

Increasing the accuracy of protein loop structure prediction with predicted contacts

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1. Training set details

Target	Length
1SMRA_113_118	6
4J3VA_313_318	6
3U1LA_78_83	6
2JC5A_150_155	6
4L6DA_270_275	6
1TRBA_289_294	6
1Q35A_237_242	6
1VHEA_267_272	6
1S9RA_348_353	6
1OFDA_218_223	6
4X00A_175_182	8
3PVKA_176_183	8
1TKEA_47_54	8
3GVEA_59_66	8
1F46A_118_125	8
2CARA_103_110	8
2YNAA_241_248	8
2BW4A_221_228	8
2Z9WA_115_122	8
1N08A_85_92	8
3KHYA_165_174	10
2CFCA_208_217	10
4CI7A_480_489	10
2OEMA_271_280	10
2DRIA_89_98	10
3KWEA_130_139	10
1PG4A_450_459	10
1NHSA_362_371	10
4GEKA_116_125	10
3DCIA_117_126	10
2DDXA_155_166	12
2NUWA_7_18	12
1EOKA_170_181	12
4I3GA_198_209	12
4G29A_294_305	12
1VHQA_148_159	12
4GWIA_81_92	12
3AMNA_121_132	12
4AG1A_56_67	12
4MJKA_145_156	12

Target	Length
3W8KA_200_213	14
4R3FA_66_79	14
1GPOA_1593_1606	14
2GDMA_44_57	14
4P6BA_277_290	14
2Q4WA_422_435	14
1KV9A_288_301	14
4WKSC_715_728	14
3F4LA_153_166	14
2AXQA_321_334	14
2R16A_857_872	16
4FE9A_326_341	16
1EI5A_139_154	16
2DDBA_18_33	16
1RGZA_112_127	16
4J94A_133_148	16
1QCXA_12_27	16
3R6AA_26_41	16
1EOKA_127_142	16
4LIHA_453_468	16
4X84A_86_103	18
2Y8TA_127_144	18
1RP0A_71_88	18
4P3FA_96_113	18
4CC2A_1521_1538	18
2OCGA_78_95	18
2OCTA_32_49	18
3T8WA_133_150	18
4JICA_268_285	18
1V4AA_212_229	18

2. General target set results

(a) MetaPSICOV contact prediction results - contacts involving at least one target loop residue

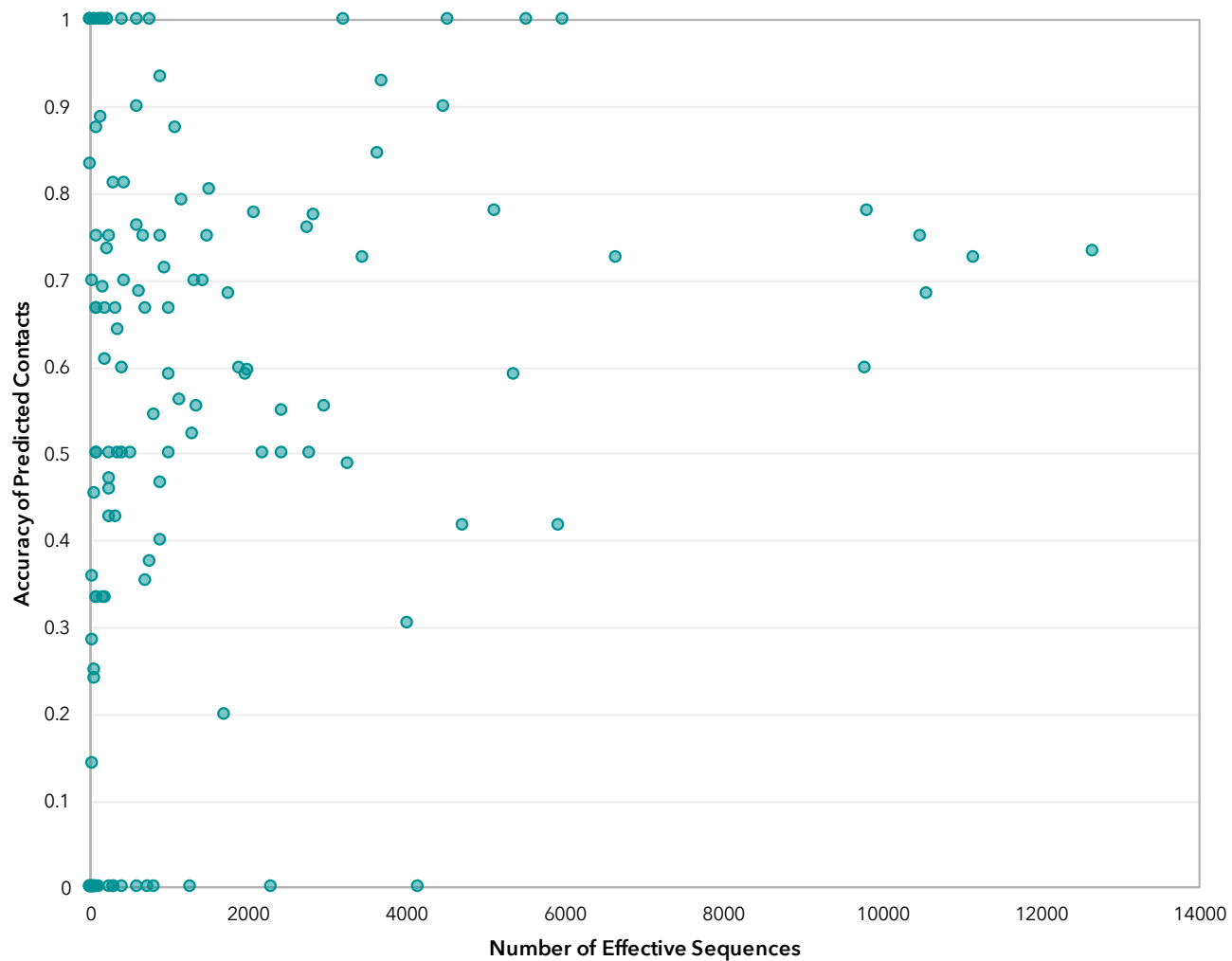
Target	Length	No Predicted	No Correct	Target	Length	No Predicted	No Correct
1F74A_105_114	10	22	13	3UN7A_461_474	14	18	10
1NU4A_73_82	10	26	22	3ZO9A_554_567	14	5	0
1YOPA_168_177	10	6	4	4AUKA_27_40	14	27	18
1ZJCA_18_27	10	16	13	4B4DA_236_249	14	1	1
2IVFA_677_686	10	7	3	4MDYA_204_217	14	6	3
2PN1A_95_104	10	31	24	4NOGA_100_113	14	1	1
3JQYA_109_118	10	21	7	4P5PA_183_196	14	52	26
3PHXB_127_136	10	10	9	1APYA_49_63	15	23	14
4FFJA_164_173	10	14	9	1KQPA_205_219	15	18	9
4MGQA_173_182	10	16	13	1N5UA_490_504	15	2	1
4N68A_955_964	10	35	24	1ODMA_74_88	15	-	-
4RMXA_413_422	10	-	-	1YSQA_87_101	15	10	5
4W8HA_194_203	10	4	2	1ZUOA_333_347	15	2	1
5J41A_140_149	10	22	13	2Q0LA_43_57	15	1	1
5JRHA_331_340	10	5	3	2RB9A_189_203	15	12	8
1KGDG_854_864	11	9	5	2VNGA_125_139	15	17	8
1Y9LA_87_97	11	1	1	2WW8A_501_515	15	-	-
2D5BA_9_19	11	15	6	3IT3A_60_74	15	10	7
2Y78A_17_27	11	36	29	4A4AA_818_832	15	12	4
3L5LA_65_75	11	29	23	4ANOA_123_137	15	3	3
3PMEA_1048_1058	11	7	1	4E9XA_1073_1087	15	21	16
3VKWA_891_901	11	6	4	4LZKA_32_46	15	3	3
4DV8A_488_498	11	2	0	1IUJA_75_90	16	11	8
4ITBA_102_112	11	9	7	1NFPA_49_64	16	-	-
4LGYA_831_841	11	1	1	2BGKA_99_114	16	30	22
4UZGA_426_436	11	10	7	2FVYA_274_289	16	1	1
4YFUA_620_630	11	16	11	2Q88A_192_207	16	59	46
4ZMYA_40_50	11	12	5	3G06A_652_667	16	1	1
5CENA_253_263	11	49	15	3ZX4A_219_234	16	15	9
5IOJA_406_416	11	10	7	4E8DA_330_345	16	1	0
1DJ7A_51_62	12	25	9	4LM8A_125_140	16	11	5
1JS1X_273_284	12	24	11	4U9HL_231_246	16	1	1
1OO0B_104_115	12	25	19	5DAWA_162_177	16	84	60
1UF5A_66_77	12	5	1	5KKQA_375_390	16	22	16
1W2WB_367_378	12	10	6	5LX8A_538_553	16	8	6
2C4EA_278_289	12	14	13	5M6QA_55_70	16	-	-
2ICGA_16_27	12	4	3	5XNHA_116_131	16	-	-
3F58A_227_238	12	-	-	1GQIA_550_566	17	4	3
3NIOA_45_56	12	10	9	1U7BA_118_134	17	8	7
3UUEA_57_68	12	7	3	2DSKA_626_642	17	12	9
4B6IA_85_96	12	2	1	2I5VO_248_264	17	18	15
5AVDA_224_235	12	11	8	2P9BA_386_402	17	62	37
5C9LA_103_114	12	31	11	3DCMX_11_27	17	15	7
5HWAA_212_223	12	-	-	3F2VA_85_101	17	19	13
5MZWB_95_106	12	34	25	3VENA_464_480	17	4	3
2CB1A_200_212	13	20	14	3VMNA_326_342	17	-	-
2IXMA_59_71	13	1	1	4AGKA_143_159	17	1	1
3AYRA_109_121	13	23	12	4HDRB_125_141	17	6	4
3EF6A_53_65	13	-	-	4R12A_491_507	17	-	-
3PT5A_258_270	13	-	-	5B0NA_124_140	17	50	39
3QY9A_165_177	13	-	-	5CDKA_105_121	17	13	9
3TN4A_229_241	13	16	9	5LSVA_26_42	17	3	1
4B2ZA_307_319	13	1	1	1GAIA_254_271	18	4	2
4ETNA_111_123	13	22	12	1HQ0A_741_758	18	-	-
4EUUA_189_201	13	3	0	1QQFA_1058_1075	18	15	14
4P8NA_370_382	13	1	1	1UM0A_211_228	18	3	1
4QV2A_536_548	13	7	2	2GGSA_111_128	18	4	3
5E56A_53_65	13	12	5	2XZIA_39_56	18	3	3
5IRCA_1276_1288	13	22	13	3UV0A_26_43	18	43	21
5KF9A_62_74	13	1	0	3VSA_6_23	18	9	8
2HC9A_258_271	14	29	7	4AK2A_555_572	18	-	-
2OZLA_55_68	14	36	18	4B4HA_526_543	18	8	7
2VHKA_177_190	14	5	0	4QO5A_294_311	18	1	1
2YIMA_113_126	14	16	6	4R9OA_85_102	18	20	11
2ZFNH_121_134	14	1	0	5A7MA_584_601	18	-	-
3ACHA_69_82	14	2	0	5GN2A_204_221	18	1	1
3QFTA_354_367	14	1	1	5H3ZA_1072_1089	18	12	3
3QLIA_262_275	14	27	18				

