Supporting Information

Table of Contents

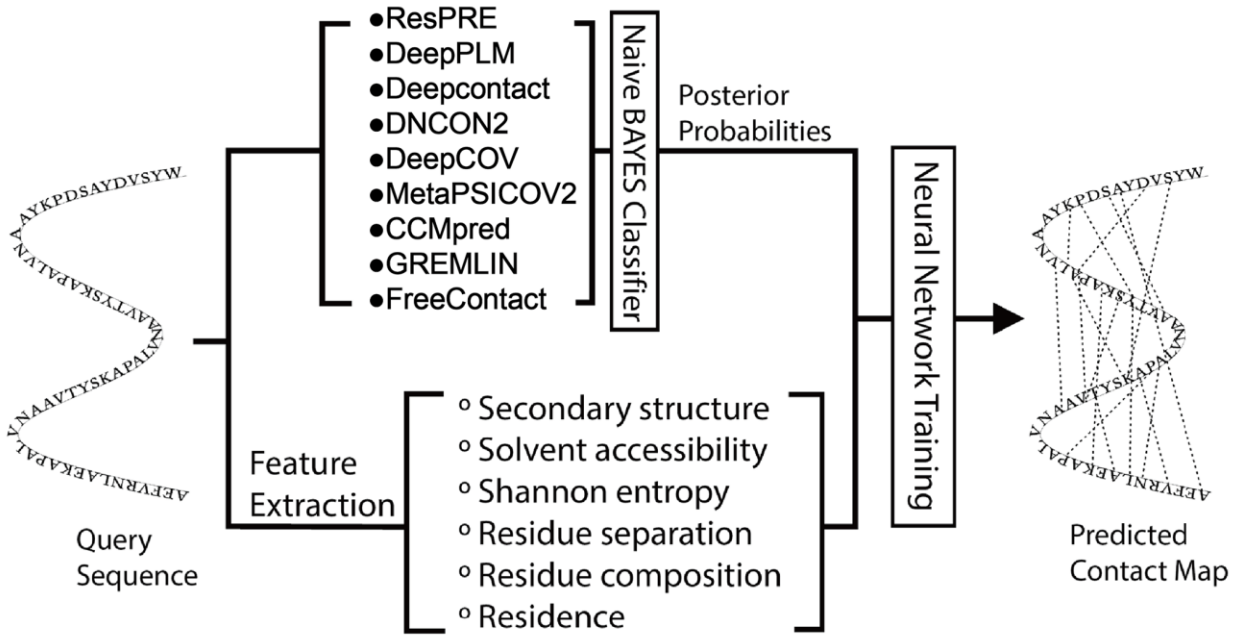

Figure S1. NeBcon flowchart.

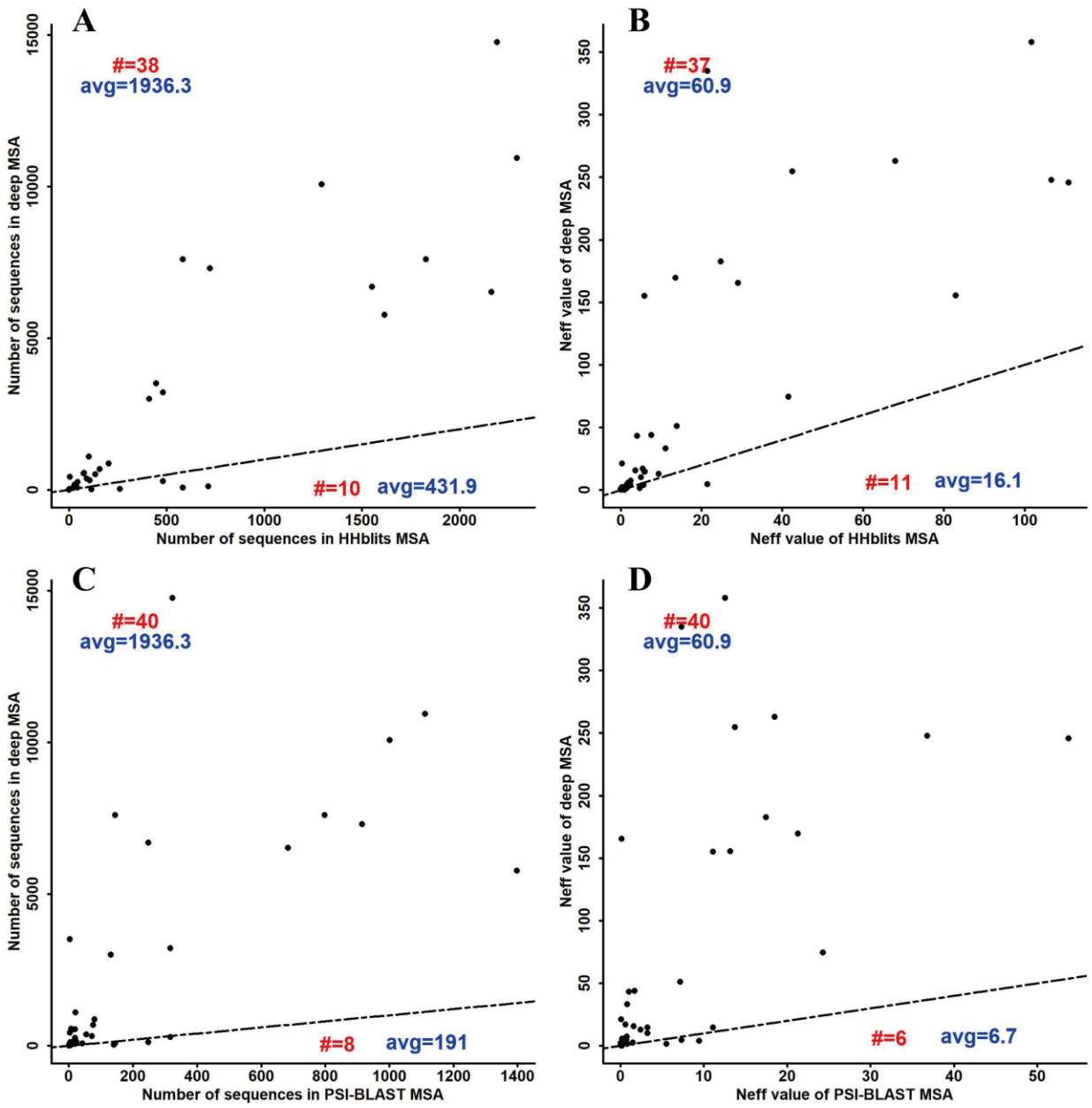

Figure S2. Comparison of homologous sequences detected by DeepMSA, HHblits and PSI-BLAST for the 50 FM targets. (A) Number of sequences detected by DeepMSA and HHblits; (B) Number of effective sequence (*Neff*) detected by DeepMSA and HHblits; (C) Number of sequences detected by DeepMSA and PSI-BLAST; (D) *Neff* detected by DeepMSA and PSI-BLAST. The black dashed-dotted line represents the diagonal line (i.e. $y = x$). The red numbers are the number of points above or below the diagonal line. Here, HHblits was used with the default parameters to search the Uniclust30 database, while PSI-BLAST was used with the default parameters to search the NR (Dec 2017) database.

Table S1. Comparison between the first models built by I-TASSER and C-I-TASSER for the 121 CASP13 targets. The "Target" column contains the name of each target, the "Domain" column includes the domain information for each target, and the "Type" column contains the category of each target. The "I-TASSER first model" columns include the TM-scores, GDT-HA scores, and RMSDs of the first models built by I-TASSER, while the "C-I-TASSER first model" columns include the TM-scores, GDT-HA scores, and RMSDs of the first models built by C-I-TASSER.

