

Supplemental Data for Distance-based Reconstruction of Protein Quaternary Structures from Inter-Chain Contacts

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Supplementary Figures

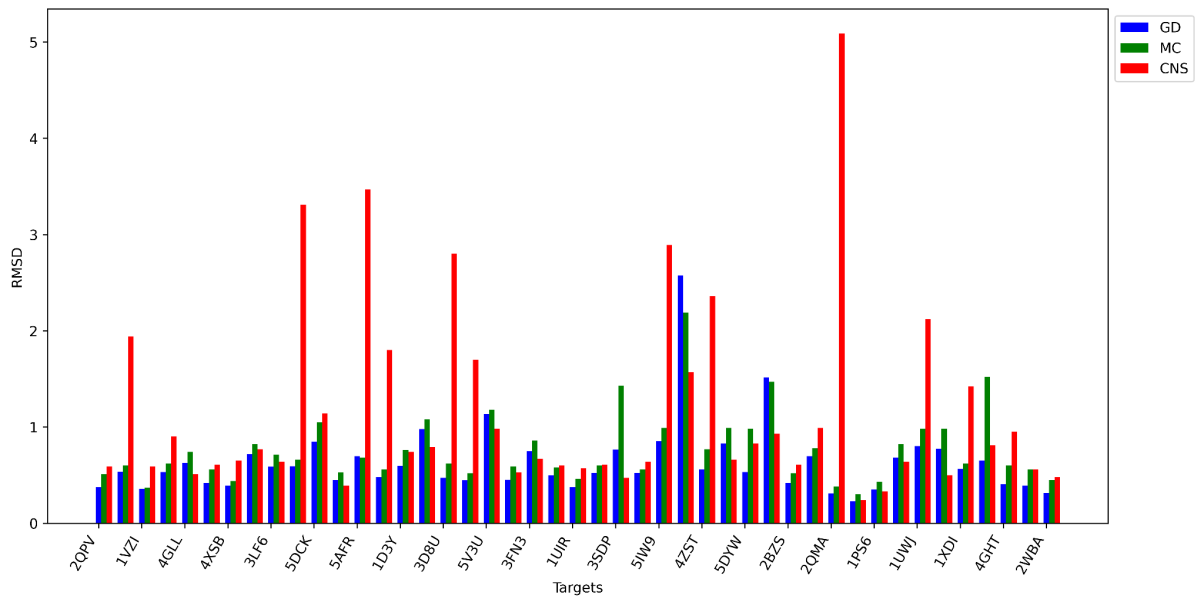


Figure S1. RMSD of GD, MC, and CNS on a dataset of 44 homodimers with known inter-protein contacts. The average RMSD of GD, MC, and CNS is 0.63, 0.76, and 1.16.

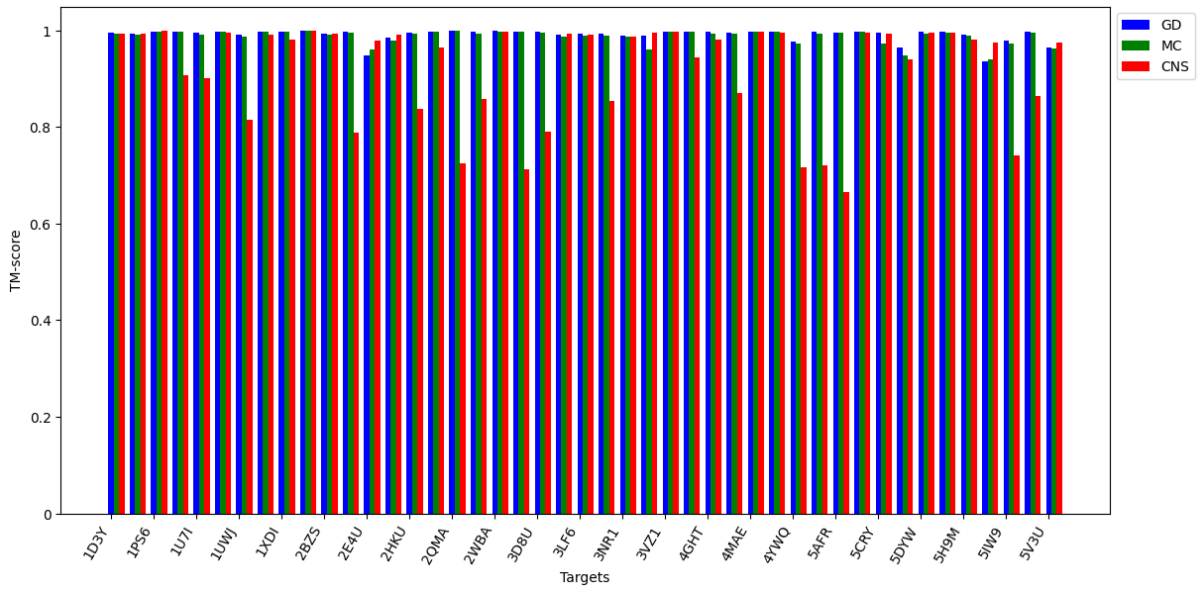


Figure S2. TM-score of GD, MC, and CNS on a dataset of 44 protein complexes with known inter-protein contacts. The average TM-score of GD, MC, and CNS is 0.99, 0.98, and 0.91.

