLS Lysozyme NPT equilibration

; Run parameters

integrator = md ; leap-frog integrator

*nsteps = 500000 ; 2 * 500000 = 1000 ps (1 ns)*

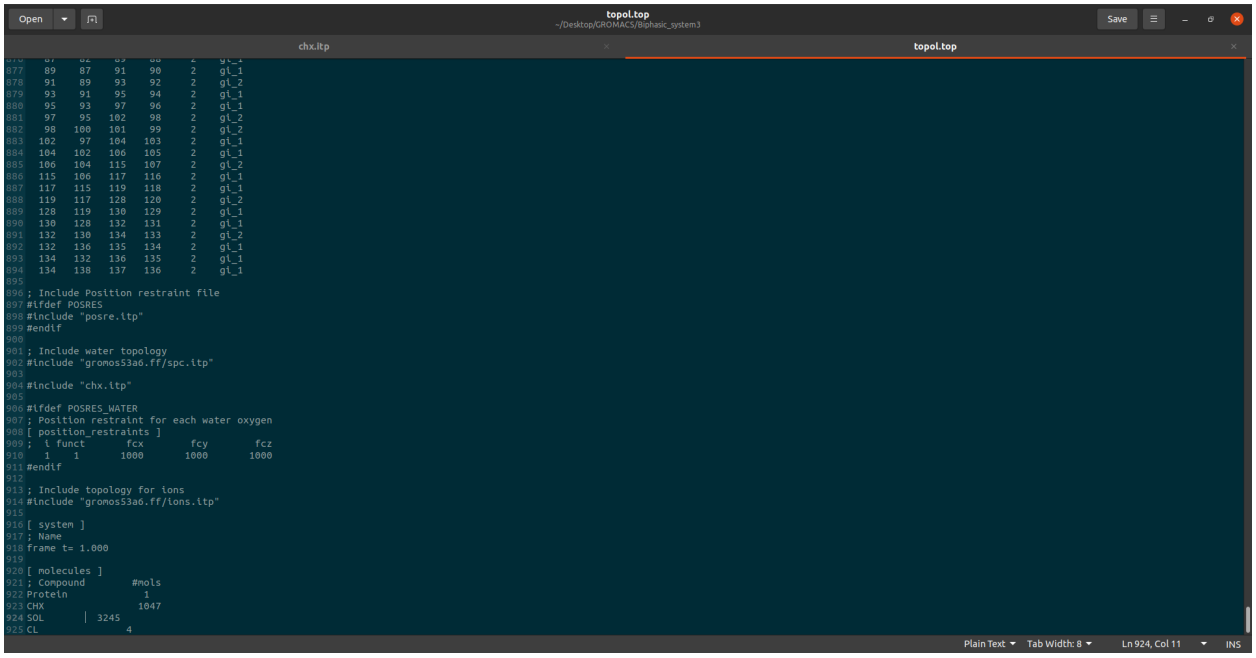
dt = 0.002 ; 2 fs

EXPERIMENT 3 : Biphasic System Protein in Aqueous Layer 30 Nov 2022

Construct chx.itp file:

```
[ moleculetype ]
; Name nrexcl
CHX      3

[ atoms ]
;   nr       type  resnr resid  atom  cgnr   charge     mass
     1       CH2     1  CHX     CAA     1    0.000  14.0270
     2       CH2     1  CHX     CAB     2    0.000  14.0270
     3       CH2     1  CHX     CAD     3    0.000  14.0270
     4       CH2     1  CHX     CAF     4    0.000  14.0270
     5       CH2     1  CHX     CAE     5    0.000  14.0270
     6       CH2     1  CHX     CAC     6    0.000  14.0270

[ bonds ]
; ai  aj  fu    c0, c1, ...
   1   2   2    0.152   5430000.0    0.152   5430000.0 ;   CAA  CAB
   1   6   2    0.152   5430000.0    0.152   5430000.0 ;   CAA  CAC
   2   3   2    0.152   5430000.0    0.152   5430000.0 ;   CAB  CAD
   3   4   2    0.152   5430000.0    0.152   5430000.0 ;   CAD  CAF
   4   5   2    0.152   5430000.0    0.152   5430000.0 ;   CAF  CAE
   5   6   2    0.152   5430000.0    0.152   5430000.0 ;   CAE  CAC

[ pairs ]
; ai  aj  fu    c0, c1, ...
   1   4   1                                       ;   CAA  CAF
   2   5   1                                       ;   CAB  CAE
   3   6   1                                       ;   CAD  CAC

[ angles ]
; ai  aj  ak  fu    c0, c1, ...
   2   1   6   2    109.5       520.0    109.5       520.0 ;   CAB  CAA  CAC
   1   2   3   2    109.5       520.0    109.5       520.0 ;   CAA  CAB  CAD
   2   3   4   2    109.5       520.0    109.5       520.0 ;   CAB  CAD  CAF
   3   4   5   2    109.5       520.0    109.5       520.0 ;   CAD  CAF  CAE
   4   5   6   2    109.5       520.0    109.5       520.0 ;   CAF  CAE  CAC
   1   6   5   2    109.5       520.0    109.5       520.0 ;   CAA  CAC  CAE

[ dihedrals ]
; ai  aj  ak  al  fu    c0, c1, m, ...
   3   2   1   6   1      0.0    5.9 3      0.0    5.9 3 ; dih   CAD  CAB  CAA  CAC
   5   6   1   2   1      0.0    5.9 3      0.0    5.9 3 ; dih   CAE  CAC  CAA  CAB
   4   3   2   1   1      0.0    5.9 3      0.0    5.9 3 ; dih   CAF  CAD  CAB  CAA
   5   4   3   2   1      0.0    5.9 3      0.0    5.9 3 ; dih   CAE  CAF  CAD  CAB
   6   5   4   3   1      0.0    5.9 3      0.0    5.9 3 ; dih   CAC  CAE  CAF  CAD
   1   6   5   4   1      0.0    5.9 3      0.0    5.9 3 ; dih   CAA  CAC  CAE  CAF

; include water


Plain Text  Tab Width: 8  Ln 1, Col 1  INS
```

Make changes in the topology file: #include chx.itp



Make index file

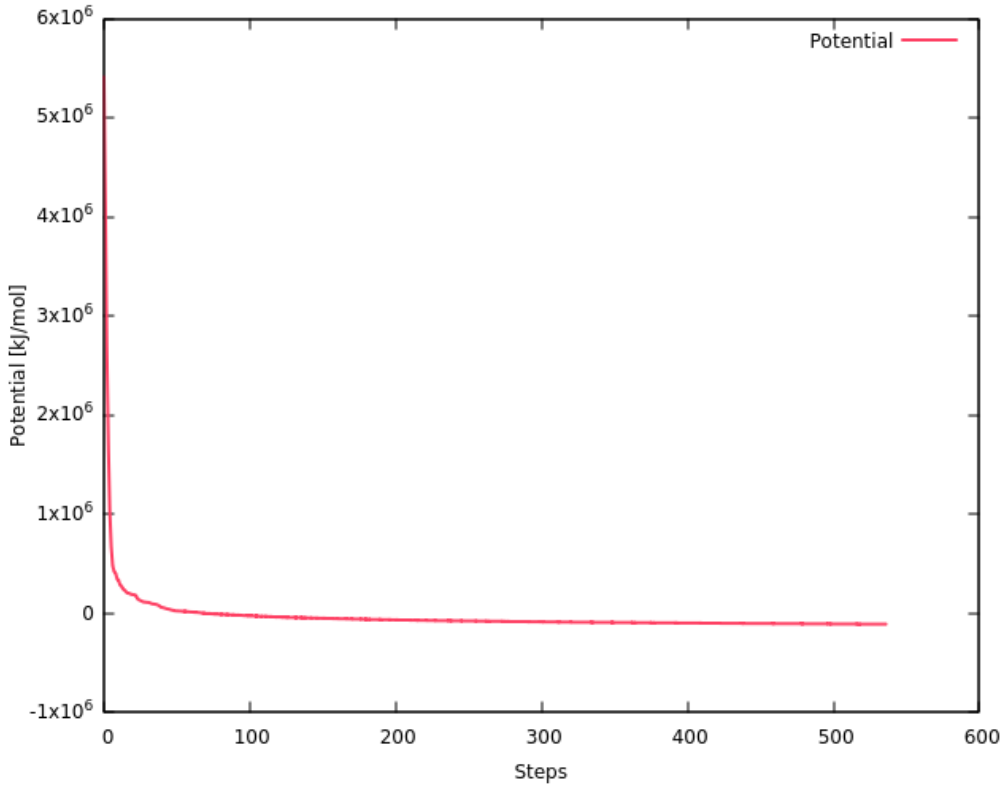
1 Protein 13 CHX 21 Water_and_ions

Energy Minimization

Before we can begin dynamics, we must ensure that the system has no steric clashes or inappropriate geometry. harmonic force constants of 1000 kJ mol^{-1} nm^{-2}