Target	Domain	Type	I-TASSER first model			C-I-TASSER first model		
			TM-score	GDT-HA	RMSD(Å)	TM-score	GDT-HA	RMSD(Å)
T0949	T0949-D1	FM/TBM	0.673	0.448	7.364	0.665	0.424	6.568
T0950	T0950-D1	FM	0.178	0.076	50.588	0.441	0.144	15.398
T0951	T0951-D1	TBM-easy	0.973	0.776	1.034	0.972	0.760	1.065
T0953s1	T0953s1-D1	FM	0.252	0.164	10.749	0.397	0.287	11.026
T0953s2	T0953s2-D1	FM/TBM	0.268	0.261	9.086	0.358	0.318	6.737
T0953s2	T0953s2-D2	FM	0.228	0.128	15.617	0.590	0.313	5.282
T0953s2	T0953s2-D3	FM	0.201	0.117	12.589	0.310	0.162	6.778
T0954	T0954-D1	TBM-hard	0.807	0.372	4.651	0.810	0.390	5.294
T0955	T0955-D1	FM/TBM	0.753	0.707	1.263	0.755	0.689	1.337
T0957s1	T0957s1-D1	FM	0.283	0.176	12.266	0.380	0.215	10.201
T0957s1	T0957s1-D2	TBM-hard	0.374	0.333	8.271	0.495	0.435	5.995
T0957s2	T0957s2-D1	FM	0.511	0.253	5.830	0.532	0.279	5.928
T0958	T0958-D1	FM/TBM	0.454	0.334	5.049	0.547	0.406	4.108
T0959	T0959-D1	TBM-hard	0.632	0.357	7.282	0.725	0.394	4.181
T0960	T0960-D1	FM	0.153	0.203	9.907	0.166	0.219	8.792
T0960	T0960-D2	FM	0.322	0.188	10.441	0.392	0.247	9.451
T0960	T0960-D3	TBM-hard	0.740	0.553	3.018	0.765	0.570	2.702
T0960	T0960-D4	FM	0.155	0.148	22.936	0.230	0.203	21.549
T0960	T0960-D5	TBM-easy	0.729	0.498	3.341	0.713	0.507	3.493
T0961	T0961-D1	TBM-easy	0.961	0.700	2.115	0.960	0.694	2.135
T0962	T0962-D1	TBM-easy	0.826	0.573	4.630	0.866	0.589	3.866
T0963	T0963-D1	FM	0.208	0.250	9.214	0.151	0.234	8.557
T0963	T0963-D2	FM	0.329	0.186	9.243	0.481	0.305	4.899
T0963	T0963-D3	TBM-hard	0.715	0.470	2.698	0.756	0.546	4.470
T0963	T0963-D4	FM	0.168	0.145	22.089	0.239	0.219	23.204
T0963	T0963-D5	TBM-easy	0.757	0.580	2.674	0.784	0.590	2.389
T0964	T0964-D1	TBM-hard	0.759	0.550	3.931	0.687	0.482	5.989
T0965	T0965-D1	TBM-hard	0.825	0.407	3.981	0.828	0.393	3.885
T0966	T0966-D1	TBM-hard	0.840	0.339	3.862	0.839	0.335	3.906
T0967	T0967-D1	TBM-easy	0.852	0.665	1.561	0.834	0.639	1.708
T0968s1	T0968s1-D1	FM	0.319	0.159	12.364	0.556	0.292	5.832
T0968s2	T0968s2-D1	FM	0.325	0.170	12.513	0.621	0.357	3.875
T0969	T0969-D1	FM	0.531	0.209	9.207	0.729	0.288	6.077
T0970	T0970-D1	FM/TBM	0.495	0.309	5.399	0.583	0.374	4.694
T0971	T0971-D1	TBM-easy	0.941	0.714	1.130	0.921	0.662	1.318
T0973	T0973-D1	TBM-easy	0.811	0.525	2.706	0.618	0.377	10.191
T0974s1	T0974s1-D1	TBM-easy	0.723	0.598	2.453	0.716	0.591	2.252
T0974s2	T0974s2-D1	TBM-easy	0.905	0.866	2.282	0.897	0.838	2.507
T0975	T0975-D1	FM	0.541	0.242	15.449	0.669	0.277	6.442
T0976	T0976-D1	TBM-easy	0.838	0.588	2.166	0.832	0.573	2.200
T0976	T0976-D2	TBM-easy	0.824	0.577	2.697	0.828	0.575	2.681
T0977	T0977-D1	TBM-easy	0.897	0.551	2.677	0.900	0.545	2.561
T0977	T0977-D2	TBM-easy	0.796	0.468	5.113	0.759	0.404	4.527
T0978	T0978-D1	FM/TBM	0.574	0.242	14.792	0.527	0.237	17.747
T0979	T0979-D1	TBM-hard	0.352	0.304	40.548	0.441	0.321	6.487
T0980s1	T0980s1-D1	FM	0.352	0.243	14.489	0.290	0.190	10.158
T0980s2	T0980s2-D1	FM	0.175	0.242	12.840	0.153	0.226	14.251
T0981	T0981-D1	TBM-hard	0.578	0.372	3.089	0.629	0.439	3.802
T0981	T0981-D2	FM	0.293	0.175	10.631	0.262	0.150	9.058
T0981	T0981-D3	FM/TBM	0.644	0.303	6.139	0.677	0.308	5.308
T0981	T0981-D4	TBM-hard	0.586	0.399	4.896	0.591	0.394	8.213
T0981	T0981-D5	TBM-hard	0.575	0.366	12.507	0.659	0.402	6.050
T0982	T0982-D1	TBM-easy	0.863	0.602	2.321	0.888	0.630	1.894
T0982	T0982-D2	TBM-hard	0.541	0.301	7.293	0.626	0.358	7.043
T0983	T0983-D1	TBM-easy	0.942	0.714	1.680	0.947	0.733	1.599
T0984	T0984-D1	TBM-easy	0.869	0.418	3.750	0.874	0.420	3.874
T0984	T0984-D2	TBM-easy	0.790	0.549	3.679	0.782	0.535	3.493
T0985	T0985-D1	TBM-hard	0.856	0.352	5.855	0.854	0.347	5.685
T0986s1	T0986s1-D1	FM/TBM	0.555	0.345	5.232	0.648	0.413	3.684

