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Supporting information for article:

Using iterative fragment assembly and progressive sequence truncation to facilitate phasing and crystal structure determination of distantly related proteins

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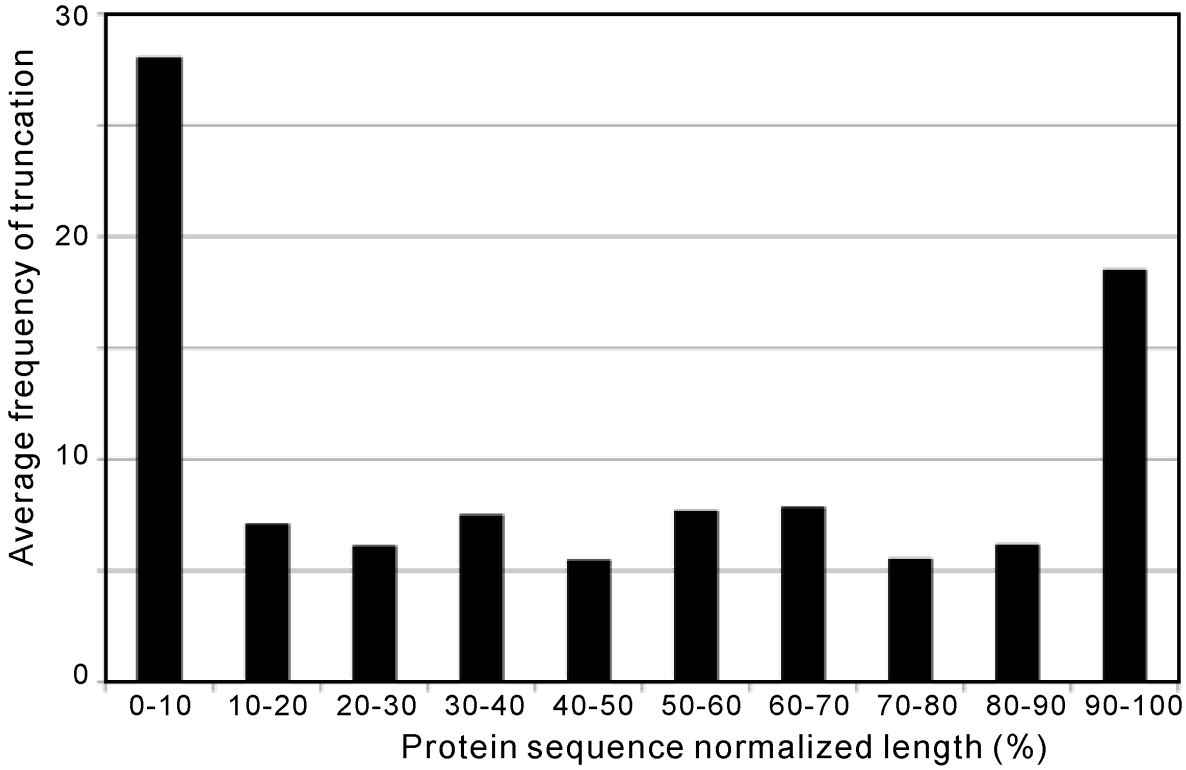

Figure S1. Average frequency of residue truncation in different regions of the protein sequence. The target sequences are evenly split into 10 bins and the number of trancated residues is then averaged in each bin for all target proteins.

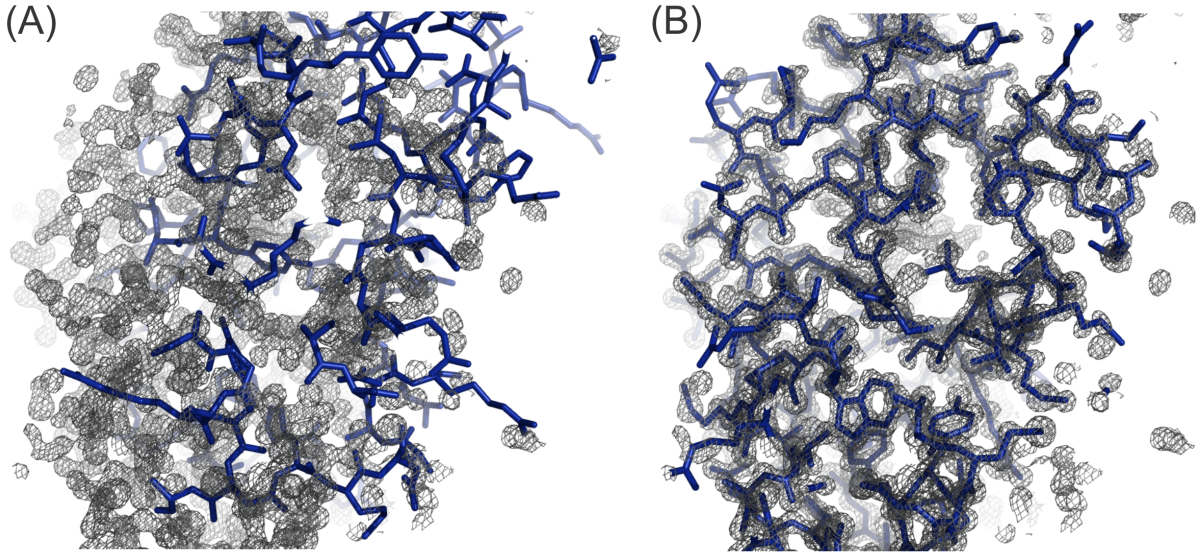

Figure S2. Comparison of LOMETS and I-TASSER models for molecular replacement. (A) Overlay of the MR solution built from LOMETS template on the 2m$|F_o|$-D$|F_c|$ σ^A-weighted map of PDB entry 1tu9 contoured at 2σ. (B) Overlay of the final I-TASSER-MR model.

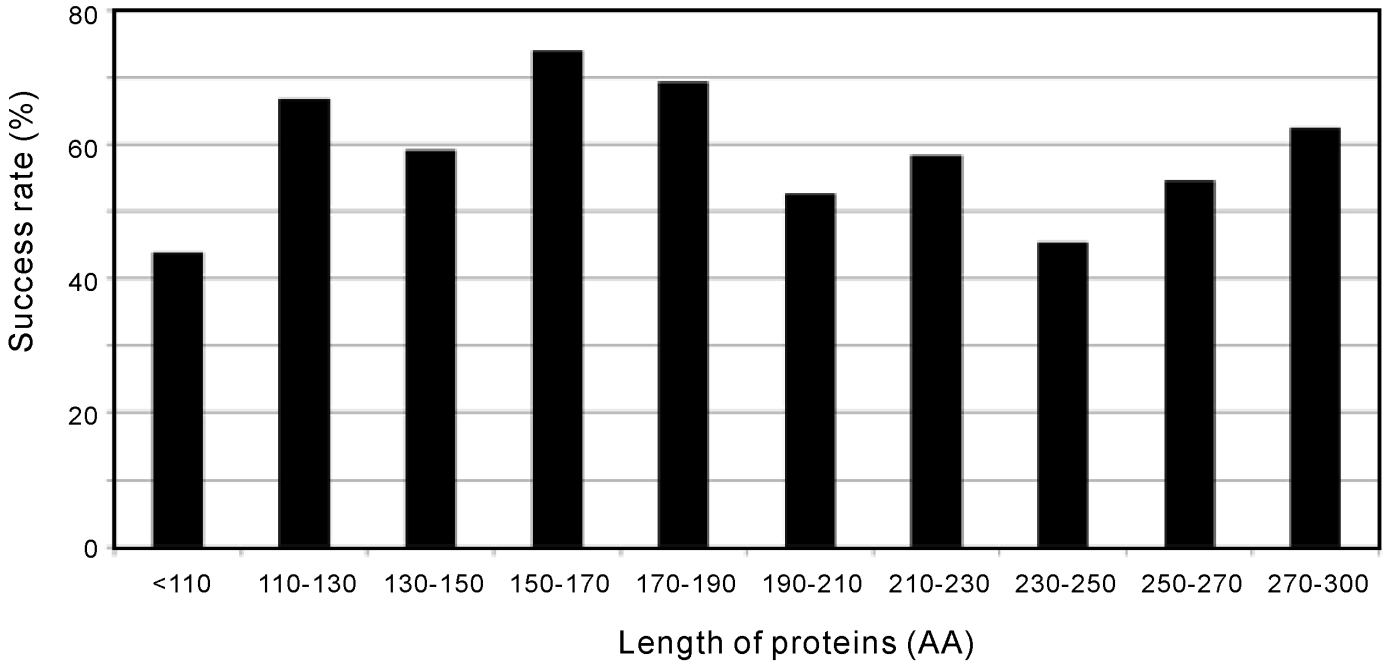

Figure S3. Success rate of I-TASSER-MR as a function of the number of amino acides (AA) in the target proteins.

