Finding protonation states - PDB2PQR tutorial

Visit the APBS-PDB2PQR server at https://server.poissonboltzmann.org/

Under “Getting Started”, click “PDB2PQR”.

Under “PDB Selection”, click “Upload a PDB File”

Select your 1ubq.pdb file.

Under pKa options, make sure that pH is 7.0, and make sure that “Use PROPKA to assign protonation states at provided pH” is selected.

Under “Forcefield Options” select “CHARMM”.

For the output naming scheme, use “CHARMM”

Click “Start Job”.

Find the PQR file and download it. View the PQR file to see the histidine protonation states.

Though not necessary for CHARMM-GUI, some MD preparation software (like AMBERTOOLS) requires your input PDB to have the correct histidine protonation state residue naming. Optionally modify your PDB file to have the correct protonated residues (Change “HIS” to “HID” or other residue name).