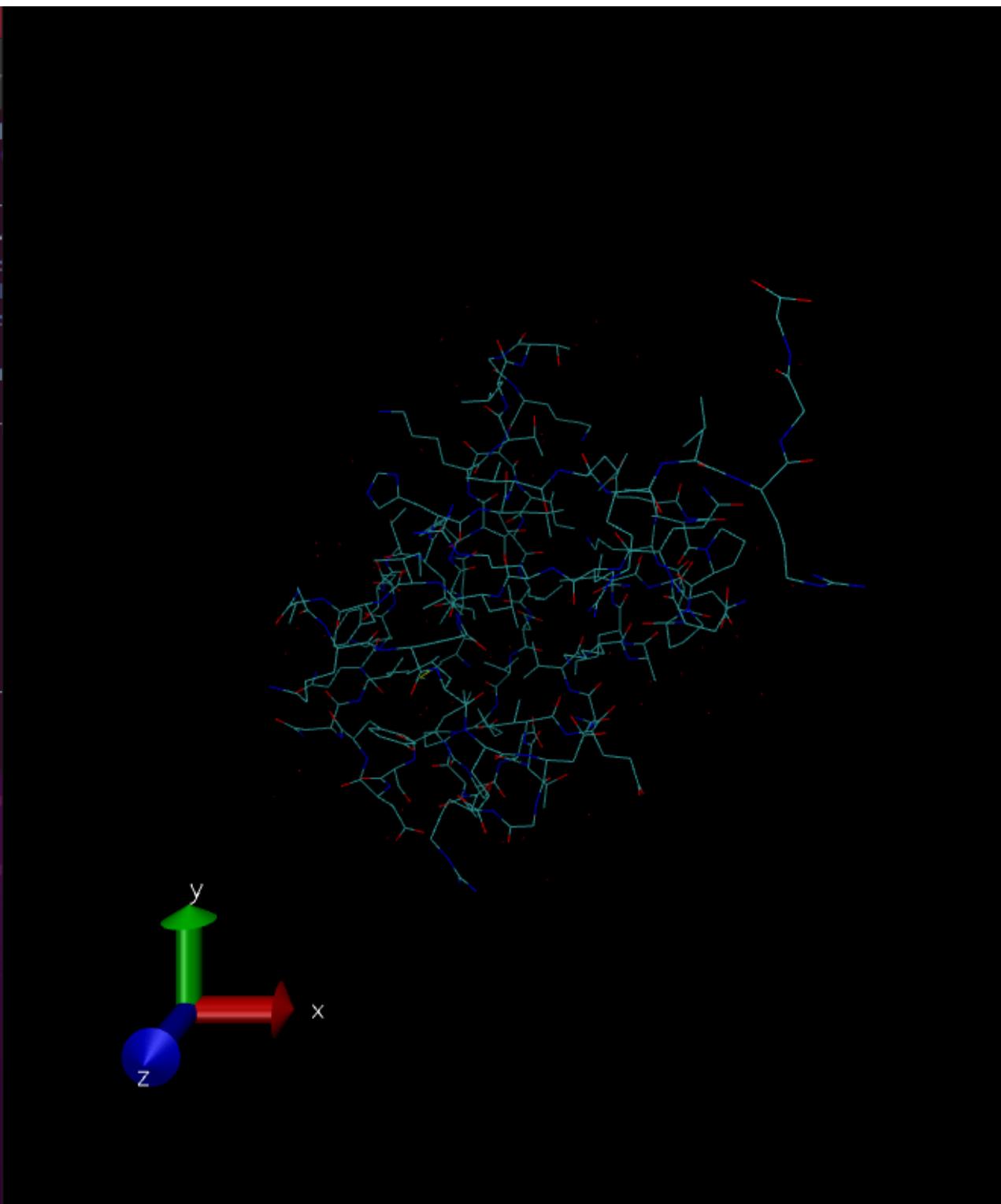


# **RESULTS OF THE NAMD TUTORIAL FILE**

## 1UBQ.pdb

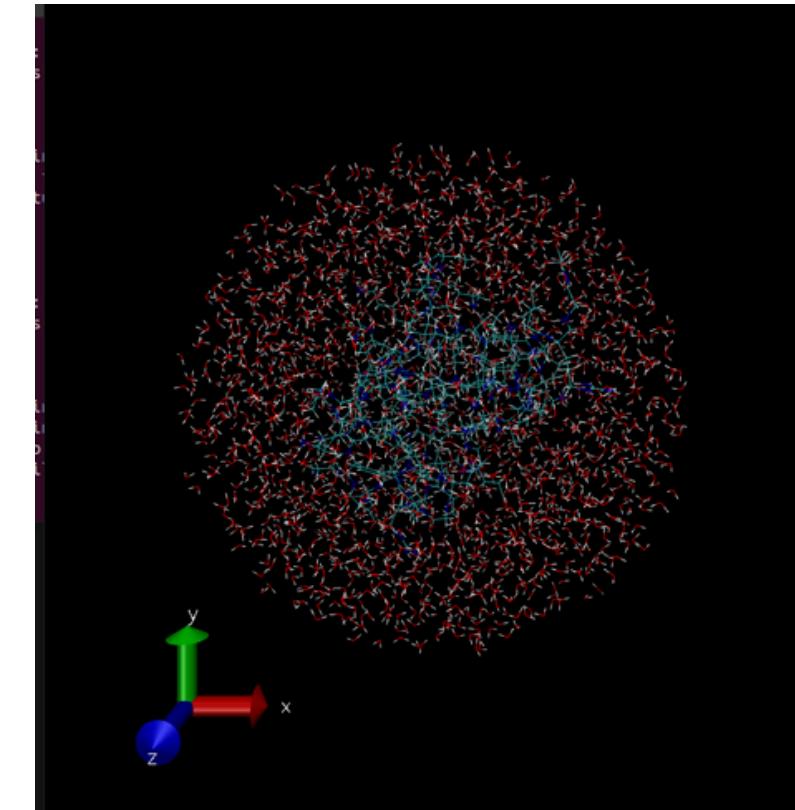


Ubiquitin X-Ray structure obtained from Protein Data Bank and visualised on VMD

```
5
Info) Using plugin pdb for coordinates from file ubq_ws.pdb
Info) Finished with coordinate file ubq_ws.pdb.
5
CENTER OF MASS OF SPHERE IS: 30.313770294189453 28.9261531829834 15.284436225891
113
RADIUS_OF_SPHERE IS: 25.33897531251609
vmd > █
```

Radius of Water Sphere obtained (to be used later on in the minimization and equilibration step)

