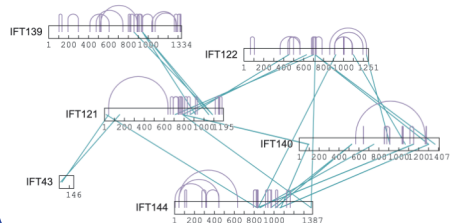


Gathering data into spatial restraints

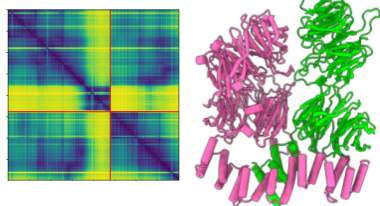
Chemical crosslinking

98 DSSO crosslinks

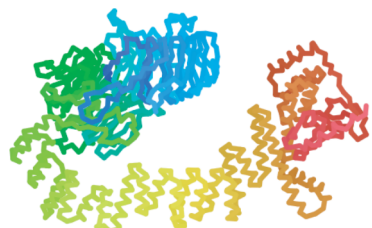


AlphaFold predicted interfaces

7 predicted interfaces

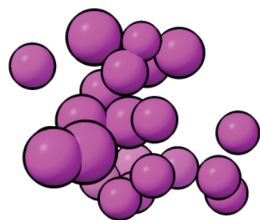


AlphaFold predicted structures



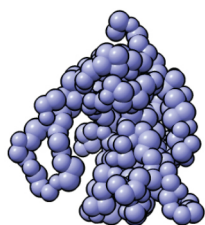
Steric effects

Excluded volume restraint



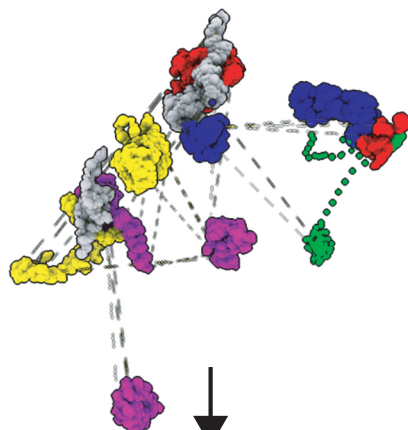
Sequence connectivity

Sequence connectivity restraint

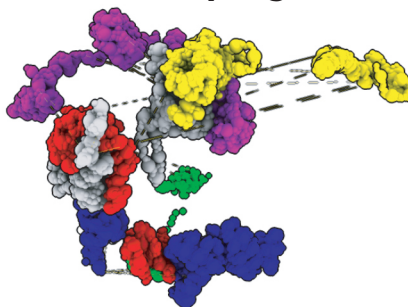


Optimized sampling

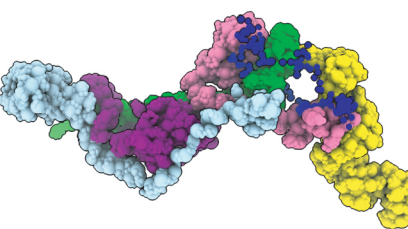
Initial random



Sampling

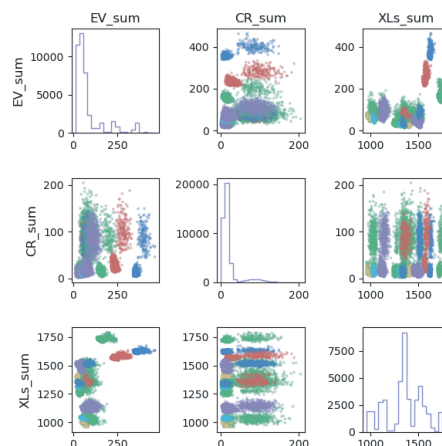


Ensemble of models

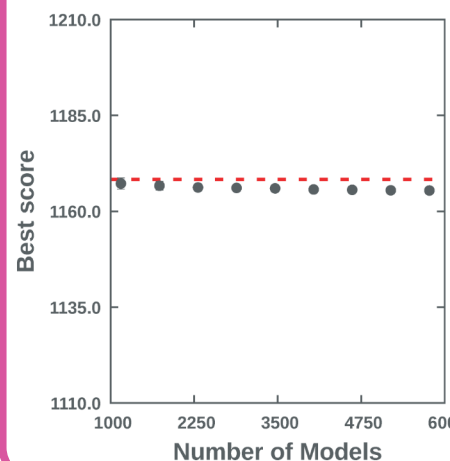
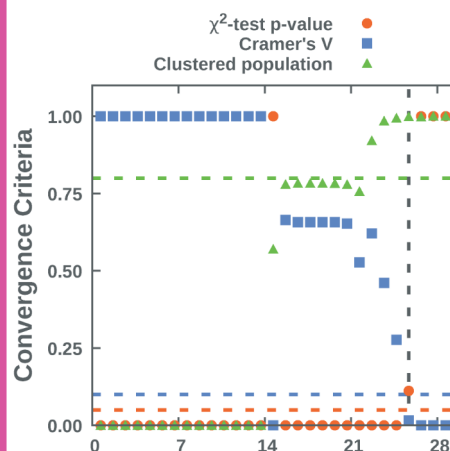


Ensemble analysis

Initial clustering and selection

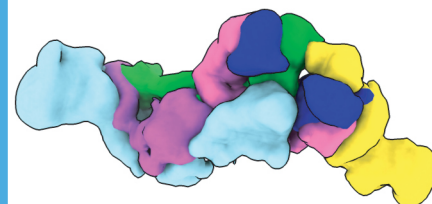


Sampling exhaustiveness

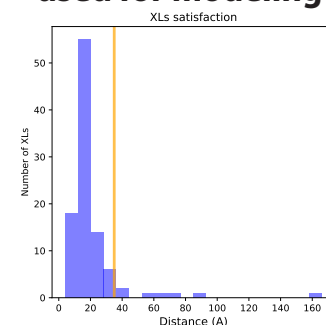


Ensemble validation

Localized probability densities



Validation with data used for modeling



Validation with data from literature

