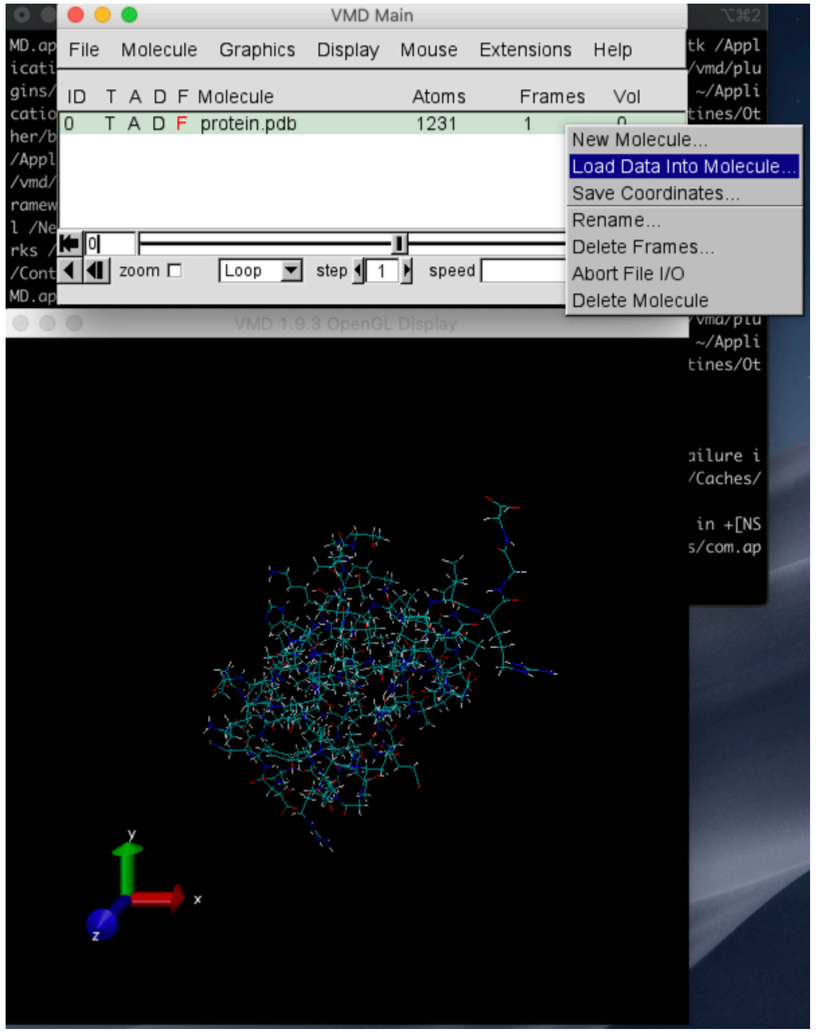
Visualizing Trajectories

- can be done by
  - loading a model into VMD
  - loading the trajectory into the model
- I will show you unaligned and aligned trajectories of ubiquitin without water
- For an unaligned simulation in explicit solvent
  - molecules, especially water, can be split across a periodic box
  - you probably don't need to see all water



Root mean square analysis

$$\text{RMSD}(v, w) = \sqrt{\frac{1}{n}\sum_{i=1}^{n} ||\, v_i - w_i \,||^2}$$

- Root mean square deviation (RMSD)
  - describes the difference between two structures
  - usually based on a subset of atoms
  - *i* is an index over atoms
- Root mean square fluctuation (RMSF)
  - describes the fluctuations of a specific atom, e.g. alpha carbon, over the course of a simulation
  - usually described per residue, identifying relatively flexible regions of a protein
  - *i* is an index over configurations
- Both require structural alignment

- See RMS.ipynb, which shows different types of RMS analysis for a simulation of ubiquitin.