SUPPORTING INFORMATION

Table S1: Normalization parameters (Eq. 1 in the main text) for surface area, desolvation, and contact energy terms.

Term	FSA				PSA			
	α	β	X_0	sgn	α	β	X_0	sgn
ΔSASA	5.2300	0.0047	0	+1	5.3700	0.0045	0	+1
E_{des}	8.0990	0.3112	10	+1	8.7069	0.3148	10	+1
E_{AACE18}	6.4403	0.0797	50	–1	5.8480	0.0695	50	–1

Table S2. Top ten template-based docking predictions for dimeric T119/T0917.

No.	Protein model	Template	Rank by F(S)	F(S)	AACE18	TM-score [(1)]	f_{nat}	*i*-RMSD, Å [(2)]	CAPRI class [(3)]
1	35[(4)]	3iv7AB	22	0.967	-85.7	0.77	0.62	2.3	A
2	51[(5)]	3iv7AB	6	0.981	-109.6	0.77	0.45	2.4	M
3	67[(6)]	5br4AB	749	0.517	38.8	0.90	0.00	24.9	I
4	71[(7)]	4rflAB	245	0.850	-91.4	0.66	0.12	6.8	I
5	100[(8)]	3iv7AB	49	0.952	-103.2	0.77	0.49	2.0	M
6	154[(9)]	$1jq5A_1A_7$[(13)]	9	0.975	-83.8	0.76	0.58	3.5	A
7	154[(9)]	3ox4BC	734	0.530	-5.6	0.92	0.00	24.8	I
8	174[(10)]	$1jq5A_1A_7$[(13)]	15	0.969	-76.8	0.74	0.66	3.2	A
9	176[(11)]	$1jq5A_1A_7$[(13)]	25	0.965	-78.7	0.75	0.59	3.6	A
10	177[(12)]	1vljAB	49	0.952	-103.2	0.77	0.45	3.3	A

[(1)] Score of the structural alignment of protein model and one of the template chains.
[(2)] C^{α} root-mean-square deviation of the ligand interface.
[(3)] I – incorrect; A – acceptable-, M – medium-, H – high-quality model.
[(4)] Model 5 of DISTILL server.[1]
[(5)] Model 4 of Princeton TIGRESS (FLOUDAS) server.[2]
[(6)] Model 5 of GOAL server.[3]
[(7)] Model 4 of HHGG server.[4]
[(8)] Model 5 of MULTICOM-CONSTRUCT server.[5]
[(9)] Model 3 of SEOK-naïve-assembly server.[6]
[(10)] Model 2 of YASARA server.[7]
[(11)] Model 4 of YASARA server.
[(12)] Model 5 of YASARA server.
[(13)] Models 1 and 7 in the PDB biological unit.

Table S3. Top ten template-based docking predictions for trimeric T110/T0860.
Characteristics of the predictions are for the interface obtained by superimposition of target models onto chains A_1 and A_2 of the templates (other interfaces are nearly identical).

No.	Protein model	Template	F(S)	AACE18	TM-score	f_{nat}	*i*-RMSD, Å	CAPRI class
1	1[(2)]	3zpe$A_1A_2A_3$[(1)]	0.963	-25.1	0.96	0.31	2.76	M
2	1[(2)]	4cw8 $A_1A_2A_3$[(1)]	0.965	-25.8	0.97	0.29	2.80	A
3	2[(3)]	3zpe $A_1A_2A_3$	0.957	-19.7	0.97	0.27	2.70	A
4	2[(3)]	4cw8 $A_1A_2A_3$	0.961	-22.3	0.96	0.29	2.70	A
5	3[(4)]	3zpe $A_1A_2A_3$	0.988	-45.7	0.87	0.58	1.86	M
6	3[(4)]	4cw8$A_1A_2A_3$	0.989	-50.3	0.87	0.58	1.87	M
7	4[(5)]	3zpe $A_1A_2A_3$	0.986	-48.5	0.89	0.62	1.57	M
8	4[(5)]	4cw8 $A_1A_2A_3$	0.988	-51.3	0.88	0.62	1.60	M
9	5[(6)]	3zpe $A_1A_2A_3$	0.991	-39.7	0.98	0.47	2.25	M
10	5[(6)]	4cw8 $A_1A_2A_3$	0.991	-40.8	0.98	0.43	2.28	M

[(1)] Models of 1, 2 and 3 in the PDB biounit.
[(2)] Model 1 of ZHANG server.[8]
[(3)] Model 2 of ZHANG server.
[(4)] Model 1 of BAKER-ROSETTA server.[9]
[(5)] Model 5 of BAKER-ROSETTA server.
[(6)] Model 1 of HHPRED0 server.[10]

Table S4. Top ten template-based docking predictions for trimeric T111/T0867.
Characteristics of the predictions are for the interface obtained by superimposition of target models onto the first two chains of the templates.