✗ = Omitted due to having <2 predicted contacts

● = Omitted due to having <2 predicted contacts remaining after ignoring those which were never satisfied (Sphinx only)

2. General target set results

(b) N_{eff} vs accuracy of predicted contacts

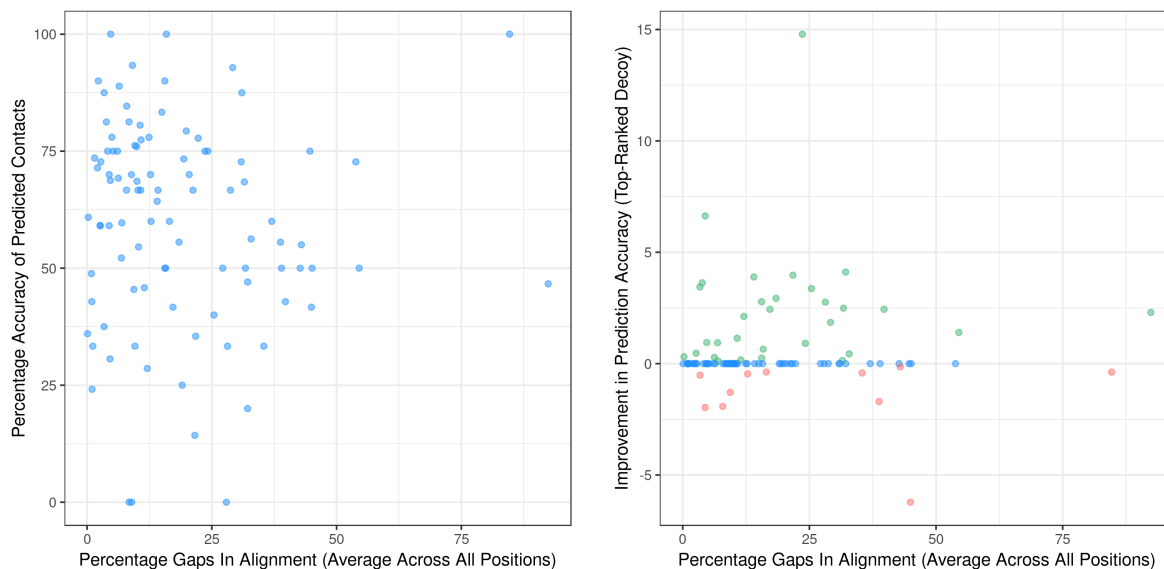


The number of effective sequences in the alignment (N_{eff}) used to predict contacts by MetaPSICOV, vs. the accuracy of the predicted contacts. N_{eff} values are taken directly from the MetaPSICOV output.

2. General target set results

(c) Alignment gaps vs. accuracy of predicted contacts/loop structure prediction

To investigate the effect of the alignments in more detail, we looked at each position in the loop and calculated the percentage of sequences in the alignment that feature a gap at that location. For each target loop, we averaged the values for each position to give a single value indicating the prevalence of gaps in the alignment for that target. Plotting this value against the accuracy of contact prediction and the improvement in the accuracy of structure prediction (Sphinx results) shows no clear relationship (see below). Targets with high gap occurrence may have a near-perfect set of predicted contacts, leading to improved structure prediction, while the contacts for some targets with few gaps in the alignment are predicted poorly and hence the accuracy of structure prediction is made worse.



Average gap percentage vs. accuracy of predicted contacts (left) and improvement in the accuracy of loop structure prediction after incorporation of contact information (right). In the right-hand plot, the 'improvement' in accuracy of structure prediction refers to the RMSD of the top-ranked decoy. Targets whose models were improved by contact information are coloured green, those that were not affected are in blue, and those that were made worse are in red.

2. General target set results

(d) Full Sphinx results

Best = RMSD of the best (i.e. closest to native) decoy generated

Best of Top 500 = RMSD of the best decoy remaining in the set after filtering using Sphinx's scoring function

Top Ranked = RMSD of the decoy predicted to be the best by the SOAP-Loop scoring function

Best of Top 5 = RMSD of the best decoy in the top five as ranked by SOAP-Loop

All RMSDs are global backbone RMSDs.

Target	Length	Best	Best of Top 500		Top Ranked		Best of Top 5	
			Normal	Contacts	Normal	Contacts	Normal	Contacts
1F74A_105_114	10	0.33	0.34	0.39	0.87	0.40	0.51	0.40
1NU4A_73_82	10	0.31	0.44	0.44	0.63	0.63	0.62	0.63
1Y0PA_168_177	10	0.36	0.36	0.36	0.42	0.42	0.38	0.38
1ZJCA_18_27	10	1.59	1.84	1.84	5.58	1.95	5.07	1.95
2IVFA_677_686	10	0.41	0.41	0.41	0.57	0.57	0.44	0.44
2PN1A_95_104	10	0.88	0.88	0.88	0.88	0.88	0.88	0.88
3JQYA_109_118	10	0.54	0.54	0.54	0.66	0.66	0.54	0.54
3PHXB_127_136	10	0.34	0.36	0.34	0.45	0.45	0.45	0.45
4FFJA_164_173	10	1.56	1.90	1.83	7.41	3.52	6.78	3.05
4MGQA_173_182	10	1.28	1.40	1.28	2.16	2.16	2.03	2.03
4N68A_955_964	10	0.43	0.43	0.43	0.57	0.57	0.43	0.43
4W8HA_194_203	10	1.05	1.66	1.05	4.86	3.46	3.46	3.46
5J41A_140_149	10	0.26	0.26	0.26	6.89	0.26	6.89	0.26
5JRHA_331_340	10	0.26	0.26	0.86	0.78	1.16	0.26	1.15
1KGDA_854_864	11	1.47	1.63	2.13	4.05	5.75	3.01	3.01
2D5BA_9_19	11	1.51	1.87	1.52	5.27	1.90	4.59	1.90
2Y78A_17_27	11	0.22	0.22	0.22	0.36	0.36	0.22	0.22
3L5LA_65_75	11	0.16	0.16	0.16	0.20	0.20	0.20	0.20
3PMEA_1048_1058	11	0.46	0.46	0.46	0.71	0.71	0.54	0.54
3VKWA_891_901	11	1.54	1.57	1.57	4.09	4.09	2.40	2.43
4DV8A_488_498	11	0.47	0.47	0.47	0.58	0.58	0.54	0.54
4ITBA_102_112	11	0.18	0.18	0.18	0.36	0.36	0.23	0.23
4UZGA_426_436	11	1.08	2.23	2.05	3.93	5.90	3.93	2.55
4YFUA_620_630	11	0.19	0.23	0.19	0.23	0.23	0.23	0.23
4ZMYA_40_50	11	0.19	0.20	3.50	0.39	6.61	0.38	5.89
5CENA_253_263	11	1.74	1.76	1.74	3.55	3.55	3.14	3.14
5IOJA_406_416	11	1.68	1.68	1.89	2.91	2.91	2.19	2.19
1DJ7A_51_62	12	0.30	0.30	0.30	0.49	0.49	0.30	0.30
1JS1X_273_284	12	0.27	0.40	0.29	0.46	0.29	0.40	0.29
1OO0B_104_115	12	0.53	0.53	0.53	0.89	0.89	0.58	0.58
1UF5A_66_77	12	1.09	3.41	1.46	5.57	1.46	3.41	1.46
1W2WB_367_378	12	0.64	0.64	0.64	0.64	1.10	0.64	1.03
2C4EA_278_289	12	1.70	2.86	2.17	8.61	6.76	6.76	4.83
2ICGA_16_27	12	1.69	2.25	2.54	6.33	6.33	4.81	3.53
3NIOA_45_56	12	0.87	0.87	0.87	5.39	5.14	4.65	2.11
3UUEA_57_68	12	0.68	0.85	0.68	3.26	0.82	0.85	0.68
5AVDA_224_235	12	0.33	0.33	0.33	0.67	0.67	0.41	0.41
5C9LA_103_114	12	1.85	3.18	2.84	8.71	4.74	4.14	3.45
5MZWB_95_106	12	1.14	1.14	1.14	2.64	2.64	1.62	1.62
2CB1A_200_212	13	0.51	0.51	0.51	0.90	0.90	0.56	0.56
3AYRA_109_121	13	0.94	3.60	2.83	6.20	5.26	6.20	4.89
3TN4A_229_241	13	0.49	0.59	0.73	3.07	2.63	0.59	2.63
4ETNA_111_123	13	0.82	0.91	0.82	0.98	0.98	0.95	0.95
4EUUA_189_201	13	0.59	0.59	0.59	1.81	1.81	0.59	0.59
4QV2A_536_548	13	1.92	2.46	2.31	5.99	3.87	3.72	2.46
5E56A_53_65	13	1.92	2.85	2.56	5.62	3.18	2.90	3.18
5IRCA_1276_1288	13	0.42	0.42	0.42	0.51	0.51	0.47	0.47
2HC9A_258_271	14	2.92	3.79	3.79	6.43	6.43	6.10	5.46
2OZLA_55_68	14	0.29	0.29	0.29	0.33	0.33	0.33	0.33
2VHKA_177_190	14	1.62	3.33	3.87	7.58	7.58	6.37	6.37
2YIMA_113_126	14	2.24	2.69	2.30	8.15	4.71	3.91	2.69
3QLIA_262_275	14	0.22	0.22	0.22	0.33	0.33	0.33	0.33
3UN7A_461_474	14	1.39	1.81	1.73	7.00	4.07	1.87	1.87
4AUKA_27_40	14	1.62	1.62	1.62	1.78	1.78	1.77	1.77
4MDYA_204_217	14	1.49	2.61	2.61	9.51	6.73	5.55	5.37
4P5PA_183_196	14	1.68	3.39	1.68	5.94	5.94	5.80	4.78
1APYA_49_63	15	0.97	0.97	0.97	1.42	1.11	1.10	1.00
1KQPA_205_219	15	2.38	8.34	2.38	10.14	7.65	10.14	4.02
1YSQA_87_101	15	2.87	2.95	2.95	5.48	5.48	5.48	4.24
1ZUOA_333_347	15	1.92	1.92	1.92	1.97	1.97	1.92	1.92
2RB9A_189_203	15	2.29	3.13	2.67	4.96	3.82	4.08	3.61

