

Supporting Information

Improved consensus-fragment selection in template-assisted prediction of protein structures with the UNRES force field in CASP13

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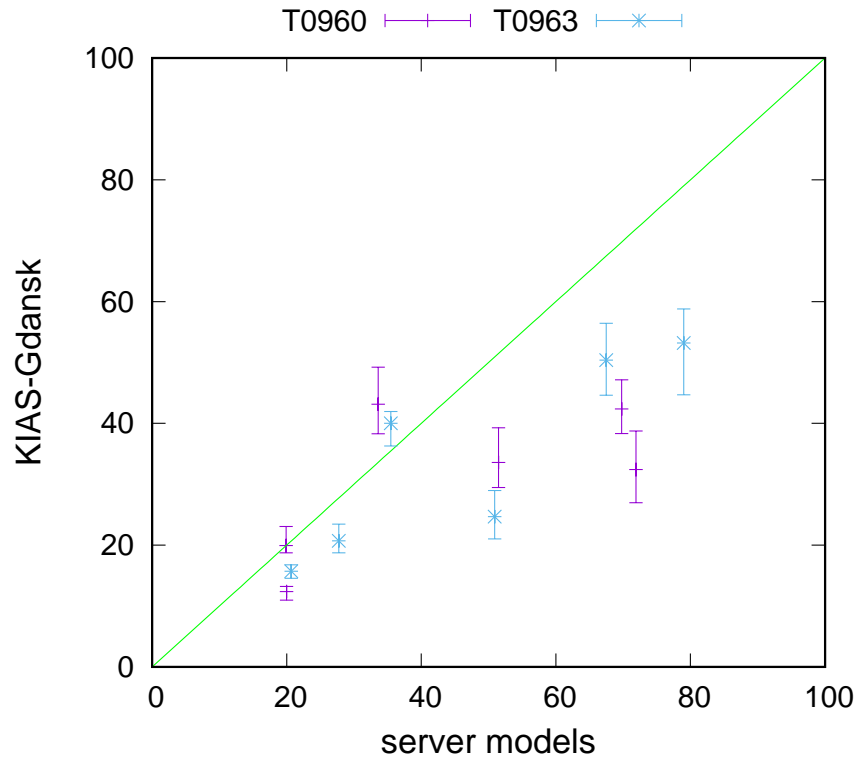


Figure S1: A whiskered scatter plot of the GDT_TS of initial models vs. KIAS-Gdansk predictions of the T0960 and T0963 targets.

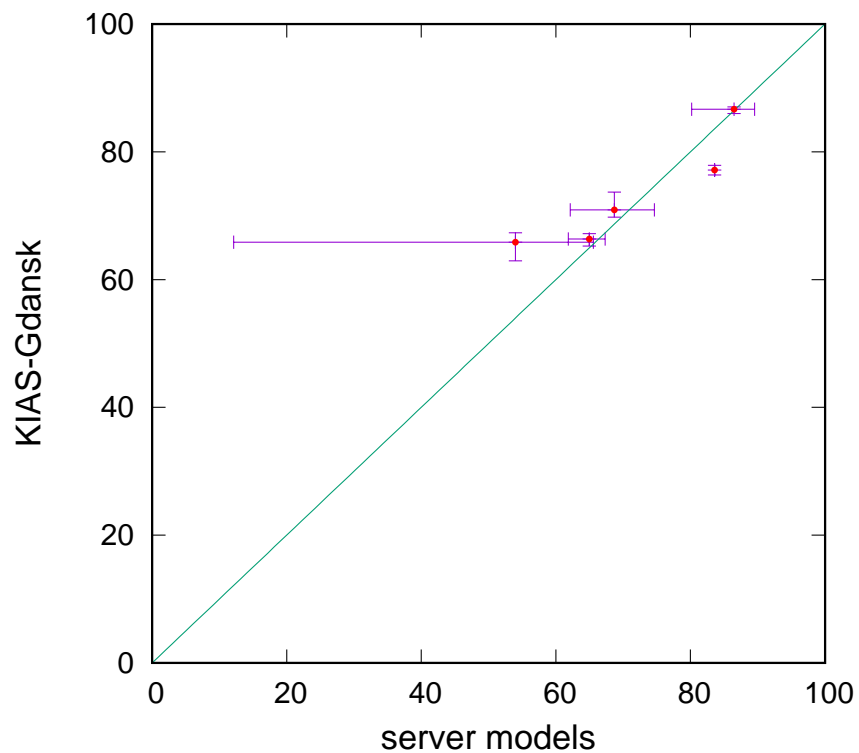


Figure S2: A whiskered scatter plot of the GDT_TS of the models from the selected servers vs. that of the KIAS-Gdansk predictions for the large-size regular targets (T0984, T0995, T1003 and T1009), for which the server models selected based on DeepQA score²⁵ were used as initial models.