gmx grompp -f minim.mdp -c chx_solv.gro -n choco.ndx -p chx.top -o em.tpr

gmx mdrun -v -deffnm em



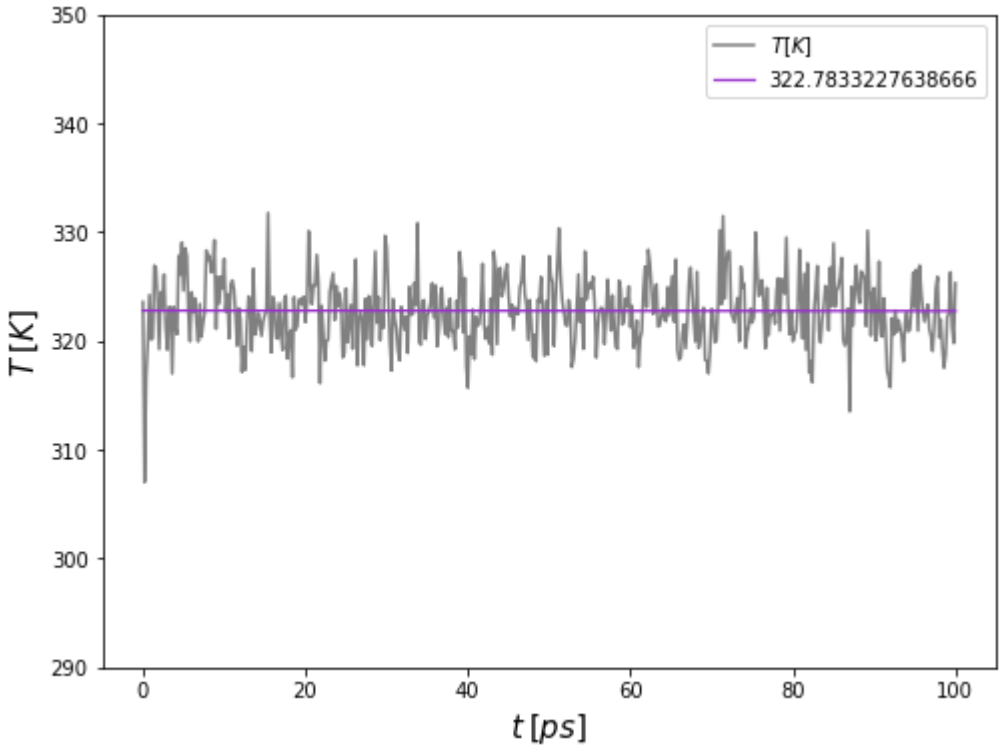
NVT

This will help the added water molecules find a stable (equilibrium) distribution around the protein.

gmx grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -o nvt.tpr

gmx mdrun -deffnm nvt

```
; Temperature coupling is on
tcoupl                  = V-rescale             ; modified Berendsen
thermostat
tc-grps                 = Protein CHX   Water_and_ions   ; two coupling
groups - more accurate
tau_t                   = 0.1       0.1   0.1   ; time constant, in ps
ref_t                   = 300       300   300   ; reference temperature, one
for each group, in K
```



$$T = 300.109 \pm 3.049\ [K]$$

NPT

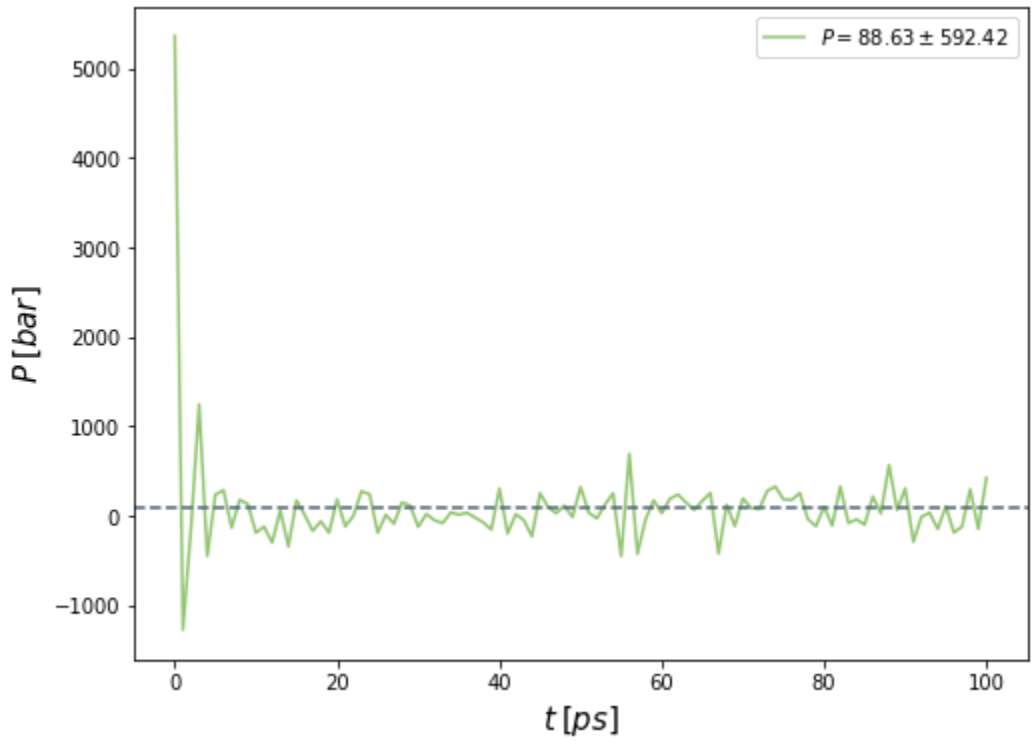
This will adjust the box size, ensuring that the density of water in the periodic box is correct for the simulation temperature and pressure.

gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -o npt.tpr

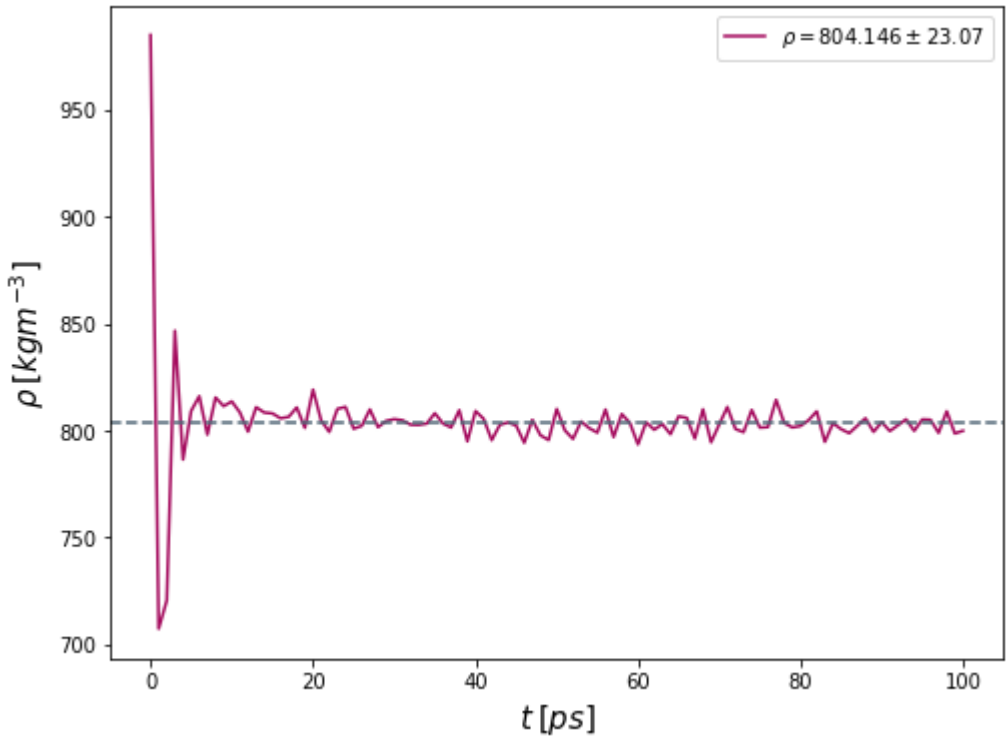
gmx mdrun -deffnm npt

```
; Temperature coupling is on
tcoupl                  = V-rescale             ; modified Berendsen thermostat
tc-grps                 = Protein CHX   Water_and_ions   ; two coupling groups - more accurate
tau_t                   = 0.1   0.1     0.1     ; time constant, in ps
ref_t                   = 300   300     300     ; reference temperature, one for each group, in K
```

