

CASP16_TWO-STATE_TABLES

Tiburon Leon Benavides

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Supplementary Table S1: Results for M1228 BestDockQ Two-State Score

Group	Group_Name	Two-State_Score	V1_BestDockQ	V2_BestDockQ	V1_Model	V2_Model
TS294	KiharaLab	1.61	0.79	0.82	TS294.v1.1	TS294.v2.1
TS033	Diff	1.52	0.73	0.79	TS033.v1.4	TS033.v2.5
TS462	Zheng	1.49	0.81	0.68	TS462.v1.3	TS462.v2.3
TS204	Zou	1.48	0.65	0.83	TS204.v1.2	TS204.v2.2
TS325	405	1.42	0.61	0.81	TS325.v1.1	TS325.v2.1
TS159	406	1.42	0.61	0.81	TS159.v1.1	TS159.v2.1
TS304	AF3-server	1.40	0.59	0.81	TS304.v1.2	TS304.v2.3
TS241	elofsson	1.37	0.58	0.78	TS241.v1.3	TS241.v2.1
TS091	Huang-HUST	1.36	0.75	0.61	TS091.v1.3	TS091.v2.2
TS262	CoDock	1.31	0.69	0.62	TS262.v1.1	TS262.v2.3
TS231	B-LAB	1.29	0.53	0.77	TS231.v1.2	TS231.v2.1
TS489	Fernandez-Recio	1.29	0.65	0.64	TS489.v1.1	TS489.v2.1
TS481	Vfold	1.26	0.60	0.65	TS481.v1.4	TS481.v2.2
TS208	falcon2	1.24	0.50	0.74	TS208.v1.1	TS208.v2.5
TS286	CSSB_experimental	1.19	0.59	0.60	TS286.v1.1	TS286.v2.1
TS110	MIEnsembles-Server	1.19	0.55	0.63	TS110.v1.3	TS110.v2.5
TS028	NKRNA-s	1.16	0.55	0.61	TS028.v1.4	TS028.v2.4
TS450	OpenComplex_Server	1.07	0.51	0.56	TS450.v1.1	TS450.v2.2
TS167	OpenComplex	1.07	0.51	0.56	TS167.v1.1	TS167.v2.2
TS022	Yang	0.38	0.18	0.20	TS022.v1.4	TS022.v2.5
TS052	Yang-Server	0.38	0.18	0.20	TS052.v1.3	TS052.v2.5
TS456	Yang-Multimer	0.36	0.17	0.18	TS456.v1.4	TS456.v2.5
TS494	ClusPro	0.34	0.17	0.17	TS494.v1.2	TS494.v2.3
TS274	kozakovvajda	0.34	0.17	0.17	TS274.v1.2	TS274.v2.3
TS014	Cool-PSP	0.32	0.18	0.14	TS014.v1.4	TS014.v2.4

Supplementary Table S2: Results for M1228 GDT TS Two-State Score

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS294	KiharaLab	0.71	36.90	34.50	TS294_v1.1	TS294_v2.1
TS204	Zou	0.71	36.40	35.00	TS204_v1.1	TS204_v2.2
TS033	Diff	0.69	34.30	34.90	TS033_v2.5	TS033_v1.5
TS304	AF3-server	0.69	35.50	33.70	TS304_v1.3	TS304_v2.3
TS052	Yang-Server	0.69	33.70	35.40	TS052_v1.4	TS052_v2.4
TS286	CSSB_experimental	0.69	33.80	35.00	TS286_v2.4	TS286_v1.1
TS481	Vfold	0.67	35.50	31.80	TS481_v1.3	TS481_v2.1
TS456	Yang-Multimer	0.66	30.70	35.60	TS456_v1.3	TS456_v2.3
TS241	elofsson	0.66	30.60	35.10	TS241_v2.5	TS241_v1.1
TS022	Yang	0.66	33.30	32.30	TS022_v1.4	TS022_v2.4
TS462	Zheng	0.65	36.70	28.50	TS462_v1.3	TS462_v2.1
TS494	ClusPro	0.65	30.80	34.10	TS494_v1.2	TS494_v2.1
TS274	kozakovvajda	0.65	30.80	34.10	TS274_v1.2	TS274_v2.1
TS091	Huang-HUST	0.65	34.00	30.80	TS091_v1.3	TS091_v2.2
TS323	Yan	0.63	29.70	32.90	TS323_v1.1	TS323_v2.1
TS167	OpenComplex	0.62	30.60	31.70	TS167_v1.1	TS167_v2.4
TS450	OpenComplex_Server	0.62	30.60	31.70	TS450_v1.1	TS450_v2.4
TS028	NKRNA-s	0.61	31.90	29.40	TS028_v2.5	TS028_v1.2
TS489	Fernandez-Recio	0.61	31.20	29.40	TS489_v1.2	TS489_v2.2
TS014	Cool-PSP	0.60	25.30	34.60	TS014_v1.1	TS014_v2.5
TS110	MIEnsembles-Server	0.59	31.20	28.00	TS110_v2.4	TS110_v1.1
TS159	406	0.59	26.00	33.00	TS159_v1.1	TS159_v2.1
TS325	405	0.59	26.00	33.00	TS325_v1.1	TS325_v2.1
TS262	CoDock	0.55	34.00	21.30	TS262_v1.1	TS262_v2.2
TS231	B-LAB	0.47	11.70	35.80	TS231_v1.5	TS231_v2.1
TS208	falcon2	0.45	11.60	33.60	TS208_v2.5	TS208_v1.1

Supplementary Table S3: Results for M1228 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS204	Zou	1.33	0.65	0.68	TS204.v1.5	TS204.v2.5
TS294	KiharaLab	1.32	0.66	0.66	TS294.v1.1	TS294.v2.3
TS091	Huang-HUST	1.31	0.66	0.64	TS091.v1.3	TS091.v2.2
TS033	Diff	1.29	0.65	0.65	TS033.v1.4	TS033.v2.4
TS462	Zheng	1.29	0.67	0.62	TS462.v1.3	TS462.v2.2
TS241	elofsson	1.28	0.62	0.66	TS241.v1.3	TS241.v2.1
TS325	405	1.27	0.62	0.65	TS325.v1.1	TS325.v2.1
TS159	406	1.27	0.62	0.65	TS159.v1.1	TS159.v2.1
TS110	MIEnsembles-Server	1.27	0.62	0.65	TS110.v1.4	TS110.v2.3
TS028	NKRNA-s	1.27	0.62	0.65	TS028.v1.5	TS028.v2.4
TS481	Vfold	1.26	0.62	0.64	TS481.v1.1	TS481.v2.1
TS304	AF3-server	1.26	0.61	0.65	TS304.v1.3	TS304.v2.1
TS286	CSSB_experimental	1.26	0.63	0.63	TS286.v1.1	TS286.v2.1
TS208	falcon2	1.25	0.61	0.64	TS208.v1.1	TS208.v2.5
TS262	CoDock	1.25	0.63	0.62	TS262.v1.1	TS262.v2.3
TS231	B-LAB	1.25	0.61	0.64	TS231.v1.2	TS231.v2.5
TS450	OpenComplex_Server	1.23	0.62	0.61	TS450.v1.4	TS450.v2.5
TS167	OpenComplex	1.23	0.62	0.61	TS167.v1.4	TS167.v2.5
TS489	Fernandez-Recio	1.20	0.62	0.57	TS489.v1.2	TS489.v2.1
TS022	Yang	1.04	0.53	0.52	TS022.v1.3	TS022.v2.3
TS323	Yan	1.04	0.52	0.52	TS323.v1.1	TS323.v2.1
TS456	Yang-Multimer	1.04	0.52	0.52	TS456.v1.1	TS456.v2.5
TS052	Yang-Server	1.03	0.52	0.52	TS052.v1.1	TS052.v2.5
TS014	Cool-PSP	1.03	0.52	0.51	TS014.v1.3	TS014.v2.3
TS494	ClusPro	1.00	0.50	0.50	TS494.v1.2	TS494.v2.3
TS274	kozakovvajda	1.00	0.50	0.50	TS274.v1.2	TS274.v2.3

Supplementary Table S4: Results for M1228 GlobDockQ Two-State Score

Group	Group_Name	Two-State_Score	V1_GlobDockQ	V2_GlobDockQ	V1_Model	V2_Model
TS294	KiharaLab	0.72	0.34	0.37	TS294_v1.1	TS294_v2.1
TS033	Diff	0.68	0.32	0.36	TS033_v1.4	TS033_v2.5
TS462	Zheng	0.66	0.35	0.31	TS462_v1.3	TS462_v2.3
TS204	Zou	0.66	0.28	0.38	TS204_v1.2	TS204_v2.2
TS022	Yang	0.64	0.30	0.34	TS022_v1.4	TS022_v2.5
TS159	406	0.64	0.27	0.37	TS159_v1.1	TS159_v2.1
TS325	405	0.64	0.27	0.37	TS325_v1.1	TS325_v2.1
TS052	Yang-Server	0.63	0.29	0.34	TS052_v1.3	TS052_v2.5
TS304	AF3-server	0.62	0.26	0.37	TS304_v1.2	TS304_v2.3
TS241	elofsson	0.61	0.25	0.35	TS241_v1.3	TS241_v2.1
TS091	Huang-HUST	0.60	0.32	0.28	TS091_v1.3	TS091_v2.2
TS456	Yang-Multimer	0.59	0.29	0.30	TS456_v1.4	TS456_v2.5
TS262	CoDock	0.58	0.30	0.28	TS262_v1.1	TS262_v2.3
TS231	B-LAB	0.58	0.23	0.35	TS231_v1.5	TS231_v2.1
TS489	Fernandez-Recio	0.57	0.28	0.29	TS489_v1.1	TS489_v2.1
TS494	ClusPro	0.56	0.28	0.29	TS494_v1.2	TS494_v2.3
TS274	kozakovvajda	0.56	0.28	0.29	TS274_v1.2	TS274_v2.3
TS481	Vfold	0.56	0.26	0.30	TS481_v1.4	TS481_v2.2
TS208	falcon2	0.55	0.22	0.34	TS208_v1.1	TS208_v2.5
TS286	CSSB_experimental	0.53	0.26	0.27	TS286_v1.1	TS286_v2.1
TS110	MIEnsembles-Server	0.53	0.24	0.29	TS110_v1.3	TS110_v2.5
TS014	Cool-PSP	0.53	0.29	0.23	TS014_v1.4	TS014_v2.4
TS028	NKRNA-s	0.52	0.24	0.28	TS028_v1.4	TS028_v2.4
TS450	OpenComplex_Server	0.48	0.22	0.25	TS450_v1.4	TS450_v2.2
TS167	OpenComplex	0.48	0.22	0.25	TS167_v1.4	TS167_v2.2

Supplementary Table S5: Results for M1228 TMscore Two-State Score

Group	Group_Name	Two-State_Score	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS028	NKRNA-s	1.56	0.80	0.76	TS028_v2_5	TS028_v1_5
TS462	Zheng	1.55	0.77	0.78	TS462_v1_1	TS462_v2_1
TS481	Vfold	1.54	0.74	0.79	TS481_v1_4	TS481_v2_1
TS286	CSSB_experimental	1.52	0.75	0.77	TS286_v2_5	TS286_v1_3
TS091	Huang-HUST	1.50	0.71	0.79	TS091_v2_1	TS091_v1_2
TS052	Yang-Server	1.50	0.69	0.81	TS052_v2_3	TS052_v1_1
TS033	Diff	1.50	0.71	0.79	TS033_v1_5	TS033_v2_2
TS022	Yang	1.50	0.70	0.80	TS022_v1_4	TS022_v2_2
TS450	OpenComplex_Server	1.49	0.79	0.71	TS450_v2_4	TS450_v1_1
TS167	OpenComplex	1.49	0.79	0.71	TS167_v2_4	TS167_v1_1
TS304	AF3-server	1.49	0.71	0.78	TS304_v1_4	TS304_v2_5
TS262	CoDock	1.49	0.80	0.70	TS262_v1_1	TS262_v2_3
TS494	ClusPro	1.46	0.69	0.77	TS494_v2_2	TS494_v1_3
TS274	kozakovvajda	1.46	0.69	0.77	TS274_v2_2	TS274_v1_3
TS456	Yang-Multimer	1.46	0.67	0.78	TS456_v2_3	TS456_v1_1
TS204	Zou	1.45	0.73	0.73	TS204_v1_1	TS204_v2_1
TS241	elofsson	1.44	0.69	0.76	TS241_v1_3	TS241_v2_3
TS110	MIEnsembles-Server	1.44	0.66	0.79	TS110_v1_2	TS110_v2_3
TS294	KiharaLab	1.44	0.72	0.72	TS294_v1_5	TS294_v2_1
TS369	Bhattacharya	1.40	0.72	0.69	TS369_v2_5	TS369_v1_2
TS231	B-LAB	1.40	0.68	0.72	TS231_v1_2	TS231_v2_1
TS208	falcon2	1.37	0.70	0.67	TS208_v2_5	TS208_v1_1
TS489	Fernandez-Recio	1.37	0.67	0.70	TS489_v2_2	TS489_v1_2
TS323	Yan	1.33	0.65	0.68	TS323_v1_1	TS323_v2_1
TS325	405	1.32	0.63	0.69	TS325_v1_1	TS325_v2_1
TS159	406	1.32	0.63	0.69	TS159_v1_1	TS159_v2_1
TS014	Cool-PSP	1.31	0.61	0.71	TS014_v1_4	TS014_v2_5

Supplementary Table S6: Results for M1239 BestDockQ Two-State Score

Group	Group_Name	Two-State_Score	V1_BestDockQ	V2_BestDockQ	V1_Model	V2_Model
TS294	KiharaLab	1.53	0.79	0.74	TS294_v1.4	TS294_v2.3
TS286	CSSB_experimental	1.49	0.76	0.74	TS286_v1.4	TS286_v2.1
TS110	MIEnsembles-Server	1.47	0.82	0.65	TS110_v1.1	TS110_v2.4
TS489	Fernandez-Recio	1.34	0.77	0.57	TS489_v1.5	TS489_v2.4
TS208	falcon2	1.34	0.73	0.61	TS208_v1.2	TS208_v2.4
TS481	Vfold	1.32	0.77	0.55	TS481_v1.4	TS481_v2.2
TS325	405	1.27	0.70	0.58	TS325_v1.2	TS325_v2.2
TS159	406	1.27	0.70	0.58	TS159_v1.2	TS159_v2.2
TS167	OpenComplex	1.24	0.76	0.49	TS167_v1.4	TS167_v2.5
TS450	OpenComplex_Server	1.24	0.76	0.49	TS450_v1.4	TS450_v2.5
TS091	Huang-HUST	1.22	0.66	0.56	TS091_v1.5	TS091_v2.5
TS262	CoDock	1.21	0.67	0.54	TS262_v1.5	TS262_v2.4
TS033	Diff	1.20	0.66	0.54	TS033_v1.3	TS033_v2.3
TS028	NKRNA-s	1.17	0.59	0.58	TS028_v1.3	TS028_v2.3
TS462	Zheng	1.15	0.59	0.57	TS462_v1.4	TS462_v2.5
TS231	B-LAB	1.13	0.65	0.48	TS231_v1.2	TS231_v2.5
TS235	isyslab-hust	0.90	0.46	0.44	TS235_v1.1	TS235_v2.5
TS272	GromihaLab	0.78	0.45	0.34	TS272_v1.3	TS272_v2.3
TS241	elofsson	0.68	0.36	0.32	TS241_v1.3	TS241_v2.3
TS304	AF3-server	0.64	0.32	0.32	TS304_v1.1	TS304_v2.4
TS014	Cool-PSP	0.27	0.15	0.12	TS014_v1.1	TS014_v2.2

Supplementary Table S7: Results for M1239 GDT TS Two-State Score

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS235	isyslab-hust	0.59	30.00	28.80	TS235_v2_4	TS235_v1_2
TS462	Zheng	0.59	30.60	28.20	TS462_v2_2	TS462_v1_4
TS028	NKRNA-s	0.57	29.80	27.70	TS028_v1_4	TS028_v2_2
TS110	MIEnsembles-Server	0.56	29.40	26.50	TS110_v1_1	TS110_v2_4
TS481	Vfold	0.54	27.40	27.00	TS481_v1_4	TS481_v2_5
TS286	CSSB_experimental	0.54	26.60	27.50	TS286_v1_5	TS286_v2_1
TS262	CoDock	0.54	28.00	26.00	TS262_v2_2	TS262_v1_4
TS294	KiharaLab	0.53	25.60	26.90	TS294_v2_2	TS294_v1_1
TS033	Diff	0.51	25.90	25.40	TS033_v2_1	TS033_v1_3
TS231	B-LAB	0.51	27.90	23.00	TS231_v2_1	TS231_v1_2
TS091	Huang-HUST	0.51	25.50	25.30	TS091_v1_2	TS091_v2_2
TS489	Fernandez-Recio	0.51	25.60	24.90	TS489_v1_3	TS489_v2_5
TS208	falcon2	0.46	29.70	16.70	TS208_v1_4	TS208_v2_1
TS167	OpenComplex	0.44	27.90	16.40	TS167_v1_5	TS167_v2_5
TS450	OpenComplex_Server	0.44	27.90	16.40	TS450_v1_5	TS450_v2_5
TS325	405	0.41	25.20	15.50	TS325_v1_2	TS325_v2_2
TS159	406	0.41	25.20	15.50	TS159_v1_2	TS159_v2_2
TS014	Cool-PSP	0.40	19.40	20.20	TS014_v1_5	TS014_v2_4
TS241	elofsson	0.37	18.10	18.70	TS241_v2_1	TS241_v1_3
TS304	AF3-server	0.37	19.20	17.60	TS304_v2_5	TS304_v1_1
TS272	GromihaLab	0.29	14.60	14.60	TS272_v1_3	TS272_v2_5

Supplementary Table S8: Results for M1239 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS286	CSSB_experimental	1.47	0.73	0.73	TS286.v1.4	TS286.v2.1
TS294	KiharaLab	1.45	0.74	0.71	TS294.v1.5	TS294.v2.5
TS110	MIEnsembles-Server	1.40	0.73	0.67	TS110.v1.1	TS110.v2.5
TS489	Fernandez-Recio	1.40	0.72	0.68	TS489.v1.5	TS489.v2.4
TS208	falcon2	1.40	0.70	0.70	TS208.v1.1	TS208.v2.5
TS262	CoDock	1.39	0.70	0.69	TS262.v1.2	TS262.v2.1
TS462	Zheng	1.38	0.69	0.69	TS462.v1.4	TS462.v2.2
TS028	NKRNA-s	1.38	0.69	0.69	TS028.v1.3	TS028.v2.3
TS481	Vfold	1.37	0.71	0.66	TS481.v1.1	TS481.v2.4
TS159	406	1.36	0.68	0.68	TS159.v1.1	TS159.v2.1
TS325	405	1.35	0.68	0.67	TS325.v1.1	TS325.v2.2
TS450	OpenComplex_Server	1.35	0.69	0.66	TS450.v1.1	TS450.v2.5
TS167	OpenComplex	1.35	0.69	0.66	TS167.v1.1	TS167.v2.5
TS231	B-LAB	1.32	0.68	0.64	TS231.v1.1	TS231.v2.1
TS091	Huang-HUST	1.31	0.66	0.65	TS091.v1.5	TS091.v2.5
TS033	Diff	1.30	0.66	0.65	TS033.v1.4	TS033.v2.4
TS235	isyslab-hust	1.30	0.65	0.65	TS235.v1.1	TS235.v2.2
TS272	GromihaLab	1.27	0.64	0.63	TS272.v1.4	TS272.v2.4
TS014	Cool-PSP	1.01	0.51	0.50	TS014.v1.4	TS014.v2.6
TS241	elofsson	0.74	0.38	0.36	TS241.v1.2	TS241.v2.3
TS304	AF3-server	0.72	0.36	0.36	TS304.v1.3	TS304.v2.2

Supplementary Table S9: Results for M1239 GlobDockQ Two-State Score

Group	Group_Name	Two-State_Score	V1_GlobDockQ	V2_GlobDockQ	V1_Model	V2_Model
TS294	KiharaLab	0.71	0.36	0.35	TS294_v1.4	TS294_v2.3
TS286	CSSB_experimental	0.69	0.34	0.35	TS286_v1.4	TS286_v2.1
TS110	MIEnsembles-Server	0.68	0.37	0.31	TS110_v1.1	TS110_v2.4
TS241	elofsson	0.65	0.33	0.32	TS241_v1.3	TS241_v2.3
TS235	isyslab-hust	0.64	0.33	0.32	TS235_v1.1	TS235_v2.5
TS489	Fernandez-Recio	0.62	0.35	0.27	TS489_v1.5	TS489_v2.4
TS208	falcon2	0.62	0.33	0.29	TS208_v1.2	TS208_v2.4
TS304	AF3-server	0.61	0.29	0.32	TS304_v1.1	TS304_v2.4
TS481	Vfold	0.61	0.35	0.26	TS481_v1.4	TS481_v2.2
TS325	405	0.59	0.32	0.28	TS325_v1.2	TS325_v2.2
TS159	406	0.59	0.32	0.28	TS159_v1.2	TS159_v2.2
TS167	OpenComplex	0.58	0.34	0.23	TS167_v1.4	TS167_v2.5
TS450	OpenComplex_Server	0.58	0.34	0.23	TS450_v1.4	TS450_v2.5
TS091	Huang-HUST	0.57	0.30	0.27	TS091_v1.5	TS091_v2.5
TS262	CoDock	0.56	0.30	0.26	TS262_v1.5	TS262_v2.4
TS033	Diff	0.56	0.30	0.26	TS033_v1.3	TS033_v2.3
TS028	NKRNA-s	0.54	0.27	0.28	TS028_v1.3	TS028_v2.3
TS462	Zheng	0.54	0.27	0.27	TS462_v1.4	TS462_v2.5
TS231	B-LAB	0.52	0.30	0.23	TS231_v1.2	TS231_v2.5
TS014	Cool-PSP	0.46	0.25	0.21	TS014_v1.1	TS014_v2.2
TS272	GromihaLab	0.36	0.20	0.16	TS272_v1.3	TS272_v2.3