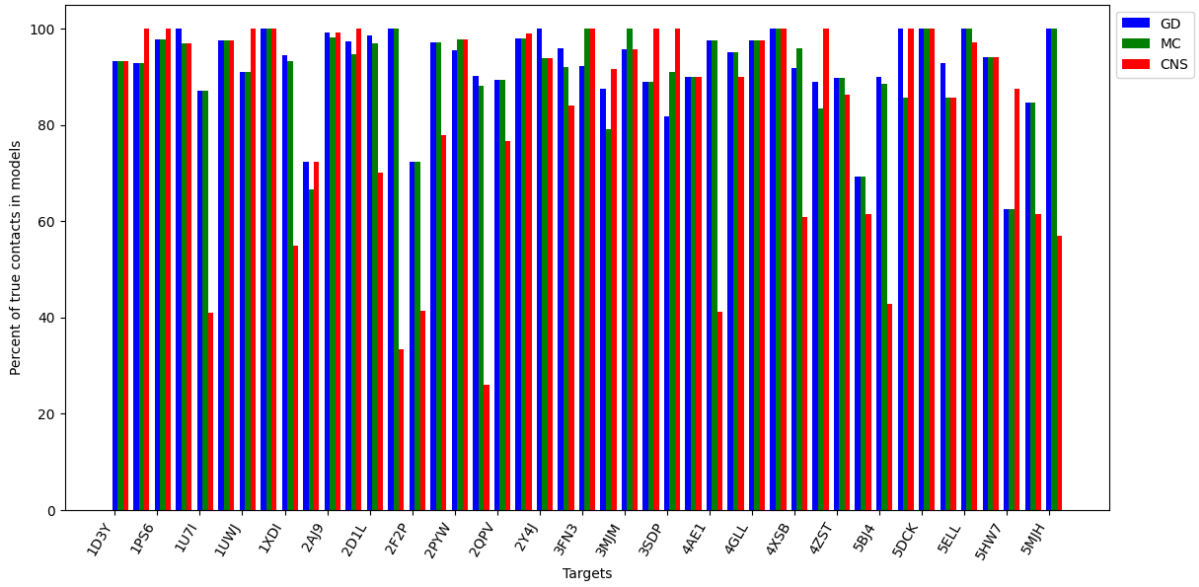


Figure S3. The f_{nat} of GD, MC, and CNS on a dataset of 44 homodimers with known inter-protein contacts. The average f_{nat} of GD, MC, and CNS is 92.19, 91.39, and 82.49.

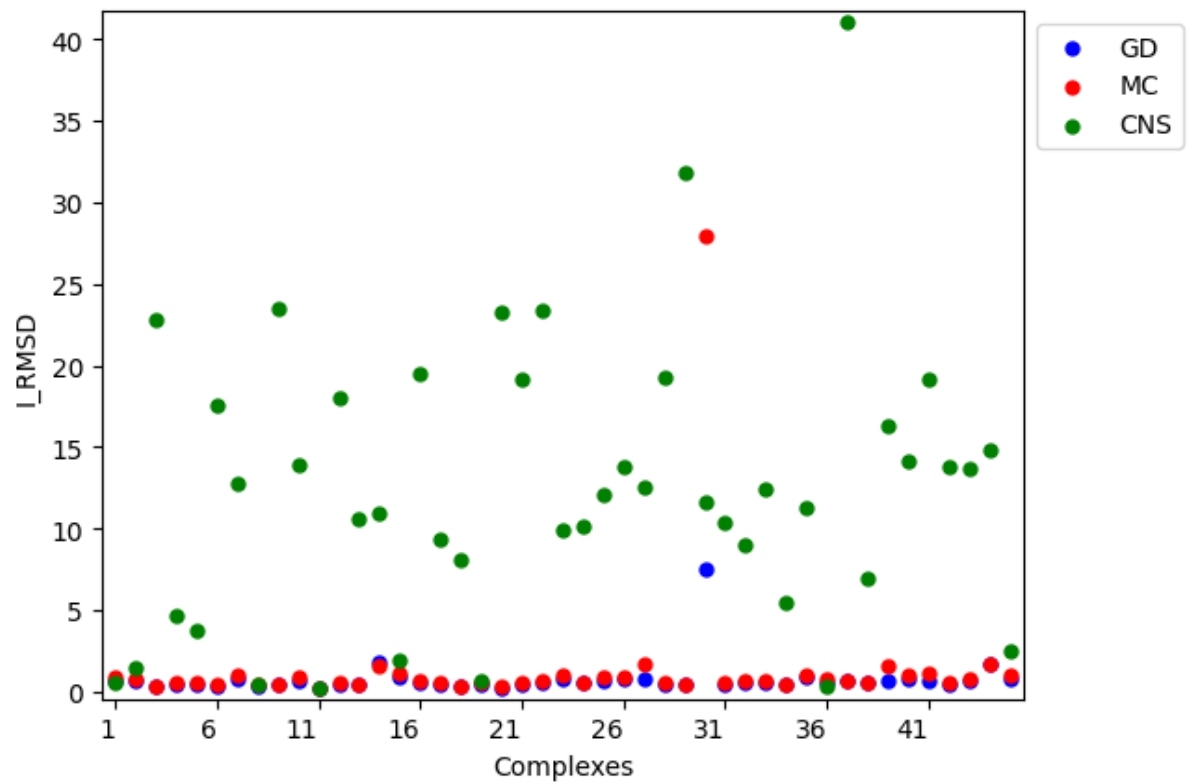


Figure S4. I_RMSD of GD, MC, and CNS on a dataset of 44 homodimers with known inter-protein contacts. The average I_RMSD of GD, MC, and CNS is 0.77, 1.35, and 12.46.

