

Table 1. Average GDT_TS scores for the different types of models obtained (domains only) for CASP14 dataset.

Targets	Structural classification by DSSP	Average GDT_TS score for AF2, ranked	Average GDT_TS score for AlphaMod 5ranked, unsupervised	Average GDT_TS score for AlphaMod 2best, supervised	Average GDT_TS score for AlphaMod 2best, unsupervised
T1024-D1	>40 helices	90.00 \pm 0.35 *	89.28 \pm 0.82	89.61 \pm 0.31	89.61 \pm 0.31
T1024-D2	>40 helices	90.61 \pm 0.73	90.59 \pm 0.74	90.66 \pm 0.68 *	90.51 \pm 0.78
T1025-D1	>40 helices	97.30 \pm 1.08	98.15 \pm 0.12	98.17 \pm 0.11 *	97.88 \pm 0.17
T1026-D1	>40 beta, >40 irregular	92.47 \pm 0.12	92.47 \pm 0.52	92.09 \pm 0.33	92.67 \pm 0.14 *
T1028-D1	>40 irregular	92.17 \pm 0.64	91.92 \pm 0.29	92.84 \pm 0.20 *	92.84 \pm 0.20 *
T1029-D1	No class	45.52 \pm 0.54 *	44.92 \pm 0.33	45.28 \pm 0.59	45.28 \pm 0.59
T1030-D1	>40 helices	69.32 \pm 1.79	67.73 \pm 1.69	69.55 \pm 1.15 *	65.88 \pm 1.80
T1030-D2	>40 helices	87.69 \pm 1.08 *	79.70 \pm 1.82	80.84 \pm 2.78	82.31 \pm 2.53
T1031-D1	>40 irregular	90.16 \pm 3.62	88.95 \pm 0.62	94.31 \pm 0.40 *	91.31 \pm 2.85
T1032-D1	>40 irregular	65.03 \pm 0.34 *	61.41 \pm 4.72	59.76 \pm 4.45	61.53 \pm 4.83
T1033-D1	>40 helices	42.50 \pm 6.16 *	42.50 \pm 5.74 *	39.60 \pm 4.65	40.25 \pm 1.22
T1034-D1	>40 beta, >40 irregular	95.29 \pm 0.14 *	95.00 \pm 0.21	95.03 \pm 0.25	95.03 \pm 0.16
T1035-D1	>40 helices, >40 irregular	86.42 \pm 1.51	85.64 \pm 1.57	87.11 \pm 0.77 *	87.11 \pm 0.77 *
T1036s1-D1	>40 irregular	68.68 \pm 12.68	59.14 \pm 2.57	69.24 \pm 4.25 *	69.24 \pm 4.25 *
T1037-D1	>40 helices	81.48 \pm 3.10	85.68 \pm 0.42	85.94 \pm 0.14 *	83.02 \pm 0.96
T1038-D1	>40 beta, >40 irregular	69.74 \pm 19.20	82.15 \pm 0.69	84.21 \pm 1.60 *	80.83 \pm 0.46
T1038-D2	>40 irregular	89.14 \pm 3.05	89.87 \pm 0.43	90.59 \pm 0.50 *	89.54 \pm 0.75
T1039-D1	>40 helices	80.03 \pm 3.24	80.31 \pm 0.28	82.39 \pm 0.37	82.89 \pm 0.76 *
T1040-D1	>40 helices	54.54 \pm 1.44	54.46 \pm 0.91	55.69 \pm 0.94 *	54.39 \pm 1.38
T1041-D1	>40 helices, >40 irregular	83.86 \pm 1.40	84.60 \pm 0.79	84.56 \pm 0.34	84.69 \pm 0.54 *
T1042-D1	>40 helices	59.91 \pm 1.09 *	58.86 \pm 0.81	57.32 \pm 2.32	58.90 \pm 0.76