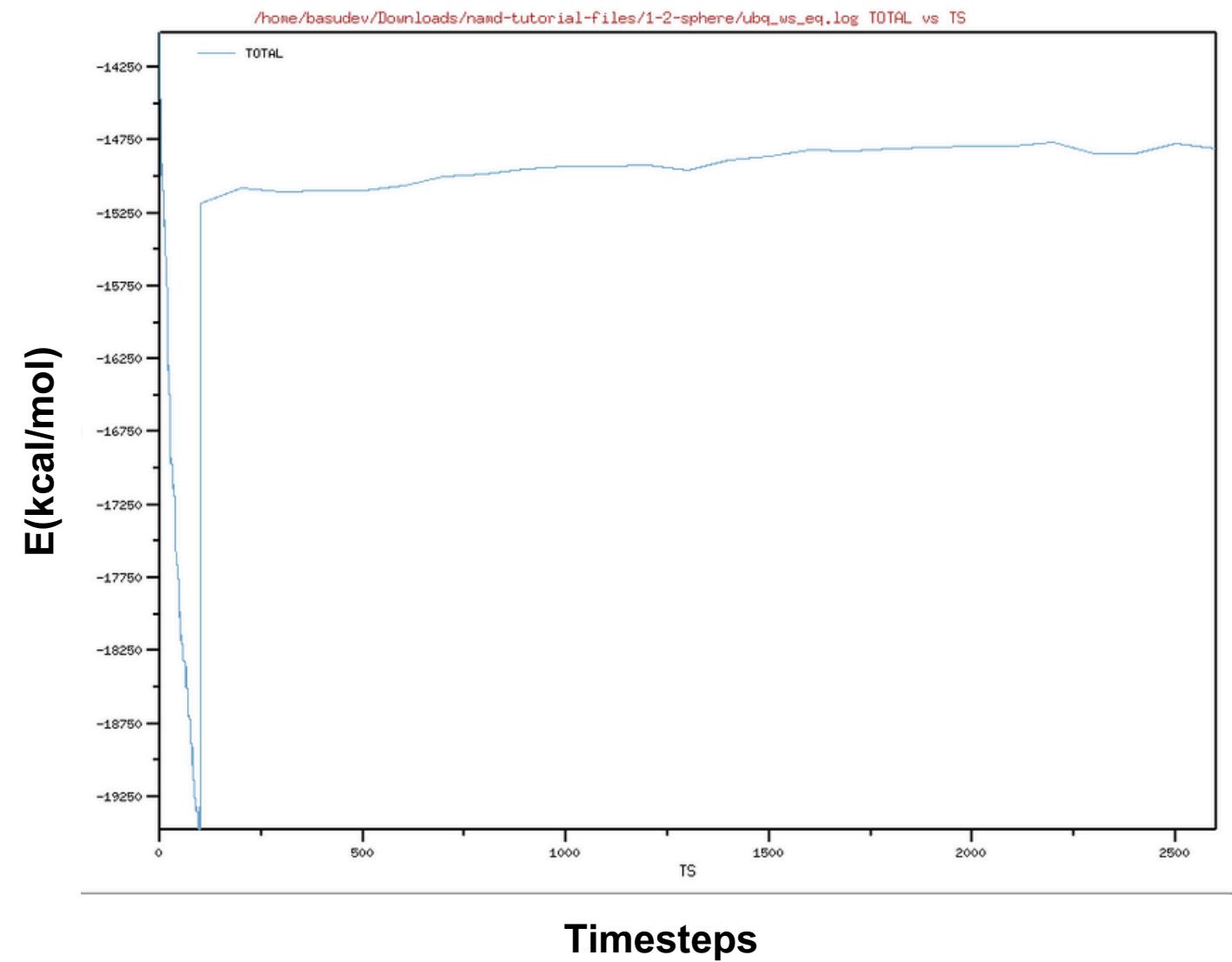
## ubq\_ws.psf



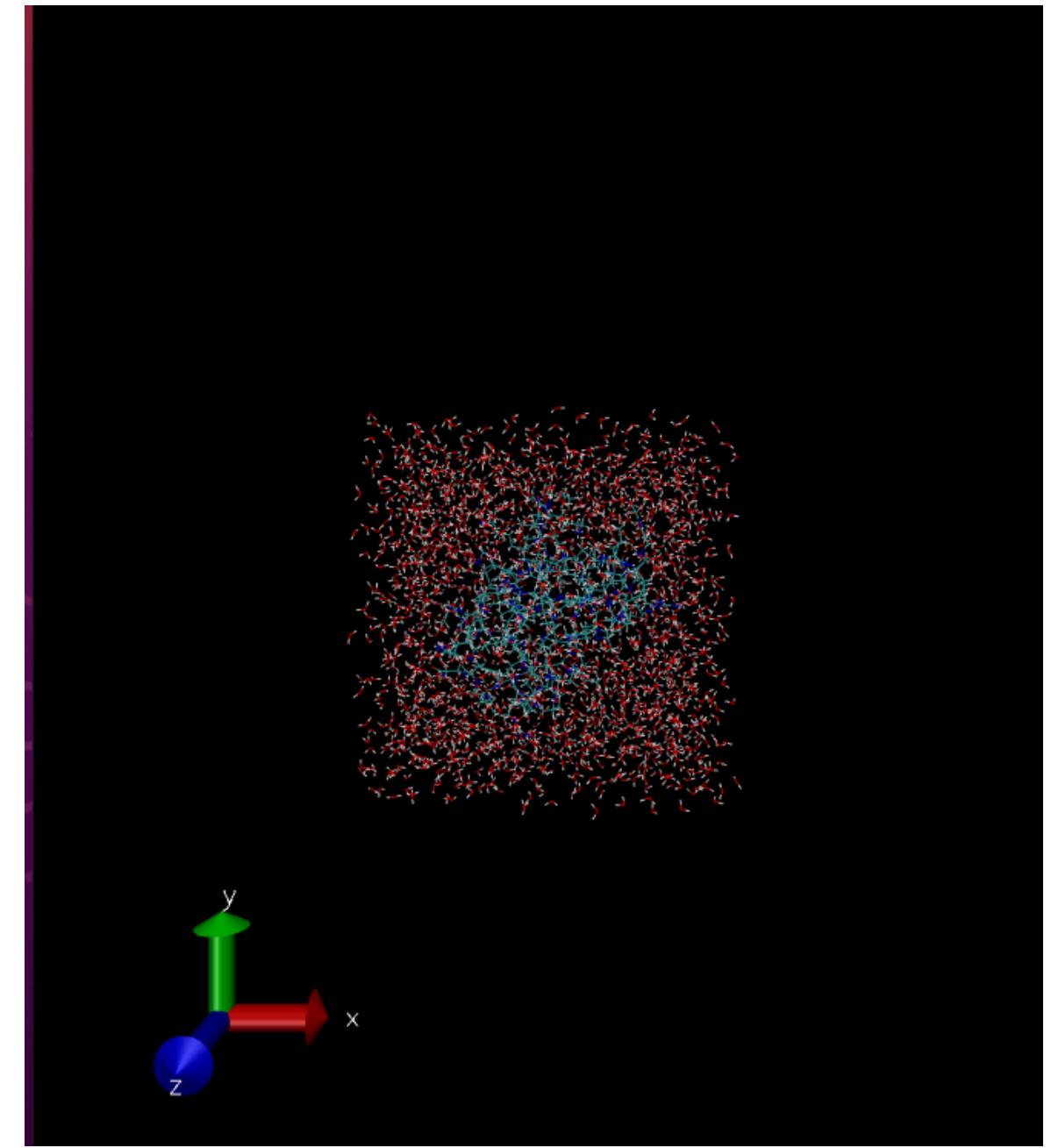
Creation of ubiquitin water sphere to simulate the protein surrounded by water in vacuum

**ubq\_wb.psf**

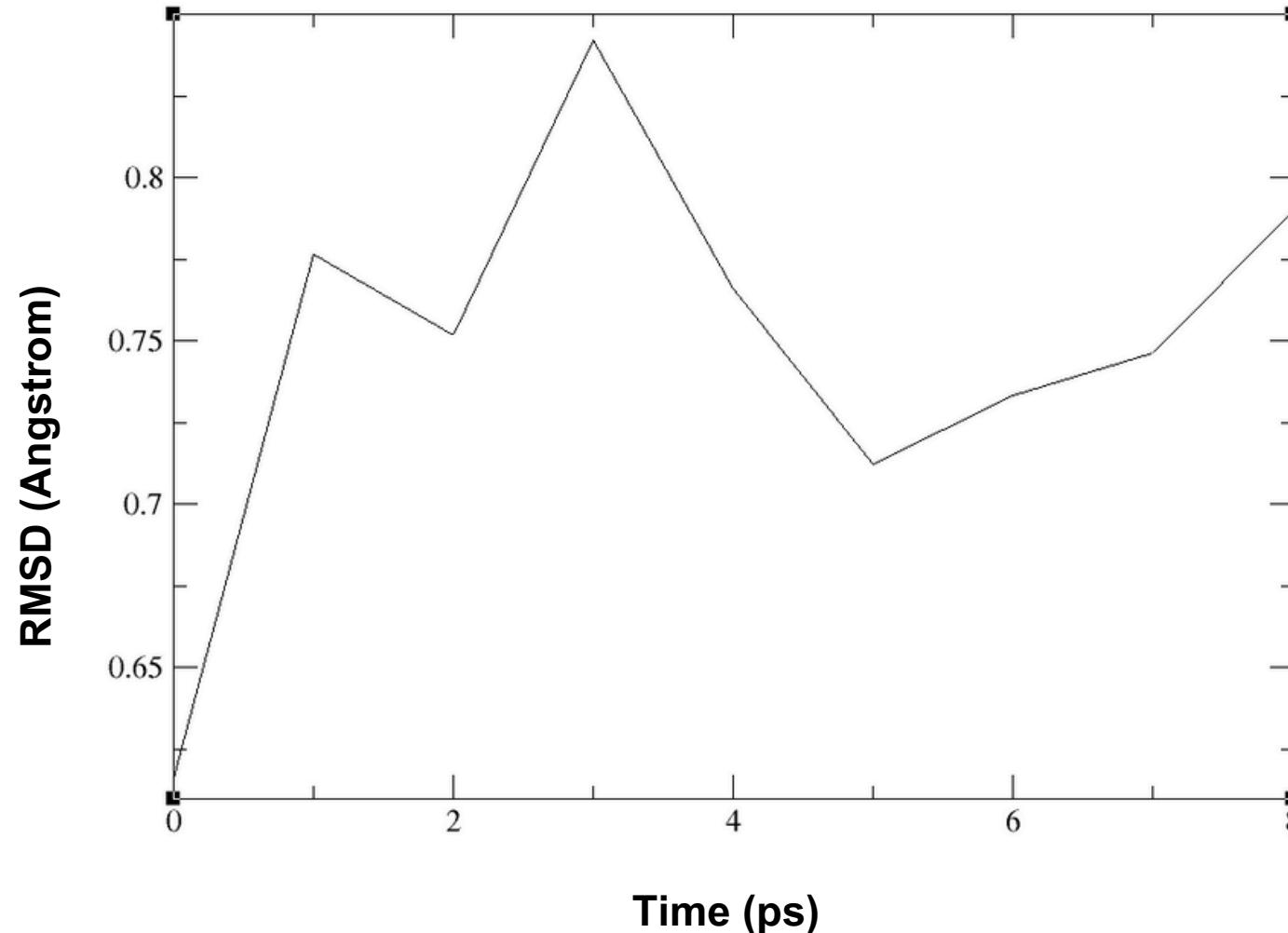
### Temperature vs Time Steps for ubq\_ws\_eq.log



**Analysis of water-sphere equilibrium (E(kcal-mol) vs TS)**  
**(Variable converging to an average value to signify an equilibrated system)**