Table S1: GDT_TS values and rankings of the KIAS-Gdansk first and the best (highest GDT_TS) models of the CASP13 regular targets.

EU ^a	#res ^b	type ^c	Model 1		best model		
			GDT_TS	rank ^d	model# ^e	GDT_TS	rank ^d
T0949-D1	139	TBM/FM	61.24	69/395	5	62.79	30/395
T0953s1-D1	67	FM	47.76	16/419	5	49.63	9/419
T0953s2-D1	44	FM/TBM	28.41	357/412	4	30.68	311/412
T0953s2-D23	204	other	30.39	98/412	5	32.23	73/412
T0953s2-D2	111	FM	48.23	78/412	5	50.39	69/412
T0953s2-D3	93	FM	20.45	215/410	1	20.45	215/410
T0953s2	249	other	25.61	88/412	5	26.91	70/412
T0954-D1	336	TBM-hard	52.23	220/390	5	53.94	193/390
T0955-D1	41	FM/TBM	92.68	19/413	4	93.29	15/413
T0957s1-D1	108	FM	40.74	98/435	4	41.44	94/435
T0957s1-D2	54	TBM-hard	56.02	87/435	1	56.02	87/435
T0957s1	163	other	27.32	151/435	2	29.32	96/435
T0957s2-D1	155	FM	45.81	94/431	1	45.81	94/431
T0958-D1	77	FM/TBM	61.36	103/420	3	61.69	97/420
T0959-D1	180	TBM-hard	59.31	103/392	5	60.56	80/392
T0960-D1	32	other	42.19	99/391	3	49.22	12/391
T0960-D2	84	FM	39.29	68/395	1	39.29	68/395
T0960-D3	89	TBM-hard	38.76	209/397	1	38.76	209/397
T0960-D4	64	other	18.75	306/395	5	23.05	164/395
T0960-D5	105	TBM-easy	45.00	232/395	3	47.14	229/395
T0960	384	other	13.17	249/399	3	13.23	247/399
T0961-D1	503	TBM-easy	88.97	50/402	1	88.97	50/402
T0963-D1	31	other	41.13	102/382	4	41.94	69/382
T0963-D2	82	FM	21.04	266/383	3	28.96	157/383
T0963-D3	93	TBM-hard	44.62	182/387	3	56.45	107/387
T0963-D4	64	other	19.53	285/382	2	23.44	129/382
T0963-D5	94	TBM-easy	55.59	204/392	3	58.78	189/392
T0963	372	other	16.35	206/392	3	16.76	198/392
T0964-D1	95	TBM-hard	70.79	73/401	4	71.58	68/401
T0965-D1	313	TBM-hard	63.98	106/411	2	65.02	50/411
T0966-D1	492	TBM-hard	53.40	210/403	1	53.40	210/403