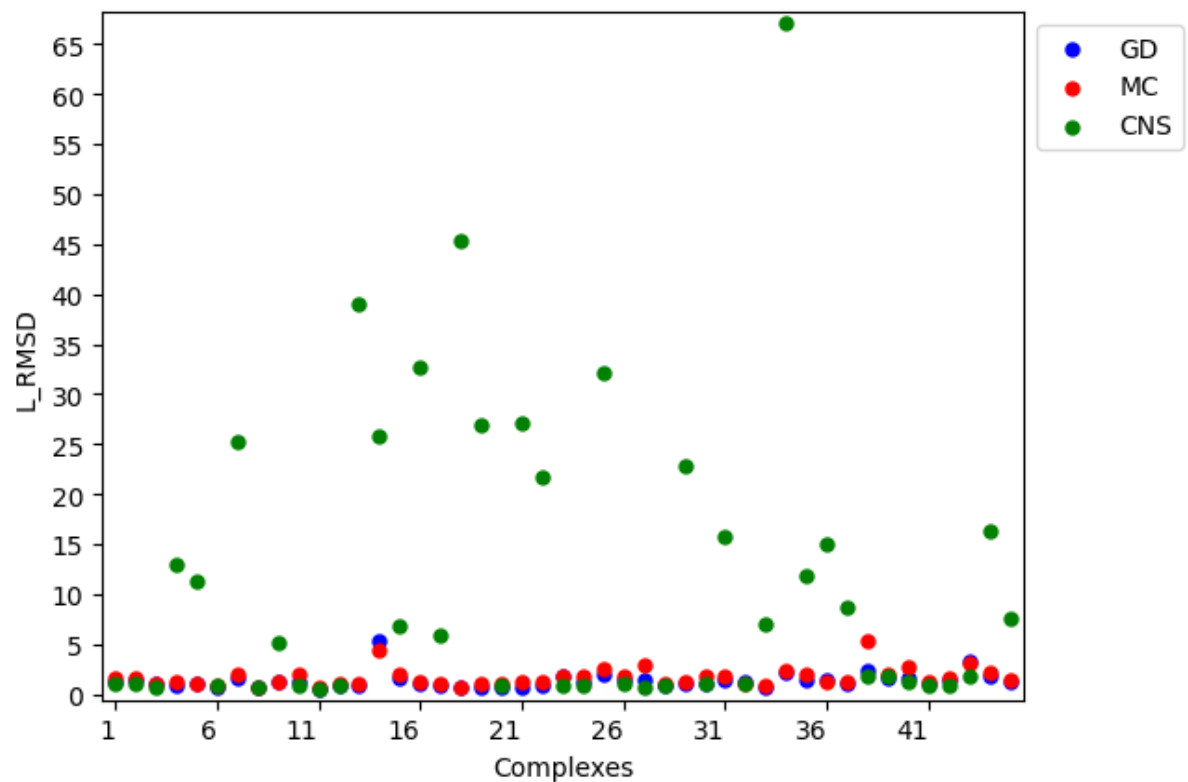


Figure S5. L_RMSD of GD, MC, and CNS on a dataset of 44 homodimers with known inter-protein contacts. The average L_RMSD of GD, MC, and CNS is 1.38, 1.7, and 11.18.

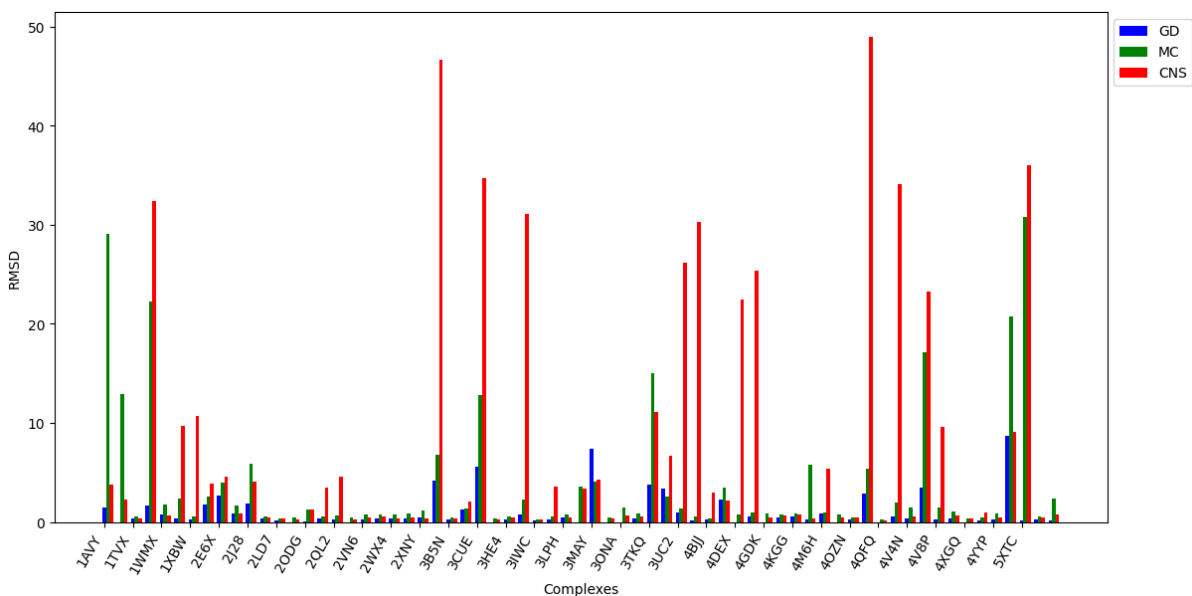


Figure S6. RMSD of GD, MC, and CNS on 73 heterodimers with known inter-protein contacts. The average RMSD of GD, MC, and CNS is 1.23, 4.76, and 7.7.