T0986s2	T0986s2-D1	FM	0.335	0.177	11.091	0.594	0.266	5.887
T0987	T0987-D1	FM	0.243	0.089	15.493	0.620	0.262	5.811
T0987	T0987-D2	FM	0.293	0.093	14.700	0.378	0.145	14.869
T0989	T0989-D1	FM	0.541	0.280	9.886	0.547	0.302	11.475
T0989	T0989-D2	FM	0.246	0.143	14.379	0.342	0.172	13.152
T0990	T0990-D1	FM	0.378	0.286	10.896	0.567	0.415	5.348
T0990	T0990-D2	FM	0.246	0.118	13.646	0.382	0.156	23.564
T0990	T0990-D3	FM	0.211	0.103	16.560	0.212	0.090	18.412
T0991	T0991-D1	FM	0.218	0.151	18.974	0.223	0.158	18.604
T0992	T0992-D1	FM/TBM	0.704	0.456	4.940	0.722	0.463	3.272
T0993s1	T0993s1-D1	TBM-easy	0.835	0.516	8.828	0.843	0.542	8.877
T0993s2	T0993s2-D1	TBM-easy	0.694	0.462	4.073	0.704	0.475	3.620
T0995	T0995-D1	TBM-easy	0.878	0.605	2.229	0.904	0.638	3.833
T0996	T0996-D1	TBM-easy	0.782	0.568	4.161	0.778	0.554	4.155
T0996	T0996-D2	TBM-easy	0.823	0.620	2.857	0.815	0.598	3.190
T0996	T0996-D3	TBM-easy	0.820	0.603	2.991	0.823	0.605	3.003
T0996	T0996-D4	TBM-easy	0.739	0.521	3.345	0.750	0.547	7.353
T0996	T0996-D5	TBM-easy	0.739	0.533	4.043	0.738	0.531	4.100
T0996	T0996-D6	TBM-easy	0.866	0.654	1.923	0.879	0.676	1.840
T0997	T0997-D1	FM/TBM	0.585	0.338	5.807	0.613	0.342	6.919
T0998	T0998-D1	FM	0.177	0.075	21.969	0.206	0.095	22.314
T0999	T0999-D1	TBM-easy	0.985	0.825	0.958	0.986	0.832	0.943
T0999	T0999-D2	TBM-hard	0.785	0.341	4.581	0.795	0.346	4.813
T0999	T0999-D3	TBM-easy	0.784	0.494	3.816	0.793	0.499	3.664
T0999	T0999-D4	TBM-easy	0.971	0.757	1.064	0.964	0.758	1.320
T0999	T0999-D5	TBM-easy	0.889	0.524	2.522	0.888	0.518	2.517
T1000	T1000-D1	TBM-easy	0.946	0.871	1.030	0.945	0.874	1.098
T1000	T1000-D2	FM	0.258	0.082	22.708	0.814	0.387	9.726
T1001	T1001-D1	FM	0.637	0.338	4.341	0.631	0.336	4.360
T1002	T1002-D1	TBM-easy	0.795	0.678	1.817	0.794	0.661	1.694
T1002	T1002-D2	TBM-easy	0.797	0.678	2.182	0.803	0.712	2.256
T1002	T1002-D3	TBM-easy	0.781	0.632	3.334	0.792	0.622	6.496
T1003	T1003-D1	TBM-easy	0.935	0.761	7.678	0.934	0.737	7.736
T1004	T1004-D1	TBM-easy	0.769	0.587	2.824	0.775	0.587	2.692
T1004	T1004-D2	TBM-easy	0.675	0.484	2.726	0.705	0.474	2.463
T1004	T1004-D3	TBM-easy	0.909	0.764	2.239	0.925	0.830	3.446
T1005	T1005-D1	FM/TBM	0.683	0.318	6.009	0.697	0.311	8.001
T1006	T1006-D1	TBM-easy	0.947	0.838	0.764	0.954	0.844	0.698
T1008	T1008-D1	FM/TBM	0.366	0.263	9.971	0.362	0.263	9.030
T1009	T1009-D1	TBM-hard	0.875	0.445	5.073	0.876	0.442	5.063
T1010	T1010-D1	FM	0.247	0.062	20.352	0.561	0.208	8.523
T1011	T1011-D1	TBM-hard	0.800	0.402	4.486	0.806	0.407	4.697
T1011	T1011-D2	TBM-easy	0.880	0.727	1.864	0.866	0.697	1.991
T1013	T1013-D1	TBM-easy	0.934	0.666	2.418	0.927	0.620	2.452
T1014	T1014-D1	TBM-easy	0.906	0.654	2.515	0.889	0.637	2.491
T1014	T1014-D2	TBM-easy	0.801	0.551	3.020	0.805	0.581	3.002
T1015s1	T1015s1-D1	FM	0.256	0.168	12.424	0.466	0.332	9.767
T1015s2	T1015s2-D1	TBM-hard	0.653	0.421	5.945	0.716	0.465	4.303
T1016	T1016-D1	TBM-easy	0.880	0.614	3.786	0.880	0.614	3.654
T1017s1	T1017s1-D1	TBM-easy	0.758	0.543	3.060	0.764	0.536	2.941
T1017s2	T1017s2-D1	FM	0.421	0.222	6.891	0.697	0.420	4.114
T1018	T1018-D1	TBM-easy	0.938	0.617	1.914	0.940	0.604	1.871
T1019s1	T1019s1-D1	FM/TBM	0.391	0.319	6.761	0.596	0.483	2.569
T1019s2	T1019s2-D1	TBM-easy	0.691	0.472	3.627	0.773	0.560	3.142
T1020	T1020-D1	TBM-easy	0.872	0.454	3.075	0.879	0.455	2.999
T1021s1	T1021s1-D1	TBM-hard	0.810	0.525	3.633	0.822	0.532	3.418
T1021s2	T1021s2-D1	TBM-hard	0.858	0.440	3.338	0.797	0.415	15.146
T1021s3	T1021s3-D1	FM	0.630	0.327	7.606	0.633	0.309	7.252
T1021s3	T1021s3-D2	FM	0.356	0.199	7.042	0.436	0.271	10.858
T1022s1	T1022s1-D1	FM	0.657	0.383	8.650	0.694	0.401	8.313
T1022s1	T1022s1-D2	TBM-hard	0.621	0.496	5.578	0.626	0.508	6.822
T1022s2	T1022s2-D1	TBM-hard	0.681	0.302	5.314	0.772	0.319	7.334
Average			**0.624**	**0.417**	**7.396**	**0.674**	**0.444**	**6.193**

Table S2. Comparison between the first models built by QUARK and C-QUARK for the 121 CASP13 targets. The "Target" column contains the name of each target, the "Domain" column includes the domain information for each target, and the "Type" column contains the category of each target. The "QUARK first model" columns include the TM-scores, GDT-HA scores, and RMSDs of the first models built by QUARK, while the "C-QUARK first model" columns include the TM-scores, GDT-HA scores, and RMSDs of the first models built by C-QUARK.