gmx energy -f npt.edr -o pressure.xvg

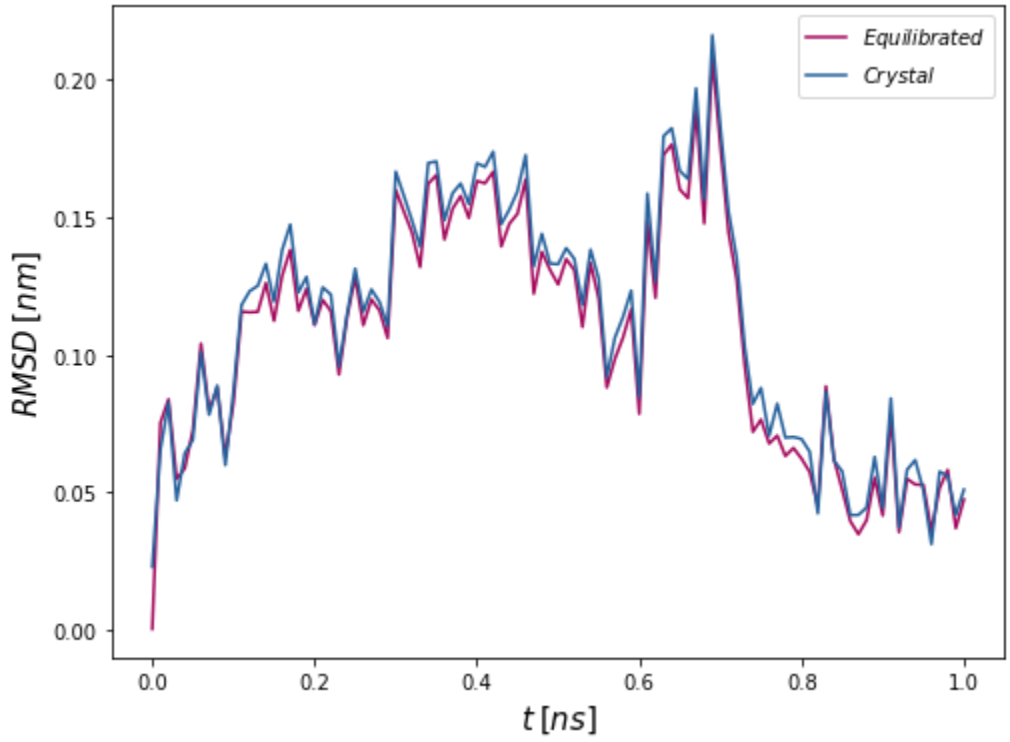


$P = 88.637 \pm 592.423\ [bar]$



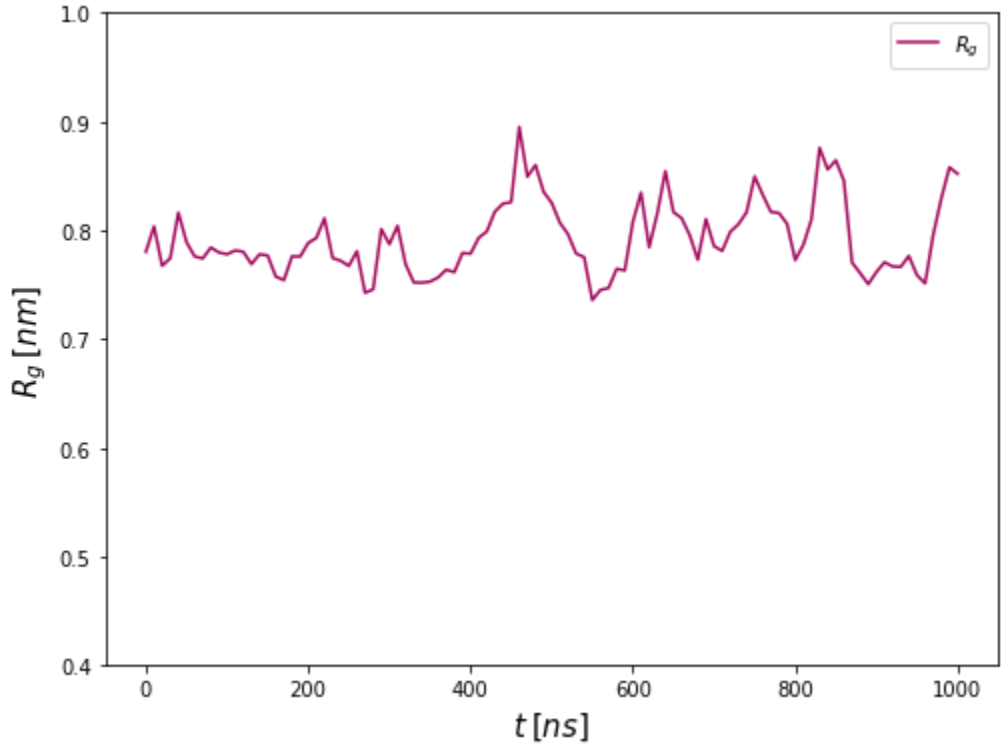
$\rho = 804.146 \pm 23.07\ [kgm^{-3}]$

Analysis



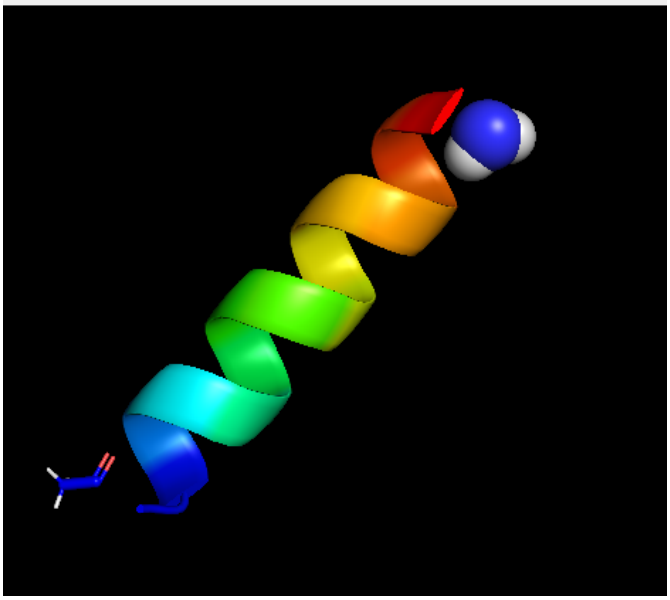
$\rho_{RMSD} = 0.1065 \pm 0.043\ [nm]$

Radius of gyration



$R_g = 0.792 \pm 0.033\ [nm]$

EXPERIMENT 4 : Membrane Protein Jan 2023

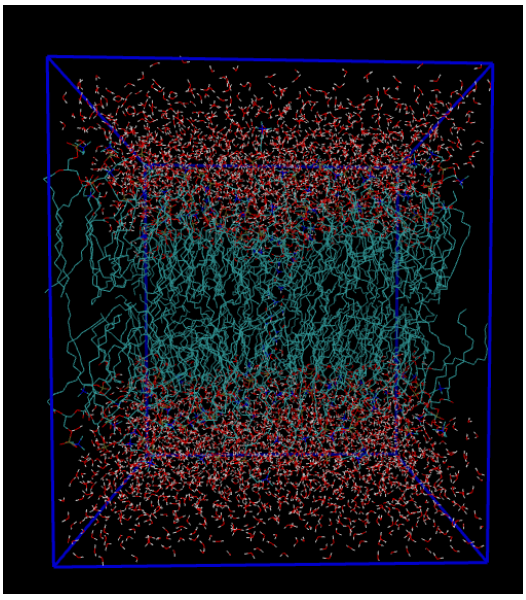


KALP-15

1. Orient the protein and membrane

gmx grompp -f minim.mdp -c dppc128.pdb -p topol_dppc.top -o dppc.tpr

gmx trjconv -s dppc.tpr -f dppc128.pdb -o dppc128_whole.gro -pbc mol -ur compact

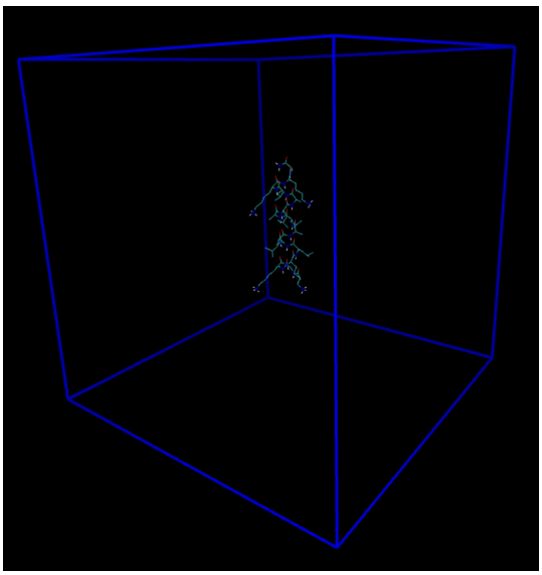


dppc128_whole.gro

Use trjconv to remove periodicity (select group 0, "System" for output):

place the center of mass of the peptide at the center of this box

gmx editconf -f KALP-15_processed.gro -o KALP_newbox.gro -c -box 6.41840 6.44350 6.59650



center of our system now lies at (3.20920, 3.22175, 3.29825)

Pack the lipids around the protein

cat KALP_newbox.gro dppc128_whole.gro > system.gro

```
; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif


; Strong position restraints for InflateGRO
#ifdef STRONG_POSRES
#include "strong_posre.itp"
#endif
#include "dppc.itp"

; Include water topology
#include "gromos53a6.ff/spc.itp"

#ifdef POSRES_WATER
; Position restraint for each water oxygen
[ position_restraints ]
;  i funct       fcx        fcy        fcz
   1    1       1000       1000       1000
#endif

; Include topology for ions
#include "gromos53a6.ff/ions.itp"

[ system ]
; Name
frame t= 1.000 in water

[ molecules ]
; Compound        #mols
Protein             1
DPPC                126
SOL         4176
CL               4
```

generate this new position restraint file using genrestr:

gmx genrestr -f KALP_newbox.gro -o strong_posre.itp -fc 100000 100000 100000

perl inflategro.pl system.gro 4 DPPC 14 system_inflated.gro 5 area.dat

inflategro.perl

```
$areaprotein_lower=($gridsize)**2 *$howmany *0.01;
$arealipid_lower=($box_x * $box_y - $areaprotein_lower)/($newlower);
print "Area per protein: $areaprotein_total nm^2\n";
print "Area per lipid: $arealipid_total nm^2\n\n";

print "Area per protein, upper half: $areaprotein_upper nm^2\n";
print "Area per lipid, upper leaflet : $arealipid_upper nm^2\n\n";

print "Area per protein, lower half: $areaprotein_lower nm^2\n";
print "Area per lipid, lower leaflet : $arealipid_lower nm^2\n\n";
```

```
; minim.mdp - used as input into grompp to generate em.tpr
; Parameters describing what to do, when to stop and what to save
define          = -DSTRONG_POSRES   ; Prevent protein from moving
integrator      = steep     ; Algorithm (steep = steepest descent minimization)
emtol           = 1000.0    ; Stop minimization when the maximum force < 1000.0
kJ/mol/nm
emstep          = 0.01      ; Energy step size
nsteps          = 50000     ; Maximum number of (minimization) steps to perform
```

gmx grompp -f minim_inflategro.mdp -c system_inflated.gro -p topol.top -r system_inflated.gro -o system_inflated_em.tpr

gmx mdrun -deffnm system_inflated_em

reconstruct with trjconv before attempting to use such coordinates with InflateGRO:

gmx trjconv -s system_inflated_em.tpr -f system_inflated_em.gro -o tmp.gro -pbc mol

mv tmp.gro system_inflated_em.gro

begin packing the lipids around the protein by applying a scaling factor that is < 1

perl inflategro.pl system_inflated_em.gro 0.95 DPPC 0 system_shrink1.gro 5 area_shrink1.dat

run_inflategro.sh

```
# loop over 26 shrinking iterations
for curr in {1..26}
do
      prev=$((curr - 1))
.
.
.
      # otherwise use minimized coordinates from previous iteration
      perl inflategro.pl system_shrink${prev}_em.gro 0.95 DPPC 0
system_shrink${curr}.gro 5 area_shrink${curr}.dat
      fi

      # run grompp and mdrun to carry out energy minimization
```

```
      gmx grompp -f minim_inflategro.mdp -c system_shrink${curr}.gro -r
system_shrink${curr}.gro -p topol.top -o system_shrink${curr}_em.tpr
-maxwarn 2
      gmx mdrun -deffnm system_shrink${curr}_em

      # make molecules whole
      gmx trjconv -s system_shrink${curr}_em.tpr -f
system_shrink${curr}_em.gro -o tmp.gro -pbc mol
      mv tmp.gro system_shrink${curr}_em.gro
```

Solvate with water

gmx solvate -cp system_shrink26_em.gro -cs spc216.gro -o system_solv.gro -p topol.top

waterdeletor.perl

```
# Report what happened
print "$ndel water molecules have been deleted.\n";
my $watnew = $nwater_start - $ndel;
print "$watnew water molecules remain. Update your topology!\n";

# print the cleaned output
my $natoms_clean = scalar(@clean_atoms);
```

perl water_deletor.pl -in system_solv.gro -out system_solv_fix.gro -ref O33 -middle C50 -nwater 3