## RMSD for protein (xmgrace rmsd.dat)



## Average rmsd per residue

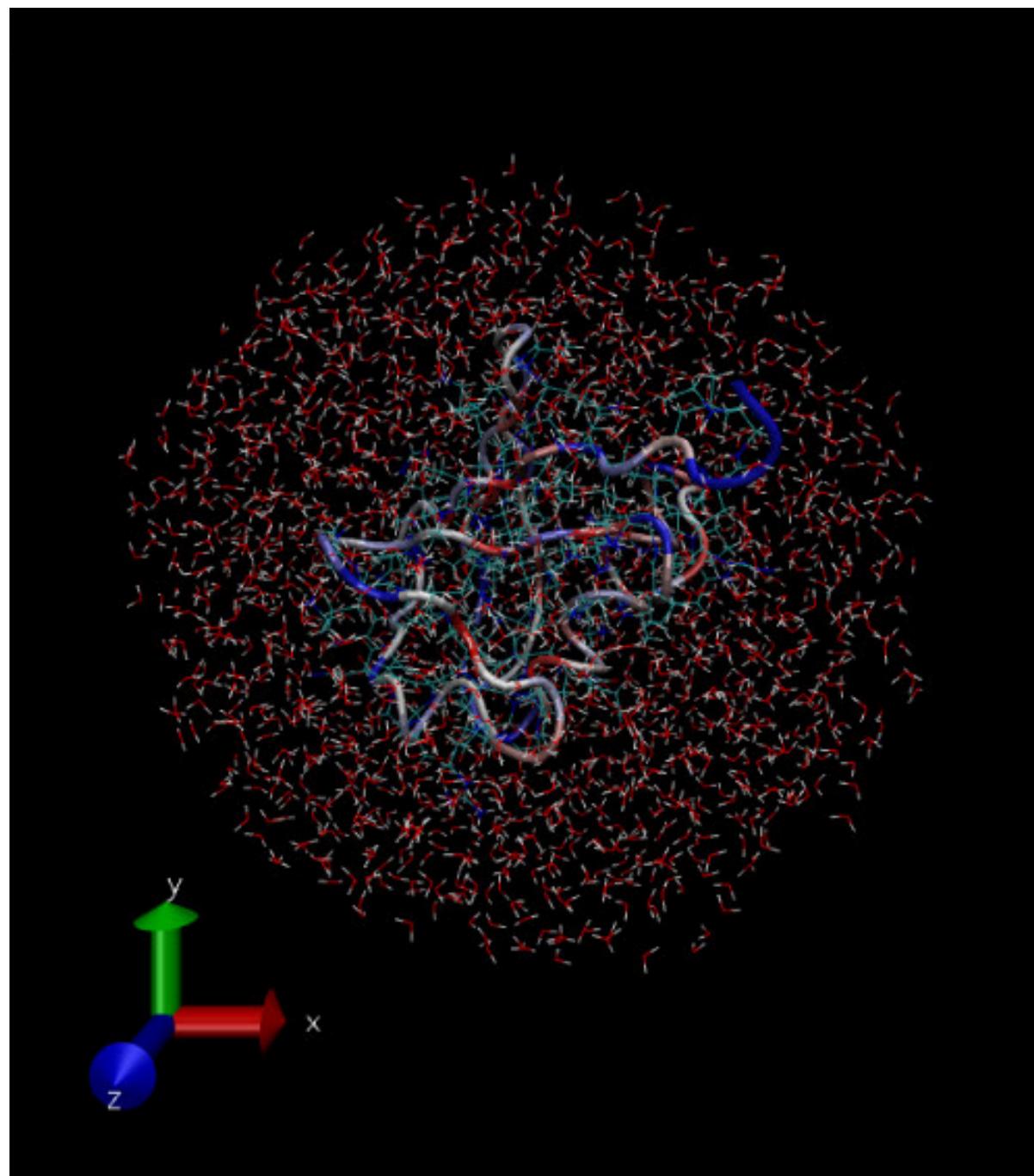
VMD TkConsole window showing the command-line interface for VMD. The console output lists the RMSD for each residue (59 to 76) and calculates the average RMSD per residue.

```
RMSD of residue 59 is 0.7257629722356796
RMSD of residue 60 is 1.2666749477386474
RMSD of residue 61 is 0.7317290157079697
RMSD of residue 62 is 0.7977995157241822
RMSD of residue 63 is 0.7634912967681885
RMSD of residue 64 is 1.145518308877945
RMSD of residue 65 is 0.6974837124347687
RMSD of residue 66 is 0.769138103723526
RMSD of residue 67 is 0.37842662930488585
RMSD of residue 68 is 0.7963787376880646
RMSD of residue 69 is 0.43906342685222627
RMSD of residue 70 is 0.5518958061933518
RMSD of residue 71 is 1.3126765608787536
RMSD of residue 72 is 0.840199601650238
RMSD of residue 73 is 0.624832421541214
RMSD of residue 74 is 1.0111189842224122
RMSD of residue 75 is 1.573327511548996
RMSD of residue 76 is 1.4230657696723938
Average rmsd per residue: 0.749431367257708
>Main< (2-1-rmsd) 19 %
```

This procedure is further used to colour the protein with respect to this average value (it helps us to see how much each residue deviates from a reference structure)

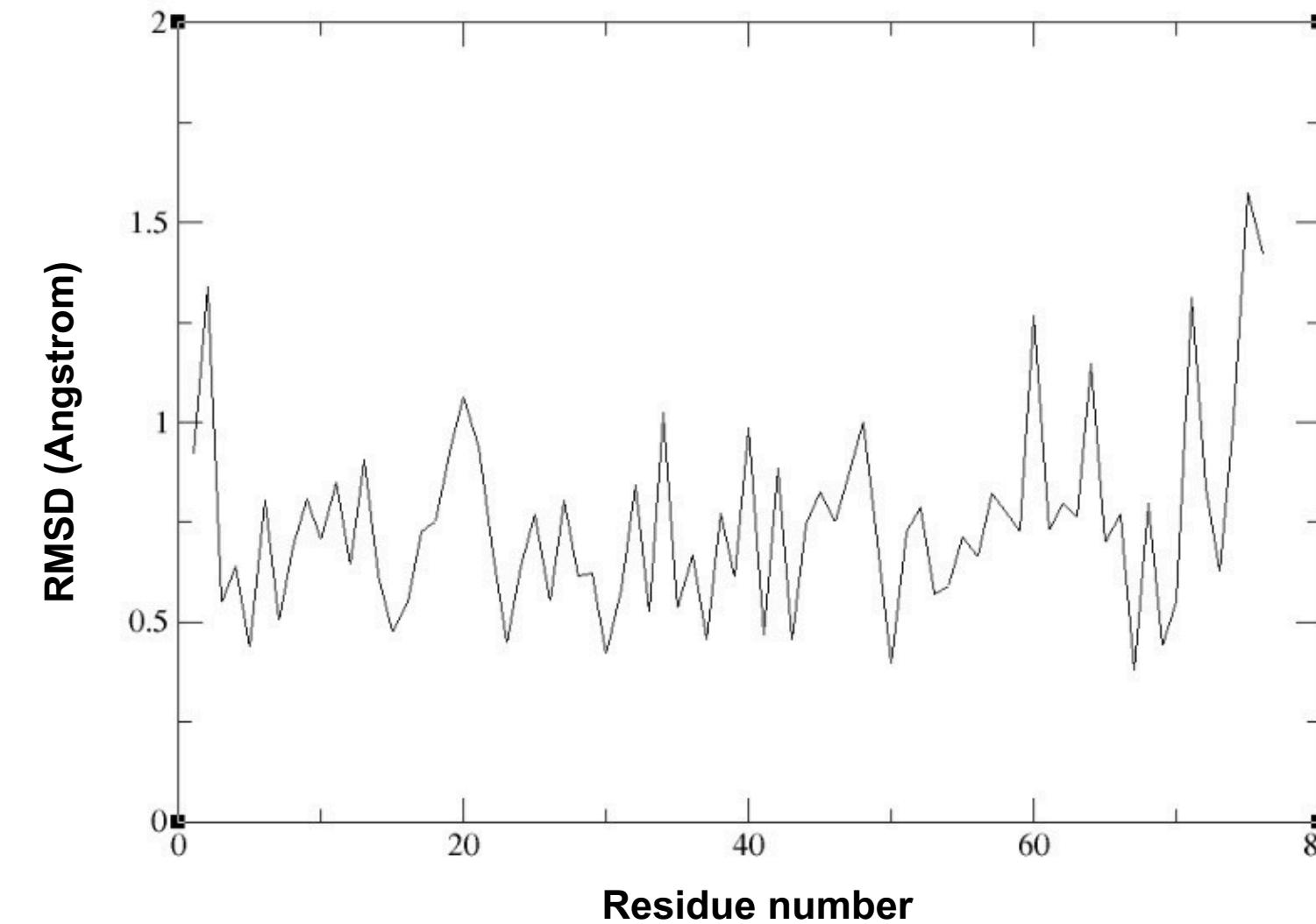
RMSD Curve Flattening (initially rises and then flattens) : protein moving away from it's initial state and then attaining equilibrium

## ubq\_ws.psf with BGR Color Scale



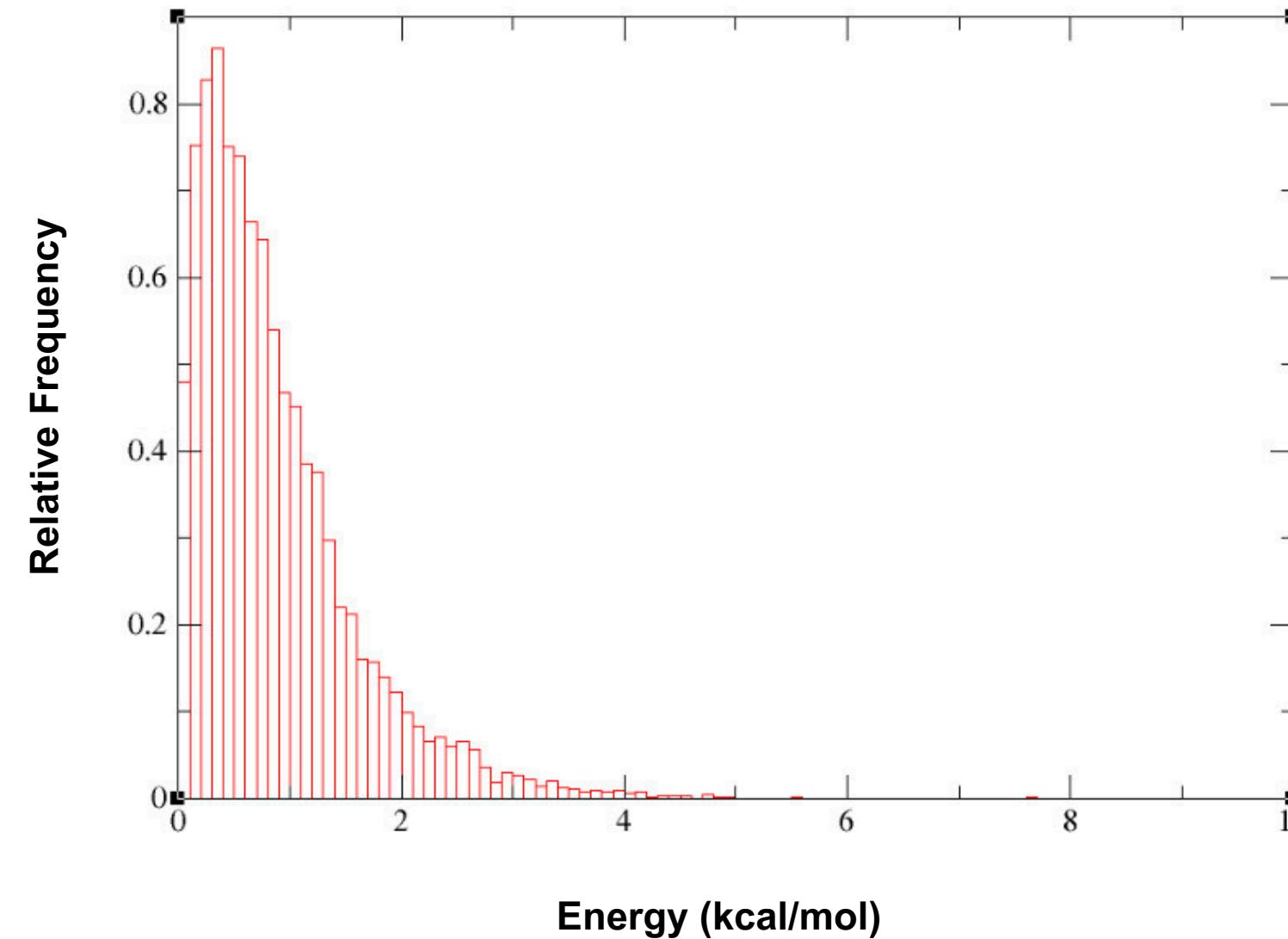
Coloured ubiquitin with respect to average value  
(Helps us see which residues are free to move more  
and which ones less during equilibration) Blue: more  
mobile, Red: Less Mobile