Table S1. The X-Ray structures and I-TASSER model of the 33 successful targets from the CASP8 test set.

X-Ray Structure					I-TASSER Model			
PDBID	**D_{min}[a]**	**SG[b]**	**Len[c]**	**#Copy[e]**	**RMSD[f]**	**PBS[g]**	**TM-score[h]**	**GDT**
2vsw	2	$P2_12_12$	153	2	2.44 (810)	1.82	0.77	0.72
2vwr	1.3	$C121$	95	1	2.47(666)	1.57	0.85	0.85
3cyn	2	$C121$	174	3	2.22 (1293)	1.63	0.83	0.75
3d1p	0.98	$C121$	139	1	2.79(753)	1.69	0.77	0.74
3d6j	2	$P4_12_12$	222	1	2.13(1621)	1.63	0.93	0.83
3d6w	2.4	$P4_222$	109	2	2.59(834)	2.16	0.81	0.77
3d89	2.07	$P4_32_12$	157	1	2.76(821)	1.78	0.7	0.66
3d8h	2.01	$C222_1$	267	2	2.8(1471)	1.96	0.81	0.69
3d8p	2.2	$I422$	162	2	2.68(1100)	1.96	0.78	0.72
3da2	2.05	$C121$	283	2	2.46(1728)	1.56	0.88	0.79
3dai	1.95	$P6_522$	130	1	2.19(919)	1.36	0.86	0.84
3db0	2	$C121$	139	2	2.37(856)	1.78	0.84	0.78
3db5	2.15	$I422$	151	2	2.16(927)	1.15	0.85	0.83
3dcp	2.1	$P6_4$	275	3	2.45(1902)	1.66	0.86	0.75
3df8	1.65	$C121$	111	1	2.31(703)	1.52	0.78	0.76
3dfa	2.45	$P4_32_12$	286	1	2.98(1761)	2.36	0.83	0.68
3dh1	2.8	$P12_11$	189	4	2.25(1177)	1.54	0.89	0.83
3dhn	2	$P2_12_12_1$	219	1	2.62(1374)	1.86	0.83	0.71
3dka	2.3	$P2_12_12_1$	154	2	2.32(1021)	1.93	0.81	0.74
3dkp	2.1	$P12_11$	242	1	2.54(1563)	1.88	0.82	0.7
3dkz	2.4	$P3_121$	134	2	1.97(862)	1.38	0.9	0.89
3dm3	2.4	$P6_522$	105	3	2.4(694)	1.69	0.79	0.79
3dmb	2.3	$P3_221$	146	3	2.35(978)	1.4	0.83	0.8
3dmc	1.65	$P1$	133	2	2.78(963)	2.09	0.8	0.73
3dmn	1.66	$P6_522$	174	1	2.88(1174)	2.07	0.87	0.76
3dnh	1.94	$P12_11$	254	2	2.93(1475)	2.73	0.79	0.65
3dou	1.45	$C121$	197	1	2.25(1357)	1.38	0.94	0.88
3dr5	2.25	$P6_122$	213	1	2.34(1502)	1.76	0.9	0.78
3e03	1.69	$C121$	271	3	2.25(1460)	1.54	0.77	0.67
3gwl	2.1	$P2_12_12_1$	105	2	2.31(865)	1.45	0.89	0.88
3klw	2	$P6_3$	115	2	2.04(718)	1.43	0.91	0.9
3czx	1.6	$P12_11$	181	4	2.33(1218)	1.75	0.84	0.74
3djb	2.9	$P4_3$	223	2	2.75(1289)	1.98	0.84	0.73

[a]Resolution of the X-ray structure.

[b]Space group of the entry

[c]Length of the PDB structure (including unstructured residues)

[d]Number of monomers in the asymmetric unit of the target

[e]RMSD of the initial I-TASSER model to the PDB entry

[f]PBS of the initial I-TASSER model to the PDB entry
[g]TM-score of the initial I-TASSER model
[h]GDT-TS score of the initial I-TASSER model

Table S2. Summary of the first successful search models and the statistics for the 33 successful I-TASSER-MR solutions from the CASP8 test set (extension of Table S1).

PDB structure		Search model after truncation[m]					Phaser		I-TASSER-MR Model			
ID	Len[a]	Trun[b]	RMS[c]	PBS[d]	TM[e]	GT[f]	LLG[g]	TFZ[h]	R_{free}[i]	#built[j]	TM[k]	PBS[l]
2vsw	87	0.43	1.56(534)	1.02	0.49	0.49	72	10.5	0.31	86/92	0.64/0.68	0.29/0.29
2vwr	89	0.06	2.41(649)	1.51	0.83	0.83	34	4.2	0.25	89	0.94	0.09
3cyn	174	0.00	2.22 (1293)	1.63	0.83	0.75	189	13.2	0.24	146/158/158	0.83/0.91/0.9	0.18 /0.18 /0.13
3czx[n]	177	0.02	2.34(1210)	1.74	0.84	0.74	353	40.8	0.53	80	0.39	3.05
3d1p	133	0.04	2.79(753)	1.69	0.77	0.74	15	4.1	0.41	96	0.66	0.75
3d6j	222	0.00	2.13(1621)	1.63	0.93	0.83	79	12.1	0.29	204	0.97	0.18
3d6w	105	0.04	2.54(800)	2.09	0.78	0.75	78	9.8	0.29	95/96	0.87/0.88	0.19 /0.19
3d89	111	0.29	2.70(781)	1.68	0.67	0.63	41	5.3	0.36	100	0.73	0.24
3d8h	255	0.04	2.77(1426)	2.05	0.15	0.08	82	7.2	0.33	134	0.58	0.35 /0.35
3d8p	158	0.02	2.71(1102)	1.97	0.77	0.71	57	5.2	0.24	158/158	0.97/0.98	0.12 /0.12
3da2	283	0.00	2.46(1728)	1.56	0.88	0.79	112	8.3	0.26	247/246	0.93/0.93	0.37 /0.37
3dai	130	0.00	2.19(919)	1.36	0.86	0.84	50	9.4	0.26	120	0.92	0.12
3db0	120	0.14	2.36(830)	1.69	0.79	0.74	52	4.5	0.27	124/57	0.99/0.45	0.14 /0.48
3db5	151	0.00	2.16(927)	1.15	0.85	0.83	226	17.4	0.3	125/125	0.92/0.93	0.33 /0.33
3dcp	237	0.14	2.41(1809)	1.6	0.79	0.71	366	23.4	0.4	273/190/196	0.98/0.59/0.62	0.28/0.26 /0.25
3df8	102	0.08	2.22(684)	1.44	0.77	0.76	54	4.9	0.25	89	0.7	0.11
3dfa	226	0.21	2.80(1627)	2.25	0.55	0.49	65	8.2	0.36	167	0.63	0.24
3dh1	163	0.14	2.20(1119)	1.46	0.85	0.81	208	8.4	0.28	158/158/145	0.97/0.97/0.89	0.36 /0.35 /0.35
3dhn	219	0.00	2.62(1374)	1.86	0.83	0.71	23	7.5	0.4	218	0.83	0.44
3djb[n]	163	0.27	2.79(1125)	1.88	0.75	0.68	65	8.8	0.53	97	0.44	4.09
3dka	132	0.14	2.29(992)	1.87	0.77	0.71	94	8.3	0.3	117/114	0.81/0.79	0.26 /0.20
3dkp	236	0.02	2.54(1563)	1.88	0.81	0.7	27	4	0.34	163	0.66	0.26
3dkz	134	0.00	1.97(862)	1.38	0.9	0.89	96	11.2	0.32	120/110	0.93/0.87	0.31 /0.27
3dm3	93	0.11	1.98(655)	1.51	0.76	0.76	64	6.6	0.31	96	0.97	0.25
3dmb	142	0.03	2.35(978)	1.4	0.83	0.8	173	7.3	0.34	131/121/123	0.87/0.76/0.8	0.32 /0.65 /0.69
3dmc	119	0.11	2.75(861)	2.03	0.76	0.69	46	5.8	0.25	127/130	0.95/0.98	0.13 /0.13
3dmn	172	0.01	2.87(1181)	2.09	0.87	0.76	39	7	0.25	137	0.84	0.11
3dnh	218	0.14	2.97(1524)	2.7	0.76	0.63	61	6.5	0.36	139/117	0.57/0.41	0.67 /0.18
3dou	197	0.00	2.25(1357)	1.38	0.94	0.88	64	7.1	0.23	164	0.94	0.09
3dr5	213	0.00	2.34(1502)	1.76	0.9	0.78	70	10.7	0.35	202	0.94	0.34
3e03	115	0.58	1.73(700)	1.03	0.41	0.39	340	10.3	0.4	163/164	0.6/0.6	0.23 /0.16
3gwl	101	0.04	2.30(861)	1.44	0.88	0.87	91	10.7	0.32	99/105	0.92/0.80	0.17
3klw	115	0.00	2.04(718)	1.43	0.91	0.9	25	6.2	0.33	94	0.96	0.24

