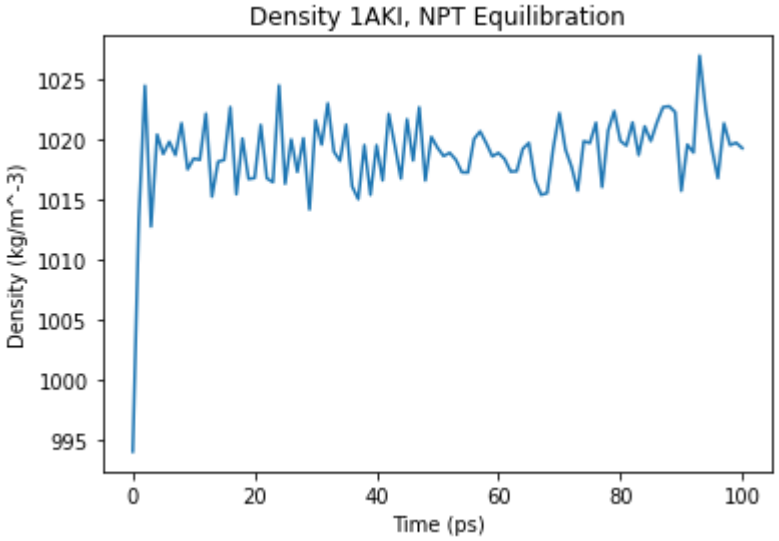
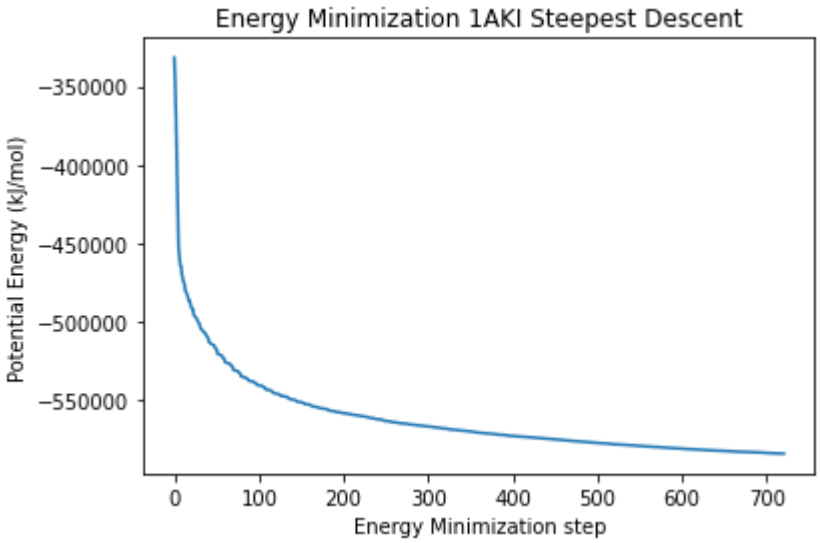
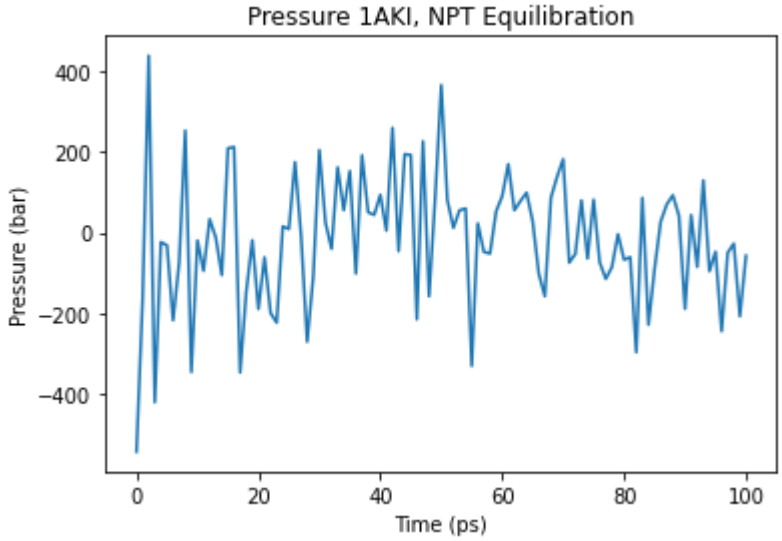
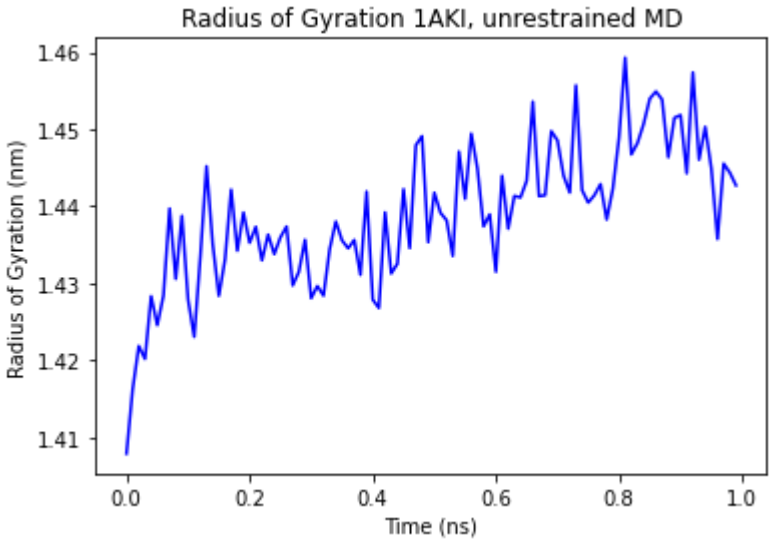
In [1]:
```
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
data = pd.read_csv('../Week3/density_1AKI_equil.xvg', sep='\s+', skiprows=24, header=No
data.columns = ['Time (ps)', 'Density (kg/m^-3)']
plt.plot(data['Time (ps)'], data['Density (kg/m^-3)'])
plt.xlabel('Time (ps)')
plt.ylabel('Density (kg/m^-3)')
plt.title('Density 1AKI, NPT Equilibration')
plt.show()

data = pd.read_csv('../Week3/minimization_potential_energy.xvg', sep='\s+', skiprows=24
data.columns = ['Energy Minimization step', 'Potential Energy (kJ/mol)']
plt.plot(data['Energy Minimization step'], data['Potential Energy (kJ/mol)'])
plt.xlabel('Energy Minimization step')
plt.ylabel('Potential Energy (kJ/mol)')
plt.title('Energy Minimization 1AKI Steepest Descent')
plt.show()

data = pd.read_csv('../Week3/pressure_npt_equil.xvg', sep='\s+', skiprows=24, header=No
data.columns = ['Time (ps)', 'Pressure (bar)']
plt.plot(data['Time (ps)'], data['Pressure (bar)'])
plt.xlabel('Time (ps)')
plt.ylabel('Pressure (bar)')
plt.title('Pressure 1AKI, NPT Equilibration')
plt.show()

#read data from file
data = np.genfromtxt('r_gyrate_1AKI.xvg', skip_header=27, skip_footer=1)

#plot data
plt.plot(data[:,0]/1000, data[:,1], 'b-')
plt.xlabel('Time (ns)')
plt.ylabel('Radius of Gyration (nm)')
plt.title('Radius of Gyration 1AKI, unrestrained MD')
plt.show()

#read data from rmsd.xvg
data = np.genfromtxt('rmsd.xvg', skip_header=18, skip_footer=1)
time = data[:,0]
rmsd = data[:,1]

#read data from rmsd_crystal.xvg
data = np.genfromtxt('rmsd_crystal.xvg', skip_header=18, skip_footer=1)
time_crystal = data[:,0]
rmsd_crystal = data[:,1]

#plot
plt.plot(time, rmsd, label='Equilibrated')
plt.plot(time_crystal, rmsd_crystal, label='Crystal')
plt.xlabel('Time (ps)')
plt.ylabel('RMSD (nm)')
plt.legend()
plt.title('RMSD 1AKI, Backbone')
plt.savefig('rmsd.png')
plt.show()

data = pd.read_csv('../Week3/temperature_progression_1AKI.xvg', sep='\s+', skiprows=24,
data.columns = ['Time (ps)', 'Temperature (K)']
```

