

combined-clustering.in

#load prmtops for each sys (can use same prmtop, only difference is force fields)

parm /uufs/chpc.utah.edu/common/home/cheatham-group5/james/e2-dna/new-hmr-18mer/dna/analysis/nowat.dna.hmr.prmtop

#load the trajectories, every 1ns

trajin /uufs/chpc.utah.edu/common/home/cheatham-group5/james/e2-dna/new-hmr-18mer/dna/analysis/dna.1.nc 1 last 25

trajin /uufs/chpc.utah.edu/common/home/cheatham-group5/james/e2-dna/new-hmr-18mer/dna/analysis/dna.2.nc 1 last 25

trajin /uufs/chpc.utah.edu/common/home/cheatham-group5/james/e2-dna/new-hmr-18mer/dna/analysis/dna.3.nc 1 last 25

trajin /uufs/chpc.utah.edu/common/home/cheatham-group5/james/e2-dna/new-hmr-18mer/dna-decoy1/analysis/dna-decoy1.1.nc 1 last 25

trajin /uufs/chpc.utah.edu/common/home/cheatham-group5/james/e2-dna/new-hmr-18mer/dna-decoy1/analysis/dna-decoy1.2.nc 1 last 25

trajin /uufs/chpc.utah.edu/common/home/cheatham-group5/james/e2-dna/new-hmr-18mer/dna-decoy1/analysis/dna-decoy1.3.nc 1 last 25

trajin /uufs/chpc.utah.edu/common/home/cheatham-group5/james/e2-dna/new-hmr-18mer/dna-decoy2/analysis/dna-decoy2.1.nc 1 last 25

trajin /uufs/chpc.utah.edu/common/home/cheatham-group5/james/e2-dna/new-hmr-18mer/dna-decoy2/analysis/dna-decoy2.2.nc 1 last 25

trajin /uufs/chpc.utah.edu/common/home/cheatham-group5/james/e2-dna/new-hmr-18mer/dna-decoy2/analysis/dna-decoy2.3.nc 1 last 25

#cluster on backbone

cluster :1-36@P,O5',C5',C4',C3',O3' kmeans clusters 3 randpoint \

sieve 100 random \

out dna_combine-cluster_cnumvtime.dat summary dna_combine-cluster_avg-summary.dat \

cpopvtime dna_combine-cluster_cpopvtime.dat normframe \

summarysplit dna_combine-cluster_summarysplit.dat splitframe '120000,170400' \

savepairdist pairdist dna_combine-cluster.pairdist