

Integration of QUARK and I-TASSER for *ab initio* protein structure prediction in CASP11

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SUPPLEMENTARY INFORMATION

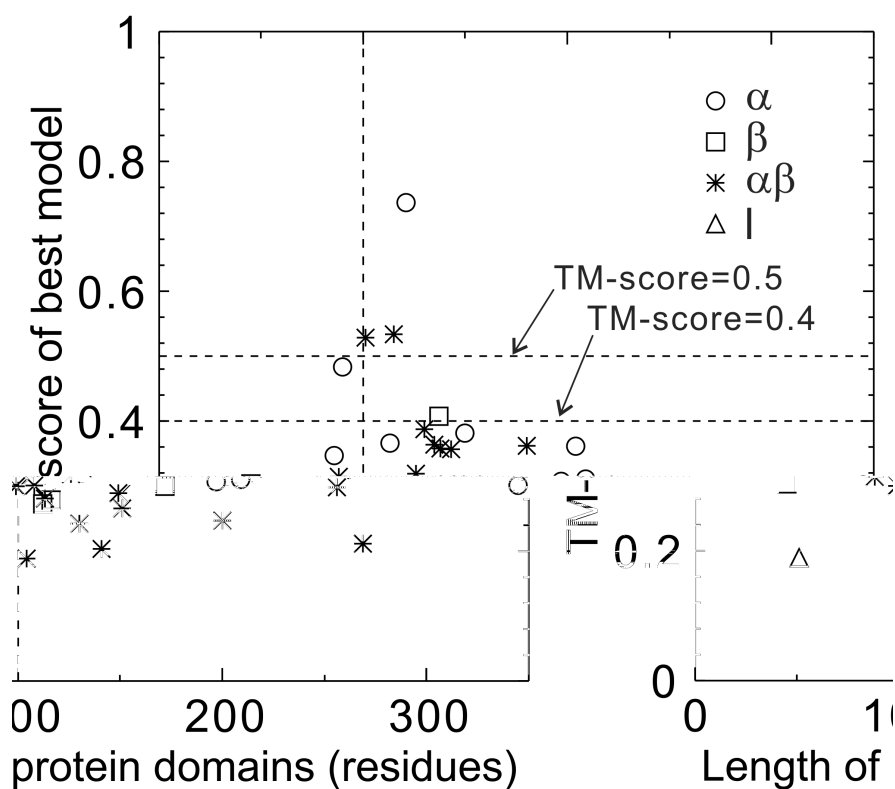


Figure S1. TM-score of the best QUARK models for 35 FM domains versus protein length.