## residue\_rmsd.dat



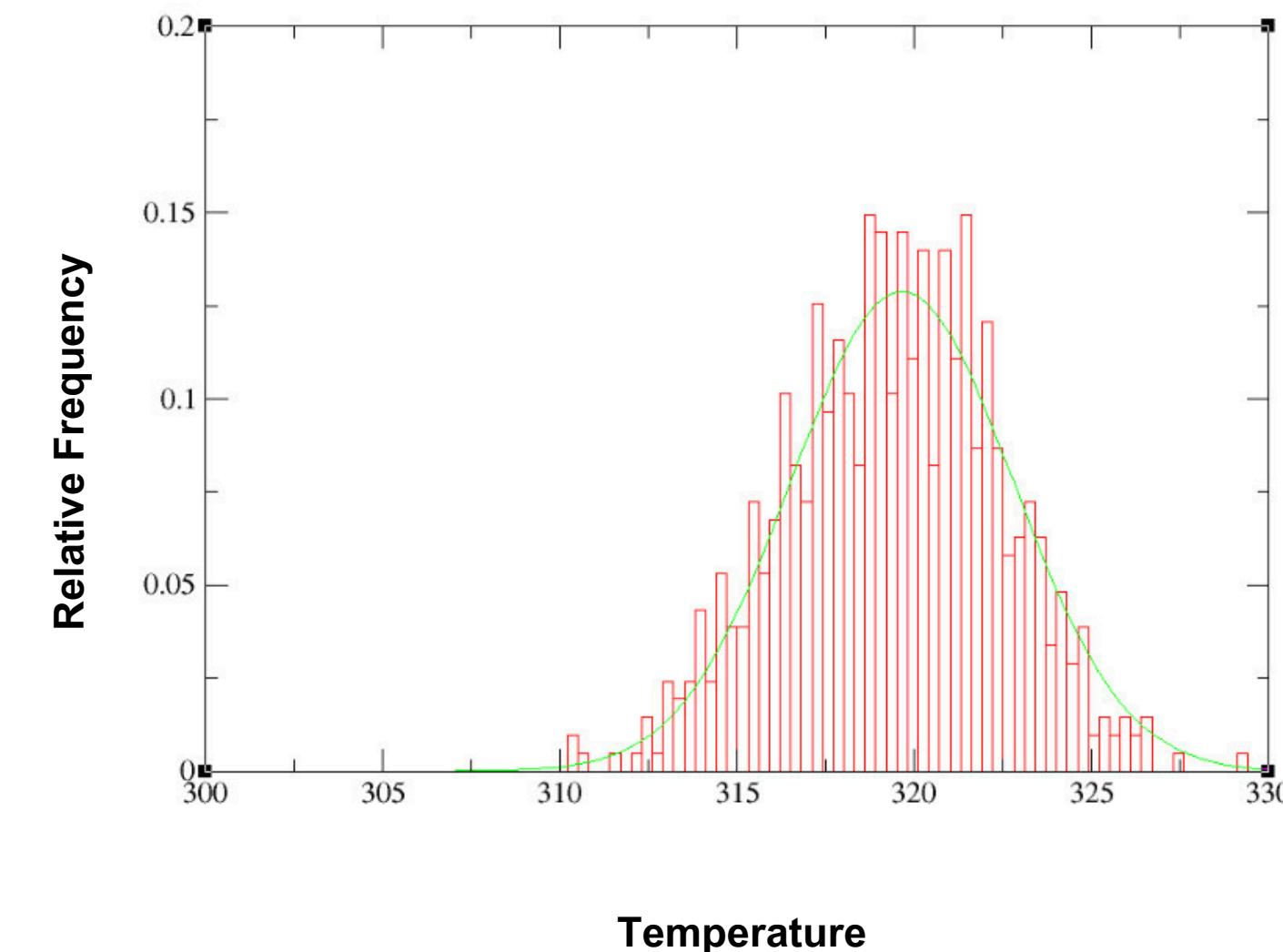
RMSD value per residue: Helps us see where a set  
of residues shows lesser mobility

## Maxwell Boltzmann Distribution of KE among particles (Relative freq vs energy)



The Maxwell Boltzmann Distribution is the expected statistical behavior for a system at thermal equilibrium at a given temperature. Therefore our system shows realistic dynamics

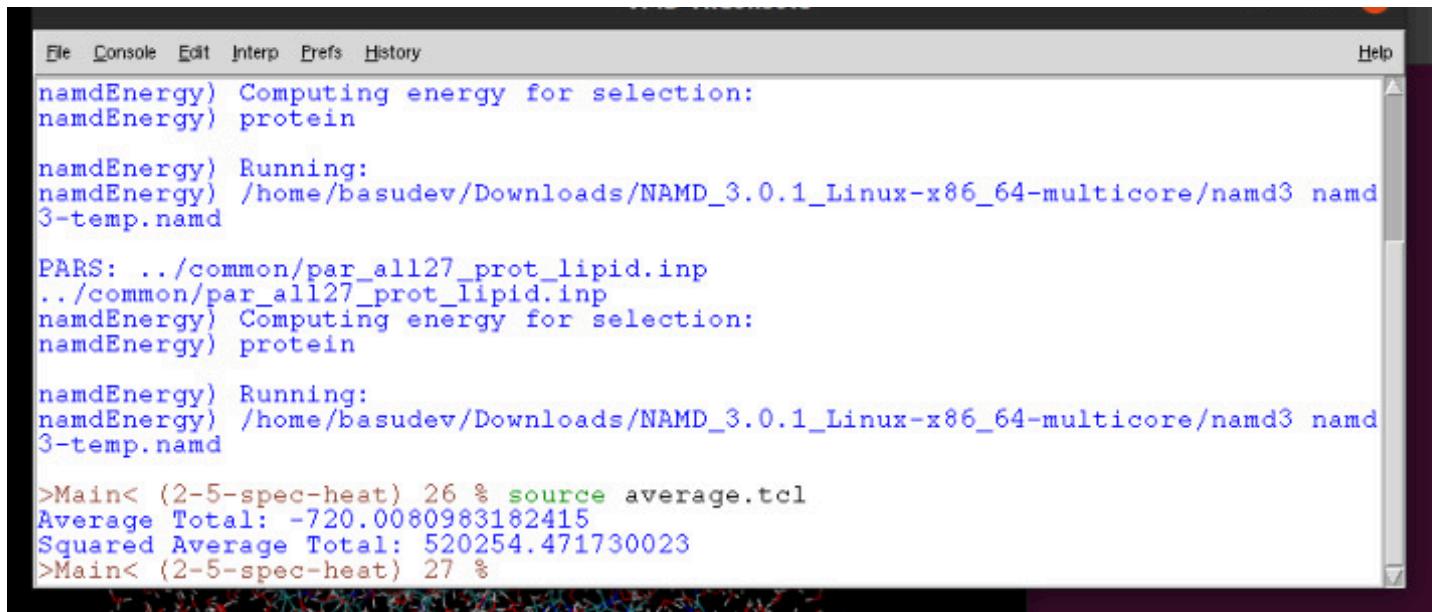
## Fluctuation of Temperature in a finite sample (Relative Freq vs temperature)



The Gaussian Distribution signifies that most of the single proteins cluster around a mean temperature but show finiteness in the form of temperature fluctuations