No.	Protein model	Template	F(S)	AACE18	TM-score	f_{nat}	*i*-RMSD, Å	CAPRI class
1	1[(1)]	4d0uABC	0.940	-22.7	0.99	0.67	0.92	H
2	1[(1)]	4d0uADB	0.832	-24.6	0.97	0.65	0.92	H
3	1[(1)]	4d0uACD	0.944	-24.7	0.97	0.02	8.32	I
4	1[(1)]	4d1fABE	0.952	-24.9	0.99	0.63	1.00	M
5	1[(1)]	4d1fACE	0.954	-25.9	0.87	0.02	8.35	I
6	1[(1)]	4d1fAEL	0.804	2.8	0.99	0.00	20.15	I
7	2[(2)]	4d0uABC	0.977	-26.2	0.96	0.87	0.71	H
8	3[(3)]	4d0uABC	0.919	-25.0	0.95	0.60	1.19	M
9	4[(4)]	4d0uABC	0.910	-26.1	0.95	0.62	0.96	H
10	5[(5)]	4d0uABC	0.929	-25.7	0.97	0.58	1.01	M

[(1)] Model 4 of HHGG server.[4]
[(2)] Model 1 of BAKER-ROSETTA servr.[9]
[(3)] Model 1 of GOAL server.[3]
[(4)] Model 3 of SEOK server.[6]
[(5)] Model 1 of ZHANG server.[8]

Table S5. Top ten template-based docking predictions for trimeric T112/T0881.
Characteristics of the predictions are for the interface obtained by superimposition of target models onto the first two chains of the templates.

No.	Protein model	Template	F(S)	AACE18	TM-score	f_{nat}	*i*-RMSD, Å	CAPRI class
1	1[(1)]	2iumABC	0.661	-15.03	0.82	0.53	3.99	A
2	1[(1)]	2vtwAEF	0.807	-9.56	0.84	0.51	4.27	A
3	2[(2)]	2vtwAEF	0.829	-15.28	0.92	0.38	4.27	A
4	3[(3)]	2vtwAEF	0.873	-17.78	0.92	0.26	4.33	A
5	4[(4)]	2vtwAEF	0.885	-14.68	0.93	0.38	4.15	A
6	5[(5)]	2vtwAEF	0.831	-6.83	0.89	0.43	4.32	A
7	6[(6)]	2vtwAEF	0.800	-14.56	0.91	0.45	4.83	I
8	7[(7)]	2vtwAEF	0.778	-7.92	0.89	0.53	4.85	A
9	9[(8)]	2iumABC	0.795	-18.62	0.90	0.55	3.83	A
10	10[(9)]	2vtwAEF	0.796	-12.79	0.90	0.53	4.85	I

[(1)] Model 1 of BAKER-ROSETTA server.[9]
[(2)] Model 3 of MUFOLD1 server.[11]
[(3)] Model 3 of MULTICOM-NOVEL server.[5]
[(4)] Model 1 of CHUO-U server.[12]
[(5)] Model 2 of QUARK server.[13]
[(6)] Model 2 of ZHANG server.[8]
[(7)] Model 4 of RBO_ALEPH server.[14]
[(8)] Model 1 of RAPTOR-X server.[15]
[(9)] Model 2 of SEOK server.[6]

Table S6. Top ten template-based docking predictions for octameric T118/T0906.
Characteristics of the predictions are for the interface obtained by superimposition of target models onto models 2 and 6 of the template biounit (other interfaces are nearly identical).