Adding Ions

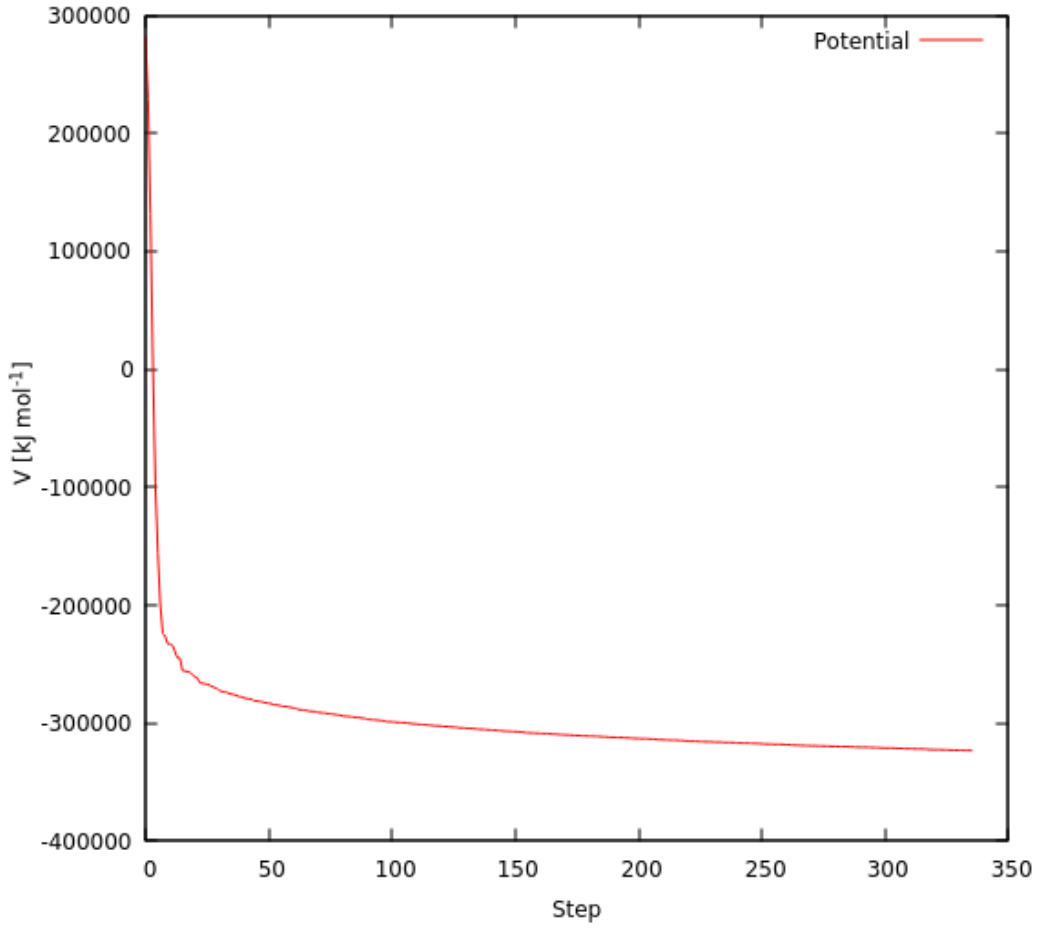
gmx grompp -f ions.mdp -c system_solv_fix.gro -p topol.top -o ions.tpr

gmx genion -s ions.tpr -o system_solv_ions.gro -p topol.top -pname NA -nname CL -neutral

Energy minimization

gmx grompp -f minim.mdp -c system_solv_ions.gro -p topol.top -o em.tpr

gmx mdrun -v -deffnm em



NVT

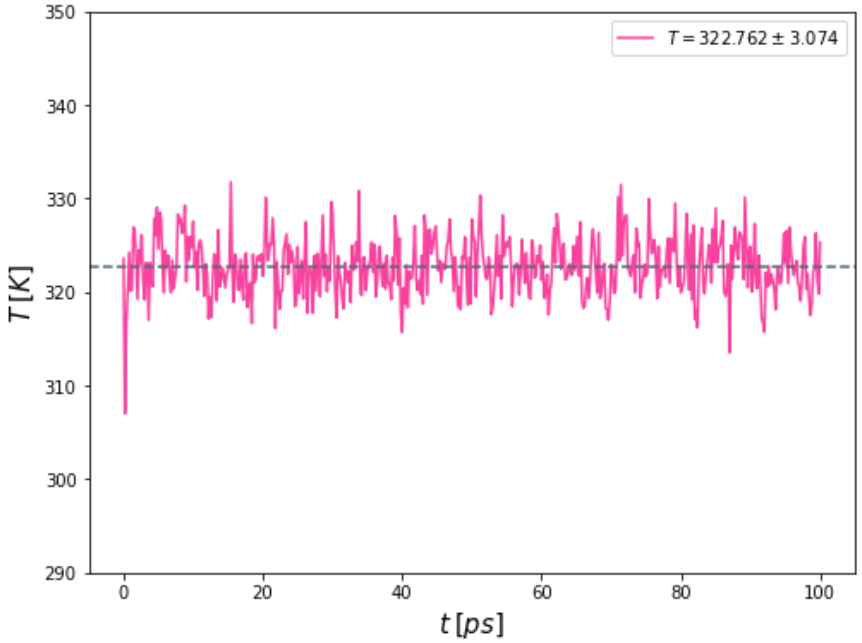
This will help the added water molecules find a stable (equilibrium) distribution around the protein.

gmx grompp -f nvt.mdp -c em.gro -r em.gro -p topol.top -n index.ndx -o nvt.tpr

gmx mdrun -deffnm nvt

```
title       = NVT equilibration for KALP15-DPPC
define      = -DPOSRES  ; position restrain the protein
; Run parameters
integrator  = md        ; leap-frog integrator
nsteps      = 50000     ; 2 * 50000 = 100 ps
dt          = 0.002     ; 2 fs
```

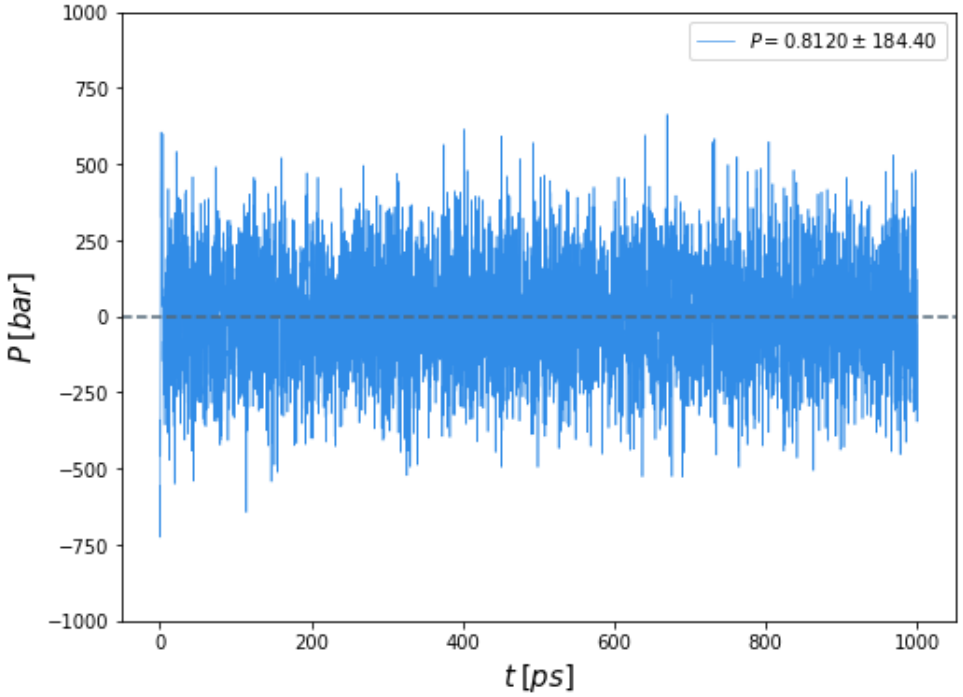
```
; Temperature coupling is on
tcoupl      = V-rescale                     ; modified Berendsen
thermostat
tc-grps     = Protein_DPPC  Water_and_ions   ; two coupling groups -
more accurate
tau_t       = 0.1           0.1             ; time constant, in ps
ref_t       = 323           323             ; reference temperature,
one for each group, in K
```



