Receptor setup

- The YANK workflow requests a PDB file for the receptor
- You have already done similar steps
- I prepared the receptor file by
  - submitting the structure 6LU7 to the PDB2PQR server
  - removing the ligand and water from the main result, 6LU7.pqr
    - results of these first steps are here: 3cl-pro/YANK/receptor
  - copying 6LU7.pqr to 6LU7.pdb to have a file name accepted by the YANK workflow

Parameterizing the ligand

- Why do we need ligand parameters?
- I am assuming that you docked the ligand using AutoDock Vina or AutoDock 4
- Parameters from docking programs
  - are not carefully assigned, e.g. charges have minimal dependence on environment
  - are not compatible with biomolecular force fields like AMBER