[a]Length of the first successful search model

[b]Fraction of truncated residues in the first successful search model

[c]RMSD of the first successful search model to the PDB entry

[d]PBS of first successful search model to the PDB entry

[e]TM-score of first successful search model

[f]GDT-TS score of first successful search model

[g]LLG of Phaser solution relative to random

[h]TFZ score of Phaser

[i]R_{free} for the refined I-TASSER-MR structure

[j]#built: Number of residues in the model constructed by I-TASSER-MR. When multiple subunits exist in the asymmetric unit of the target, a number is given for each chain

[k]TM-score of the I-TASSER-MR structure and the PDB entry

[l]PBS of the I-TASSER-MR structure and the PDB entry

[m]The first search model after editing that was successful in MR

[n]Target has a significant MR solution but failed to be autobuilt.

Table S3. Statistics for the 28 unsuccessful CASP8 targets.

X-Ray Structure					I-TASSER Model				Phaser		I-TASSER-MR structure		
PDBID	**L[a]**	**D_{min}[b]**	**#Cp[c]**	**SG[d]**	**RMS[e]**	**PBS[f]**	**TMs[g]**	**GDT[h]**	**LLG**	**TFZ**	**Rfree**	**TMs[i]**	**PBS[j]**
2vsv	109	1.82	2	$C121$	1.83 (608)	1.31	0.74	0.72	98	4.3	0.48	0.12	1.99
3d1l	263	2.19	2	$I4_1$	3.02(1298)	2.68	0.65	0.53	21	5.3	0.55	0.06	3.18
3dcy	275	1.75	1	$P2_12_12_1$	2.47(1367)	1.83	0.65	0.54	22	4.2	0.54	0.34	1.93
3d4o	292	2.1	4	$P12_11$	2.98(1587)	2.75	0.72	0.52	124	5.8	0.5	0.03	NA[k]
3d4e	206	1.4	1	$C121$	4.27(896)	3.84	0.57	0.48	22	3.5	0.54	0.34	4.19
3d5p	143	1.45	2	$P2_12_12_1$	2.95(831)	2.43	0.70	0.62	45	7	0.53	0.12	2.69
3di5	167	2.01	1	$C222_1$	2.38(1024)	1.74	0.79	0.69	45	4.6	0.51	0.32	2.46
3d7i	104	1.75	3	$C222_1$	2.33(708)	1.89	0.78	0.79	83	5.9	0.55	0.4	2.34
3d0f	103	1.64	2	$P12_11$	5.29(378)	4.68	0.45	0.44	29	5.5	0.54	0.16	2.25
3d3o	178	2.46	2	$P2_12_12_1$	2.91(1033)	1.92	0.82	0.73	38	6.4	0.54	0.04	NA
3d0j	140	1.53	1	$P3_221$	3.01(781)	2.27	0.84	0.74	26	4.8	0.53	0.59	2.48
3d3s	189	1.87	4	$P12_11$	3.23(996)	2.55	0.74	0.65	60	4.9	0.52	0.23	2.19
3db3	178	2.4	1	$P6_2$	2.04(543)	1.30	0.43	0.38	6	4.8	0.58	0.15	3.72
3dal	205	1.65	2	$P2_12_12_1$	2.74(947)	1.79	0.59	0.52	40	6.9	0.55	0.42	2.61
3db9	269	2.8	1	$P6_222$	2.07(336)	1.57	0.19	0.10	5	5.5	0.58	NA[l]	NA
3dee	248	2.1	1	$C121$	5.35(425)	5.32	0.33	0.22	3	4.2	0.53	0.05	3.24
3dao	264	1.8	2	$P4_12_12$	3.08(1887)	2.56	0.84	0.70	38	6.3	0.56	0.18	2.19
3dc7	232	2.12	3	$P2_12_12_1$	3.26(1212)	2.69	0.74	0.59	50	6.2	0.56	0.29	4.93
3dew	203	1.75	1	$P3_221$	3.50(1238)	3.20	0.76	0.61	18	5.5	0.53	0.14	3.27
3klu	157	2.2	1	$P6_5$	3.97(302)	3.49	0.23	0.20	9	4.7	0.54	NA	NA
3dlc	218	1.15	1	$P2_12_12_1$	2.76(1262)	2.00	0.84	0.73	42	5.7	0.54	0.61	2.2
3dl1	266	2.2	1	$P4_12_12$	3.67(775)	3.42	0.47	0.35	9	5.5	0.52	0.22	2.61
3dnx	150	1.94	1	$P4_122$	3.55(604)	2.91	0.49	0.44	18	4.8	0.56	NA	NA
3dn7	191	1.8	2	$P2_12_12_1$	2.59(1130)	2.06	0.83	0.75	38	5.9	0.56	0.16	NA
3dlm	208	1.77	1	$P2_12_12_1$	3.72(517)	3.19	0.34	0.26	23	5.4	0.57	0.33	2.16
3do8	148	1.6	2	$P12_11$	3.53(828)	3.03	0.63	0.57	32	5.2	0.53	0.44	4.96
3doa	288	2.81	1	$I4_122$	3.95(984)	3.46	0.49	0.32	22	5.6	0.54	0.05	NA
3dup	292	1.8	2	$P6_1$	3.09(1304)	2.41	0.59	0.44	22	6.2	0.52	0.42	2.8

[a]Length of target sequence

[b]Resolution of the X-Ray structure

[c]Number of monomers in the asymmetric unit of the target crystal

[d]Space group of X-Ray structure

[e]RMSD between the I-TASSER model and the PDB entry

[f]PBS between the I-TASSER model and the PDB entry

[g]TM-score between the I-TASSER model and the PDB entry

[h]GDT: GDT-TS score of the I-TASSER model and the PDB entry

[i]TM-score of the I-TASSER-MR structure and the PDB entry

[j]PBS of the I-TASSER-MR structure and the PDB entry

[k]No matched residues built in the final model for the target

Table S4. The X-Ray structures and I-TASSER model of the 62 successful targets from High-Res test set.