Supplementary Table S10: Results for M1239 TMscore Two-State Score

Group	Group_Name	Two-State_Score	V1-TMscore	V2-TMscore	V1_Model	V2_Model
TS294	KiharaLab	1.45	0.81	0.64	TS294_v1.1	TS294_v2.3
TS462	Zheng	1.41	0.75	0.66	TS462_v2.3	TS462_v1.1
TS110	MIEnsembles-Server	1.39	0.73	0.66	TS110_v2.5	TS110_v1.1
TS262	CoDock	1.37	0.74	0.63	TS262_v1.3	TS262_v2.4
TS028	NKRNA-s	1.37	0.72	0.64	TS028_v1.5	TS028_v2.1
TS235	isyslab-hust	1.35	0.67	0.68	TS235_v2.4	TS235_v1.5
TS489	Fernandez-Recio	1.33	0.71	0.63	TS489_v2.2	TS489_v1.3
TS481	Vfold	1.32	0.67	0.65	TS481_v1.5	TS481_v2.5
TS204	Zou	1.29	0.64	0.65	TS204_v2.1	TS204_v1.5
TS208	falcon2	1.27	0.67	0.60	TS208_v1.4	TS208_v2.1
TS325	405	1.27	0.64	0.63	TS325_v1.2	TS325_v2.2
TS159	406	1.27	0.64	0.63	TS159_v1.2	TS159_v2.2
TS286	CSSB_experimental	1.27	0.65	0.62	TS286_v1.2	TS286_v2.2
TS033	Diff	1.25	0.65	0.61	TS033_v2.4	TS033_v1.2
TS231	B-LAB	1.25	0.64	0.60	TS231_v1.2	TS231_v2.1
TS091	Huang-HUST	1.23	0.64	0.59	TS091_v2.2	TS091_v1.5
TS369	Bhattacharya	1.22	0.61	0.61	TS369_v2.3	TS369_v1.3
TS167	OpenComplex	1.19	0.57	0.62	TS167_v2.1	TS167_v1.1
TS450	OpenComplex_Server	1.19	0.57	0.62	TS450_v2.1	TS450_v1.1
TS014	Cool-PSP	1.06	0.52	0.54	TS014_v1.5	TS014_v2.4
TS272	GromihaLab	0.77	0.36	0.41	TS272_v2.1	TS272_v1.3
TS241	elofsson	0.69	0.35	0.34	TS241_v1.4	TS241_v2.1
TS304	AF3-server	0.66	0.33	0.33	TS304_v2.4	TS304_v1.1

Supplementary Table S11: Results for R1203 Composite Score 1 Two-State Score

Group	Group_Name	Two-State_Score	V1_Composite_Score_1	V2_Composite_Score_1	V1_Model	V2_Model
TS435	RNAFOLDX	106.98	55.05	51.93	TS435.v1.5	TS435.v2.6
TS304	AF3-server	100.74	57.26	43.48	TS304.v1.3	TS304.v2.2
TS241	elofsson	100.74	57.26	43.48	TS241.v1.3	TS241.v2.2
TS235	isyslab-hust	98.12	53.19	44.94	TS235.v1.2	TS235.v2.5
TS231	B-LAB	96.65	49.47	47.18	TS231.v1.1	TS231.v2.5
TS006	RNA_Dojo	95.76	46.31	49.45	TS006.v1.2	TS006.v2.5
TS159	406	95.63	39.00	56.64	TS159.v1.4	TS159.v2.1
TS369	Bhattacharya	87.97	47.35	40.62	TS369.v1.2	TS369.v2.5
TS267	kiharalab_server	86.82	41.17	45.65	TS267.v1.1	TS267.v2.3
TS417	GuangzhouRNA-meta	83.49	34.78	48.71	TS417.v1.5	TS417.v2.4
TS272	GromihaLab	83.04	38.56	44.48	TS272.v1.4	TS272.v2.1
TS286	CSSB_experimental	82.97	42.97	40.00	TS286.v1.1	TS286.v2.3
TS165	dfr	82.51	36.40	46.11	TS165.v1.3	TS165.v2.5
TS189	LCBio	82.18	46.75	35.43	TS189.v1.5	TS189.v2.1
TS052	Yang-Server	82.15	42.13	40.02	TS052.v1.2	TS052.v2.4
TS294	KiharaLab	81.15	38.56	42.59	TS294.v1.1	TS294.v2.3
TS028	NKRNA-s	80.84	44.82	36.02	TS028.v1.3	TS028.v2.2
TS238	BRIQX	80.70	36.15	44.55	TS238.v1.2	TS238.v2.5
TS156	SouthRNA	77.89	47.36	30.54	TS156.v1.1	TS156.v2.4
TS183	GuangzhouRNA-human	77.89	42.03	35.85	TS183.v1.5	TS183.v2.2
TS448	dNAfold	77.26	43.23	34.03	TS448.v1.1	TS448.v2.5
TS317	GuangzhouRNA_AI	77.25	29.80	47.45	TS317.v1.5	TS317.v2.4
TS481	Vfold	74.20	33.37	40.83	TS481.v1.4	TS481.v2.5
TS338	GeneSilico	72.59	34.78	37.81	TS338.v1.5	TS338.v2.3
TS063	RNApolis	71.28	34.87	36.41	TS063.v1.4	TS063.v2.3
TS110	MIEnsembles-Server	69.61	25.72	43.89	TS110.v1.1	TS110.v2.5
TS456	Yang-Multimer	68.91	35.66	33.25	TS456.v1.2	TS456.v2.1
TS167	OpenComplex	65.39	25.69	39.70	TS167.v1.5	TS167.v2.2
TS462	Zheng	64.06	25.74	38.32	TS462.v1.4	TS462.v2.1
TS358	PerezLab_Gators	54.15	25.70	28.45	TS358.v1.2	TS358.v2.1
TS169	thermomaps	50.29	23.20	27.09	TS169.v1.5	TS169.v2.2
TS261	UNRES	46.08	19.62	26.46	TS261.v1.1	TS261.v2.3
TS450	OpenComplex_Server	45.74	23.63	22.12	TS450.v1.2	TS450.v2.4
TS400	OmniFold	43.12	0.00	43.12	N/A ¹	TS400.v2.1
TS276	FrederickFolding	41.67	0.00	41.67	N/A ¹	TS276.v2.1
TS094	SimRNA-Server	32.49	18.13	14.36	TS094.v1.2	TS094.v2.3
TS367	AIR	31.66	0.00	31.66	N/A ¹	TS367.v2.1
TS423	ShanghaiTech-server	27.51	27.51	0.00	TS423.v1.1	N/A ¹
TS298	ShanghaiTech-human	27.51	27.51	0.00	TS298.v1.1	N/A ¹
TS403	mmagnus	22.46	22.46	0.00	TS403.v1.1	N/A ¹
TS208	falcon2	20.64	20.64	0.00	TS208.v1.1	N/A ¹
TS306	GeneSilicoRNA-server	15.63	0.00	15.63	N/A ¹	TS306.v2.1

¹ Model either not submitted or not assessed

Supplementary Table S12: Results for R1203 Composite Score 2 Two-State Score

Group	Group_Name	Two-State_Score	V1_Composite_Score_2	V2_Composite_Score_2	V1_Model	V2_Model
TS435	RNAFOLDX	133.31	68.50	64.81	TS435.v1.5	TS435.v2.6
TS304	AF3-server	124.44	71.30	53.15	TS304.v1.3	TS304.v2.2
TS241	elofsson	124.44	71.30	53.15	TS241.v1.3	TS241.v2.2
TS006	RNA_Dojo	119.67	57.89	61.78	TS006.v1.2	TS006.v2.5
TS235	isyslab-hust	119.24	66.45	52.79	TS235.v1.2	TS235.v2.5
TS231	B-LAB	113.06	61.77	51.29	TS231.v1.1	TS231.v2.5
TS159	406	112.55	63.91	48.64	TS159.v1.1	TS159.v2.4
TS267	kiharalab_server	108.53	51.47	57.06	TS267.v1.1	TS267.v2.3
TS369	Bhattacharya	108.26	58.89	49.38	TS369.v1.2	TS369.v2.5
TS417	GuangzhouRNA-meta	104.31	43.47	60.84	TS417.v1.5	TS417.v2.4
TS052	Yang-Server	102.68	52.66	50.02	TS052.v1.2	TS052.v2.4
TS165	dfr	102.63	45.05	57.58	TS165.v1.3	TS165.v2.5
TS286	CSSB_experimental	102.39	53.67	48.72	TS286.v1.1	TS286.v2.3
TS028	NKRNA-s	101.05	56.03	45.02	TS028.v1.3	TS028.v2.2
TS294	KiharaLab	100.92	47.73	53.19	TS294.v1.1	TS294.v2.3
TS238	BRIQX	100.85	45.17	55.67	TS238.v1.2	TS238.v2.5
TS189	LCBio	99.94	58.12	41.82	TS189.v1.5	TS189.v2.1
TS183	GuangzhouRNA-human	97.34	52.53	44.80	TS183.v1.5	TS183.v2.2
TS272	GromihaLab	97.29	47.53	49.76	TS272.v1.4	TS272.v2.1
TS156	SouthRNA	97.15	58.98	38.17	TS156.v1.1	TS156.v2.4
TS448	dNAfold	96.57	54.03	42.54	TS448.v1.1	TS448.v2.5
TS317	GuangzhouRNA_AI	95.74	37.24	58.50	TS317.v1.5	TS317.v2.4
TS481	Vfold	92.32	41.59	50.73	TS481.v1.4	TS481.v2.5
TS338	GeneSilico	90.02	42.87	47.15	TS338.v1.5	TS338.v2.3
TS063	RNApolis	87.78	42.26	45.51	TS063.v1.1	TS063.v2.3
TS110	MIEnsembles-Server	87.00	32.15	54.85	TS110.v1.1	TS110.v2.5
TS456	Yang-Multimer	86.14	44.58	41.56	TS456.v1.2	TS456.v2.1
TS167	OpenComplex	80.50	32.11	48.39	TS167.v1.5	TS167.v2.2
TS462	Zheng	80.07	32.17	47.90	TS462.v1.4	TS462.v2.1
TS358	PerezLab_Gators	67.69	32.12	35.56	TS358.v1.2	TS358.v2.1
TS169	thermomaps	62.86	29.00	33.86	TS169.v1.5	TS169.v2.2
TS261	UNRES	57.60	24.52	33.08	TS261.v1.1	TS261.v2.3
TS450	OpenComplex_Server	57.18	29.53	27.65	TS450.v1.2	TS450.v2.4
TS400	OmniFold	51.62	0.00	51.62	N/A ¹	TS400.v2.1
TS276	FrederickFolding	51.19	0.00	51.19	N/A ¹	TS276.v2.1
TS094	SimRNA-Server	40.61	22.66	17.95	TS094.v1.2	TS094.v2.3
TS367	AIR	39.57	0.00	39.57	N/A ¹	TS367.v2.1
TS423	ShanghaiTech-server	34.39	34.39	0.00	TS423.v1.1	N/A ¹
TS298	ShanghaiTech-human	34.39	34.39	0.00	TS298.v1.1	N/A ¹
TS403	mmagnus	28.02	0.00	28.02	N/A ¹	TS403.v2.1
TS208	falcon2	25.52	25.52	0.00	TS208.v1.1	N/A ¹
TS306	GeneSilicoRNA-server	19.54	0.00	19.54	N/A ¹	TS306.v2.1

¹ Model either not submitted or not assessed

Supplementary Table S13: Results for R1203 Composite Score 3 Two-State Score

Group	Group_Name	Two-State_Score	V1_Composite_Score_3	V2_Composite_Score_3	V1_Model	V2_Model
TS304	AF3-server	83.89	49.85	34.05	TS304.v1.3	TS304.v2.2
TS241	elofsson	83.89	49.85	34.05	TS241.v1.3	TS241.v2.2
TS235	isyslab-hust	80.87	46.39	34.48	TS235.v1.2	TS235.v2.5
TS435	RNAFOLDX	76.72	47.49	29.22	TS435.v1.5	TS435.v2.6
TS369	Bhattacharya	72.03	40.13	31.90	TS369.v1.2	TS369.v2.5
TS006	RNA_Dojo	70.26	30.77	39.49	TS006.v1.1	TS006.v2.3
TS272	GromihaLab	61.99	30.71	31.28	TS272.v1.1	TS272.v2.5
TS231	B-LAB	60.39	28.08	32.30	TS231.v1.1	TS231.v2.5
TS238	BRIQX	49.71	11.66	38.05	TS238.v1.2	TS238.v2.5
TS159	406	48.74	31.26	17.49	TS159.v1.2	TS159.v2.1
TS267	kiharalab_server	42.25	19.02	23.23	TS267.v1.1	TS267.v2.3
TS294	KiharaLab	41.90	10.15	31.75	TS294.v1.4	TS294.v2.1
TS167	OpenComplex	41.17	9.21	31.97	TS167.v1.5	TS167.v2.2
TS156	SouthRNA	40.74	24.95	15.79	TS156.v1.1	TS156.v2.4
TS052	Yang-Server	39.88	19.93	19.95	TS052.v1.2	TS052.v2.4
TS028	NKRNA-s	36.51	24.46	12.05	TS028.v1.3	TS028.v2.2
TS110	MIEnsembles-Server	35.06	7.94	27.12	TS110.v1.2	TS110.v2.5
TS165	dfr	35.04	10.85	24.19	TS165.v1.3	TS165.v2.5
TS417	GuangzhouRNA-meta	34.64	9.97	24.67	TS417.v1.5	TS417.v2.4
TS400	OmniFold	33.42	0.00	33.42	N/A ¹	TS400.v2.1
TS286	CSSB_experimental	33.03	18.74	14.28	TS286.v1.1	TS286.v2.3
TS189	LCBio	32.93	23.20	9.74	TS189.v1.5	TS189.v2.2
TS276	FrederickFolding	32.90	0.00	32.90	N/A ¹	TS276.v2.1
TS317	GuangzhouRNA_AI	32.50	9.19	23.32	TS317.v1.5	TS317.v2.4
TS448	dNAfold	30.11	20.49	9.62	TS448.v1.1	TS448.v2.5
TS169	thermomaps	28.57	12.37	16.20	TS169.v1.5	TS169.v2.2
TS462	Zheng	27.64	7.94	19.69	TS462.v1.2	TS462.v2.1
TS183	GuangzhouRNA-human	26.82	16.07	10.75	TS183.v1.5	TS183.v2.2
TS481	Vfold	26.38	9.53	16.85	TS481.v1.4	TS481.v2.5
TS358	PerezLab_Gators	25.81	11.55	14.27	TS358.v1.2	TS358.v2.1
TS261	UNRES	25.29	9.56	15.73	TS261.v1.1	TS261.v2.3
TS338	GeneSilico	24.57	10.19	14.38	TS338.v1.5	TS338.v2.3
TS456	Yang-Multimer	23.65	13.31	10.35	TS456.v1.2	TS456.v2.4
TS094	SimRNA-Server	22.53	13.25	9.28	TS094.v1.2	TS094.v2.3
TS063	RNApolis	22.07	9.95	12.12	TS063.v1.1	TS063.v2.3
TS450	OpenComplex_Server	18.83	9.97	8.86	TS450.v1.2	TS450.v2.4
TS423	ShanghaiTech-server	9.18	9.18	0.00	TS423.v1.1	N/A ¹
TS298	ShanghaiTech-human	9.18	9.18	0.00	TS298.v1.1	N/A ¹
TS367	AIR	9.14	0.00	9.14	N/A ¹	TS367.v2.1
TS306	GeneSilicoRNA-server	6.35	0.00	6.35	N/A ¹	TS306.v2.1
TS208	falcon2	4.13	4.13	0.00	TS208.v1.1	N/A ¹
TS403	mmagnus	2.85	0.00	2.85	N/A ¹	TS403.v2.1

¹ Model either not submitted or not assessed

Supplementary Table S14: Results for R1203 Composite Score 4 Two-State Score

Group	Group_Name	Two-State_Score	V1_Composite_Score_4	V2_Composite_Score_4	V1_Model	V2_Model
TS304	AF3-server	85.08	50.07	35.01	TS304.v1.3	TS304.v2.2
TS241	elofsson	85.08	50.07	35.01	TS241.v1.3	TS241.v2.2
TS235	isyslab-hust	83.60	46.42	37.18	TS235.v1.2	TS235.v2.5
TS435	RNAFOLDX	77.05	47.74	29.31	TS435.v1.5	TS435.v2.6
TS369	Bhattacharya	73.39	40.37	33.02	TS369.v1.2	TS369.v2.5
TS006	RNA_Dojo	70.31	30.80	39.51	TS006.v1.1	TS006.v2.3
TS272	GromihaLab	67.08	31.19	35.89	TS272.v1.4	TS272.v2.1
TS231	B-LAB	66.58	28.13	38.45	TS231.v1.1	TS231.v2.5
TS159	406	59.61	31.73	27.89	TS159.v1.2	TS159.v2.1
TS238	BRIQX	49.74	11.68	38.06	TS238.v1.2	TS238.v2.5
TS294	KiharaLab	42.72	10.72	31.99	TS294.v1.4	TS294.v2.1
TS267	kiharalab_server	42.25	19.02	23.23	TS267.v1.1	TS267.v2.3
TS167	OpenComplex	42.16	9.21	32.95	TS167.v1.5	TS167.v2.2
TS156	SouthRNA	40.91	25.12	15.79	TS156.v1.1	TS156.v2.4
TS052	Yang-Server	39.88	19.93	19.95	TS052.v1.2	TS052.v2.4
TS028	NKRNA-s	36.51	24.46	12.05	TS028.v1.3	TS028.v2.2
TS165	dfr	35.44	11.21	24.23	TS165.v1.3	TS165.v2.5
TS400	OmniFold	35.24	0.00	35.24	N/A ¹	TS400.v2.1
TS110	MIEnsembles-Server	35.06	7.94	27.12	TS110.v1.2	TS110.v2.5
TS189	LCBio	34.89	23.45	11.44	TS189.v1.5	TS189.v2.1
TS417	GuangzhouRNA-meta	34.68	9.97	24.71	TS417.v1.5	TS417.v2.4
TS286	CSSB_experimental	34.08	18.77	15.31	TS286.v1.1	TS286.v2.3
TS276	FrederickFolding	33.62	0.00	33.62	N/A ¹	TS276.v2.1
TS317	GuangzhouRNA_AI	33.16	9.19	23.97	TS317.v1.5	TS317.v2.4
TS448	dNAfold	30.11	20.49	9.62	TS448.v1.1	TS448.v2.5
TS169	thermomaps	28.57	12.37	16.20	TS169.v1.5	TS169.v2.2
TS462	Zheng	27.64	7.94	19.70	TS462.v1.2	TS462.v2.1
TS183	GuangzhouRNA-human	26.84	16.07	10.77	TS183.v1.5	TS183.v2.2
TS481	Vfold	26.72	9.62	17.10	TS481.v1.4	TS481.v2.5
TS358	PerezLab_Gators	25.81	11.55	14.27	TS358.v1.2	TS358.v2.1
TS261	UNRES	25.29	9.56	15.73	TS261.v1.1	TS261.v2.3
TS338	GeneSilico	25.14	10.67	14.47	TS338.v1.5	TS338.v2.3
TS456	Yang-Multimer	23.94	13.31	10.63	TS456.v1.2	TS456.v2.4
TS094	SimRNA-Server	22.53	13.25	9.28	TS094.v1.2	TS094.v2.3
TS063	RNApolis	22.33	10.21	12.13	TS063.v1.4	TS063.v2.3
TS450	OpenComplex_Server	18.83	9.97	8.86	TS450.v1.2	TS450.v2.4
TS298	ShanghaiTech-human	9.18	9.18	0.00	TS298.v1.1	N/A ¹
TS423	ShanghaiTech-server	9.18	9.18	0.00	TS423.v1.1	N/A ¹
TS367	AIR	9.14	0.00	9.14	N/A ¹	TS367.v2.1
TS306	GeneSilicoRNA-server	6.35	0.00	6.35	N/A ¹	TS306.v2.1
TS208	falcon2	4.34	4.34	0.00	TS208.v1.1	N/A ¹
TS403	mmagnus	2.86	0.00	2.86	N/A ¹	TS403.v2.1

