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: 20180326-28, LacI input structure prep)
- made a constraints file based on original structure

constraints.cst 1 kB

constraints.xlsx 40 kB

- 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

PF1_firstshell.res 151 B

PF2_firstshell.res 158 B

firstshell.res 199 B

- XML RS:

coupled_moves.xml 2 kB

- Flags file:

flags.txt 431 B

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