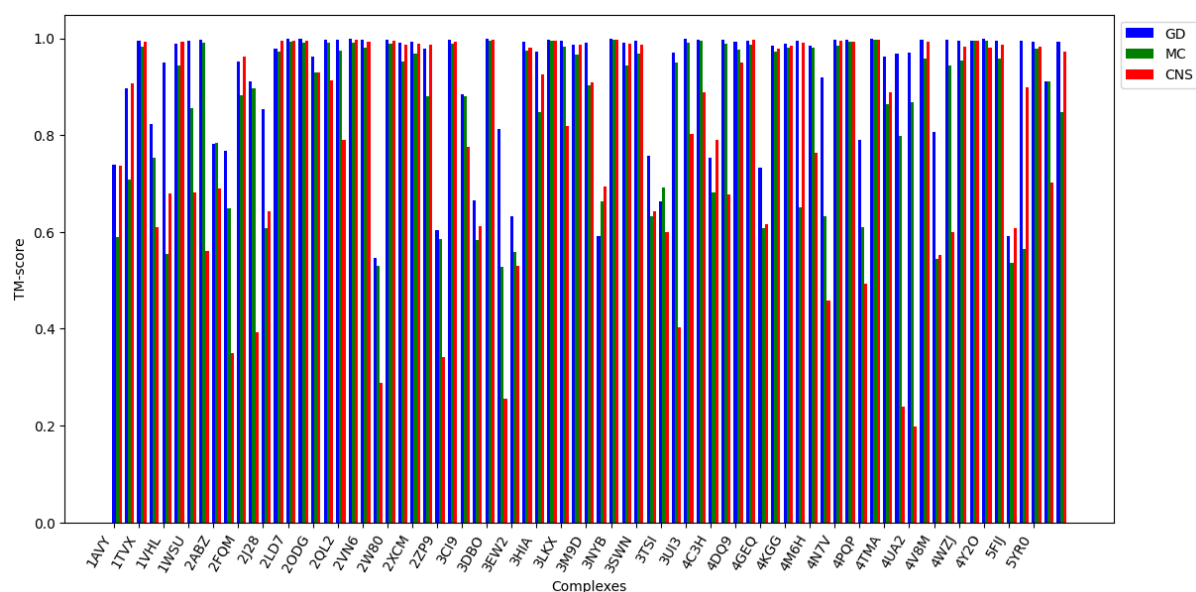


Figure S7. TM-score of GD, MC, and CNS on 73 heterodimers with known inter-protein contacts. The average TM-score of GD, MC, and CNS is 0.92, 0.85, and 0.79.

Supplementary Tables

Table S1. TM-score, RMSD, f_nat, I_RMSD, and L_RMSD of the models that GD reconstructed for each of 44 homodimers from true inter-chain contacts.

Target	Number of true contacts	Length of chain A	Length of chain B	TM-score	RMSD	f_nat (%)	I_RMSD	L_RMSD
2QMA	621	444	440	0.999	0.31	90.2	0.325	0.619
2E4U	52	512	514	0.948	2.576	100	1.85	5.314
5DCK	53	71	72	0.965	0.846	100	0.754	1.674
5CRY	59	348	348	0.995	0.652	100	0.682	2.315
5IW9	67	123	122	0.979	0.853	84.6	0.842	1.727
4GHT	77	181	181	0.997	0.407	95	0.41	1.128
3SDP	78	186	186	0.988	0.764	81.8	0.813	1.438

5V3U	83	131	123	0.965	1.135	90.9	1.12	2.64
5DYW	84	527	525	0.998	0.532	92.9	0.62	1.682
5AFR	88	327	325	0.994	0.696	69.19	0.681	1.349
4YWQ	89	147	146	0.977	0.979	88.9	0.847	2.19
3FN3	94	215	211	0.99	0.748	92.3	0.84	1.737
2Y4J	99	377	377	0.998	0.391	100	0.398	0.788
5H9M	103	190	189	0.99	0.696	94.1	0.642	1.312
3D8U	107	260	266	0.997	0.471	96	0.719	1.39
3LF6	110	154	157	0.992	0.588	87.5	0.526	0.949
1UWJ	111	264	263	0.99	0.802	90.9	0.564	1.247
1JCZ	116	260	260	0.993	0.683	92.9	0.833	1.603
3NR1	130	178	178	0.989	0.717	88.9	0.674	1.43
3MJM	132	343	342	0.993	0.773	95.7	0.748	1.512
4GLL	139	307	306	0.995	0.625	97.5	0.657	2.08
5ELL	142	231	235	0.996	0.499	100	0.558	1.423
1PS6	144	328	328	0.998	0.348	97.7	0.438	1.108
4ZST	146	328	328	0.996	0.56	89.7	0.281	0.999
2HKU	152	188	182	0.994	0.534	97.2	0.569	1.358
2F2P	155	169	169	0.985	0.827	72.39	0.603	1.047