T0968s1-D1	119	FM	55.09	113/443	3	55.93	109/443
T0968s2-D1	116	FM	64.78	39/452	1	64.78	39/452
T0969-D1	354	FM	46.40	75/389	2	48.87	46/389
T0970-D1	97	FM/TBM	45.29	96/451	5	45.59	95/451
T0973-D1	128	TBM-easy	52.15	214/440	4	57.42	156/440
T0974s1-D1	69	TBM-easy	76.81	170/444	5	78.62	114/444
T0975-D1	293	FM	34.79	152/394	2	40.75	81/394
T0976-D1	120	TBM-easy	79.17	62/407	2	79.79	56/407
T0976-D2	124	TBM-easy	72.38	164/408	4	77.62	80/408
T0976	252	other	42.30	133/410	2	42.90	125/410
T0977-D1	301	TBM-easy	74.83	144/404	4	75.17	129/404
T0977-D2	204	TBM-easy	63.85	205/404	1	63.85	205/404
T0977	566	other	41.77	193/404	5	43.65	109/404
T0979-D1	92	TBM-hard	49.46	72/453	2	58.97	21/453
T0980s1-D1	105	FM	27.16	252/449	5	43.03	34/449
T0980s2-D1	31	other	31.45	353/452	2	33.87	153/452
T0981-D1	86	TBM-hard	54.94	80/387	1	54.94	80/387
T0981-D2	80	FM	28.44	71/387	4	33.12	12/387
T0981-D3	203	FM/TBM	46.55	74/387	2	50.12	33/387
T0981-D4	111	TBM-hard	58.56	83/394	5	61.26	27/394
T0981-D5	127	TBM-hard	47.05	88/394	5	51.38	58/394
T0981	640	other	17.05	87/399	5	18.29	43/399
T0983-D1	236	TBM-easy	87.71	127/419	3	88.14	106/419
T0984-D1	504	TBM-easy	67.32	1/393	1	67.32	1/393
T0984-D2	147	TBM-easy	70.34	73/393	3	73.69	32/393
T0985-D1	842	TBM-hard	55.11	29/382	4	55.28	27/382
T0986s1-D1	92	FM/TBM	64.13	62/443	2	69.29	14/443
T0986s2-D1	155	FM	41.29	56/425	4	41.77	55/425
T0987-D1	185	FM	49.59	14/394	1	49.59	14/394
T0987-D2	207	FM	41.07	20/394	5	41.20	19/394
T0987	405	other	24.80	14/394	1	24.80	14/394
T0989-D1	134	FM	45.90	37/418	2	49.63	10/418
T0989-D2	112	FM	34.38	23/418	2	35.94	12/418
T0989	246	other	25.71	52/418	2	27.74	11/418
T0990-D1	76	FM	65.79	22/396	4	67.11	11/396
T0990-D2	231	FM	14.50	275/397	4	21.54	67/397

T0990-D3	213	FM	15.38	123/397	4	17.14	53/397
T0990	552	other	9.24	95/397	4	10.14	65/397
T0991-D1	111	FM	23.65	152/447	3	26.80	75/447
T0992-D1	107	FM/TBM	69.86	82/431	4	71.50	52/431
T0993s1-D1	263	TBM-easy	72.15	130/417	2	72.24	125/417
T0993s2-D1	98	TMB-easy	68.11	179/444	3	68.37	176/444
T0995-D1	294	TBM-easy	76.45	206/416	3	77.89	192/416
T0996-D1	107	TBM-easy	79.21	2/390	1	79.21	2/390
T0996-D2	127	TBM-easy	78.35	67/390	1	78.35	67/390
T0996-D3	100	TBM-easy	54.25	159/388	5	66.50	100/388
T0996-D4	133	TBM-easy	60.90	125/388	2	68.80	79/388
T0996-D5	121	TBM-easy	65.08	142/385	1	65.08	142/385
T0996-D6	104	TBM-easy	39.18	205/385	3	52.16	189/385
T0996-D7	140	TBM-easy	70.36	46/385	1	70.36	46/385
T0996	848	other	18.03	150/390	3	19.20	78/390
T0997-D1	185	FM/TBM	46.35	190/440	2	46.62	188/440
T0998-D1	166	FM	17.02	116/436	2	17.77	82/436
T1000-D1	83	other	93.67	198/399	5	95.78	120/399
T1000-D2	431	FM	57.06	141/401	4	59.17	31/401
T1000	514	other	46.56	140/401	4	48.28	35/401
T1001-D1	139	FM	66.73	89/442	1	66.73	89/442
T1002-D1	59	TBM-easy	59.32	239/405	4	64.41	227/405
T1002-D2	59	TBM-easy	38.56	248/405	1	38.56	248/405
T1002-D3	144	TBM-easy	71.88	168/405	4	76.04	130/405
T1002	270	other	38.33	173/405	4	41.02	120/405
T1003-D1	437	TBM-easy	87.04	82/417	1	87.04	82/417
T1004-D1	86	TBM-easy	79.07	153/402	1	79.07	153/402
T1004-D2	77	TBM-easy	72.73	46/402	3	75.00	30/402
T1004-D3	230	other	84.46	147/396	3	88.48	97/396
T1004	458	other	48.87	148/403	3	51.26	104/403
T1005-D1	326	FM/TBM	51.23	80/397	5	51.69	72/397
T1006-D1	77	TBM-easy	97.40	57/453	2	97.73	43/453
T1008-D1	77	FM/TBM	83.12	20/440	4	84.09	14/440
T1009-D1	718	TMB-hard	66.99	58/408	4	67.20	38/408
T1010-D1	210	FM	32.74	57/429	2	34.76	41/429
T1011-D1	302	TBM-hard	65.89	29/390	5	67.50	13/390