¹ Model either not submitted or not assessed

Supplementary Table S15: Results for R1203 GDT TS Two-State Score

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS272	GromihaLab	1.16	54.85	61.57	TS272.v1.4	TS272.v2.1
TS304	AF3-server	1.15	55.22	60.26	TS304.v1.4	TS304.v2.2
TS241	elofsson	1.15	55.22	60.26	TS241.v1.4	TS241.v2.2
TS159	406	1.15	50.56	64.74	TS159.v1.2	TS159.v2.1
TS369	Bhattacharya	1.11	53.73	57.46	TS369.v1.5	TS369.v2.3
TS235	isyslab-hust	1.09	51.31	58.02	TS235.v1.5	TS235.v2.2
TS006	RNA_Dojo	1.09	53.92	55.22	TS006.v1.3	TS006.v2.1
TS231	B-LAB	1.09	45.71	63.06	TS231.v1.2	TS231.v2.5
TS238	BRIQX	1.08	59.52	48.69	TS238.v1.5	TS238.v2.2
TS294	KiharaLab	1.08	51.68	56.53	TS294.v1.2	TS294.v2.1
TS448	dNAfold	1.08	48.51	59.33	TS448.v1.3	TS448.v2.4
TS165	dfr	1.07	52.05	55.41	TS165.v1.3	TS165.v2.4
TS417	GuangzhouRNA-meta	1.07	52.61	54.10	TS417.v1.5	TS417.v2.3
TS435	RNAFOLDX	1.05	44.40	60.26	TS435.v1.1	TS435.v2.5
TS317	GuangzhouRNA_AI	1.03	51.87	50.75	TS317.v1.2	TS317.v2.3
TS183	GuangzhouRNA-human	1.02	52.80	49.44	TS183.v1.5	TS183.v2.2
TS286	CSSB_experimental	0.99	46.27	52.42	TS286.v1.3	TS286.v2.2
TS456	Yang-Multimer	0.99	49.44	49.25	TS456.v1.3	TS456.v2.1
TS338	GeneSilico	0.99	49.44	49.07	TS338.v1.5	TS338.v2.1
TS063	RNApolis	0.97	48.69	48.51	TS063.v1.4	TS063.v2.1
TS052	Yang-Server	0.96	47.95	48.51	TS052.v1.5	TS052.v2.1
TS189	LCBio	0.95	45.90	49.44	TS189.v1.5	TS189.v2.1
TS267	kiharalab_server	0.93	45.90	47.58	TS267.v1.4	TS267.v2.5
TS028	NKRNA-s	0.93	42.35	50.75	TS028.v1.4	TS028.v2.2
TS481	Vfold	0.92	43.66	47.95	TS481.v1.5	TS481.v2.4
TS167	OpenComplex	0.86	33.95	52.42	TS167.v1.1	TS167.v2.2
TS156	SouthRNA	0.83	25.56	57.84	TS156.v1.4	TS156.v2.1
TS462	Zheng	0.74	36.19	38.06	TS462.v1.4	TS462.v2.5
TS110	MIEnsembles-Server	0.73	34.52	38.25	TS110.v1.3	TS110.v2.1
TS276	FrederickFolding	0.59	0.00	58.95	N/A ¹	TS276.v2.1
TS400	OmniFold	0.58	0.00	58.40	N/A ¹	TS400.v2.1
TS403	mmagnus	0.50	50.37	0.00	TS403.v1.1	N/A ¹
TS367	AIR	0.50	0.00	50.00	N/A ¹	TS367.v2.1
TS306	GeneSilicoRNA-server	0.48	48.32	0.00	TS306.v1.1	N/A ¹
TS358	PerezLab_Gators	0.47	27.43	19.59	TS358.v1.3	TS358.v2.4
TS094	SimRNA-Server	0.47	25.75	21.27	TS094.v1.5	TS094.v2.2
TS208	falcon2	0.42	42.16	0.00	TS208.v1.1	N/A ¹
TS423	ShanghaiTech-server	0.40	0.00	39.92	N/A ¹	TS423.v2.1
TS298	ShanghaiTech-human	0.40	0.00	39.92	N/A ¹	TS298.v2.1
TS169	thermomaps	0.37	19.59	17.16	TS169.v1.4	TS169.v2.2
TS261	UNRES	0.30	13.81	16.23	TS261.v1.4	TS261.v2.5
TS450	OpenComplex_Server	0.25	12.69	12.50	TS450.v1.5	TS450.v2.3

¹ Model either not submitted or not assessed

Supplementary Table S16: Results for R1203 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS304	AF3-server	1.65	0.83	0.82	TS304_v1.1	TS304_v2.3
TS241	elofsson	1.65	0.83	0.82	TS241_v1.1	TS241_v2.3
TS272	GromihaLab	1.65	0.82	0.82	TS272_v1.1	TS272_v2.5
TS369	Bhattacharya	1.64	0.82	0.81	TS369_v1.2	TS369_v2.3
TS235	isyslab-hust	1.63	0.82	0.81	TS235_v1.5	TS235_v2.2
TS006	RNA_Dojo	1.62	0.81	0.81	TS006_v1.3	TS006_v2.1
TS159	406	1.60	0.81	0.79	TS159_v1.2	TS159_v2.1
TS294	KiharaLab	1.60	0.83	0.77	TS294_v1.1	TS294_v2.2
TS238	BRIQX	1.56	0.82	0.74	TS238_v1.5	TS238_v2.2
TS183	GuangzhouRNA-human	1.54	0.77	0.77	TS183_v1.2	TS183_v2.5
TS286	CSSB_experimental	1.52	0.76	0.76	TS286_v1.1	TS286_v2.2
TS063	RNAPolis	1.51	0.77	0.75	TS063_v1.3	TS063_v2.5
TS481	Vfold	1.50	0.75	0.75	TS481_v1.3	TS481_v2.4
TS435	RNAFOLDX	1.50	0.81	0.68	TS435_v1.5	TS435_v2.1
TS165	dfr	1.45	0.71	0.74	TS165_v1.2	TS165_v2.3
TS417	GuangzhouRNA-meta	1.44	0.72	0.71	TS417_v1.2	TS417_v2.1
TS231	B-LAB	1.43	0.81	0.63	TS231_v1.5	TS231_v2.2
TS189	LCBio	1.43	0.72	0.71	TS189_v1.2	TS189_v2.4
TS338	GeneSilico	1.42	0.71	0.71	TS338_v1.2	TS338_v2.5
TS456	Yang-Multimer	1.40	0.73	0.67	TS456_v1.1	TS456_v2.2
TS052	Yang-Server	1.39	0.70	0.69	TS052_v1.1	TS052_v2.5
TS448	dNAfold	1.38	0.66	0.72	TS448_v1.1	TS448_v2.5
TS167	OpenComplex	1.38	0.81	0.56	TS167_v1.2	TS167_v2.3
TS267	kiharalab_server	1.37	0.68	0.69	TS267_v1.5	TS267_v2.1
TS317	GuangzhouRNA_AI	1.35	0.63	0.72	TS317_v1.5	TS317_v2.4
TS028	NKRNA-s	1.35	0.70	0.65	TS028_v1.2	TS028_v2.3
TS450	OpenComplex_Server	1.13	0.57	0.56	TS450_v1.2	TS450_v2.3
TS462	Zheng	1.13	0.55	0.57	TS462_v1.4	TS462_v2.1
TS110	MIEnsembles-Server	1.12	0.55	0.58	TS110_v1.5	TS110_v2.1
TS156	SoutheRNA	1.11	0.59	0.52	TS156_v1.1	TS156_v2.4
TS358	PerezLab_Gators	1.10	0.51	0.59	TS358_v1.1	TS358_v2.3
TS169	thermomaps	0.85	0.38	0.47	TS169_v1.5	TS169_v2.4
TS276	FrederickFolding	0.82	0.82	0.00	TS276_v1.1	N/A ¹
TS400	OmniFold	0.82	0.82	0.00	TS400_v1.1	N/A ¹
TS261	UNRES	0.78	0.38	0.40	TS261_v1.1	TS261_v2.3
TS367	AIR	0.63	0.00	0.63	N/A ¹	TS367_v2.1
TS423	ShanghaiTech-server	0.54	0.54	0.00	TS423_v1.1	N/A ¹
TS298	ShanghaiTech-human	0.54	0.54	0.00	TS298_v1.1	N/A ¹
TS403	mmagnus	0.49	0.00	0.49	N/A ¹	TS403_v2.1
TS208	falcon2	0.39	0.39	0.00	TS208_v1.1	N/A ¹
TS094	SimRNA-Server	0.20	0.09	0.12	TS094_v1.3	TS094_v2.5
TS306	GeneSilicoRNA-server	0.01	0.01	0.00	TS306_v1.1	N/A ¹

¹ Model either not submitted or not assessed

Supplementary Table S17: Results for R1203 TMscore Two-State Score

Group	Group_Name	Two-State_Score	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS159	406	1.27	0.56	0.72	TS159.v1.2	TS159.v2.1
TS304	AF3-server	1.23	0.59	0.63	TS304.v1.1	TS304.v2.2
TS241	elofsson	1.23	0.59	0.63	TS241.v1.1	TS241.v2.2
TS272	GromihaLab	1.20	0.59	0.60	TS272.v1.4	TS272.v2.1
TS369	Bhattacharya	1.19	0.59	0.60	TS369.v1.5	TS369.v2.3
TS238	BRIQX	1.18	0.64	0.54	TS238.v1.5	TS238.v2.3
TS448	dNAfold	1.17	0.50	0.67	TS448.v1.3	TS448.v2.4
TS231	B-LAB	1.16	0.53	0.63	TS231.v1.2	TS231.v2.5
TS006	RNA_Dojo	1.16	0.58	0.58	TS006.v1.3	TS006.v2.1
TS165	dfr	1.15	0.56	0.60	TS165.v1.3	TS165.v2.4
TS417	GuangzhouRNA-meta	1.14	0.56	0.58	TS417.v1.2	TS417.v2.3
TS235	isyslab-hust	1.14	0.54	0.59	TS235.v1.5	TS235.v2.2
TS294	KiharaLab	1.12	0.59	0.53	TS294.v1.1	TS294.v2.4
TS317	GuangzhouRNA_AI	1.12	0.57	0.55	TS317.v1.2	TS317.v2.3
TS435	RNAFOLDX	1.11	0.50	0.61	TS435.v1.4	TS435.v2.5
TS183	GuangzhouRNA-human	1.10	0.56	0.54	TS183.v1.2	TS183.v2.3
TS456	Yang-Multimer	1.09	0.56	0.53	TS456.v1.3	TS456.v2.1
TS063	RNApolis	1.08	0.56	0.53	TS063.v1.4	TS063.v2.1
TS052	Yang-Server	1.08	0.54	0.54	TS052.v1.3	TS052.v2.5
TS286	CSSB_experimental	1.06	0.49	0.57	TS286.v1.4	TS286.v2.3
TS267	kiharalab_server	1.05	0.52	0.53	TS267.v1.4	TS267.v2.5
TS189	LCBio	1.05	0.49	0.56	TS189.v1.5	TS189.v2.1
TS028	NKRNA-s	1.02	0.55	0.47	TS028.v1.2	TS028.v2.4
TS481	Vfold	1.01	0.48	0.53	TS481.v1.5	TS481.v2.4
TS338	GeneSilico	1.00	0.49	0.51	TS338.v1.5	TS338.v2.2
TS167	OpenComplex	0.98	0.41	0.57	TS167.v1.1	TS167.v2.2
TS462	Zheng	0.90	0.44	0.46	TS462.v1.4	TS462.v2.3
TS110	MIEnsembles-Server	0.89	0.42	0.47	TS110.v1.3	TS110.v2.1
TS156	SouthRNA	0.86	0.26	0.60	TS156.v1.4	TS156.v2.1
TS400	OmniFold	0.65	0.00	0.65	N/A ¹	TS400.v2.1
TS276	FrederickFolding	0.59	0.00	0.59	N/A ¹	TS276.v2.1
TS403	mmagnus	0.57	0.57	0.00	TS403.v1.1	N/A ¹
TS358	PerezLab_Gators	0.56	0.32	0.24	TS358.v1.3	TS358.v2.2
TS094	SimRNA-Server	0.56	0.30	0.26	TS094.v1.5	TS094.v2.2
TS306	GeneSilicoRNA-server	0.55	0.55	0.00	TS306.v1.1	N/A ¹
TS367	AIR	0.55	0.00	0.55	N/A ¹	TS367.v2.1
TS208	falcon2	0.50	0.50	0.00	TS208.v1.1	N/A ¹
TS298	ShanghaiTech-human	0.46	0.00	0.46	N/A ¹	TS298.v2.1
TS423	ShanghaiTech-server	0.46	0.00	0.46	N/A ¹	TS423.v2.1
TS169	thermomaps	0.42	0.23	0.19	TS169.v1.4	TS169.v2.2
TS261	UNRES	0.39	0.18	0.20	TS261.v1.4	TS261.v2.5
TS450	OpenComplex_Server	0.33	0.15	0.17	TS450.v1.5	TS450.v2.4
TS033	Diff	0.09	0.04	0.04	TS033.v1.1	TS033.v2.4

¹ Model either not submitted or not assessed

Supplementary Table S18: Results for T1214 GDT TS Two-State
Score

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS091	Huang-HUST	194.17	94.25	99.92	TS091_v1.2	TS091_v2.5
TS388	DeepFold-server	193.81	95.23	98.58	TS388_v1.4	TS388_v2.1
TS110	MIEnsembles-Server	193.63	94.67	98.97	TS110_v1.1	TS110_v2.5
TS015	PEZYZFoldings	193.26	96.41	96.86	TS015_v1.2	TS015_v2.1
TS375	milliseconds	193.14	94.25	98.89	TS375_v1.3	TS375_v2.4
TS319	MULTICOM.LLM	193.02	94.78	98.24	TS319_v1.3	TS319_v2.4
TS425	MULTICOM.GATE	192.90	94.78	98.12	TS425_v1.2	TS425_v2.4
TS462	Zheng	192.84	93.83	99.00	TS462_v1.2	TS462_v2.3
TS147	Zheng-Multimer	192.84	93.83	99.00	TS147_v1.2	TS147_v2.3
TS198	colabfold	192.42	93.38	99.04	TS198_v1.5	TS198_v2.1
TS145	colabfold_baseline	192.04	93.12	98.93	TS145_v1.2	TS145_v2.1
TS017	Seder2024hard	192.04	93.12	98.93	TS017_v1.4	TS017_v2.1
TS022	Yang	191.98	95.05	96.93	TS022_v1.4	TS022_v2.3
TS148	Guijunlab-Complex	191.92	93.87	98.04	TS148_v1.5	TS148_v2.2
TS055	LCDD-team	190.69	93.99	96.70	TS055_v1.5	TS055_v2.1
TS052	Yang-Server	190.66	93.50	97.16	TS052_v1.3	TS052_v2.2
TS456	Yang-Multimer	189.79	92.62	97.16	TS456_v1.3	TS456_v2.4
TS262	CoDock	189.52	92.44	97.09	TS262_v1.5	TS262_v2.1
TS204	Zou	189.24	90.32	98.93	TS204_v1.5	TS204_v2.3
TS019	Zheng-Server	188.81	94.21	94.59	TS019_v1.2	TS019_v2.1
TS465	Wallner	188.80	94.44	94.36	TS465_v1.4	TS465_v2.1
TS235	isyslab-hust	188.12	93.87	94.25	TS235_v1.3	TS235_v2.1
TS221	CSSB_FAKER	188.05	90.55	97.51	TS221_v1.3	TS221_v2.1
TS419	CSSB-Human	188.05	90.55	97.51	TS419_v1.3	TS419_v2.1
TS267	kiharalab_server	188.01	93.80	94.21	TS267_v1.1	TS267_v2.3
TS423	ShanghaiTech-server	187.99	94.78	93.21	TS423_v1.5	TS423_v2.4
TS286	CSSB_experimental	187.99	89.79	98.20	TS286_v1.4	TS286_v2.1
TS345	MULTICOM_human	187.88	94.33	93.56	TS345_v1.4	TS345_v2.6
TS208	falcon2	187.81	94.29	93.52	TS208_v1.4	TS208_v2.2
TS040	DELCLAB	187.78	87.94	99.85	TS040_v1.2	TS040_v2.3
TS269	CSSB_server	187.75	90.32	97.43	TS269_v1.1	TS269_v2.2
TS386	ShanghaiTech-Ligand	187.60	95.27	92.33	TS386_v1.1	TS386_v2.4
TS298	ShanghaiTech-human	187.60	95.27	92.33	TS298_v1.1	TS298_v2.4
TS311	RAGfold_Prot1	187.54	94.02	93.52	TS311_v1.2	TS311_v2.3
TS059	DeepFold	187.54	89.03	98.50	TS059_v1.1	TS059_v2.6
TS051	MULTICOM	187.51	93.91	93.60	TS051_v1.5	TS051_v2.6
TS079	MRAFold	187.50	94.21	93.29	TS079_v1.5	TS079_v2.2
TS293	MRAH	187.47	94.17	93.29	TS293_v1.3	TS293_v2.5
TS393	GuijunLab-QA	187.28	93.95	93.33	TS393_v1.5	TS393_v2.4
TS312	GuijunLab-Assembly	187.20	93.87	93.33	TS312_v1.1	TS312_v2.5
TS314	GuijunLab-Pathreader	187.20	93.87	93.33	TS314_v1.1	TS314_v2.5

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Supplementary Table S18 – continued from previous page

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS196	HYU_MLLAB	187.13	93.46	93.67	TS196_v1.2	TS196_v2.4
TS408	SNU-CHEM-lig	187.12	94.06	93.06	TS408_v1.1	TS408_v2.2
TS264	GuijunLab-Human	187.09	93.95	93.14	TS264_v1.3	TS264_v2.2
TS287	plmfold	187.05	93.53	93.52	TS287_v1.1	TS287_v2.4
TS163	MultiFOLD2	186.87	93.19	93.67	TS163_v1.3	TS163_v2.5
TS164	McGuffin	186.87	93.19	93.67	TS164_v1.3	TS164_v2.5
TS102	Psi-Phi	186.86	93.68	93.17	TS102_v1.3	TS102_v2.2
TS464	PocketTracer	186.82	93.38	93.44	TS464_v1.2	TS464_v2.1
TS475	ptq	186.82	93.76	93.06	TS475_v1.3	TS475_v2.1
TS122	MQA_server	186.78	93.68	93.10	TS122_v1.2	TS122_v2.1
TS301	GHZ-MAN	186.75	93.38	93.37	TS301_v1.1	TS301_v2.4
TS014	Cool-PSP	186.71	93.50	93.21	TS014_v1.3	TS014_v2.2
TS494	ClusPro	186.61	86.61	100.00	TS494_v1.3	TS494_v2.1
TS274	kozakovvajda	186.61	86.61	100.00	TS274_v1.3	TS274_v2.1
TS272	GromihaLab	186.60	93.31	93.29	TS272_v1.3	TS272_v2.5
TS227	KUMC	186.55	93.83	92.72	TS227_v1.1	TS227_v2.4
TS207	MULTICOM_ligand	186.44	93.42	93.02	TS207_v1.1	TS207_v2.2
TS304	AF3-server	186.21	93.15	93.06	TS304_v1.4	TS304_v2.3
TS241	elofsson	186.21	93.15	93.06	TS241_v1.4	TS241_v2.3
TS369	Bhattacharya	186.21	93.34	92.87	TS369_v1.1	TS369_v2.2
TS331	MULTICOM_AI	185.67	93.91	91.76	TS331_v1.5	TS331_v2.1
TS284	Unicorn	185.17	93.76	91.41	TS284_v1.1	TS284_v2.3
TS075	GHZ-ISM	185.17	93.76	91.41	TS075_v1.1	TS075_v2.3
TS039	arosko	184.92	87.03	97.89	TS039_v1.2	TS039_v2.1
TS020	comppharmunibas	183.54	87.14	96.40	TS020_v1.4	TS020_v2.3
TS139	DeepFold-refine	180.92	82.41	98.50	TS139_v1.3	TS139_v2.6
TS294	KiharaLab	177.92	85.55	92.37	TS294_v1.3	TS294_v2.2
TS202	test001	168.01	89.56	78.45	TS202_v1.5	TS202_v2.2
TS167	OpenComplex	164.95	94.44	70.51	TS167_v1.2	TS167_v2.3
TS461	forlilab	160.91	76.40	84.51	TS461_v1.2	TS461_v2.3
TS120	Cerebra	160.86	85.70	75.15	TS120_v1.6	TS120_v2.1
TS450	OpenComplex_Server	156.25	94.44	61.81	TS450_v1.5	TS450_v2.1
TS361	Cerebra_server	152.66	76.55	76.11	TS361_v1.3	TS361_v2.4
TS400	OmniFold	93.44	0.00	93.44	N/A ¹	TS400_v2.1
TS225	Unknown	92.93	92.93	0.00	TS225_v1.1	N/A ¹
TS275	Seminole	78.71	78.71	0.00	TS275_v1.1	N/A ¹
TS132	profold2	54.91	0.00	54.91	N/A ¹	TS132_v2.1

¹ Model either not submitted or not assessed

Supplementary Table S19: Results for T1214 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	V1_gLDDT	V2_gLDDT	V1_Model	V2_Model
TS091	Huang-HUST	1.79	0.85	0.94	TS091.v1.2	TS091.v2.1
TS110	MIEnsembles-Server	1.78	0.85	0.93	TS110.v1.2	TS110.v2.5
TS147	Zheng-Multimer	1.78	0.85	0.93	TS147.v1.1	TS147.v2.3
TS462	Zheng	1.78	0.85	0.93	TS462.v1.1	TS462.v2.3
TS375	milliseconds	1.77	0.85	0.92	TS375.v1.3	TS375.v2.4
TS319	MULTICOM_LLM	1.77	0.85	0.92	TS319.v1.3	TS319.v2.4
TS198	colabfold	1.77	0.84	0.93	TS198.v1.5	TS198.v2.1
TS425	MULTICOM_GATE	1.77	0.85	0.91	TS425.v1.2	TS425.v2.4
TS148	Guijunlab-Complex	1.77	0.85	0.92	TS148.v1.5	TS148.v2.2
TS388	DeepFold-server	1.77	0.86	0.91	TS388.v1.4	TS388.v2.1
TS017	Seder2024hard	1.77	0.84	0.93	TS017.v1.4	TS017.v2.1
TS145	colabfold_baseline	1.77	0.84	0.93	TS145.v1.2	TS145.v2.1
TS015	PEZYZFoldings	1.75	0.87	0.88	TS015.v1.5	TS015.v2.1
TS494	ClusPro	1.74	0.75	0.99	TS494.v1.4	TS494.v2.1
TS274	kozakovvajda	1.74	0.75	0.99	TS274.v1.4	TS274.v2.1
TS204	Zou	1.73	0.81	0.93	TS204.v1.5	TS204.v2.3
TS055	LCDD-team	1.72	0.82	0.90	TS055.v1.3	TS055.v2.2
TS039	arosko	1.72	0.75	0.97	TS039.v1.2	TS039.v2.3
TS022	Yang	1.71	0.85	0.86	TS022.v1.4	TS022.v2.2
TS052	Yang-Server	1.70	0.84	0.86	TS052.v1.3	TS052.v2.2
TS456	Yang-Multimer	1.70	0.83	0.86	TS456.v1.5	TS456.v2.4
TS019	Zheng-Server	1.70	0.85	0.85	TS019.v1.2	TS019.v2.1
TS040	DELCLAB	1.70	0.75	0.94	TS040.v1.2	TS040.v2.5
TS059	DeepFold	1.69	0.78	0.91	TS059.v1.5	TS059.v2.6
TS269	CSSB_server	1.69	0.81	0.88	TS269.v1.5	TS269.v2.1
TS221	CSSB_FAKER	1.69	0.81	0.88	TS221.v1.3	TS221.v2.4
TS419	CSSB-Human	1.69	0.81	0.88	TS419.v1.3	TS419.v2.4
TS262	CoDock	1.69	0.83	0.86	TS262.v1.1	TS262.v2.2
TS208	falcon2	1.69	0.86	0.83	TS208.v1.4	TS208.v2.1
TS386	ShanghaiTech-Ligand	1.68	0.86	0.82	TS386.v1.4	TS386.v2.5
TS298	ShanghaiTech-human	1.68	0.86	0.82	TS298.v1.4	TS298.v2.5
TS267	kiharalab_server	1.68	0.85	0.83	TS267.v1.1	TS267.v2.3
TS465	Wallner	1.68	0.85	0.83	TS465.v1.2	TS465.v2.1
TS393	GuijunLab-QA	1.68	0.85	0.83	TS393.v1.1	TS393.v2.2
TS312	GuijunLab-Assembly	1.68	0.85	0.83	TS312.v1.1	TS312.v2.4
TS314	GuijunLab-Pathreader	1.68	0.85	0.83	TS314.v1.1	TS314.v2.4
TS264	GuijunLab-Human	1.68	0.85	0.83	TS264.v1.1	TS264.v2.6
TS287	plmfold	1.68	0.85	0.83	TS287.v1.2	TS287.v2.4
TS235	isyslab-hust	1.68	0.84	0.83	TS235.v1.3	TS235.v2.2
TS102	Psi-Phi	1.68	0.85	0.82	TS102.v1.5	TS102.v2.2
TS207	MULTICOM_ligand	1.67	0.85	0.83	TS207.v1.2	TS207.v2.3

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Supplementary Table S19 – continued from previous page

Group	Group_Name	Two-State_Score	V1_gLDDT	V2_gLDDT	V1_Model	V2_Model
TS139	DeepFold-refine	1.67	0.76	0.91	TS139_v1_3	TS139_v2_6
TS304	AF3-server	1.67	0.84	0.83	TS304_v1_4	TS304_v2_1
TS241	elofsson	1.67	0.84	0.83	TS241_v1_4	TS241_v2_1
TS272	GromihaLab	1.67	0.84	0.83	TS272_v1_3	TS272_v2_2
TS345	MULTICOM_human	1.67	0.85	0.82	TS345_v1_4	TS345_v2_6
TS122	MQA_server	1.67	0.84	0.83	TS122_v1_5	TS122_v2_4
TS311	RAGfold_Prot1	1.67	0.85	0.82	TS311_v1_4	TS311_v2_5
TS464	PocketTracer	1.67	0.84	0.83	TS464_v1_1	TS464_v2_3
TS051	MULTICOM	1.67	0.85	0.82	TS051_v1_1	TS051_v2_6
TS369	Bhattacharya	1.67	0.85	0.82	TS369_v1_1	TS369_v2_2
TS227	KUMC	1.67	0.85	0.82	TS227_v1_3	TS227_v2_5
TS286	CSSB_experimental	1.67	0.80	0.87	TS286_v1_2	TS286_v2_4
TS301	GHZ-MAN	1.66	0.84	0.82	TS301_v1_2	TS301_v2_4
TS079	MRAFold	1.66	0.85	0.82	TS079_v1_1	TS079_v2_5
TS196	HYU_MLLAB	1.66	0.84	0.82	TS196_v1_3	TS196_v2_4
TS293	MRAH	1.66	0.85	0.81	TS293_v1_2	TS293_v2_1
TS164	McGuffin	1.66	0.84	0.82	TS164_v1_3	TS164_v2_4
TS163	MultiFOLD2	1.66	0.84	0.82	TS163_v1_3	TS163_v2_4
TS423	ShanghaiTech-server	1.66	0.85	0.81	TS423_v1_5	TS423_v2_4
TS014	Cool-PSP	1.65	0.84	0.81	TS014_v1_4	TS014_v2_3
TS331	MULTICOM_AI	1.65	0.85	0.80	TS331_v1_1	TS331_v2_5
TS075	GHZ-ISM	1.65	0.85	0.80	TS075_v1_1	TS075_v2_3
TS284	Unicorn	1.65	0.85	0.80	TS284_v1_1	TS284_v2_3
TS408	SNU-CHEM-lig	1.64	0.84	0.81	TS408_v1_3	TS408_v2_2
TS475	ptq	1.64	0.83	0.80	TS475_v1_5	TS475_v2_3
TS020	comp pharmunibas	1.62	0.77	0.85	TS020_v1_4	TS020_v2_3
TS294	KiharaLab	1.56	0.84	0.72	TS294_v1_2	TS294_v2_3
TS202	test001	1.54	0.81	0.73	TS202_v1_5	TS202_v2_2
TS461	forlilab	1.45	0.71	0.73	TS461_v1_2	TS461_v2_3
TS120	Cerebra	1.35	0.63	0.72	TS120_v1_1	TS120_v2_6
TS361	Cerebra_server	1.26	0.62	0.64	TS361_v1_4	TS361_v2_1
TS167	OpenComplex	1.24	0.85	0.39	TS167_v1_2	TS167_v2_5
TS450	OpenComplex_Server	1.20	0.85	0.35	TS450_v1_5	TS450_v2_3
TS400	OmniFold	0.84	0.84	0.00	TS400_v1_1	N/A ¹
TS225	Unknown	0.83	0.83	0.00	TS225_v1_1	N/A ¹
TS275	Seminole	0.69	0.69	0.00	TS275_v1_1	N/A ¹
TS132	profold2	0.50	0.00	0.50	N/A ¹	TS132_v2_1

¹ Model either not submitted or not assessed

Supplementary Table S20: T1214 Sigma1 Score Results

Group	Group_Name	Σ_{score}	Score	Model	Group	Group_Name	Σ_{score}	Score	Model
TS015	PEZYZFoldings		91.17	5	TS079	MRAFold		79.37	1
TS386	ShanghaiTech-Ligand		89.37	4	TS293	MRAH		79.37	2
TS298	ShanghaiTech-human		89.37	4	TS304	AF3-server		79.33	2
TS208	falcon2		87.66	4	TS241	elofsson		79.33	2
TS462	Zheng		86.42	6	TS267	kiharalab_server		79.28	2
TS022	Yang		86.26	4	TS345	MULTICOM_human		79.25	4
TS408	SNU-CHEM-lig		85.96	1	TS301	GHZ-MAN		78.96	2
TS055	LCDD-team		85.68	5	TS369	Bhattacharya		78.81	1
TS465	Wallner		85.35	3	TS284	Unicorn		78.73	2
TS110	MIEnsembles-Server		84.08	2	TS075	GHZ-ISM		78.73	2
TS202	test001		83.44	5	TS331	MULTICOM_AI		78.67	1
TS388	DeepFold-server		82.69	4	TS051	MULTICOM		78.67	1
TS423	ShanghaiTech-server		81.84	1	TS122	MQA_server		78.55	2
TS091	Huang-HUST		81.57	2	TS235	isyslab-hust		78.25	3
TS147	Zheng-Multimer		81.50	1	TS198	colabfold		77.92	3
TS102	Psi-Phi		81.34	2	TS145	colabfold_baseline		77.75	5
TS375	milliseconds		81.32	3	TS017	Seder2024hard		77.75	3
TS287	plmfold		81.25	1	TS272	GromihaLab		77.66	1
TS020	comppharmunibas		81.19	4	TS400	OmniFold		77.54	1
TS319	MULTICOM_LLM		81.15	3	TS464	PocketTracer		77.38	4
TS425	MULTICOM_GATE		81.15	2	TS139	DeepFold-refine		72.37	3
TS314	GuijunLab-Pathreader		81.13	1	TS120	Cerebra		71.99	6
TS312	GuijunLab-Assembly		81.13	1	TS275	Seminole		69.53	1
TS393	GuijunLab-QA		81.13	1	TS052	Yang-Server		69.05	1
TS148	Guijunlab-Complex		81.13	5	TS221	CSSB_FAKER		68.55	3
TS264	GuijunLab-Human		81.13	1	TS419	CSSB-Human		68.55	3
TS227	KUMC		80.86	3	TS269	CSSB_server		68.49	3
TS294	KiharaLab		80.80	3	TS456	Yang-Multimer		68.48	5
TS311	RAGfold_Prot1		80.54	4	TS059	DeepFold		67.39	6
TS207	MULTICOM_ligand		80.33	2	TS204	Zou		66.94	5
TS014	Cool-PSP		80.10	5	TS262	CoDock		66.81	3
TS163	MultiFOLD2		79.86	1	TS461	forlilab		66.23	2
TS225	TS225		79.86	1	TS286	CSSB_experimental		65.85	2
TS164	McGuffin		79.86	1	TS039	arosko		65.44	3
TS019	Zheng-Server		79.81	1	TS494	ClusPro		62.98	1
TS196	HYU_MLLAB		79.57	4	TS274	kozakovvajda		62.98	1
TS167	OpenComplex		79.46	2	TS040	DELCLAB		62.72	3
TS450	OpenComplex_Server		79.46	5	TS361	Cerebra_server		62.26	1
TS475	ptq		79.41	3	TS132	profold2		30.97	1

Supplementary Table S21: T1214 Sigma2 Score Results

Group	Group_Name	Σ_{score}	Score	Model	Group	Group_Name	Σ_{score}	Score	Model
TS015	PEZYZFoldings		90.16	5	TS304	AF3-server		76.05	2
TS386	ShanghaiTech-Ligand		88.04	4	TS475	ptq		76.01	3
TS298	ShanghaiTech-human		88.04	4	TS079	MRAFold		76.00	1
TS208	falcon2		86.01	4	TS293	MRAH		76.00	2
TS462	Zheng		84.51	6	TS267	kiharalab_server		75.92	2
TS022	Yang		84.28	4	TS345	MULTICOM_human		75.84	4
TS408	SNU-CHEM-lig		83.92	1	TS301	GHZ-MAN		75.56	2
TS055	LCDD-team		83.59	4	TS369	Bhattacharya		75.37	1
TS465	Wallner		83.15	3	TS284	Unicorn		75.26	2
TS110	MIEnsembles-Server		81.68	2	TS075	GHZ-ISM		75.26	2
TS202	test001		81.16	5	TS051	MULTICOM		75.09	1
TS388	DeepFold-server		79.88	4	TS331	MULTICOM_AI		75.09	1
TS423	ShanghaiTech-server		78.89	1	TS122	MQA_server		75.03	4
TS020	comppharmunibas		78.81	4	TS235	isyslab-hust		74.66	3
TS147	Zheng-Multimer		78.66	1	TS198	colabfold		74.33	3
TS091	Huang-HUST		78.62	2	TS145	colabfold_baseline		74.24	5
TS102	Psi-Phi		78.38	4	TS017	Seder2024hard		74.24	3
TS375	milliseconds		78.31	3	TS272	GromihaLab		74.03	1
TS294	KiharaLab		78.29	3	TS400	OmniFold		73.89	1
TS287	plmfold		78.28	1	TS464	PocketTracer		73.69	1
TS314	GuijunLab-Pathreader		78.13	1	TS120	Cerebra		68.49	6
TS312	GuijunLab-Assembly		78.13	1	TS139	DeepFold-refine		68.36	3
TS148	Guijunlab-Complex		78.13	5	TS275	Seminole		65.38	1
TS393	GuijunLab-QA		78.13	1	TS052	Yang-Server		64.23	1
TS264	GuijunLab-Human		78.13	1	TS419	CSSB-Human		63.71	3
TS319	MULTICOM_LLM		78.02	3	TS221	CSSB_FAKER		63.71	3
TS425	MULTICOM_GATE		78.02	2	TS269	CSSB_server		63.66	3
TS227	KUMC		77.81	3	TS456	Yang-Multimer		63.66	5
TS311	RAGfold_Prot1		77.44	4	TS059	DeepFold		62.49	6
TS207	MULTICOM_ligand		77.17	3	TS204	Zou		62.01	1
TS014	Cool-PSP		76.85	5	TS262	CoDock		61.92	3
TS164	McGuffin		76.67	1	TS461	forlilab		61.64	2
TS225	TS225		76.67	1	TS286	CSSB_experimental		60.78	2
TS163	MultiFOLD2		76.67	1	TS039	arosko		60.25	3
TS019	Zheng-Server		76.56	1	TS040	DELCLAB		58.05	5
TS196	HYU_MLLAB		76.32	4	TS361	Cerebra_server		58.04	1
TS450	OpenComplex_Server		76.09	5	TS494	ClusPro		57.81	1
TS167	OpenComplex		76.09	2	TS274	kozakovvajda		57.81	1
TS241	elofsson		76.05	2	TS132	profold2		37.74	1

Supplementary Table S22: T1214 Sigma3 Score Results

Group	Group_Name	Σ_{score}	Score	Model	Group	Group_Name	Σ_{score}	Score	Model
TS015	PEZYZFoldings		95.40	5	TS267	kiharalab_server		85.13	2
TS386	ShanghaiTech-Ligand		94.08	4	TS293	MRAH		85.06	2
TS298	ShanghaiTech-human		94.08	4	TS079	MRAFold		85.06	1
TS208	falcon2		92.80	4	TS167	OpenComplex		85.00	2
TS462	Zheng		92.29	6	TS450	OpenComplex_Server		85.00	5
TS408	SNU-CHEM-lig		91.80	1	TS075	GHZ-ISM		84.89	2
TS055	LCDD-team		91.58	3	TS284	Unicorn		84.89	2
TS022	Yang		91.33	4	TS345	MULTICOM_human		84.87	4
TS202	test001		90.86	5	TS017	Seder2024hard		84.76	3
TS465	Wallner		90.74	3	TS145	colabfold_baseline		84.76	5
TS110	MIEnsembles-Server		89.48	2	TS369	Bhattacharya		84.70	1
TS388	DeepFold-server		87.75	4	TS122	MQA_server		84.65	4
TS147	Zheng-Multimer		87.38	1	TS051	MULTICOM		84.56	3
TS423	ShanghaiTech-server		87.25	1	TS331	MULTICOM_AI		84.56	3
TS091	Huang-HUST		87.13	2	TS198	colabfold		84.29	4
TS287	plmfold		86.96	1	TS235	isyslab-hust		84.11	3
TS102	Psi-Phi		86.95	1	TS400	OmniFold		83.80	1
TS148	Guijunlab-Complex		86.74	5	TS272	GromihaLab		83.67	3
TS264	GuijunLab-Human		86.74	1	TS464	PocketTracer		83.44	3
TS312	GuijunLab-Assembly		86.74	1	TS269	CSSB_server		76.64	3
TS314	GuijunLab-PATHreader		86.74	1	TS221	CSSB_FAKER		76.63	3
TS393	GuijunLab-QA		86.74	1	TS419	CSSB-Human		76.63	3
TS375	milliseconds		86.73	3	TS020	comp pharmunibas		76.56	3
TS227	KUMC		86.67	3	TS052	Yang-Server		76.28	1
TS425	MULTICOM_GATE		86.39	2	TS456	Yang-Multimer		75.87	1
TS319	MULTICOM_LLM		86.39	3	TS139	DeepFold-refine		75.62	6
TS014	Cool-PSP		86.23	5	TS059	DeepFold		75.62	6
TS311	RAGfold_Prot1		86.21	4	TS204	Zou		75.40	5
TS207	MULTICOM_ligand		86.09	3	TS262	CoDock		74.54	3
TS164	McGuffin		86.06	1	TS120	Cerebra		63.21	6
TS225	TS225		86.06	1	TS039	arosko		55.81	3
TS163	MultiFOLD2		86.06	1	TS286	CSSB_experimental		54.69	4
TS294	KiharaLab		85.78	2	TS274	kozakovvajda		53.90	3
TS196	HYU_MLLAB		85.70	4	TS494	ClusPro		53.90	3
TS019	Zheng-Server		85.62	1	TS040	DELCLAB		53.84	5
TS241	elofsson		85.46	2	TS275	Seminole		42.73	1
TS475	ptq		85.46	2	TS461	forlilab		39.80	2
TS304	AF3-server		85.46	2	TS361	Cerebra_server		18.76	1
TS301	GHZ-MAN		85.17	2	TS132	profold2		9.66	1

Supplementary Table S23: T1214 Sigma4 Score Results

Group	Group_Name	Σ_{score}	Score	Model	Group	Group_Name	Σ_{score}	Score	Model
TS015	PEZYZFoldings		94.44	5	TS267	kiharalab_server		83.67	2
TS386	ShanghaiTech-Ligand		93.01	4	TS079	MRAFold		83.64	5
TS298	ShanghaiTech-human		93.01	4	TS293	MRAH		83.63	2
TS208	falcon2		91.66	4	TS167	OpenComplex		83.59	2
TS462	Zheng		91.10	6	TS450	OpenComplex_Server		83.59	5
TS408	SNU-CHEM-lig		90.61	1	TS345	MULTICOM_human		83.45	4
TS055	LCDD-team		90.40	5	TS075	GHZ-ISM		83.42	2
TS022	Yang		90.16	4	TS284	Unicorn		83.42	2
TS465	Wallner		89.57	3	TS369	Bhattacharya		83.22	1
TS202	test001		89.38	5	TS122	MQA_server		83.13	4
TS110	MIEnsembles-Server		88.23	2	TS051	MULTICOM		83.12	3
TS388	DeepFold-server		86.53	4	TS017	Seder2024hard		83.12	3
TS423	ShanghaiTech-server		85.97	1	TS145	colabfold_baseline		83.12	5
TS147	Zheng-Multimer		85.96	1	TS331	MULTICOM_AI		83.12	3
TS091	Huang-HUST		85.80	2	TS235	isyslab-hust		82.62	3
TS102	Psi-Phi		85.59	2	TS198	colabfold		82.61	4
TS287	plmfold		85.58	1	TS400	OmniFold		82.22	1
TS375	milliseconds		85.40	3	TS272	GromihaLab		82.11	1
TS148	Guijunlab-Complex		85.37	5	TS464	PocketTracer		81.87	4
TS264	GuijunLab-Human		85.37	1	TS221	CSSB_FAKER		74.21	3
TS312	GuijunLab-Assembly		85.37	1	TS419	CSSB-Human		74.21	3
TS314	GuijunLab-PATHreader		85.37	1	TS269	CSSB_server		74.20	3
TS393	GuijunLab-QA		85.37	1	TS020	comp pharmunibas		74.16	3
TS227	KUMC		85.28	3	TS052	Yang-Server		73.95	1
TS425	MULTICOM_GATE		85.12	2	TS456	Yang-Multimer		73.37	1
TS319	MULTICOM_LLM		85.12	3	TS139	DeepFold-refine		73.02	6
TS014	Cool-PSP		84.85	5	TS059	DeepFold		73.02	6
TS311	RAGfold_Prot1		84.80	4	TS204	Zou		72.76	5
TS207	MULTICOM_ligand		84.68	3	TS262	CoDock		71.81	3
TS164	McGuffin		84.58	1	TS120	Cerebra		60.41	6
TS225	TS225		84.58	1	TS039	arosko		53.05	3
TS163	MultiFOLD2		84.58	1	TS286	CSSB_experimental		51.91	2
TS294	KiharaLab		84.28	2	TS274	kozakovvajda		50.66	3
TS196	HYU_MLLAB		84.21	4	TS494	ClusPro		50.66	3
TS019	Zheng-Server		84.18	1	TS040	DELCLAB		50.16	3
TS475	ptq		84.06	3	TS275	Seminole		39.95	1
TS241	elofsson		83.94	2	TS461	forlilab		36.73	2
TS304	AF3-server		83.94	2	TS361	Cerebra_server		34.59	1
TS301	GHZ-MAN		83.68	2	TS132	profold2		10.44	1