4MAE	161	577	577	0.998	0.522	100	0.924	1.598
1U7I	164	130	129	0.994	0.48	87.2	0.601	1.219
1SOX	167	463	458	0.998	0.452	100	0.492	0.975
2QPV	169	128	128	0.996	0.375	89.4	0.46	0.964
1VZI	174	125	125	0.996	0.355	100	0.417	0.729
1UIR	179	309	313	0.998	0.376	97.6	0.373	0.717
2PYW	197	417	411	0.998	0.448	95.6	0.377	0.763
2BZS	207	230	228	0.993	0.419	97.3	0.45	0.949
2D1L	236	240	222	0.997	0.447	98.5	0.441	0.859
1D3Y	250	289	290	0.995	0.597	93.3	0.423	0.914
3VZ1	273	452	452	0.998	0.417	90.0	0.671	1.341
5MJH	320	368	368	0.996	0.593	100	0.418	0.844
4XSB	323	340	343	0.998	0.39	91.9	0.65	1.261
5BJ4	340	366	366	0.997	0.524	90	0.403	0.784
2WBA	347	489	489	0.999	0.313	98	0.535	1.049
1XDI	352	459	459	0.997	0.562	94.5	0.249	0.747
2AJ9	364	334	334	0.999	0.228	99.1	0.48	1.225
4AE1	398	501	501	0.997	0.531	97.5	0.204	0.446
5HW7	39	122	119	0.936	1.515	62.5	0.419	1.061

Table S2. TM-score, RMSD, f_nat, I_RMSD, and L_RMSD of structural models reconstructed by GD for 73 heterodimers in the Hetero73 dataset using true/native inter-chain contacts as input.

Target	Chains	Length of chain 1	Length of chain 2	Number of true contacts	TM-score	RMSD	f_nat	I_RMSD	L_RMSD
1AVY	A, B	68	54	19	0.74	1.47	92.9	0	6.91
1IS7	A, K	194	84	10	0.9	0	85.7	1.61	4.97
1TVX	A, B	64	71	86	0.99	0.33	100	0.35	0.66
1VCH	B, E	170	152	19	0.82	3.33	42.9	1.76	9.22
1VHL	B, C	208	183	22	0.95	1.65	72.7	1.53	4.04
1WMX	A, B	173	195	61	0.99	0.74	96.89	0.49	1.75
1WSU	C, D	102	121	49	0.99	0.39	100	0.38	1.21
1XBW	A, B	99	96	149	1	0.26	97.7	0.25	0.63
2ABZ	C, D	62	46	13	0.78	1.74	54.5	2	5.06
2E6X	C, D	56	66	23	0.77	2.64	85.7	0	5.38
2FQM	A, D	65	72	21	0.95	0.84	100	0.76	3.57
2IS5	A, D	156	143	43	0.91	2.01	61.9	1.88	4.04
2J28	1, 3	54	64	11	0.85	1.82	83.3	0.93	6.05

2JG8	A, B	132	129	119	0.98	0.32	98.6	0.32	0.67
2LD7	A, B	94	75	153	1	0.18	95.7	0.18	0.34
2MJF	A, B	40	95	132	1	0	97.8	0.16	0.3
2ODG	A, C	89	47	30	0.96	0.07	78.6	0	1.65
2P7M	A, B	127	122	199	1	0.33	97	0.33	0.65
2QL2	A, B	56	59	79	1	0.25	94.69	0.23	0.58
2ROZ	A, B	32	136	101	1	0	100	0.21	0.46
2VN6	A, B	151	64	80	1	0.27	100	0.3	0.61
2W80	A, D	123	244	145	1	0.39	100	0.42	0.87
2WX4	B, C	41	43	61	0.99	0.3	100	0.3	0.6
2XCM	C, E	92	74	57	0.99	0.4	100	0.37	0.81
2XNY	M, N	37	36	77	0.98	0.44	83.6	0.43	0.87
2ZP9	E, I	49	39	4	0.6	4.17	100	3.06	16.47
3B5N	B, C	69	70	149	1	0.23	100	0.23	0.45
3CI9	A, B	44	45	20	0.88	1.28	100	0.54	4.62
3CUE	B, Q	167	188	5	0.67	5.6	50	0.98	23.58
3DBO	A, B	34	126	171	1	0	98.1	0.1	0.44
3ERM	D, E	63	56	16	0.81	2.14	81.8	0.43	6.61
3EW2	C, F	124	119	10	0.63	5.36	85.7	2.06	20.79

3HE4	A, B	45	44	90	0.99	0.28	100	0.25	0.53
3HIA	B, C	83	74	38	0.97	0.8	88.5	0.69	1.72
3IWC	A, B	58	61	255	1	0.18	96.89	0.18	0.36
3LKX	A, B	65	53	123	1	0.28	100	0.28	0.54
3LPH	A, B	62	55	65	0.99	0.44	100	0.44	0.97
3M9D	A, G	186	31	29	0.99	0	90.9	0.71	1.55
3MAY	A, C	86	97	6	0.59	7.39	83.3	2.78	15.12
3NYB	A, B	323	64	173	1	0	99.2	0.27	0.57
3ONA	A, B	158	66	61	0.99	0	97.1	0.46	1.22
3SWN	R, S	76	72	98	1	0.32	100	0.32	0.66
3TKQ	A, E	191	166	5	0.76	3.8	50	4.74	10.04
3UC2	B, D	125	109	43	0.97	0.98	88.5	0.76	2.63
3UI3	A, B	142	102	177	1	0.17	99.1	0.17	0.39
4BJJ	A, B	106	85	192	1	0.28	96.5	0.29	0.56
4C3H	J, L	69	45	18	0.75	2.26	90	0	7.34
4DEX	A, B	289	45	93	1	0	96.2	0.38	1.03
4DQ9	A, B	149	141	66	0.99	0.51	98	0.49	1.02
4GDK	A, B	88	267	71	0.99	0	95.8	0.37	1.96
4GEQ	B, C	58	90	6	0.73	2.61	50	1.57	15.37

