2/11/2020 Week 5 Module 1
Interactive Exercise for Molecular Dynamics

- In this exercise we wilł
  - prepare a python script to run OpenMM using the OpenMM script builder: http://builder.openmm.org
  - run a short MD simulation on our desktops
  - visualize the simulation with VMD

- This is the default script in the OpenMM script builder: http://builder.openmm.org
- Let's go through what the parameters mean and I'll give you values for a simple simulation of ubiquitin, a protein that we looked at during the VMD tutorial
- If you hover your mouse over the parameter names, it'll also give a brief description
- A more detailed description of simulation parameters is available at http://docs.openmm.org/latest/userguide/application.html#simulation-parameters