NPT

This will adjust the box size, ensuring that the density of water in the periodic box is correct for the simulation temperature and pressure.

```
gmx grompp -f npt.mdp -c nvt.gro -r nvt.gro -t nvt.cpt -p topol.top -n
index.ndx -o npt.tpr

gmx mdrun -deffnm npt
```

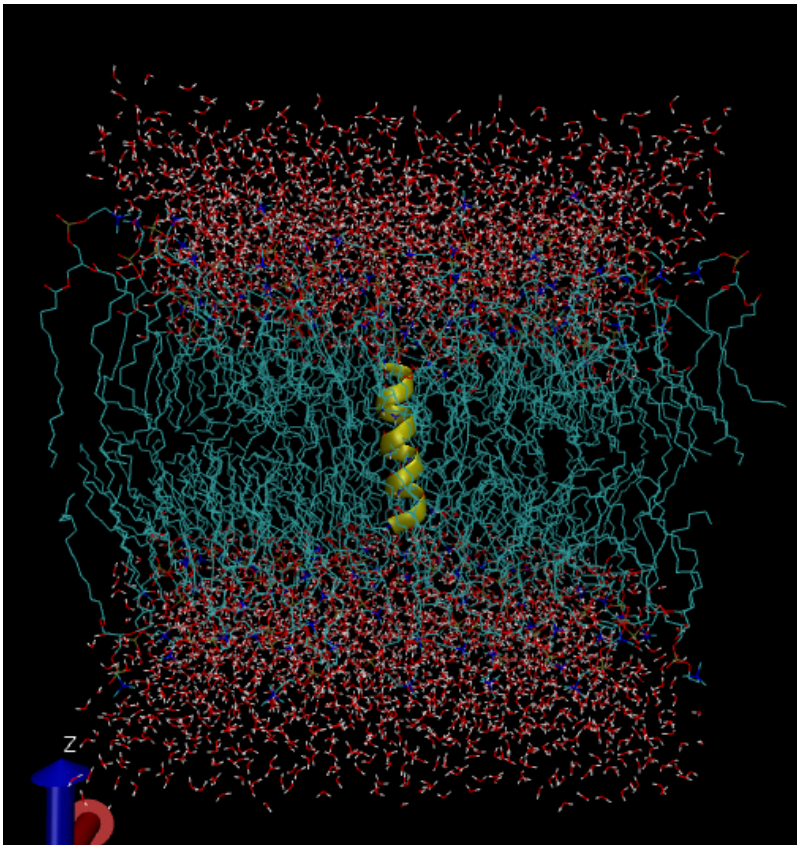


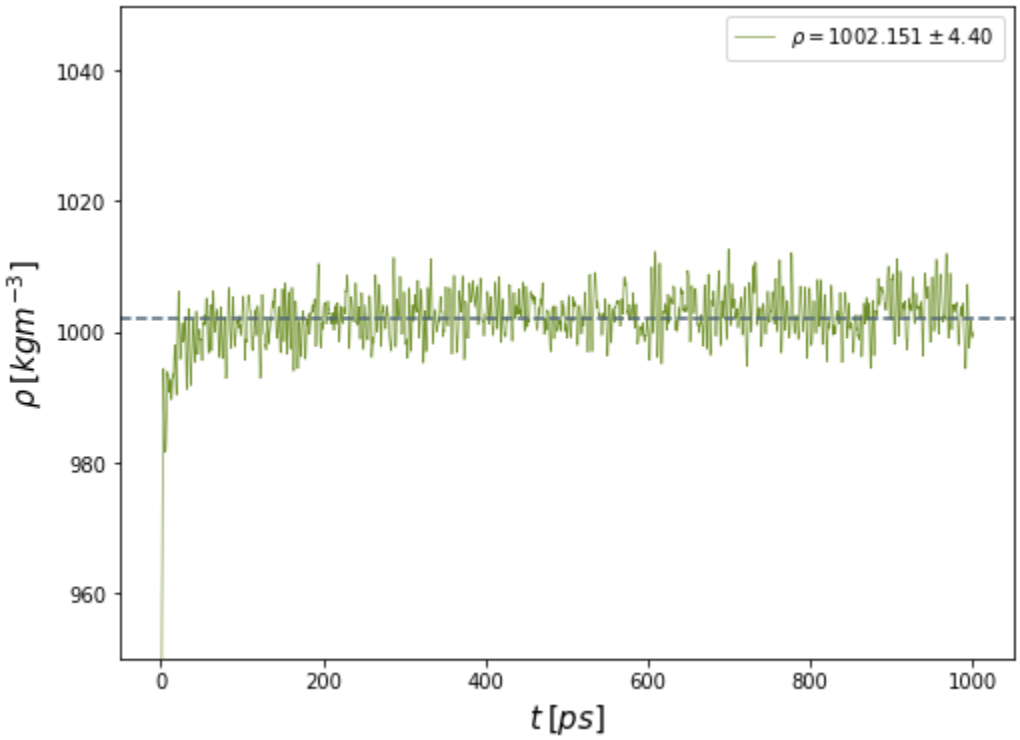
MD run

The final step is the actual molecular dynamics simulation.Upon completion of the two equilibration phases, the system is now well-equilibrated at the desired temperature and pressure.

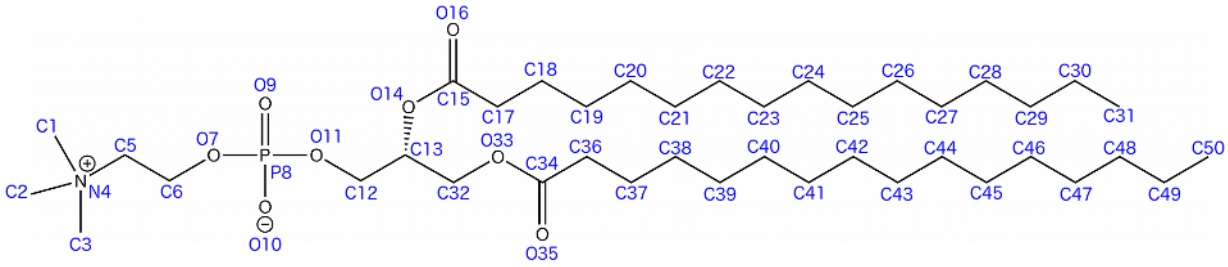
```
gmx grompp -f md.mdp -c npt.gro -t npt.cpt -p topol.top -n index.ndx -o md_0_1.tpr
```

```
gmx mdrun -deffnm md_0_1
```





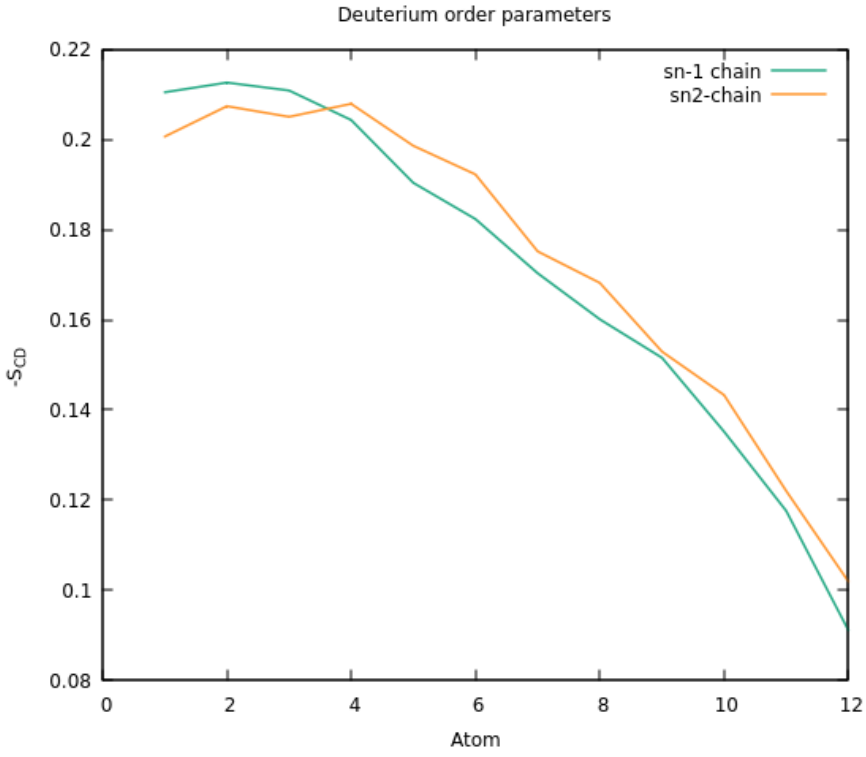
1. Deuterium Order Parameters




```
gmx make_ndx -f md_0_1.tpr -o sn1.ndx
...
 > a C34
 > a C36
 > a C37
 > a C38
...
 > a C50
 > del 0-21
 > q
```