4K12	A, B	64	82	57	0.98	0.5	100	0.45	1.71
4KGG	D, A	163	141	66	0.99	0.57	96.2	0.56	1.16
4M3L	A, D	60	53	59	0.99	0.28	100	0.3	0.67
4M6H	A, B	190	162	66	0.99	0.84	97.1	0.59	2.14
4M77	H, J	85	72	23	0.92	1.46	100	0.56	3.81
4N7V	A, C	222	33	98	1	0	100	0.2	0.76
4OZN	A, B	116	104	124	1	0.28	98.8	0.29	0.68
4PQP	A, D	102	97	17	0.79	2.89	64.3	1.24	8.39
4QFQ	A, B	101	35	250	1	0	98.4	0	0.29
4TMA	I, J	47	57	42	0.96	0.6	93.5	0.57	1.83
4U3Q	A, B	93	99	17	0.97	0.94	81.8	0.94	2.62
4UA2	A, H	115	103	27	0.97	0.95	94.1	0.59	2.08
4V4N	T, W	215	135	107	1	0.31	100	0.35	0.85
4V8P	K, M	108	143	65	1	0.28	100	0.28	0.95
4WZJ	L, M	79	79	98	0.99	0.34	98.1	0.32	0.64
4XGQ	A, B	132	30	90	1	0	98.5	0.36	0.77
4Y2O	A, B	211	142	170	1	0.19	98	0.2	0.44
4YYP	A, B	87	32	86	0.99	0.3	100	0.33	0.71
5FIJ	S, T	167	174	7	0.59	8.68	11.4	0	36.13

5XTC	B, V	124	111	64	0.99	0.17	97.1	0.44	0.61
5YR0	A, B	48	44	75	0.99	0.3	100	0.29	0.58
6UMM	D, I	81	61	23	0.99	0.11	100	0.48	0.68

Table S3. Average TM-score, RMSD, f_nat, I_RMSD, and L_RMSD) of GD on 32 heterodimers in the Std32 dataset using true contacts as input.

Target	Length of chain 1	Length of chain 2	Chains	Number of true contacts	TM-score	RMSD	f_nat	I_RMSD	L_RMSD
1W85	358	324	A, B	185	1	0.11	100	0.1	0.22
1EFP	307	246	A, B	317	1	0.07	97.8	0.08	0.18
1I1Q	512	186	A, B	153	1	0.08	100	0.08	0.18
2Y69	227	259	B, C	2	0.54	13.88	50	10	11.01
3MML	285	207	A, B	146	1	0.12	96.3	0.12	0.38
2VPZ	734	193	A, B	188	1	0.19	94.1	0.24	0.58
1TYG	65	242	B, A	114	1	0.05	98.7	0.08	0.26
3RPF	143	72	A, C	5	0.82	3.49	100	1.15	7.44
1EP3	311	261	A, B	133	1	0.05	100	0.04	0.12
2NU9	285	385	A, B	190	1	0.11	98.6	0.11	0.21
3RRL	227	197	A, B	194	1	0.14	99.3	0.14	0.45
3IP4	485	482	A, B	183	1	0.12	98.3	0.02	0.24

1RM6	761	323	A, B	129	1	0.18	100	0.1	0.28
2D1P	119	95	B, C	60	1	0.12	97.3	0.1	0.33
4HR7	443	80	A, B	36	0.99	0.78	100	0.35	2.2
2ONK	240	252	A, C	92	1	0.32	92.6	0	0.9
3A0R	334	113	A, B	60	1	0.28	100	0.06	0.71
1B70	265	775	A, B	414	1	0.07	95.7	0.08	0.23
1QOP	265	390	A, B	157	1	0.15	99	0.15	0.32
2WDQ	121	105	C, D	77	1	0.12	100	0.12	0.27
1BXR	1073	379	A, B	258	1	0.07	98.7	0.07	0.17
3G5O	92	81	A, B	143	1	0.05	97.8	0.05	0.08
3OAA	138	284	H, G	240	1	0.11	98.3	0.11	0.33
3PNL	356	211	A, B	148	1	0.2	100	0.19	0.55
1ZUN	196	382	A, B	251	1	0.14	100	0.15	0.45
1IXR	135	308	A, C	0	0.69	29.9	0	29	92.99
1W85	358	324	A, B	185	1	0.11	100	0.1	0.22
1EFP	307	246	A, B	317	1	0.07	97.8	0.08	0.18
1I1Q	512	186	A, B	153	1	0.08	100	0.08	0.18
2Y69	227	259	B, C	2	0.54	13.88	50	10	11.01
3MML	285	207	A, B	146	1	0.12	96.3	0.12	0.38

2VPZ	734	193	A, B	188	1	0.19	94.1	0.24	0.58
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Table S4. Detailed results of GD on Set A with predicted inter-chain contacts as input.

Target name	Length of chain A	Length of chain B	Number of predicted interchain contacts	Precision of predicted interchain contacts (%)	Recall of predicted interchain contacts (%)	TM-score	RMSD	f_{nat}	I_RMSD	L_RMSD
2XBQ	105	105	26	0.0	0.0	0.5	14.74	0.0	14.544	43.547
1Z9Z	60	60	32	0.0	0.0	0.55	11.27	0.0	13.191	20.364
1A19	89	89	26	0.0	0.0	0.5	14.96	0.0	14.706	39.503
1YH8	266	266	54	0.0	0.0	0.5	18.47	0.0	17.312	58.735
3N8E	159	159	53	0.0	0.0	0.51	21.39	0.0	22.79	44.298
5LLJ	57	57	41	3.12	8.0	0.53	13.20	0.0	9.685	22.742
2FU4	81	81	29	0.0	0.0	0.5	17.39	0.0	11.888	38.914
2PL7	67	67	25	1.85	3.33	0.51	10.19	0.0	9.634	28.831
4E83	31	31	41	5.08	9.68	0.55	9.36	12.5	6.373	13.754
5UZX	231	231	48	0.0	0.0	0.5	22.67	0.0	24.152	66.521

