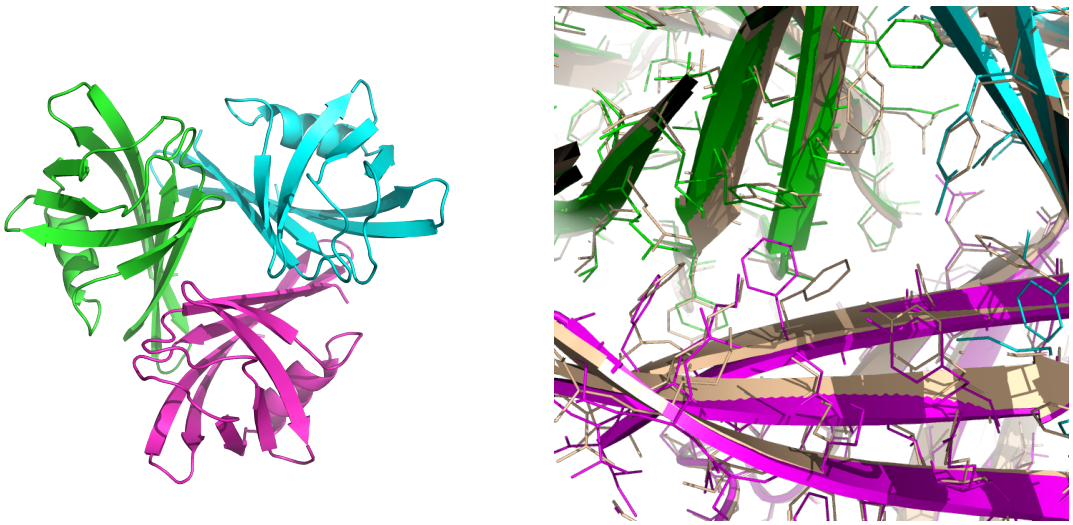

Figure S1: On the left, trimeric assembly of target T0867o, a viral fibre head with close sequence and structural templates. On the right, superposition of the top scoring prediction (0.92 ICS and 0.95 IPS), second model by BAKER-ROSETTASERVER (beige), onto the target. Despite some differences in side chain orientation, the backbone conformation and interface are predicted with high accuracy to the experimental structure.

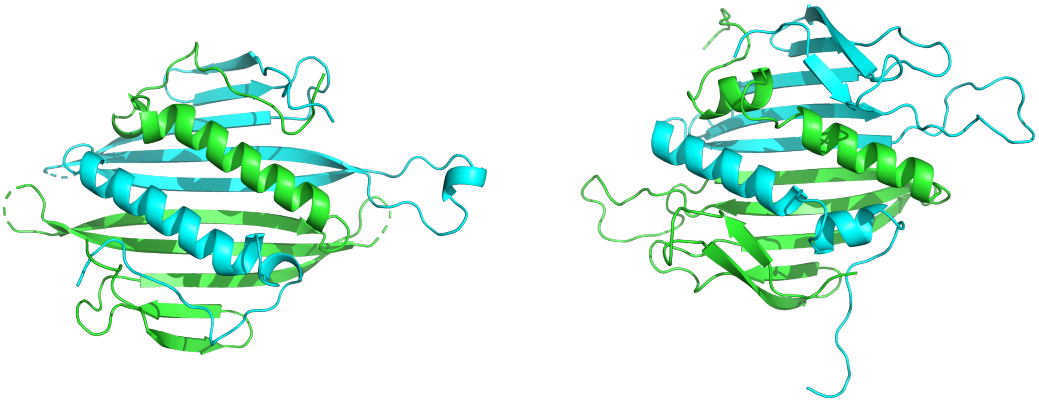

Figure S2: AP205 (T0929) is a viral coat protein with 180 subunits in the biological assembly. The experimental structure by solid-state NMR only contained a dimeric interface (left), which is significantly stronger than the others, so it was released as a dimer for prediction. Structural templates for the dimer were available during the prediction period, but they were not detectable using sequence comparison methods. The human group TSlab-assembly was able to reproduce the protein fold and dimeric assembly correctly (right), although a threading error led to poor monomeric and interface contact scores.