T1011-D2	160	other	84.06	154/390	5	87.19	111/390
T1011	534	other	45.21	42/390	1	45.21	42/390
T1013-D1	288	TBM-easy	77.34	123/388	4	79.51	96/388
T1014-D1	159	TBM-easy	82.12	156/404	4	86.26	10/404
T1014-D2	117	TBM-easy	70.94	117/398	3	74.57	29/398
T1014	276	other	46.27	155/405	4	48.60	10/405
T1015s1-D1	88	FM	35.80	123/464	2	48.86	49/464
T1015s2-D1	129	TBM-hard	48.06	292/436	5	69.96	16/436
T1016-D1	202	TBM-easy	81.06	31/439	5	81.68	11/439
T1017s1-D1	110	TBM-easy	64.09	240/441	5	68.86	211/441
T1017s2-D1	128	FM	53.80	104/438	3	55.40	90/438
T1018-D1	324	TBM-easy	85.70	59/421	1	85.70	59/421
T1019s1-D1	58	FM/TBM	50.00	146/445	4	53.02	128/445
T1019s2-D1	88	TBM-easy	53.12	273/436	1	53.12	273/436
T1020-D1	322	TBM-easy	69.97	51/410	2	70.85	36/410
T1021s1-D1	149	TBM-hard	70.47	17/422	2	70.64	16/422
T1021s2-D1	349	TBM-hard	65.04	74/406	2	65.62	61/406
T1021s3-D1	178	FM	51.05	75/413	3	52.26	54/413
T1021s3-D2	101	FM	51.03	65/411	1	51.03	65/411
T1021s3	295	other	30.71	74/413	3	31.43	64/413
T1022s1-D1	156	FM	48.72	80/423	4	51.12	65/423
T1022s1-D2	67	TBM-hard	62.31	157/422	4	63.43	135/422
T1022s1	229	other	35.31	79/428	4	36.21	67/428
T1022s2-D1	525	TBM-hard	46.63	154/404	1	46.63	154/404

^aEvaluation unit. ^bNumber of residues. ^cTarget type; TMB: Template Based Modeling, FM: Free Modeling. ^dCASP13 rank/total number of models submitted for the respective target. ^eThe numbers of the best of KIAS-Gdansk models.

Table S2: Numbers of EUs and their minimum, maximum, and average GDT_TS values, as well as the standard deviations of the GDT_TS for the respective target categories for the KIAS-Gdansk, selected server and all server first, all and best models obtained in the CASP12 and CASP13 experiments.