X-Ray Structure					I-TASSER Model			
PDBID	**D_{min}[a]**	**SG[b]**	**Len[c]**	**#Copy[d]**	**RMSD[e]**	**PBS[f]**	**TM-score[g]**	**GDT[h]**
1es5	1.4	$P2_12_12_1$	262	1	1.90(1761)	1.21	0.93	0.87
1ew4	1.4	$P3_221$	106	1	2.64(826)	1.92	0.84	0.79
1f86	1.1	$P2_12_12$	115	2	2.28(831)	1.42	0.88	0.86
1i12	1.3	$C121$	160	4	2.53(1059)	1.78	0.85	0.8
1i4u	1.15	$P2_12_12_1$	181	2	2.24(1191)	1.46	0.82	0.73
1k7c	1.12	$P2_12_12_1$	233	1	2.12(1391)	1.44	0.79	0.7
1lo7	1.5	$I222$	141	1	2.36(1056)	1.62	0.86	0.81
1mf7	1.25	$P2_12_12_1$	194	1	2.30(1411)	1.34	0.92	0.87
1nz0	1.2	$P12_11$	118	4	2.42(838)	1.67	0.87	0.83
1o7i	1.2	$P6_1$	119	2	2.51(755)	1.93	0.79	0.75
1od6	1.5	$H32$	160	2	2.72(1040)	2.12	0.78	0.7
1rg8	1.1	$C222_1$	146	3	2.60(1027)	1.2	0.87	0.85
1rw1	1.02	$C121$	114	1	2.33(839)	1.72	0.87	0.82
1tu9	1.2	$P6_122$	134	1	2.60(977)	2.03	0.83	0.75
1unq	0.98	$C121$	125	1	2.36(806)	1.6	0.69	0.66
1vd6	1.3	$P3_221$	224	1	2.26(1582)	1.67	0.92	0.81
1vdw	1.3	$P2_12_12_1$	254	2	2.57(1749)	1.96	0.88	0.75
1vkk	1.35	$P1$	154	1	2.41(1084)	1.5	0.91	0.88
1z0w	1.2	$P6_5$	207	1	2.74(1172)	2.15	0.77	0.65
1zi8	1.4	$P2_12_12_1$	236	1	2.53(1516)	1.64	0.87	0.77
2b06	1.4	$C121$	155	1	2.91(1024)	2.2	0.78	0.71
2bbr	1.2	$P2_12_12_1$	195	1	2.96(1273)	2.38	0.77	0.64
2cbz	1.5	$P3_1$	237	1	2.36(1673)	1.63	0.92	0.82
2dt8	1.48	$C121$	280	1	2.37(2026)	1.61	0.93	0.82
2ew0	1.4	$P6_1$	192	1	2.45(1077)	1.82	0.77	0.69
2hc1	1.3	$P2_12_12_1$	291	1	2.57(2104)	1.86	0.88	0.75
2i6c	1.3	$P2_12_12$	160	1	3.51(1037)	2.5	0.8	0.73
2iyv	1.35	$P12_11$	184	1	1.97(1096)	1.27	0.79	0.75
2o2x	1.5	$P12_11$	218	1	2.47(1225)	1.9	0.77	0.67
2pc1	1.28	$P1$	201	1	2.35(1187)	1.76	0.86	0.78
2qim	1.35	$P6_5$	158	1	2.47(1121)	1.97	0.85	0.76
2r0x	1.06	$C121$	158	1	1.98(1114)	1.37	0.92	0.87
2ra9	1.4	$P2_12_12_1$	150	1	2.63(857)	2.09	0.77	0.73
2rb8	1.45	$P3_221$	104	1	1.77(704)	1.06	0.93	0.94
2rkq	1.5	$P2_12_12_1$	169	1	2.24(1226)	1.53	0.89	0.83
2tnf	1.4	$P1$	156	3	2.29(998)	1.55	0.83	0.78
2v2p	1.15	$F432$	174	1	1.97(1311)	1.03	0.95	0.93
2w15	1.05	$P2_12_12_1$	202	1	2.27(1485)	1.52	0.91	0.82
2wy4	1.35	$P12_11$	140	1	2.15(1077)	1.63	0.89	0.82

2x5y	1.05	$P2_12_12_1$	173	1	2.50(1386)	1.55	0.93	0.88
2z98	1.4	$P4_22_12$	200	1	2.23(1442)	1.67	0.91	0.8
3a07	1.19	$C222_1$	118	2	2.25(846)	1.32	0.91	0.88
3ajd	1.27	$P12_11$	274	1	2.31(1828)	1.66	0.88	0.79
3bed	1.45	$C121$	142	2	2.06(802)	1.27	0.88	0.86
3bhy	1.24	$P12_11$	283	1	2.08(1975)	1.57	0.91	0.81
3bt5	1.35	$P4_1$	177	1	2.12(1082)	1.33	0.88	0.84
3bwh	1	$P2_12_12_1$	245	1	2.37(1729)	1.69	0.89	0.77
3cbz	1.38	$P2_12_12_1$	108	1	2.17(611)	1.29	0.77	0.77
3eer	1.45	$I2_12_12_1$	148	1	2.27(813)	1.8	0.74	0.66
3eln	1.42	$P4_32_12$	200	1	2.40(1250)	1.88	0.75	0.67
3frh	1.2	$P12_11$	253	1	2.47(1277)	1.72	0.68	0.59
3fsa	0.98	$P2_12_12_1$	125	1	2.50(825)	1.98	0.83	0.77
3fuc	1.45	$C121$	284	4	2.52(1654)	1.88	0.83	0.69
3gfa	1.35	$C121$	198	2	2.77(1175)	1.88	0.81	0.73
3gg7	1.5	$P4_1$	254	1	2.60(1767)	1.84	0.9	0.78
3gr3	1.45	$P2_12_12_1$	230	2	2.21(1554)	1.51	0.93	0.85
3h79	1.5	$P2_12_12_1$	127	1	2.44(911)	1.72	0.89	0.85
3hm4	1.3	$P2_12_12_1$	156	2	2.46(943)	1.93	0.88	0.8
3l8w	1	$I222$	296	1	2.59(2034)	1.86	0.87	0.73
3m1x	1.2	$H32$	148	1	2.13(887)	1.42	0.91	0.89
3mmh	1.25	$P1$	167	2	2.54(1124)	1.96	0.81	0.72
2qjz	1.25	$P12_11$	123	2	3.40(832)	2.85	0.69	0.65

[a]Resolution of the X-ray structure.

[b]Space group of the entry

[c]Length of the PDB structure (including unstructured residues)

[d]Number of monomers in the asymmetric unit of the target

[e]RMSD of the initial I-TASSER model and the PDB entry

[f]PBS of the initial I-TASSER model and the PDB entry

[g]TM-score of the initial I-TASSER model

[h]GDT-TS score of the initial I-TASSER model

Table S5. Summary of the first successful search models and the statistics of the 62 successful I-TASSER-MR solutions in test set-II (extension from Table S4).

PDB structure		Search model after truncation[m]					Phaser		I-TASSER-MR model			
ID	Len[a]	Trun[b]	RMS[c]	PBS[d]	TM[e]	GT[f]	LLG[g]	TFZ[h]	R_{free}[i]	#built[j]	TM[k]	PBS[l]
1es5	262	0	1.90(1761)	1.21	0.93	0.87	168	12.2	0.25	247	0.95	0.09
1ew4	106	0	2.64(826)	1.92	0.84	0.79	36	6.5	0.26	96	0.9	0.13
1f86	113	0.02	2.26(828)	1.42	0.86	0.84	216	7.6	0.31	97/95	0.82/0.78	0.13/0.43
1i12	160	0	2.53(1059)	1.78	0.85	0.8	167	10.7	0.28	147/125/138/142	0.91/0.81/0.89/0.91	0.26 /0.27 /0.26 /0.26
1i4u	181	0	2.24(1191)	1.46	0.82	0.73	82	9.9	0.24	165/165	0.91/0.91	0.10 /0.17
1k7c	229	0.02	2.25(1395)	1.44	0.79	0.71	47	8	0.25	186	0.8	0.06
1lo7	132	0.06	2.12(1011)	1.52	0.84	0.79	30	6.3	0.27	122	0.77	0.15
1mf7	194	0	2.30(1411)	1.34	0.92	0.87	94	9.9	0.3	165	0.83	0.12
1nz0	114	0.03	2.36(841)	1.72	0.86	0.82	352	9.1	0.26	100/98/98/99	0.93/0.89/0.89/0.9	0.10/0.62/0.57
1o7i	119	0	2.51(755)	1.93	0.79	0.75	22	6.1	0.31	102/111	0.84/0.94	0.37 /0.37
1od6	159	0.01	2.72(1035)	2.1	0.78	0.7	28	6.9	0.22	0.059	0.92	0.1
1rg8	126	0.14	2.36(984)	1.15	0.83	0.82	62	6	0.31	121/117/28	0.71/0.77/0.20	0.22 /0.12 /0.19
1rw1	114	0	2.33(839)	1.72	0.87	0.82	39	6	0.25	108	0.93	0.45
1tu9	102	0.24	2.51(816)	1.82	0.69	0.64	24	6.2	0.28	129	0.98	0.08
1unq	98	0.22	1.92(559)	1.5	0.48	0.48	22	3.2	0.35	76	0.45	0.14
1vd6	214	0.04	2.37(1535)	1.67	0.89	0.79	46	8.4	0.3	196	0.89	0.18
1vdw	254	0	2.57(1749)	1.96	0.88	0.75	92	10.6	0.26	186/161	0.75/0.64	0.08 /0.68
1vkk	154	0	2.41(1084)	1.5	0.91	0.88	55	0	0.24	130	0.95	0.08
1z0w	187	0.1	2.74(1172)	2.15	0.75	0.65	29	6.5	0.27	157	0.66	0.09
1zi8	236	0	2.53(1516)	1.64	0.87	0.77	32	7.2	0.21	217	0.93	0.06
2b06	111	0.28	2.39(841)	1.69	0.66	0.62	16	4.3	0.42	47	0.31	0.28
2bbr	161	0.17	2.81(1155)	2.23	0.7	0.59	21	6.4	0.28	152	0.7	0.12
2cbz	237	0	2.36(1673)	1.63	0.92	0.82	103	10.6	0.24	218	0.95	0.05
2dt8	280	0	2.37(2026)	1.61	0.93	0.82	73	7	0.33	276	0.96	0.2
2ew0	164	0.15	2.27(1014)	1.69	0.73	0.67	13	6	0.21	173	0.96	0.12
2hc1	231	0.21	2.56(1722)	1.67	0.74	0.65	77	9.3	0.31	267	0.53	0.1
2i6c	122	0.24	3.02(816)	2	0.68	0.63	29	6	0.25	151	0.98	0.18
2iyv	176	0.04	2.02(1108)	1.29	0.79	0.75	82	6	0.26	154	0.86	0.1
2o2x	212	0.03	2.47(1225)	1.9	0.77	0.67	78	7	0.31	142	0.66	0.67
2pc1	201	0	2.35(1187)	1.76	0.86	0.78	27	0	0.24	147	0.87	0.06
2qim	158	0	2.47(1121)	1.97	0.85	0.76	23	5.9	0.26	135	0.86	0.08
2qjz[n]	118	0.04	3.40(832)	2.85	0.69	0.65	120	17.3	0.53	54	0.39	2.18
2r0x	154	0.03	1.98(1114)	1.37	0.92	0.88	123	7.8	0.32	91	0.59	0.2
2ra9	96	0.36	2.45(723)	1.83	0.65	0.62	32	4.7	0.21	121	0.96	0.09
2rb8	104	0	1.77(704)	1.06	0.93	0.94	50	8.9	0.32	91	0.97	0.24
2rkq	169	0	2.24(1226)	1.53	0.89	0.83	24	5.7	0.23	167	0.98	0.12
2tnf	156	0	2.29(998)	1.55	0.83	0.78	71	6.7	0.28	138/142/127	0.83/0.82/0.83	0.40 /0.47 /0.30
2v2p	174	0	1.97(1311)	1.03	0.95	0.93	151	15	0.28	169	0.97	0.06
2w15	178	0.12	1.97(1369)	1.39	0.83	0.77	49	7.3	0.31	115	0.57	0.24

