

Structure Preparation

- None of the structures were ready for electrostatic potential calculation
- The human structure, 1HVV
 - has 4 chains, but we are only interested in 2
 - I used MultiSeq to write separate files for each chain, merged the files for chains A and B, and then modified “END” after chain A into “TER”
- The E. coli structure, 6NNR
 - is not aligned with the human structure
 - I used MultiSeq to write separate files for each chain, used MultiSeq STAMP structural alignment to superpose E. coli chains A and B on top of the respective human chains, wrote the aligned files, and merged and modified them as with 1HVV
- The W.g.b. homology model
 - is not aligned with the human structure
 - I used MultiSeq STAMP structural alignment to superpose W.g.b. chains A and B on top of the respective human chains, wrote the aligned files, and merged and modified them as with 1HVV

Electrostatics Calculations

- I ran electrostatic potential calculations with PDB2PQR and APBS (<http://www.poissonboltzmann.org>) on the PDB2PQR server (http://nbc-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.

The screenshot displays the PDB2PQR Server interface, which is used for performing electrostatic calculations. It is divided into three main sections:

- PDB2PQR Server:** The top section shows the server version (2.1.1) and provides a link to the homepage. It explains that the server converts PDB files into PQR files, replacing occupancy and B-factor columns with per-atom charge and radius. It also mentions that pKa calculations are performed by PROPKA. A list of links (Home Page, Register, User Guide, Examples, Release Notes) is provided. A citation for Dolinsky TJ, Nielsen JE, McCammon JA, Baker NA (2004) is included. A note states that the server is limited to a maximum size of 10000 atoms per protein. A form for entering a PDB ID or uploading a PDB file is shown.
- Status: complete ✓:** The middle section shows the results of a calculation. It includes the run time (0:00:34) and current time (Mon Jan 20 13:52:26 2020). The results are listed under "Here are the results:" and include input files (TS_human.pdb), output files (TS_human.propka, TS_human.pqr, TS_human.in), and runtime and debugging information (Program output (stdout), Program errors and warnings (stderr)). A link to "Click here to run APBS with your results." is provided.
- Status: complete ✓:** The bottom section shows the results of another calculation. It includes the run time (0:01:35) and current time (Mon Jan 20 13:57:47 2020). The results are listed under "Here are the results:" and include input files (15795571126.pqr, apbsinput.in), output files (15795571126-pot-PEO.dx.gz, 15795571126.cube.gz), and runtime and debugging information (Program output (stdout), Program errors and warnings (stderr)). A link to "Visualize your results online:" is provided, with options for 3Dmol and Jmol.