Type	#EU ^a	GDT_TS, first models				#EU ^a	GDT_TS, all models				#EU ^a	GDT_TS, best models			
		min ^b	max ^c	ave ^d	std ^e		min ^b	max ^c	ave ^d	std ^e		min ^b	max ^c	ave ^d	std ^e
CASP12 KIAS-Gdansk															
TBM	12	32.25	87.03	62.51	15.13	60	19.60	87.66	62.03	14.76	12	50.35	87.66	65.95	11.29
FM/TBM	17	16.81	82.25	47.97	19.40	85	16.81	82.25	47.82	18.51	17	17.24	82.25	50.21	18.34
FM	38	9.46	71.15	29.88	13.50	190	8.14	71.64	29.62	13.30	38	9.82	71.64	32.47	13.73
other	18	8.68	53.67	24.66	11.70	90	7.65	54.52	25.36	12.13	18	8.68	54.52	27.90	13.52
CASP12 selected servers															
TBM	48	34.10	87.66	65.86	9.88	240	19.22	90.82	61.31	13.77	48	35.12	90.82	67.20	9.99
FM/TBM	68	20.35	80.17	51.32	13.80	340	12.07	81.16	47.32	13.50	68	20.64	81.16	56.09	12.04
FM	150	7.77	77.16	30.61	12.87	750	6.96	79.57	29.23	11.91	150	9.16	79.57	35.09	13.25
other	71	7.52	50.87	26.97	11.89	355	5.84	52.33	25.26	11.08	71	8.16	52.33	29.27	12.27
CASP12 all servers															
TBM	471	5.13	87.66	49.86	20.19	2056	4.53	90.82	45.94	20.65	474	5.43	90.82	52.27	19.19
FM/TBM	668	6.08	80.17	36.83	15.25	2924	4.96	81.16	34.88	14.95	670	6.16	81.16	40.03	15.19
FM	1448	3.79	77.16	23.16	11.16	6330	2.88	79.57	22.50	10.65	1458	3.93	79.57	25.26	11.88
other	697	0.79	50.87	19.48	11.23	3047	0.79	52.33	18.56	10.64	702	2.53	52.33	21.01	11.39

Type	#EU ^a	GDT_TS, first models				#EU ^a	GDT_TS, all models				#EU ^a	GDT_TS, best models			
		min ^b	max ^c	ave ^d	std ^e		min ^b	max ^c	ave ^d	std ^e		min ^b	max ^c	ave ^d	std ^e
CASP13 KIAS-Gdansk															
TBM	57	38.56	97.40	65.23	13.75	285	21.61	97.73	64.53	14.91	57	38.56	97.73	67.76	12.67
FM/TBM	11	28.41	92.68	59.44	18.14	55	25.57	93.29	56.78	17.59	11	30.68	93.29	61.25	17.84
FM	31	14.50	66.73	40.82	14.78	155	14.50	67.11	40.70	14.24	31	17.14	67.11	43.56	13.72
other	27	9.24	93.67	36.97	21.43	135	9.24	95.78	37.18	21.25	27	10.14	95.78	38.89	21.95
CASP13 selected servers															
TBM	276	20.36	99.03	68.01	12.95	987	12.11	99.03	66.63	14.43	344	15.16	99.03	69.38	13.38
FM/TBM	47	32.65	92.68	58.64	15.88	186	29.41	95.12	55.75	14.86	56	29.41	95.12	59.87	17.10
FM	140	7.20	73.02	38.99	13.82	510	7.20	73.20	37.14	13.18	167	7.20	73.20	38.90	14.45
other	101	5.82	96.72	39.72	24.17	394	5.82	97.29	40.20	24.27	119	5.82	97.29	38.25	23.60
CASP13 all servers															
TBM	2271	2.35	99.03	50.46	24.86	10917	2.10	99.03	47.60	24.81	2125	3.15	99.03	53.93	24.37
FM/TBM	395	5.06	92.68	42.33	17.73	1931	4.53	95.12	40.38	17.02	395	6.77	95.12	45.65	17.76
FM	1202	3.60	73.02	24.82	12.48	5920	3.60	73.20	23.93	11.83	1130	6.14	73.20	27.41	13.13
other	1204	2.10	99.53	26.89	19.85	5855	1.92	99.53	25.77	19.53	986	2.10	99.53	29.52	21.79

^aNumber of models of the evaluation units of a given type, pool (first, all or best), from a given source and from a given CASP experiment. ^bMinimum over all models specified in point a. ^cMaximum over all models specified in point a. ^dAverage over all models specified in point a. ^eStandard deviation over all models specified in point a.

Table S3: The differences of the mean GDT_TS values corresponding to the CASP12 and CASP13 experiments, for the respective target categories for the KIAS-Gdansk, selected server and all server models (first, all, and best), the standard deviations of these differences, and their statistical significances.

