Homework 2

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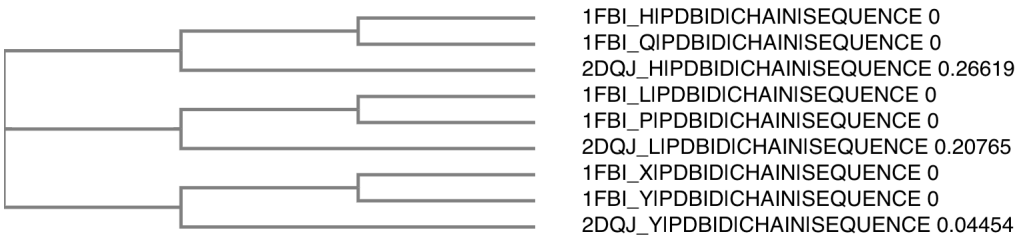
1. (a) Please refer to Problem1.pse and look at F1.

   (b) From It looks like F05 and Y41 are aligned. From a pure pairwise sequence alignment standpoint, every amino acid aligns with each other. This was confirmed through NEEDLE which is an online pairwise alignment program.

   (c) Please refer to Problem1.pse and look at F2. The aligned Tyrosines (Y38 and Y02) have a dihedral angle of $\sim 120°$. The aligned Glycine (G40 and G5) have a dihedral angle of $\sim 120°$. The angle that I calculated was the τ angles.

2. (a) To figure out some of the better alignments, I initially did a multiple sequence alignment to see which residues had the most homology and may be candidates for piecewise alignment. This was done using T-Coffee, an online multiple sequence alignment program from Phylogenetic tree calculated via the Neighbor Joining approach from EMBOSS NEEDLE is shown below.



   From this, I chose to align the 1FBI:H sequence to the 2DQJ:H sequence. These two sequences can be found in the FASTA files from RCSB. The resulting alignment can be found on F1 in Problem2.pse.

   Though sequence homology alone is not always a good fit for protein structure alignment, it worked out okay here.

   (b) Preset is F1 AND F2 for 1FBI and 2DQJ in PreAligned_1FBI_2DQJ.pse, repsectively. For N77 in 1FBI, the only main interaction I see with the antibody is with a corresponding N59, an asparagine. Similarly, the only main interaction for N77 in 2DQJ with the antibody is D99, an aspartate. In 1FBI, the distance between the amino group of the sidechain carboxamide of N77 and the carbonyl of the of the sidechain carboxamide of N59 is 2.7 Å. In 2DQJ, the distance between the amino group of the sidechain carboxamide of N77 and the carbonyl of the of the sidechain carboxamide of D99 is 2.7 Å. This would suggest hydrogen bonding is happening in both complexes. Because the interactions happening are the same in each of the lysozymes, mutagenesis of these regions would not create a more effective super antibody.