20180328: CM with 2P9H_correctNPF & 2P9H_correctNPF_relaxed

Input files (on guybrush: /home/anum/20180328):

- also created relaxed version of original 2p9h_redo file
- scored both PDBs (see Evernote: <u>20180326-28, Lacl input structure prep</u>)
- · made a constraints file based on original structure



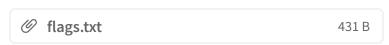
 made resfiles: used create_first_shell_resfile.py script to generate lists of residues for the resfiles for each ligand (PF1 & PF2), got rid of any that I had constrained in the cst file, and made a master resfile with matched up linked residues between monomers



XML RS:



Flags file:



Running CM on guybrush overnight:

- ntrials = 10000
- nstruct = 20
- relaxed and non-relaxed input files
- constraints +/- atompair constraint on N125 residues (rosetta res# 64, 333)

Screens as follows:

- 6474.relax-fewerconstraints (folder: 20180328-relax-fewerconstraints)
- 6133.relax-constraints (folder: 20180328-relax)
- 5923.orig-fewerconstraints (folder: 20180328-orig-fewerconstraints)
- 5751.orig-constraints (folder: 20180328)

TODO tomorrow: analyze results from these runs and and try to run HBNet