Target	Domain	Type	QUARK first model			C-QUARK first model		
			TM-score	GDT-HA	RMSD(Å)	TM-score	GDT-HA	RMSD(Å)
T0949	T0949-D1	FM/TBM	0.667	0.424	6.556	0.672	0.450	6.778
T0950	T0950-D1	FM	0.197	0.072	38.466	0.444	0.142	15.417
T0951	T0951-D1	TBM-easy	0.965	0.698	1.189	0.971	0.746	1.093
T0953s1	T0953s1-D1	FM	0.396	0.299	11.395	0.399	0.284	10.859
T0953s2	T0953s2-D1	FM/TBM	0.283	0.301	7.369	0.361	0.341	6.529
T0953s2	T0953s2-D2	FM	0.176	0.108	17.029	0.469	0.191	5.938
T0953s2	T0953s2-D3	FM	0.149	0.094	13.408	0.286	0.156	6.923
T0954	T0954-D1	TBM-hard	0.803	0.365	4.633	0.808	0.380	5.279
T0955	T0955-D1	FM/TBM	0.696	0.652	1.551	0.731	0.671	1.464
T0957s1	T0957s1-D1	FM	0.293	0.176	10.123	0.397	0.236	9.697
T0957s1	T0957s1-D2	TBM-hard	0.391	0.375	7.788	0.378	0.338	6.810
T0957s2	T0957s2-D1	FM	0.395	0.195	11.983	0.532	0.302	6.135
T0958	T0958-D1	FM/TBM	0.348	0.286	10.486	0.548	0.409	4.029
T0959	T0959-D1	TBM-hard	0.637	0.343	7.001	0.711	0.375	4.391
T0960	T0960-D1	FM	0.185	0.273	8.268	0.158	0.211	8.841
T0960	T0960-D2	FM	0.330	0.182	8.172	0.437	0.256	5.955
T0960	T0960-D3	TBM-hard	0.480	0.292	6.410	0.768	0.570	2.559
T0960	T0960-D4	FM	0.172	0.125	20.746	0.236	0.207	21.746
T0960	T0960-D5	TBM-easy	0.697	0.507	3.914	0.714	0.486	3.353
T0961	T0961-D1	TBM-easy	0.962	0.675	1.963	0.962	0.689	1.948
T0962	T0962-D1	TBM-easy	0.815	0.540	4.767	0.839	0.571	3.937
T0963	T0963-D1	FM	0.200	0.234	7.605	0.160	0.218	9.277
T0963	T0963-D2	FM	0.314	0.171	8.429	0.459	0.265	4.913
T0963	T0963-D3	TBM-hard	0.316	0.167	8.904	0.773	0.586	4.505
T0963	T0963-D4	FM	0.196	0.176	21.781	0.250	0.227	22.591
T0963	T0963-D5	TBM-easy	0.799	0.604	2.405	0.786	0.598	2.474
T0964	T0964-D1	TBM-hard	0.740	0.566	5.373	0.767	0.584	4.775
T0965	T0965-D1	TBM-hard	0.818	0.391	4.025	0.825	0.397	3.952
T0966	T0966-D1	TBM-hard	0.846	0.343	3.806	0.843	0.340	3.803
T0967	T0967-D1	TBM-easy	0.854	0.671	1.460	0.820	0.623	1.787
T0968s1	T0968s1-D1	FM	0.375	0.220	11.194	0.563	0.305	5.660
T0968s2	T0968s2-D1	FM	0.356	0.189	11.233	0.647	0.370	3.766
T0969	T0969-D1	FM	0.186	0.061	18.466	0.752	0.302	5.410
T0970	T0970-D1	FM/TBM	0.255	0.194	11.505	0.506	0.329	5.959
T0971	T0971-D1	TBM-easy	0.917	0.673	1.381	0.924	0.675	1.290
T0973	T0973-D1	TBM-easy	0.828	0.572	2.731	0.678	0.426	9.922
T0974s1	T0974s1-D1	TBM-easy	0.746	0.634	2.451	0.741	0.623	2.320
T0974s2	T0974s2-D1	TBM-easy	0.898	0.800	2.114	0.904	0.803	2.353
T0975	T0975-D1	FM	0.469	0.199	15.776	0.667	0.273	6.549
T0976	T0976-D1	TBM-easy	0.832	0.594	2.188	0.839	0.590	2.136
T0976	T0976-D2	TBM-easy	0.816	0.552	2.670	0.830	0.597	2.677
T0977	T0977-D1	TBM-easy	0.882	0.493	2.760	0.899	0.549	2.634
T0977	T0977-D2	TBM-easy	0.794	0.461	4.751	0.777	0.415	3.679
T0978	T0978-D1	FM/TBM	0.541	0.215	14.871	0.530	0.240	18.101
T0979	T0979-D1	TBM-hard	0.410	0.361	41.212	0.501	0.359	6.559
T0980s1	T0980s1-D1	FM	0.233	0.190	12.627	0.540	0.339	7.124
T0980s2	T0980s2-D1	FM	0.204	0.242	11.768	0.188	0.226	13.975
T0981	T0981-D1	TBM-hard	0.331	0.195	8.941	0.535	0.334	5.210
T0981	T0981-D2	FM	0.235	0.156	10.506	0.246	0.156	9.399
T0981	T0981-D3	FM/TBM	0.624	0.275	6.283	0.669	0.296	5.334
T0981	T0981-D4	TBM-hard	0.578	0.381	5.169	0.591	0.392	7.282
T0981	T0981-D5	TBM-hard	0.422	0.309	16.665	0.640	0.382	6.625
T0982	T0982-D1	TBM-easy	0.888	0.630	1.887	0.867	0.609	3.299
T0982	T0982-D2	TBM-hard	0.301	0.184	14.183	0.590	0.309	7.122
T0983	T0983-D1	TBM-easy	0.947	0.714	1.591	0.946	0.724	1.615
T0984	T0984-D1	TBM-easy	0.867	0.393	4.149	0.875	0.413	3.798
T0984	T0984-D2	TBM-easy	0.775	0.524	3.713	0.789	0.550	3.524
T0985	T0985-D1	TBM-hard	0.810	0.306	7.378	0.810	0.303	7.473
T0986s1	T0986s1-D1	FM/TBM	0.396	0.269	8.484	0.691	0.459	3.148

T0986s2	T0986s2-D1	FM	0.230	0.150	17.058	0.598	0.279	6.719
T0987	T0987-D1	FM	0.221	0.088	18.996	0.581	0.211	6.457
T0987	T0987-D2	FM	0.166	0.073	20.548	0.440	0.163	15.237
T0989	T0989-D1	FM	0.252	0.129	14.723	0.477	0.237	10.499
T0989	T0989-D2	FM	0.234	0.134	12.956	0.313	0.172	13.109
T0990	T0990-D1	FM	0.360	0.283	13.791	0.577	0.411	5.438
T0990	T0990-D2	FM	0.249	0.123	8.672	0.371	0.157	19.744
T0990	T0990-D3	FM	0.202	0.097	5.240	0.223	0.089	17.292
T0991	T0991-D1	FM	0.214	0.155	18.137	0.269	0.180	15.107
T0992	T0992-D1	FM/TBM	0.321	0.164	11.019	0.732	0.481	3.334
T0993s1	T0993s1-D1	TBM-easy	0.839	0.517	8.419	0.846	0.547	8.884
T0993s2	T0993s2-D1	TBM-easy	0.692	0.457	4.031	0.704	0.472	3.487
T0995	T0995-D1	TBM-easy	0.891	0.617	2.043	0.900	0.631	4.308
T0996	T0996-D1	TBM-easy	0.778	0.558	4.127	0.779	0.563	4.126
T0996	T0996-D2	TBM-easy	0.803	0.579	3.022	0.820	0.604	3.059
T0996	T0996-D3	TBM-easy	0.813	0.583	3.151	0.816	0.598	2.986
T0996	T0996-D4	TBM-easy	0.749	0.538	3.190	0.750	0.540	7.248
T0996	T0996-D5	TBM-easy	0.735	0.510	4.141	0.737	0.535	4.134
T0996	T0996-D6	TBM-easy	0.860	0.666	2.118	0.865	0.651	1.935
T0997	T0997-D1	FM/TBM	0.565	0.332	5.957	0.612	0.350	6.788
T0998	T0998-D1	FM	0.228	0.108	21.221	0.199	0.087	18.877
T0999	T0999-D1	TBM-easy	0.980	0.762	1.086	0.986	0.833	0.927
T0999	T0999-D2	TBM-hard	0.761	0.323	5.037	0.769	0.326	5.694
T0999	T0999-D3	TBM-easy	0.787	0.496	3.868	0.792	0.493	3.684
T0999	T0999-D4	TBM-easy	0.971	0.744	1.044	0.964	0.757	1.320
T0999	T0999-D5	TBM-easy	0.893	0.513	2.391	0.890	0.522	2.501
T1000	T1000-D1	TBM-easy	0.929	0.810	1.136	0.948	0.886	1.097
T1000	T1000-D2	FM	0.183	0.062	24.872	0.851	0.426	4.249
T1001	T1001-D1	FM	0.292	0.171	13.017	0.614	0.331	4.201
T1002	T1002-D1	TBM-easy	0.785	0.653	1.797	0.782	0.636	1.764
T1002	T1002-D2	TBM-easy	0.807	0.682	1.995	0.802	0.670	2.189
T1002	T1002-D3	TBM-easy	0.781	0.616	3.214	0.777	0.602	7.012
T1003	T1003-D1	TBM-easy	0.933	0.726	7.691	0.936	0.746	7.695
T1004	T1004-D1	TBM-easy	0.759	0.581	2.934	0.793	0.616	2.606
T1004	T1004-D2	TBM-easy	0.631	0.435	2.900	0.673	0.464	2.701
T1004	T1004-D3	TBM-easy	0.905	0.715	2.104	0.926	0.832	3.570
T1005	T1005-D1	FM/TBM	0.669	0.301	6.110	0.699	0.313	7.741
T1006	T1006-D1	TBM-easy	0.946	0.828	0.773	0.957	0.844	0.679
T1008	T1008-D1	FM/TBM	0.348	0.244	9.066	0.353	0.253	9.156
T1009	T1009-D1	TBM-hard	0.854	0.377	5.641	0.875	0.437	5.081
T1010	T1010-D1	FM	0.181	0.050	17.840	0.513	0.168	8.362
T1011	T1011-D1	TBM-hard	0.805	0.414	4.460	0.794	0.387	4.748
T1011	T1011-D2	TBM-easy	0.843	0.641	2.220	0.874	0.709	1.924
T1013	T1013-D1	TBM-easy	0.923	0.626	3.238	0.929	0.633	2.360
T1014	T1014-D1	TBM-easy	0.883	0.626	2.550	0.897	0.646	3.351
T1014	T1014-D2	TBM-easy	0.803	0.577	2.944	0.800	0.556	2.960
T1015s1	T1015s1-D1	FM	0.367	0.267	10.472	0.524	0.372	5.880
T1015s2	T1015s2-D1	TBM-hard	0.705	0.457	4.317	0.713	0.469	4.293
T1016	T1016-D1	TBM-easy	0.879	0.589	3.724	0.881	0.597	3.683
T1017s1	T1017s1-D1	TBM-easy	0.749	0.541	3.317	0.770	0.552	2.895
T1017s2	T1017s2-D1	FM	0.443	0.248	8.733	0.768	0.466	3.353
T1018	T1018-D1	TBM-easy	0.937	0.595	1.910	0.938	0.604	1.907
T1019s1	T1019s1-D1	FM/TBM	0.407	0.341	8.196	0.597	0.491	2.491
T1019s2	T1019s2-D1	TBM-easy	0.579	0.415	11.392	0.705	0.494	3.515
T1020	T1020-D1	TBM-easy	0.880	0.480	2.946	0.879	0.463	3.012
T1021s1	T1021s1-D1	TBM-hard	0.795	0.513	3.538	0.827	0.549	3.331
T1021s2	T1021s2-D1	TBM-hard	0.846	0.405	3.462	0.799	0.419	15.149
T1021s3	T1021s3-D1	FM	0.249	0.121	18.187	0.636	0.313	7.216
T1021s3	T1021s3-D2	FM	0.288	0.196	10.234	0.452	0.286	6.838
T1022s1	T1022s1-D1	FM	0.196	0.096	20.711	0.555	0.297	10.751
T1022s1	T1022s1-D2	TBM-hard	0.307	0.261	11.733	0.632	0.511	6.524
T1022s2	T1022s2-D1	TBM-hard	0.104	0.051	16.187	0.769	0.317	7.390
Average			**0.577**	**0.386**	**8.241**	**0.673**	**0.442**	**6.002**