2. General target set results
(d) Full Sphinx results (cont.)

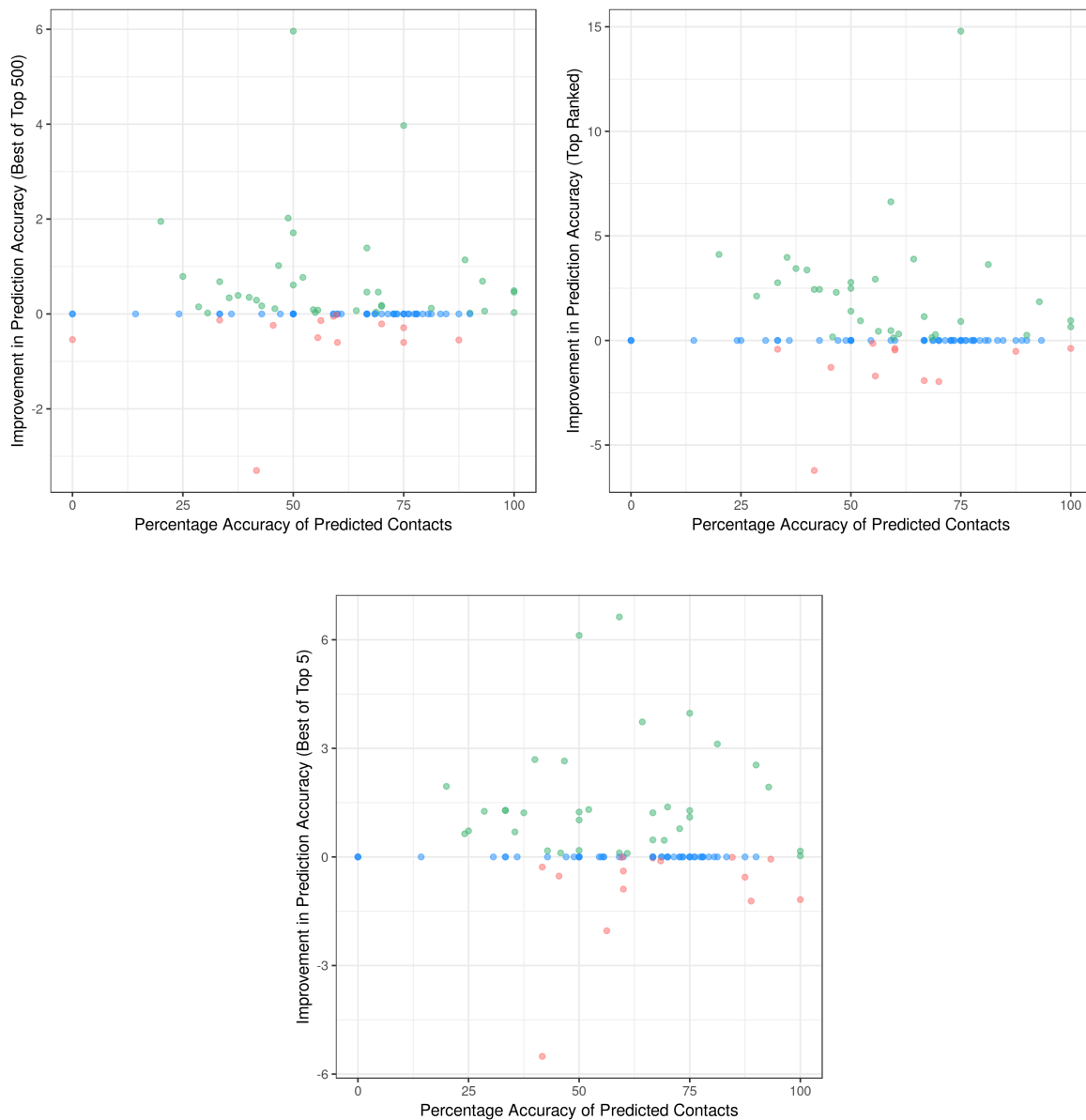
Target	Length	Best	Best of Top 500		Top Ranked		Best of Top 5	
			Normal	Contacts	Normal	Contacts	Normal	Contacts
2VNGA_125_139	15	2.45	2.92	2.92	4.03	4.03	3.65	3.65
3IT3A_60_74	15	1.14	1.30	1.14	1.30	1.30	1.30	1.30
4A4AA_818_832	15	0.60	0.60	0.60	0.86	0.86	0.60	0.60
4ANOA_123_137	15	3.01	4.38	3.89	6.46	5.51	5.67	5.51
4E9XA_1073_1087	15	0.40	0.40	0.40	0.47	0.47	0.40	0.40
4LZKA_32_46	15	2.50	3.73	3.27	12.21	11.56	7.67	8.85
1IUJA_75_90	16	2.94	3.13	3.13	3.91	3.91	3.91	3.13
2BGKA_99_114	16	2.05	2.05	2.05	3.57	3.57	3.57	3.57
2Q88A_192_207	16	1.94	1.94	1.94	1.94	1.94	1.94	1.94
3ZX4A_219_234	16	2.53	2.68	2.68	10.16	10.16	4.90	4.90
4LM8A_125_140	16	2.20	2.61	2.85	4.82	6.11	4.82	5.35
5DAWA_162_177	16	1.13	1.13	1.13	1.13	1.13	1.13	1.13
5KKQA_375_390	16	0.72	0.72	0.72	0.72	0.72	0.72	0.72
5LX8A_538_553	16	2.19	2.23	2.83	6.51	5.60	4.93	3.83
1GQIA_550_566	17	0.15	0.15	0.15	0.29	0.29	0.15	0.15
1U7BA_118_134	17	0.90	0.90	1.45	1.50	2.02	1.20	1.76
2DSKA_626_642	17	0.19	0.19	0.19	0.21	0.21	0.19	0.19
2I5VO_248_264	17	0.24	0.24	0.24	0.41	0.41	0.24	0.24
2P9BA_386_402	17	0.28	0.28	0.30	0.42	0.30	0.29	0.30
3DCMX_11_27	17	2.84	5.06	4.04	13.60	11.30	10.41	7.76
3F2VA_85_101	17	0.79	0.79	0.79	1.36	1.22	0.93	1.04
3VENA_464_480	17	0.27	0.27	0.27	0.28	0.28	0.28	0.28
4HDRB_125_141	17	3.43	6.41	5.02	11.30	13.22	10.67	9.45
5B0NA_124_140	17	0.63	0.63	0.63	0.71	0.71	0.67	0.67
5CDKA_105_121	17	1.38	2.00	1.54	2.08	1.80	2.00	1.54
5LSVA_26_42	17	2.79	4.46	4.59	9.96	10.38	7.11	5.83
1GAIA_254_271	18	0.63	0.63	0.63	1.22	1.22	0.63	0.63
1QQFA_1058_1075	18	0.21	0.28	0.22	0.49	0.49	0.35	0.41
1UM0A_211_228	18	3.17	3.85	3.17	7.41	4.65	5.94	4.65
2GGSA_111_128	18	0.79	5.35	1.38	16.17	1.38	5.35	1.38
2XZIA_39_56	18	0.45	0.48	0.45	0.48	0.86	0.48	0.45
3UV0A_26_43	18	3.92	6.61	4.59	13.89	13.89	10.65	10.65
3VSVA_6_23	18	2.95	7.06	5.92	11.37	11.37	9.15	10.37
4B4HA_526_543	18	0.27	0.27	0.27	0.70	0.70	0.45	0.45
4R9OA_85_102	18	0.50	0.53	0.50	0.53	0.67	0.53	0.53
5H3ZA_1072_1089	18	4.18	5.14	4.35	8.57	8.57	7.78	7.06

Average results:

Length	No. Targets	Best	Best of Top 500		Top Ranked		Best of Top 5	
			Normal	Contacts	Normal	Contacts	Normal	Contacts
10	14	0.69	0.79	0.78	2.34	1.22	2.05	1.15
11	13	0.84	0.97	1.24	2.05	2.55	1.66	1.77
12	12	0.93	1.40	1.15	3.64	2.61	2.38	1.69
13	8	0.95	1.49	1.35	3.13	2.39	2.00	1.97
14	9	1.49	2.19	2.01	5.23	4.21	3.56	3.22
15	11	1.87	2.79	2.10	4.48	3.98	3.82	3.19
16	8	1.96	2.06	2.17	4.09	4.14	3.24	3.07
17	12	1.16	1.78	1.60	3.51	3.51	2.85	2.43
18	10	1.71	3.02	2.15	6.08	4.38	4.13	3.66
ALL	97	1.24	1.76	1.55	3.71	3.11	2.79	2.37

2. General target set results

(e) Accuracy of predicted contacts vs. improvement in structure prediction



Plots of the accuracy of predicted contacts for each target vs. the improvement observed in the accuracy of structure prediction using Sphinx. The colour of each point relates to whether the accuracy of structure prediction was improved (green), remained the same (blue) or was made worse (red) when contact information was used. There is no clear relationship - improvements in structure prediction are still observed for targets for which contacts were predicted poorly.

2. General target set results

(f) Inclusion of trivial contacts

MetaPSICOV does not predict trivial contacts (those between residues fewer than 5 residues apart in the protein sequence). To test whether contacts between residues that are close in sequence ('trivial' contacts) have an effect on the accuracy of loop structure prediction, we used the method CCMpred, which does allow the user to specify a minimum residue separation. Using CCMpred resulted in predicted contacts for 42 of the 135 targets of the test set - this is far fewer than MetaPSICOV, which gave contacts for 97. Of these, 30 targets had both trivial and non-trivial contacts. The results achieved for this set using Sphinx, and using the contacts predicted by CCMpred, are given in the table below:

	Best Top 500	Top Ranked	Best Top 5
No Contacts	1.38 Å	2.97 Å	2.16 Å
Non-Trivial Only	1.12 Å	2.16 Å	1.63 Å
All Contacts	1.17 Å	2.02 Å	1.69 Å

Using all predicted contacts (both trivial and non-trivial) produces very similar results to using non-trivial contacts only.

2. General target set results

(g) Location of predicted contact residues

We have examined whether the accuracy of predicted contacts is different depending on the location of the contacting residues. Comparing predicted contacts between two target loop residues to those between one loop residue and one residue located elsewhere in the protein showed no difference in accuracy (62.3% and 62.0% respectively).

For those predicted contacts featuring only one target loop residue, we investigated whether the accuracy differed for contacts where the loop residue was located in the middle, the beginning ('N-end') or end ('C-end') of the loop, according to the table below.

Loop Length	Number of Residues		
	N-end	Middle	C-end
10	3	4	3
11	4	3	4
12	4	4	4
13	4	5	4
14	5	4	5
15	5	5	5
16	5	6	5
17	6	5	6
18	6	6	6

We found slight differences in the accuracy of predicted contacts: 59.4%, 64.4% and 62.4% for the middle, N-end and C-end contacts, respectively. Re-running our ranking method omitting each type of contact revealed little difference in Sphinx prediction accuracy (see table below). We therefore cannot conclude that contacts involving residues from a particular loop region are more/less useful.

	Best Top 500	Top Ranked	Best Top 5
Excluding 'middle'	1.54 Å	3.06 Å	2.35 Å
Excluding 'N-end'	1.51 Å	3.15 Å	2.39 Å
Excluding 'C-end'	1.54 Å	2.99 Å	2.39 Å

2. General target set results

(h) Full MODELLER results

Best = RMSD of the best (i.e. closest to native) decoy generated

Top Ranked = RMSD of the decoy predicted to be the best by the SOAP-Loop scoring function

Best of Top 5 = RMSD of the best decoy in the top five as ranked by SOAP-Loop

All RMSDs are global backbone RMSDs.