Supplementary Table S24: Results for T1214 TMscore Two-State
Score

Group	Group_Name	Two-State_Score	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS091	Huang-HUST	1.99	0.99	1.00	TS091_v1.2	TS091_v2.4
TS462	Zheng	1.98	0.99	1.00	TS462_v1.6	TS462_v2.3
TS015	PEZYFoldings	1.98	0.99	0.99	TS015_v1.2	TS015_v2.1
TS388	DeepFold-server	1.98	0.99	1.00	TS388_v1.4	TS388_v2.1
TS110	MIEnsembles-Server	1.98	0.99	1.00	TS110_v1.2	TS110_v2.5
TS319	MULTICOM.LLM	1.98	0.99	0.99	TS319_v1.3	TS319_v2.4
TS425	MULTICOM.GATE	1.98	0.99	0.99	TS425_v1.2	TS425_v2.4
TS375	milliseconds	1.98	0.99	1.00	TS375_v1.3	TS375_v2.4
TS147	Zheng-Multimer	1.98	0.99	1.00	TS147_v1.4	TS147_v2.3
TS022	Yang	1.98	0.99	0.99	TS022_v1.4	TS022_v2.2
TS148	Guijunlab-Complex	1.98	0.99	0.99	TS148_v1.5	TS148_v2.2
TS198	colabfold	1.98	0.98	1.00	TS198_v1.5	TS198_v2.1
TS017	Seder2024hard	1.98	0.98	1.00	TS017_v1.4	TS017_v2.1
TS145	colabfold_baseline	1.98	0.98	1.00	TS145_v1.2	TS145_v2.1
TS055	LCDD-team	1.98	0.99	0.99	TS055_v1.3	TS055_v2.1
TS465	Wallner	1.97	0.99	0.99	TS465_v1.3	TS465_v2.1
TS208	falcon2	1.97	0.99	0.98	TS208_v1.4	TS208_v2.2
TS287	plmfold	1.97	0.99	0.99	TS287_v1.2	TS287_v2.5
TS408	SNU-CHEM-lig	1.97	0.99	0.98	TS408_v1.1	TS408_v2.2
TS423	ShanghaiTech-server	1.97	0.99	0.98	TS423_v1.1	TS423_v2.4
TS235	isyslab-hust	1.97	0.99	0.99	TS235_v1.3	TS235_v2.5
TS314	GuijunLab-Pathreader	1.97	0.99	0.98	TS314_v1.1	TS314_v2.5
TS312	GuijunLab-Assembly	1.97	0.99	0.98	TS312_v1.1	TS312_v2.5
TS393	GuijunLab-QA	1.97	0.99	0.98	TS393_v1.1	TS393_v2.4
TS019	Zheng-Server	1.97	0.99	0.98	TS019_v1.2	TS019_v2.1
TS051	MULTICOM	1.97	0.99	0.98	TS051_v1.1	TS051_v2.6
TS267	kiharalab_server	1.97	0.99	0.98	TS267_v1.1	TS267_v2.3
TS345	MULTICOM_human	1.97	0.99	0.98	TS345_v1.4	TS345_v2.1
TS311	RAGfold_Prot1	1.97	0.99	0.98	TS311_v1.1	TS311_v2.2
TS264	GuijunLab-Human	1.97	0.99	0.98	TS264_v1.1	TS264_v2.6
TS475	ptq	1.97	0.99	0.98	TS475_v1.3	TS475_v2.1
TS014	Cool-PSP	1.97	0.99	0.98	TS014_v1.4	TS014_v2.2
TS020	comppharmunibas	1.97	0.98	0.99	TS020_v1.4	TS020_v2.3
TS164	McGuffin	1.97	0.98	0.98	TS164_v1.1	TS164_v2.5
TS163	MultiFOLD2	1.97	0.98	0.98	TS163_v1.1	TS163_v2.5
TS052	Yang-Server	1.97	0.98	0.99	TS052_v1.1	TS052_v2.5
TS122	MQA_server	1.97	0.99	0.98	TS122_v1.2	TS122_v2.1
TS204	Zou	1.97	0.97	1.00	TS204_v1.3	TS204_v2.5
TS196	HYU_MLLAB	1.97	0.98	0.98	TS196_v1.2	TS196_v2.1
TS079	MRAFold	1.97	0.99	0.98	TS079_v1.5	TS079_v2.2
TS456	Yang-Multimer	1.97	0.98	0.99	TS456_v1.5	TS456_v2.4

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Supplementary Table S24 – continued from previous page

Group	Group_Name	Two-State_Score	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS293	MRAH	1.97	0.99	0.98	TS293_v1_3	TS293_v2_1
TS301	GHZ-MAN	1.97	0.98	0.98	TS301_v1_2	TS301_v2_4
TS369	Bhattacharya	1.97	0.98	0.98	TS369_v1_1	TS369_v2_5
TS304	AF3-server	1.97	0.98	0.98	TS304_v1_2	TS304_v2_1
TS241	elofsson	1.97	0.98	0.98	TS241_v1_2	TS241_v2_1
TS272	GromihaLab	1.97	0.98	0.98	TS272_v1_4	TS272_v2_1
TS227	KUMC	1.97	0.99	0.98	TS227_v1_2	TS227_v2_1
TS464	PocketTracer	1.97	0.98	0.98	TS464_v1_3	TS464_v2_5
TS419	CSSB-Human	1.97	0.97	0.99	TS419_v1_3	TS419_v2_1
TS221	CSSB_FAKER	1.97	0.97	0.99	TS221_v1_3	TS221_v2_1
TS102	Psi-Phi	1.97	0.99	0.98	TS102_v1_1	TS102_v2_3
TS269	CSSB_server	1.97	0.97	0.99	TS269_v1_3	TS269_v2_1
TS207	MULTICOM_ligand	1.97	0.99	0.98	TS207_v1_3	TS207_v2_1
TS331	MULTICOM_AI	1.97	0.99	0.98	TS331_v1_1	TS331_v2_5
TS139	DeepFold-refine	1.97	0.97	1.00	TS139_v1_3	TS139_v2_6
TS298	ShanghaiTech-human	1.97	0.99	0.98	TS298_v1_1	TS298_v2_5
TS386	ShanghaiTech-Ligand	1.97	0.99	0.98	TS386_v1_1	TS386_v2_5
TS059	DeepFold	1.97	0.97	1.00	TS059_v1_3	TS059_v2_6
TS284	Unicorn	1.97	0.99	0.98	TS284_v1_3	TS284_v2_5
TS075	GHZ-ISM	1.97	0.99	0.98	TS075_v1_3	TS075_v2_5
TS286	CSSB_experimental	1.97	0.97	0.99	TS286_v1_2	TS286_v2_4
TS262	CoDock	1.97	0.97	0.99	TS262_v1_5	TS262_v2_2
TS040	DELCLAB	1.96	0.96	1.00	TS040_v1_5	TS040_v2_3
TS494	ClusPro	1.95	0.95	1.00	TS494_v1_3	TS494_v2_1
TS274	kozakovvajda	1.95	0.95	1.00	TS274_v1_3	TS274_v2_1
TS039	arosko	1.95	0.96	0.99	TS039_v1_1	TS039_v2_2
TS294	KiharaLab	1.94	0.98	0.96	TS294_v1_2	TS294_v2_1
TS202	test001	1.94	0.98	0.95	TS202_v1_5	TS202_v2_2
TS461	forlilab	1.93	0.96	0.97	TS461_v1_2	TS461_v2_3
TS167	OpenComplex	1.92	0.99	0.94	TS167_v1_2	TS167_v2_1
TS120	Cerebra	1.92	0.97	0.95	TS120_v1_6	TS120_v2_1
TS450	OpenComplex_Server	1.90	0.99	0.92	TS450_v1_5	TS450_v2_1
TS361	Cerebra_server	1.89	0.94	0.95	TS361_v1_3	TS361_v2_1
TS225	Unknown	0.98	0.98	0.00	TS225_v1_1	N/A ¹
TS400	OmniFold	0.98	0.98	0.00	TS400_v1_1	N/A ¹
TS275	Seminole	0.96	0.96	0.00	TS275_v1_1	N/A ¹
TS132	profold2	0.80	0.00	0.80	N/A ¹	TS132_v2_1

¹ Model either not submitted or not assessed

Supplementary Table S25: Results for T1228 GDT TS Two-State
Score

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS462	Zheng	116.15	63.11	53.04	TS462.v1.3	TS462.v2.5
TS264	GuijunLab-Human	116.01	55.95	60.07	TS264.v1.6	TS264.v2.2
TS147	Zheng-Multimer	115.68	62.31	53.37	TS147.v1.1	TS147.v2.1
TS148	Guijunlab-Complex	114.51	54.45	60.07	TS148.v2.3	TS148.v1.3
TS481	Vfold	112.45	61.80	50.66	TS481.v1.3	TS481.v2.5
TS167	OpenComplex	112.41	57.07	55.34	TS167.v1.1	TS167.v2.3
TS450	OpenComplex_Server	112.41	57.07	55.34	TS450.v1.1	TS450.v2.3
TS022	Yang	112.13	57.21	54.92	TS022.v1.4	TS022.v2.5
TS052	Yang-Server	111.89	59.50	52.39	TS052.v1.4	TS052.v2.2
TS456	Yang-Multimer	110.72	58.33	52.39	TS456.v1.3	TS456.v2.2
TS204	Zou	110.58	62.17	48.41	TS204.v1.1	TS204.v2.2
TS241	elofsson	110.39	58.57	51.83	TS241.v2.1	TS241.v1.2
TS294	KiharaLab	109.41	59.97	49.44	TS294.v2.5	TS294.v1.2
TS091	Huang-HUST	109.18	54.54	54.63	TS091.v1.2	TS091.v2.5
TS033	Diff	108.71	56.88	51.83	TS033.v2.1	TS033.v1.4
TS262	CoDock	108.24	55.90	52.34	TS262.v1.2	TS262.v2.1
TS212	PIEFold_human	107.58	55.10	52.48	TS212.v2.4	TS212.v1.2
TS375	milliseconds	106.98	59.41	47.57	TS375.v2.4	TS375.v1.3
TS028	NKRNA-s	106.69	51.31	55.38	TS028.v1.2	TS028.v2.5
TS301	GHZ-MAN	106.65	55.95	50.70	TS301.v1.3	TS301.v2.4
TS110	MIEnsembles-Server	105.81	52.25	53.56	TS110.v1.2	TS110.v2.5
TS304	AF3-server	104.59	57.73	46.86	TS304.v1.4	TS304.v2.5
TS331	MULTICOM_AI	103.98	56.65	47.33	TS331.v1.2	TS331.v2.4
TS319	MULTICOM_LLM	103.98	56.65	47.33	TS319.v1.2	TS319.v2.4
TS345	MULTICOM_human	103.98	56.65	47.33	TS345.v1.3	TS345.v2.2
TS051	MULTICOM	103.98	56.65	47.33	TS051.v1.3	TS051.v2.2
TS274	kozakovvajda	103.84	56.32	47.52	TS274.v1.2	TS274.v2.2
TS494	ClusPro	103.84	56.32	47.52	TS494.v1.2	TS494.v2.2
TS231	B-LAB	103.60	56.27	47.33	TS231.v2.4	TS231.v1.4
TS314	GuijunLab-Pathreader	103.56	48.55	55.01	TS314.v2.3	TS314.v1.1
TS286	CSSB_experimental	103.46	56.13	47.33	TS286.v1.5	TS286.v2.4
TS425	MULTICOM_GATE	103.18	55.85	47.33	TS425.v1.1	TS425.v2.1
TS198	colabfold	102.58	56.41	46.16	TS198.v2.2	TS198.v1.2
TS419	CSSB-Human	102.29	55.52	46.77	TS419.v2.4	TS419.v1.3
TS221	CSSB_FAKER	102.20	55.57	46.63	TS221.v2.2	TS221.v1.5
TS369	Bhattacharya	102.11	54.82	47.28	TS369.v1.2	TS369.v2.1
TS019	Zheng-Server	101.97	51.69	50.28	TS019.v1.4	TS019.v2.4
TS475	ptq	101.12	58.43	42.70	TS475.v2.5	TS475.v1.2
TS014	Cool-PSP	101.12	58.57	42.56	TS014.v2.6	TS014.v1.6
TS287	plmfold	101.08	54.07	47.00	TS287.v1.2	TS287.v2.1
TS267	kiharalab_server	100.05	54.68	45.37	TS267.v1.1	TS267.v2.5

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Supplementary Table S25 – continued from previous page

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS079	MRAFold	99.77	54.82	44.94	TS079_v1.2	TS079_v2.2
TS293	MRAH	99.77	54.82	44.94	TS293_v1.2	TS293_v2.2
TS489	Fernandez-Recio	99.67	55.48	44.20	TS489_v1.2	TS489_v2.2
TS208	falcon2	99.20	54.54	44.66	TS208_v2.5	TS208_v1.1
TS196	HYU_MLLAB	98.74	53.37	45.37	TS196_v1.5	TS196_v2.5
TS312	GuijunLab-Assembly	98.50	53.84	44.66	TS312_v1.1	TS312_v2.2
TS112	Seder2024easy	97.99	54.35	43.63	TS112_v1.4	TS112_v2.3
TS017	Seder2024hard	97.99	54.35	43.63	TS017_v1.5	TS017_v2.5
TS145	colabfold_baseline	97.89	54.35	43.54	TS145_v1.3	TS145_v2.3
TS465	Wallner	97.47	50.00	47.47	TS465_v1.5	TS465_v2.1
TS235	isyslab-hust	96.63	50.80	45.83	TS235_v1.1	TS235_v2.3
TS311	RAGfold_Prot1	96.58	49.86	46.72	TS311_v1.2	TS311_v2.5
TS163	MultiFOLD2	96.02	53.23	42.79	TS163_v1.5	TS163_v2.2
TS015	PEZYZFoldings	95.55	51.12	44.43	TS015_v2.2	TS015_v1.5
TS298	ShanghaiTech-human	95.04	54.35	40.68	TS298_v1.1	TS298_v2.3
TS284	Unicorn	94.90	44.20	50.70	TS284_v1.3	TS284_v2.4
TS075	GHZ-ISM	94.90	44.20	50.70	TS075_v1.3	TS075_v2.4
TS122	MQA_server	94.90	44.20	50.70	TS122_v1.3	TS122_v2.4
TS164	McGuffin	94.76	48.03	46.72	TS164_v1.1	TS164_v2.2
TS325	405	94.29	49.34	44.94	TS325_v1.1	TS325_v2.1
TS159	406	94.29	49.34	44.94	TS159_v1.1	TS159_v2.1
TS269	CSSB_server	92.98	50.70	42.27	TS269_v1.1	TS269_v2.1
TS059	DeepFold	91.53	46.91	44.62	TS059_v2.3	TS059_v1.3
TS388	DeepFold-server	89.23	44.10	45.13	TS388_v1.3	TS388_v2.3
TS023	FTBiot0119	85.63	45.79	39.84	TS023_v1.1	TS023_v2.3
TS139	DeepFold-refine	80.15	40.59	39.56	TS139_v1.4	TS139_v2.2
TS120	Cerebra	76.08	38.34	37.73	TS120_v1.4	TS120_v2.1
TS361	Cerebra_server	66.11	32.77	33.33	TS361_v1.1	TS361_v2.1

Supplementary Table S26: Results for T1228 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	V1_gLDDT	V2_gLDDT	V1_Model	V2_Model
TS314	GuijunLab-PAthreader	1.51	0.77	0.74	TS314_v1.4	TS314_v2.5
TS028	NKRNA-s	1.51	0.77	0.75	TS028_v1.5	TS028_v2.4
TS110	MIEnsembles-Server	1.51	0.77	0.75	TS110_v1.3	TS110_v2.3
TS051	MULTICOM	1.51	0.77	0.74	TS051_v1.1	TS051_v2.3
TS345	MULTICOM_human	1.51	0.77	0.74	TS345_v1.1	TS345_v2.3
TS331	MULTICOM_AI	1.51	0.77	0.74	TS331_v1.1	TS331_v2.2
TS319	MULTICOM_LLM	1.51	0.77	0.74	TS319_v1.1	TS319_v2.2
TS147	Zheng-Multimer	1.51	0.77	0.74	TS147_v2.4	TS147_v1.5
TS425	MULTICOM_GATE	1.50	0.77	0.73	TS425_v2.4	TS425_v1.4
TS462	Zheng	1.50	0.77	0.73	TS462_v2.2	TS462_v1.2
TS022	Yang	1.50	0.77	0.74	TS022_v1.3	TS022_v2.5
TS204	Zou	1.50	0.76	0.74	TS204_v1.4	TS204_v2.5
TS075	GHZ-ISM	1.50	0.76	0.74	TS075_v1.2	TS075_v2.4
TS122	MQA_server	1.50	0.76	0.74	TS122_v1.2	TS122_v2.4
TS284	Unicorn	1.50	0.76	0.74	TS284_v1.2	TS284_v2.4
TS145	colabfold_baseline	1.50	0.77	0.73	TS145_v1.3	TS145_v2.3
TS450	OpenComplex_Server	1.50	0.76	0.73	TS450_v1.1	TS450_v2.5
TS167	OpenComplex	1.50	0.76	0.73	TS167_v1.1	TS167_v2.5
TS198	colabfold	1.50	0.77	0.73	TS198_v1.3	TS198_v2.2
TS475	ptq	1.50	0.76	0.73	TS475_v1.5	TS475_v2.4
TS017	Seder2024hard	1.50	0.77	0.73	TS017_v1.4	TS017_v2.2
TS301	GHZ-MAN	1.49	0.76	0.74	TS301_v1.3	TS301_v2.4
TS325	405	1.49	0.76	0.73	TS325_v1.1	TS325_v2.1
TS159	406	1.49	0.76	0.73	TS159_v1.1	TS159_v2.1
TS456	Yang-Multimer	1.49	0.76	0.73	TS456_v1.1	TS456_v2.2
TS231	B-LAB	1.49	0.76	0.73	TS231_v2.4	TS231_v1.1
TS033	Diff	1.49	0.76	0.73	TS033_v2.1	TS033_v1.4
TS164	McGuffin	1.49	0.76	0.73	TS164_v2.5	TS164_v1.2
TS148	Guijunlab-Complex	1.49	0.76	0.74	TS148_v2.2	TS148_v1.2
TS298	ShanghaiTech-human	1.49	0.77	0.73	TS298_v1.3	TS298_v2.3
TS465	Wallner	1.49	0.76	0.73	TS465_v1.1	TS465_v2.4
TS052	Yang-Server	1.49	0.76	0.73	TS052_v1.1	TS052_v2.2
TS294	KiharaLab	1.49	0.76	0.73	TS294_v2.4	TS294_v1.4
TS375	milliseconds	1.49	0.76	0.73	TS375_v2.4	TS375_v1.2
TS264	GuijunLab-Human	1.49	0.76	0.73	TS264_v2.4	TS264_v1.6
TS196	HYU_MLLAB	1.49	0.76	0.73	TS196_v1.2	TS196_v2.4
TS241	elofsson	1.49	0.76	0.73	TS241_v2.1	TS241_v1.2
TS489	Fernandez-Recio	1.49	0.77	0.72	TS489_v1.2	TS489_v2.2
TS019	Zheng-Server	1.49	0.76	0.73	TS019_v1.4	TS019_v2.4
TS369	Bhattacharya	1.49	0.76	0.73	TS369_v1.1	TS369_v2.1
TS269	CSSB_server	1.49	0.76	0.73	TS269_v1.1	TS269_v2.1

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Supplementary Table S26 – continued from previous page

Group	Group_Name	Two-State_Score	V1_gLDDT	V2_gLDDT	V1_Model	V2_Model
TS481	Vfold	1.49	0.76	0.73	TS481_v2_1	TS481_v1_4
TS287	plmfold	1.49	0.76	0.73	TS287_v1_4	TS287_v2_3
TS312	GuijunLab-Assembly	1.49	0.76	0.73	TS312_v2_5	TS312_v1_1
TS208	falcon2	1.49	0.76	0.72	TS208_v2_5	TS208_v1_1
TS235	isyslab-hust	1.49	0.76	0.73	TS235_v1_2	TS235_v2_2
TS267	kiharalab_server	1.49	0.76	0.72	TS267_v2_3	TS267_v1_3
TS015	PEZYZFoldings	1.48	0.76	0.72	TS015_v1_5	TS015_v2_2
TS304	AF3-server	1.48	0.76	0.72	TS304_v2_1	TS304_v1_3
TS388	DeepFold-server	1.48	0.75	0.73	TS388_v1_3	TS388_v2_3
TS023	FTBiot0119	1.48	0.76	0.73	TS023_v1_3	TS023_v2_4
TS014	Cool-PSP	1.48	0.76	0.72	TS014_v1_5	TS014_v2_5
TS059	DeepFold	1.48	0.75	0.73	TS059_v1_4	TS059_v2_4
TS091	Huang-HUST	1.48	0.75	0.73	TS091_v1_3	TS091_v2_4
TS419	CSSB-Human	1.47	0.75	0.72	TS419_v2_3	TS419_v1_2
TS079	MRAFold	1.47	0.76	0.72	TS079_v1_1	TS079_v2_1
TS221	CSSB_FAKER	1.47	0.75	0.72	TS221_v2_4	TS221_v1_2
TS311	RAGfold_Prot1	1.47	0.75	0.73	TS311_v1_4	TS311_v2_5
TS163	MultiFOLD2	1.47	0.75	0.72	TS163_v1_1	TS163_v2_2
TS293	MRAH	1.47	0.75	0.72	TS293_v1_4	TS293_v2_4
TS112	Seder2024easy	1.47	0.75	0.71	TS112_v1_1	TS112_v2_2
TS286	CSSB_experimental	1.47	0.75	0.72	TS286_v2_3	TS286_v1_4
TS262	CoDock	1.46	0.74	0.71	TS262_v1_4	TS262_v2_2
TS274	kozakovvajda	1.45	0.74	0.71	TS274_v1_1	TS274_v2_3
TS494	ClusPro	1.45	0.74	0.71	TS494_v1_1	TS494_v2_3
TS139	DeepFold-refine	1.45	0.75	0.70	TS139_v1_6	TS139_v2_6
TS212	PIEFold_human	1.37	0.70	0.67	TS212_v2_5	TS212_v1_2
TS120	Cerebra	1.28	0.65	0.63	TS120_v2_5	TS120_v1_2
TS361	Cerebra_server	1.27	0.65	0.62	TS361_v1_2	TS361_v2_1

Supplementary Table S27: Results for T1228 TMscore Two-State
Score

Group	Group_Name	Two-State_Score	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS264	GuijunLab-Human	1.61	0.78	0.82	TS264_v1.6	TS264_v2.1
TS148	Guijunlab-Complex	1.59	0.77	0.83	TS148_v2.3	TS148_v1.2
TS147	Zheng-Multimer	1.55	0.83	0.72	TS147_v1.1	TS147_v2.1
TS167	OpenComplex	1.55	0.80	0.75	TS167_v1.1	TS167_v2.3
TS450	OpenComplex_Server	1.55	0.80	0.75	TS450_v1.1	TS450_v2.3
TS022	Yang	1.55	0.78	0.76	TS022_v1.3	TS022_v2.5
TS481	Vfold	1.54	0.82	0.71	TS481_v1.3	TS481_v2.5
TS462	Zheng	1.53	0.83	0.70	TS462_v1.3	TS462_v2.5
TS091	Huang-HUST	1.51	0.77	0.74	TS091_v1.3	TS091_v2.5
TS241	elofsson	1.51	0.79	0.71	TS241_v2.1	TS241_v1.2
TS456	Yang-Multimer	1.50	0.80	0.70	TS456_v1.3	TS456_v2.2
TS052	Yang-Server	1.50	0.79	0.70	TS052_v1.4	TS052_v2.2
TS033	Diff	1.48	0.80	0.68	TS033_v2.1	TS033_v1.4
TS262	CoDock	1.48	0.77	0.71	TS262_v1.2	TS262_v2.1
TS028	NKRNA-s	1.47	0.72	0.76	TS028_v1.2	TS028_v2.4
TS212	PIEFold_human	1.47	0.77	0.71	TS212_v2.3	TS212_v1.2
TS110	MIEnsembles-Server	1.47	0.73	0.74	TS110_v1.2	TS110_v2.3
TS314	GuijunLab-Pathreader	1.46	0.69	0.77	TS314_v2.3	TS314_v1.1
TS019	Zheng-Server	1.41	0.73	0.68	TS019_v1.4	TS019_v2.3
TS204	Zou	1.39	0.83	0.56	TS204_v1.1	TS204_v2.2
TS301	GHZ-MAN	1.38	0.72	0.67	TS301_v1.3	TS301_v2.5
TS294	KiharaLab	1.38	0.82	0.56	TS294_v2.5	TS294_v1.1
TS375	milliseconds	1.38	0.81	0.56	TS375_v2.4	TS375_v1.2
TS345	MULTICOM_human	1.36	0.80	0.56	TS345_v1.3	TS345_v2.5
TS051	MULTICOM	1.36	0.80	0.56	TS051_v1.3	TS051_v2.5
TS274	kozakovvajda	1.36	0.80	0.56	TS274_v1.1	TS274_v2.2
TS494	ClusPro	1.36	0.80	0.56	TS494_v1.1	TS494_v2.2
TS331	MULTICOM_AI	1.36	0.80	0.56	TS331_v1.2	TS331_v2.1
TS319	MULTICOM_LLM	1.36	0.80	0.56	TS319_v1.2	TS319_v2.1
TS231	B-LAB	1.35	0.79	0.56	TS231_v2.2	TS231_v1.4
TS425	MULTICOM_GATE	1.35	0.79	0.56	TS425_v1.1	TS425_v2.2
TS419	CSSB-Human	1.35	0.79	0.56	TS419_v1.1	TS419_v2.2
TS198	colabfold	1.34	0.78	0.56	TS198_v1.2	TS198_v2.2
TS221	CSSB_FAKER	1.34	0.78	0.56	TS221_v1.1	TS221_v2.1
TS014	Cool-PSP	1.34	0.79	0.55	TS014_v2.5	TS014_v1.5
TS286	CSSB_experimental	1.34	0.78	0.56	TS286_v1.1	TS286_v2.4
TS489	Fernandez-Recio	1.34	0.79	0.55	TS489_v1.2	TS489_v2.5
TS287	plmfold	1.34	0.76	0.58	TS287_v1.2	TS287_v2.1
TS235	isyslab-hust	1.33	0.72	0.61	TS235_v1.1	TS235_v2.3
TS304	AF3-server	1.33	0.77	0.56	TS304_v2.2	TS304_v1.4
TS312	GuijunLab-Assembly	1.33	0.76	0.56	TS312_v1.5	TS312_v2.2

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Supplementary Table S27 – continued from previous page

Group	Group_Name	Two-State_Score	V1.TMscore	V2.TMscore	V1_Model	V2_Model
TS293	MRAH	1.32	0.76	0.56	TS293_v1_2	TS293_v2_2
TS079	MRAFold	1.32	0.76	0.56	TS079_v1_2	TS079_v2_2
TS267	kiharalab_server	1.32	0.76	0.57	TS267_v1_1	TS267_v2_5
TS369	Bhattacharya	1.32	0.76	0.56	TS369_v1_2	TS369_v2_1
TS208	falcon2	1.32	0.76	0.55	TS208_v2_5	TS208_v1_1
TS112	Seder2024easy	1.31	0.76	0.55	TS112_v1_4	TS112_v2_3
TS017	Seder2024hard	1.31	0.76	0.55	TS017_v1_5	TS017_v2_5
TS145	colabfold_baseline	1.31	0.76	0.55	TS145_v1_3	TS145_v2_3
TS015	PEZYZFoldings	1.31	0.74	0.56	TS015_v2_2	TS015_v1_3
TS163	MultiFOLD2	1.30	0.76	0.54	TS163_v1_5	TS163_v2_2
TS269	CSSB_server	1.29	0.75	0.54	TS269_v1_1	TS269_v2_1
TS465	Wallner	1.28	0.71	0.58	TS465_v1_3	TS465_v2_1
TS298	ShanghaiTech-human	1.28	0.76	0.52	TS298_v1_3	TS298_v2_3
TS475	ptq	1.27	0.73	0.54	TS475_v2_5	TS475_v1_2
TS325	405	1.27	0.71	0.55	TS325_v1_1	TS325_v2_1
TS159	406	1.27	0.71	0.55	TS159_v1_1	TS159_v2_1
TS196	HYU_MLLAB	1.26	0.70	0.56	TS196_v1_5	TS196_v2_5
TS164	McGuffin	1.25	0.67	0.58	TS164_v1_1	TS164_v2_2
TS075	GHZ-ISM	1.23	0.54	0.69	TS075_v2_4	TS075_v1_3
TS122	MQA_server	1.23	0.54	0.69	TS122_v2_4	TS122_v1_3
TS284	Unicorn	1.23	0.54	0.69	TS284_v2_4	TS284_v1_3
TS059	DeepFold	1.21	0.61	0.60	TS059_v1_5	TS059_v2_4
TS023	FTBiot0119	1.19	0.66	0.53	TS023_v1_1	TS023_v2_1
TS311	RAGfold_Prot1	1.18	0.58	0.60	TS311_v1_4	TS311_v2_5
TS388	DeepFold-server	1.18	0.58	0.61	TS388_v2_3	TS388_v1_3
TS139	DeepFold-refine	1.17	0.61	0.56	TS139_v1_6	TS139_v2_2
TS120	Cerebra	1.12	0.55	0.56	TS120_v1_4	TS120_v2_3
TS361	Cerebra_server	1.06	0.51	0.55	TS361_v1_1	TS361_v2_1

Supplementary Table S28: Results for T1239 GDT TS Two-State
Score

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS462	Zheng	119.79	70.81	48.98	TS462.v2.2	TS462.v1.1
TS235	isyslab-hust	114.17	71.31	42.85	TS235.v2.4	TS235.v1.1
TS419	CSSB-Human	114.04	71.10	42.94	TS419.v2.1	TS419.v1.5
TS221	CSSB_FAKER	114.04	71.10	42.94	TS221.v2.1	TS221.v1.5
TS028	NKRNA-s	113.49	71.36	42.13	TS028.v2.2	TS028.v1.2
TS345	MULTICOM_human	113.32	71.23	42.09	TS345.v1.4	TS345.v2.5
TS051	MULTICOM	113.32	71.23	42.09	TS051.v1.4	TS051.v2.5
TS286	CSSB_experimental	112.64	69.87	42.77	TS286.v2.1	TS286.v1.2
TS208	falcon2	108.53	66.99	41.54	TS208.v1.4	TS208.v2.4
TS425	MULTICOM_GATE	107.68	63.22	44.46	TS425.v1.2	TS425.v2.4
TS019	Zheng-Server	106.22	54.02	52.20	TS019.v1.5	TS019.v2.5
TS022	Yang	105.14	60.72	44.42	TS022.v1.5	TS022.v2.4
TS204	Zou	104.76	61.23	43.53	TS204.v1.5	TS204.v2.2
TS110	MIEnsembles-Server	104.72	63.01	41.71	TS110.v1.1	TS110.v2.2
TS456	Yang-Multimer	104.50	60.21	44.29	TS456.v1.3	TS456.v2.2
TS147	Zheng-Multimer	103.35	56.27	47.08	TS147.v1.3	TS147.v2.5
TS167	OpenComplex	102.59	54.07	48.52	TS167.v1.5	TS167.v2.3
TS450	OpenComplex_Server	102.59	54.07	48.52	TS450.v1.5	TS450.v2.3
TS294	KiharaLab	101.71	59.58	42.13	TS294.v1.1	TS294.v2.2
TS314	GuijunLab-Pathreader	101.54	58.77	42.77	TS314.v2.5	TS314.v1.2
TS052	Yang-Server	100.05	55.93	44.12	TS052.v1.5	TS052.v2.2
TS481	Vfold	99.67	56.57	43.10	TS481.v2.5	TS481.v1.2
TS091	Huang-HUST	99.24	52.08	47.17	TS091.v1.5	TS091.v2.3
TS319	MULTICOM_LLM	98.53	55.64	42.89	TS319.v1.2	TS319.v2.5
TS262	CoDock	98.36	57.63	40.74	TS262.v1.2	TS262.v2.1
TS033	Diff	97.93	53.94	43.99	TS033.v2.2	TS033.v1.1
TS331	MULTICOM_AI	97.73	55.64	42.09	TS331.v1.2	TS331.v2.2
TS325	405	97.47	55.21	42.26	TS325.v1.2	TS325.v2.2
TS159	406	97.47	55.21	42.26	TS159.v1.2	TS159.v2.2
TS369	Bhattacharya	97.17	54.07	43.10	TS369.v1.4	TS369.v2.4
TS489	Fernandez-Recio	96.71	54.96	41.75	TS489.v1.3	TS489.v2.4
TS298	ShanghaiTech-human	96.00	61.74	34.26	TS298.v1.1	TS298.v2.1
TS212	PIEFold_human	95.91	55.21	40.69	TS212.v2.1	TS212.v1.3
TS241	elofsson	95.14	54.32	40.82	TS241.v1.1	TS241.v2.5
TS231	B-LAB	94.34	54.07	40.27	TS231.v2.1	TS231.v1.2
TS304	AF3-server	94.04	50.89	43.15	TS304.v2.5	TS304.v1.2
TS465	Wallner	92.97	48.14	44.84	TS465.v1.4	TS465.v2.2
TS358	PerezLab_Gators	92.78	54.96	37.82	TS358.v2.2	TS358.v1.4
TS293	MRAH	91.92	49.91	42.01	TS293.v1.2	TS293.v2.3
TS079	MRAFold	91.92	49.91	42.01	TS079.v1.2	TS079.v2.3
TS272	GromihaLab	91.33	50.09	41.24	TS272.v1.1	TS272.v2.1

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Supplementary Table S28 – continued from previous page

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS423	ShanghaiTech-server	91.08	51.91	39.17	TS423_v2.4	TS423_v1.1
TS267	kiharalab_server	89.30	50.00	39.30	TS267_v1.1	TS267_v2.4
TS148	Guijunlab-Complex	88.53	48.94	39.59	TS148_v2.5	TS148_v1.4
TS287	plmfold	88.49	49.32	39.17	TS287_v1.3	TS287_v2.4
TS198	colabfold	88.11	50.34	37.77	TS198_v1.2	TS198_v2.1
TS375	milliseconds	87.73	47.16	40.57	TS375_v2.3	TS375_v1.4
TS112	Seder2024easy	86.88	48.09	38.79	TS112_v1.4	TS112_v2.5
TS014	Cool-PSP	86.84	49.49	37.35	TS014_v2.3	TS014_v1.3
TS301	GHZ-MAN	86.84	46.65	40.19	TS301_v2.4	TS301_v1.1
TS163	MultiFOLD2	86.72	48.39	38.33	TS163_v1.3	TS163_v2.3
TS040	DELCLAB	86.50	48.09	38.41	TS040_v1.3	TS040_v2.3
TS145	colabfold_baseline	86.46	47.67	38.79	TS145_v1.2	TS145_v2.1
TS023	FTBiot0119	86.46	47.67	38.79	TS023_v1.2	TS023_v2.1
TS264	GuijunLab-Human	86.20	47.54	38.66	TS264_v2.2	TS264_v1.5
TS312	GuijunLab-Assembly	85.86	46.27	39.59	TS312_v2.4	TS312_v1.4
TS122	MQA_server	85.78	46.65	39.13	TS122_v1.3	TS122_v2.2
TS139	DeepFold-refine	84.76	45.93	38.83	TS139_v1.6	TS139_v2.6
TS059	DeepFold	84.76	45.93	38.83	TS059_v1.6	TS059_v2.6
TS017	Seder2024hard	84.52	48.05	36.46	TS017_v1.5	TS017_v2.4
TS397	smg_ulaval	84.13	45.00	39.13	TS397_v1.1	TS397_v2.1
TS164	McGuffin	83.83	45.47	38.37	TS164_v2.2	TS164_v1.3
TS015	PEZYZFoldings	83.79	45.00	38.79	TS015_v1.4	TS015_v2.1
TS196	HYU_MLLAB	78.41	38.94	39.47	TS196_v1.2	TS196_v2.2
TS388	DeepFold-server	75.91	37.92	37.99	TS388_v1.3	TS388_v2.2
TS120	Cerebra	61.43	31.48	29.95	TS120_v1.3	TS120_v2.2
TS475	ptq	49.20	49.20	0.00	TS475_v2.1	N/A ¹
TS351	digiwiser-ensemble	48.73	24.45	24.28	TS351_v1.1	TS351_v2.1
TS269	CSSB_server	48.18	48.18	0.00	TS269_v2.4	N/A ¹
TS075	GHZ-ISM	46.65	46.65	0.00	TS075_v2.4	N/A ¹
TS284	Unicorn	46.65	46.65	0.00	TS284_v2.4	N/A ¹
TS311	RAGfold_Prot1	42.25	42.25	0.00	TS311_v1.1	N/A ¹
TS361	Cerebra_server	31.40	31.40	0.00	TS361_v1.2	N/A ¹
TS105	PFSC-PFVM	4.20	4.20	0.00	TS105_v1.3	N/A ¹

¹ Model either not submitted or not assessed

Supplementary Table S29: Results for T1239 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	V1_gLDDT	V2_gLDDT	V1_Model	V2_Model
TS028	NKRNA-s	1.67	0.82	0.85	TS028.v1.4	TS028.v2.1
TS208	falcon2	1.66	0.81	0.85	TS208.v1.4	TS208.v2.4
TS051	MULTICOM	1.66	0.81	0.85	TS051.v1.3	TS051.v2.2
TS345	MULTICOM_human	1.66	0.81	0.85	TS345.v1.1	TS345.v2.2
TS425	MULTICOM_GATE	1.65	0.81	0.85	TS425.v1.2	TS425.v2.1
TS456	Yang-Multimer	1.65	0.81	0.84	TS456.v1.3	TS456.v2.4
TS462	Zheng	1.65	0.81	0.84	TS462.v1.4	TS462.v2.2
TS235	isyslab-hust	1.65	0.81	0.84	TS235.v2.4	TS235.v1.2
TS110	MIEnsembles-Server	1.65	0.80	0.85	TS110.v2.5	TS110.v1.2
TS019	Zheng-Server	1.64	0.79	0.85	TS019.v1.1	TS019.v2.5
TS489	Fernandez-Recio	1.64	0.79	0.85	TS489.v1.3	TS489.v2.5
TS331	MULTICOM_AI	1.64	0.80	0.85	TS331.v1.2	TS331.v2.1
TS319	MULTICOM_LLM	1.64	0.80	0.85	TS319.v1.2	TS319.v2.1
TS022	Yang	1.64	0.80	0.84	TS022.v1.5	TS022.v2.1
TS052	Yang-Server	1.64	0.79	0.84	TS052.v1.1	TS052.v2.4
TS419	CSSB-Human	1.63	0.80	0.84	TS419.v1.2	TS419.v2.2
TS221	CSSB_FAKER	1.63	0.80	0.84	TS221.v1.2	TS221.v2.2
TS314	GuijunLab-Pathreader	1.63	0.79	0.84	TS314.v1.5	TS314.v2.5
TS294	KiharaLab	1.63	0.79	0.84	TS294.v2.1	TS294.v1.4
TS325	405	1.63	0.79	0.84	TS325.v2.2	TS325.v1.1
TS159	406	1.63	0.79	0.84	TS159.v1.2	TS159.v2.1
TS481	Vfold	1.63	0.79	0.84	TS481.v1.4	TS481.v2.4
TS272	GromihaLab	1.61	0.78	0.83	TS272.v1.3	TS272.v2.4
TS262	CoDock	1.61	0.78	0.83	TS262.v1.2	TS262.v2.5
TS147	Zheng-Multimer	1.60	0.76	0.85	TS147.v2.4	TS147.v1.1
TS286	CSSB_experimental	1.60	0.77	0.83	TS286.v1.4	TS286.v2.1
TS241	elofsson	1.60	0.75	0.85	TS241.v2.3	TS241.v1.2
TS204	Zou	1.58	0.75	0.83	TS204.v2.1	TS204.v1.5
TS298	ShanghaiTech-human	1.57	0.74	0.83	TS298.v2.1	TS298.v1.1
TS167	OpenComplex	1.57	0.74	0.83	TS167.v1.1	TS167.v2.5
TS450	OpenComplex_Server	1.57	0.74	0.83	TS450.v1.1	TS450.v2.5
TS304	AF3-server	1.54	0.74	0.81	TS304.v1.1	TS304.v2.2
TS033	Diff	1.54	0.73	0.81	TS033.v1.1	TS033.v2.4
TS231	B-LAB	1.54	0.74	0.80	TS231.v1.2	TS231.v2.5
TS091	Huang-HUST	1.52	0.74	0.78	TS091.v1.4	TS091.v2.4
TS264	GuijunLab-Human	1.51	0.72	0.79	TS264.v2.6	TS264.v1.5
TS198	colabfold	1.50	0.72	0.79	TS198.v1.5	TS198.v2.4
TS023	FTBiot0119	1.50	0.71	0.79	TS023.v1.5	TS023.v2.4
TS145	colabfold_baseline	1.50	0.71	0.79	TS145.v1.2	TS145.v2.4
TS164	McGuffin	1.50	0.73	0.78	TS164.v1.5	TS164.v2.5
TS017	Seder2024hard	1.50	0.71	0.79	TS017.v1.1	TS017.v2.5

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Supplementary Table S29 – continued from previous page