Table S3. Template information for all 121 CASP13 targets. The "Target" column is the name of each target. The "Server group deadline" is the Server group submission deadline for each target. The "Domain" is the domain information for each target. The "Type" is the category each target falls into. The "TM-score" is the TM-score of the first model built by "Zhang-server". The "TM-align template" columns include the best template identified by TM-align, the TM-score of the best template, and the PDB release date of the best template. The "LOMETS template" columns include the first template identified by LOMETS and the TM-score of the first template.

Target	Server group deadline	Domain	Type	TM-score (Zhang-Server first model)	TM-align template			LOMETS template	
					Best template	TM-score	PDB Released date	First template	TM-score
T0949	5/4/2018	T0949-D1	FM/TBM	0.665	3gyrL	0.714	4/28/2009	3cg8B	0.552
T0950	5/5/2018	T0950-D1	FM	0.441	5j65A	0.566	5/25/2016	1qoyA	0.285
T0951	5/9/2018	T0951-D1	TBM-easy	0.972	5cbkA	0.970	10/21/2015	5cbkA	0.970
T0953s1	5/10/2018	T0953s1-D1	FM	0.397	4uxeA	0.710	8/19/2015	4ld1A	0.364
T0953s2	5/10/2018	T0953s2-D1	FM/TBM	0.358	2f96A	0.589	2/14/2006	2ic7A	0.146
T0953s2	5/10/2018	T0953s2-D2	FM	0.590	1jtaA	0.686	6/19/2002	2ic7A	0.210
T0953s2	5/10/2018	T0953s2-D3	FM	0.310	2i3oD	0.596	8/29/2006	2ic7A	0.150
T0954	5/13/2018	T0954-D1	TBM-hard	0.810	5e6rA	0.814	3/2/2016	2h9lA	0.654
T0955	5/14/2018	T0955-D1	FM/TBM	0.755	3b35A	0.711	11/27/2007	4at7B	0.657
T0957s1	5/15/2018	T0957s1-D1	FM	0.380	5sy5B	0.512	11/9/2016	4ifdD	0.229
T0957s1	5/15/2018	T0957s1-D2	TBM-hard	0.495	4l5gA	0.764	7/31/2013	4ifdD	0.234
T0957s2	5/15/2018	T0957s2-D1	FM	0.532	4f52E	0.682	9/19/2012	3qkyA	0.348
T0958	5/15/2018	T0958-D1	FM/TBM	0.547	4v0pA	0.626	10/1/2014	3duwA	0.412
T0959	5/15/2018	T0959-D1	TBM-hard	0.725	4oltA	0.647	4/30/2014	2nr7A	0.569
T0960	5/16/2018	T0960-D1	FM	0.166	1w18B	0.451	5/11/2005	5hqgA	0.191
T0960	5/16/2018	T0960-D2	FM	0.392	5m9fA	0.708	12/20/2017	1uynX	0.284
T0960	5/16/2018	T0960-D3	TBM-hard	0.765	5efvA	0.764	5/25/2016	5efvA	0.693
T0960	5/16/2018	T0960-D4	FM	0.230	3tj1A	0.504	9/28/2011	1oa8D	0.146
T0960	5/16/2018	T0960-D5	TBM-easy	0.713	4mtmA	0.723	10/1/2014	4mtmA	0.666
T0961	5/24/2018	T0961-D1	TBM-easy	0.960	4y9jA	0.958	6/3/2015	4y9jA	0.952
T0962	5/24/2018	T0962-D1	TBM-easy	0.866	4ok7A	0.860	3/19/2014	4ok7A	0.835
T0963	5/18/2018	T0963-D1	FM	0.151	1w18B	0.471	5/11/2005	4unmA	0.152
T0963	5/18/2018	T0963-D2	FM	0.481	5m9fA	0.692	12/20/2017	2qomB	0.243
T0963	5/18/2018	T0963-D3	TBM-hard	0.756	5efvA	0.780	5/25/2016	5efvA	0.679
T0963	5/18/2018	T0963-D4	FM	0.239	3tj1A	0.507	9/28/2011	4unmA	0.137
T0963	5/18/2018	T0963-D5	TBM-easy	0.784	4mtmA	0.807	10/1/2014	4mtmA	0.762
T0964	5/19/2018	T0964-D1	TBM-hard	0.687	5t7aA	0.762	8/23/2017	5t7aA	0.724
T0965	5/19/2018	T0965-D1	TBM-hard	0.828	1orrA	0.831	8/26/2003	2p5uA	0.769
T0966	5/20/2018	T0966-D1	TBM-hard	0.839	2ebfX	0.841	3/6/2007	2ebfX	0.779
T0967	5/20/2018	T0967-D1	TBM-easy	0.834	3j1zP	0.819	10/10/2012	5ho1A	0.809
T0968s1	5/21/2018	T0968s1-D1	FM	0.556	3ujhA	0.518	11/16/2011	1xksA	0.368
T0968s2	5/21/2018	T0968s2-D1	FM	0.621	3ty1A	0.553	12/28/2011	4ygtA	0.310
T0969	5/25/2018	T0969-D1	FM	0.729	4k3uA	0.489	9/3/2014	1escA	0.407
T0970	5/26/2018	T0970-D1	FM/TBM	0.583	1wplK	0.648	9/28/2004	1vx7W	0.317
T0971	5/26/2018	T0971-D1	TBM-easy	0.921	3ebtA	0.934	9/30/2008	3ebtA	0.917
T0973	5/27/2018	T0973-D1	TBM-easy	0.618	1qbeB	0.855	7/11/1996	3rz3A	0.179
T0974s1	5/28/2018	T0974s1-D1	TBM-easy	0.716	3vk0A	0.748	3/14/2012	3bs3A	0.621
T0974s2	5/28/2018	T0974s2-D1	TBM-easy	0.897	3zhiA	0.867	12/25/2013	3zhiA	0.868
T0975	6/1/2018	T0975-D1	FM	0.669	3u44B	0.542	3/21/2012	3l0aA	0.418
T0976	6/1/2018	T0976-D1	TBM-easy	0.832	2hhgA	0.845	7/25/2006	1yt8A	0.716
T0976	6/1/2018	T0976-D2	TBM-easy	0.828	2hhgA	0.825	7/25/2006	1yt8A	0.787
T0977	6/2/2018	T0977-D1	TBM-easy	0.900	5efvA	0.881	5/25/2016	5efvA	0.843
T0977	6/2/2018	T0977-D2	TBM-easy	0.759	5efvA	0.830	5/25/2016	5efvA	0.789
T0978	6/3/2018	T0978-D1	FM/TBM	0.527	1q2rA	0.643	9/9/2003	1enuA	0.414
T0979	6/3/2018	T0979-D1	TBM-hard	0.441	5apzA	0.770	1/27/2016	3na7A	0.390
T0980s1	6/4/2018	T0980s1-D1	FM	0.290	4kmaA	0.524	11/20/2013	2v64A	0.255
T0980s2	6/4/2018	T0980s2-D1	FM	0.153	3gedB	0.477	3/17/2009	3evzA	0.166
T0981	6/7/2018	T0981-D1	TBM-hard	0.629	5efvA	0.696	5/25/2016	3bs0A	0.392
T0981	6/7/2018	T0981-D2	FM	0.262	5efvA	0.686	5/25/2016	2oajA	0.234
T0981	6/7/2018	T0981-D3	FM/TBM	0.677	3seeA	0.644	8/3/2011	5e7tB	0.458
T0981	6/7/2018	T0981-D4	TBM-hard	0.591	5m9fA	0.647	12/20/2017	5m9fA	0.557
T0981	6/7/2018	T0981-D5	TBM-hard	0.659	5m9fA	0.741	12/20/2017	5m9fA	0.600
T0982	6/8/2018	T0982-D1	TBM-easy	0.888	2luzA	0.849	10/3/2012	3q63A	0.800
T0982	6/8/2018	T0982-D2	TBM-hard	0.626	2rezA	0.751	4/22/2008	4xrtA	0.457