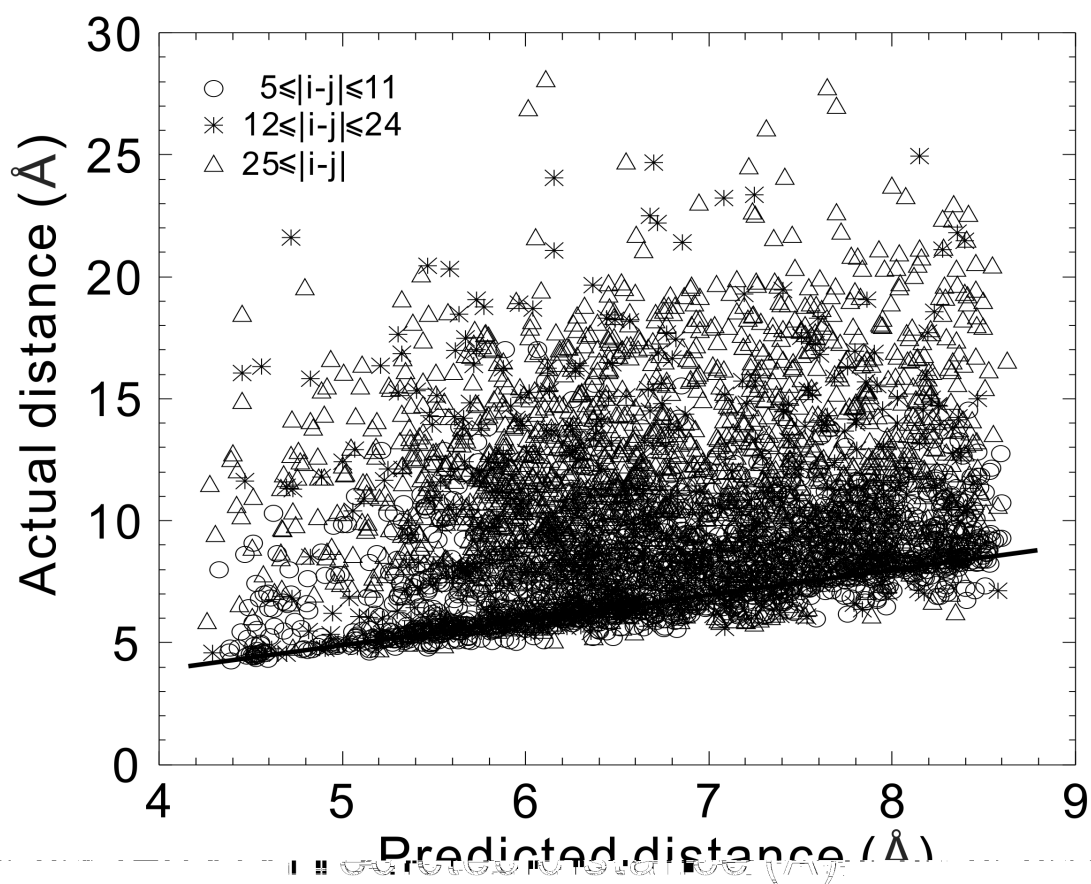


Figure S2. Predicted distance of the residue pairs by QUARK as in contact versus the actual distance of the residue pairs in the native structure. Points in different shapes indicate data from residue pairs of different contact order. The solid line shows the position with identical distances to guide the eye.

Table S1. RMSD of the fragments identified by QUARK for T0837-D1. The ten best fragments are counted at each position and the average RMSD is calculated along the positions for a given fragment size.

Size of fragments (residues)	Average RMSD (Å)	Standard deviation (Å)
2	0.011	0.010
3	0.113	0.078
4	0.789	0.226
5	1.372	0.303
6	1.470	0.310
7	1.548	0.298
8	1.612	0.296
9	1.729	0.300
10	1.803	0.346
11	1.874	0.376
12	1.948	0.393
13	2.031	0.415
14	2.103	0.425
15	2.181	0.441
16	2.259	0.446
17	2.341	0.454
18	2.436	0.450
19	2.530	0.437
20	2.637	0.421

Table S2. Contact prediction results using fragment-based distance profile by QUARK for T0837-D1.

#	i	j	i-j	$d_{\text{pred}} (\text{\AA})^a$	$d_{\text{exp}} (\text{\AA})^b$	$ d_{\text{pred}} - d_{\text{exp}} (\text{\AA})$
1	7	18	11	7.923	6.150	1.773
2	8	17	9	8.435	9.035	0.600
3	10	15	5	8.201	8.143	0.058
4	10	16	6	8.350	8.636	0.286
5	11	18	7	6.708	5.498	1.210
6	11	17	6	6.255	6.220	0.035
7	11	16	5	5.072	5.360	0.288
8	12	18	6	7.996	8.540	0.544
9	12	17	5	7.969	8.391	0.422
10	19	24	5	7.319	8.555	1.236
11	20	56	36	7.942	10.250	2.308
12	20	52	32	8.224	11.178	2.954
13	24	55	31	6.921	7.102	0.181
14	24	59	35	7.542	8.047	0.505
15	38	43	5	8.419	8.117	0.302
16	39	44	5	6.097	8.835	2.738
17	40	45	5	7.980	8.856	0.876
18	42	47	5	8.052	8.455	0.403
19	43	48	5	6.650	6.687	0.037
20	64	70	6	8.067	7.862	0.205
21	64	69	5	6.915	6.665	0.250
22	65	70	5	6.773	6.108	0.665
23	77	83	6	8.136	6.806	1.330
24	77	82	5	5.544	5.231	0.313
25	78	83	5	6.206	6.340	0.134
26	78	84	6	7.299	6.294	1.005
27	86	91	5	6.463	7.956	1.493
28	92	97	5	8.528	9.030	0.502
29	98	103	5	7.908	7.326	0.582
30	99	104	5	7.595	9.826	2.231
31	102	107	5	7.834	11.721	3.887
32	103	108	5	7.359	7.724	0.365
33	115	120	5	7.809	7.523	0.286
34	116	121	5	7.361	8.190	0.829
Average						0.934

^a d_{pred} : predicted distance by QUARK.

^b d_{exp} : actual distance in experimental structure.