No.	Protein model	Template	F(S)	AACE18	TM-score	f_{nat}	*i*-RMSD, Å	CAPRI class
1	1[(2)]	3t2c[(1)]	0.998	-72.25	0.97	0.68	0.88	H
2	2[(3)]		0.996	-52.36	0.96	0.55	0.99	H
3	3[(4)]		0.998	-70.84	0.97	0.61	0.03	H
4	4[(5)]		0.995	-41.39	0.97	0.62	0.93	H
5	5[(6)]		0.997	-72.42	0.94	0.55	1.04	M
6	6[(7)]		0.993	-57.43	0.98	0.59	1.06	M
7	7[(8)]		0.990	-48.84	0.97	0.59	1.06	M
8	8[(9)]		0.998	-58.78	0.98	0.62	1.04	M
9	9[(10)]		0.997	-67.39	0.94	0.58	1.03	M
10	10[(11)]		0.990	-42.93	0.97	0.65	1.23	M

[(1)] The same template (octameric in biological unit, monomeric in the asymmetric unit) was used for all docking models.
[(2)] Model 5 of BAKER-ROSETTA server.[9]
[(3)] Model 1 of YASARA server.[7]
[(4)] Model 1 of QUARK server.[13]
[(5)] Model 5 of HHGG server.[4]
[(6)] Model 2 of ZHANG server.[8]
[(7)] Model 3 of SLBIO server (reference not available).
[(8)] Model 1of TSSPRED2 server (reference not available)
[(9)] Model 1of HHPRED1 server.[10]
[(10)] Model 5 of MULTICOM-CONSTRUCT server.[5]
[(11)] Model 1 of DISTILL server.[1]

Table S7. Top ten template-based docking predictions for hetero-dimeric T120/T0921-T0922.

No.	T0921 model	T0922 model	Template	F(S)	AACE18	TM-score [1]	TM-score [2]	f_{nat}	*i*-RMSD, Å	CAPRI class
1	21[4]	89[13]	4dh2AB	0.765	4.05	0.94	0.98	0.26	3.63	A
2[3]	21[4]	89[13]	4dh2AB	–	–	–	–	0.22	6.55	I
3	73[5]	98[14]	2cclAB	0.637	-3.92	0.85	0.60	0.26	3.61	A
4	74[6]	24[15]	2cclAB	0.645	-10.24	0.83	0.59	0.33	3.47	M
5	87[7]	29[16]	2cclAB	0.624	-14.41	0.83	0.59	0.26	4.28	A
6	95[8]	51[17]	2cclAB	0.602	-23.20	0.84	0.57	0.36	3.63	M
7	142[9]	174[18]	2cclAB	0.725	-10.99	0.79	0.71	0.32	3.12	M
8	145[10]	24[15]	2cclAB	0.667	-15.03	0.80	0.59	0.33	3.41	A
9	169[11]	46[19]	4uypAB	0.604	-0.33	0.85	0.95	0.03	12.69	I
10	186[12]	143[20]	4dh2AB	0.638	-7.57	0.92	0.72	0.24	3.50	A

[1] TM-score of alignment of T0921 model and first template chain.
[2] TM-score of alignment of T0922 model and second template chain.
[3] Prediction obtained from prediction 1 by manual shift of the T0922 model.
[4] Model 1 of CHUO-U2 server.[12]
[5] Model 4 of INTFOLD4 server.[16]
[6] Model 5 of INTFOLD4 server.
[7] Model 3 of MUFOLD2 server.[11]
[8] Model 1 of MULTICOM-CONSTRUCT server.[5]
[9] Model 2 of RBO-ALEPH server.[14]
[10] Model 5 of RBO-ALEPH server.
[11] Model 3 of TSSPRED2 server (reference and link are not available).
[12] Model 5 of ZHOU-SPARKS-X server.[17]
[13] Model 4 of MUFOLD1 server.[11]
[14] Model 4 of MULTICOM-CONSTRUCT server.[5]
[15] Model 4 of CHUO-U2 server.[12]
[16] Model 4 of CHUO-U server.[12]
[17] Model 4 of FLOUDAS server.[2]
[18] Model 3 of YASARA server.[7]
[19] Model 1 of FFAS03 server.[18]
[20] Model 3 of RBO-ALEPH server.[14]

Table S8. Top ten template-based (1-6) and free (7-10) docking predictions for homodimeric T114/T0875.

No.	Protein model	Template	F(S)	AACE18	TM-score or Rank[(1)]	f_{nat}	*i*-RMSD, Å	CAPRI class
1	1[(2)]	2fbqA_1A_2	0.056	-83.04	0.34	0.00	9.67	I
2	2[(3)]	1mscA_1A_2	0.239	-77.24	0.33	0.00	17.27	I
3	4[(4)]	3f13A_1A_2	0.120	-76.98	0.36	0.00	8.80	I
4	7[(5)]	4q95AB	0.832	-1.56	0.78/0.66	0.00	9.88	I
5	8[(6)]	4dpzA_1A_4	0.246	-6.79	0.81	0.00	9.91	I
6	10[(7)]	4dotA_1A_3	0.302	-0.93	0.79	0.00	19.61	I
7	3[(8)]	–	–	-67.54	4759	0.27	15.61	I
8	4[(4)]	–	–	-70.05	7629	0.00	6.64	I
9	6[(9)]	–	–	-96.80	14270	0.04	19.02	I
10	7[(5)]	–	–	-118.38	26793	0.04	8.13	I