T0983	6/8/2018	T0983-D1	TBM-easy	0.947	3pfgA	0.945	12/15/2010	3pfgA	0.936
T0984	6/9/2018	T0984-D1	TBM-easy	0.874	6c96A	0.873	4/4/2018	6c96A	0.847
T0984	6/9/2018	T0984-D2	TBM-easy	0.782	5e1jA	0.815	12/16/2015	6c96A	0.757
T0985	6/10/2018	T0985-D1	TBM-hard	0.854	2cqtA	0.836	5/16/2006	2cqtA	0.771
T0986s1	6/11/2018	T0986s1-D1	FM/TBM	0.648	1v74A	0.652	3/30/2004	5ts4A	0.280
T0986s2	6/11/2018	T0986s2-D1	FM	0.594	4wj3B	0.592	12/31/2014	1iruW	0.269
T0987	6/14/2018	T0987-D1	FM	0.620	3htlX	0.580	9/15/2009	4ypjA	0.316
T0987	6/14/2018	T0987-D2	FM	0.378	3uxfA	0.574	11/28/2012	2y7lA	0.309
T0989	6/15/2018	T0989-D1	FM	0.547	5efvA	0.590	5/25/2016	2ra5A	0.301
T0989	6/15/2018	T0989-D2	FM	0.342	5m9fA	0.591	12/20/2017	2wjqA	0.232
T0990	6/16/2018	T0990-D1	FM	0.567	1ciiA	0.592	1/14/1998	5ctqA	0.340
T0990	6/16/2018	T0990-D2	FM	0.382	3s27A	0.483	8/24/2011	1tjfB	0.207
T0990	6/16/2018	T0990-D3	FM	0.212	1o0sA	0.449	7/22/2003	5ijnD	0.207
T0991	6/17/2018	T0991-D1	FM	0.223	5jzrA	0.672	8/10/2016	2m47A	0.212
T0992	6/17/2018	T0992-D1	FM/TBM	0.722	3uc2A	0.710	11/23/2011	4bffA	0.523
T0993s1	6/18/2018	T0993s1-D1	TBM-easy	0.843	4u00A	0.811	5/13/2015	3dhwC	0.770
T0993s2	6/18/2018	T0993s2-D1	TBM-easy	0.704	1tilD	0.767	6/15/2004	1vc1A	0.685
T0995	6/22/2018	T0995-D1	TBM-easy	0.904	3wuyA	0.892	12/31/2014	3wuyA	0.881
T0996	6/23/2018	T0996-D1	TBM-easy	0.778	5uvnA	0.774	4/12/2017	5uvnA	0.764
T0996	6/23/2018	T0996-D2	TBM-easy	0.815	5uvnA	0.820	4/12/2017	5uvnA	0.817
T0996	6/23/2018	T0996-D3	TBM-easy	0.823	5uvnA	0.808	4/12/2017	5uvnA	0.805
T0996	6/23/2018	T0996-D4	TBM-easy	0.750	5uvnA	0.797	4/12/2017	5uvnA	0.717
T0996	6/23/2018	T0996-D5	TBM-easy	0.7380	5uvnA	0.747	4/12/2017	5uvnA	0.728
T0996	6/23/2018	T0996-D6	TBM-easy	0.879	5uvnA	0.846	4/12/2017	5uvnA	0.820
T0997	6/24/2018	T0997-D1	FM/TBM	0.613	4xzzA	0.618	9/2/2015	4xzzA	0.503
T0998	6/24/2018	T0998-D1	FM	0.206	2vf9A	0.536	9/23/2008	2vqiA	0.159
T0999	6/25/2018	T0999-D1	TBM-easy	0.986	1nr5A	0.986	3/18/2003	1nr5A	0.983
T0999	6/25/2018	T0999-D2	TBM-hard	0.795	5xwbA	0.871	9/6/2017	1x8rA	0.726
T0999	6/25/2018	T0999-D3	TBM-easy	0.793	4y0aA	0.789	8/12/2015	4y0aA	0.724
T0999	6/25/2018	T0999-D4	TBM-easy	0.964	5swuA	0.963	9/7/2016	5swvC	0.955
T0999	6/25/2018	T0999-D5	TBM-easy	0.888	5swvC	0.870	12/21/2016	5swvC	0.860
T1000	6/28/2018	T1000-D1	TBM-easy	0.945	3lazA	0.935	1/19/2010	3lazA	0.922
T1000	6/28/2018	T1000-D2	FM	0.814	3lq2A	0.438	3/2/2010	1jqkA	0.230
T1001	6/29/2018	T1001-D1	FM	0.631	4rpwA	0.690	5/11/2016	5akpA	0.533
T1002	6/29/2018	T1002-D1	TBM-easy	0.794	4krtA	0.900	4/2/2014	3npfA	0.686
T1002	6/29/2018	T1002-D2	TBM-easy	0.803	4krtA	0.899	4/2/2014	3npfA	0.741
T1002	6/29/2018	T1002-D3	TBM-easy	0.792	4xxtA	0.790	2/18/2015	4xxtA	0.728
T1003	6/30/2018	T1003-D1	TBM-easy	0.934	5txrB	0.922	3/28/2018	5txrB	0.908
T1004	7/1/2018	T1004-D1	TBM-easy	0.775	5efvA	0.818	5/25/2016	5efvA	0.748
T1004	7/1/2018	T1004-D2	TBM-easy	0.705	6cl6A	0.805	6/27/2018	5efvA	0.574
T1004	7/1/2018	T1004-D3	TBM-easy	0.925	5m9fA	0.911	12/20/2017	5m9fA	0.909
T1005	7/2/2018	T1005-D1	FM/TBM	0.697	4nuyA	0.694	4/9/2014	4nuyA	0.570
T1006	7/5/2018	T1006-D1	TBM-easy	0.954	3w5xA	0.959	4/16/2014	3w5xA	0.937
T1008	7/6/2018	T1008-D1	FM/TBM	0.362	1ry6A	0.704	4/13/2004	4proC	0.246
T1009	7/6/2018	T1009-D1	TBM-hard	0.876	2x2hA	0.842	1/19/2011	2xvgA	0.809
T1010	7/8/2018	T1010-D1	FM	0.561	1i78A	0.538	10/3/2001	1ekmA	0.158
T1011	7/9/2018	T1011-D1	TBM-hard	0.806	4zwjA	0.841	7/29/2015	4n6hA	0.749
T1011	7/9/2018	T1011-D2	TBM-easy	0.866	4k5yA	0.988	7/17/2013	5x33A	0.963
T1013	7/12/2018	T1013-D1	TBM-easy	0.927	4n6hA	0.919	12/25/2013	4n6hA	0.916
T1014	7/12/2018	T1014-D1	TBM-easy	0.889	3dgeA	0.894	7/7/2009	3dgeA	0.859
T1014	7/12/2018	T1014-D2	TBM-easy	0.805	1a2oA	0.806	4/29/1998	1m5tA	0.724
T1015s1	7/13/2018	T1015s1-D1	FM	0.466	1dp4C	0.518	7/12/2000	3v9fA	0.252
T1015s2	7/13/2018	T1015s2-D1	TBM-hard	0.716	4g6vA	0.717	12/12/2012	4g6vA	0.616
T1016	7/13/2018	T1016-D1	TBM-easy	0.880	4embA	0.874	4/25/2012	4ij5A	0.864
T1017s1	7/14/2018	T1017s1-D1	TBM-easy	0.764	2o5hA	0.777	1/9/2007	2o5hA	0.684
T1017s2	7/14/2018	T1017s2-D1	FM	0.697	2zzgA	0.504	7/21/2009	2gzaC	0.361
T1018	7/14/2018	T1018-D1	TBM-easy	0.940	3iarA	0.926	8/11/2009	3rysA	0.894
T1019s1	7/15/2018	T1019s1-D1	FM/TBM	0.596	4uzjA	0.500	2/25/2015	5tdwA	0.272
T1019s2	7/15/2018	T1019s2-D1	TBM-easy	0.773	1v74A	0.660	3/30/2004	1v74A	0.597
T1020	7/15/2018	T1020-D1	TBM-easy	0.879	3m71A	0.843	5/12/2010	3m71A	0.835
T1021s1	7/16/2018	T1021s1-D1	TBM-hard	0.822	5iv5W	0.796	5/18/2016	5w5fA	0.755
T1021s2	7/16/2018	T1021s2-D1	TBM-hard	0.797	3j9qA	0.851	4/1/2015	3j9qA	0.792
T1021s3	7/16/2018	T1021s3-D1	FM	0.633	2gjvA	0.581	4/11/2006	4hudA	0.408
T1021s3	7/16/2018	T1021s3-D2	FM	0.436	3ievA	0.604	8/25/2009	3kzfA	0.241
T1022s1	7/19/2018	T1022s1-D1	FM	0.694	5iv5U	0.703	5/18/2016	5iv5U	0.566
T1022s1	7/19/2018	T1022s1-D2	TBM-hard	0.626	5jceA	0.666	6/8/2016	2l9yA	0.520
T1022s2	7/19/2018	T1022s2-D1	TBM-hard	0.772	4mtkA	0.830	10/1/2014	4mtkA	0.727
Average				**0.674**		**0.732**			**0.567**