Target	Length	Best		Top Ranked		Best of Top 5	
		Normal	Contacts	Normal	Contacts	Normal	Contacts
1F74A_105_114	10	1.00	1.01	2.61	3.31	2.07	1.30
1NU4A_73_82	10	0.78	0.77	0.79	0.82	0.79	0.82
1Y0PA_168_177	10	0.76	0.76	0.93	0.85	0.90	0.84
1ZJCA_18_27	10	0.94	0.37	1.51	0.37	0.94	0.37
2IVFA_677_686	10	1.72	0.80	2.12	2.29	2.12	1.11
2PN1A_95_104	10	0.47	0.45	0.48	0.50	0.48	0.47
3JQYA_109_118	10	0.56	0.62	0.56	0.62	0.56	0.62
3PHXB_127_136	10	0.60	0.58	0.60	0.58	0.60	0.58
4FFJA_164_173	10	1.73	1.57	8.19	3.22	1.83	2.47
4MGQA_173_182	10	0.56	0.41	0.56	0.53	0.56	0.41
4N68A_955_964	10	0.49	0.50	0.53	0.54	0.49	0.50
4W8HA_194_203	10	1.64	1.19	1.64	1.19	1.64	1.19
5J41A_140_149	10	1.02	0.83	1.25	1.21	1.02	1.03
5JRHA_331_340	10	1.67	1.75	3.93	1.89	1.71	1.89
1KGDA_854_864	11	1.82	1.97	6.15	2.47	4.56	2.41
2D5BA_9_19	11	1.08	1.19	1.32	4.99	1.16	1.25
2Y78A_17_27	11	2.54	0.77	3.08	0.82	3.06	0.80
3L5LA_65_75	11	0.55	0.47	0.69	0.47	0.55	0.47
3PMEA_1048_1058	11	1.59	1.88	2.48	4.20	2.48	2.53
3VKWA_891_901	11	1.63	1.64	1.99	3.13	1.64	2.42
4DV8A_488_498	11	1.11	1.63	1.11	4.32	1.11	2.78
4ITBA_102_112	11	0.42	0.48	0.60	3.06	0.60	0.48
4UZGA_426_436	11	0.76	0.75	0.76	1.91	0.76	0.75
4YFUA_620_630	11	2.61	1.14	4.04	1.39	3.60	1.14
4ZMYA_40_50	11	3.98	2.10	5.00	5.61	5.00	5.54
5CENA_253_263	11	1.29	2.03	6.52	5.14	6.15	2.59
5IOJA_406_416	11	1.13	1.14	2.53	1.36	2.31	1.36
1DJ7A_51_62	12	1.25	1.20	1.64	1.35	1.41	1.35
1JS1X_273_284	12	2.05	1.73	4.09	2.04	2.48	2.04
1OO0B_104_115	12	2.35	1.79	11.40	8.80	5.32	3.70
1UF5A_66_77	12	1.62	1.59	4.55	1.59	1.62	1.59
1W2WB_367_378	12	1.44	1.30	3.61	5.89	1.94	2.34
2C4EA_278_289	12	2.17	1.37	3.65	3.36	3.65	1.60
2ICGA_16_27	12	1.26	0.84	1.26	1.26	1.26	1.26
3NIOA_45_56	12	1.58	1.52	3.46	2.48	1.91	2.15
3UUEA_57_68	12	1.53	1.46	2.52	3.11	1.53	1.46
4B6IA_85_96	12	2.16	1.72	8.19	7.20	4.46	4.49
5AVDA_224_235	12	3.66	2.01	4.83	2.91	4.83	2.91
5C9LA_103_114	12	1.90	2.88	3.02	3.13	1.90	2.88
5MZWB_95_106	12	0.87	0.54	2.76	0.84	1.63	0.54
2CB1A_200_212	13	2.83	2.49	6.52	3.30	4.36	3.30
3AYRA_109_121	13	2.61	2.07	3.17	9.84	3.17	4.56
3TN4A_228_241	13	1.55	1.65	6.80	1.65	1.77	1.65
4ETNA_111_123	13	1.04	0.56	1.33	0.56	1.04	0.56
4EUUA_189_201	13	1.12	0.87	1.90	1.91	1.12	0.97
4QV2A_536_548	13	0.66	1.55	0.66	3.13	0.66	1.89
5E56A_53_65	13	3.50	3.37	4.48	6.28	4.07	5.11
5IRCA_1276_1288	13	3.18	1.63	8.80	3.25	3.75	2.70
2HC9A_258_271	14	3.63	4.55	5.71	7.70	5.71	4.98
2OZLA_55_68	14	2.12	1.50	2.60	5.24	2.12	2.41
2VHKA_177_190	14	2.82	4.09	5.98	7.50	5.10	6.62
2YIMA_113_126	14	2.76	2.56	3.30	10.89	3.30	4.14
3ACHA_69_82	14	2.23	2.83	5.53	5.67	4.15	2.88
3QLIA_262_275	14	2.17	2.56	6.67	5.70	2.17	3.15
3UN7A_461_474	14	3.66	3.18	9.37	15.50	6.77	5.11
3ZO9A_554_567	14	1.86	2.44	1.86	6.08	1.86	2.58
4AUKA_27_40	14	2.51	1.73	2.59	2.87	2.51	2.87
4MDYA_204_217	14	1.25	2.00	1.92	5.03	1.25	2.14
4P5PA_183_196	14	2.81	2.51	7.04	3.45	3.47	3.45
1APYA_49_63	15	3.24	2.67	5.38	8.94	5.38	3.11
1KQPA_205_219	15	2.12	1.62	4.10	1.77	2.46	1.77
1N5UA_490_504	15	1.94	2.42	3.01	3.43	2.51	2.65

2. General target set results

(h) Full MODELLER results (cont.)

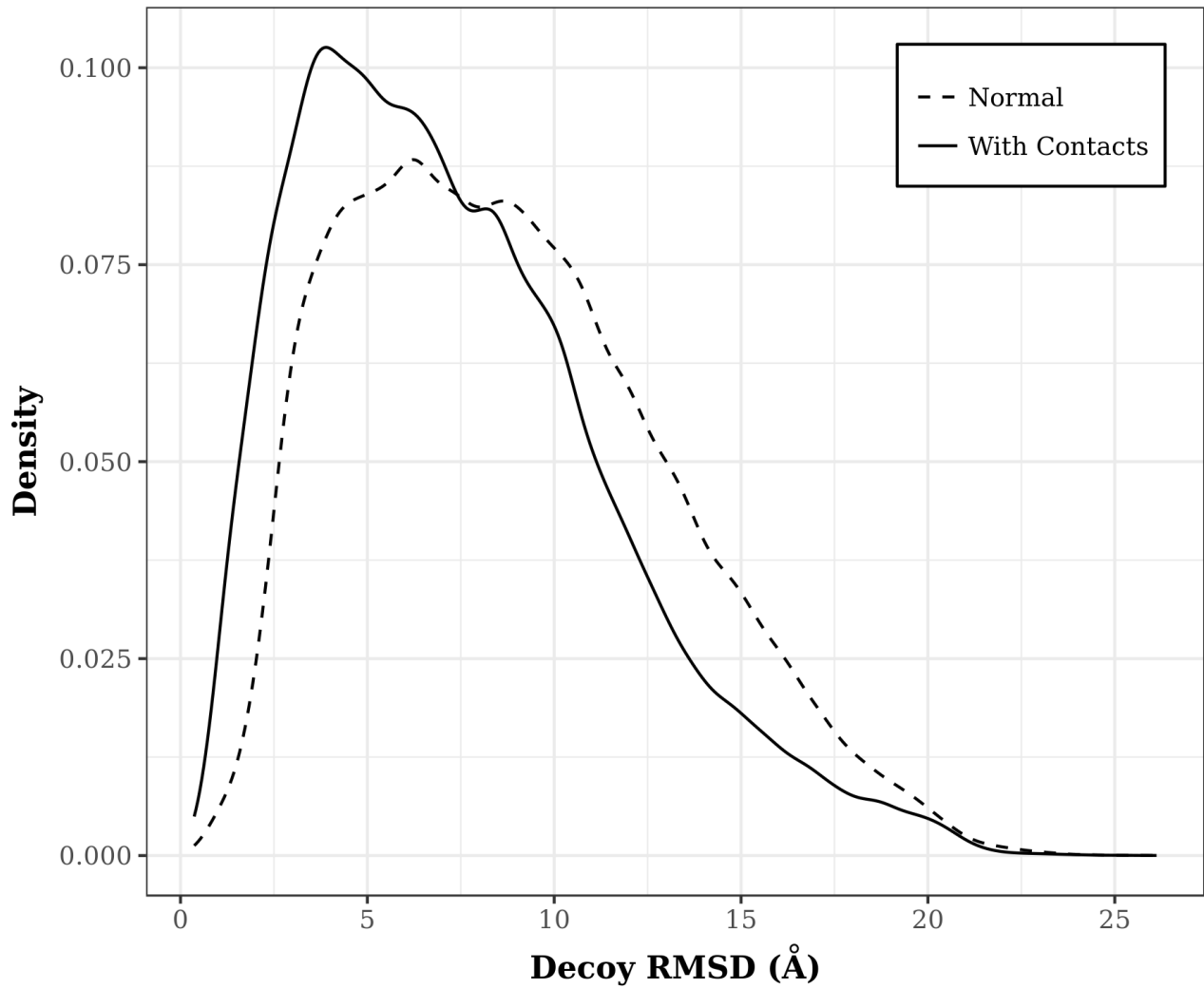
Target	Length	Best		Top Ranked		Best of Top 5	
		Normal	Contacts	Normal	Contacts	Normal	Contacts
1YSQA_87_101	15	2.57	2.95	4.75	6.21	4.75	3.46
1ZUOA_333_347	15	1.95	2.19	2.98	2.42	2.22	2.34
2RB9A_189_203	15	2.23	2.03	3.25	2.69	2.23	2.69
2VNGA_125_139	15	2.99	2.99	7.21	6.25	2.99	4.96
3IT3A_60_74	15	2.76	0.56	2.76	0.56	2.76	0.56
4A4AA_818_832	15	1.74	1.49	1.74	4.07	1.74	2.16
4ANOA_123_137	15	3.09	3.28	8.14	5.26	3.09	5.26
4E9XA_1073_1087	15	3.42	1.70	5.70	1.70	4.31	1.70
4LZKA_32_46	15	2.59	2.39	6.56	5.16	3.27	2.39
1IUJA_75_90	16	3.81	4.07	10.96	8.32	4.75	4.46
2BGKA_99_114	16	2.73	2.48	10.54	8.44	4.91	5.05
2Q88A_192_207	16	1.40	1.27	3.06	1.59	2.16	1.59
3ZX4A_219_234	16	2.02	1.35	2.02	1.52	2.02	1.35
4LM8A_125_140	16	2.49	2.83	3.74	3.38	3.08	2.85
5DAWA_162_177	16	3.37	0.58	6.48	4.85	4.60	0.58
5KKQA_375_390	16	2.43	1.61	7.28	11.56	7.28	2.53
5LX8A_538_553	16	3.27	2.76	4.23	5.28	4.04	4.05
1GQIA_550_566	17	3.87	3.17	3.87	4.48	3.87	3.54
1U7BA_118_134	17	1.25	1.29	1.86	2.05	1.43	1.43
2DSKA_626_642	17	1.35	2.15	1.35	2.70	1.35	2.15
2I5VO_248_264	17	3.38	2.36	6.99	4.34	5.53	3.57
2P9BA_386_402	17	3.57	1.85	7.35	2.83	7.35	2.83
3DCMX_11_27	17	5.17	4.91	5.55	11.44	5.55	4.91
3F2VA_85_101	17	4.49	4.29	7.97	5.77	5.55	5.77
3VENA_464_480	17	3.96	2.15	5.74	4.52	4.31	2.15
4HDRB_125_141	17	3.59	3.81	12.08	7.18	11.65	6.14
5B0NA_124_140	17	2.40	1.48	4.07	2.14	2.83	1.93
5CDKA_105_121	17	4.22	1.56	16.96	3.81	4.89	2.81
5LSVA_26_42	17	2.94	3.28	2.94	12.77	2.94	10.76
1GAIA_254_271	18	3.12	2.68	4.09	2.68	3.97	2.68
1QQFA_1058_1075	18	4.75	2.43	10.34	10.10	7.65	2.97
1UM0A_211_228	18	3.83	3.08	13.68	6.04	3.83	4.42
2GGSA_112_128	18	3.89	3.30	11.89	4.34	4.40	3.35
2XZIA_39_56	18	3.79	3.35	8.95	9.41	4.33	9.41
3UV0A_26_43	18	3.95	2.83	10.19	2.83	10.19	2.83
3VSVA_6_23	18	7.44	4.24	10.96	5.79	9.33	4.37
4B4HA_526_543	18	3.82	3.08	4.27	7.27	4.27	5.52
4R9OA_85_102	18	4.24	4.14	10.83	9.82	8.56	6.18
5H3ZA_1072_1089	18	4.22	4.14	10.76	8.18	6.37	6.46

