Template-based and free modeling of I-TASSER and QUARK pipelines using predicted contact maps in CASP12

Chengxin Zhang, S. M. Mortuza, Baoji He, Yanting Wang, Yang Zhang

Supplemental Materials

Table S1. Comparison of template quality before and after QUARK-based sorting using domains defined by CASP12 accessors. The number outside parentheses is TM-score, while the number inside parenthesis is GDT_TS.

target domain	"QUARK" with contact		QUARK without contact	
	first model	best model in top 5	first model	best model in top 5
T0859-D1	0.26 (25)	0.28 (27)	0.23 (24)	0.26 (26)
T0862-D1	0.37 (41)	0.54 (59)	0.41 (40)	0.50 (50)
T0863-D1	0.30 (23)	0.30 (23)	0.25 (21)	0.27 (22)
T0864-D1	0.19 (13)	0.36 (22)	0.23 (14)	0.23 (14)
T0866-D1	0.49 (46)	0.56 (56)	0.32 (33)	0.47 (47)
T0869-D1	0.32 (36)	0.34 (36)	0.25 (26)	0.27 (27)
T0870-D1	0.21 (21)	0.39 (34)	0.21 (20)	0.28 (26)
T0878-D1	0.20 (12)	0.20 (12)	0.15 (9)	0.17 (10)
T0880-D2	0.23 (16)	0.24 (19)	0.20 (15)	0.23 (19)
T0886-D1	0.29 (36)	0.35 (41)	0.28 (33)	0.30 (35)
T0886-D2	0.41 (35)	0.47 (41)	0.36 (32)	0.38 (34)
T0888-D1	0.25 (22)	0.26 (22)	0.19 (18)	0.22 (20)
T0890-D1	0.56 (62)	0.61 (63)	0.47 (51)	0.57 (60)
T0892-D1	0.74 (76)	0.74 (76)	0.78 (80)	0.78 (80)
T0892-D2	0.33 (31)	0.51 (48)	0.35 (33)	0.35 (34)
T0894-D2	0.60 (73)	0.60 (73)	0.55 (69)	0.55 (69)
T0896-D1	0.20 (20)	0.56 (55)	0.16 (17)	0.18 (18)
T0896-D2	0.56 (46)	0.56 (46)	0.21 (15)	0.22 (16)
T0896-D3	0.19 (14)	0.20 (15)	0.17 (13)	0.18 (13)
T0897-D1	0.24 (19)	0.24 (21)	0.28 (25)	0.28 (25)
T0897-D2	0.59 (52)	0.59 (52)	0.22 (21)	0.23 (21)
T0898-D1	0.35 (33)	0.39 (39)	0.39 (36)	0.39 (36)
T0899-D1	0.50 (35)	0.59 (41)	0.18 (11)	0.20 (13)
T0900-D1	0.43 (42)	0.43 (42)	0.35 (32)	0.36 (34)
T0901-D1	0.57 (43)	0.66 (49)	0.23 (15)	0.23 (15)
T0904-D1	0.45 (37)	0.46 (39)	0.42 (31)	0.48 (34)
T0905-D1	0.53 (38)	0.59 (43)	0.18 (13)	0.24 (15)
T0912-D1	0.72 (54)	0.74 (56)	0.16 (6)	0.17 (7)
T0914-D1	0.33 (31)	0.34 (32)	0.29 (25)	0.32 (31)
T0914-D2	0.32 (27)	0.35 (30)	0.31 (25)	0.35 (29)
T0915-D1	0.49 (42)	0.51 (42)	0.46 (39)	0.46 (39)
T0918-D1	0.49 (46)	0.49 (46)	0.32 (28)	0.33 (31)
T0918-D2	0.39 (34)	0.42 (37)	0.28 (26)	0.30 (28)
T0918-D3	0.45 (40)	0.50 (45)	0.24 (23)	0.35 (30)
T0923-D1	0.20 (17)	0.20 (18)	0.12 (11)	0.21 (18)
T0941-D1	0.21 (9)	0.21 (11)	0.16 (8)	0.18 (9)
T0946-D2	0.74 (59)	0.74 (59)	0.26 (18)	0.26 (18)

Table S2. Comparison between quality of the first model for "hard" and "very hard" targets generated by QUARK with NeBcon predicted contacts ("QUARK" server group in CASP12) and that by original QUARK without contacts (post-CASP experiment). The number outside parentheses is TM-score, while the number inside parenthesis is GDT_TS. The domains are defined from the CASP12 assessors.

target domain	LOMETS templates before sorting		Template after sorting (excluding QUARK models)		Template after sorting (including QUARK models)	
	first template	best template in top 20	first template	best template in top 20	first template	best template in top 20
T0859-D1	0.25 (25)	0.27 (25)	0.18 (18)	0.29 (27)	0.26 (25)	0.29 (27)
T0862-D1	0.41 (48)	0.49 (51)	0.40 (41)	0.41 (42)	0.37 (41)	0.41 (42)
T0863-D1	0.17 (16)	0.27 (22)	0.23 (18)	0.27 (22)	0.30 (23)	0.30 (23)
T0864-D1	0.13 (8)	0.18 (12)	0.17 (11)	0.21 (13)	0.19 (13)	0.22 (14)
T0866-D1	0.40 (40)	0.46 (45)	0.46 (45)	0.47 (45)	0.49 (46)	0.49 (46)
T0869-D1	0.20 (22)	0.36 (36)	0.32 (32)	0.34 (34)	0.32 (36)	0.34 (36)
T0870-D1	0.18 (17)	0.38 (34)	0.35 (31)	0.44 (37)	0.21 (21)	0.44 (37)
T0878-D1	0.12 (7)	0.16 (9)	0.12 (7)	0.16 (9)	0.20 (12)	0.20 (12)
T0880-D2	0.16 (13)	0.37 (31)	0.19 (14)	0.19 (14)	0.23 (16)	0.23 (17)
T0886-D1	0.19 (24)	0.27 (33)	0.24 (28)	0.28 (33)	0.29 (36)	0.29 (36)
T0886-D2	0.17 (18)	0.41 (38)	0.41 (38)	0.41 (38)	0.41 (35)	0.41 (38)
T0888-D1	0.14 (13)	0.30 (30)	0.19 (17)	0.30 (30)	0.25 (22)	0.30 (30)
T0890-D1	0.09 (11)	0.48 (50)	0.39 (49)	0.54 (57)	0.56 (62)	0.56 (62)
T0892-D1	0.26 (33)	0.55 (61)	0.60 (64)	0.60 (64)	0.74 (76)	0.74 (76)
T0892-D2	0.33 (32)	0.44 (41)	0.29 (28)	0.44 (41)	0.33 (31)	0.44 (41)
T0894-D2	0.39 (53)	0.41 (53)	0.34 (50)	0.39 (53)	0.60 (73)	0.60 (73)
T0896-D1	0.50 (50)	0.57 (56)	0.17 (17)	0.18 (19)	0.20 (20)	0.20 (20)
T0896-D2	0.56 (48)	0.56 (48)	0.56 (48)	0.56 (48)	0.56 (46)	0.56 (48)
T0896-D3	0.12 (10)	0.18 (14)	0.16 (13)	0.18 (14)	0.19 (14)	0.19 (14)
T0897-D1	0.15 (14)	0.21 (19)	0.19 (16)	0.27 (22)	0.24 (19)	0.27 (22)
T0897-D2	0.45 (41)	0.45 (41)	0.49 (45)	0.49 (45)	0.59 (52)	0.59 (52)
T0898-D1	0.23 (23)	0.25 (26)	0.26 (26)	0.31 (30)	0.35 (33)	0.37 (38)
T0899-D1	0.59 (41)	0.59 (41)	0.59 (41)	0.59 (41)	0.50 (35)	0.59 (41)
T0900-D1	0.23 (23)	0.45 (45)	0.45 (45)	0.45 (45)	0.43 (42)	0.45 (45)
T0901-D1	0.63 (48)	0.63 (48)	0.63 (48)	0.63 (48)	0.57 (43)	0.65 (49)
T0904-D1	0.44 (36)	0.44 (36)	0.44 (36)	0.44 (36)	0.45 (37)	0.45 (37)
T0905-D1	0.62 (46)	0.62 (46)	0.51 (37)	0.53 (38)	0.53 (38)	0.59 (42)
T0912-D1	0.74 (58)	0.74 (58)	0.48 (35)	0.74 (58)	0.72 (54)	0.74 (58)
T0914-D1	0.18 (16)	0.26 (22)	0.25 (22)	0.28 (25)	0.33 (31)	0.33 (31)
T0914-D2	0.16 (15)	0.26 (21)	0.21 (17)	0.32 (28)	0.32 (27)	0.32 (28)
T0915-D1	0.30 (24)	0.48 (39)	0.43 (36)	0.50 (41)	0.49 (42)	0.51 (42)
T0918-D1	0.29 (30)	0.42 (41)	0.40 (37)	0.42 (41)	0.49 (46)	0.49 (46)
T0918-D2	0.33 (30)	0.40 (35)	0.34 (32)	0.38 (34)	0.39 (34)	0.39 (34)
T0918-D3	0.28 (24)	0.34 (33)	0.36 (33)	0.38 (34)	0.45 (40)	0.45 (40)
T0923-D1	0.14 (12)	0.16 (13)	0.18 (15)	0.20 (16)	0.20 (17)	0.20 (17)
T0941-D1	0.09 (6)	0.19 (8)	0.16 (7)	0.19 (10)	0.21 (9)	0.21 (10)
T0946-D2	0.69 (55)	0.69 (55)	0.69 (55)	0.69 (55)	0.74 (59)	0.74 (59)