Table S4. Contact prediction results for NeBcon and its component contact prediction methods for the 50 FM targets.

method	short range contacts			medium range contacts			long range contacts		
	top L/5	top L/2	top L	top L/5	top L/2	top L	top L/5	top L/2	top L
FreeContact	0.189	0.140	0.118	0.193	0.138	0.105	0.220	0.163	0.120
GREMLIN	0.234	0.163	0.110	0.222	0.152	0.101	0.265	0.198	0.145
CCMpred	0.247	0.163	0.110	0.228	0.152	0.102	0.269	0.196	0.146
MetaPSICOV2	0.492	0.371	0.253	0.472	0.355	0.254	0.352	0.283	0.222
DeepCOV*	0.529	0.386	0.258	0.519	0.396	0.276	0.447	0.353	0.272
DNCON2*	0.508	0.380	0.258	0.520	0.392	0.280	0.458	0.360	0.277
Deepcontact*	0.496	0.371	0.258	0.545	0.426	0.301	0.447	0.361	0.284
DeepPLM*,+	0.571	0.415	0.274	0.595	0.450	0.308	0.520	0.421	0.326
ResPRE*,+	0.590	0.431	0.286	0.621	0.457	0.314	0.530	0.431	0.342
NeBcon	0.607	0.439	0.293	0.643	0.470	0.319	0.534	0.453	0.357

* Indicates the approach uses a deep-learning framework.
+ Indicates the approach is one of our in-house methods.

Table S5. Comparison between the contact prediction results for NeBcon with HHblits MSAs as input or DeepMSA MSAs as input for the 50 FM targets. Single-tailed Student's t-test is used here to evaluate the statistical significance.

range	contacts	NeBcon based on HHblits MSAs	NeBcon based on DeepMSA MSAs	p-value
short range	top *L*/5	0.541	0.607	5.73E-04
	top *L*/2	0.391	0.439	5.43E-04
	top *L*	0.268	0.293	8.17E-04
medium range	top *L*/5	0.540	0.643	1.20E-04
	top *L*/2	0.405	0.470	3.13E-04
	top *L*	0.294	0.319	1.13E-02
long range	top *L*/5	0.474	0.534	1.86E-02
	top *L*/2	0.393	0.453	7.68E-03
	top *L*	0.302	0.357	1.48E-03

Table S6. The DeepMSA, contact prediction and structure modeling information for the 50 FM targets. The "Domain" is the domain name of each target. The "Class" is the fold class of each protein. The "N_{msa}" is the number of sequences in the MSA. The "*Neff*" is the *Neff* value of the deep MSA for each target. The "Precision" is the precision of the top L long-range contact prediction by NeBcon. The "TM-score" is the TM-score of the best model from "Zhang-Server" or "QUARK" corresponding to the information from the "Model" column.