Average results:

Length	No. Targets	Best		Top Ranked		Best of Top 5	
		Normal	Contacts	Normal	Contacts	Normal	Contacts
10	14	1.00	0.83	1.83	1.28	1.12	0.97
11	13	1.58	1.32	2.79	2.99	2.54	1.89
12	13	1.83	1.53	4.23	3.38	2.61	2.18
13	8	2.06	1.77	4.21	3.74	2.49	2.59
14	11	2.53	2.72	4.78	6.87	3.49	3.66
15	12	2.55	2.19	4.63	4.04	3.14	2.76
16	8	2.69	2.12	6.04	5.62	4.11	2.81
17	12	3.35	2.69	6.39	5.34	4.77	4.00
18	10	4.31	3.33	9.60	6.65	6.29	4.82
ALL	101	2.36	2.00	4.75	4.26	3.28	2.76

2. General target set results

(i) MODELLER RMSD distributions



Distributions of RMSDs for decoy ensembles produced by MODELLER, comparing those generated normally, i.e. without predicted contact information, with those produced using constraints based on the results of contact prediction. Each distribution shown is a combination of those from the 101 individual targets (1000 decoys per target).

3. General target set results - non-native environment

(a) Accuracy of MODELLER-generated protein models

Anchor RMSDs were calculated across backbone atoms only, after superposition of the entire model with TAlign. Anchor residues are defined as the two residues on each side of the target loop.

Target	Length	TM score	Anchor RMSD	Target	Length	TM score	Anchor RMSD
1F74A_105_114	10	0.98	0.19	2YIMA_113_126	14	0.96	0.69
1NU4A_73_82	10	0.91	0.48	✗ 3ACHA_69_82	14	0.31	18.46
1Y0PA_168_177	10	1.00	0.21	3QLIA_262_275	14	0.99	0.28
1ZJCA_18_27	10	0.97	0.63	3UN7A_461_474	14	0.96	0.15
2IVFA_677_686	10	0.92	0.84	● 3ZO9A_554_567	14	0.99	0.53
✗ 2PN1A_95_104	10	0.62	4.14	✗ 4AUKA_27_40	14	0.28	395.50
3JQYA_109_118	10	0.85	2.44	4MDYA_204_217	14	0.98	0.78
3PHXB_127_136	10	0.75	1.89	4P5PA_183_196	14	0.92	0.76
4FFJA_164_173	10	0.95	0.78	1APYA_49_63	15	0.80	2.36
✗ 4MGQA_173_182	10	0.20	18.83	1KQPA_205_219	15	0.99	0.68
4N68A_955_964	10	0.86	0.45	● 1N5UA_490_504	15	0.99	0.94
4W8HA_194_203	10	0.97	0.95	1YSQA_87_101	15	0.83	2.70
5J41A_140_149	10	0.99	0.48	1ZUOA_333_347	15	0.95	0.70
5JRHA_331_340	10	1.00	0.12	2RB9A_189_203	15	0.85	1.53
1KGDA_854_864	11	0.90	1.50	2VNGA_125_139	15	0.93	0.27
2D5BA_9_19	11	0.99	0.36	3IT3A_60_74	15	0.98	0.23
2Y78A_17_27	11	0.78	1.43	4A4AA_818_832	15	1.00	0.18
3L5LA_65_75	11	1.00	0.21	✗ 4ANOA_123_137	15	0.24	18.95
3PMEA_1048_1058	11	0.96	0.29	4E9XA_1073_1087	15	0.99	0.47
3VKWA_891_901	11	0.86	1.02	✗ 4LZKA_32_46	15	0.78	5.13
4DV8A_488_498	11	0.91	0.57	✗ 1IUJA_75_90	16	0.54	24.35
4ITBA_102_112	11	1.00	0.37	2BGKA_99_114	16	0.83	1.80
✗ 4UZGA_426_436	11	0.38	8.31	✗ 2Q88A_192_207	16	0.67	5.68
4YFUA_620_630	11	0.98	0.58	✗ 3ZX4A_219_234	16	0.84	5.63
4ZMYA_40_50	11	0.81	1.21	✗ 4LM8A_125_140	16	0.77	7.08
✗ 5CENA_253_263	11	0.90	8.45	5DAWA_162_177	16	0.92	0.89
5IOJA_406_416	11	1.00	0.23	5KKQA_375_390	16	0.72	1.77
1DJ7A_51_62	12	0.97	0.64	5LX8A_538_553	16	0.99	0.42
1JS1X_273_284	12	0.95	1.08	1GQIA_550_566	17	1.00	0.15
1O00B_104_115	12	0.96	0.24	1U7BA_118_134	17	0.99	0.34
1UF5A_66_77	12	1.00	0.19	2DSKA_626_642	17	1.00	0.18
✗ 1W2WB_367_378	12	0.83	3.12	2I5VO_248_264	17	0.95	0.99
2C4EA_278_289	12	0.88	2.23	2P9BA_386_402	17	0.85	0.68
2ICGA_16_27	12	0.80	2.35	✗ 3DCMX_11_27	17	0.31	16.65
3NIOA_45_56	12	0.93	1.02	3F2VA_85_101	17	0.93	0.45
3UUEA_57_68	12	1.00	0.30	3VENA_464_480	17	0.99	1.50
4B6IA_85_96	12	0.85	2.37	4HDRB_125_141	17	0.93	0.82
5AVDA_224_235	12	0.98	0.51	5B0NA_124_140	17	0.80	2.66
5C9LA_103_114	12	0.99	0.19	5CDKA_105_121	17	0.91	2.01
5MZWB_95_106	12	0.99	0.41	✗ 5LSVA_26_42	17	0.27	21.45
2CB1A_200_212	13	0.95	0.35	1GAIA_254_271	18	1.00	0.12
3AYRA_109_121	13	0.98	0.19	1QQFA_1058_1075	18	0.99	0.20
3TN4A_228_241	13	0.99	0.19	✗ 1UM0A_211_228	18	0.78	3.59
4ETNA_111_123	13	0.99	0.36	2GGSA_112_128	18	0.85	0.32
4EUUA_189_201	13	0.98	0.61	2XZIA_39_56	18	1.00	0.15
4QV2A_536_548	13	0.92	0.47	✗ 3UV0A_26_43	18	0.35	6.33
5E56A_53_65	13	0.91	0.39	✗ 3VSVA_6_23	18	0.47	2.13
5IRCA_1276_1288	13	0.96	0.52	4B4HA_526_543	18	0.99	1.68
2HC9A_258_271	14	0.88	0.56	4R9OA_85_102	18	0.99	0.19
2OZLA_55_68	14	1.00	0.22	✗ 5H3ZA_1072_1089	18	0.59	12.06
2VHKA_177_190	14	1.00	0.21				

✗ = Omitted due to poor model quality (TM score < 0.5 or anchor RMSD > 3Å)

● = Omitted due to having <2 predicted contacts remaining after ignoring those which were never satisfied (Sphinx only)

3. General target set results - non-native environment

(b) Full Sphinx results

Best = RMSD of the best (i.e. closest to native) decoy generated

Best of Top 500 = RMSD of the best decoy remaining in the set after filtering using Sphinx's scoring function

Top Ranked = RMSD of the decoy predicted to be the best by the SOAP-Loop scoring function

Best of Top 5 = RMSD of the best decoy in the top five as ranked by SOAP-Loop

All RMSDs are global backbone RMSDs.

Target	Length	Best	Best of Top 500		Top Ranked		Best of Top 5	
			Normal	Contacts	Normal	Contacts	Normal	Contacts
1F74A_105_114	10	0.25	0.25	0.25	0.45	0.45	0.45	0.45
1NU4A_73_82	10	0.36	0.46	0.46	0.57	0.57	0.57	0.57
1Y0PA_168_177	10	0.24	0.24	0.24	0.29	0.29	0.29	0.29
1ZJCA_18_27	10	1.86	3.03	1.86	6.95	5.29	5.67	3.03
2IVFA_677_686	10	0.44	0.44	0.44	0.65	0.65	0.65	0.65
3JQYA_109_118	10	2.51	2.51	2.51	3.52	3.52	2.70	2.70
3PHXB_127_136	10	0.90	0.96	0.90	2.64	2.64	1.80	1.80
4FFJA_164_173	10	1.38	2.13	1.38	8.84	3.41	7.38	2.13
4N68A_955_964	10	0.46	0.47	0.46	0.57	0.57	0.47	0.47
4W8HA_194_203	10	1.22	1.34	1.22	3.23	3.23	3.23	3.23
5J41A_140_149	10	0.90	1.23	0.90	1.23	1.23	1.23	1.05
5JRHA_331_340	10	0.36	0.36	1.29	1.53	1.93	0.46	1.78
1KGDA_854_864	11	1.53	2.04	1.95	7.25	7.98	5.24	3.49
2D5BA_9_19	11	1.73	2.00	2.00	4.77	4.77	4.77	2.80
2Y78A_17_27	11	1.26	1.42	1.41	2.38	2.38	2.05	1.99
3L5LA_65_75	11	0.12	0.12	0.12	0.12	0.12	0.12	0.12
3PMEA_1048_1058	11	0.37	0.37	0.37	0.82	0.82	0.60	0.60
3VKWA_891_901	11	1.85	2.05	2.01	4.49	4.49	3.42	4.36
4DV8A_488_498	11	0.69	0.69	0.69	0.84	0.84	0.84	0.84
4ITBA_102_112	11	0.37	0.37	0.37	0.49	0.49	0.37	0.37
4YFUA_620_630	11	0.32	0.42	0.33	0.63	0.42	0.63	0.42
4ZMYA_40_50	11	0.46	0.63	2.52	1.74	7.68	1.48	6.75
5IOJA_406_416	11	1.87	1.87	2.39	3.06	3.06	1.87	2.44
1DJ7A_51_62	12	0.30	0.53	0.30	0.96	0.83	0.53	0.71
1JS1X_273_284	12	0.51	0.84	0.71	1.02	1.02	1.02	0.90
1OO0B_104_115	12	0.37	0.37	0.37	0.87	0.87	0.37	0.37
1UF5A_66_77	12	0.44	4.70	0.44	6.28	0.44	6.28	0.44
2C4EA_278_289	12	2.19	4.87	2.76	10.19	10.19	6.82	6.82
2ICGA_16_27	12	2.43	4.74	3.10	11.78	6.94	5.98	5.98
3NIOA_45_56	12	2.17	2.46	2.30	4.30	3.26	2.74	2.74
3UUEA_57_68	12	0.84	0.96	0.84	0.96	0.96	0.96	0.84
4B6IA_85_96	12	2.76	3.95	3.01	7.63	8.11	4.09	4.50
5AVDA_224_235	12	0.54	0.79	0.54	1.17	1.17	1.00	1.00
5C9LA_103_114	12	1.96	3.62	2.56	3.62	3.62	3.62	3.62
5MZWB_95_106	12	1.15	1.15	1.15	3.01	2.84	2.47	2.47
2CB1A_200_212	13	0.56	0.56	0.56	0.88	0.88	0.56	0.56
3AYRA_109_121	13	1.10	3.61	3.65	7.83	6.22	5.60	5.46
3TN4A_229_241	13	0.48	0.79	0.79	3.52	0.79	2.77	0.79
4ETNA_111_123	13	0.91	0.96	0.91	1.45	1.45	1.16	1.16
4EUUA_189_201	13	1.10	1.10	1.10	1.88	1.88	1.88	1.88
4QV2A_536_548	13	2.44	2.77	2.44	6.83	6.83	6.61	3.83
5E56A_53_65	13	2.09	2.88	2.79	3.46	3.46	3.46	3.46
5IRCA_1276_1288	13	0.40	0.40	0.40	0.44	0.44	0.44	0.44
2HC9A_258_271	14	3.35	4.34	4.72	9.65	8.03	5.24	7.41
2OZLA_55_68	14	0.27	0.27	0.27	0.59	0.59	0.27	0.27
2VHKA_177_190	14	1.92	3.51	5.22	7.59	7.59	7.59	7.59
2YIMA_113_126	14	0.94	0.94	0.94	0.94	0.94	0.94	0.94
3QLIA_262_275	14	0.21	0.21	0.21	0.39	0.39	0.26	0.26
3UN7A_461_474	14	1.69	4.56	3.98	7.47	10.29	6.14	4.56
4MDYA_204_217	14	2.47	4.98	4.77	10.23	10.39	10.23	7.89
4P5PA_183_196	14	1.76	3.22	2.96	6.78	6.78	6.78	6.78
1APYA_49_63	15	1.04	1.25	1.04	1.63	1.30	1.36	1.30
1KQPA_205_219	15	1.98	4.57	1.98	10.84	12.79	10.21	4.28
1YSQA_87_101	15	2.42	2.73	2.73	13.54	5.94	10.02	4.73
1ZUOA_333_347	15	1.26	1.26	1.26	1.53	1.53	1.27	1.27
2RB9A_189_203	15	2.53	2.97	2.58	6.18	5.11	2.97	2.97
2VNGA_125_139	15	3.16	3.79	3.58	5.37	4.77	5.05	4.77
3IT3A_60_74	15	1.36	1.36	1.36	4.86	4.86	1.36	1.36
4A4AA_818_832	15	0.56	0.56	0.56	0.56	0.56	0.56	0.56
4E9XA_1073_1087	15	0.60	0.60	0.60	0.68	0.68	0.60	0.60
2BGKA_99_114	16	2.45	2.45	2.45	9.71	11.61	8.06	7.00

