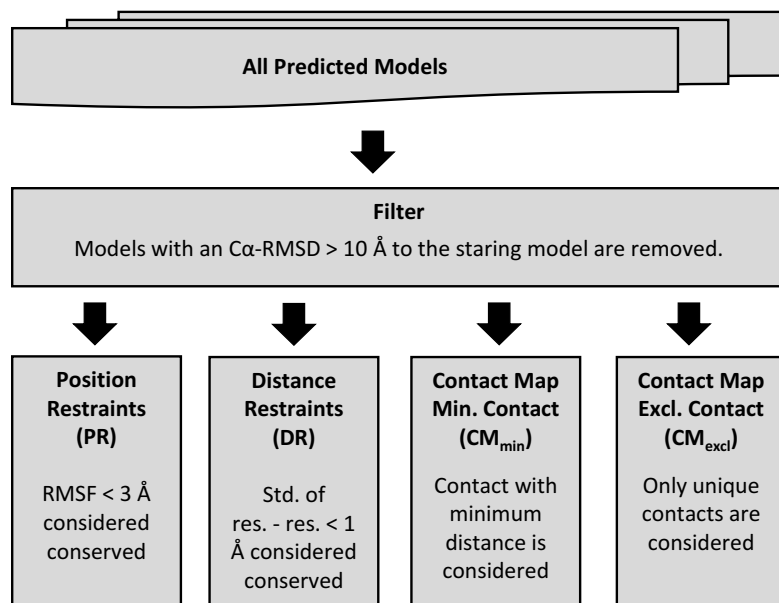
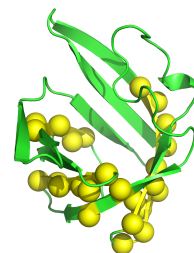


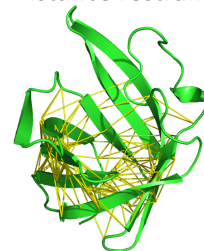
### A Generation of restraints and contact maps



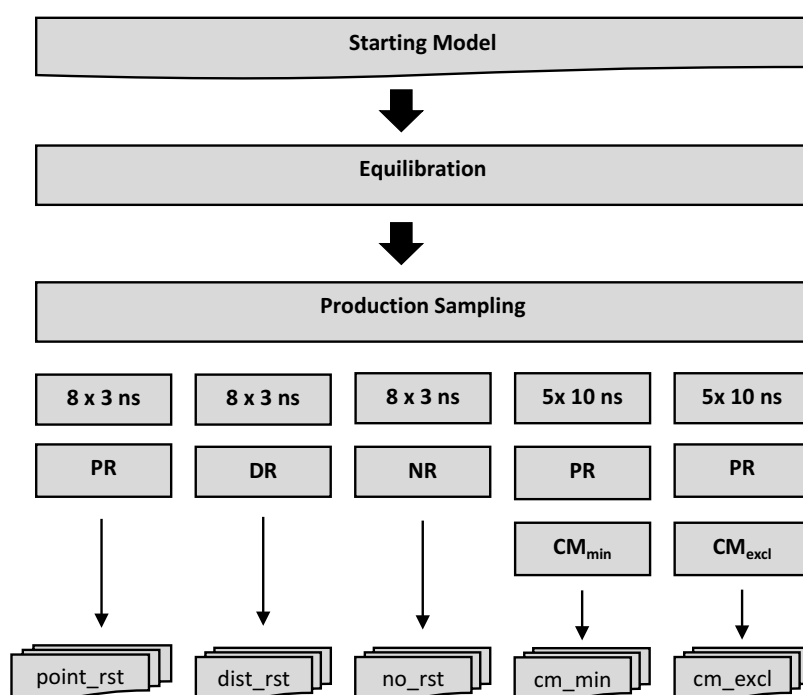
### C Point restraints



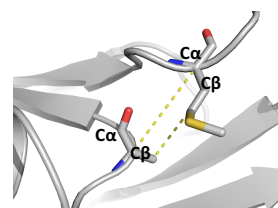
### D Distance restraints



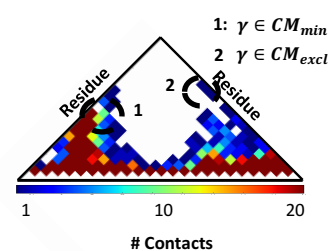
### B Sampling procedure



### E Residue-residue contact



### F Contact map



S2 Fig. : Sampling Protocol. (A) Flowchart outlining the generation of the restraints and contact maps. (B) Flowchart outlining the different MD sampling procedures (C) Example of point restraints applied to a protein. (D) Example of residue-residue distance restraints applied to a protein. (E) Definition of residue-residue contact (F) Contact map definition for  $CM_{excl}$  and  $CM_{min}$ .