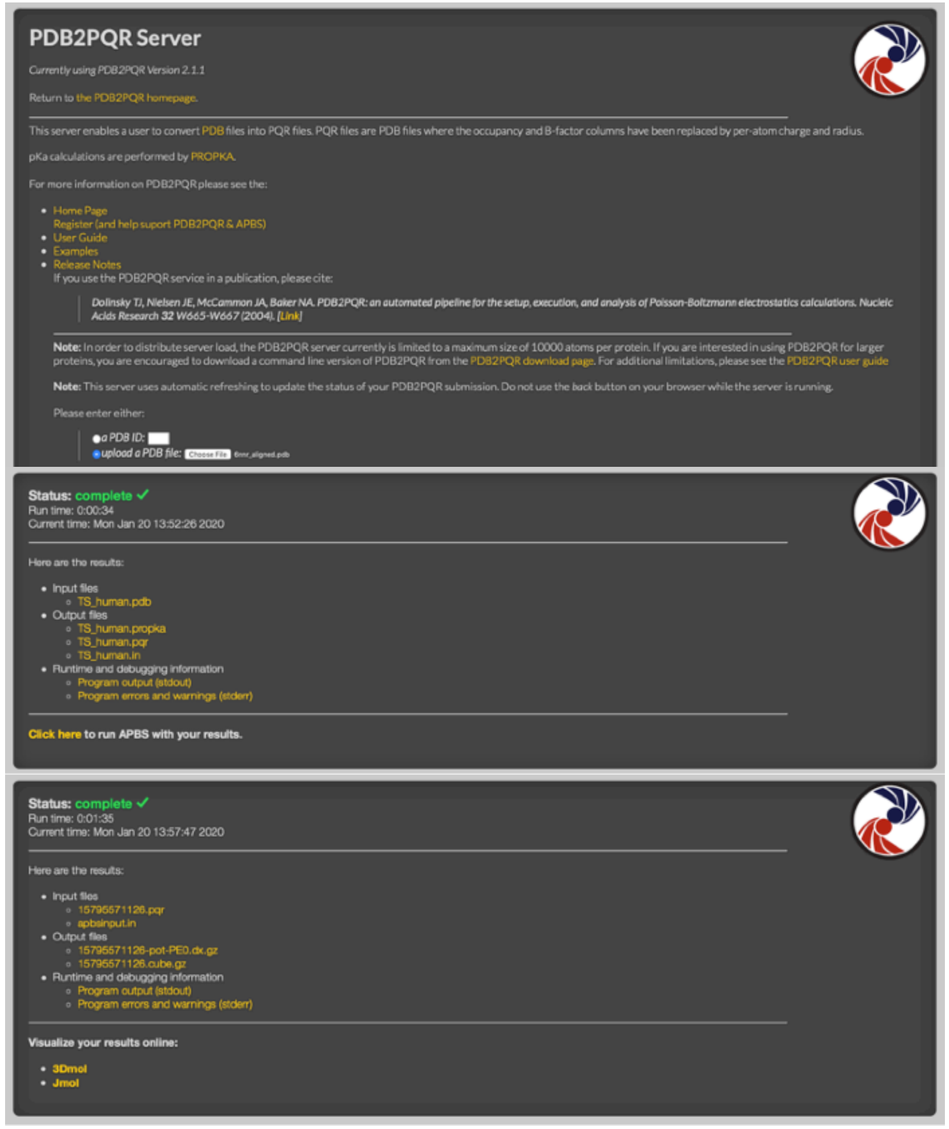
Electrostatics Calculations

- I ran electrostatic potential calculations with PDB2PQR and APBS (http://www.poissonboltzmann.org) on the PDB2PQR server (http://nbcr-222.ucsd.edu/pdb2pqr_2.1.1/). There were three steps:
  - Uploading the PDB file and selecting parameters. I used the defaults.
  - Running PDB2PQR by pressing “Submit”. This performs some basic structural preparation, e.g. adding missing atoms and optimizing hydrogen positions.
  - Running APBS by following “Click here to run APBS with your results”. This actually solves the PB equation.
- For TS, none of these calculations took a very long time.



Visualizing Electrostatic Potentials with VMD