3. General target set results - non-native environment
(b) Full Sphinx results (cont.)

Target	Length	Best	Best of Top 500		Top Ranked		Best of Top 5	
			Normal	Contacts	Normal	Contacts	Normal	Contacts
5DAWA_162_177	16	0.95	0.95	0.95	1.01	1.01	0.99	0.99
5KKQA_375_390	16	1.35	1.35	1.35	4.38	4.38	1.76	1.76
5LX8A_538_553	16	1.88	3.49	3.23	5.05	8.26	4.97	4.98
1GQIA_550_566	17	0.14	0.14	0.14	0.30	0.30	0.14	0.14
1U7BA_118_134	17	0.93	0.93	1.45	1.48	1.48	1.22	1.48
2DSKA_626_642	17	0.18	0.18	0.18	0.32	0.32	0.18	0.18
2I5VO_248_264	17	0.61	0.68	0.64	1.84	1.84	1.16	1.16
2P9BA_386_402	17	0.29	0.29	0.49	0.82	0.66	0.68	0.66
3F2VA_85_101	17	0.98	0.98	0.98	4.13	4.13	1.17	1.17
3VENA_464_480	17	0.59	0.59	0.59	1.05	1.05	0.75	0.75
4HDRB_125_141	17	3.48	7.32	5.79	11.70	13.85	11.70	6.52
5B0NA_124_140	17	1.58	1.78	1.58	5.32	6.68	2.72	2.72
5CDKA_105_121	17	2.09	4.28	2.13	9.67	9.67	6.30	2.67
1GAIA_254_271	18	0.77	0.77	0.77	0.77	0.77	0.77	0.77
1QQFA_1058_1075	18	0.24	0.26	0.24	0.41	0.41	0.40	0.37
2GGSA_111_128	18	0.88	5.64	1.58	17.47	1.58	15.99	1.58
2XZIA_39_56	18	0.51	0.51	0.51	1.16	0.89	0.51	0.51
4B4HA_526_543	18	0.81	0.81	0.81	1.00	1.00	0.88	0.96
4R9OA_85_102	18	0.44	0.69	0.44	11.39	0.59	0.70	0.59

Average results:

Length	No. Targets	Best	Best of Top 500		Top Ranked		Best of Top 5	
			Normal	Contacts	Normal	Contacts	Normal	Contacts
10	12	0.91	1.12	0.99	2.54	1.98	2.07	1.51
11	11	0.96	1.09	1.29	2.42	3.00	1.94	2.20
12	12	1.31	2.41	1.51	4.32	3.35	2.99	2.53
13	8	1.13	1.63	1.58	3.29	2.74	2.81	2.20
14	8	1.57	2.75	2.88	5.45	5.62	4.68	4.46
15	9	1.66	2.12	1.74	5.02	4.17	3.71	2.43
16	4	1.66	2.06	2.00	5.04	6.31	3.94	3.68
17	10	1.09	1.72	1.40	3.66	4.00	2.60	1.75
18	6	0.61	1.45	0.72	5.37	0.87	3.21	0.80
ALL	80	1.19	1.78	1.52	3.91	3.40	2.96	2.31

4. Membrane protein target set results

(a) MetaPSICOV contact prediction results - contacts involving at least one target loop residue

Target	Length	No Predicted	No Correct
✗ 1SUMB_108_117	10	0	0
2ERVA_129_138	10	19	15
2RH1A_137_146	10	6	2
2YNKA_225_234	10	5	4
2ZXEA_353_362	10	7	6
✗ 3M73A_130_139	10	1	0
✗ 3QAPA_56_65	10	1	1
✗ 3WFDB_416_425	10	0	0
4AL0A_53_62	10	4	4
4BVNA_195_204	10	2	1
4C9GA_258_267	10	10	6
✗ 4J05A_196_205	10	0	0
✗ 4JKVA_433_442	10	1	0
✗ 4OGQA_22_31	10	0	0
✗ 4US3A_124_133	10	1	1
✗ 5C78A_278_287	10	0	0
5HVXA_154_163	10	4	2
5KLBA_1153_1162	10	6	2
5LWEA_244_253	10	3	1
✗ 5MKKA_55_64	10	0	0
✗ 1FOEC_1107_1117	11	0	0
✗ 1JB0B_27_37	11	1	1
✗ 1QD6C_46_56	11	0	0
✗ 1RKPA_695_705	11	0	0
2E3QA_407_417	11	16	7
3GIAA_173_183	11	4	4
3QE7A_145_155	11	2	1
✗ 3RGBA_221_231	11	1	1
✗ 3WXXA_20_30	11	1	1
✗ 4AFKA_55_65	11	0	0
4D65A_25_35	11	14	11
✗ 4FC4A_126_136	11	0	0
4FSPA_331_341	11	9	7
✗ 4GCOA_187_197	11	0	0
4IKVA_52_62	11	2	2
4KT0F_94_104	11	2	2
✗ 4TQ3A_267_277	11	0	0
4U4VA_285_295	11	15	11
5D91A_139_149	11	2	2
5DL5A_390_400	11	3	3
✗ 1A0TP_169_180	12	1	0
1KF6C_94_105	12	6	3
2GSMA_215_226	12	4	3
✗ 2HDIA_345_356	12	1	1
2R83A_298_309	12	30	21
2W16A_699_710	12	22	14
✗ 2YEVA_226_237	12	1	1
✗ 3DWOX_126_137	12	0	0
✗ 3HD6A_110_121	12	0	0
3W54A_229_240	12	3	3
✗ 3ZOJA_70_81	12	0	0
✗ 4HYJA_66_77	12	0	0
4KNFA_168_179	12	2	1
4Q35A_220_231	12	19	9
4UVMA_397_408	12	7	3
✗ 5A1SA_253_264	12	1	1
5C6PA_46_57	12	28	3
5DL6A_236_247	12	10	4
5GLIA_204_215	12	14	2
5SYTA_148_159	12	5	5
1JB0F_90_102	13	4	1
1PPJC_204_216	13	2	1
1ZHXA_252_264	13	18	11
✗ 2A65A_153_165	13	1	0
2CFQA_137_149	13	12	5
✗ 2GSMA_79_91	13	0	0
✗ 2MPRA_198_210	13	0	0
2QKSA_66_78	13	2	2
2WSWA_163_175	13	12	3
✗ 2XOVA_124_136	13	0	0
3ABMJ_13_25	13	5	2

Target	Length	No Predicted	No Correct
✗ 3B9WA_161_173	13	0	0
3CN5A_148_160	13	3	2
3RKOD_58_70	13	2	1
● 3V2YA_281_293	13	2	1
3VY8X_20_32	13	5	2
✗ 4XNJA_201_213	13	0	0
✗ 4XP9C_541_553	13	1	0
✗ 4ZP0A_192_204	13	1	1
✗ 5G28A_80_92	13	0	0
1OKCA_239_252	14	10	9
✗ 3VY8X_198_211	14	0	0
4CU4A_513_526	14	16	11
4RJWA_349_362	14	2	2
● 4XK8L_13_26	14	2	1
5AEZA_366_379	14	3	2
5C6PA_314_327	14	21	17
✗ 5FVNA_199_212	14	0	0
5IVAA_112_125	14	6	5
✗ 1JB0B_104_118	15	0	0
1U7GA_333_347	15	3	3
2B2HA_320_334	15	2	2
2E3QA_507_521	15	23	18
2FGRA_156_170	15	12	8
✗ 2GSMB_83_97	15	0	0
2WSWA_302_316	15	5	3
✗ 3FIDA_236_250	15	1	1
✗ 3HB3B_60_74	15	0	0
3NSGA_194_208	15	5	4
✗ 3RKOC_50_64	15	0	0
3RSTA_195_209	15	4	2
4CU4A_651_665	15	26	23
4D65A_238_252	15	12	7
✗ 4DX5A_497_511	15	0	0
✗ 4XK8F_184_198	15	1	1
4YMKA_300_314	15	11	5
2W16A_595_610	16	11	8
✗ 2YEVA_443_458	16	1	1
3PBLA_170_185	16	10	3
✗ 4GCOA_104_119	16	0	0
✗ 4MKQA_56_71	16	0	0
5LX9A_331_346	16	8	6
1FOEC_1250_1266	17	5	4
✗ 2YEVB_64_80	17	0	0
3DWOX_361_377	17	11	9
3RKOB_356_372	17	19	15
3RKOC_367_383	17	16	8
✗ 3RQWA_286_302	17	0	0
3UG9A_140_156	17	23	17
3W4TA_219_235	17	2	0
✗ 4AFKA_231_247	17	0	0
4C7RA_210_226	17	25	10
✗ 5AWWY_134_150	17	0	0
✗ 5CXVA_169_185	17	0	0
5DSGA_176_192	17	6	3
✗ 1JB0A_228_245	18	1	0
✗ 1P6DA_123_140	18	1	1
2BHVA_199_216	18	29	23
✗ 3D34A_24_41	18	0	0
✗ 3DDLA_73_90	18	1	0
3FHHA_76_93	18	20	11
3NSGA_233_250	18	13	9
✗ 3RLFG_63_80	18	0	0
4C7RA_120_137	18	11	3
✗ 4LCZA_106_123	18	0	0
4UVMA_197_214	18	2	2
✗ 5B66B_45_62	18	1	1
2B2HA_138_156	19	23	14
✗ 2R9RB_183_201	19	0	0
3D9SA_109_127	19	3	3
3GD8A_137_155	19	3	3
✗ 3RLFF_448_466	19	0	0

4. Membrane protein target set results

(a) MetaPSICOV contact prediction results (cont.)

Target	Length	No Predicted	No Correct	Target	Length	No Predicted	No Correct
3VY8X_152_170	19	12	5	2WJNM_91_110	20	4	4
3WQJA_67_85	19	9	9	3BS0A_109_128	20	3	1
✘ 4EZCA_346_364	19	0	0	3FHHA_612_631	20	22	15
4FBZA_61_79	19	11	11	3WO6A_156_175	20	6	3
4PXZA_162_180	19	7	3	4D65A_153_172	20	6	6
✘ 4Q35A_585_603	19	0	0	4IB4A_107_126	20	15	8
4QIDB_70_88	19	12	12	4RDQA_255_274	20	4	1
✘ 5B66C_135_153	19	1	0	✘ 4RI2A_59_78	20	1	1
2F2BA_123_142	20	3	3	5AEZA_202_221	20	12	1

✘ = Omitted due to having <2 predicted contacts

● = Omitted due to having <2 predicted contacts remaining after ignoring those which were never satisfied (Sphinx only)

4. Membrane protein target set results

(b) Full Sphinx results

Best = RMSD of the best (i.e. closest to native) decoy generated

Best of Top 500 = RMSD of the best decoy remaining in the set after filtering using Sphinx's scoring function

Top Ranked = RMSD of the decoy predicted to be the best by the SOAP-Loop scoring function

Best of Top 5 = RMSD of the best decoy in the top five as ranked by SOAP-Loop

All RMSDs are global backbone RMSDs.

Target	Length	Best	Best of Top 500		Top Ranked		Best of Top 5	
			Normal	Contacts	Normal	Contacts	Normal	Contacts
4BVNA_195_204	10	0.20	0.20	0.20	0.30	0.30	0.30	0.20
5LWEA_244_253	10	0.94	1.09	1.18	1.27	1.35	1.27	1.35
2ZXEA_353_362	10	0.33	0.33	0.41	0.49	0.41	0.41	0.41
5HVXA_154_163	10	0.23	0.23	0.23	0.37	0.52	0.32	0.38
2ERVA_129_138	10	1.88	2.16	2.00	8.43	4.51	7.55	4.36
5KLBA_1153_1162	10	0.22	0.30	0.24	0.45	0.45	0.45	0.38
4C9GA_258_267	10	0.35	0.40	0.35	0.92	0.92	0.44	0.51
4ALOA_53_62	10	0.30	0.30	0.30	0.45	0.45	0.41	0.41
2YNKA_225_234	10	1.43	1.77	1.43	4.11	6.41	4.11	4.84
2RH1A_137_146	10	0.52	0.52	3.91	4.89	4.95	4.83	4.87
2E3QA_407_417	11	0.92	2.70	2.15	5.27	8.13	3.25	2.15
3GIAA_173_183	11	0.59	0.59	0.59	0.92	0.92	0.59	0.59
3QE7A_145_155	11	1.45	3.02	2.60	8.52	8.58	8.23	8.23
4D65A_25_35	11	0.87	1.00	0.87	1.47	1.47	1.47	1.47
4FSPA_331_341	11	1.91	5.87	5.99	7.50	7.50	7.50	5.99
4IKVA_52_62	11	0.26	0.49	0.26	9.71	0.42	5.75	0.42
4KT0F_94_104	11	1.00	1.03	1.00	7.69	1.54	1.06	1.06
4U4VA_285_295	11	0.34	0.34	0.34	0.54	0.54	0.54	0.54
5D91A_139_149	11	0.64	0.64	0.64	0.70	0.76	0.67	0.67
5DL5A_390_400	11	1.70	1.78	1.78	2.66	2.66	2.66	2.66
1KF6C_94_105	12	0.71	3.27	0.89	6.39	6.39	5.03	4.83
2GSMA_215_226	12	0.24	0.24	0.39	0.30	0.70	0.28	0.51
2R83A_298_309	12	2.07	3.12	2.14	7.84	6.90	6.67	6.59
2W16A_699_710	12	1.53	1.57	1.53	1.90	1.90	1.67	1.67
3W54A_229_240	12	1.60	2.89	2.11	4.39	3.97	3.76	2.58
4KNFA_168_179	12	1.25	1.27	1.76	4.89	5.02	3.84	4.95
4Q35A_220_231	12	1.99	2.54	2.85	6.77	6.77	5.83	5.45
4UVMA_397_408	12	1.80	2.06	1.83	2.06	1.83	2.06	1.83
5C6PA_46_57	12	1.66	2.43	2.84	3.71	3.68	3.25	3.68
5DL6A_236_247	12	0.88	0.88	0.88	7.00	9.76	7.00	3.95
5GLIA_204_215	12	1.60	1.99	4.17	5.35	6.06	5.00	5.24
5SYTA_148_159	12	0.47	0.47	0.47	0.60	0.60	0.47	0.47
1JB0F_90_102	13	1.03	2.01	1.57	5.32	8.47	2.01	3.32
1PPJC_204_216	13	0.42	0.42	0.51	0.57	0.57	0.57	0.51
1ZHXA_252_264	13	0.30	0.30	0.30	0.30	0.30	0.30	0.30
2CFQA_137_149	13	0.89	0.89	0.91	0.97	1.04	0.94	0.97
2QKSA_66_78	13	2.63	3.98	4.35	7.10	9.43	5.26	7.90
2WSWA_163_175	13	0.37	0.37	0.37	0.64	0.64	0.41	0.41
3ABMJ_13_25	13	0.84	1.07	1.69	8.63	6.88	3.07	1.70
3CN5A_148_160	13	0.37	0.46	0.37	0.50	0.40	0.46	0.37
3RKOD_58_70	13	2.71	3.39	2.71	8.81	8.97	7.78	8.52
3VY8X_20_32	13	2.28	3.99	3.45	5.72	6.81	5.72	5.54
1OKCA_239_252	14	1.62	1.62	1.62	6.09	4.26	3.14	2.39
4CU4A_513_526	14	0.35	0.40	0.35	0.52	0.52	0.52	0.52
4RJWA_349_362	14	0.41	0.41	0.41	0.84	0.84	0.41	0.41
5AEZA_366_379	14	0.14	0.14	0.14	0.34	0.34	0.26	0.26
5C6PA_314_327	14	1.37	1.37	1.37	5.76	1.37	5.57	1.37
5IVAA_112_125	14	2.44	3.36	6.85	12.30	14.36	9.48	10.84
1U7GA_333_347	15	0.67	0.67	0.67	9.21	0.77	0.77	0.69
2B2HA_320_334	15	3.02	4.89	4.93	7.97	7.97	7.33	7.84
2E3QA_507_521	15	2.54	3.48	3.27	7.72	7.06	4.25	4.34
2FGRA_156_170	15	0.21	0.21	0.41	0.41	0.41	0.33	0.41
2WSWA_302_316	15	0.60	0.60	0.60	0.64	0.64	0.64	0.64
3NSGA_194_208	15	1.78	2.51	3.44	2.89	4.09	2.51	3.87
3RSTA_195_209	15	0.22	0.22	0.22	11.33	0.39	0.39	0.22
4CU4A_651_665	15	0.35	0.49	0.35	0.96	0.68	0.49	0.40
4D65A_238_252	15	1.98	2.32	2.16	19.93	19.93	3.03	19.01
4YMKA_300_314	15	0.91	0.91	0.91	1.03	1.03	0.91	0.91
2W16A_595_610	16	0.79	3.62	0.79	8.29	1.06	6.47	0.79
3PBLA_170_185	16	2.67	3.05	3.05	11.44	11.44	8.42	8.42
5LX9A_331_346	16	0.47	5.30	0.47	7.93	1.40	6.41	0.54

4. Membrane protein target set results (b) Full Sphinx results (cont.)

Target	Length	Best	Best of Top 500		Top Ranked		Best of Top 5	
			Normal	Contacts	Normal	Contacts	Normal	Contacts
1FOEC_1250_1266	17	2.15	3.68	3.51	7.73	5.15	4.94	4.97
3DWOX_361_377	17	2.23	8.62	3.80	15.50	9.88	9.50	9.88
3RKOB_356_372	17	1.40	1.40	1.40	1.61	1.61	1.52	1.52
3RKOC_367_383	17	1.66	1.66	1.66	16.63	16.67	15.25	11.43
3UG9A_140_156	17	0.41	0.41	0.41	0.42	0.42	0.41	0.41
3W4TA_219_235	17	0.54	0.54	0.54	1.37	1.37	0.67	0.65
4C7RA_210_226	17	0.53	0.53	0.53	0.67	0.67	0.53	0.53
5DSGA_176_192	17	0.69	0.69	0.69	9.23	0.69	0.69	0.69
2BHVA_199_216	18	1.99	2.81	2.81	12.08	20.83	6.57	14.92
3FHHA_76_93	18	4.12	4.12	4.12	13.54	13.54	4.43	4.43
3NSGA_233_250	18	0.96	0.96	0.96	1.05	1.05	1.04	0.96
4C7RA_120_137	18	0.68	0.68	0.68	0.68	0.68	0.68	0.68
4UVMA_197_214	18	2.34	2.34	2.34	3.46	3.46	3.46	3.46
2B2HA_138_156	19	0.71	0.71	0.79	1.01	1.01	0.71	0.79
3D9SA_109_127	19	0.33	0.33	0.33	0.41	0.41	0.36	0.36
3GD8A_137_155	19	0.89	0.89	0.89	4.86	1.05	1.05	1.05
3VY8X_152_170	19	2.81	4.99	4.58	11.84	8.08	5.21	5.19
3WQJA_67_85	19	0.59	0.59	0.59	1.09	1.09	0.78	0.78
4FBZA_61_79	19	0.80	0.80	0.80	1.34	1.34	0.91	0.91
4PXZA_162_180	19	3.78	5.00	5.00	8.15	8.15	5.81	5.81
4QIDB_70_88	19	0.62	0.62	0.62	0.94	0.94	0.94	0.94
2F2BA_123_142	20	0.45	0.45	0.45	0.48	0.48	0.45	0.45
2WJNM_91_110	20	0.44	0.44	0.44	0.58	0.58	0.44	0.44
3BS0A_109_128	20	1.55	7.62	7.83	12.16	16.06	10.57	12.71
3FHHA_612_631	20	3.37	11.17	9.30	18.70	12.43	17.00	12.43
3WO6A_156_175	20	1.05	1.05	1.05	9.08	9.08	8.20	9.08
4IB4A_107_126	20	1.23	1.23	1.23	10.31	6.02	4.54	1.23
4RDQA_255_274	20	0.95	1.15	1.47	10.47	1.59	2.81	1.59
5AEZA_202_221	20	0.29	0.29	0.34	0.62	0.49	0.29	0.44