Type				KIAS-Gdansk models					
	Δ^a	σ_{Δ}^b	$P(\%)^c$	Δ^a	σ_{Δ}^b	$P(\%)^c$	Δ^a	σ_{Δ}^b	$P(\%)^c$
KIAS-Gdansk models									
TBM	2.72	4.44	92	2.50	2.11	100	1.81	3.96	89
FM/TBM	11.47	7.32	97	8.96	3.14	100	11.04	7.02	97
FM	10.94	3.41	100	11.08	1.49	100	11.09	3.32	100
other	12.31	5.54	100	11.82	2.47	100	10.99	5.80	100
selected server models									
TBM	2.15	1.96	100	5.32	1.03	100	2.18	2.01	100
FM/TBM	7.32	2.79	100	8.43	1.28	100	3.78	2.62	100
FM	8.38	1.57	100	7.91	0.71	100	3.81	1.56	100
other	12.75	3.10	100	14.94	1.40	100	8.98	3.02	100
all server models									
TBM	0.60	1.22	92	1.66	0.58	100	1.66	1.19	100
FM/TBM	5.50	1.03	100	5.50	0.46	100	5.62	1.03	100
FM	1.66	0.46	100	1.43	0.20	100	2.15	0.49	100
other	7.41	0.82	100	7.21	0.38	100	8.51	0.90	100

^a $\Delta = \text{GDT_TS}(\text{CASP13}) - \text{GDT_TS}(\text{CASP12})$. ^bStandard deviation of Δ . ^cStatistical significance of Δ assessed by means of the Student's test.

Table S4: Differences of the mean GDT_TS values along, with their standard deviations and statistical significances, corresponding to the the KIAS-Gdansk models and selected server models, the KIAS-Gdansk models and all server models, and selected server models and all server models (first, all and best).

Type	first models			all models			best models		
	Δ^a	σ_{Δ}^b	$P(\%)^c$	Δ^a	σ_{Δ}^b	$P(\%)^c$	Δ^a	σ_{Δ}^b	$P(\%)^c$
CASP12									
KIAS-Gdansk models and selected server models									
TBM	-3.35	3.57	94	0.72	2.02	78	-1.25	3.31	78
FM/TBM	-3.35	4.08	92	0.50	1.77	69	-5.88	3.66	100
FM	-0.73	2.36	75	0.39	0.99	79	-2.62	2.42	99
other	-2.31	3.13	95	0.10	1.33	56	-1.37	3.31	81
KIAS-Gdansk models and all server models									
TBM	12.65	5.87	100	16.09	2.69	100	13.68	5.57	100
FM/TBM	11.14	3.77	100	12.94	1.66	100	10.18	3.75	100
FM	6.72	1.84	100	7.12	0.79	100	7.21	1.96	100
other	5.18	2.68	100	6.80	1.14	100	6.89	2.73	100
selected server models and all server models									
TBM	16.00	2.95	100	15.37	1.37	100	14.93	2.81	100
FM/TBM	14.49	1.93	100	12.44	0.85	100	16.06	1.90	100
FM	7.45	0.97	100	6.73	0.42	100	9.83	1.03	100
other	7.49	1.41	100	6.70	0.60	100	8.26	1.43	100
CASP13									
KIAS-Gdansk models and selected server models									
TBM	-2.78	1.90	100	-2.10	0.98	100	-1.62	1.90	99
FM/TBM	0.80	5.46	62	1.03	2.38	79	1.38	5.68	72
FM	1.83	2.78	93	3.56	1.23	100	4.66	2.80	100
other	-2.75	5.12	90	-3.02	2.35	100	0.64	4.97	63
KIAS-Gdansk models and all server models									
TBM	14.77	3.31	100	16.93	1.48	100	13.83	3.24	100
FM/TBM	17.11	5.42	100	16.40	2.33	100	15.60	5.43	100
FM	16.00	2.28	100	16.77	0.97	100	16.15	2.39	100
other	10.08	3.87	100	11.41	1.70	100	9.37	4.25	100
selected server models and all server models									
TBM	17.55	1.52	100	19.03	0.80	100	15.45	1.35	100
FM/TBM	16.31	2.71	100	15.37	1.29	100	14.22	2.52	100
FM	14.17	1.13	100	13.21	0.55	100	11.49	1.10	100
other	12.83	2.09	100	14.43	1.03	100	8.73	2.13	100

^a $\Delta = \text{GDT_TS}(\text{CASP13}) - \text{GDT_TS}(\text{CASP12})$. ^bStandard deviation of Δ . ^cStatistical significance of Δ assessed by means of the Student's test.

Table S5: Difficulties, measures of the fit to the experimental structures and rankings of the KIAS-Gdansk first and the best (highest GDT_TS) models of the CASP13 oligomeric targets.

