Start from Cn multimer pdb, extract asymmetric unit

Mutate n res from “designable” selection

Calculate score for all residues minus “exclude\_from\_score\_calculation” selection

chargedesign.assign\_symmetric\_pose(pdb\_in, symm, pose\_symm)

chargedesign(pdb\_in, designable, exclude)

chargedesign.do\_step()

if chargedesign.last\_step\_accepted:

chargedesign.save\_step()

anneal