1A2D	130	130	53	2.35	5.88	0.67	6.44	10	6.57	11.312
1RRG	177	177	62	0.0	0.0	0.64	8.71	0.0	7.635	16.947
3JSL	308	308	29	0.0	0.0	0.5	23.37	0.0	24.824	55.067
3LO2	30	30	43	37.5	50	0.86	1.1	75	1.048	2.201
4Q1R	130	130	24	46.34	52.78	0.98	0.62	84. 6	0.614	1.78
1VH9	138	138	82	3.48	10.81	0.5	13.97	16. 7	13.865	35.895
1D8U	165	165	48	8.86	18.42	0.6	7.48	0.0	7.45	17.776
4GA9	134	134	58	54.69	85.37	0.9	2.06	57. 1	2.083	3.787
1IU8	206	206	38	8.97	14.89	0.61	18.85	0.0	16.81	26.005
2R74	142	142	61	0.0	0.0	0.5	15.99	0.0	15.796	45.492
5C39	51	51	90	34.67	52	0.99	0.26	92. 3	0.196	0.518
1F86	115	115	82	32.67	63.46	0.99	0.36	100	0.397	0.724
2ZWM	120	120	21	1.39	1.92	0.62	11.58	0.0	11.444	18.365
1M0U	203	203	94	46.08	85.45	0.99	0.7	100	0.766	1.427
1PD3	54	54	28	1.22	1.82	0.94	0.94	20. 8	1.2	1.98
2D4G	165	165	98	2.68	7.27	0.6	19.53	0.0	12.094	28.873
3F08	135	135	113	0.58	1.67	0.53	16.71	0.0	17.982	32.181
2CC3	144	144	28	2.3	3.28	0.62	9.01	0.0	7.978	15.46
1GNW	210	210	34	28	33.87	0.99	0.54	60. 9	0.562	1.046

2CCY	127	127	53	11.65	19.35	0.64	17.74	0.0	19.329	25.58
5F5X	333	333	30	13.41	17.46	0.7	5.38	0.0	5.183	11.139
5JYB	344	344	37	14.77	20.31	0.97	1.61	11.8	1.668	4.962
1EOG	208	208	99	51.85	86.15	0.99	0.29	96.2	0.311	0.629
1MK4	157	157	24	0.0	0.0	0.6	12.29	0.0	12.115	20.927
1HNB	217	217	58	40.45	53.73	0.99	0.61	81	0.526	1.348
2CVI	83	83	40	5.94	8.96	0.62	6.19	0.0	6.193	11.909
1V8F	276	276	35	17.05	22.06	0.5	26.92	0.0	21.932	56.044
1YQ1	198	198	51	36.78	47.06	1	0.11	95.7	0.118	0.214
3BBH	204	204	22	8.43	10.29	0.92	2.11	29.4	2.423	4.107
3RHU	141	141	49	0.0	0.0	0.5	21.20	0.0	22.02	57.47

Table S5. Detailed results of GD on Set B with predicted inter-chain contacts as input.

Target name	Length of chain A	Length of chain B	Number of predicted interchain contacts	Precision of predicted interchain contacts (%)	Recall of predicted interchain contacts (%)	TM-score	RMSD	f_nat	I_RMSD	L_RMSD
1LBK	208	208	94	52.34	81.16	0.99	0.26	96.6	0.27	0.56
2YYB	242	242	31	3.06	4.29	0.5	25.28	0.0	23.48	53.45

1T92	108	108	29	3.06	4.17	0.64	5.97	0.0	5.58	14.56
2QY6	244	244	28	0.0	0.0	0.5	25.84	0.0	21.64	72.11
1ML6	219	219	72	51.04	67.12	1	0.1	96.6	0.12	0.22
5AIF	124	124	22	6.52	7.89	0.94	1.36	24	1.38	2.80
2YR1	257	257	26	8.42	10.39	0.96	1.51	22.2	1.59	4.12
1B48	221	221	68	55.32	66.67	0.99	0.24	100	0.26	0.5
3F1V	366	366	39	27.17	32.05	0.99	0.77	56	0.76	2.47
3KXO	198	198	86	47.75	67.95	0.99	0.28	100	0.29	0.53
1ECS	120	120	94	25.38	44.3	0.97	0.91	71.4	0.80	1.90
3EE2	198	198	90	46.69	68.35	0.99	0.33	92	0.37	0.74
3WVA	163	163	24	1.92	2.44	0.92	1.98	13.6	1.99	4.58
4Q97	108	108	39	3.42	4.88	0.64	19.77	0.0	6.71	25.11
4DBH	269	269	26	7.92	9.64	0.75	5.51	0.0	6.13	12.03
2FHE	216	216	84	47.46	62.22	0.99	0.51	93.8	0.58	1.1
1DUG	234	234	35	35.11	35.87	0.98	0.83	61.3	0.83	1.93
3SW1	134	134	57	0.0	0.0	0.57	12.93	0.0	13.37	21.55
3MMH	167	166	26	2.5	3.09	0.57	13.97	0.0	13.47	22.6
4RAZ	134	134	52	26.27	31.96	0.59	9.55	5	7.02	21.66
3GW7	215	215	23	0.0	0.0	0.5	24.05	0.0	24.7	55.64

