Supplementary Information

Protein oligomer modeling guided by predicted inter-chain contacts in CASP14

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Supplementary figures

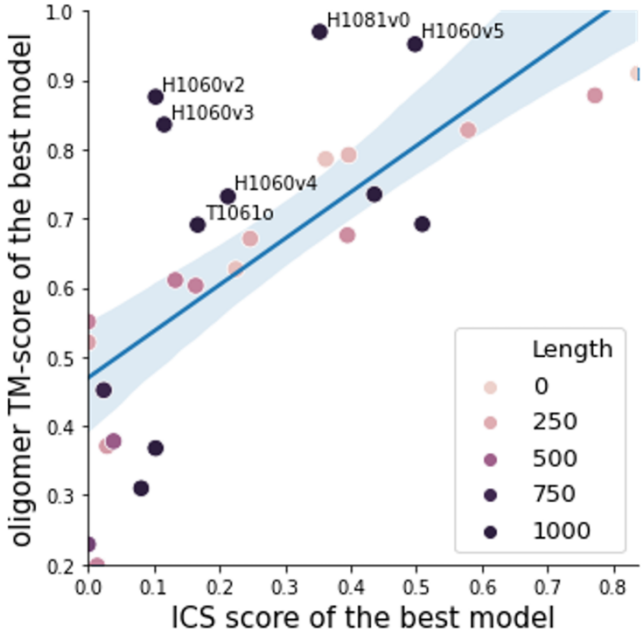

Figure S1. Relationship between ICS score and oligomer TM-score for the best model. Larger complexes (over 750 residues) tend to have significantly higher oligomer TM-scores compared to ICS scores.

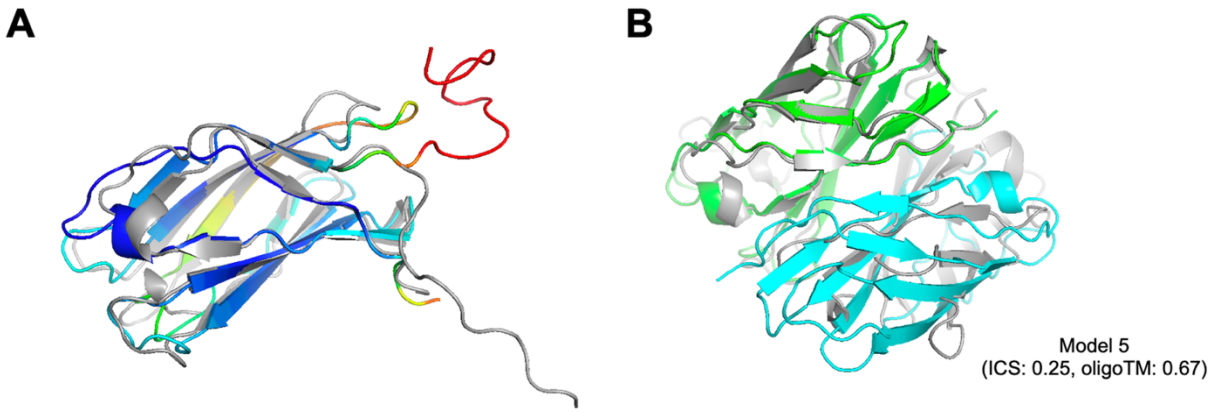

Figure S2. A successful example (T1078) of *ab initio* docking with a reasonable subunit structure. A) Quality of the predicted subunit structure (BAKER model 1). The subunit model is colored in rainbow with Cα RMS error predicted by DeepAccNet ranging from 1.0 Å (blue) to 5.0 Å (red). N-terminus (residue 1-13, colored in red) was removed before docking. B) The predicted homo-dimer model (colored in green and cyan) has a reasonable quality. Native structures are colored in gray for both panels.

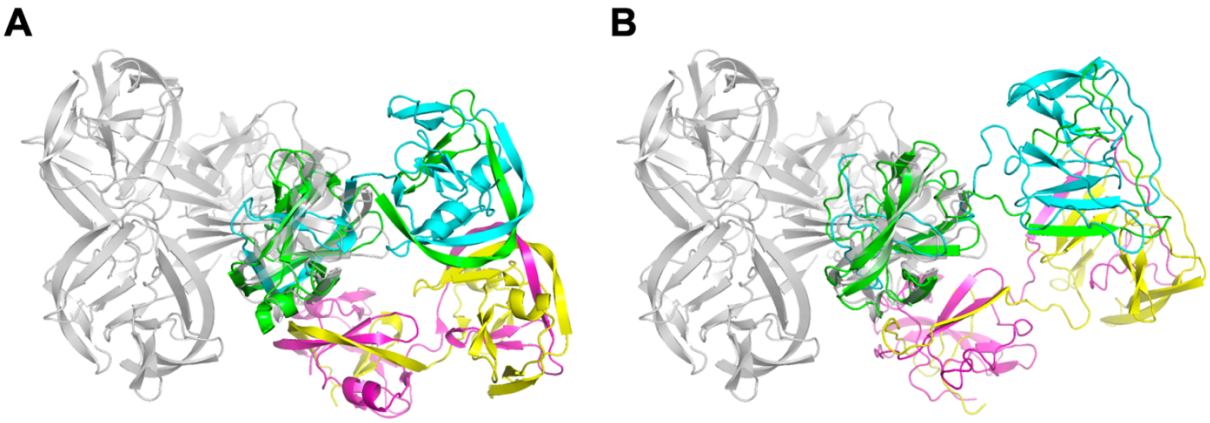

Figure S3. The wrong oligomer template led to the poor subunit quality (T1034). A) Native structure (gray) and the oligomer template (PDB ID: 4KL6, colored by chain) used to model homo-tetramer structures are shown. The oligomer template has a wrong interface. B) The predicted oligomer model (colored by chain) forms domain-swapped homo-tetramer structures with wrong interfaces resulting in the worse subunit quality.