gmx order -s md_0_1.tpr -f md_0_1.xtc -n sn1.ndx -d z -od deuter_sn1.xvg

repeat for the *sn-2* chain carbons C15, C17-C31 to give "sn2.ndx"



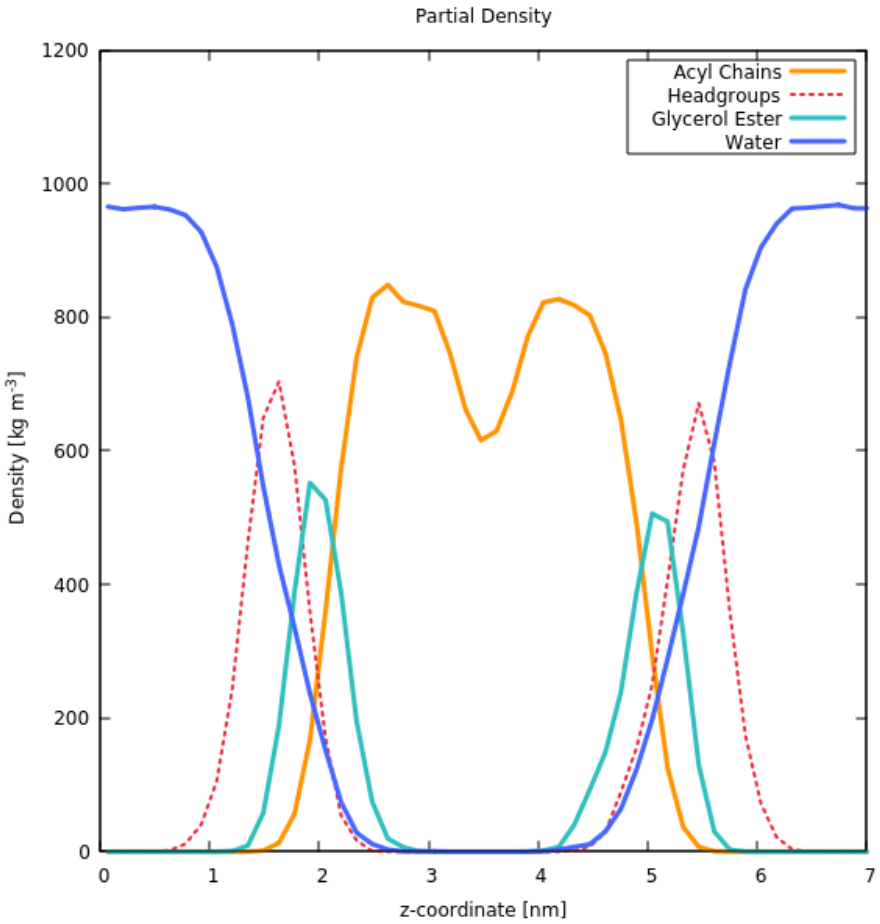
2.Density of the Membrane

```
gmx make_ndx -f md_0_1.tpr -o density_groups.ndx
...
 > 13 & a C1 | a C2 | a C3 | a N4 | ... | a O11
 > name 22 Headgroups
 > 13 & a C12 | a C13 | a O14 | a C15 | a O16 | a C32 | a O33 | a C34 | a
O35
 > name 23 Glycerol_Ester
 > 13 & ! 22 & ! 23
 > name 24 Acyl_Chains
 > q
```

gmx density -s md_0_1.tpr -f md_0_1.xtc -n density_groups.ndx -o dens_headgroups.xvg -d Z

gmx density -s md_0_1.tpr -f md_0_1.xtc -n density_groups.ndx -o dens_glycerolester.xvg -d Z

gmx density -s md_0_1.tpr -f md_0_1.xtc -n density_groups.ndx -o dens_acylchains.xvg -d Z



Generate a centered trajectory in the primary unit cell

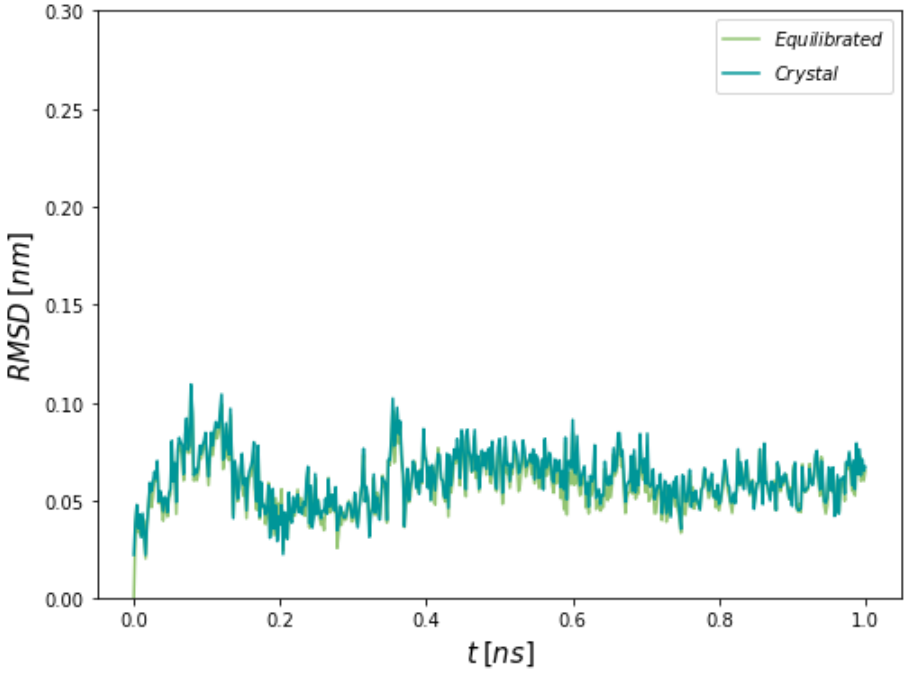
gmx trjconv -s md_0_1.tpr -f md_0_1.xtc -o md_0_1_noPBC.xtc -pbc mol -center

Select 1 ("Protein") as the group to be centered and 0 ("System") for output.

RMSD

gmx rms -s md_0_1.tpr -f md_0_1_noPBC.xtc -o rmsd.xvg -tu ns

Select 4 ("Backbone") as the group to be centered and 4 ("Backbone") for output.