[(1)] Integer numbers are GRAMM ranking by shape complementarity.
[(2)] Model 1 of BAKER-ROSETTA server.[9]
[(3)] Model 3 of INTFOLD4 server.[16]
[(4)] Model 4 of SEOK server.[6]
[(5)] Model 3 of ZHANG server.[8]
[(6)] Model 3 of ATOME2-CBS server.[19]
[(7)] Model 3 of FFAS03 server.[18]
[(8)] Model 1 of ZHANG server.

Table S9. Top ten template-based docking predictions for homodimeric T116/T0893.

No.	Protein model	Template	F(S)	AACE18	TM-score[11]	f_{nat}	*i*-RMSD, Å	CAPRI class
1	9[1]	3d36AB	0.996	-62.09	0.82	0.09	11.48	I
2	21[2]	3a0rA_1A_2	0.969	-105.95	0.72	0.10	15.26	I
3	26[3]	4bixAB	0.837	-94.64	0.75/0.70	0.40	14.47	I
4	44[4]	4mpcA_1A_2	0.946	-31.62	0.83	0.00	27.79	I
5	49[5]	3a0rA_1A_2	0.965	-85.26	0.75	0.08	15.13	I
6	105[6]	4q20AB	0.935	-68.71	0.90/0.75	0.09	15.69	I
7	116[7]	4mpcA_1A_2	0.987	-42.27	0.83	0.00	27.24	I
8	120[8]	4ctiBD	0.722	-74.04	0.53	0.01	19.04	I
9	140[9]	3d36AB	0.998	-71.73	0.84	0.07	11.60	I
10	141[10]	3d36AB	0.991	-79.13	0.81	0.14	11.68	I

[1] Model 1 of BHAGEERATHH-PLUS server.[20]
[2] Model 2 of DISTILL server.[1]
[3] Model 2 of FALCON-TOPO server.[21]
[4] Model 3 of GOAL-COMPLEX server.[3]
[5] Model 3 of GOAL server.[3]
[6] Model 5 of QUARK server.[13]
[7] Model 5 of SEOK-ASSEMBLY server.[6]
[8] Model 4 of SEOK-NAIVE server.[6]
[9] Model 5 of YASARA server.[7]
[10] Model 1 of ZHANG server.[8]
[11] Two values indicate heterodimeric template.

Table S10. Top ten docking predictions for hetero-dimeric T113/T0884-T0885.

No.	T0885 model	T0884 model	AACE18	Rank	f_{nat}	*i*-RMSD, Å	CAPRI class
1	1[(1)]	8[(5)]	-54.63	21004	0.052	12.72	I
2[(3)]	1[(1)]	29[(6)]	-58.90	19488	0.169	7.28	I
3	2[(2)]	13[(7)]	-51.22	20900	0.039	11.58	I
4	3[(3)]	12[(8)]	-51.61	12491	0.104	7.11	I
5	3[(3)]	12[(8)]	-50.27	24146	0.026	10.52	I
6	3[(3)]	16[(9)]	-51.17	28463	0.065	8.48	I
7	4[(4)]	13[(7)]	-61.44	5017	0.117	9.76	I
8	4[(4)]	16[(9)]	-50.71	4871	0.078	8.22	I
9	4[(4)]	27[(10)]	-50.19	8290	0.130	8.52	I
10	4[(4)]	29[(6)]	-50.90	23951	0.130	7.27	I

[(1)] Model 1 of BAKER-ROSETTA server.[9]
[(2)] Model 2 of ZHANG server.[8]
[(3)] Model 4 of GOAL-COMPLEX server.[3]
[(4)] Model 1 of QUARK server.[13]
[(5)] Model 2 of PCONS-NET server.[22]
[(6)] Model 5 of MULTICOM-CONSTRUCT server.[5]
[(7)] Model 1 of MULTICOM-NOVEL server.[5]
[(8)] Model 5 of ZHANG server.
[(9)] Model 5 of GOAL-COMPLEX server.
[(10)] Model 5 of PCONS-NET server.

