Why write a script?

- Molecular dynamics simulations require a lot of information about
  - Input data
    - coordinates
    - topology
      - which atoms are included in energy terms
      - parameters for functions in energy terms
  - System description
    - periodicity
    - constraints
  - Integrators
    - algorithms to propagate forward in time
    - adjust box size
    - adjust kinetic energy (temperature)
  - Simulation
    - how long to run
    - how much output data to store
- OpenMM can be run from widely-used computer programming languages, python and C++, facilitating extension and combination with other code

- 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