

- 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

```
12  pdb = app.PDBFile('1ubq.pdb')~
13  forcefield = app.ForceField('amber99sbildn.xml', 'amber99_abc.xml')~
14  ~
15  modeller = app.Modeller(pdb.topology, pdb.positions)~
16  modeller.deleteWater()~
17  modeller.addHydrogens(forcefield)~
18  pdb = modeller~
19  app.PDBFile.writeFile(pdb.topology, pdb.positions, open('ubq_mod.pdb', 'w'))~
20  ~
21  system = forcefield.createSystem(pdb.topology,~
22  ...nonbondedMethod=app.CutoffNonPeriodic, nonbondedCutoff=1.0*unit.nanometers,~
23  ...constraints=app.HBonds, rigidWater=True)~
24  integrator = mm.LangevinIntegrator(300*unit.kelvin, 1.0/unit.picoseconds,~
25  ...2.0*unit.femtoseconds)
```

# Additional Resources

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