2wy4	132	0.06	2.14(1028)	1.63	0.85	0.8	24	4.5	0.32	136	0.98	0.1
2x5y	173	0	2.50(1386)	1.55	0.93	0.88	106	10.9	0.31	167	0.94	0.27
2z98	200	0	2.23(1442)	1.67	0.91	0.8	69	10	0.27	187	0.96	0.1
3a07	100	0.15	1.82(759)	1.23	0.8	0.78	64	7.2	0.27	99/99	0.85/0.85	0.07/0.07
3ajd	274	0	2.31(1828)	1.66	0.88	0.79	53	6.5	0.24	236	0.88	0.06
3bed	142	0	2.06(802)	1.27	0.88	0.86	106	9.6	0.27	123/126	0.92/0.96	0.19 /0.19
3bhy	281	0.01	2.08(1975)	1.57	0.92	0.82	64	8	0.31	250	0.87	0.26
3bt5	151	0.15	2.00(1062)	1.31	0.87	0.83	64	6.7	0.24	146	0.96	0.1
3bwh	243	0.01	2.34(1722)	1.67	0.88	0.77	40	8.3	0.23	232	0.95	0.07
3cbz	103	0.05	2.17(611)	1.29	0.77	0.75	21	5.3	0.26	92	0.84	0.12
3eer	122	0.18	2.32(734)	1.79	0.65	0.61	12	5	0.31	137	0.99	0.09
3eln	164	0.18	2.25(1177)	1.69	0.71	0.64	47	6.7	0.28	164	0.88	0.07
3frh	211	0.17	2.47(1277)	1.72	0.67	0.59	29	6.9	0.24	218	0.9	0.06
3fsa	120	0.04	2.41(787)	1.98	0.79	0.74	20	5.5	0.33	66	0.37	0.11
3fuc	216	0.24	2.24(1514)	1.64	0.71	0.63	156	5.5	0.23	269/270/268	0.98/0.98/0.98	0.16 /0.16 /0.17
3gfa	198	0	2.77(1175)	1.88	0.81	0.73	54	6.8	0.23	168/181	0.88/0.95	0.13 /0.22
3gg7	254	0	2.60(1767)	1.84	0.9	0.78	27	6.6	0.27	214	0.88	0.07
3gr3	162	0.3	2.00(1121)	1.25	0.69	0.65	252	12.2	0.25	204/197	0.93/0.9	0.1/0.21
3h79	105	0.17	2.37(861)	1.61	0.83	0.79	34	5.4	0.22	111	0.97	0.07
3hm4	146	0.06	2.46(905)	1.83	0.83	0.77	70	5.4	0.26	114/119	0.77/0.8	0.35/0.35
3l8w	292	0.01	2.61(2037)	1.86	0.86	0.73	55	10	0.27	284	0.95	0.13
3m1x	130	0.12	2.13(887)	1.42	0.91	0.89	69	6.8	0.31	112	0.87	0.19
3mmh	161	0.04	2.54(1124)	1.96	0.81	0.73	32	6.5	0.23	150/154	0.89/0.91	0.11 /0.11

[a]Length of the first successful search model

[b]Fraction of truncated residues in the first successful search model

[c]RMSD of the first successful search model to the PDB entry

[d]PBS of first successful search model to the PDB entry

[e]TM-score of first successful search model

[f]GDT-TS score of first successful search model

[g]LLG of Phaser solution relative to random

[h]TFZ score of Phaser

[i]R_{free} for the refined I-TASSER-MR structure

[j]Number of residues in the model constructed by I-TASSER-MR. When multiple subunits exist in the asymmetric unit of the target, a number is given for each chain

[k]TM-score of the I-TASSER-MR structure and the PDB entry

[l]PBS of the I-TASSER-MR structure and the PDB entry

[m]The first search model after editing which was successful in MR

[n]The targets which has a clear MR solution but failed to be rebuilt

Table S6. Statistics of the 38 unsuccessful targets from the High-Res test set.