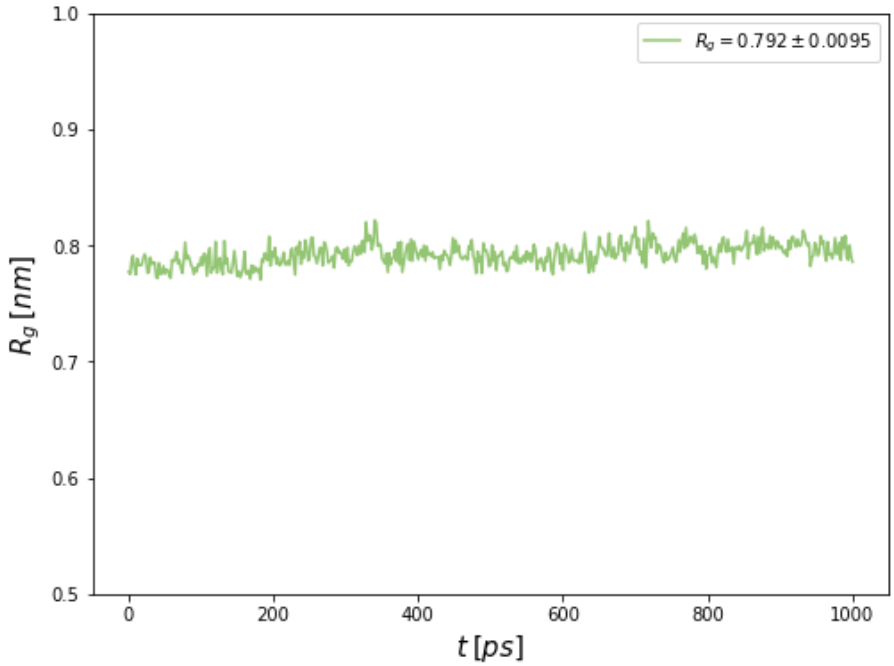


Radius of Gyration

gmx gyrate -s md_0_1.tpr -f md_0_1_noPBC.xtc -o gyrate.xvg

group 1 (Protein) for analysis

$$R_{\mathrm{gyr}}^2 = \frac{1}{M}\sum_{i=1}^{N} m_i(\mathbf{r}_i - \mathbf{R})^2 \qquad \text{where} \qquad \mathbf{R} = N^{-1}\sum_{i=1}^{N}\mathbf{r}_i$$



Acyl chain order parameter profiles in phospholipid bilayers:computation from molecular dynamics simulations and comparison with $_2$H NMR experiments

Louic S. Vermeer et.al

https://www3.mpibpc.mpg.de/groups/de_groot/pdf/Vermeer_EBJ_2007.pdf

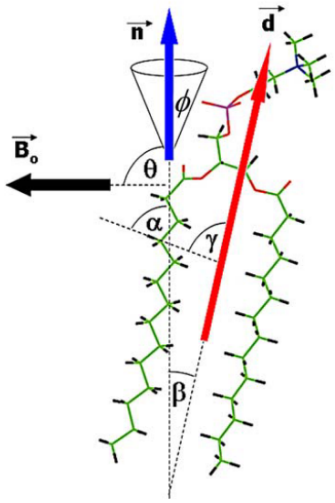


Fig. 1 Visual representation of different contributions to the observed order parameter S (Eq. 2a). Fast rotations of lipids about the vector normal to the bilayer permit to separate the contribution to

$$S_{CD} = \left\langle \frac{3\cos^2\alpha - 1}{2} \right\rangle \quad (2d)$$

$$S_{CD} = S_{coll} \cdot S_{mol} \cdot S_{intra} \quad (2e)$$

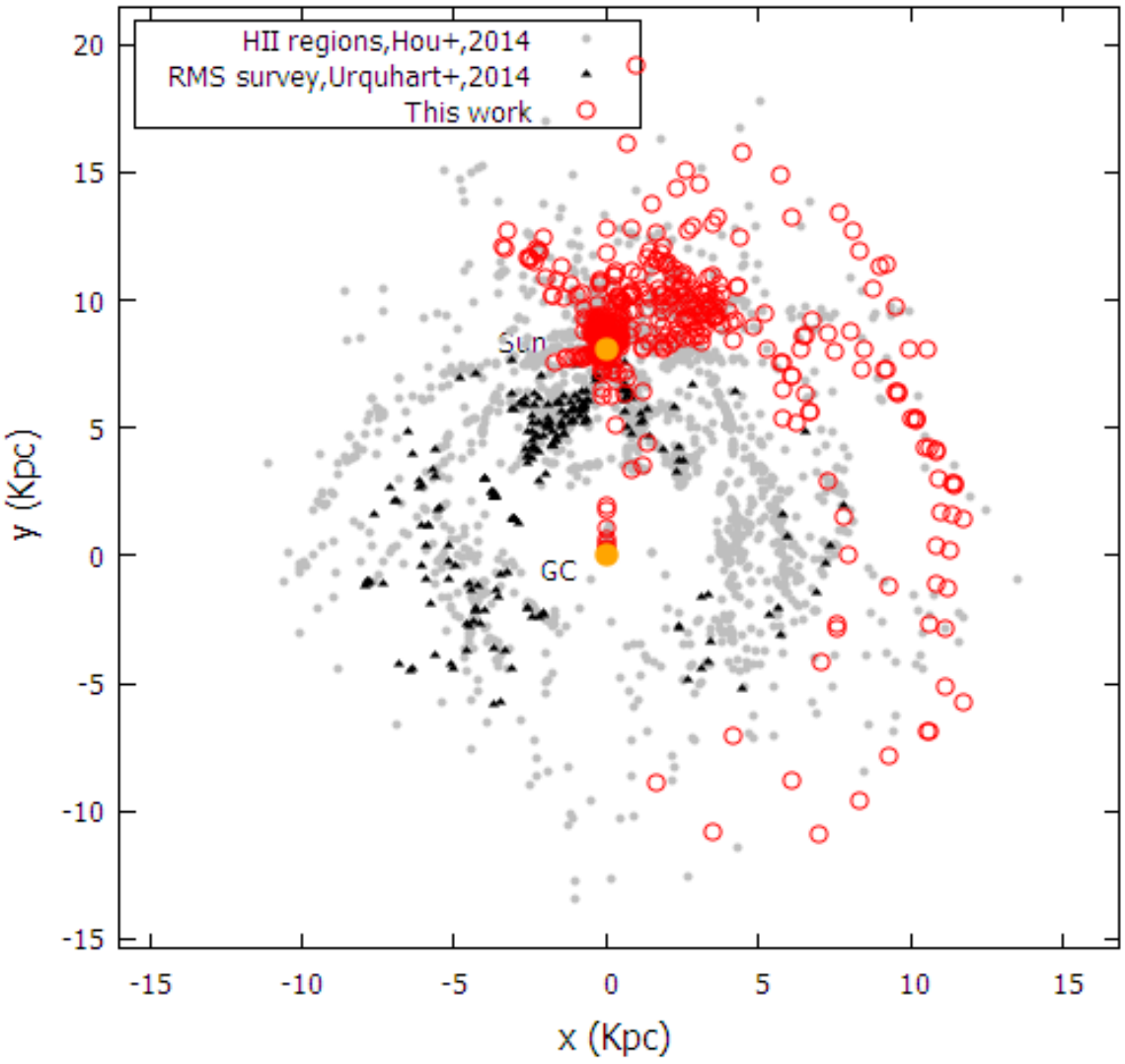
$$S_{coll} = \left\langle \frac{3\cos^2\varphi - 1}{2} \right\rangle \quad (2f)$$

$$S_{mol} = \left\langle \frac{3\cos^2\beta - 1}{2} \right\rangle \quad (2g)$$

$$S_{intra} = \left\langle \frac{3\cos^2\gamma - 1}{2} \right\rangle \quad (2h)$$

Calculating order parameters from MD simulations

gmx editconf -f myprotein_processed.gro -rotate 0 90 0 -o myprotein_newbox.gro -c -box 6.41840 6.44350 6.59650


HII regions,Hou+,2014
RMS survey,Urquhart+,2014
This work
Sun
GC
y (Kpc)
x (Kpc)
20
15
10
5
0
-5
-10
-15
-15
-10
-5
0
5
10
15