## Cooling of ubiquitin in a water sphere

### Average and squared average total energy over all timesteps



```
File Console Edit Interp Prefs History Help
namdEnergy) Computing energy for selection:
namdEnergy) protein

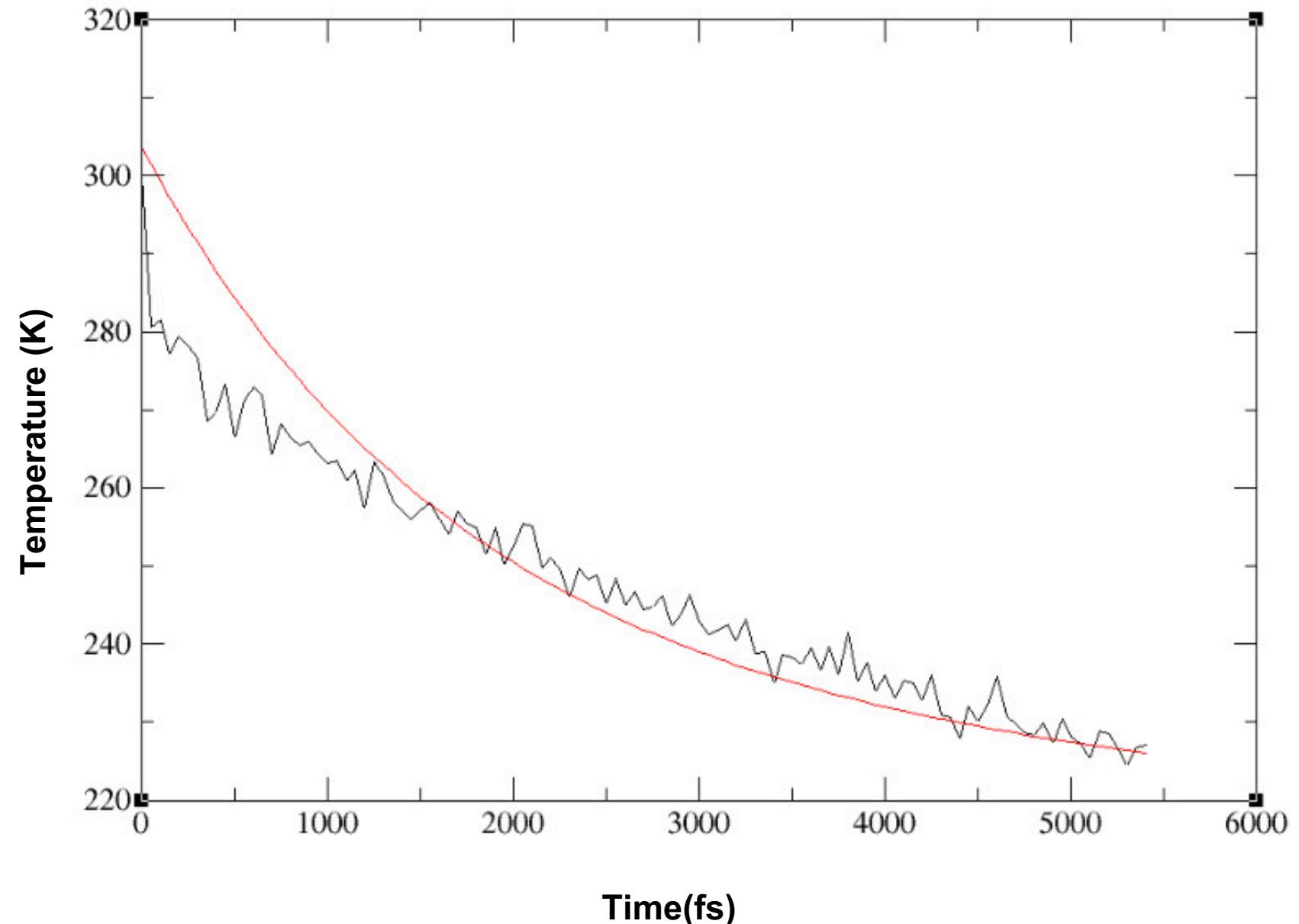
namdEnergy) Running:
namdEnergy) /home/basudev/Downloads/NAMD_3.0.1_Linux-x86_64-multicore/namd3 namd3-temp.namd

PARS: .../common/par_all27_prot_lipid.inp
.../common/par_all27_prot_lipid.inp
namdEnergy) Computing energy for selection:
namdEnergy) protein

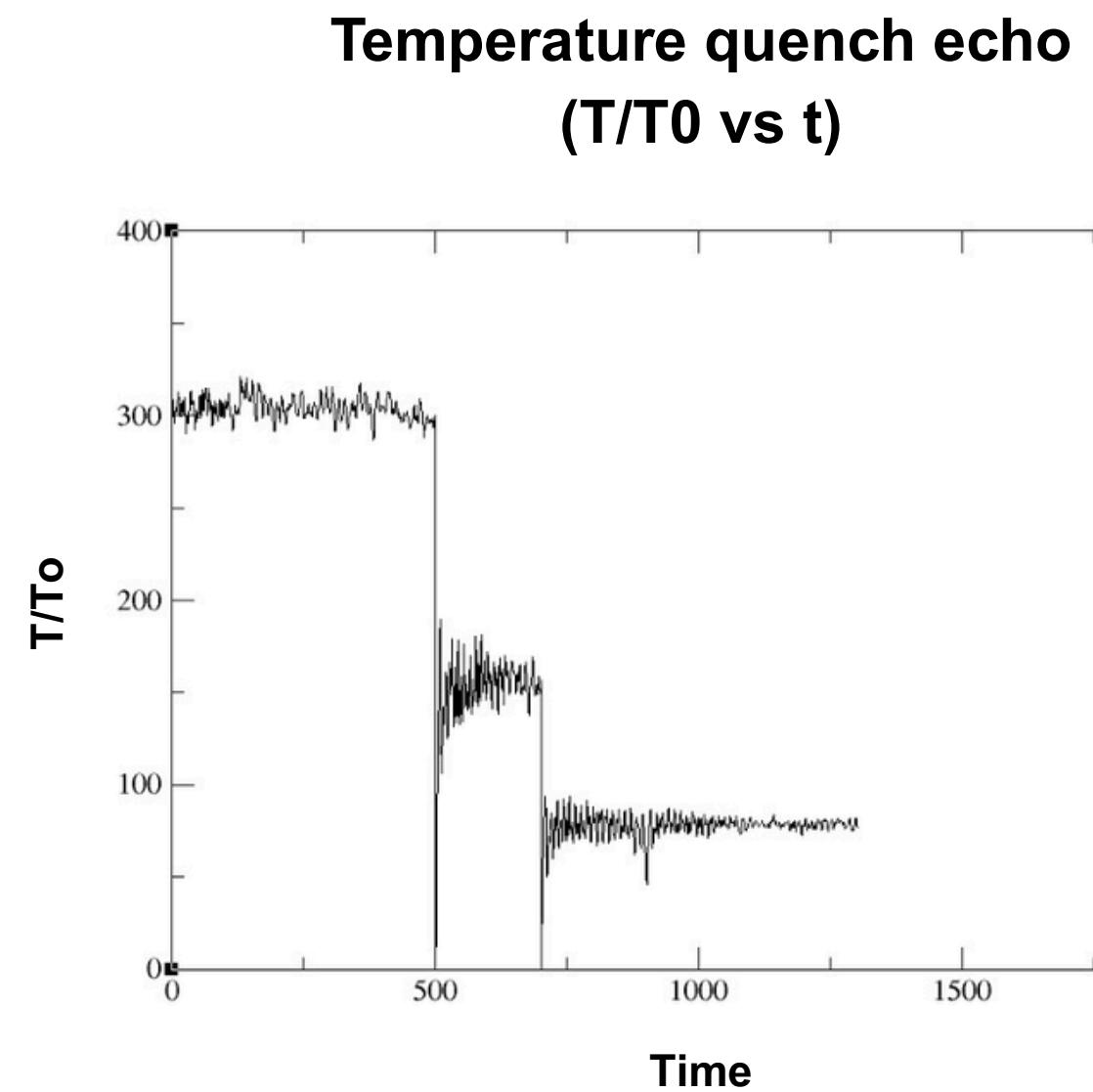
namdEnergy) Running:
namdEnergy) /home/basudev/Downloads/NAMD_3.0.1_Linux-x86_64-multicore/namd3 namd3-temp.namd

>Main< (2-5-spec-heat) 26 % source average.tcl
Average Total: -720.0080983182415
Squared Average Total: 520254.471730023
>Main< (2-5-spec-heat) 27 %
```

These values are calculated in order to further compute the variance and to track how much energy deviates from its mean value during the process of equilibration

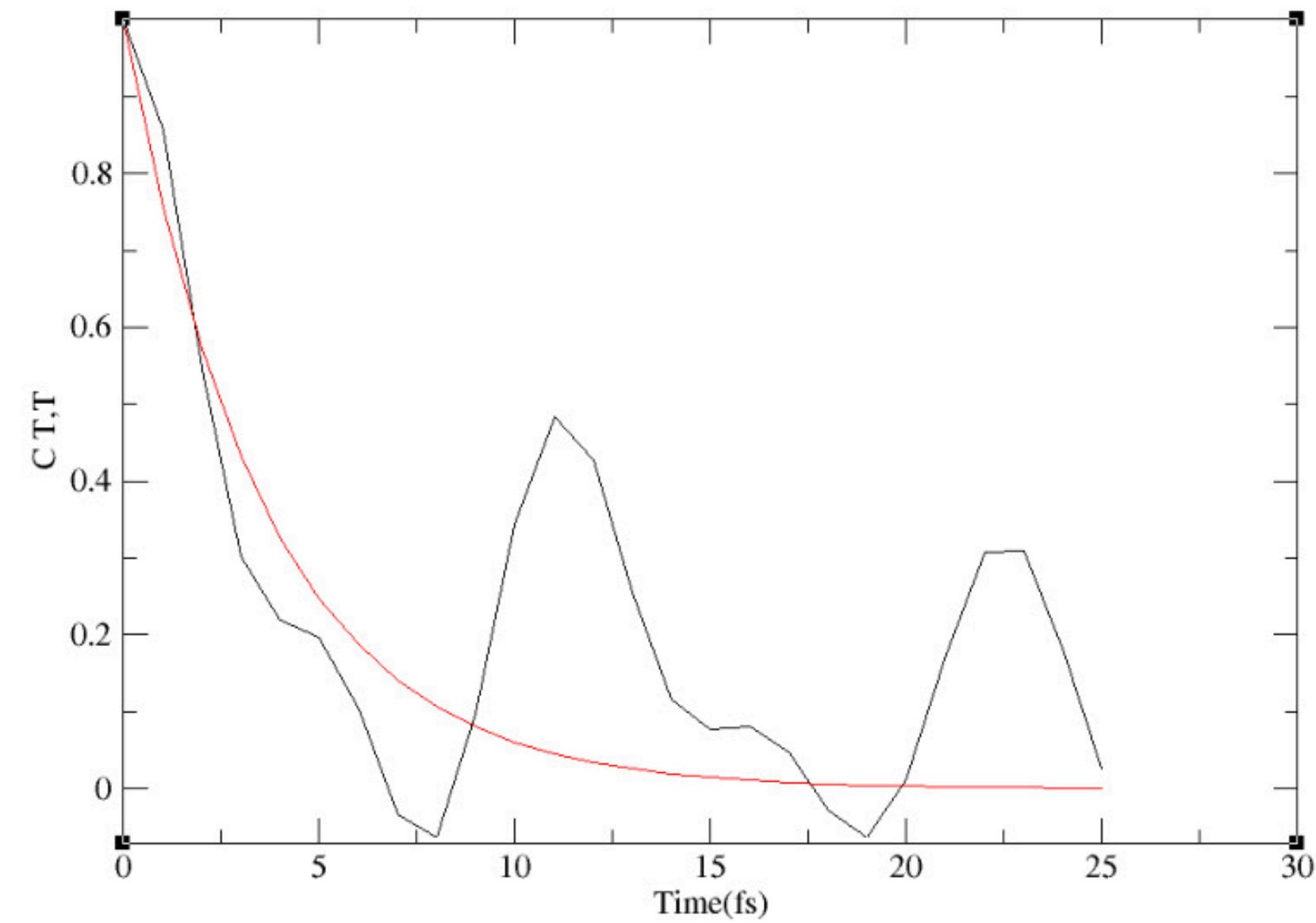


Simulating cooling will help in understanding how the protein molecule responds to temperature changes. We see there is an exponential decay and fluctuations decay with time as system comes to equilibrium)



