

A

NumPy

```
import numpy as np
import MDAnalysis as mda
```

```
u = mda.Universe("topol.tpr", "trj.xtc")
```

```
ca = u.select_atoms("name CA")
```

```
means = np.zeros((len(ca), 3))
```

```
sumsq = np.zeros_like(means)
```

```
for k, ts in enumerate(u.trajectory):
```

```
    sumsq += (k/(k+1.0)) *
```

```
        (ca.positions - means)**2
```

```
    means[:] = (k*means + ca.positions)/(k+1.0)
```

```
rmsf = np.sqrt(sumsq.sum(axis=1)/(k+1.0))
```

```
matplotlib.pyplot.plot(ca.residues.resids, rmsf)
```

B