X-Ray Structure					I-TASSER Model				Phaser		I-TASSER-MR structure		
PDBID	**L[a]**	**Res[b]**	**#Cp[c]**	**SG[d]**	**RMS[e]**	**PBS[f]**	**TMs[g]**	**GDT[h]**	**LLG**	**TFZ**	**Rfree**	**TMs[i]**	**PBS[j]**
1c7k	132	1	1	$P2_12_12_1$	2.97(876)	2.14	0.77	0.7	19	5.1	0.55	0.21	2.15
1i1j	108	1.39	2	$P2_12_12_1$	3.04(541)	2.24	0.54	0.52	39	6.6	0.57	0.51	2.27
1i8o	114	1.15	1	$P3_221$	2.27(585)	1.67	0.63	0.59	20	5.4	0.56	0.39	2.75
1j77	209	1.5	1	$P4_32_12$	2.66(1287)	2.09	0.77	0.64	20	5.4	0.56	0.22	3.87
1jhg	101	1.3	1	$P2_122_1$	2.87(618)	2.38	0.71	0.69	17	4.9	0.54	0.16	1.77
1kq6	141	1.18	1	$I4_1$	2.99(897)	2.26	0.75	0.7	15	4.7	0.5	0.21	1.7
1ls1	295	1.1	1	$C121$	3.49(1926)	2.92	0.8	0.59	11	4.5	0.52	0.48	2.19
1lv7	257	1.5	1	$P4_12_12$	3.51(1383)	3.1	0.69	0.48	10	5.6	0.58	0.2	3.63
1mg4	113	1.5	1	$C121$	2.78(673)	2.05	0.76	0.72	16	4.1	0.51	0.44	2.15
1mwq	101	0.99	2	$P2_12_12_1$	2.67(660)	2.11	0.73	0.7	29	5.4	0.57	0.58	2.28
1nki	135	0.95	2	$P2_12_12_1$	2.80(959)	1.95	0.83	0.77	38	5.6	0.56	0.44	2.3
1nnx	109	1.45	1	$C222_1$	3.25(642)	2.31	0.73	0.72	19	5.1	0.53	0.51	1.85
1qwy	291	1.3	1	$P12_11$	2.05(836)	1.18	0.47	0.43	15	4.8	0.52	0.22	4.53
1tp6	128	1.5	1	$C121$	2.89(764)	2.3	0.71	0.63	19	4.1	0.51	0.26	2.56
1tt8	164	1	1	$P1$	3.05(1027)	2.75	0.7	0.58	9	0	0.54	0.61	2.79
1w66	232	1.08	1	$P2_12_12_1$	2.83(1326)	2.19	0.8	0.66	21	5	0.55	0.56	2.1
1x8q	184	0.85	1	$C121$	3.10(1040)	2.57	0.7	0.54	21	3.1	0.53	0.2	2.64
1xmt	103	1.15	1	$P12_11$	2.53(670)	1.97	0.77	0.76	20	5.4	0.52	0.22	2.5
1y93	159	1.03	1	$C121$	2.63(960)	2.11	0.73	0.64	10	4.7	0.51	0.3	1.74
2b82	211	1.25	2	$C121$	3.55(953)	3.09	0.56	0.41	42	5.9	0.53	0.35	2.82
2fcj	119	1.3	3	$P2_12_12_1$	3.33(726)	2.75	0.68	0.65	52	6.3	0.55	0.61	2.6
2imj	166	1.5	4	$P12_11$	3.02(954)	2.16	0.67	0.6	51	6.9	0.54	0.44	5.01
2ivy	101	1.4	1	$P6_2$	2.67(570)	1.55	0.71	0.72	17	5.2	0.53	0.15	2.87
2jfr	234	0.83	1	$P2_12_12$	2.48(1428)	1.94	0.79	0.66	19	5.4	0.58	0.6	2.11
2o1q	145	1.5	2	$P4_12_12$	2.73(912)	1.88	0.83	0.76	27	5.4	0.53	0.37	4.97
2prx	160	1.5	2	$P3_1$	2.70(767)	1.92	0.84	0.79	36	5.4	0.45	0.26	NA
2qt1	207	1.32	1	$C222_1$	2.92(1072)	2.12	0.74	0.63	19	5.1	0.53	0.39	3.01
2vv6	119	1.5	4	$P1$	2.76(799)	2.14	0.81	0.83	36	5.1	0.52	0.57	1.35
3a2z	197	1.5	1	$P6_422$	3.22(748)	2.52	0.46	0.38	17	6.1	0.58	0.44	2.35
3ach	203	1.4	1	$P2_12_12_1$	3.31(1073)	2.76	0.68	0.53	20	5	0.58	0.44	3.68
3b79	129	1.37	1	$P4_32_12$	2.70(879)	1.99	0.83	0.76	26	5.4	0.53	0.25	4.06
3buu	229	1.2	2	$P12_11$	3.40(1472)	2.97	0.76	0.59	34	6.2	0.52	0.11	2.31
3fci	223	1.27	1	$P2_12_12_1$	3.14(1516)	2.67	0.81	0.61	28	6.4	0.57	0.32	2.53
3fk8	133	1.3	1	$P2_12_12_1$	2.58(716)	2.06	0.72	0.65	18	5.7	0.54	0.48	2.07
3fss	237	1.43	1	$C121$	3.26(1379)	2.49	0.75	0.59	12	4.6	0.51	0.48	3.88
3gnl	244	1.5	2	$P2_12_12_1$	3.01(886)	2.53	0.46	0.36	20	5.8	0.55	0.21	3.05
3hvi	221	1.2	1	$P2_12_12_1$	2.64(1259)	2.05	0.68	0.58	30	5.5	0.56	0.49	2.04
3n08	153	1.25	2	$P1$	2.91(890)	2.45	0.68	0.6	34	5	0.53	0.32	3.29

[b]Resolution of the X-Ray structure

[c]Number of monomers in the asymmetric unit of the target crystal

[d]Space group of X-Ray structure
[e]RMSD between the I-TASSER model and the PDB entry
[f]PBS between the I-TASSER model and the PDB entry
[g]TM-score between the I-TASSER model and the PDB entry
[h]GDT: GDT-TS score of the I-TASSER model and the PDB entry
[i]TM-score of the I-TASSER-MR structure and the PDB entry
[j]PBS of the I-TASSER-MR structure and the PDB entry

Table S7. MR results with the best LOMETS templates modified by CHAINSAW and Sculptor on the CASP8 test set.

PDBID	Search Model					Phaser		Phenix.autobuild model		
	Tem[a]	L[b]	RMS[c]	PBS[d]	TM[e]	LLG	TFZ	R_{free}	#built[f]	TMS[g]
2vsv	1whdA	100	1.77(471)	1.47	0.69	43	5	0.53	63	0.52
2vsw	1whbA	131	2.24(676)	1.77	0.75	52	5.3	0.52	21	0.06
2vwr	2iwqA	91	1.97(508)	1.36	0.78	40	5.2	0.28	66	0.69
3cyn	2rm6A	162	2.29(844)	1.79	0.72	63	6.2	0.51	36	0.1
3czx	1jwqA	172	2.09(951)	1.86	0.79	299	25.2	0.55	30	0.15
3d0f	2rcnA	61	1.92(302)	1.47	0.4	34	6.6	0.55	11	0.05
3d0j	1v70A	102	2.26(518)	1.46	0.51	41	5.9	0.24	98	0.71
3d1l	2i76A	238	3.57(1178)	3.27	0.63	58	4.9	53	34	0.08
3d1p	2hhgA	121	2.09(618)	1.44	0.74	19	4.1	0.55	47	0.09
3d3o	1tf1A	176	2.18(869)	1.88	0.79	50	5.8	0.52	37	0.11
3d3s	1mk4A	157	2.17(737)	1.83	0.71	61	5.9	0.52	63	0.26
3d4e	3c7uB	150	3.25(719)	3.09	0.56	38	2.6	0.52	36	0.06
3d4o	1pjcA	267	3.73(1246)	3.62	0.61	138	4.5	0.5	36	0.07
3d5p	2prvA	127	2.70(612)	2.44	0.61	45	5.8	0.55	14	0.06
3d6j	2nyvA	215	1.87(1170)	1.56	0.86	60	10.1	0.33	212	0.95
3d6w	3bs1A	97	2.25(581)	1.66	0.72	40	5.2	0.5	11	0.05
3d7i	1p8cC	103	2.77(525)	2.67	0.71	49	4.5	0.54	62	0.46
3d89	2qpzA	101	1.65(558)	1.16	0.63	88	10.5	0.34	94	0.69
3d8h	2a6pA	192	2.68(1072)	2.08	0.72	122	9.4	0.33	183	0.78
3d8p	1yx0A	149	2.72(762)	2.28	0.59	51	5.2	0.55	28	0.06
3da2	1kopA	219	1.46(1338)	0.89	0.77	761	22	0.25	230	0.88
3dai	1eqfA	122	1.60(698)	1.08	0.77	142	8.8	0.26	122	0.94
3dal	2jv0A	161	2.63(691)	2.04	0.54	46	6.2	0.58	114	0.49
3dao	1rkqA	261	3.08(1381)	2.88	0.79	43	6.4	0.54	53	0.08
3db0	2i02A	131	2.07(596)	1.53	0.74	46	4.9	0.54	40	0.29
3db3	2r17A	160	4.63(226)	4.46	0.16	26	4	0.58	NA[h]	NA
3db5	2jv0A	146	2.89(678)	2.14	0.71	42	6.2	0.58	13	0.06
3db9	1us4A	251	3.69(285)	3.43	0.15	13	3.9	0.57	NA	NA
3dc7	1yzfA	188	2.56(929)	1.91	0.66	57	5.7	0.53	31	0.05
3dcp	2yxoB	241	1.93(1461)	1.37	0.8	783	29.9	0.5	54	0.11
3dcy	1yjxA	239	2.24(1053)	1.79	0.58	23	6.3	0.53	46	0.16
3dee	2qenA	241	4.56(380)	4.39	0.25	43	3.1	0.5	18	0.05
3dew	1pb6A	190	3.22(922)	3.04	0.72	18	4.4	0.58	38	0.08
3df8	2fswB	92	1.78(477)	1.06	0.65	61	5.4	0.25	100	0.92
3dfa	1tkiA	265	2.53(1450)	2.12	0.81	73	6.9	0.32	228	0.86
3dh1	2nx8A	166	1.63(902)	1.22	0.85	102	12.6	0.44	88/111	0.54/0.67
3dhn	1hdoA	201	2.09(1062)	1.73	0.77	59	8.8	0.3	193	0.76
3di5	2qe9A	155	1.85(525)	1.74	0.65	43	4.7	0.48	54	0.27

