February 8

Retrieved structures, centers and selections from the "paper corrections/hydropobicity moment" subfolder of my earlier work

Looked up in "hhomp location of dataset/search results" the clusters including 1A0S (ScrY), 1QD6 (OMPLA), and 1QJP (OmpA)

ScrY: 18.1.1

OMPLA: 12.6.1

OmpA: 8.1.1

Looked up their sequences in "hhomp location of dataset/sequences.csv"

ScrY:

SGFEFHGYARSGVIMNDSGASTKSGAYITPAGETGGAIGRLGNQADTYVEMNLEHKQTLDNGATTRFKVMVADGQTSYNDWTASTSDLNVRQAFVELGNLPTFAGPFKGSTLWAGKRFDRDNFDIHWIDSDVVFLAGTGGGIYDVKWNDGLRSNFSLYGRNFGDIDDSSNSVQNYILTMNHFAGPLQMMVSGLRAKDNDERKDSNGNLAKGDAANTGVHALLGLHNDSFYGLRDGSSKTALLYGHGLGAEVKGIGSDGALRPGADTWRIASYGTTPLSENWSVAPAMLAQRSKDRYADGDSYQWATFNLRLIQAINQNFALAYEGSYQYMDLKPEGYNDRQAVNGSFYKLTFAPTFKVGSIGDFFSRPEIRFYTSWMDWSKKLNNYASDDALGSDGFNSGGEWSFGVQMETWF

OMPLA:  
FTLYPYDTNYLIYTQTSDLNKEAIASYDWAENARKDEVKFQLSLAFPLWRGILGPNSVLGASYTQKSWWQLSNSEESSPFRETNYEPQLFLGFATDYRFAGWTLRDVEMGYNHDSNGRSDPTSRSWNRLYTRLMAENGNWLVEVKPWYVVGNTDDNPDITKYMGYYQLKIGYHLGDAVLSAKGQYNWNTGYGGAELGLSYPITKHVRLYTQVYSGYGESLIDYNFNQTRVGVGVMLNDLF

OmpA:

APKDNTWYTGAKLGWSQHENKLGAGAFGGYQVNPYVGFEMGYDWLGRMPYAYKAQGVQLTAKLGYPITDDLDIYTRLGGMVWRADTYSNVYGKNHDTGVSPVFAGGVEYAITPEIATRLEYQWTNGMLSLGVSYRFG

Downloaded the alignments for those clusters as "OMPLA without pdb.clu" etc.

Added the sequences above to these alignments with the identifiers "chaina\_ompla" etc. (since these were taken from chain A of the pdb file, according to what I remember reading of how Daniel made the aligned pdb files), removed anything that wasn't actually a protein sequence (ss pred, ss conf, bb pred, bb conf, cluster name), and aligned, outputting as "OMPLA with pdb.aln" etc.

Copied "published params.csv", containing the ez-beta parameters from the first ez-beta paper, from "paper corrections/ompla moments"