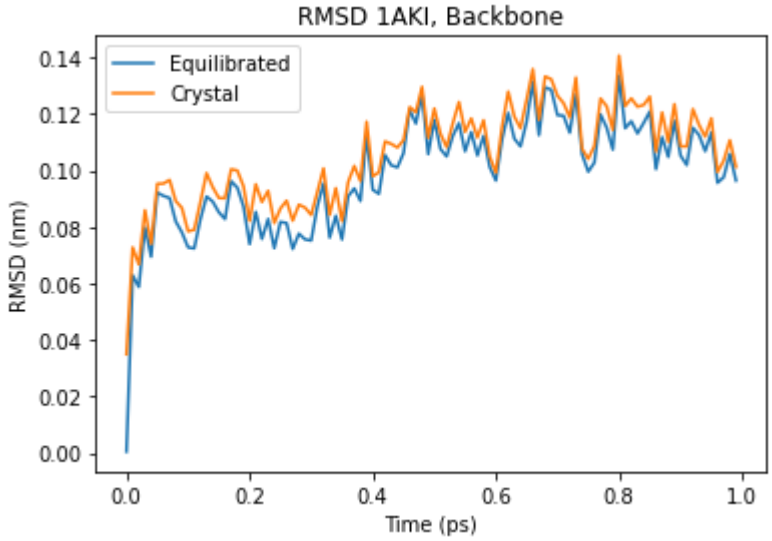
```
plt.plot(data['Time (ps)'], data['Temperature (K)'])
plt.xlabel('Time (ps)')
plt.ylabel('Temperature (K)')
plt.title('Temperature 1AKI, NVT Equilibration')
plt.show()
```