3djb	2pq7A	160	1.90(802)	1.68	0.67	70	9.2	0.51	22	0.08
3dka	2qe9A	147	2.02(507)	1.99	0.65	71	5.1	0.54	68	0.12
3dkp	3berA	214	2.02(1148)	1.62	0.75	65	5	0.32	170	0.71
3dkz	1q4sA	133	1.72(674)	1.25	0.86	108	12.1	0.34	110/103	0.78/0.72
3dl1	1j7nA	207	3.08(631)	2.8	0.44	23	4.3	0.54	NA	NA
3dlc	3dh0B	187	2.27(939)	1.84	0.66	28	4.7	0.53	75	0.22
3dlm	2qqrA	92	1.83(245)	1.51	0.13	20	5	0.55	11	0.03
3dm3	2k50A	105	1.94(555)	1.67	0.75	36	5.5	0.55	10	0.06
3dmb	2i02A	134	3.16(686)	2.54	0.67	54	7	0.52	8	0.03
3dmc	1tuhA	126	2.33(676)	2.08	0.73	43	5.2	0.52	60	0.3
3dmn	1uaaA	166	2.84(432)	2.19	0.42	22	4.2	0.58	NA	NA
3dn7	4ev0A	181	2.57(707)	2.13	0.69	35	4.9	0.57	10	0.05
3dnh	2arzA	227	2.57(1223)	2.41	0.78	80	6.3	0.28	188/199	0.8/0.83
3dnx	2eo0A	120	2.87(406)	2.07	0.4	21	5.5	0.53	44	0.11
3do8	1cozA	124	2.47(592)	1.87	0.6	37	5	0.54	23	0.06
3doa	1pieA	275	5.46(392)	5.38	0.2	21	4.1	0.53	29	0.07
3dou	2plwA	172	1.88(1066)	1.43	0.88	117	7.9	0.22	162	0.93
3dr5	2avdA	208	2.15(1128)	1.83	0.85	31	7.3	0.41	129	0.61
3dup	1q27A	171	4.10(650)	3.69	0.35	194	5.2	0.51	42	0.09
3e03	4dmlA	240	1.86(1198)	1.46	0.75	228	5.7	0.5	120	0.42
3gwl	2hj3A	100	1.60(614)	1.27	0.85	154	11.7	0.3	90/86	0.88/0.84
3klu	3dfdA	135	2.78(212)	2.71	0.18	19	4.7	0.54	19	0.07
3klw	2iheA	100	2.44(545)	1.85	0.77	64	10.3	0.27	95/80	0.97/0.67

[a]PDB id of the template

[b]Length of the LOMETS models used for search

[c]RMSD of the search model

[d]PBS of the search model

[e]TM-score of the search model

[f]Number of residues in the model constructed by Phenix.autobuild. When multiple subunits exist in the asymmetric unit of the target, a number is given for each chain

[g]TM-score of the final model

[h]'NA' indicates that there are no match residues built in the final model for the target

Table S8. MR results with the best LOMETS templates modified by CHAINSAW and Sculptor on the High-Res test set.

PDBID	Search Model					Phaser		Phenix.autobuild model		
	Tem[a]	L[b]	RMS[c]	PBS[d]	TM[e]	LLG	TFZ	R_{free}	#built[f]	TMS[g]
1c7k	1slmA	129	2.43(660)	2.08	0.7	51	5	0.53	28	0.1
1es5	2bcfA	236	1.58(1308)	1.03	0.81	246	11.2	0.25	246	0.95
1ew4	1ly7A	106	2.39(620)	1.91	0.77	35	6	0.26	98	0.92
1f86	3qvaA	102	1.27(586)	0.88	0.82	508	17.3	0.29	74/90	0.64/0.78
1i12	2dxqA	141	2.01(832)	1.61	0.74	109	6.1	0.29	139/106/89/95	0.9/0.69/0.58/0.61
1i1j	2i0nA	80	2.23(366)	1.61	0.46	39	5.2	0.55	39	0.13
1i4u	2hzqA	162	1.73(915)	1.2	0.75	209	9.9	0.25	159/163	0.88/0.9
1i8o	1w2lA	91	1.89(403)	1.38	0.58	21	5.7	0.55	64	0.23
1j77	1iw1A	189	2.28(976)	1.81	0.75	25	5.5	0.55	41	0.19
1jhg	3g1cA	97	2.37(515)	1.93	0.7	16	4.6	0.53	NA[h]	NA
1k7c	2o14A	168	1.84(876)	1.41	0.63	86	9.5	0.23	194	0.83
1kq6	2l73A	138	3.09(722)	2.46	0.69	13	4.2	0.51	18	0.12
1lo7	1s5uE	132	1.74(777)	1.2	0.82	278	7.1	0.25	122	0.87
1ls1	2px0A	256	2.89(1399)	2.82	0.71	8	3.4	0.52	107	0.25
1lv7	1d2nA	232	3.16(1116)	2.79	0.59	16	5.7	0.57	105	0.26
1mf7	1v7pC	185	1.50(1094)	1.07	0.87	185	10.1	0.27	162	0.83
1mg4	2dnfA	107	2.09(513)	1.76	0.72	19	4.1	0.53	22	0.17
1mwq	1s7iA	98	2.47(489)	1.81	0.67	38	5.4	0.55	39	0.32
1nki	1r9cA	118	1.87(723)	1.37	0.75	40	5.7	0.55	13	0.06
1nnx	2xgtA	83	3.22(608)	2.26	0.7	21	6.3	0.33	62	0.51
1nz0	1a6fA	110	2.01(674)	1.6	0.83	407	8.4	0.23	98/99/99/99	0.89/0.92/0.9/0.9
1o7i	2k5vA	96	1.98(534)	1.54	0.65	38	6.8	0.3	110/107	0.92/0.73
1od6	1f9aA	148	2.08(779)	1.76	0.68	74	7	0.5	37	0.06
1qwy	2gu1A	267	1.54(683)	1.02	0.44	23	3.5	0.52	67	0.2
1rg8	2fdbM	142	1.65(779)	1.01	0.84	103	14.1	0.27	138/130	0.95/0.86
1rw1	3gkxB	113	2.02(628)	1.5	0.81	35	4.8	0.25	85	0.69
1tp6	3gzrA	122	2.30(616)	1.97	0.63	17	3.5	0.53	16	6.2
1tt8	2nwiA	143	2.66(757)	2.25	0.66	13	0	0.52	45	0.17
1tu9	3s1iA	125	2.03(743)	1.65	0.81	70	5.2	0.58	71	0.41
1unq	1plsA	113	2.26(618)	1.73	0.63	30	3.9	0.53	6	0.05
1vd6	3no3A	215	2.15(1199)	1.77	0.84	34	6.7	0.32	175	0.55
1vdw	2bjiA	183	1.89(1047)	1.45	0.65	99	10	0.29	186/194	0.72/0.68
1vkk	1cnuA	131	1.63(792)	1.32	0.86	131	0	0.23	132	0.96
1w66	2artA	216	2.38(1054)	1.97	0.74	20	4.6	0.55	36	0.06
1x8q	1gkaB	161	3.00(815)	2.66	0.59	21	4.2	0.53	45	0.14
1xmt	1r57A	99	2.22(509)	1.86	0.66	21	3.1	0.51	11	0.09
1y93	1aklA	149	1.93(727)	1.19	0.68	18	4.1	0.53	13	0.04
1z0w	2x36A	183	2.33(958)	1.81	0.74	49	5.3	0.25	156	0.77