Table S11. Top ten docking predictions for hetero-tetrameric T117/T0903-T0904.
Characteristics of the predictions are with respect to the interface of chains H and R in the native target 5a7d (blue and yellow in Figure 6A, main text). Predictions with identical docking parameters (columns 2 – 5) differ by arrangement of the truncated parts of the ligand (see main text).

No.	T0903 model	T0904 model	AACE18	Rank	f_{nat}	*i*-RMSD, Å	CAPRI class
1	15[(1)]	1[(2)]	-87.3	18244	0.556	16.13	I
2	15[(1)]	1[(2)]	-87.3	18244	0.000	16.13	I
3	15[(1)]	93[(3)]	-94.1	66805	0.000	16.15	I
4	15[(1)]	93[(3)]	-94.1	66805	0.641	16.13	I
5	15[(1)]	24[(4)]	-35.7	2190	0.578	9.64	I
6	15[(1)]	24[(4)]	-35.7	2190	0.000	9.64	I
7	15[(1)]	68[(5)]	-65.0	1027	0.000	10.34	I
8	15[(1)]	84[(6)]	-55.5	600	0.000	10.95	I
9	15[(1)]	68[(5)]	-74.6	480	0.000	21.44	I
10	15[(1)]	106[(7)]	-47.0	64/61976[(8)]	0.007	11.01	I

[(1)] Model 3 of BHAGEERATHH-PLUS server.[20]
[(2)] Model 1 of ATOME2-CBS server.[19]
[(3)] Model 3 of MYPROTEIN-ME server (reference not available).
[(4)] Model 4 of DISTILL server.[1]
[(5)] Model 1 of MUFOLD2 server.[11]
[(6)] Model 4 of MULTICOM-NOVEL server.[5]
[(7)] Model 3 of PHYRETOPOALPHA server.[23]
[(8)] Rank 61976 of the docking prediction consists of two docking predictions with rank 64 between models of receptor 15 and ligand 106.

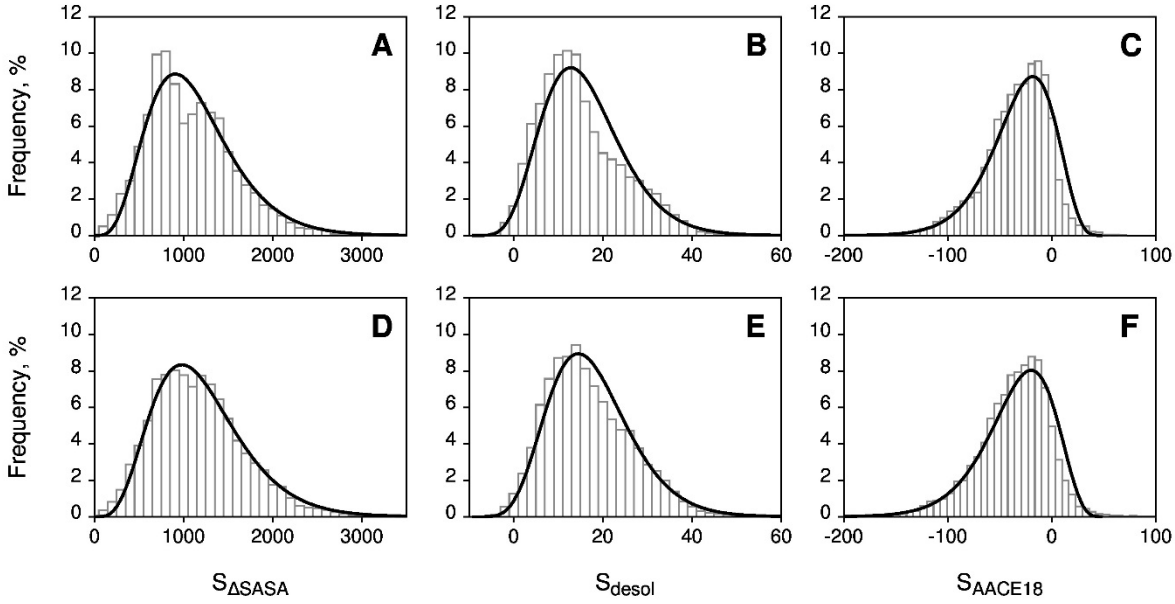

Figure S1. Raw-value histograms of buried surface area (A, D), desolvation energy (B, E) and interface contact potential AACE18 (C, F) for 7,056 FSA (A–C) and 11,400 PSA (D–F) near-native models. The data is fitted by gamma distributions (see main text for details).

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