Personal report

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Modelado Molecular

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Tripeptides

Tripeptide

ACE-R_1-R_2-R_3-NME

ACE: CH_3-CO-
NME: -NH-CH_3
R_i: Residue

> `cd for-students/tripeptides` (pdb files)

Basic report

Basic report

- Make simulations at 298 K and 400 K following the equivalent steps detailed during the practical classes.
- Show the time evolution of the total and kinetic energies, the temperature of the system, two selected bond distances, two angles and two dihedrals, the radius of gyration, and the velocities of 5 different atoms . Compare the results for both temperatures.
- Evaluate the mean values of the kinetic energy of the system at both temperatures and compare them with the expected results from statistichal thermodynamic.
- Write a report in pdf format describing the steps and including plots.
- Appropiate use of scales, units, and formats will be taken into account.
- 70 % weight

Extended report (optional)

Extended report (optional)

- Run a 500 ps simulation at 298K exporting the results every 10 fs. runNVT.mdp

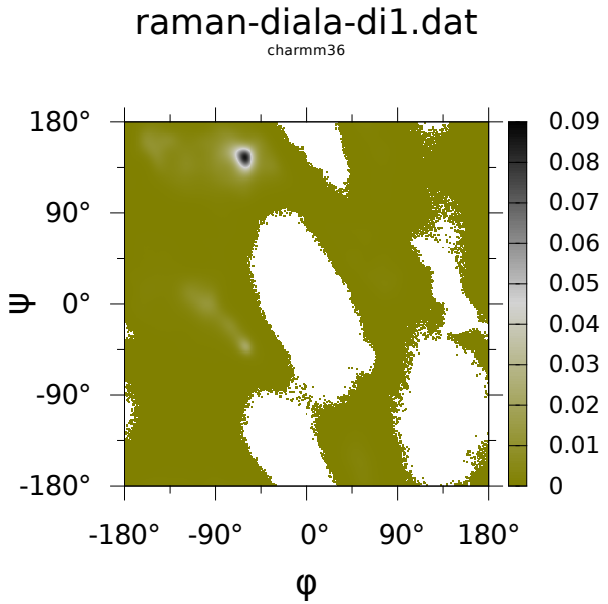
```
nsteps = 1000000 ; 500 ps
nstxout = 20 ; Save coordinates every 10 fs
nstvout = 20 ; Save velocities every 10 fs
nstlog = 20 ; Update log every 10 fs
nstenergy = 20 ; Save energies every 10 fs
```

- CPU time $\sim$ 30'
- Storage $\sim$ 30 Gb

Extended report (optional)

Extended report (optional)

- Plot histograms for the temperature and the three components of the velocity of a selected atom.
- Create Ramachandran plots for the three residues



- Identify the conformations with higher probability (α_R, β, ...)
- 30 % weight