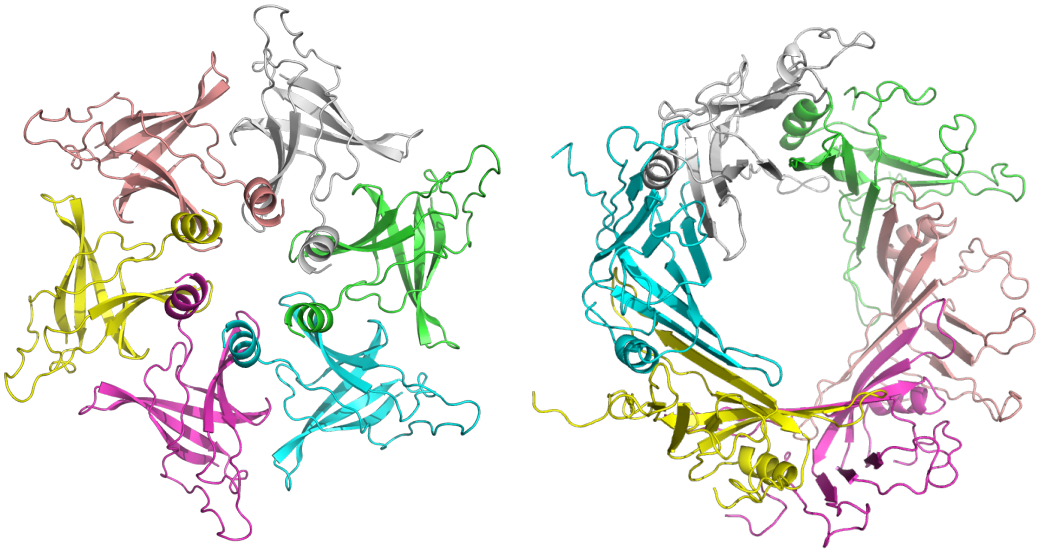

Figure S3: Biological assembly of oligomeric target T0866o (left) and first model by TSlab-assembly (right). Although the model correctly reproduces the symmetry of the target, both the tertiary structure of the monomers and the mode of association are incorrect. While the target forms the assembly through a central swapped helical interaction, the model contains beta-pairings with a central hole.