1VRW	289	289	25	2.4	2.91	0.58	12.4	0.0	12.98	31.98
4EC7	108	108	22	0.81	0.97	0.54	12.89	2.9	12.4	23.7
2C2X	280	280	40	6.62	8.57	0.97	1.22	22.2	1.34	2.41
1VJ2	114	114	27	3.85	4.63	0.98	0.65	15.2	0.67	1.32
4EP4	166	166	27	5.47	6.48	0.56	15.9	0.0	14.81	29.29
1Z3A	156	156	23	7.32	8.26	0.92	1.84	11.4	1.91	3.7
4ZBD	219	219	84	20.61	24.55	0.98	1.06	42.6	0.76	2.2
1PM7	199	199	105	30.95	45.22	0.98	0.91	55.9	0.78	1.87
2JL4	212	212	71	30.14	36.97	0.97	1.1	65.7	1.17	2.44
3NYG	93	93	99	40.4	51.26	0.99	0.51	69.8	0.53	1.03
2HIQ	96	96	29	2	2.42	0.58	16.31	0	11.67	22.65
1Q7G	358	358	43	7.64	9.52	0.97	1.51	12.5	1.61	2.97
1ITU	369	369	27	5.48	6.3	0.74	6.33	1.9	6.15	14.41
3ZJL	191	191	28	6.16	7.09	0.84	3.28	2	3.05	7.66
1DC4	323	323	38	5.7	6.98	0.51	22.53	0.0	20.69	56.98
1SW7	245	245	154	42.21	65.12	0.99	0.31	88.4	0.31	0.68

Table S6. Detailed results of GD on Set C with predicted inter-chain contacts as input.

Target name	Length of chain A	Length of chain B	Number of predicted interchain contacts	Precision of predicted interchain contacts (%)	Recall of predicted interchain contacts (%)	TM-score	RMSD	f_nat	I_RMSD	L_RMSD
3KRS	249	249	88	37.74	45.8	0.975	1.287	56	1.325	2.726
1WYI	248	248	141	46.28	64.93	1	0.159	88.9	0.166	0.375
3OGQ	112	112	21	5.37	5.88	0.525	14.553	0	12.173	31.829
1C6X	99	99	151	40.24	49.28	0.994	0.403	84.6	0.4	0.915
2BTM	250	250	121	38.5	52.17	0.998	0.392	67.3	0.433	0.825
4LUL	189	189	60	22.84	26.62	0.981	0.975	37.8	1.026	2.47
2YPI	247	247	107	40.34	50.71	0.995	0.569	65.9	0.595	1.174
3MWS	99	99	140	38.95	47.86	0.994	0.392	76.8	0.375	1.021
2FDE	99	99	157	38.73	47.52	0.993	0.435	77.8	0.418	0.896
3EM6	99	99	149	39.31	47.89	0.995	0.39	80.4	0.376	0.913
3LZU	99	99	157	40.46	48.61	0.991	0.492	84.5	0.466	0.94
3S45	99	99	147	45.51	52.78	0.991	0.501	84	0.439	1.014
4M8Y	100	100	142	39.43	47.92	0.991	0.492	87.5	0.439	1.056
2AOG	99	99	150	41.04	48.97	0.993	0.44	77.4	0.392	0.956
4M8X	99	99	161	40.8	48.63	0.993	0.446	86.2	0.391	0.974
3U7S	99	99	166	37.43	45.58	0.991	0.504	82.7	0.426	1.112

4YMZ	250	250	104	40	48.65	0.988	0.876	78.9	0.881	2.044
2FDD	99	99	160	40.11	47.65	0.99	0.538	81.8	0.492	1.27
4COB	206	206	38	5.98	7.01	0.602	16.34 7	0	11.31 2	24.4
3SK2	132	132	44	16.2	17.68	0.587	18.45 3	0	11.87 1	27.072
3DSB	146	146	34	3.11	3.64	0.557	11.25 9	1.9	11.62	25.167
1KPB	113	113	48	16.22	17.96	0.728	4.262	1.6	4.578	7.736
5CPG	155	155	97	2.33	3.59	0.616	21.86 5	0	15.81 4	29.212
2E8Q	265	265	81	21.74	26.32	0.959	1.705	32.8	0.729	3.307
1A05	357	357	24	10.73	11.05	0.59	11.66 3	4.3	9.941	25.136
2E8S	265	265	77	21.84	25.86	0.961	1.655	34.4	0.77	3.184
1LQO	134	134	60	15.11	17.09	0.621	7.869	0	7.883	15.129
1XSE	274	274	70	19.21	21.67	0.985	1.02	29.3	1.06	2.13
1EQU	284	284	21	7.58	7.77	0.963	1.639	9.1	1.603	3.361
3I3G	143	143	69	18.03	20.39	0.54	7.959	0	8.721	19.465
1V5Z	217	217	23	7.44	7.69	0.579	14.49 6	0	15.79 6	28.149
3X22	217	217	52	9.7	11.06	0.59	12.98 6	3	13.98	25.484
3TY2	245	245	57	3.41	4.17	0.584	13.64 7	0	11.13	26.812
3BM4	197	197	60	3.53	4.29	0.591	19.67 4	0	7.361	28.718

4R5M	369	369	29	5.22	5.53	0.58	11.06 1	4.5	8.494	25.924
1MB4	369	369	29	5.07	5.36	0.659	10.76 4	2.3	6.349	18.931
1QIN	176	176	46	12.32	12.82	0.54	11.6	0	9.482	23.708
4TTB	189	189	33	6.46	6.79	0.591	14.13 5	0.9	10.90 7	25.925