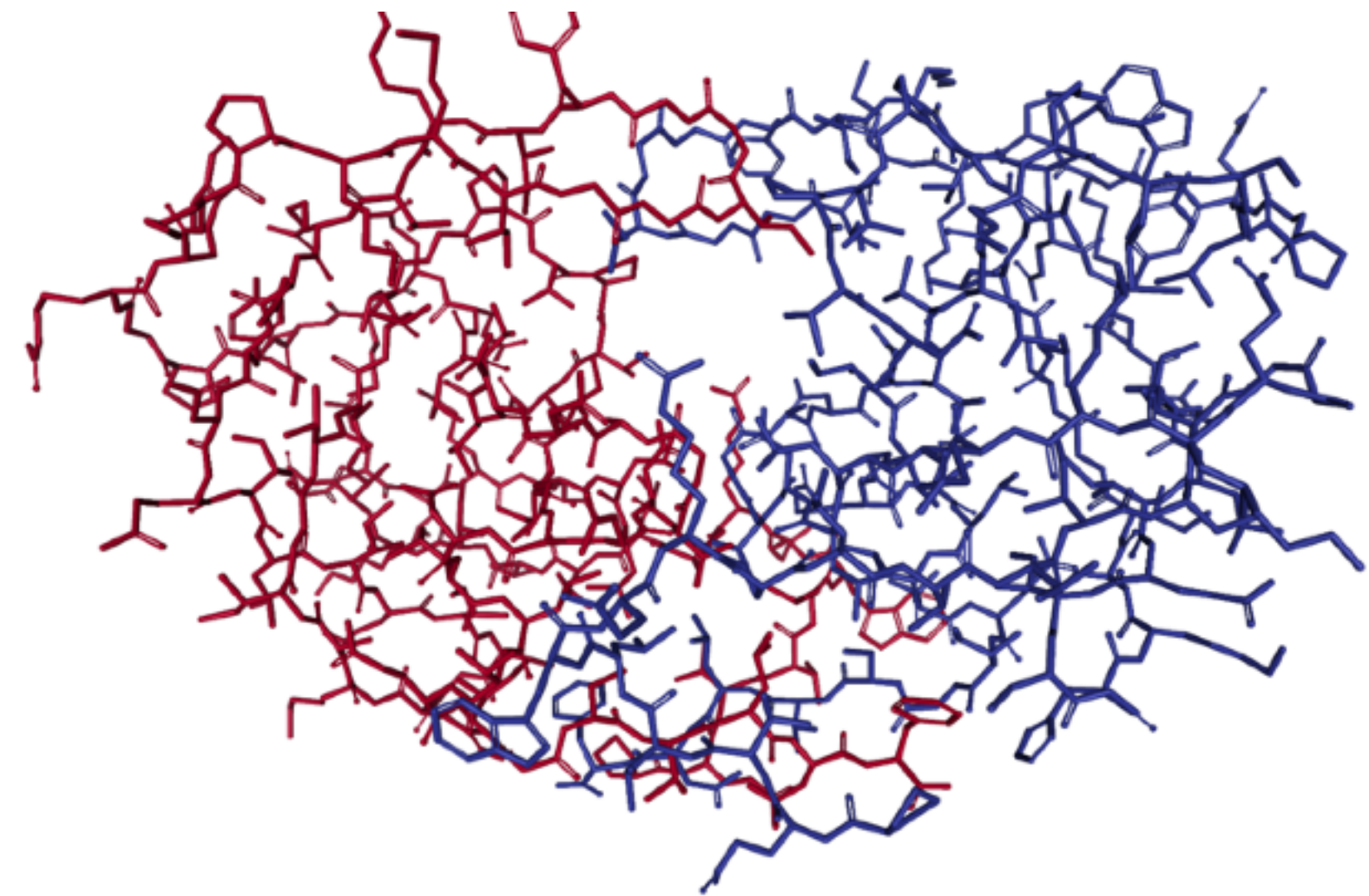
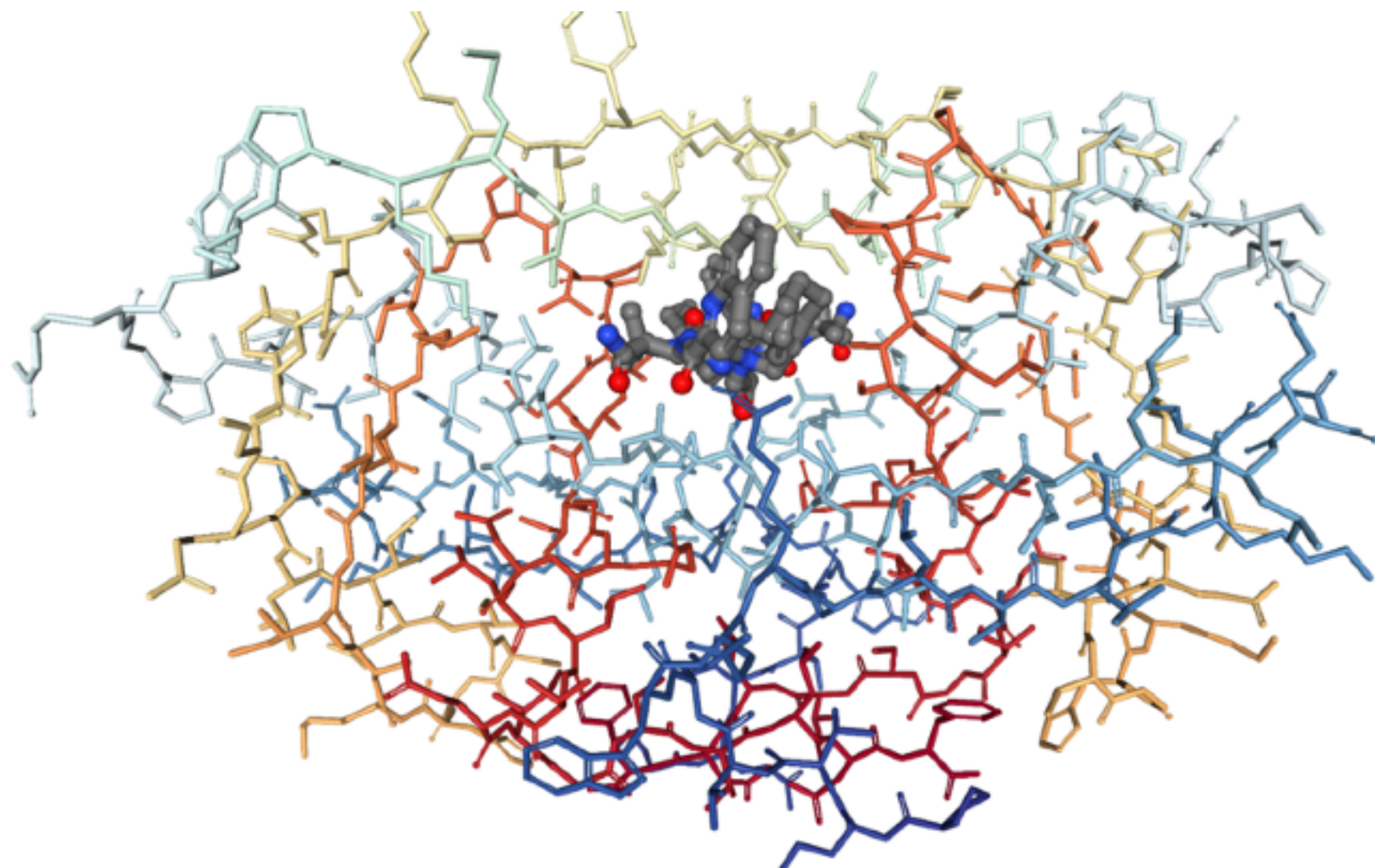


What is molecular docking?

- To predict
 - the 3D structure of a noncovalent complex
 - protein-ligand
 - protein-protein
 - the binding affinity of the partners (scoring)
- Prior to prediction, structure of binding partner(s) may be known, but
 - could be affected by binding
 - may be bound to different partners



What is molecular docking good for?

- Predicted structure can
 - explain behavior, e.g. mutagenesis
 - facilitate molecular design, e.g. of pharmaceuticals
- Predicted scores can be used for virtual screening