Structural alignment

- Other than identifying equilibration time, structural alignment is usually one of the first tasks of MD analysis
- Why?
  - In most MD simulations, molecules freely diffuse around the box
  - We are usually
    - uninterested in the overall translation and rotation,
    - interested in fluctuations relative to the macromolecule
- Alignment is often based on a rigid-body translation and rotation to minimize the root mean square deviation (RMSD)

- See Alignment.py, which performs a structural alignment for a series of simulations of ubiquitin and outputs a trajectory of the protein by itself.

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