Report

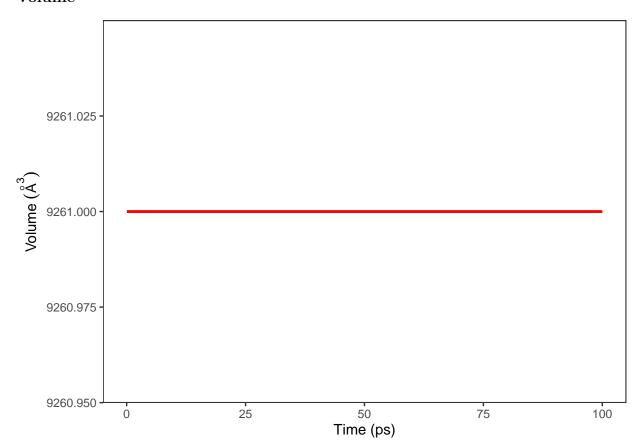
This report represents a statistical analysis of the main thermodynamic variables. The figures below show the time evolution of Volume, temperature, pressure and density followed by the linear regression (red line).

Parameters

Host: undefined ## Date: 20200901

Number of frames: 2000
Ensemble: nvt hoover
Timestep: 0.001 ps
Number of atoms: 936

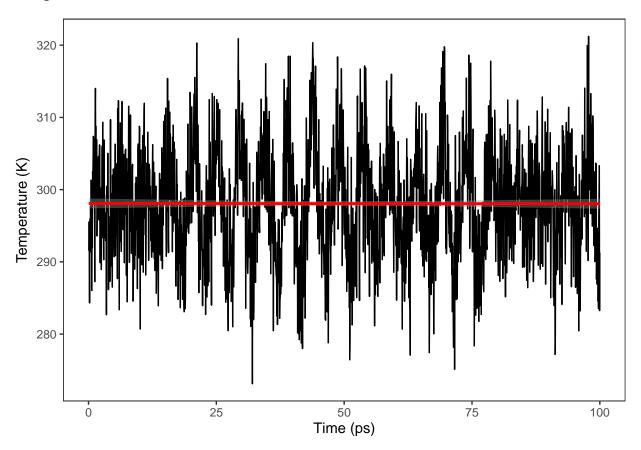
Volume



Here is the statistical values of the volume of the unit cell.

Min. 1st Qu. Median Mean 3rd Qu. Max. ## 9261 9261 9261 9261 9261 9261

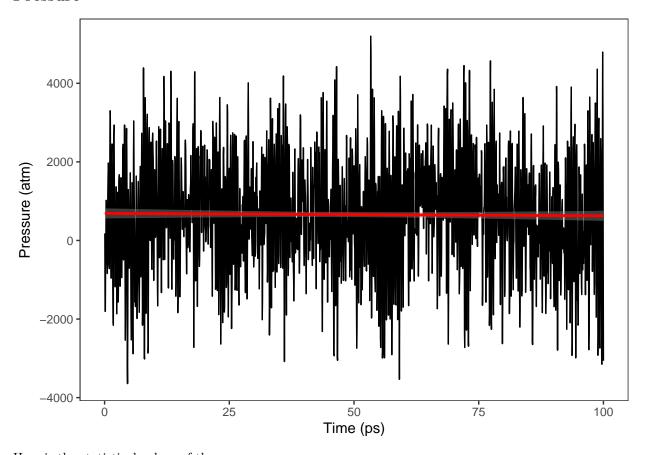
Temperature



Here is the statistical values of the temperature.

Min. 1st Qu. Median Mean 3rd Qu. Max. ## 273.1 292.6 298.0 298.1 303.1 321.2

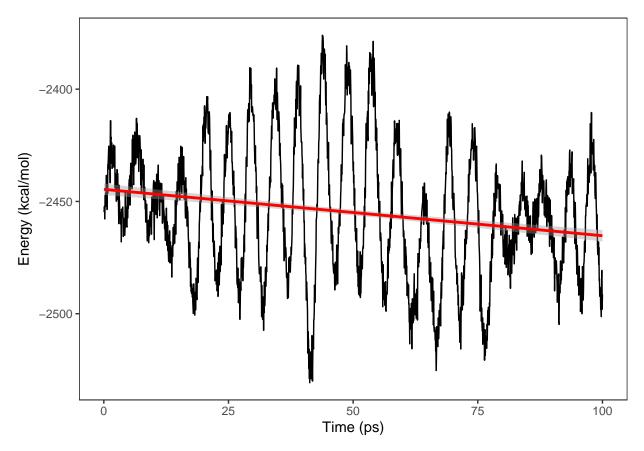
Pressure



Here is the statistical values of the pressure.

Min. 1st Qu. Median Mean 3rd Qu. Max. ## -3642.6 -345.2 684.7 657.6 1691.3 5199.7

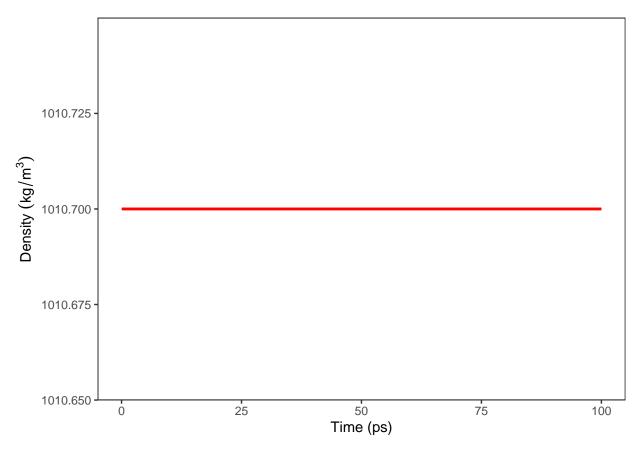
Energy



Here is the statistical values of the energy.

```
## Min. 1st Qu. Median Mean 3rd Qu. Max.
## -2531 -2477 -2455 -2456 -2436 -2376
```

Density



Here is the statistical values of the density.

```
## Min. 1st Qu. Median Mean 3rd Qu. Max.
## 1011 1011 1011 1011 1011 1011
```