- We are not completely ready for the simulation because 1ubq.pdb
  - does not have hydrogen molecules
  - includes water, which does not help when we have an implicit solvent model
- OpenMM provides a package that does some simple modeling, including these required tasks.
- To make our script use this capability, open a text editor and add the five lines shown in the box

```
pdb = app.PDBFile('1ubq.pdb')
forcefield = app.ForceField('amber99sbildn.xml', 'amber99_obc.xml')

modeller = app.Modeller(pdb.topology, pdb.positions)
modeller.deleteWater()
modeller.addHydrogens(forcefield)
pdb = modeller
app.PDBFile.writeFile(pdb.topology, pdb.positions, open('ubq_mod.pdb', 'w'))

system = forcefield.createSystem(pdb.topology,
    nonbondedMethod=app.CutoffNonPeriodic, nonbondedCutoff=1.0*unit.nanometers,
    constraints=app.HBonds, rigidWater=True)
integrator = mm.LangevinIntegrator(300*unit.kelvin, 1.0/unit.picoseconds,
```

Additional Resources

- In “Introduction to OpenMM” on http://openmm.org/documentation.html, Peter Eastman describes an OpenMM script from 5:00 to 15:03