# Structure Preparation

- None of the structures were ready for electrostatic potential calculation
- The human structure, 1HVY
  - 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 1HVY
- 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 1HVY

# 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.