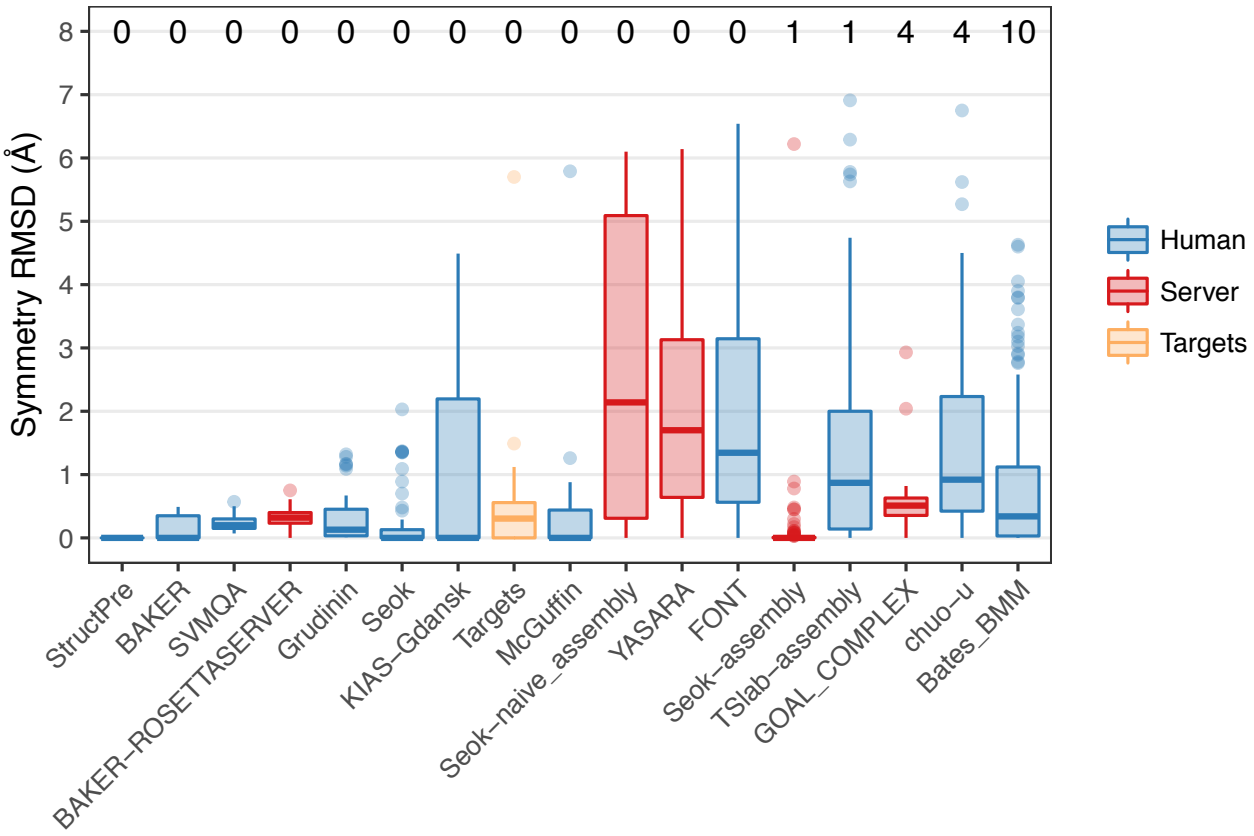

Figure S4: Distribution of symmetry RMSD for all oligomeric models of the symmetric targets submitted by each group. Number of asymmetric models is shown at the top. Groups are sorted increasingly by the number of asymmetric models, first, and by the median of the symmetry RMSD, second. The distribution of symmetry RMSD of the target experimental structures is shown for comparison.

Table S1: Sequence templates for the oligomeric target assemblies used to compute the baseline performance. The QS-score of each template to their corresponding target assembly is shown.

Target	Difficulty	Template	QS-Score
T0860o	Easy	3ZPE	0.41
T0861o-T0862o-T0870o	Medium	1Y7L	0.29
T0867o	Easy	4UMI	0.70
T0873o	Medium	4IP2	0.32
T0880o	Medium		0.00
T0881o	Easy	2VTW	0.34
T0888o	Medium		0.00
T0889o	Easy	4ZA2	0.40
T0893o	Easy	4I5S	0.04
T0903o-T0904o	Medium	4A1S	0.16
T0906o	Easy	3R1M	0.73
T0909o	Easy	2INU	0.02
T0917o	Easy	3BFJ	0.10
T0921-T0922	Easy	2CCL	0.02
T0931o	Medium	3OAO	0.39

Table S2: Symmetry of the target assemblies in CASP12. The macromolecular size (Size), chains of the experimental structure in the assembly (Chains), stoichiometry (Stoich.), symmetry (Symm.) and the symmetry RMSD and TM-score deviations are shown. There are no asymmetric assemblies, except for the heterodimers, and targets range from perfect symmetry to about 1.5Å RMSD.

Target	**Size**	**Chains**	**Stoich.**	**Symm.**	**RMSD**	**TM-Sc.**
T0860o	3	C A B	A3	C3	0.00	1.00
T0866o	6	A F E D C B	A6	C6	0.30	0.99
T0867o	3	A B C	A3	C3	0.44	0.99
T0875o	2	A B	A2	C2	1.12	0.94
T0880o	3	A C B	A3	C3	0.83	0.98
T0881o	3	A C B	A3	C3	0.49	0.99
T0873o	4	A D C B	A4	D2	0.00	1.00
T0888o	3	A C B	A3	C3	0.31	0.99
T0884-T0885	2	A B	AB	C1	0.00	1.00
T0868-T0869	2	A B	AB	C1	0.00	1.00
T0893o	2	A B	A2	C2	0.00	1.00
T0889o	4	A D C B	A4	D2	0.00	1.00
T0894-T0895	2	A B	AB	C1	0.00	1.00
T0861o-T0862o-T0870o	6	A C B D E F	A2B2C2	C2	0.34	0.99
T0909o	3	A C B	A3	C3	0.30	1.00
T0912o	2	A B	A2	C2	0.23	1.00
T0906o	8	A B H D C G F E	A8	D4	0.88	0.99
T0913o	6	A F E D C B	A6	D3	0.00	1.00
T0917o	2	A B	A2	C2	0.00	1.00
T0897-T0898	2	A B	AB	C1	0.00	1.00
T0929o	2	A B	A2	C2	0.58	0.98
T0921-T0922	2	A B	AB	C1	0.00	1.00
T0930o	2	A B	A2	C2	0.15	1.00
T0931o	2	A B	A2	C2	0.55	0.99
T0932o	2	A B	A2	C2	1.49	0.94
T0934o	2	A B	A2	C2	0.39	1.00
T0933o	6	A F E D C B	A6	C6	0.00	1.00
T0945o	2	A B	A2	C2	0.00	1.00
T0914-T0915	2	A B	AB	C1	0.00	1.00
T0903o-T0904o	4	B H R L	A2B2	C2	5.70	0.68