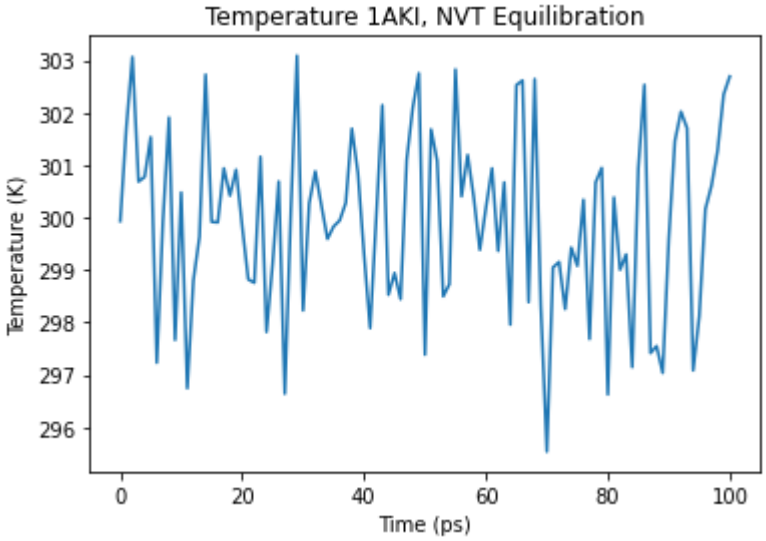







Radius of Gyration 1AKI, unrestrained MD
Radius of Gyration (nm)
1.46
1.45
1.44
1.43
1.42
1.41
0.0
0.2
0.4
0.6
0.8
1.0
Time (ns)


RMSD 1AKI, Backbone
Equilibrated
Crystal
RMSD (nm)
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
0.0
0.2
0.4
0.6
0.8
1.0
Time (ps)


Temperature 1AKI, NVT Equilibration
Temperature (K)
303
302
301
300
299
298
297
296
0
20
40
60
80
100
Time (ps)

In [ ]:

In [ ]: