Supplementary Material: Contact Prediction for Beta and Alpha-Beta Proteins Using Integer Linear Optimization and its Impact on the First Principles 3D Structure Prediction Method ASTRO-FOLD

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Table 1: Residue contact prediction results when tested on 8 β proteins of test set 1.

		Residue Separation=6			ResSep=12	ResSep=24
PDB ID	Length	Accuracy	AvgTPdis	AvgFPdis	Accuracy	Accuracy
1QJPA	137	0.810(111/137)	6.2	21.1	0.764(84/110)	1.000(28/28)
1D2SA	170	0.606(77/127)	7.1	22.1	0.383(31/81)	0.344(22/64)
1CQYA	99	0.606(60/99)	7.2	15.9	0.663(59/89)	0.694(59/85)
1BMGA	98	0.510(50/98)	9.4	14.1	0.513(41/80)	0.640(32/50)
1MAI_	119	0.328(39/119)	8.0	15.3	0.252(26/103)	0.193(17/88)
1AMX_	150	0.567(85/150)	7.7	17.1	0.568(75/132)	0.558(72/129)
1RSY_	135	0.437(59/135)	8.6	16.3	0.437(59/135)	0.567(55/97)
1HE7A	107	0.636(68/107)	7.7	13.5	0.682(60/88)	0.907(39/43)
Average		**0.563**	**7.7**	**16.9**	**0.532**	**0.612**

Table 2: Residue contact prediction results when tested on 21 $\alpha + \beta$, and α/β proteins of test set 1.

		Residue Separation=6			ResSep=12	ResSep=24
PDB ID	Length	Accuracy	AvgTPdis	AvgFPdis	Accuracy	Accuracy
1MWP	96	0.475 (38/80)	7.7	17.8	0.600 (27/45)	0.634 (26/41)
1QGV	130	0.737 (84/114)	7.2	14.8	0.737 (84/114)	0.814 (79/97)
1DBU	152	0.517 (60/116)	8.0	17.2	0.514 (57/111)	0.542 (45/83)
1XER	103	0.353 (18/51)	7.8	14.7	0.233 (10/43)	0.091 (2/22)
1JSF	130	0.667 (16/24)	7.8	17.7	0.462 (6/13)	0.167 (1/6)
1DZO	120	0.865 (64/74)	6.7	13.4	0.857 (48/56)	NA (0/0)
1GRJ	76	0.672 (41/61)	7.1	13.6	0.689 (31/45)	0.654 (17/26)
1MSC	129	0.566 (73/129)	8.5	17.0	0.539 (62/115)	0.523 (46/88)
1CEW	108	0.611 (66/108)	7.3	18.8	0.581 (50/86)	0.408 (20/49)
1VHH	157	0.424 (39/92)	7.6	16.7	0.329 (26/79)	0.246 (15/61)
1BUO	121	0.655 (36/55)	8.0	18.9	0.667 (24/36)	0.643 (18/28)
1G2R	94	0.763 (29/38)	7.5	14.1	0.720 (18/25)	1.000 (2/2)
1E9M	106	0.880 (44/50)	6.6	16.3	0.861 (31/36)	0.966 (28/29)
1E87	117	0.514 (55/107)	6.9	17.8	0.519 (55/106)	0.524 (54/103)
1H9O	108	0.500 (36/72)	7.6	16.0	0.632 (12/19)	NA (0/0)
1IDO	184	0.529 (73/138)	8.4	15.1	0.512 (63/123)	0.530 (61/115)
1CHD	198	0.534 (79/148)	7.4	17.9	0.489 (66/135)	0.402 (45/112)
1FUE	163	0.551 (54/98)	7.6	16.8	0.552 (53/96)	0.552 (53/96)
1CXQ	143	0.711 (59/83)	7.0	15.2	0.619 (39/63)	0.211 (4/19)
1ES8	196	0.556 (80/144)	7.4	19.7	0.522 (60/115)	0.653 (49/75)
1DMG	172	0.556 (65/117)	8.6	15.0	0.575 (65/113)	0.619 (52/84)
Average		**0.602**	**7.6**	**16.4**	**0.581**	**0.536**

Table 3: Residue contact prediction results when tested on 25 β test proteins of test set 2.

		Residue Separation=6			ResSep=8	ResSep=12	ResSep=24
PDB ID	Length	Accuracy	AvgTPdis	AvgFPdis	Accuracy	Accuracy	Accuracy
1PRR	90	0.602 (50/83)	7.3	14.8	0.602 (50/83)	0.568 (42/74)	0.605 (26/43)
3PCG	200	0.300 (45/150)	7.7	16.3	0.300 (45/150)	0.297 (44/148)	0.299 (44/147)
1GOF	150	0.518 (73/141)	7.1	15.1	0.518 (73/141)	0.514 (72/140)	0.514 (72/140)
1TSR	196	0.299 (44/147)	8.2	15.6	0.270 (38/141)	0.233 (30/129)	0.252 (27/107)
1IS6	134	0.261 (35/134)	7.5	17.4	0.171 (19/111)	0.073 (6/82)	0.000 (0/55)
1C5H	185	0.594 (82/138)	7.3	16.9	0.560 (70/125)	0.505 (48/95)	0.553 (26/47)
1ESO	154	0.643 (74/115)	7.2	15.4	0.631 (70/111)	0.606 (63/104)	0.437 (31/71)
1F3Z	150	0.280 (42/150)	7.8	19.0	0.284 (40/141)	0.308 (40/130)	0.347 (35/101)
1CDQ	77	0.919 (34/37)	6.9	13.6	0.903 (28/31)	0.857 (18/21)	0.813 (13/16)
1A5M	100	0.588 (30/51)	8.6	15.4	0.575 (23/40)	0.846 (11/13)	NA (0/0)
1PDG	87	0.448 (39/87)	7.8	22.9	0.443 (35/79)	0.418 (28/67)	0.178 (8/45)
1IU0	91	0.442 (38/86)	7.5	15.9	0.442 (38/86)	0.493 (36/73)	0.418 (23/55)
2DYN	111	0.523 (58/111)	7.4	16.3	0.546 (53/97)	0.500 (39/78)	0.429 (18/42)
1AUU	55	1.000 (28/28)	6.4	0.0	1.000 (23/23)	1.000 (14/14)	1.000 (5/5)
1AN7	136	0.421 (56/133)	7.2	20.3	0.403 (48/119)	0.359 (37/103)	0.176 (13/74)
1BBZ	58	0.810 (47/58)	6.9	14.6	0.896 (43/48)	0.895 (34/38)	0.813 (13/16)
1A1R	152	0.693 (79/114)	7.3	15.4	0.632 (60/95)	0.517 (31/60)	0.385 (10/26)
1KDU	85	0.800 (16/20)	6.4	10.9	0.733 (11/15)	0.400 (2/5)	0.500 (1/2)
2SNS	141	0.653 (32/49)	8.9	13.2	0.653 (32/49)	0.543 (19/35)	0.515 (17/33)
1WHI	122	0.627(74/118)	8.5	13.3	0.627(74/118)	0.610(64/105)	0.521(37/71)
1OCA	165	0.537 (66/123)	7.5	15.9	0.509 (59/116)	0.472 (51/108)	0.325 (25/77)
6I1B	153	0.789 (90/114)	6.7	16.0	0.753 (73/97)	0.682 (45/66)	0.609 (14/23)
1JAC	133	0.398 (53/133)	7.4	15.9	0.376 (44/117)	0.360 (27/75)	0.125 (4/32)
1JPC	108	0.861 (93/108)	7.1	14.3	0.838 (62/74)	0.636 (21/33)	0.538 (14/26)
1RIE	127	0.467 (56/120)	8.2	17.2	0.443 (51/115)	0.429 (48/112)	0.418 (46/110)
Average		**0.579**	**7.5**	**15.3**	**0.564**	**0.525**	**0.449**

Table 4: Residue contact prediction results when tested on 29 $\alpha+\beta$, and α/β test proteins of test set 2.

		Residue Separation=6			ResSep=8	ResSep=12	ResSep=24
PDB ID	Length	Accuracy	AvgTPdis	AvgFPdis	Accuracy	Accuracy	Accuracy
1FRD	98	0.490 (48/98)	7.6	16.3	0.495 (48/97)	0.493 (35/71)	0.500 (32/64)
1TIF	76	0.853 (58/68)	7.5	16.2	0.836 (51/61)	0.756 (31/41)	0.630 (17/27)
1B5M	84	0.842 (32/38)	7.6	10.3	0.818 (27/33)	0.833 (25/30)	0.833 (25/30)
1DMX	237	0.424 (75/177)	7.7	21.6	0.429 (70/163)	0.424 (61/144)	0.346 (44/127)
1BP1	217	0.333 (54/162)	7.8	28.1	0.300 (45/150)	0.275 (36/131)	0.252 (27/107)
1YDV	246	0.457 (63/138)	7.4	15.9	0.456 (62/136)	0.456 (62/136)	0.470 (62/132)
1ONE	141	0.761 (51/67)	7.4	14.4	0.746 (44/59)	0.722 (26/36)	NA (0/0)
1EAF	243	0.497 (87/175)	7.9	20.4	0.519 (83/160)	0.560 (75/134)	0.584 (66/113)
1GLU	81	0.615 (8/13)	9.8	16.2	0.667 (8/12)	0.600 (6/10)	0.556 (5/9)
1BHP	45	0.947 (18/19)	7.6	12.3	0.941 (16/17)	1.000 (12/12)	1.000 (10/10)
1RIS	97	0.526 (51/97)	6.8	16.4	0.526 (51/97)	0.526 (51/97)	0.526 (51/97)
1MLA	70	0.943 (66/70)	6.6	11.3	0.938 (61/65)	0.927 (51/55)	0.957 (45/47)
1DBD	100	0.962 (51/53)	6.4	19.7	0.962 (51/53)	0.962 (51/53)	1.000 (51/51)
1F5M	176	0.591 (78/132)	6.6	15.8	0.583 (74/127)	0.541 (60/111)	0.420 (34/81)
1APY	161	0.880 (44/50)	7.3	19.2	0.870 (40/46)	0.882 (30/34)	0.727 (8/11)
1QNX	209	0.327 (51/156)	9.3	18.4	0.327 (51/156)	0.333 (43/129)	0.343 (37/108)
1JUL	247	0.261 (37/142)	8.1	16.0	0.250 (35/140)	0.246 (34/138)	0.252 (34/135)
2HGF	97	0.926 (50/54)	6.7	10.1	0.918 (45/49)	0.900 (36/40)	0.892 (33/37)
1DIV	55	1.000 (24/24)	6.6	0.0	1.000 (24/24)	1.000 (23/23)	1.000 (11/11)
1BLE	161	0.533 (64/120)	7.9	18.0	0.533 (64/120)	0.533 (64/120)	0.536 (59/110)
1IOW	96	0.886 (39/44)	7.0	14.5	0.886 (39/44)	0.949 (37/39)	0.974 (37/38)
2PIA	103	0.584 (59/101)	8.0	15.3	0.577 (56/97)	0.568 (46/81)	0.565 (35/62)
2SCU	121	0.604 (58/96)	7.8	16.7	0.604 (58/96)	0.600 (57/95)	0.500 (26/52)
1LFA	183	0.574 (78/136)	7.6	18.8	0.574 (78/136)	0.578 (78/135)	0.486 (53/109)
1A1S	150	0.512 (42/82)	9.1	14.4	0.512 (42/82)	0.512 (42/82)	0.522 (35/67)
1O7B	98	0.623 (33/53)	6.7	14.8	0.635 (33/52)	0.673 (33/49)	0.594 (19/32)
1DEF	147	0.576 (38/66)	7.2	14.8	0.691 (38/55)	0.644 (29/45)	0.568 (21/37)
1MLD	144	0.640 (73/114)	8.9	13.5	0.640 (73/114)	0.637 (72/113)	0.625 (60/96)
1FIB	249	0.505 (94/186)	7.6	17.6	0.497 (91/183)	0.463 (74/160)	0.253 (24/95)
Average		**0.643**	**7.6**	**15.8**	**0.646**	**0.641**	**0.604**

Table 5: Residue contact prediction results when tested on 29 $\alpha + \beta$, and α/β test proteins of test set 2 with secondary structure information derived using PSIPRED.

		Residue Separation=6			ResSep=8	ResSep=12	ResSep=24
PDB ID	Length	Accuracy	AvgTPdis	AvgFPdis	Accuracy	Accuracy	Accuracy
1FRD	98	0.488 (40/82)	7.3	16.3	0.488 (39/80)	0.460 (29/63)	0.423 (22/52)
1TIF	76	0.903 (28/31)	8.4	12.1	0.903 (28/31)	0.833 (15/18)	0.800 (12/15)
1B5M	84	0.830 (39/47)	7.6	12.8	0.810 (34/42)	0.788 (26/33)	0.788 (26/33)
1DMX	237	0.537 (95/177)	8.3	19.8	0.541 (92/170)	0.525 (85/162)	0.511 (71/139)
1BP1	217	0.333 (54/162)	9.3	40.1	0.325 (52/160)	0.307 (46/150)	0.287 (41/143)
1YDV	246	0.426 (60/141)	8.7	15.1	0.429 (60/140)	0.429 (60/140)	0.361 (44/122)
1ONE	141	0.511 (45/88)	9.2	17.4	0.488 (40/82)	0.491 (27/55)	0.565 (13/23)
1EAF	243	0.302 (55/182)	8.6	26.6	0.269 (45/167)	0.257 (38/148)	0.295 (38/129)
1GLU	81	0.563 (18/32)	8.1	21.0	0.548 (17/31)	0.517 (15/29)	0.500 (5/10)
1BHP	45	0.769 (10/13)	8.5	14.1	0.727 (8/11)	0.750 (3/4)	NA (0/0)
1RIS	97	0.567 (55/97)	7.9	14.6	0.567 (55/97)	0.567 (55/97)	0.587 (54/92)
1MLA	70	0.613 (38/62)	7.7	13.8	0.607 (37/61)	0.585 (31/53)	0.686 (24/35)
1DBD	100	0.650 (65/100)	7.9	16.9	0.684 (65/95)	0.707 (65/92)	0.846 (55/65)
1F5M	176	0.538 (71/132)	8.4	16.8	0.528 (67/127)	0.483 (56/116)	0.422 (38/90)
1APY	161	0.579 (44/76)	7.9	20.3	0.563 (40/71)	0.500 (28/56)	0.265 (9/34)
1QNX	209	0.568 (50/88)	7.8	15.2	0.548 (46/84)	0.541 (40/74)	0.491 (27/55)
1JUL	247	0.570 (90/158)	8.2	15.1	0.570 (90/158)	0.577 (90/156)	0.622 (89/143)
2HGF	97	0.754 (49/65)	7.7	13.7	0.738 (45/61)	0.756 (31/41)	0.744 (29/39)
1DIV	55	0.875 (14/16)	7.0	12.3	0.875 (14/16)	0.867 (13/15)	NA (0/0)
1BLE	161	0.542 (65/120)	8.2	16.1	0.542 (65/120)	0.565 (65/115)	0.616 (61/99)
1IOW	96	0.830 (39/47)	7.8	13.6	0.830 (39/47)	0.830 (39/47)	0.826 (38/46)
2PIA	103	0.631 (65/103)	7.4	16.2	0.616 (61/99)	0.624 (53/85)	0.698 (44/63)
2SCU	121	0.423 (47/111)	9.0	16.6	0.423 (47/111)	0.423 (47/111)	0.429 (45/105)
1LFA	183	0.832 (114/137)	6.9	16.3	0.827 (110/133)	0.816 (102/125)	0.848 (84/99)
1A1S	150	0.789 (60/76)	6.7	17.0	0.789 (60/76)	0.789 (60/76)	0.769 (40/52)
1O7B	98	0.493 (36/73)	6.9	15.5	0.500 (36/72)	0.522 (35/67)	0.536 (15/28)
1DEF	147	0.422 (62/147)	8.1	18.3	0.439 (61/139)	0.408 (53/130)	0.350 (41/117)
1MLD	144	0.671 (55/82)	7.9	15.1	0.671 (55/82)	0.667 (54/81)	0.667 (50/75)
1FIB	249	0.522 (97/186)	8.0	16.1	0.519 (95/183)	0.488 (78/160)	0.446 (58/130)
Average		**0.605**	**7.9**	**17.0**	**0.599**	**0.589**	**0.570**

Table 6: Residue contact prediction results when tested on 100 β and mixed α/β proteins of test set 3.

		Residue Separation=6			ResSep=12	ResSep=24
PDB ID	Length	Accuracy	AvgTPdis	AvgFPdis	Accuracy	Accuracy
1QLD	50	0.833 (20/24)	7.1	12.1	0.733 (11/15)	1.000 (1/1)
1Z0R	53	1.000 (15/15)	6.2	NA	1.000 (1/1)	NA (0/0)
1S0Y	55	0.552 (16/29)	7.5	15.3	0.552 (16/29)	0.552 (16/29)
1P65	57	0.875 (14/16)	7.6	14.8	0.750 (3/4)	1.000 (3/3)
1CXW	60	0.786 (22/28)	6.5	12.8	0.739 (17/23)	1.000 (1/1)
1HX2	60	0.810 (17/21)	5.9	13.3	0.813 (13/16)	0.857 (12/14)
1DTD	61	0.754 (46/61)	8.5	13.2	0.681 (32/47)	0.634 (26/41)
1HZ6	63	0.556 (35/63)	7.6	15.7	0.500 (19/38)	0.593 (16/27)
2FQM	64	0.621 (18/29)	6.3	22.5	0.000 (0/11)	0.000 (0/11)
2A50	64	0.557 (34/61)	7.8	14.4	0.548 (17/31)	1.000 (2/2)
1F02	66	0.727 (16/22)	8.6	13.2	0.900 (9/10)	1.000 (4/4)
1UW1	67	0.966 (28/29)	6.2	11.3	1.000 (21/21)	1.000 (11/11)
1VBW	68	0.667 (16/24)	7.0	12.9	0.667 (16/24)	1.000 (1/1)
4ULL	69	0.744 (32/43)	6.3	12.5	0.737 (28/38)	0.929 (13/14)
1BB8	71	0.667 (16/24)	7.7	14.2	0.750 (3/4)	NA (0/0)
1KN6	73	0.966 (28/29)	6.9	3.9	0.966 (28/29)	0.966 (28/29)
1I27	73	1.000 (10/10)	6.4	NA	NA (0/0)	NA (0/0)
1OK0	74	0.541 (40/74)	8.8	14.1	0.529 (36/68)	0.667 (26/39)
1TH5	74	0.818 (18/22)	7.5	13.4	0.800 (16/20)	0.800 (16/20)
1HLQ	75	1.000 (2/2)	8.8	NA	1.000 (2/2)	1.000 (1/1)
1LJO	75	0.760 (57/75)	7.3	14.2	0.691 (38/55)	0.444 (12/27)
1KVD	77	0.531 (34/64)	8.7	13.9	0.531 (34/64)	0.531 (34/64)
1KP6	79	0.613 (38/62)	8.9	14.7	0.607 (37/61)	0.684 (26/38)
1ZT3	80	0.714 (10/14)	6.3	14.4	0.636 (7/11)	0.000 (0/3)
1XS3	80	0.794 (27/34)	7.7	12.4	0.794 (27/34)	0.708 (17/24)
1IS7	84	0.845 (71/84)	7.1	13.4	0.814 (57/70)	0.794 (50/63)
1F53	84	0.651 (41/63)	8.0	13.3	0.553 (21/38)	0.214 (3/14)
2A6S	84	0.934 (57/61)	7.3	13.6	0.840 (21/25)	0.778 (14/18)
1E44	84	0.869 (73/84)	7.0	16.2	0.941 (64/68)	1.000 (50/50)
1Y96	85	0.624 (53/85)	7.2	14.0	0.630 (29/46)	0.500 (6/12)
1OPD	85	0.655 (36/55)	7.7	14.8	0.655 (36/55)	0.655 (36/55)
1X9A	87	0.712 (37/52)	7.8	12.4	0.712 (37/52)	0.545 (12/22)
1GH8	89	0.976 (80/82)	6.6	16.4	0.976 (80/82)	0.976 (80/82)
						Continued..

Table 7: Residue contact prediction results when tested on 100 β and mixed α/β proteins of test set 3.

		Residue Separation=6			ResSep=12	ResSep=24
PDB ID	Length	Accuracy	AvgTPdis	AvgFPdis	Accuracy	Accuracy
1U07	90	0.452 (38/84)	8.2	15.5	0.452 (38/84)	0.535 (38/71)
1F60	90	0.911 (82/90)	7.1	12.5	0.900 (72/80)	0.867 (52/60)
1XEE	91	0.653 (47/72)	7.0	15.4	0.565 (26/46)	0.441 (15/34)
1FUW	91	0.857 (42/49)	6.6	11.6	0.813 (26/32)	1.000 (1/1)
1T23	93	0.548 (51/93)	7.5	16.2	0.437 (31/71)	0.311 (14/45)
2A8K	94	0.767 (46/60)	8.5	12.2	0.711 (32/45)	0.815 (22/27)
1PYT	94	0.694 (50/72)	8.6	19.3	0.694 (50/72)	0.791 (34/43)
1IM3	95	0.558 (53/95)	6.8	14.2	0.425 (31/73)	0.030 (1/33)
1JO0	96	0.741 (43/58)	7.2	14.1	0.727 (32/44)	0.886 (31/35)
2HGF	97	0.926 (50/54)	6.7	10.1	0.900 (36/40)	0.892 (33/37)
1OVY	97	0.636 (28/44)	7.9	14.1	0.571 (8/14)	1.000 (2/2)
1PRT	98	0.592 (58/98)	7.3	13.8	0.529 (37/70)	0.200 (5/25)
1LM0	101	0.683 (69/101)	7.3	13.1	0.579 (44/76)	0.429 (24/56)
1ZDX	101	0.813 (78/96)	7.3	12.9	0.778 (63/81)	0.717 (43/60)
3EZM	101	0.406 (41/101)	6.5	24.5	0.161 (9/56)	0.000 (0/37)
1GO1	102	0.783 (54/69)	7.1	21.0	0.783 (54/69)	0.907 (49/54)
1JT8	102	0.696 (71/102)	8.5	15.6	0.644 (56/87)	0.631 (53/84)
1Z5F	104	0.489 (44/90)	8.1	16.3	0.375 (27/72)	0.419 (13/31)
1N6Z	105	0.698 (67/96)	7.5	15.9	0.708 (51/72)	0.708 (51/72)
1EW4	106	0.651 (69/106)	8.0	15.5	0.493 (33/67)	0.143 (2/14)
1KAF	108	0.731 (79/108)	7.8	14.9	0.629 (44/70)	0.636 (21/33)
1YH5	108	0.686 (35/51)	8.3	13.6	0.594 (19/32)	0.478 (11/23)
2D0P	110	0.620 (57/92)	8.0	14.2	0.581 (43/74)	0.688 (33/48)
2BHO	110	0.536 (59/110)	7.5	15.4	0.444 (24/54)	0.447 (21/47)
1WWQ	111	0.781 (50/64)	7.3	13.2	0.702 (33/47)	0.667 (14/21)
1D4U	111	0.923 (12/13)	6.5	26.6	0.909 (10/11)	NA (0/0)
1NYC	111	0.820 (91/111)	6.7	14.3	0.775 (69/89)	0.661 (39/59)
1O5P	113	0.372 (42/113)	8.0	16.1	0.370 (34/92)	0.430 (34/79)
1N3G	113	0.470 (39/83)	8.7	16.2	0.500 (22/44)	1.000 (11/11)
1WHG	113	0.593 (54/91)	8.2	14.6	0.600 (48/80)	0.627 (37/59)
1F86	115	0.791 (91/115)	6.7	13.5	0.745 (70/94)	0.586 (34/58)
2B7F	116	0.595 (66/111)	8.0	15.2	0.564 (53/94)	0.547 (29/53)
1WN2	118	0.541 (53/98)	8.5	14.1	0.526 (50/95)	0.516 (47/91)

Continued..

Table 8: Residue contact prediction results when tested on 100 β and mixed α/β proteins of test set 3.

		Residue Separation=6			ResSep=12	ResSep=24
PDB ID	Length	Accuracy	AvgTPdis	AvgFPdis	Accuracy	Accuracy
1K3B	119	0.429 (51/119)	7.1	18.4	0.319 (23/72)	0.294 (10/34)
1SSF	123	0.439 (54/123)	7.4	16.8	0.341 (31/91)	0.319 (22/69)
1MAE	124	0.395 (34/86)	7.6	17.7	0.481 (25/52)	0.429 (18/42)
1HKQ	125	0.656 (61/93)	7.3	20.3	0.795 (31/39)	0.742 (23/31)
1SZV	125	0.563 (63/112)	7.3	15.6	0.474 (36/76)	0.395 (15/38)
1EIO	127	0.622 (79/127)	7.3	15.4	0.606 (40/66)	0.621 (18/29)
1A63	130	0.625 (40/64)	7.9	13.7	0.613 (38/62)	0.545 (12/22)
1Z1D	131	0.439 (54/123)	7.9	17.1	0.355 (38/107)	0.354 (29/82)
1C7K	132	0.617 (58/94)	7.7	16.0	0.614 (51/83)	0.431 (22/51)
1TQZ	133	0.451 (51/113)	7.0	16.7	0.400 (32/80)	0.228 (13/57)
1IS3	134	0.261 (35/134)	7.5	17.5	0.073 (6/82)	0.000 (0/55)
1QYN	136	0.647 (88/136)	7.3	22.6	0.584 (66/113)	0.444 (32/72)
1CL3	138	0.669 (81/121)	7.8	15.1	0.622 (56/90)	0.476 (38/66)
1WKI	141	0.694 (43/62)	7.5	17.2	0.694 (43/62)	0.694 (43/62)
1KTU	143	0.410 (32/78)	7.2	14.5	0.188 (9/48)	0.000 (0/24)
1W4S	146	0.541 (79/146)	6.9	17.0	0.484 (59/122)	0.159 (11/69)
1IDP	147	0.483 (71/147)	7.8	15.4	0.400 (50/125)	0.253 (24/95)
1JL1	152	0.605 (69/114)	7.0	17.0	0.660 (66/100)	1.000 (45/45)
1HQK	154	0.514 (55/107)	7.7	17.9	0.514 (55/107)	0.519 (55/106)
1P6O	156	0.586 (65/111)	8.1	16.6	0.575 (61/106)	0.564 (44/78)
1ZWT	158	0.977 (42/43)	7.3	11.6	0.971 (34/35)	0.968 (30/31)
1AX3	162	0.240 (29/121)	7.7	17.0	0.278 (25/90)	0.284 (25/88)
1SK3	165	0.632 (72/114)	7.5	18.2	0.604 (64/106)	0.610 (64/105)
1XPN	170	0.740 (94/127)	7.5	11.9	0.778 (77/99)	0.815 (53/65)
1OQV	171	0.513 (60/117)	7.2	17.2	0.513 (60/117)	0.588 (47/80)
1CV8	173	0.271 (35/129)	9.0	16.5	0.256 (31/121)	0.248 (26/105)
1C5F	173	0.550 (71/129)	6.8	16.7	0.487 (55/113)	0.345 (29/84)
1OH4	174	0.292 (38/130)	8.6	18.4	0.269 (29/108)	0.305 (29/95)
1I40	175	0.374 (49/131)	8.8	19.3	0.374 (49/131)	0.300 (30/100)
1BNL	178	0.625 (45/72)	7.5	17.3	0.625 (45/72)	0.672 (45/67)
1UCD	190	0.401 (57/142)	8.7	18.6	0.416 (57/137)	0.414 (55/133)
2CAR	194	0.497 (72/145)	6.8	21.5	0.478 (65/136)	0.348 (31/89)
1K4I	216	0.358 (43/120)	7.8	19.9	0.321 (36/112)	0.277 (28/101)
2BO9	217	0.660 (107/162)	8.4	14.6	0.635 (87/137)	0.544 (43/79)
Average		**0.646**	**7.5**	**15.0**	**0.603**	**0.675**

Table 9: Residue contact prediction results for 20 selected CASP8 proteins.

		Residue Separation=6			ResSep=8	ResSep=12	ResSep=24
PDB ID	Length	Accuracy	AvgTPdis	AvgFPdis	Accuracy	Accuracy	Accuracy
t389	134	0.607 (37/61)	7.2	19.4	0.600 (36/60)	0.596 (34/57)	0.733 (33/45)
t399	162	0.603 (73/121)	6.8	17.8	0.577 (60/104)	0.566 (43/76)	0.000 (0/32)
t401	132	0.378 (34/90)	7.3	15.7	0.382 (34/89)	0.254 (16/63)	0.078 (4/51)
t411	120	0.769 (30/39)	7.2	18.1	0.763 (29/38)	0.763 (29/38)	0.857 (24/28)
t415	109	0.491 (53/108)	6.9	18.4	0.487 (38/78)	0.310 (13/42)	0.216 (8/37)
t417	159	0.580 (69/119)	7.6	16.6	0.569 (66/116)	0.533 (57/107)	0.453 (39/86)
t425	181	0.430 (52/121)	8.1	15.5	0.415 (49/118)	0.436 (48/110)	0.488 (41/84)
t437	99	0.175 (17/97)	7.0	20.4	0.140 (13/93)	0.079 (5/63)	0.044 (2/45)
t451	133	0.576 (76/132)	7.9	17.3	0.598 (70/117)	0.612 (60/98)	0.429 (27/63)
t460	111	0.836 (51/61)	7.4	13.0	0.815 (44/54)	0.800 (36/45)	0.750 (21/28)
t466	108	0.250 (27/108)	7.7	18.1	0.247 (22/89)	0.227 (15/66)	0.375 (9/24)
t468	109	0.443 (39/88)	7.1	16.6	0.443 (39/88)	0.443 (39/88)	0.414 (24/58)
t469	65	0.900 (9/10)	9.9	12.4	0.900 (9/10)	0.900 (9/10)	0.900 (9/10)
t471	133	0.373 (47/126)	7.3	16.7	0.342 (41/120)	0.225 (23/102)	0.111 (8/72)
t474	80	0.833 (5/6)	9.8	14.5	0.833 (5/6)	1.000 (2/2)	NA (0/0)
t476	87	0.167 (3/18)	9.6	18.7	0.167 (3/18)	0.167 (3/18)	0.167 (3/18)
t480	55	0.152 (7/46)	9.4	19.1	0.189 (7/37)	0.214 (6/28)	NA (0/0)
t482	120	0.507 (38/75)	7.2	16.5	0.507 (38/75)	0.486 (35/72)	0.176 (3/17)
t492	73	0.575 (42/73)	7.3	15.2	0.551 (38/69)	0.481 (26/54)	0.516 (16/31)
t495	146	0.707 (87/123)	7.9	15.0	0.681 (77/113)	0.622 (51/82)	0.294 (5/17)
Average		**0.518**	**7.8**	**16.8**	**0.510**	**0.486**	**0.389**

Table 10: A comparison of RMSD, TM score and GDT score distributions for predicted tertiary structures of proteins generated 1) using predicted residue contacts and 2) without using predicted contacts.

Proteins	With Predicted Contacts			Without Predicted Contacts		
	RMSD range	TM range	GDT range	RMSD range	TM range	GDT range
1J75	2.98-12.15	0.24-0.57	0.33-0.67	5.06-22.56	0.24-0.52	0.30-0.61
1CTJ	5.26-17.76	0.21-0.44	0.23-0.45	7.99-33.05	0.20-0.40	0.22-0.40
1ELR	4.59-18.12	0.20-0.57	0.20-0.49	8.63-33.45	0.16-0.41	0.17-0.36
1R69	3.74-12.55	0.21-0.49	0.28-0.56	4.58-22.32	0.20-0.44	0.25-0.54
1AUU	4.31-15.33	0.18-0.48	0.24-0.59	6.93-42.28	0.11-0.31	0.16-0.38
T499	5.20-11.73	0.22-0.39	0.29-0.54	6.58-30.58	0.22-0.38	0.27-0.46
T473	5.01-12.44	0.23-0.42	0.30-0.54	5.90-27.87	0.22-0.40	0.26-0.47
1C75	5.11-13.38	0.20-0.41	0.23-0.47	5.91-26.45	0.19-0.39	0.22-0.44
1HCR	4.05-15.20	0.22-0.62	0.29-0.70	4.83-18.55	0.21-0.49	0.28-0.59
1ROP	0.99-6.53	0.33-0.90	0.49-0.96	1.34-23.96	0.37-0.85	0.46-0.93

Table 11: A comparison of the numbers of the meaningful structures of proteins generated 1) using predicted residue contacts and 2) without using predicted contacts.

Proteins	With Predicted Contacts			Without Predicted Contacts		
	RMSD < 6Å	TM > 0.4	GDT > 0.4	RMSD < 6Å	TM > 0.4	GDT > 0.4
1J75	14262	5999	25361	383	18	13742
1CTJ	10	30	103	0	0	0
1ELR	10	359	132	0	1	0
1R69	2520	280	7268	264	26	1946
1AUU	497	700	7980	0	0	0
T499	244	0	3194	0	0	2077
T473	108	11	4060	1	2	266
1C75	8	1	313	4	0	134
1HCR	418	2458	19390	102	206	11967
1ROP	32409	32290	32481	31144	35042	35108