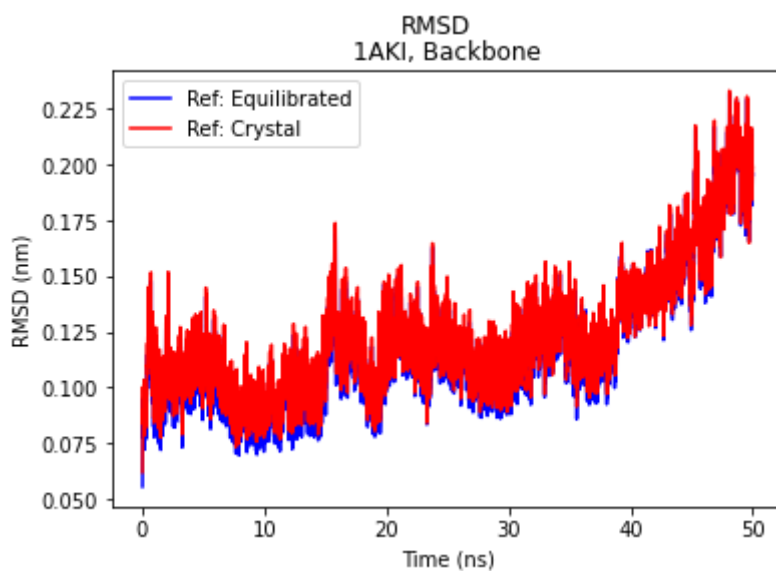


```
In [4]: import matplotlib.pyplot as plt
import numpy as np

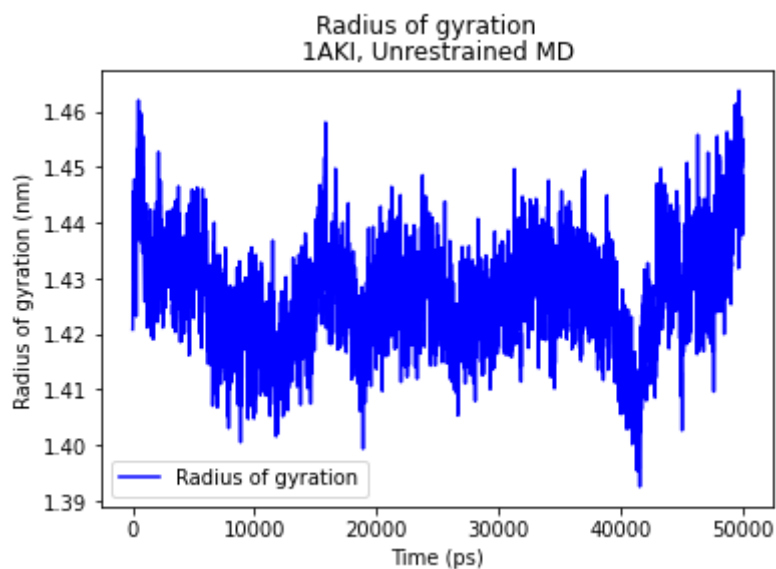
# open RMSD.xvg and RMSD_xtal.xvg and read from line 19
rmsd_xtc = np.loadtxt('RMSD.xvg', skiprows=19)
rmsd_xtal = np.loadtxt('RMSD_xtal.xvg', skiprows=19)

# plot RMSD (nm) from both files vs time (ns)
plt.plot(rmsd_xtc[:,0], rmsd_xtc[:,1], label='Ref: Equilibrated', color='blue')
plt.plot(rmsd_xtal[:,0], rmsd_xtal[:,1], label='Ref: Crystal', color='red')
plt.xlabel('Time (ns)')
plt.ylabel('RMSD (nm)')
plt.suptitle('RMSD')
plt.title('1AKI, Backbone')
plt.legend()
plt.show()
```



```
In [5]: # open gyrate.xvg and read from line 28
gyrate = np.loadtxt('gyrate.xvg', skiprows=28)

# plot radius of gyration (nm) vs time (ps)
plt.plot(gyrate[:,0], gyrate[:,1], label='Radius of gyration', color='blue')
plt.xlabel('Time (ps)')
plt.ylabel('Radius of gyration (nm)')
plt.suptitle('Radius of gyration')
plt.title('1AKI, Unrestrained MD')
plt.legend()
plt.show()
```



```
In [ ]:
```