Group	Group_Name	Two-State_Score	V1_gLDDT	V2_gLDDT	V1_Model	V2_Model
TS358	PerezLab_Gators	1.50	0.71	0.78	TS358.v1.5	TS358.v2.1
TS369	Bhattacharya	1.50	0.72	0.77	TS369.v1.4	TS369.v2.1
TS148	Guijunlab-Complex	1.49	0.71	0.78	TS148.v2.5	TS148.v1.3
TS312	GuijunLab-Assembly	1.49	0.71	0.78	TS312.v2.5	TS312.v1.3
TS287	plmfold	1.49	0.71	0.77	TS287.v2.4	TS287.v1.5
TS163	MultiFOLD2	1.49	0.71	0.78	TS163.v1.3	TS163.v2.5
TS112	Seder2024easy	1.48	0.70	0.79	TS112.v1.2	TS112.v2.1
TS301	GHZ-MAN	1.48	0.71	0.77	TS301.v2.5	TS301.v1.4
TS375	milliseconds	1.48	0.71	0.77	TS375.v2.3	TS375.v1.2
TS397	smg_ulaval	1.47	0.71	0.77	TS397.v1.1	TS397.v2.1
TS122	MQA_server	1.47	0.71	0.76	TS122.v1.4	TS122.v2.2
TS423	ShanghaiTech-server	1.44	0.68	0.76	TS423.v2.3	TS423.v1.2
TS465	Wallner	1.43	0.68	0.75	TS465.v1.3	TS465.v2.2
TS212	PIEFold_human	1.43	0.66	0.77	TS212.v1.3	TS212.v2.1
TS267	kiharalab_server	1.42	0.68	0.74	TS267.v1.5	TS267.v2.4
TS388	DeepFold-server	1.41	0.65	0.76	TS388.v1.2	TS388.v2.3
TS014	Cool-PSP	1.41	0.68	0.73	TS014.v2.6	TS014.v1.1
TS059	DeepFold	1.41	0.67	0.74	TS059.v1.6	TS059.v2.3
TS293	MRAH	1.39	0.67	0.72	TS293.v1.3	TS293.v2.3
TS079	MRAFold	1.39	0.67	0.72	TS079.v1.3	TS079.v2.3
TS139	DeepFold-refine	1.39	0.67	0.72	TS139.v1.6	TS139.v2.6
TS040	DELCLAB	1.34	0.65	0.70	TS040.v1.2	TS040.v2.3
TS015	PEZYZFoldings	1.34	0.65	0.70	TS015.v2.6	TS015.v1.6
TS196	HYU_MLLAB	1.27	0.60	0.66	TS196.v1.1	TS196.v2.3
TS351	digiwiser-ensemble	1.23	0.59	0.64	TS351.v1.1	TS351.v2.1
TS120	Cerebra	1.12	0.54	0.58	TS120.v1.4	TS120.v2.3
TS475	ptq	0.77	0.00	0.77	N/A ¹	TS475.v2.5
TS269	CSSB_server	0.76	0.00	0.76	N/A ¹	TS269.v2.2
TS075	GHZ-ISM	0.76	0.00	0.76	N/A ¹	TS075.v2.2
TS284	Unicorn	0.76	0.00	0.76	N/A ¹	TS284.v2.2
TS311	RAGfold_Prot1	0.76	0.00	0.76	N/A ¹	TS311.v1.1
TS361	Cerebra_server	0.58	0.00	0.58	N/A ¹	TS361.v1.3
TS105	PFSC-PFVM	0.07	0.00	0.07	N/A ¹	TS105.v1.3

¹ Model either not submitted or not assessed

Supplementary Table S30: Results for T1239 TMscore Two-State
Score

Group	Group_Name	Two-State_Score	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS462	Zheng	1.58	0.91	0.67	TS462_v2.2	TS462_v1.1
TS019	Zheng-Server	1.54	0.76	0.77	TS019_v1.1	TS019_v2.5
TS425	MULTICOM_GATE	1.52	0.88	0.64	TS425_v1.2	TS425_v2.4
TS481	Vfold	1.47	0.81	0.65	TS481_v1.5	TS481_v2.4
TS147	Zheng-Multimer	1.44	0.80	0.64	TS147_v1.3	TS147_v2.5
TS221	CSSB_FAKER	1.43	0.91	0.52	TS221_v2.1	TS221_v1.4
TS419	CSSB-Human	1.43	0.91	0.52	TS419_v2.1	TS419_v1.4
TS028	NKRNA-s	1.43	0.92	0.51	TS028_v2.2	TS028_v1.4
TS051	MULTICOM	1.43	0.92	0.51	TS051_v1.4	TS051_v2.4
TS345	MULTICOM_human	1.43	0.92	0.51	TS345_v1.4	TS345_v2.4
TS286	CSSB_experimental	1.42	0.91	0.52	TS286_v2.1	TS286_v1.5
TS235	isyslab-hust	1.42	0.91	0.51	TS235_v2.4	TS235_v1.1
TS208	falcon2	1.40	0.90	0.50	TS208_v1.4	TS208_v2.4
TS204	Zou	1.39	0.87	0.52	TS204_v1.5	TS204_v2.2
TS456	Yang-Multimer	1.38	0.86	0.52	TS456_v1.3	TS456_v2.2
TS450	OpenComplex_Server	1.38	0.72	0.65	TS450_v1.1	TS450_v2.4
TS167	OpenComplex	1.38	0.72	0.65	TS167_v1.1	TS167_v2.4
TS110	MIEnsembles-Server	1.36	0.85	0.51	TS110_v1.1	TS110_v2.2
TS022	Yang	1.34	0.82	0.52	TS022_v1.5	TS022_v2.4
TS298	ShanghaiTech-human	1.34	0.87	0.47	TS298_v1.1	TS298_v2.1
TS052	Yang-Server	1.34	0.81	0.53	TS052_v1.5	TS052_v2.3
TS294	KiharaLab	1.34	0.83	0.51	TS294_v1.1	TS294_v2.2
TS262	CoDock	1.34	0.83	0.50	TS262_v1.2	TS262_v2.2
TS033	Diff	1.33	0.70	0.62	TS033_v2.2	TS033_v1.1
TS091	Huang-HUST	1.32	0.71	0.61	TS091_v1.5	TS091_v2.3
TS314	GuijunLab-Pathreader	1.32	0.82	0.51	TS314_v2.5	TS314_v1.5
TS319	MULTICOM_LLM	1.32	0.81	0.51	TS319_v1.2	TS319_v2.5
TS331	MULTICOM_AI	1.32	0.81	0.51	TS331_v1.2	TS331_v2.5
TS159	406	1.31	0.80	0.51	TS159_v1.2	TS159_v2.2
TS325	405	1.31	0.80	0.51	TS325_v1.2	TS325_v2.2
TS212	PIEFold_human	1.30	0.80	0.50	TS212_v2.1	TS212_v1.4
TS465	Wallner	1.30	0.66	0.63	TS465_v1.4	TS465_v2.2
TS489	Fernandez-Recio	1.28	0.78	0.50	TS489_v1.3	TS489_v2.4
TS241	elofsson	1.27	0.76	0.51	TS241_v1.4	TS241_v2.5
TS423	ShanghaiTech-server	1.23	0.72	0.51	TS423_v1.4	TS423_v2.5
TS369	Bhattacharya	1.22	0.71	0.51	TS369_v1.3	TS369_v2.4
TS231	B-LAB	1.21	0.71	0.50	TS231_v2.1	TS231_v1.2
TS358	PerezLab_Gators	1.21	0.72	0.49	TS358_v2.2	TS358_v1.4
TS272	GromihaLab	1.21	0.70	0.50	TS272_v1.1	TS272_v2.1
TS040	DELCLAB	1.21	0.70	0.51	TS040_v1.3	TS040_v2.3
TS112	Seder2024easy	1.20	0.69	0.51	TS112_v1.4	TS112_v2.4

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Supplementary Table S30 – continued from previous page

Group	Group_Name	Two-State_Score	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS017	Seder2024hard	1.20	0.69	0.51	TS017_v1_1	TS017_v2_4
TS145	colabfold_baseline	1.20	0.69	0.51	TS145_v1_2	TS145_v2_3
TS079	MRAFold	1.20	0.67	0.53	TS079_v1_2	TS079_v2_3
TS293	MRAH	1.20	0.67	0.53	TS293_v1_2	TS293_v2_3
TS023	FTBiot0119	1.20	0.69	0.51	TS023_v1_2	TS023_v2_3
TS304	AF3-server	1.20	0.67	0.52	TS304_v2_4	TS304_v1_2
TS198	colabfold	1.19	0.70	0.49	TS198_v1_2	TS198_v2_1
TS148	Guijunlab-Complex	1.19	0.69	0.50	TS148_v2_5	TS148_v1_3
TS059	DeepFold	1.19	0.67	0.52	TS059_v1_6	TS059_v2_3
TS014	Cool-PSP	1.19	0.69	0.50	TS014_v2_3	TS014_v1_5
TS163	MultiFOLD2	1.19	0.69	0.50	TS163_v1_2	TS163_v2_3
TS139	DeepFold-refine	1.18	0.67	0.52	TS139_v1_6	TS139_v2_2
TS375	milliseconds	1.18	0.68	0.50	TS375_v1_3	TS375_v2_3
TS301	GHZ-MAN	1.16	0.65	0.51	TS301_v2_4	TS301_v1_1
TS312	GuijunLab-Assembly	1.16	0.66	0.50	TS312_v2_4	TS312_v1_3
TS264	GuijunLab-Human	1.16	0.65	0.50	TS264_v2_2	TS264_v1_5
TS267	kiharalab_server	1.16	0.66	0.50	TS267_v1_1	TS267_v2_4
TS122	MQA_server	1.15	0.65	0.50	TS122_v1_3	TS122_v2_3
TS287	plmfold	1.15	0.64	0.51	TS287_v1_3	TS287_v2_4
TS015	PEZYFoldings	1.14	0.62	0.52	TS015_v2_3	TS015_v1_4
TS164	McGuffin	1.14	0.64	0.50	TS164_v2_2	TS164_v1_2
TS397	smg_ulaval	1.12	0.61	0.50	TS397_v2_1	TS397_v1_1
TS196	HYU_MLLAB	1.08	0.52	0.56	TS196_v1_2	TS196_v2_3
TS388	DeepFold-server	1.05	0.52	0.53	TS388_v1_3	TS388_v2_2
TS120	Cerebra	1.02	0.52	0.50	TS120_v1_4	TS120_v2_4
TS351	digiwiser-ensemble	0.71	0.35	0.36	TS351_v1_2	TS351_v2_5
TS269	CSSB_server	0.69	0.69	0.00	TS269_v2_4	N/A ¹
TS475	ptq	0.67	0.67	0.00	TS475_v2_1	N/A ¹
TS075	GHZ-ISM	0.65	0.65	0.00	TS075_v2_4	N/A ¹
TS284	Unicorn	0.65	0.65	0.00	TS284_v2_4	N/A ¹
TS311	RAGfold_Prot1	0.53	0.00	0.53	N/A ¹	TS311_v1_1
TS361	Cerebra_server	0.52	0.52	0.00	TS361_v1_3	N/A ¹
TS105	PFSC-PFVM	0.14	0.14	0.00	TS105_v1_3	N/A ¹

¹ Model either not submitted or not assessed

Supplementary Table S31: Results for T1249 AvgDockQ Two-State Score

Group	Group_Name	Two-State_Score	V1_AvgDockQ	V2_AvgDockQ	V1_Model	V2_Model
TS393	GuijunLab-QA	0.97	0.47	0.50	TS393.v1.3o	TS393.v2.6o
TS304	AF3-server	0.94	0.43	0.51	TS304.v1.2o	TS304.v2.1o
TS314	GuijunLab-Pathreader	0.88	0.37	0.52	TS314.v1.2o	TS314.v2.1o
TS345	MULTICOM_human	0.87	0.69	0.19	TS345.v2.4o	TS345.v1.5o
TS397	smg_ulaval	0.87	0.65	0.21	TS397.v2.1o	TS397.v1.1o
TS015	PEZYZFoldings	0.86	0.71	0.14	TS015.v1.2o	TS015.v2.1o
TS456	Yang-Multimer	0.81	0.65	0.15	TS456.v1.2o	TS456.v2.2o
TS051	MULTICOM	0.79	0.61	0.18	TS051.v1.6o	TS051.v2.5o
TS293	MRAH	0.78	0.62	0.16	TS293.v1.2o	TS293.v2.5o
TS079	MRAFold	0.78	0.62	0.16	TS079.v1.2o	TS079.v2.5o
TS014	Cool-PSP	0.77	0.65	0.12	TS014.v1.1o	TS014.v2.1o
TS322	XGroup	0.76	0.49	0.26	TS322.v1.4o	TS322.v2.1o
TS219	XGroup-Server	0.76	0.49	0.26	TS219.v1.4o	TS219.v2.1o
TS465	Wallner	0.73	0.58	0.15	TS465.v1.1o	TS465.v2.3o
TS241	elofsson	0.73	0.55	0.18	TS241.v2.5o	TS241.v1.1o
TS052	Yang-Server	0.72	0.46	0.26	TS052.v1.3o	TS052.v2.1o
TS091	Huang-HUST	0.71	0.49	0.23	TS091.v2.5o	TS091.v1.1o
TS462	Zheng	0.71	0.45	0.26	TS462.v2.1o	TS462.v1.6o
TS290	Pierce	0.71	0.46	0.25	TS290.v1.5o	TS290.v2.4o
TS167	OpenComplex	0.70	0.48	0.22	TS167.v2.2o	TS167.v1.5o
TS450	OpenComplex_Server	0.70	0.48	0.22	TS450.v2.2o	TS450.v1.5o
TS008	HADDOCK	0.70	0.46	0.24	TS008.v1.1o	TS008.v2.5o
TS059	DeepFold	0.68	0.47	0.21	TS059.v2.3o	TS059.v1.5o
TS369	Bhattacharya	0.66	0.44	0.22	TS369.v1.3o	TS369.v2.2o
TS022	Yang	0.64	0.46	0.18	TS022.v1.5o	TS022.v2.1o
TS425	MULTICOM_GATE	0.64	0.46	0.18	TS425.v2.3o	TS425.v1.4o
TS331	MULTICOM_AI	0.64	0.46	0.18	TS331.v2.3o	TS331.v1.4o
TS319	MULTICOM_LLM	0.64	0.46	0.18	TS319.v2.3o	TS319.v1.4o
TS301	GHZ-MAN	0.64	0.50	0.14	TS301.v1.4o	TS301.v2.1o
TS267	kiharalab_server	0.64	0.48	0.15	TS267.v1.2o	TS267.v2.5o
TS375	milliseconds	0.64	0.45	0.18	TS375.v2.1o	TS375.v1.4o
TS423	ShanghaiTech-server	0.63	0.49	0.14	TS423.v1.2o	TS423.v2.2o
TS294	KiharaLab	0.62	0.46	0.17	TS294.v2.4o	TS294.v1.5o
TS204	Zou	0.62	0.51	0.11	TS204.v2.5o	TS204.v1.1o
TS145	colabfold_baseline	0.62	0.38	0.24	TS145.v1.2o	TS145.v2.5o
TS380	mialab_prediction	0.62	0.38	0.24	TS380.v1.4o	TS380.v2.5o
TS311	RAGfold_Prot1	0.62	0.47	0.14	TS311.v1.2o	TS311.v2.1o
TS148	Guijunlab-Complex	0.62	0.58	0.03	TS148.v2.2o	TS148.v1.3o
TS264	GuijunLab-Human	0.61	0.58	0.03	TS264.v2.2o	TS264.v1.4o
TS312	GuijunLab-Assembly	0.61	0.58	0.03	TS312.v2.2o	TS312.v1.4o
TS287	plmfold	0.60	0.47	0.12	TS287.v2.2o	TS287.v1.5o

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Supplementary Table S31 – continued from previous page

Group	Group_Name	Two-State_Score	V1_AvgDockQ	V2_AvgDockQ	V1_Model	V2_Model
TS198	colabfold	0.60	0.39	0.21	TS198_v2.2o	TS198_v1.3o
TS122	MQA_server	0.59	0.57	0.02	TS122_v2.2o	TS122_v1.3o
TS075	GHZ-ISM	0.59	0.57	0.02	TS075_v2.1o	TS075_v1.2o
TS475	ptq	0.59	0.57	0.02	TS475_v2.1o	TS475_v1.2o
TS284	Unicorn	0.59	0.57	0.02	TS284_v2.1o	TS284_v1.2o
TS031	MassiveFold	0.56	0.42	0.14	TS031_v2.4o	TS031_v1.5o
TS163	MultiFOLD2	0.55	0.36	0.19	TS163_v1.3o	TS163_v2.5o
TS494	ClusPro	0.55	0.35	0.20	TS494_v1.4o	TS494_v2.4o
TS261	UNRES	0.55	0.29	0.26	TS261_v1.1o	TS261_v2.1o
TS187	Ayush	0.53	0.36	0.17	TS187_v2.1o	TS187_v1.1o
TS274	kozakovvajda	0.52	0.36	0.15	TS274_v2.1o	TS274_v1.5o
TS272	GromihaLab	0.52	0.06	0.46	TS272_v2.1o	TS272_v1.2o
TS164	McGuffin	0.52	0.39	0.12	TS164_v2.5o	TS164_v1.4o
TS028	NKRNA-s	0.49	0.46	0.03	TS028_v2.1o	TS028_v1.4o
TS208	falcon2	0.48	0.37	0.10	TS208_v2.4o	TS208_v1.5o
TS110	MIEnsembles-Server	0.48	0.45	0.03	TS110_v2.1o	TS110_v1.4o
TS147	Zheng-Multimer	0.48	0.45	0.03	TS147_v2.1o	TS147_v1.3o
TS117	Vakser	0.41	0.02	0.39	TS117_v1.2o	TS117_v2.3o
TS040	DELCLAB	0.39	0.39	0.00	TS040_v2.3o	N/A ¹
TS419	CSSB-Human	0.39	0.26	0.12	TS419_v1.3o	TS419_v2.1o
TS221	CSSB_FAKER	0.39	0.26	0.12	TS221_v1.3o	TS221_v2.1o
TS286	CSSB_experimental	0.39	0.26	0.12	TS286_v1.3o	TS286_v2.1o
TS323	Yan	0.33	0.31	0.02	TS323_v2.1o	TS323_v1.1o
TS262	CoDock	0.33	0.24	0.09	TS262_v2.5o	TS262_v1.1o
TS489	Fernandez-Recio	0.20	0.15	0.05	TS489_v1.1o	TS489_v2.5o
TS196	HYU_MLLAB	0.07	0.01	0.05	TS196_v1.3o	TS196_v2.5o
TS114	COAST	0.04	0.02	0.01	TS114_v1.5o	TS114_v2.1o
TS337	APOLLO	0.03	0.02	0.02	TS337_v1.1o	TS337_v2.4o
TS139	DeepFold-refine	0.03	0.01	0.02	TS139_v1.4o	TS139_v2.3o
TS300	ARC	0.03	0.01	0.01	TS300_v1.2o	TS300_v2.2o
TS085	Bates	0.03	0.01	0.01	TS085_v1.5o	TS085_v2.4o
TS023	FTBiot0119	0.02	0.01	0.01	TS023_v1.3o	TS023_v2.1o

¹ Model either not submitted or not assessed

Supplementary Table S32: Results for T1249 GDT TS Two-State
Score

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS393	GuijunLab-QA	1.51	79.50	71.70	TS393.v1.2	TS393.v2.6
TS304	AF3-server	1.46	70.80	75.00	TS304.v1.2	TS304.v2.1
TS059	DeepFold	1.44	84.80	59.00	TS059.v2.3	TS059.v1.5
TS345	MULTICOM_human	1.42	88.00	53.60	TS345.v2.4	TS345.v1.2
TS052	Yang-Server	1.41	82.50	58.30	TS052.v1.3	TS052.v2.1
TS079	MRAFold	1.40	86.40	53.20	TS079.v2.1	TS079.v1.4
TS091	Huang-HUST	1.40	78.80	60.80	TS091.v2.1	TS091.v1.1
TS293	MRAH	1.40	86.40	53.20	TS293.v2.1	TS293.v1.4
TS314	GuijunLab-Pathreader	1.39	61.60	77.60	TS314.v1.2	TS314.v2.1
TS015	PEZYFoldings	1.39	86.60	52.20	TS015.v1.2	TS015.v2.5
TS456	Yang-Multimer	1.38	87.30	51.00	TS456.v1.1	TS456.v2.2
TS397	smg.ulaval	1.38	82.40	55.70	TS397.v2.1	TS397.v1.1
TS241	elofsson	1.38	79.10	58.40	TS241.v1.3	TS241.v2.4
TS014	Cool-PSP	1.37	85.60	51.30	TS014.v1.1	TS014.v2.1
TS375	milliseconds	1.37	79.90	56.90	TS375.v1.3	TS375.v2.2
TS423	ShanghaiTech-server	1.37	84.60	52.20	TS423.v1.2	TS423.v2.4
TS008	HADDOCK	1.37	78.00	58.70	TS008.v1.4	TS008.v2.5
TS290	Pierce	1.36	82.70	53.80	TS290.v2.3	TS290.v1.5
TS462	Zheng	1.36	78.30	58.10	TS462.v2.3	TS462.v1.6
TS167	OpenComplex	1.36	77.60	58.60	TS167.v2.2	TS167.v1.5
TS294	KiharaLab	1.36	84.10	52.10	TS294.v2.4	TS294.v1.4
TS267	kiharalab_server	1.36	83.20	53.00	TS267.v2.3	TS267.v1.1
TS450	OpenComplex_Server	1.36	77.60	58.60	TS450.v2.2	TS450.v1.5
TS145	colabfold_baseline	1.36	71.50	64.40	TS145.v1.2	TS145.v2.5
TS380	mialab_prediction	1.36	71.50	64.40	TS380.v1.4	TS380.v2.5
TS198	colabfold	1.36	75.20	60.60	TS198.v1.2	TS198.v2.3
TS301	GHZ-MAN	1.35	83.90	51.50	TS301.v1.2	TS301.v2.1
TS031	MassiveFold	1.35	82.60	52.30	TS031.v2.3	TS031.v1.5
TS022	Yang	1.35	82.50	52.20	TS022.v1.3	TS022.v2.5
TS051	MULTICOM	1.34	80.50	53.60	TS051.v1.6	TS051.v2.2
TS311	RAGfold_Prot1	1.31	77.20	53.90	TS311.v1.2	TS311.v2.1
TS163	MultiFOLD2	1.30	71.20	59.30	TS163.v1.3	TS163.v2.5
TS319	MULTICOM_LLM	1.30	77.90	52.30	TS319.v2.3	TS319.v1.5
TS425	MULTICOM_GATE	1.30	77.90	52.30	TS425.v2.3	TS425.v1.5
TS331	MULTICOM_AI	1.30	77.90	52.30	TS331.v2.3	TS331.v1.5
TS219	XGroup-Server	1.30	71.90	58.20	TS219.v1.3	TS219.v2.4
TS322	XGroup	1.30	71.90	58.20	TS322.v1.3	TS322.v2.4
TS204	Zou	1.30	84.00	46.00	TS204.v2.4	TS204.v1.2
TS369	Bhattacharya	1.29	74.90	54.40	TS369.v1.3	TS369.v2.2
TS187	Ayush	1.26	70.80	55.20	TS187.v1.1	TS187.v2.1
TS494	ClusPro	1.26	67.90	58.00	TS494.v1.3	TS494.v2.4