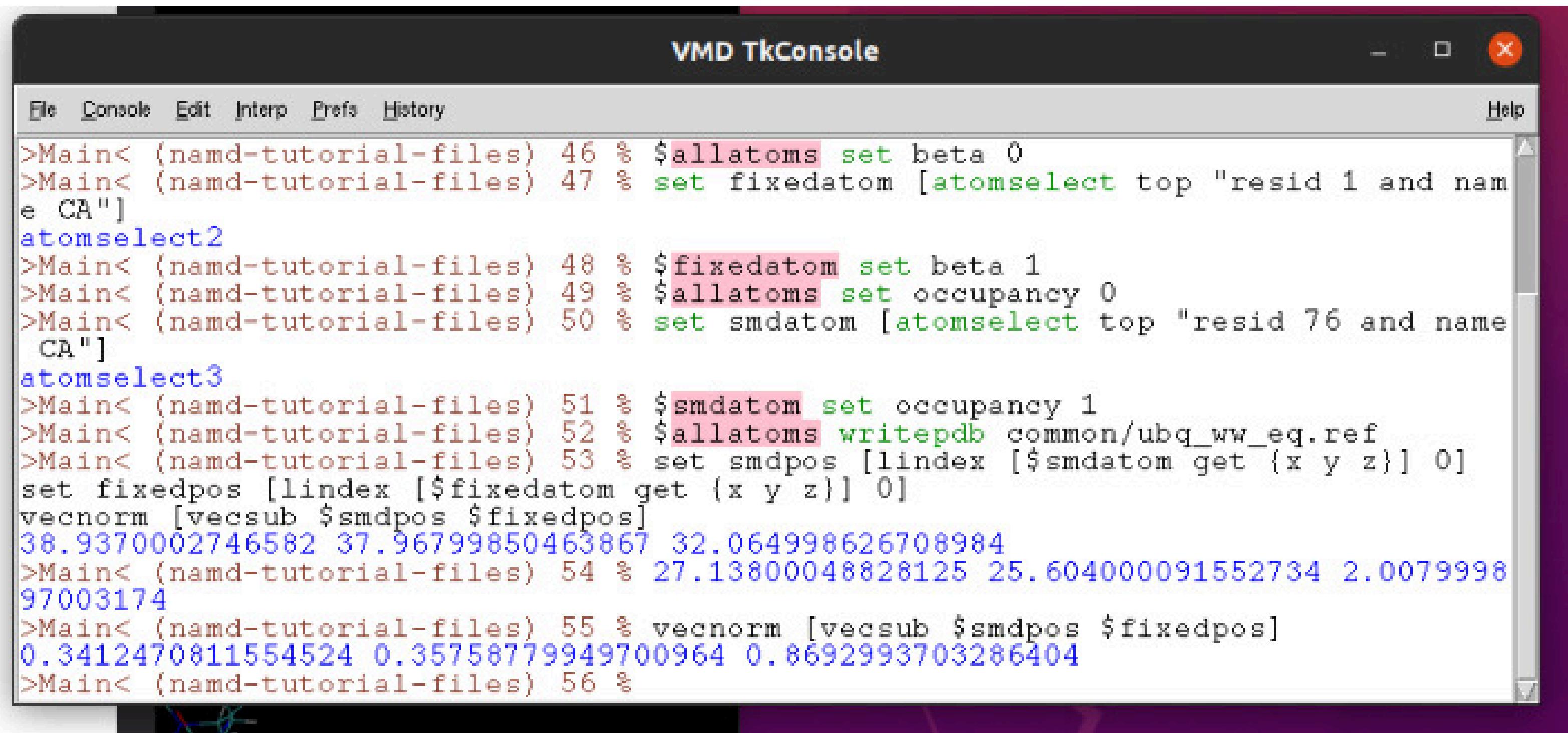
**The temperature echo plot shows how the system goes back to its initial state after velocity reassessments or temperature quenches (shows coordination and phase coherence of the protein's molecules)**

### Temperature Autocorrelation Function



**The autocorrelation helps us in analyzing the temperature echoes later on and can be fit to a decaying approximation (producing the new simulations)**

## Normalized direction between fixed and SMD atom



The image shows a screenshot of the VMD TkConsole window. The title bar reads "VMD TkConsole". The menu bar includes "File", "Console", "Edit", "Interp", "Prefs", "History", and "Help". The main console area displays a series of NAMD command-line inputs and their outputs. The commands involve selecting atoms (e.g., CA), setting occupancy, and calculating normalized directions between atoms. The output includes numerical values for the direction vector components.

```
>Main< (namd-tutorial-files) 46 % $allatoms set beta 0
>Main< (namd-tutorial-files) 47 % set fixedatom [atomselect top "resid 1 and name CA"]
atomselect2
>Main< (namd-tutorial-files) 48 % $fixedatom set beta 1
>Main< (namd-tutorial-files) 49 % $allatoms set occupancy 0
>Main< (namd-tutorial-files) 50 % set smdatom [atomselect top "resid 76 and name CA"]
atomselect3
>Main< (namd-tutorial-files) 51 % $smdatom set occupancy 1
>Main< (namd-tutorial-files) 52 % $allatoms writepdb common/ubq_ww_eq.ref
>Main< (namd-tutorial-files) 53 % set smdpos [lindex [$smdatom get {x y z}] 0]
set fixedpos [lindex [$fixedatom get {x y z}] 0]
vecnorm [vecsub $smdpos $fixedpos]
38.9370002746582 37.96799850463867 32.064998626708984
>Main< (namd-tutorial-files) 54 % 27.13800048828125 25.604000091552734 2.007998
97003174
>Main< (namd-tutorial-files) 55 % vecnorm [vecsub $smdpos $fixedpos]
0.3412470811554524 0.35758779949700964 0.8692993703286404
>Main< (namd-tutorial-files) 56 %
```

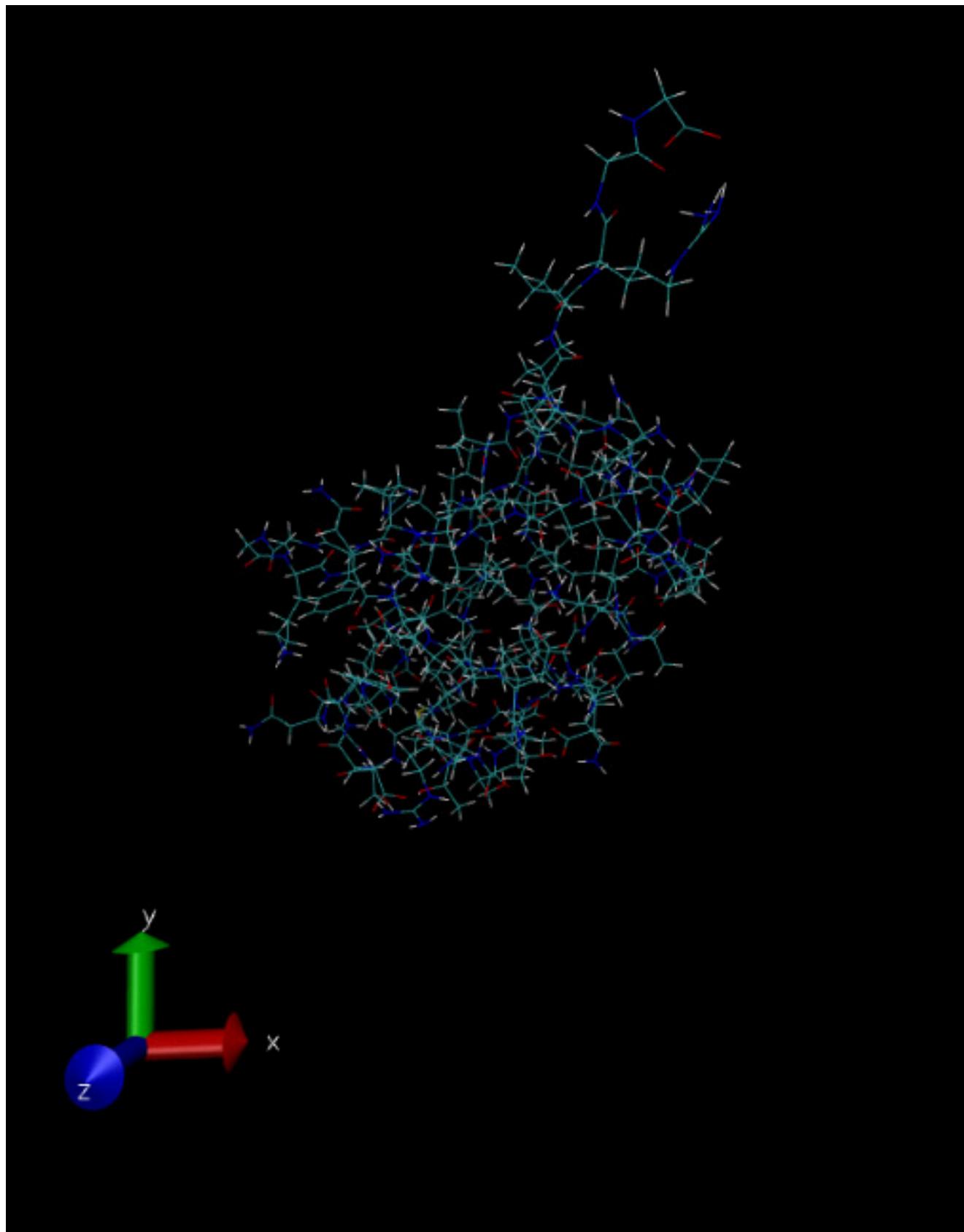
Normalized direction between fixed and SMD atom which is used to create the NAMD configuration file to perform steered molecular dynamics. This is the direction between the fixed and SMD atom.