T1043-D1	>40 irregular	24.60 \pm 1.00	20.03 \pm 5.83	24.90 \pm 3.98 *	24.39 \pm 1.34
T1045s1-D1	>40 irregular	95.20 \pm 0.27	95.91 \pm 0.48	96.14 \pm 0.51 *	95.75 \pm 0.24
T1045s2-D1	>40 irregular	92.29 \pm 1.03	91.99 \pm 0.39	92.68 \pm 0.43 *	91.45 \pm 0.48
T1046s1-D1	>40 helices	96.94 \pm 0.45	96.73 \pm 0.39	97.08 \pm 0.53 *	96.53 \pm 0.24
T1046s2-D1	>40 irregular	97.59 \pm 1.33	98.30 \pm 0.09	98.54 \pm 0.15 *	98.44 \pm 0.15
T1047s1-D1	>40 beta, >40 irregular	46.02 \pm 1.15	44.72 \pm 1.35	46.12 \pm 1.49 *	45.45 \pm 1.27
T1047s2-D1	>40 irregular	87.48 \pm 1.05 *	86.56 \pm 0.52	86.56 \pm 0.72	87.38 \pm 0.90
T1047s2-D3	>40 irregular	48.62 \pm 1.76	48.66 \pm 0.77	49.53 \pm 0.56 *	48.66 \pm 1.22
T1049-D1	>40 irregular	92.69 \pm 0.58	92.42 \pm 0.21	92.76 \pm 0.08 *	92.69 \pm 0.15
T1053-D1	>40 helices, >40 irregular	88.77 \pm 0.29	88.92 \pm 0.26 *	88.89 \pm 0.37	88.67 \pm 0.42
T1053-D2	>40 helices	82.78 \pm 1.08	82.22 \pm 0.08	84.80 \pm 0.74 *	82.08 \pm 0.25
T1054-D1	No class	88.53 \pm 0.80	88.22 \pm 0.46	88.67 \pm 0.29 *	88.67 \pm 0.29 *
T1055-D1	>40 helices	86.84 \pm 0.85	87.66 \pm 0.27	88.20 \pm 0.43 *	88.20 \pm 0.43 *
T1056-D1	>40 irregular	93.25 \pm 4.21	95.12 \pm 0.18	95.92 \pm 0.13 *	95.59 \pm 0.13
T1065s1-D1	No class	92.69 \pm 0.18	92.90 \pm 0.69 *	92.61 \pm 0.48	92.19 \pm 0.58
T1065s2-D1	>40 helices	97.65 \pm 0.28	97.60 \pm 0.50	97.91 \pm 0.56 *	97.60 \pm 0.53
T1074-D1	>40 beta	91.82 \pm 1.45 *	90.87 \pm 0.69	91.82 \pm 0.49 *	91.33 \pm 1.49
T1076-D1	>40 helices	98.93 \pm 0.07	98.90 \pm 0.15	98.94 \pm 0.17	98.96 \pm 0.11 *
T1078-D1	>40 beta, >40 irregular	94.61 \pm 0.29 *	93.56 \pm 0.65	94.07 \pm 0.22	93.80 \pm 1.12
T1082-D1	>40 helices	90.33 \pm 1.18 *	89.73 \pm 0.55	89.93 \pm 0.28	89.86 \pm 0.51
T1090-D1	>40 irregular	88.43 \pm 1.00	88.82 \pm 0.12	89.42 \pm 0.34 *	89.06 \pm 0.40
T1099-D1	>40 helices	75.53 \pm 6.37	80.11 \pm 2.82 *	78.96 \pm 1.70	78.48 \pm 1.52
Global average GDT_TS		81.01 \pm 18.25	80.77 \pm 18.62	81.61 \pm 18.28 *	81.18 \pm 18.21

Results in bold represent pair-to-pair models obtained with either AlphaMod procedure with a GDT_TS score higher than the one obtained by AF2 alone. Results with * represent, for each target, the best result in terms of GDT_TS score.