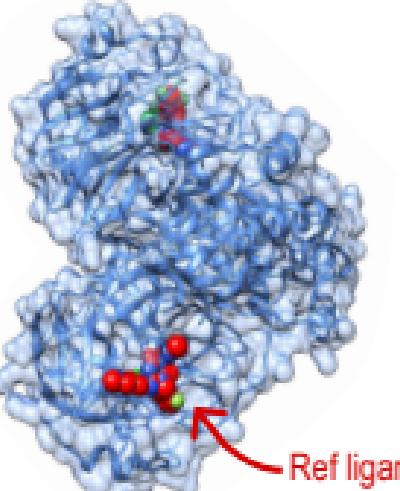
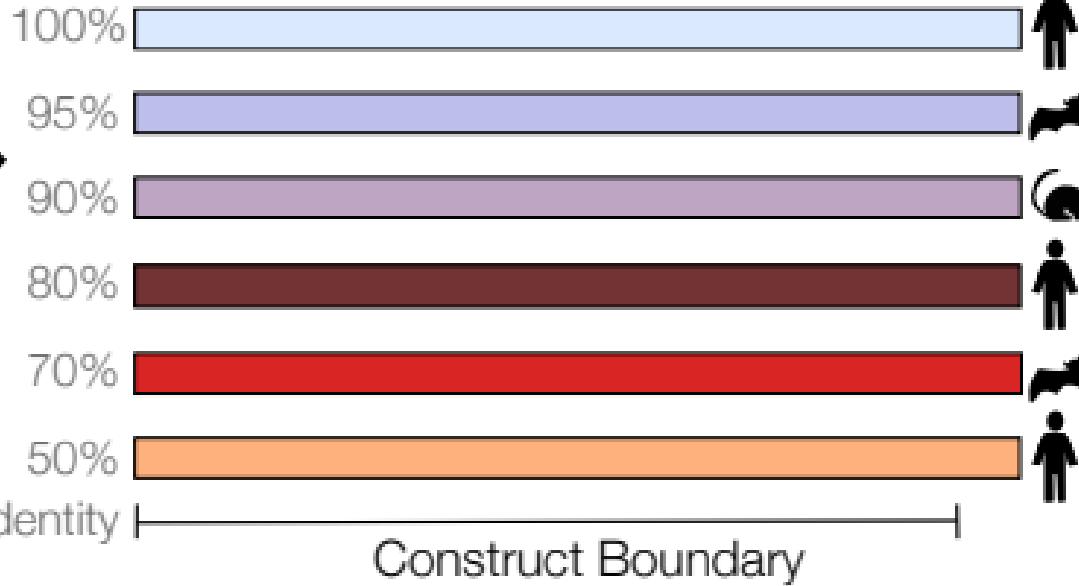


**Reference structure**  
  
PDB of protein-ligand complex  
Ref ligand

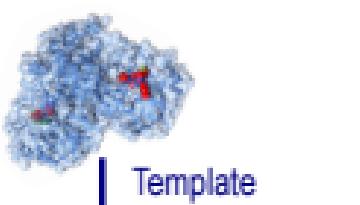
## 1) BLAST Query

>SARS-CoV-2  
SGFRKMAFP<sup>S</sup>GKVEGCMVQVTC<sup>T</sup>TLNGLWLDDVVYCP  
RHVI<sup>C</sup>TSEDMLNP<sup>N</sup>YEDLLIRKSNNFLVQAGNVQLRVI  
GHSMQN<sup>C</sup>VILKLKVDTANPKTPKYKFVRIQPGQTF<...>

Filter by species



## 2) Template-based AlphaFold



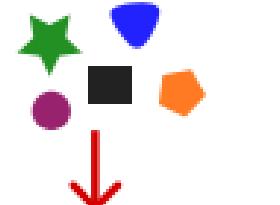
## 3) Transfer docking



## 4) Refinement



## 5) Docking of new compounds



## 6) Score ligands

- RMSD
- Seq Similarity
- Fingerprints
- ChemGauss4
- Auto-dock Vina
- Gnina