1zi8	3f67A	156	1.85(764)	1.45	0.58	36	7.1	0.21	230	0.99
2b06	1iryA	147	2.80(801)	1.96	0.71	14	3.3	0.52	69	0.39
2b82	2i33A	195	2.77(619)	2.48	0.49	39	5.9	0.53	19	0.05
2bbr	3cl3A	168	2.48(961)	2.13	0.71	21	5.3	0.56	37	0.09
2cbz	1mv5A	226	2.76(1246)	2.38	0.79	82	6.2	0.48	93	0.36
2dt8	1pzxB	278	2.16(1590)	1.58	0.9	91	7.8	0.27	235	0.84
2ew0	2gs5A	173	2.17(835)	1.52	0.75	21	5.4	0.53	19	0.11
2fcj	2au3A	99	2.78(536)	2.46	0.58	87	6.6	0.58	9	0.05
2hc1	1yguB	258	1.65(1468)	1.25	0.79	91	9.6	0.3	121	0.42
2i6c	2cnmA	147	2.76(785)	1.89	0.76	43	5.8	0.24	150	0.97
2imj	2geyA	89	2.09(345)	1.94	0.35	85	5.6	0.54	9	0.05
2ivy	3oq2A	34	1.65(254)	1.28	0.17	22	4.4	0.52	13	0.07
2iyv	2pt5B	165	1.94(864)	1.62	0.75	38	4.5	0.52	92	0.4
2jfr	3rnrA	167	2.26(617)	1.98	0.44	53	4.4	0.53	54	0.17
2o1q	3ebrA	133	2.06(704)	1.48	0.79	104	4.8	0.27	118/119	0.82/0.83
2o2x	3l8hA	173	2.21(868)	1.51	0.64	30	3.9	0.33	82	0.4
2pc1	2fiaB	151	1.60(800)	1.29	0.76	41	0	0.22	143	0.85
2prx	2ov9C	136	2.29(591)	1.74	0.79	56	6.4	0.42	17	0.11
2qim	2flhD	150	2.80(824)	1.8	0.78	29	6.1	0.27	136	0.86
2qjz	1wypA	119	3.02(547)	2.82	0.61	35	6.4	0.54	22	0.14
2qt1	3asyA	186	2.38(829)	1.78	0.69	22	4.7	0.52	13	0.05
2r0x	1yoaA	156	2.12(795)	1.59	0.83	89	4.3	0.38	40	0.26
2ra9	2re3B	146	2.14(643)	1.65	0.71	20	4	0.54	51	0.36
2rb8	1fnfA	90	1.04(561)	0.66	0.93	433	18.5	0.32	88	0.94
2rkq	3ep1A	157	1.59(874)	1.16	0.82	61	8.7	0.22	161	0.95
2tnf	3ugnA	139	1.97(789)	1.4	0.78	86	8.4	0.31	94/82/93	0.59/0.39/0.38
2v2p	1z6oX	174	1.40(978)	0.87	0.92	598	10.2	0.27	168	0.99
2vv6	1s67L	107	1.78(633)	1.47	0.84	46	5.8	0.53	44	0.36
2w15	3g5cA	196	1.68(1177)	1.26	0.89	85	8.3	0.31	140	0.7
2wy4	3s1iA	129	1.87(807)	1.56	0.81	59	4.5	0.29	132	0.95
2x5y	3hkvA	161	1.66(951)	1.12	0.84	160	13.3	0.27	164	0.94
2z98	3p0rA	199	2.11(1147)	1.68	0.86	75	7.2	0.25	188	0.97
3a07	1ce7B	116	1.94(660)	1.16	0.86	66	7.8	0.24	111	0.93
3a2z	2k3aA	151	2.31(492)	1.6	0.33	17	3.7	0.58	NA	NA
3ach	1j83A	167	3.08(845)	2.76	0.42	11	5.8	0.56	36	0.1
3ajd	2b9eA	253	1.79(1375)	1.24	0.84	90	7.2	0.23	229	0.9
3b79	3k8uA	125	2.08(666)	1.65	0.8	25	4.2	0.26	83	0.68
3bed	3lfhA	125	1.66(651)	1.26	0.83	187	12.4	0.23	105/118	0.85/0.97
3bhy	2vgpB	267	2.18(1542)	1.81	0.82	39	5.3	0.3	164	0.61
3bt5	2qf9A	147	2.84(681)	2.29	0.62	35	2.5	0.52	26	0.07
3buu	3bk5A	220	3.00(1192)	2.61	0.73	49	5.4	0.54	62	0.27
3bwh	1rl0A	214	2.35(1209)	1.73	0.73	20	5.2	0.56	59	0.22
3cbz	1u3bA	102	1.94(484)	1.36	0.72	22	4.8	0.56	17	0.15

3eer	1nyeD	145	2.23(663)	1.87	0.7	15	4.2	0.56	33	0.19
3eln	3ussA	180	1.88(958)	1.38	0.72	76	9.6	0.27	168	0.9
3fci	2owqB	201	2.50(1079)	2.19	0.72	19	5.5	0.55	40	0.1
3fk8	1uc7A	123	2.52(602)	2.17	0.64	19	5.4	0.53	33	0.11
3frh	3lcuA	163	1.74(962)	1.23	0.6	116	9.2	0.27	194	0.8
3fsa	2aanA	117	2.04(685)	1.66	0.78	33	5.9	0.32	54	0.44
3fss	2gcjC	212	2.47(1050)	2.06	0.68	23	4.3	0.52	28	0.06
3fuc	1k27A	247	1.93(1282)	1.38	0.77	213	9.3	0.23	244/268	0.89/0.98
3gfa	1noxA	196	1.82(872)	1.28	0.65	230	8.7	0.23	182/181	0.96/0.95
3gg7	1yixA	251	1.82(1381)	1.52	0.85	53	7	0.27	189	0.78
3gnl	3bkx_	237	2.88(769)	2.45	0.5	11	4.8	0.55	210	0.43
3gr3	2wzvA	216	1.77(1221)	1.25	0.86	377	8.4	0.26	192/187	0.88/0.95
3h79	3uemA	119	1.54(656)	1.04	0.83	102	9.8	0.23	112	0.97
3hm4	1xkoB	154	2.25(778)	1.87	0.84	20	6	0.53	88	0.53
3hvi	3r3hA	210	2.47(1015)	2.06	0.64	18	5.1	0.56	42	0.09
3l8w	1j2gA	282	1.81(1612)	1.31	0.85	669	10.9	0.25	257	0.54
3m1x	3lmeA	124	1.79(715)	1.23	0.89	97	8.2	0.33	54	0.43
3mmh	3trcA	111	2.20(519)	1.64	0.54	74	4.4	0.52	56	0.31
3n08	2jyzA	137	3.62(679)	3.32	0.52	28	4.5	0.54	7	0.04

[a]PDB id of the template

[b]Length of the LOMETS models used for search

[c]RMSD of the search model

[d]PBS of the search model

[e]TM-score of the search model

[f]Number of residues in the model constructed by Phenix.autobuild. When multiple subunits exist in the asymmetric unit of the target, a number is given for each chain

[g]TM-score of the final model

[h]'NA' indicates that there are no match residues built in the final model for the target

Table S9. Statistics of I-TASSER-MR on the 14 PSI targets.

Target	X-Ray Structure					I-TASSER models			Phaser		I-TASSER-MR structure			
	L[a]	Res[b]	Cp[c]	SG[d]	Meth[e]	PBS[f]	TM[g]	GDT[h]	LLG	TFZ	R_{free}[i]	#built[j]	TM[k]	PBS[l]
4p47	345	1.3	1	$P2_12_12_1$	SAD	2.24	0.86	0.72	40	7.7	0.26	274	0.86	0.06
4ps6	130	1.25	1	$P12_11$	SAD	1.41	0.92	0.88	76	5.5	0.27	101	0.79	0.08
4pux	160	1.43	1	$C222$	MAD	1.48	0.83	0.78	28	5.1	0.26	120	0.77	0.13
4pw0	283	1.48	1	$P6_2$	SAD	1.95	0.81	0.67	45	9.4	0.22	267	0.99	0.06
4pxy	250	1.5	2	$H3$	SAD	1.02	0.98	0.96	528	18.6	0.23	231/235	0.96/0.96	0.07/0.06
4pz0	324	1.25	1	$P12_11$	SAD	1.36	0.96	0.88	158	9.8	0.21	305	0.96	0.16
4pqx	217	2.39	4	$P2_12_12_2$	MAD	1.93	0.85	0.74	109	9.2	0.51	64	0.16	NA[m]
4p7c	322	1.85	2	$P2_12_12_1$	SAD	2.33	0.51	0.38	18	6.2	0.46	138	0.22	0.36
4p56	343	1.9	3	$P12_11$	SAD	2.58	0.88	0.67	50	6.2	0.53	48	0.3	4.34
4pup	131	2.75	3	$C121$	SAD	2.68	0.49	0.45	39	6.4	0.53	12	0.06	NA[m]
4pyr	305	1.45	1	$P12_11$	SAD	3.55	0.67	0.52	13	3.9	0.52	85	0.09	3.81
4jqs	250	2.3	3	$C222_1$	MAD	2.47	0.78	0.61	63	6.5	0.55	74	0.19	2.93
4pwu	98	2.45	4	$C121$	MAD	2.70	0.59	0.62	14	5.1	0.5	15	0.07	NA[m]
4pw1	252	2.1	2	$P4_12_12$	MAD	3.64	0.26	0.17	34	5.4	0.54	40	0.12	5.35

[a]Length of target sequence

[b]Resolution of the X-Ray structure

[c]Number of subunits in the asymmetric unit of the target crystal

[d]Space group of X-Ray structure

[e]Phasing method used for solving the structure. 'SAD' refers to single-wavelength anomalous diffraction and 'MAD' refers to multi-wavelength anomalous diffraction.

[f]PBS of the I-TASSER model

[g]TM-score of the I-TASSER model

[h]GDT-TS score of the I-TASSER model

[i]R_{free} of the final I-TASSER-MR structure

[j]Number of residues in the model constructed by Phenix.autobuild. When multiple subunits exist in the asymmetric unit of the target, a number is given for each chain

[k]TM-score of the final I-TASSER-MR structure

[l]PBS of the final I-TASSER-MR structure

[m]'NA' indicates that there are no match residues built in the final model for the target