## Typical Output of an SMD simulation

```
GPRESSURE: 500 0 0 0 0 0 0 0 0 0  
PRESSAVG: 500 0 0 0 0 0 0 0 0 0  
GPRESSAVG: 500 0 0 0 0 0 0 0 0 0  
ENERGY: 500 275.2359 897.9273 396.7279 54.1967 -2469.9322 -218.0132 0.0000 12.6223 1249.5765 198.3413 410.8563 -1051.2>  
  
WRITING EXTENDED SYSTEM TO RESTART FILE AT STEP 500  
OPENING COORDINATE DCD FILE  
WRITING COORDINATES TO DCD FILE ubq_ww_pcv.dcd AT STEP 500  
WRITING COORDINATES TO RESTART FILE AT STEP 500  
FINISHED WRITING RESTART COORDINATES  
The last position output (seq=500) takes 0.000 seconds, 0.693 MB of memory in use  
WRITING VELOCITIES TO RESTART FILE AT STEP 500  
FINISHED WRITING RESTART VELOCITIES  
The last velocity output (seq=500) takes 0.000 seconds, 0.693 MB of memory in use  
SMD 510 39.2586 33.1048 34.5066 341.352 357.698 869.568  
SMD 520 39.4017 32.8221 34.4714 363.418 380.821 925.778  
SMD 530 39.5809 32.7546 34.4073 374.811 392.759 954.8  
SMD 540 39.7058 32.8015 34.5599 351.23 368.049 894.73  
SMD 550 39.7882 32.8767 34.7259 326.447 342.079 831.596  
SMD 560 39.986 32.8959 34.9396 291.581 305.544 742.779  
SMD 570 40.2042 32.9651 35.0103 273.207 286.289 695.972  
SMD 580 40.3262 33.0019 34.9785 277.002 290.266 705.64  
SMD 590 40.4512 33.1192 34.9855 270.252 283.193 688.445  
SMD 600 40.5601 33.2372 35.077 252.189 264.265 642.431  
PRESSURE: 600 0 0 0 0 0 0 0 0  
GPRESSURE: 600 0 0 0 0 0 0 0 0  
PRESSAVG: 600 0 0 0 0 0 0 0 0  
GPRESSAVG: 600 0 0 0 0 0 0 0 0  
ENERGY: 600 285.2216 882.0459 398.9113 59.1983 -2458.8546 -182.5428 0.0000 8.0812 1212.4543 204.5153 398.6506 -1007.9>  
  
SMD 610 40.7199 33.3866 35.0827 241.739 253.315 615.812  
SMD 620 40.8222 33.5995 35.2239 211.236 221.351 538.107  
SMD 630 40.8528 33.7857 35.2643 200.92 210.541 511.828  
SMD 640 40.9549 33.9223 35.2031 204.159 213.935 520.078  
SMD 650 40.8714 34.0238 35.2324 206.94 216.849 527.163  
SMD 660 40.7733 34.0397 35.2422 218.429 228.889 556.431  
SMD 670 40.8148 34.0839 35.2283 223.763 234.478 570.017  
SMD 680 40.8023 34.1109 35.0814 252.366 264.451 642.882  
SMD 690 40.7871 34.1966 35.0035 267.669 280.487 681.865  
SMD 700 40.7978 34.2034 34.7933 305.297 319.916 777.719  
PRESSURE: 700 0 0 0 0 0 0 0 0  
GPRESSURE: 700 0 0 0 0 0 0 0 0  
PRESSAVG: 700 0 0 0 0 0 0 0 0  
GPRESSAVG: 700 0 0 0 0 0 0 0 0  
ENERGY: 700 294.6659 887.0051 393.2648 52.0373 -2480.9782 -190.4471 0.0000 11.8433 1242.3470 209.7381 408.4792 -1032.6>  
  
SMD 710 40.9059 34.0305 34.834 311.855 326.789 794.426  
SMD 720 40.9012 33.8826 35.0417 299.235 313.564 762.277  
SMD 730 40.9963 33.7357 35.1049 301.74 316.189 768.658  
SMD 740 41.2585 33.6651 35.0469 307.754 322.491 783.979  
  
^G Get Help ^O Write Out ^W Where Is ^K Cut Text ^J Justify ^C Cur Pos ^M-U Undo ^M-A Mark Text ^M-] To Bracket ^M-Q Previous ^B Back ^E Prev Word  
^X Exit ^R Read File ^\ Replace ^U Paste Text ^T To Spell ^A Go To Line ^M-E Redo ^M-6 Copy Text ^O Where Was ^M-W Next ^F Forward ^L Next Word
```

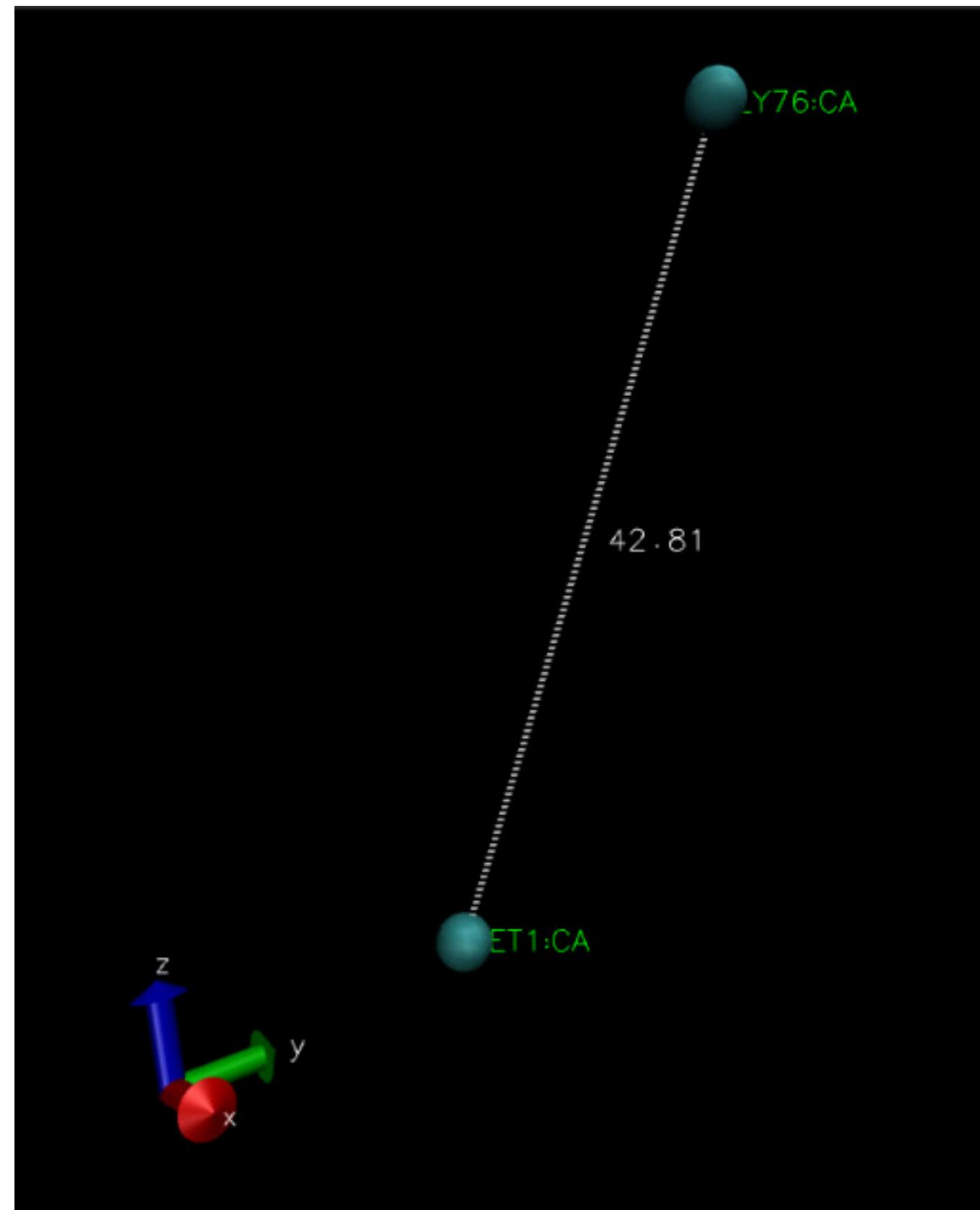
The columns show the word ‘SMD’, the number of timesteps, the coordinates of the atoms (3) and components of the current force applied to the SMD atom in pN (3)