Average results:

Length	No. Targets	Best	Best of Top 500		Top Ranked		Best of Top 5	
			Normal	Contacts	Normal	Contacts	Normal	Contacts
10	10	0.64	0.73	1.02	2.17	2.03	2.01	1.77
11	10	0.97	1.75	1.62	4.50	3.25	3.17	2.38
12	12	1.32	1.89	1.82	4.27	4.47	3.74	3.48
13	10	1.18	1.69	1.62	3.85	4.35	2.65	2.95
14	6	1.05	1.22	1.79	4.31	3.61	3.23	2.63
15	10	1.23	1.63	1.70	6.21	4.30	2.07	3.83
16	3	1.31	3.99	1.44	9.22	4.63	7.10	3.25
17	8	1.20	2.19	1.57	6.65	4.56	4.19	3.76
18	5	2.02	2.18	2.18	6.16	7.91	3.24	4.89
19	8	1.32	1.74	1.70	3.71	2.76	1.97	1.98
20	8	1.17	2.92	2.76	7.80	5.84	5.54	4.80
ALL	90	1.18	1.84	1.73	4.98	4.15	3.27	3.17

4. Membrane protein target set results (c) Full MODELLER results

Best = RMSD of the best (i.e. closest to native) decoy generated

Top Ranked = RMSD of the decoy predicted to be the best by the SOAP-Loop scoring function

Best of Top 5 = RMSD of the best decoy in the top five as ranked by SOAP-Loop

All RMSDs are global backbone RMSDs.

Target	Length	Best		Top Ranked		Best of Top 5	
		Normal	Contacts	Normal	Contacts	Normal	Contacts
4BVNA_195_204	10	1.13	1.02	2.61	2.14	2.02	1.29
5LWEA_244_253	10	1.70	2.52	2.85	5.66	2.27	2.52
2ZXEA_353_362	10	0.58	0.39	0.83	0.45	0.58	0.45
5HVXA_154_163	10	1.44	1.38	1.44	2.68	1.44	1.92
2ERVA_129_138	10	2.33	1.94	7.58	5.55	3.17	2.96
5KLBA_1153_1162	10	2.01	1.27	4.37	3.39	3.27	2.40
4C9GA_258_267	10	1.49	1.66	3.34	2.90	2.73	2.89
4AL0A_53_62	10	2.10	1.41	2.20	2.38	2.20	1.41
2YNKA_225_234	10	1.36	1.48	2.42	2.37	2.42	1.48
2RH1A_137_146	10	1.34	1.35	6.28	5.84	5.15	1.97
2E3QA_407_417	11	1.20	1.16	1.20	1.16	1.20	1.16
3GIAA_173_183	11	2.02	1.08	2.57	1.09	2.02	1.08
3QE7A_145_155	11	1.47	1.39	8.40	4.39	7.74	3.74
4D65A_25_35	11	1.54	1.46	1.78	2.13	1.78	1.86
4FSPA_331_341	11	4.45	3.67	13.54	10.51	10.18	9.22
4IKVA_52_62	11	2.62	3.00	7.06	9.52	3.68	8.12
4KT0F_94_104	11	2.67	2.77	3.59	5.39	3.59	3.41
4U4VA_285_295	11	2.06	1.54	2.06	2.34	2.06	1.61
5D91A_139_149	11	1.37	1.30	5.14	4.33	4.69	4.13
5DL5A_390_400	11	1.69	2.14	3.74	3.61	1.69	2.95
1KF6C_94_105	12	1.78	1.31	5.72	3.08	5.72	3.08
2GSMA_215_226	12	1.97	1.61	3.65	4.52	2.73	4.52
2R83A_298_309	12	2.18	1.73	2.68	4.84	2.68	2.50
2W16A_699_710	12	2.60	1.64	3.94	1.80	3.33	1.64
3W54A_229_240	12	1.77	1.77	2.31	2.86	1.77	1.88
4KNFA_168_179	12	2.90	2.64	5.45	6.06	5.45	4.53
4Q35A_220_231	12	1.65	2.27	5.14	4.40	4.35	2.89
4UVMA_397_408	12	2.48	2.60	2.48	2.68	2.48	2.68
5C6PA_46_57	12	3.04	3.28	11.43	9.99	5.25	3.28
5DL6A_236_247	12	3.73	3.64	7.60	7.59	7.60	7.59
5GLIA_204_215	12	1.25	1.81	5.59	6.43	1.54	6.43
5SYTA_148_159	12	1.49	1.32	4.64	2.29	1.49	1.40
1JB0F_90_102	13	3.26	2.83	4.94	3.94	4.19	3.47
1PPJC_204_216	13	2.60	2.72	3.95	3.71	3.95	2.72
1ZHXA_252_264	13	3.10	3.18	10.09	7.90	4.24	7.08
2CFQA_137_149	13	3.73	3.44	5.32	3.69	5.04	3.69
2QKSA_66_78	13	2.97	2.90	9.19	8.34	5.15	5.50
2WSWA_163_175	13	2.34	1.51	5.18	1.51	2.34	1.51
3ABMJ_13_25	13	3.27	3.39	10.94	5.78	6.93	5.51
3CN5A_148_160	13	1.44	0.68	1.74	0.68	1.74	0.68
3RKOD_58_70	13	0.68	0.85	0.68	0.88	0.68	0.85
3V2YA_281_293	13	2.90	2.60	5.57	2.60	2.90	2.60
3VY8X_20_32	13	3.82	4.73	6.23	6.03	5.89	6.03
1OKCA_239_252	14	1.83	2.00	1.83	2.90	1.83	2.76
4CU4A_513_526	14	3.05	1.79	4.86	7.08	3.05	1.79
4RJWA_349_362	14	3.39	3.96	7.27	8.76	6.42	5.96
4XK8L_13_26	14	3.01	2.88	4.86	5.52	4.86	4.56
5AEZA_366_379	14	2.54	2.21	9.82	4.60	4.19	3.23
5C6PA_314_327	14	3.57	2.48	3.76	3.84	3.76	2.48
5IVAA_112_125	14	2.34	2.55	4.87	3.77	2.66	2.55
1U7GA_333_347	15	2.75	3.74	4.55	5.09	4.55	3.87
2B2HA_320_334	15	5.82	5.90	7.34	10.01	6.92	8.91
2E3QA_507_521	15	2.29	2.12	5.02	3.92	4.60	3.92
2FGRA_156_170	15	3.23	3.07	12.10	10.54	11.87	10.23
2WSWA_302_316	15	3.24	3.02	8.34	4.11	4.98	3.92
3NSGA_194_208	15	2.71	2.31	3.44	5.01	3.16	2.44
3RSTA_195_209	15	2.25	2.81	9.07	3.31	3.51	3.31
4CU4A_651_665	15	4.66	2.13	7.50	2.13	5.05	2.13
4D65A_238_252	15	2.73	2.70	3.55	3.14	3.55	3.14
4YMKA_300_314	15	3.62	2.47	5.65	4.18	4.34	3.53
2W16A_595_610	16	3.68	3.76	5.98	9.23	5.98	8.05
3PBLA_170_185	16	2.88	2.53	8.11	7.53	4.71	3.37

4. Membrane protein target set results (c) Full MODELLER results (cont.)

Target	Length	Best		Top Ranked		Best of Top 5	
		Normal	Contacts	Normal	Contacts	Normal	Contacts
5LX9A_331_346	16	4.63	4.07	14.76	11.46	7.20	4.92
1FOEC_1250_1266	17	4.60	3.72	6.10	7.86	5.80	5.90
3DWOX_361_377	17	2.15	1.65	4.47	3.42	2.15	1.65
3RKOB_356_372	17	3.70	1.84	4.54	2.09	4.54	2.01
3RKOC_367_383	17	3.04	2.06	8.64	2.12	3.04	2.06
3UG9A_140_156	17	3.80	2.59	5.79	2.59	5.79	2.59
3W4TA_219_235	17	2.88	2.68	9.67	7.18	2.88	4.91
4C7RA_210_226	17	3.22	3.50	4.80	4.50	3.32	4.50
5DSGA_176_192	17	4.06	3.52	12.16	9.63	9.98	4.85
2BHVA_199_216	18	3.97	2.10	17.16	4.44	8.58	2.55
3FHHA_76_93	18	2.09	2.24	4.65	4.51	3.55	4.30
3NSGA_233_250	18	2.64	3.57	5.61	4.90	2.64	3.57
4C7RA_120_137	18	4.17	3.32	7.45	10.62	7.45	5.04
4UVMA_197_214	18	3.00	3.04	6.30	5.70	5.27	4.49
2B2HA_138_156	19	4.47	3.17	8.33	3.78	8.33	3.39
3D9SA_109_127	19	3.21	2.81	7.64	6.22	7.64	3.87
3GD8A_137_155	19	3.72	2.81	7.30	5.18	4.03	3.21
3VY8X_152_170	19	5.48	4.24	11.18	14.69	7.86	7.82
3WQJA_67_85	19	3.96	3.35	6.60	4.28	3.96	4.28
4FBZA_61_79	19	3.33	2.50	5.01	3.43	3.75	2.73
4PXZA_162_180	19	3.86	3.08	17.09	8.57	8.61	4.41
4QIDB_70_88	19	4.23	3.74	10.83	8.62	6.67	8.62
2F2BA_123_142	20	4.36	3.85	4.36	4.60	4.36	4.60
2WJNM_91_110	20	4.90	2.80	14.32	13.04	7.30	2.80
3BS0A_109_128	20	4.75	4.00	11.25	17.78	7.41	7.97
3FHHA_612_631	20	3.52	1.91	11.91	5.39	6.26	3.16
3WO6A_156_175	20	4.78	4.73	14.24	7.48	10.66	7.48
4IB4A_107_126	20	4.39	3.89	12.24	7.87	11.86	7.87
4RDQA_255_274	20	3.43	3.50	9.26	10.46	7.70	7.44
5AEZA_202_221	20	3.69	4.21	12.29	5.77	4.92	5.15

Average results:

Length	No. Targets	Best		Top Ranked		Best of Top 5	
		Normal	Contacts	Normal	Contacts	Normal	Contacts
10	10	1.55	1.44	3.39	3.34	2.53	1.93
11	10	2.11	1.95	4.91	4.45	3.86	3.73
12	12	2.24	2.14	5.05	4.71	3.70	3.54
13	11	2.74	2.62	5.80	4.09	3.91	3.60
14	7	2.82	2.55	5.32	5.21	3.82	3.33
15	10	3.33	3.03	6.66	5.14	5.25	4.54
16	3	3.73	3.45	9.61	9.40	5.96	5.45
17	8	3.43	2.70	7.02	4.92	4.69	3.56
18	5	3.18	2.85	8.23	6.04	5.50	3.99
19	8	4.03	3.21	9.25	6.85	6.36	4.79
20	8	4.23	3.61	11.23	9.05	7.56	5.81
ALL	92	2.90	2.58	6.54	5.35	4.62	3.88