Continued on next page

Supplementary Table S32 – continued from previous page

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS261	UNRES	1.22	58.30	63.40	TS261_v2.4	TS261_v1.5
TS465	Wallner	1.20	75.30	44.20	TS465_v1.1	TS465_v2.3
TS287	plmfold	1.19	70.50	48.50	TS287_v2.1	TS287_v1.5
TS274	kozakovvajda	1.18	67.50	50.80	TS274_v2.1	TS274_v1.4
TS264	GuijunLab-Human	1.18	86.40	31.10	TS264_v2.2	TS264_v1.3
TS312	GuijunLab-Assembly	1.18	86.40	31.10	TS312_v2.2	TS312_v1.3
TS148	Guijunlab-Complex	1.17	86.40	30.50	TS148_v2.2	TS148_v1.4
TS164	McGuffin	1.15	68.30	46.20	TS164_v2.5	TS164_v1.4
TS208	falcon2	1.13	66.70	46.20	TS208_v2.4	TS208_v1.5
TS110	MIEnsembles-Server	1.09	78.30	31.00	TS110_v2.4	TS110_v1.4
TS028	NKRNA-s	1.09	78.80	30.50	TS028_v2.1	TS028_v1.1
TS147	Zheng-Multimer	1.09	78.30	31.00	TS147_v2.3	TS147_v1.4
TS075	GHZ-ISM	1.05	74.00	30.70	TS075_v2.2	TS075_v1.1
TS122	MQA_server	1.05	74.00	30.70	TS122_v2.3	TS122_v1.1
TS284	Unicorn	1.05	74.00	30.70	TS284_v2.2	TS284_v1.1
TS475	ptq	1.05	74.00	30.70	TS475_v2.2	TS475_v1.1
TS272	GromihaLab	1.04	35.90	68.40	TS272_v2.1	TS272_v1.2
TS286	CSSB_experimental	0.97	53.90	43.10	TS286_v2.1	TS286_v1.1
TS221	CSSB_FAKER	0.97	53.90	43.10	TS221_v2.1	TS221_v1.1
TS419	CSSB-Human	0.97	53.90	43.10	TS419_v2.1	TS419_v1.1
TS117	Vakser	0.77	15.70	61.30	TS117_v1.2	TS117_v2.4
TS323	Yan	0.76	59.60	16.00	TS323_v2.1	TS323_v1.1
TS262	CoDock	0.75	42.40	32.60	TS262_v2.1	TS262_v1.2
TS040	DELCLAB	0.72	72.20	0.00	TS040_v2.3	N/A ¹
TS489	Fernandez-Recio	0.59	39.10	19.70	TS489_v1.1	TS489_v2.5
TS196	HYU_MLLAB	0.39	18.10	21.20	TS196_v2.5	TS196_v1.1
TS085	Bates	0.34	16.10	18.10	TS085_v1.5	TS085_v2.2
TS139	DeepFold-refine	0.22	15.30	6.80	TS139_v1.3	TS139_v2.4
TS114	COAST	0.08	4.10	4.20	TS114_v1.3	TS114_v2.3
TS337	APOLLO	0.08	4.10	4.20	TS337_v1.1	TS337_v2.1
TS023	FTBiot0119	0.08	3.60	4.50	TS023_v1.3	TS023_v2.2
TS300	ARC	0.07	3.60	3.90	TS300_v1.2	TS300_v2.4

¹ Model either not submitted or not assessed

Supplementary Table S33: Results for T1249 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	V1_gLDDT	V2_gLDDT	V1_Model	V2_Model
TS304	AF3-server	1.60	0.79	0.81	TS304_v1_2o	TS304_v2_1o
TS393	GuijunLab-QA	1.57	0.78	0.79	TS393_v1_6o	TS393_v2_6o
TS462	Zheng	1.57	0.79	0.78	TS462_v1_6o	TS462_v2_6o
TS314	GuijunLab-Pathreader	1.56	0.76	0.81	TS314_v1_2o	TS314_v2_1o
TS241	elofsson	1.55	0.79	0.76	TS241_v2_5o	TS241_v1_3o
TS015	PEZYZFoldings	1.55	0.81	0.74	TS015_v1_2o	TS015_v2_1o
TS345	MULTICOM_human	1.55	0.79	0.76	TS345_v1_5o	TS345_v2_5o
TS272	GromihaLab	1.55	0.74	0.80	TS272_v2_1o	TS272_v1_2o
TS375	milliseconds	1.55	0.79	0.76	TS375_v1_3o	TS375_v2_2o
TS284	Unicorn	1.54	0.80	0.75	TS284_v2_1o	TS284_v1_4o
TS475	ptq	1.54	0.80	0.75	TS475_v2_1o	TS475_v1_4o
TS075	GHZ-ISM	1.54	0.80	0.75	TS075_v2_1o	TS075_v1_4o
TS110	MIEnsembles-Server	1.54	0.79	0.76	TS110_v2_5o	TS110_v1_3o
TS122	MQA_server	1.54	0.80	0.75	TS122_v2_2o	TS122_v1_5o
TS052	Yang-Server	1.54	0.78	0.76	TS052_v1_1o	TS052_v2_1o
TS051	MULTICOM	1.54	0.79	0.76	TS051_v1_3o	TS051_v2_5o
TS290	Pierce	1.54	0.78	0.76	TS290_v1_5o	TS290_v2_1o
TS319	MULTICOM_LLM	1.54	0.78	0.76	TS319_v1_4o	TS319_v2_2o
TS425	MULTICOM_GATE	1.54	0.78	0.76	TS425_v1_4o	TS425_v2_2o
TS331	MULTICOM_AI	1.54	0.78	0.76	TS331_v1_4o	TS331_v2_2o
TS028	NKRNA-s	1.54	0.79	0.76	TS028_v2_4o	TS028_v1_2o
TS287	plmfold	1.54	0.79	0.75	TS287_v2_1o	TS287_v1_4o
TS147	Zheng-Multimer	1.54	0.79	0.76	TS147_v2_3o	TS147_v1_1o
TS397	smg_ulaval	1.54	0.79	0.75	TS397_v2_1o	TS397_v1_1o
TS167	OpenComplex	1.54	0.78	0.76	TS167_v2_2o	TS167_v1_5o
TS450	OpenComplex_Server	1.54	0.78	0.76	TS450_v2_2o	TS450_v1_5o
TS293	MRAH	1.54	0.80	0.74	TS293_v1_2o	TS293_v2_5o
TS079	MRAFold	1.54	0.80	0.74	TS079_v1_2o	TS079_v2_5o
TS369	Bhattacharya	1.54	0.78	0.76	TS369_v1_3o	TS369_v2_2o
TS456	Yang-Multimer	1.53	0.79	0.74	TS456_v1_2o	TS456_v2_5o
TS312	GuijunLab-Assembly	1.53	0.77	0.76	TS312_v2_1o	TS312_v1_5o
TS264	GuijunLab-Human	1.53	0.77	0.76	TS264_v2_1o	TS264_v1_5o
TS294	KiharaLab	1.53	0.79	0.75	TS294_v2_3o	TS294_v1_1o
TS022	Yang	1.53	0.78	0.75	TS022_v1_5o	TS022_v2_1o
TS091	Huang-HUST	1.53	0.77	0.76	TS091_v2_4o	TS091_v1_1o
TS148	Guijunlab-Complex	1.52	0.77	0.75	TS148_v2_1o	TS148_v1_1o
TS204	Zou	1.52	0.78	0.74	TS204_v2_3o	TS204_v1_3o
TS008	HADDOCK	1.52	0.77	0.75	TS008_v1_4o	TS008_v2_5o
TS059	DeepFold	1.52	0.77	0.74	TS059_v1_1o	TS059_v2_6o
TS267	kiharalab_server	1.51	0.78	0.73	TS267_v2_3o	TS267_v1_3o
TS145	colabfold_baseline	1.51	0.76	0.76	TS145_v1_1o	TS145_v2_5o

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Supplementary Table S33 – continued from previous page

Group	Group_Name	Two-State_Score	V1_gLDDT	V2_gLDDT	V1_Model	V2_Model
TS164	McGuffin	1.51	0.77	0.74	TS164_v2_5o	TS164_v1_2o
TS380	mialab_prediction	1.51	0.76	0.76	TS380_v1_3o	TS380_v2_5o
TS311	RAGfold_Prot1	1.51	0.76	0.75	TS311_v1_3o	TS311_v2_1o
TS198	colabfold	1.51	0.76	0.75	TS198_v2_2o	TS198_v1_3o
TS301	GHZ-MAN	1.51	0.77	0.74	TS301_v2_1o	TS301_v1_3o
TS014	Cool-PSP	1.51	0.80	0.71	TS014_v1_1o	TS014_v2_1o
TS208	falcon2	1.51	0.76	0.74	TS208_v2_4o	TS208_v1_5o
TS163	MultiFOLD2	1.50	0.76	0.74	TS163_v1_3o	TS163_v2_3o
TS494	ClusPro	1.49	0.75	0.74	TS494_v1_2o	TS494_v2_5o
TS187	Ayush	1.49	0.75	0.74	TS187_v1_1o	TS187_v2_1o
TS322	XGroup	1.48	0.74	0.74	TS322_v1_4o	TS322_v2_1o
TS219	XGroup-Server	1.48	0.74	0.74	TS219_v1_4o	TS219_v2_1o
TS274	kozakovvajda	1.48	0.75	0.73	TS274_v2_1o	TS274_v1_5o
TS423	ShanghaiTech-server	1.47	0.75	0.72	TS423_v2_2o	TS423_v1_4o
TS031	MassiveFold	1.47	0.75	0.71	TS031_v2_5o	TS031_v1_5o
TS261	UNRES	1.44	0.72	0.72	TS261_v1_3o	TS261_v2_1o
TS465	Wallner	1.43	0.74	0.69	TS465_v1_1o	TS465_v2_3o
TS262	CoDock	1.32	0.61	0.72	TS262_v2_2o	TS262_v1_5o
TS323	Yan	1.24	0.76	0.49	TS323_v2_1o	TS323_v1_1o
TS419	CSSB-Human	1.22	0.65	0.57	TS419_v1_1o	TS419_v2_1o
TS221	CSSB_FAKER	1.22	0.65	0.57	TS221_v1_1o	TS221_v2_1o
TS286	CSSB_experimental	1.22	0.65	0.57	TS286_v1_1o	TS286_v2_1o
TS489	Fernandez-Recio	1.08	0.55	0.53	TS489_v1_3o	TS489_v2_3o
TS117	Vakser	1.07	0.65	0.42	TS117_v2_2o	TS117_v1_2o
TS196	HYU_MLLAB	1.07	0.51	0.56	TS196_v2_3o	TS196_v1_1o
TS085	Bates	0.98	0.43	0.55	TS085_v1_5o	TS085_v2_5o
TS040	DELCLAB	0.72	0.72	0.00	TS040_v2_3o	N/A ¹
TS139	DeepFold-refine	0.65	0.25	0.40	TS139_v2_4o	TS139_v1_5o
TS114	COAST	0.36	0.18	0.18	TS114_v1_4o	TS114_v2_4o
TS337	APOLLO	0.35	0.17	0.18	TS337_v1_1o	TS337_v2_1o
TS300	ARC	0.34	0.17	0.17	TS300_v1_1o	TS300_v2_1o
TS023	FTBiot0119	0.32	0.16	0.16	TS023_v1_3o	TS023_v2_3o

¹ Model either not submitted or not assessed

Supplementary Table S34: Results for T1249 TMscore Two-State
Score

Group	Group_Name	Two-State_Score	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS304	AF3-server	1.91	0.95	0.97	TS304_v1_2o	TS304_v2_1o
TS393	GuijunLab-QA	1.91	0.96	0.95	TS393_v1_2o	TS393_v2_6o
TS314	GuijunLab-Pathreader	1.90	0.94	0.96	TS314_v1_2o	TS314_v2_1o
TS145	colabfold_baseline	1.88	0.95	0.93	TS145_v2_1o	TS145_v1_5o
TS380	mialab_prediction	1.88	0.95	0.93	TS380_v2_3o	TS380_v1_5o
TS091	Huang-HUST	1.88	0.96	0.92	TS091_v2_4o	TS091_v1_1o
TS052	Yang-Server	1.88	0.96	0.91	TS052_v1_3o	TS052_v2_1o
TS059	DeepFold	1.87	0.96	0.91	TS059_v2_3o	TS059_v1_5o
TS198	colabfold	1.87	0.95	0.92	TS198_v1_2o	TS198_v2_3o
TS450	OpenComplex_Server	1.87	0.96	0.91	TS450_v2_2o	TS450_v1_5o
TS167	OpenComplex	1.87	0.96	0.91	TS167_v2_2o	TS167_v1_5o
TS462	Zheng	1.87	0.96	0.91	TS462_v2_3o	TS462_v1_6o
TS008	HADDOCK	1.87	0.96	0.91	TS008_v2_1o	TS008_v1_5o
TS345	MULTICOM_human	1.86	0.98	0.89	TS345_v2_4o	TS345_v1_2o
TS322	XGroup	1.86	0.94	0.92	TS322_v1_3o	TS322_v2_4o
TS219	XGroup-Server	1.86	0.94	0.92	TS219_v1_3o	TS219_v2_4o
TS015	PEZYZFoldings	1.86	0.98	0.88	TS015_v1_2o	TS015_v2_3o
TS293	MRAH	1.86	0.98	0.88	TS293_v1_2o	TS293_v2_5o
TS079	MRAFold	1.86	0.98	0.88	TS079_v1_2o	TS079_v2_5o
TS163	MultiFOLD2	1.86	0.95	0.91	TS163_v1_3o	TS163_v2_5o
TS311	RAGfold_Prot1	1.86	0.97	0.89	TS311_v1_2o	TS311_v2_1o
TS375	milliseconds	1.86	0.96	0.90	TS375_v1_3o	TS375_v2_2o
TS290	Pierce	1.86	0.96	0.89	TS290_v2_2o	TS290_v1_5o
TS494	ClusPro	1.85	0.94	0.91	TS494_v1_4o	TS494_v2_4o
TS397	smg_ulaval	1.85	0.97	0.88	TS397_v2_1o	TS397_v1_1o
TS456	Yang-Multimer	1.85	0.98	0.87	TS456_v1_2o	TS456_v2_2o
TS051	MULTICOM	1.85	0.96	0.89	TS051_v1_6o	TS051_v2_2o
TS241	elofsson	1.85	0.96	0.89	TS241_v2_1o	TS241_v1_1o
TS369	Bhattacharya	1.85	0.95	0.90	TS369_v1_3o	TS369_v2_2o
TS267	kiharalab_server	1.85	0.96	0.88	TS267_v2_3o	TS267_v1_1o
TS022	Yang	1.85	0.96	0.88	TS022_v1_3o	TS022_v2_5o
TS294	KiharaLab	1.85	0.96	0.88	TS294_v2_4o	TS294_v1_5o
TS187	Ayush	1.84	0.95	0.90	TS187_v1_1o	TS187_v2_1o
TS014	Cool-PSP	1.84	0.98	0.87	TS014_v1_1o	TS014_v2_1o
TS423	ShanghaiTech-server	1.84	0.97	0.88	TS423_v1_2o	TS423_v2_4o
TS319	MULTICOM_LLM	1.84	0.96	0.88	TS319_v2_3o	TS319_v1_5o
TS425	MULTICOM_GATE	1.84	0.96	0.88	TS425_v2_3o	TS425_v1_5o
TS331	MULTICOM_AI	1.84	0.96	0.88	TS331_v2_3o	TS331_v1_5o
TS301	GHZ-MAN	1.84	0.97	0.87	TS301_v1_5o	TS301_v2_1o
TS261	UNRES	1.84	0.91	0.93	TS261_v1_1o	TS261_v2_5o
TS031	MassiveFold	1.84	0.96	0.87	TS031_v2_5o	TS031_v1_5o

Continued on next page

Supplementary Table S34 – continued from previous page

Group	Group_Name	Two-State_Score	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS274	kozakovvajda	1.82	0.94	0.88	TS274_v2_1o	TS274_v1_4o
TS287	plmfold	1.82	0.95	0.87	TS287_v2_1o	TS287_v1_5o
TS204	Zou	1.81	0.96	0.84	TS204_v2_3o	TS204_v1_2o
TS465	Wallner	1.80	0.95	0.84	TS465_v1_1o	TS465_v2_3o
TS164	McGuffin	1.79	0.94	0.84	TS164_v2_5o	TS164_v1_4o
TS208	falcon2	1.78	0.94	0.83	TS208_v2_4o	TS208_v1_5o
TS286	CSSB_experimental	1.68	0.86	0.82	TS286_v1_3o	TS286_v2_3o
TS419	CSSB-Human	1.68	0.86	0.82	TS419_v1_3o	TS419_v2_3o
TS221	CSSB_FAKER	1.68	0.86	0.82	TS221_v1_3o	TS221_v2_3o
TS272	GromihaLab	1.63	0.69	0.94	TS272_v2_1o	TS272_v1_2o
TS262	CoDock	1.56	0.82	0.74	TS262_v2_1o	TS262_v1_1o
TS122	MQA_server	1.41	0.95	0.46	TS122_v2_2o	TS122_v1_2o
TS475	ptq	1.41	0.95	0.46	TS475_v2_1o	TS475_v1_5o
TS075	GHZ-ISM	1.41	0.95	0.46	TS075_v2_1o	TS075_v1_5o
TS284	Unicorn	1.41	0.95	0.46	TS284_v2_1o	TS284_v1_5o
TS264	GuijunLab-Human	1.40	0.97	0.43	TS264_v2_2o	TS264_v1_6o
TS110	MIEnsembles-Server	1.40	0.96	0.44	TS110_v2_5o	TS110_v1_4o
TS312	GuijunLab-Assembly	1.36	0.97	0.39	TS312_v2_2o	TS312_v1_1o
TS148	Guijunlab-Complex	1.36	0.97	0.39	TS148_v2_2o	TS148_v1_3o
TS147	Zheng-Multimer	1.35	0.96	0.39	TS147_v2_3o	TS147_v1_4o
TS028	NKRNA-s	1.34	0.96	0.38	TS028_v2_1o	TS028_v1_1o
TS117	Vakser	1.30	0.37	0.93	TS117_v1_2o	TS117_v2_4o
TS323	Yan	1.23	0.92	0.32	TS323_v2_1o	TS323_v1_1o
TS489	Fernandez-Recio	1.21	0.74	0.46	TS489_v1_1o	TS489_v2_5o
TS040	DELCLAB	0.95	0.95	0.00	TS040_v2_3o	N/A ¹
TS196	HYU_MLLAB	0.86	0.39	0.47	TS196_v1_4o	TS196_v2_5o
TS085	Bates	0.73	0.29	0.44	TS085_v2_4o	TS085_v1_1o
TS139	DeepFold-refine	0.60	0.27	0.33	TS139_v2_1o	TS139_v1_1o
TS023	FTBiot0119	0.58	0.28	0.30	TS023_v1_3o	TS023_v2_1o
TS114	COAST	0.57	0.29	0.28	TS114_v1_1o	TS114_v2_4o
TS300	ARC	0.55	0.29	0.26	TS300_v1_1o	TS300_v2_4o
TS337	APOLLO	0.53	0.26	0.27	TS337_v1_1o	TS337_v2_1o

¹ Model either not submitted or not assessed