## Ubiquitin pulling with constant velocity



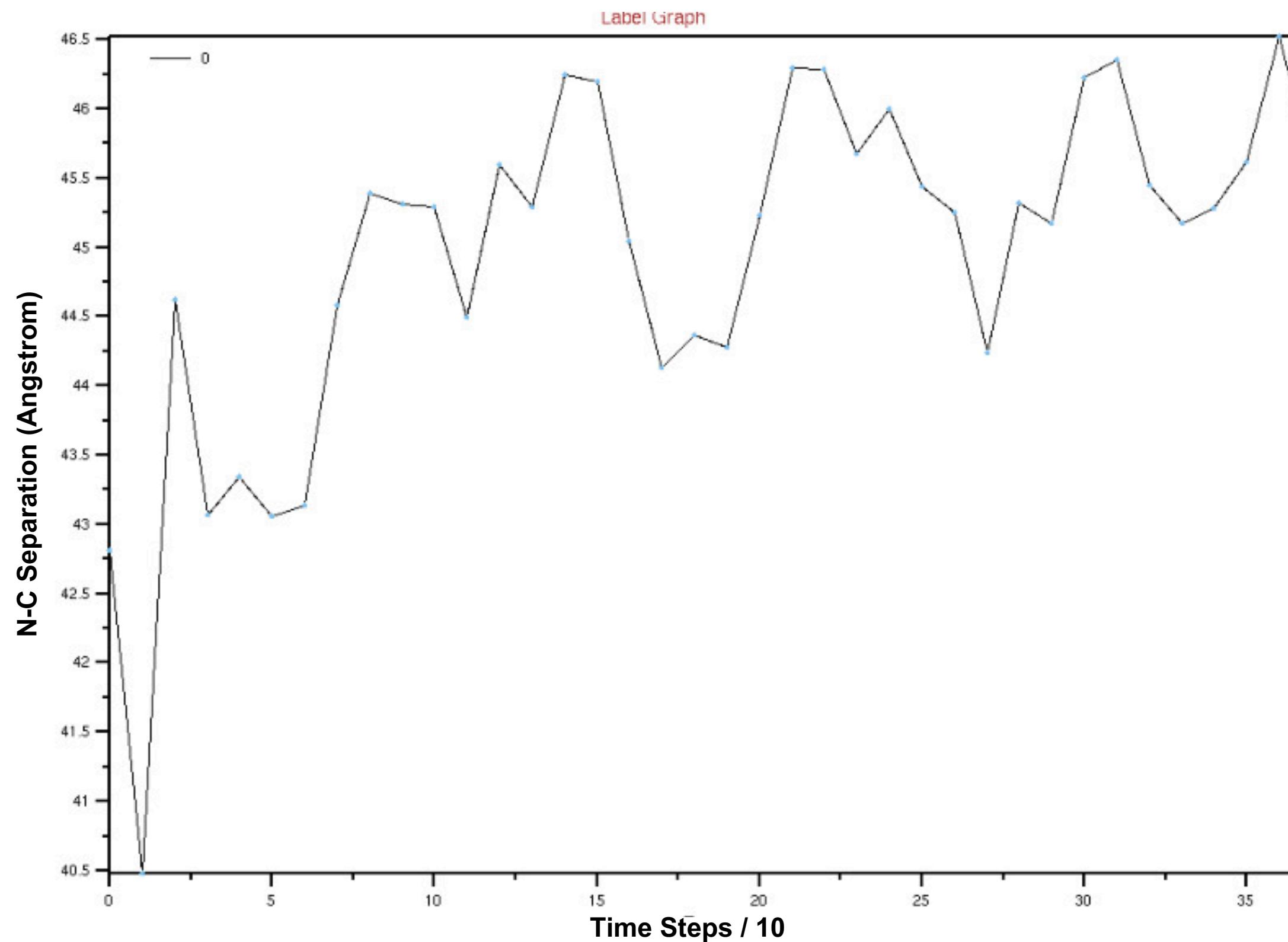
Trajectory of the pulling with constant velocity of the molecular dynamics simulations (Both are the same structure but with different drawing methods)

## Distance between two C alpha atoms



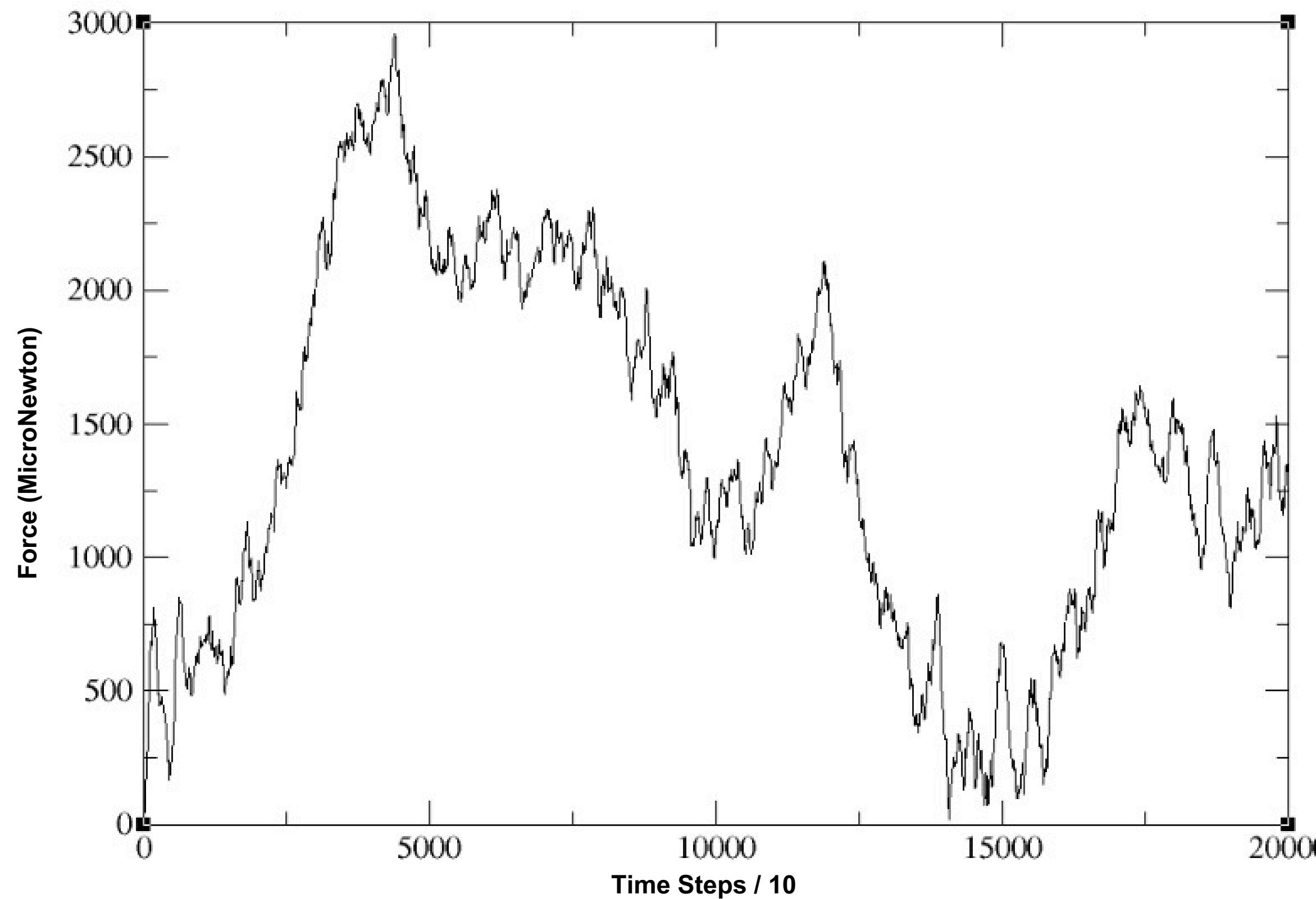
Distance between two C-alpha atoms after pulling of ubiquitin

## N-C Termini Constant force pull



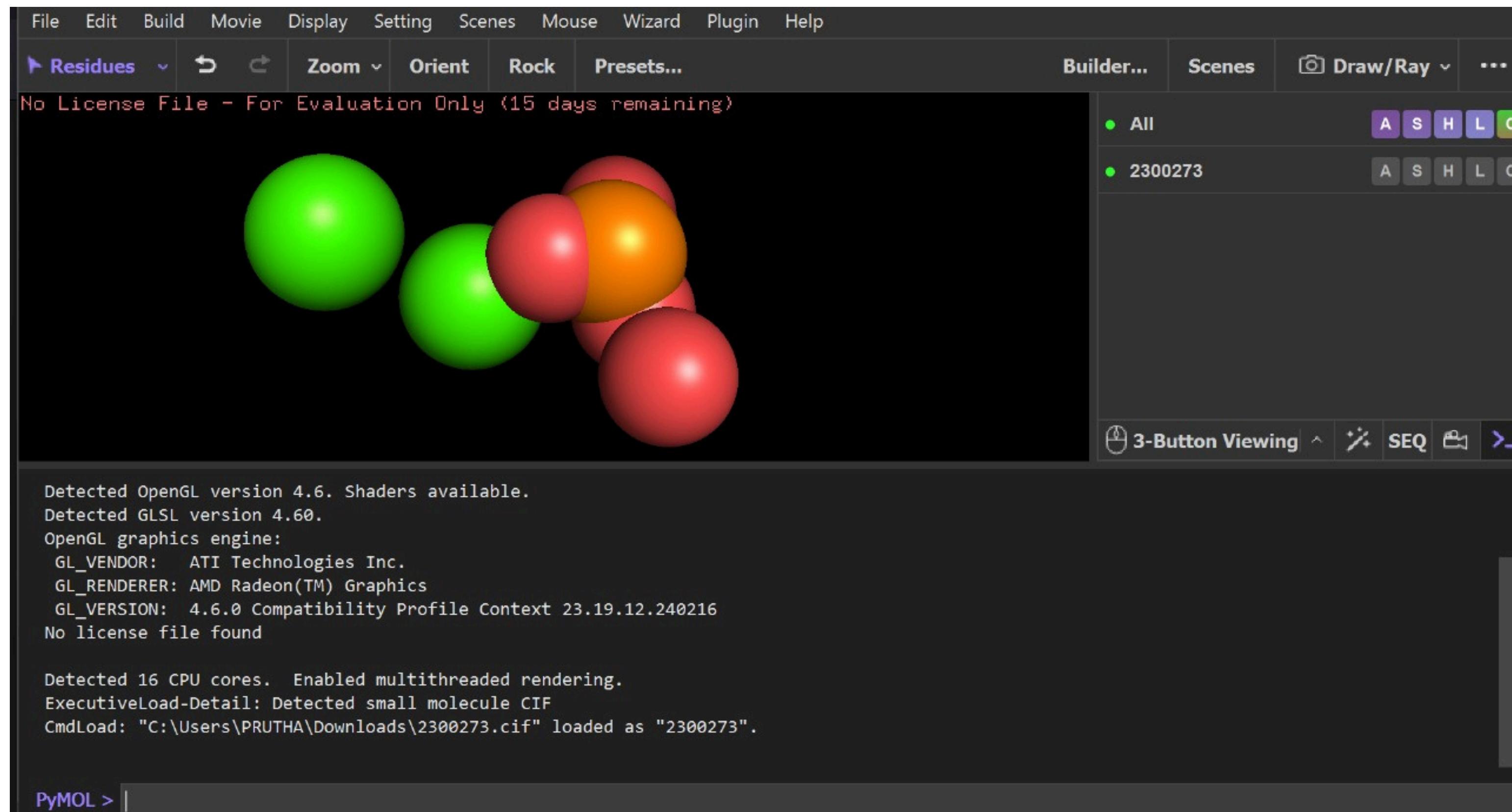
This is the trajectory of the constant force pulling simulation. The multiple plateaus observed signify intermediate states that occur during protein unfolding.

**N-C Termini constant velocity pull  
(Force vs timestep/10)**



A series of peaks and plateaus with each peak representing a key unfolding event/breaking of hydrogen bonds followed by a return to lower force as the protein extends

# CIF File for Hydroxyapatite



# CIF File generation for layer of Hydroxyapatite