Domain	Class	N_{msa}	*Neff*	Precision	TM-score	Model
T0949-D1	β	5760	245.757	0.892	0.689	QUARK model4
T0950-D1	α	304	10.012	0.509	0.506	QUARK model2
T0953s1-D1	β	548	16.987	0.000	0.433	Zhang-Server model4
T0953s2-D1	α	1093	43.132	0.250	0.464	QUARK model2
T0953s2-D2	αβ	1093	43.132	0.819	0.590	Zhang-Server model1
T0953s2-D3	αβ	1093	43.132	0.753	0.310	Zhang-Server model1
T0955-D1	αβ	1	0.156	0.098	0.824	QUARK model2
T0957s1-D1	αβ	109	5.436	0.287	0.462	QUARK model5
T0957s2-D1	α	84	4.529	0.303	0.635	QUARK model4
T0958-D1	αβ	58	2.567	0.416	0.548	QUARK model1
T0960-D1	αβ	118	3.957	0.000	0.188	QUARK model2
T0960-D2	β	118	3.957	0.048	0.454	Zhang-Server model2
T0960-D4	α	118	3.957	0.000	0.256	QUARK model2
T0963-D1	αβ	276	14.572	0.000	0.189	Zhang-Server model3
T0963-D2	β	276	14.572	0.037	0.481	Zhang-Server model1
T0963-D4	α	3208	155.175	0.000	0.250	QUARK model1
T0968s1-D1	αβ	256	15.588	0.288	0.566	Zhang-Server model2
T0968s2-D1	β	510	33.033	0.252	0.647	QUARK model1
T0969-D1	αβ	7589	74.493	0.661	0.752	QUARK model1
T0970-D1	αβ	673	12.928	0.518	0.583	Zhang-Server model1
T0975-D1	αβ	14749	357.906	0.545	0.751	Zhang-Server model5
T0978-D1	αβ	10073	182.546	0.489	0.661	Zhang-Server model3
T0980s1-D1	αβ	172	7.429	0.308	0.540	QUARK model1
T0980s2-D1	αβ	126	4.670	0.000	0.206	Zhang-Server model4
T0981-D2	αβ	9	0.198	0.063	0.302	Zhang-Server model2
T0981-D3	αβ	9	0.198	0.163	0.677	Zhang-Server model1
T0986s1-D1	αβ	862	51.067	0.359	0.692	QUARK model2
T0986s2-D1	αβ	94	5.684	0.568	0.598	QUARK model1
T0987-D1	αβ	122	2.404	0.687	0.620	Zhang-Server model1
T0987-D2	αβ	122	2.404	0.500	0.543	Zhang-Server model2
T0989-D1	αβ	20	1.275	0.291	0.547	Zhang-Server model1
T0989-D2	β	20	1.275	0.098	0.371	Zhang-Server model4
T0990-D1	α	68	1.496	0.342	0.653	QUARK model4
T0990-D2	αβ	68	1.496	0.234	0.382	Zhang-Server model1
T0990-D3	αβ	68	1.496	0.216	0.294	Zhang-Server model2
T0991-D1	αβ	3	0.276	0.126	0.279	Zhang-Server model2
T0992-D1	β	3506	165.324	0.701	0.746	QUARK model5
T0997-D1	αβ	6683	155.400	0.730	0.695	Zhang-Server model4
T0998-D1	αβ	10	0.699	0.102	0.274	Zhang-Server model5
T1000-D2	αβ	7302	169.641	0.829	0.851	QUARK model1
T1001-D1	αβ	24	2.028	0.201	0.631	Zhang-Server model1
T1005-D1	αβ	10926	247.590	0.718	0.706	QUARK model5
T1008-D1	αβ	1	0.112	0.429	0.659	QUARK model3
T1010-D1	β	421	21.083	0.538	0.561	Zhang-Server model1
T1015s1-D1	αβ	534	43.643	0.534	0.524	QUARK model1
T1017s2-D1	αβ	366	14.615	0.280	0.768	QUARK model1
T1019s1-D1	αβ	2994	254.684	0.207	0.597	QUARK model1
T1021s3-D1	αβ	7592	334.750	0.729	0.643	Zhang-Server model3
T1021s3-D2	αβ	68	4.442	0.083	0.530	Zhang-Server model5
T1022s1-D1	β	6518	263.019	0.635	0.694	Zhang-Server model1
Average		**1936.3**	**60.918**	**0.357**	**0.536**	

Table S7. Domain partition information for the 21 multi-domain targets. The "Target" column is the name of each target. The "CASP domain partition" columns include the number of domains and the domain boundaries given by the CASP13 assessors for each target. The "Zhang-server domain partition" columns include the number of domains and the domain boundaries predicted by ThreaDom for each target. The "NDO-score" is the normalized domain overlap (NDO) score. The "DBD-score" is the domain boundary distance (DBD) score. The "TM-score" is the TM-score of the first full-length model built by "Zhang-Server" for each multi-domain target.

Target	CASP domain partition		Zhang-Server domain partition		NDO-score	DBD-score	TM-score
	No.	boundary	No.	boundary			
T0953s2	3	2-45;46-151,229-249;152-228;	1	1-249;	0.418	0.000	0.445
T0957s1	2	2-37,92-163;38-91;	1	1-163;	0.629	0.000	0.303
T0960	5	11-42;43-126;127-215;216-279;280-384;	4	1-135;136-218;219-293;294-384;	0.663	0.281	0.271
T0963	5	9-39;40-121;122-214;215-278;279-372;	4	1-135;136-215;216-280;281-372;	0.776	0.500	0.242
T0976	2	9-128;129-252;	1	1-252;	0.478	0.000	0.707
T0977	2	59-359;360-563;	1	1-566;	0.516	0.000	0.624
T0981	5	34-119;120-190,394-402;191-393;403-513;514-640;	4	1-110;111-195;196-422;423-640;	0.686	0.325	0.312
T0982	2	11-145;146-277;	2	1-150;151-283;	0.941	1.000	0.497
T0984*	2	39-406,565-700;417-563;	1	1-752;	0.658	0.000	0.861
T0987	2	11-195;196-402;	2	1-215;216-405;	0.882	0.000	0.420
T0989	2	1-134;135-246;	2	1-136;137-246;	1.000	1.000	0.378
T0990	3	1-76;77-134,348-520;135-347;	4	1-136;137-289;290-406;407-552;	0.408	0.333	0.257
T0996	6	17-123;124-250;251-350;351-483;484-604;605-708;	7	12-130;131-252;253-363;364-483;484-604;605-714;715-848;	0.794	0.688	0.360
T0999	5	15-400;401-853;866-1045;1046-1289;1290-1577;	4	1-402;403-849;850-1050;1051-1589;	0.789	0.406	0.392
T1000*	2	10-92;93-523;	2	1-98;99-523;	0.936	0.625	0.680
T1002*	3	1-59;60-118;127-270;	2	1-150;151-270;	0.609	0.063	0.450
T1004	3	66-151;152-228;229-458;	2	1-247;248-458;	0.607	0.063	0.550
T1011	2	55-268,433-520;271-430;	2	8-270,434-519;271-433;	0.879	0.750	0.585
T1014	2	1-159;160-276;	2	1-164;165-276;	1.000	1.000	0.529
T1021s3	2	4-181;195-295;	2	1-181;182-295;	0.989	1.000	0.424
T1022s1	2	2-157;158-224;	2	1-171;172-229;	0.856	0.375	0.534
Average					**0.739**	**0.400**	**0.468**

Targets with '*' mark are assessed as FM-sp targets which means the CASP assessor assessed the model quality using the full-length structure.