Target	Composition ^a	Difficulty ^b	Model 1				best model				
			F1 ^c	JC ^d	I-RMSD ^e	Rank ^h	Model ^f	F1 ^c	JC ^d	I-RMSD ^e	Rank ^f
H0953	3 × 72 + 249	Hard	2.6	0.27	15.19	27/62	4	5.5	0.26	13.43	22/62
H0957	163 + 164	Hard	0.0	0.07	21.55	47/61	5	0.0	0.29	16.55	19/61
H0968	2 × 126 + 2 × 116	Hard	2.4	0.25	10.42	10/63	4	5.3	0.30	1.33	1/63
H0974	72 + 95	Easy	0.0	0.11	9.43	117/177	4	16.2	0.33	10.69	55/177
H0980	2 × 111 + 2 × 52	Hard	0.0	0.13	11.25	52/73	4	3.0	0.20	7.04	4/73
H0986	96 + 155	Hard	1.5	0.09	21.57	13/77	3	2.9	0.35	18.45	7/77
H0993	2 × 269 + 2 × 109	Medium	9.0	0.24	13.36	14/148	5	10.8	0.24	11.97	10/148
H1015	89 + 129	Hard	0.0	0.17	15.52	154/158	3	7.4	0.21	13.76	10/158
H1017	111 + 129	Medium	5.4	0.25	15.30	19/159	1	5.4	0.25	15.30	19/159
H1019	58 + 88	Hard	8.8	0.26	11.54	41/161	1	8.8	0.26	11.54	41/161
T0961o	4 × 505	Easy	62.9	0.65	1.09	33/151	1	62.9	0.65	1.09	33/151
T0965o	2 × 334	Medium	0.0	0.09	21.46	133/152	2	0.0	0.18	15.24	131/152
T0966o	2 × 494	Medium	0.0	0.00	26.68	67/155	5	0.0	0.00	36.76	34/155
T0973o	2 × 146	Easy	10.9	0.70	7.58	107/162	1	10.9	0.70	7.58	107/162
T0976o	2 × 252	Medium	0.7	0.16	19.28	45/162	5	2.7	0.20	20.61	32/162
T0983o	2 × 245	Easy	86.1	0.77	0.87	23/158	1	86.1	0.77	0.87	23/158
T0984o	2 × 752	Easy	28.2	0.37	6.41	116/157	2	35.9	0.50	5.47	89/157
T0995o	8 × 330	Easy	18.9	0.36	4.78	84/147	2	18.1	0.35	5.27	80/147
T0997o	2 × 228	Medium	0.0	0.00	32.59	97/163	2	26.3	0.24	14.46	1/163
T1003o	2 × 474	Easy	1.2	0.30	10.75	138/164	4	61.5	0.69	5.27	73/164
T1006o	2 × 79	Easy	0.0	0.00	19.03	169/189	2	28.3	0.35	2.54	110/189
T1009o	2 × 718	Medium	0.0	0.10	19.01	72/166	4	4.8	0.39	9.03	12/166
T1020o	3 × 577	Easy	0.0	0.12	10.23	112/144	2	0.0	0.12	9.87	108/144

^aComposition of the oligomers; $m1 \times n1 + m2 \times n2$ indicates that it consists of $m1$ molecules of monomer 1, each containing $n1$ residues and $m2$ molecules of monomer 2, each containing $n2$ residues. ^bTarget difficulties taken from Table S1 of the Supporting Information of ref 35 of the main text (file: prot25795-sup-0005-TableS1.xlsx). ^cInterface Contact Similarity (ICS) quantified as the $F1$ score,³⁴ see eq 4 in the main text. ^dInterface Patch Similarity (IPS) quantified as the Jaccard coefficient,³⁴ see eq 3 in the main text. The corresponding values reported in CASP12 were the Jaccard distances (J_D), and were converted to the Jaccard coefficients by using the relationship $J_C = 1 - J_D$.³⁴ ^eInterface residue RMSD, defined as the minimum RMSD of the superposition between target and model chains based on the interacting residues in the target; ^fCASP13 rank of the KIAS-Gdansk model/all models submitted for the respective target; ^gThe number of the best of the KIAS-Gdansk models for the respective target.