

CASP16_TWO-STATE_TABLES

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

Group	Group_Name	Two-State_Score	Balance	V1_BestDockQ	V2_BestDockQ	V1_Model	V2_Model
TS294	KiharaLab	1.61	0.98	0.79	0.82	TS294_v1_1	TS294_v2_1
TS033	Diff	1.52	0.96	0.73	0.79	TS033_v1_4	TS033_v2_5
TS462	Zheng	1.49	0.91	0.81	0.68	TS462_v1_3	TS462_v2_3
TS204	Zou	1.48	0.88	0.65	0.83	TS204_v1_2	TS204_v2_2
TS325	405	1.42	0.86	0.61	0.81	TS325_v1_1	TS325_v2_1
TS159	406	1.42	0.86	0.61	0.81	TS159_v1_1	TS159_v2_1
TS304	AF3-server	1.40	0.85	0.59	0.81	TS304_v1_2	TS304_v2_3
TS241	elofsson	1.37	0.86	0.58	0.78	TS241_v1_3	TS241_v2_1
TS091	Huang-HUST	1.36	0.90	0.75	0.61	TS091_v1_3	TS091_v2_2
TS262	CoDock	1.31	0.95	0.69	0.62	TS262_v1_1	TS262_v2_3
TS231	B-LAB	1.29	0.81	0.53	0.77	TS231_v1_2	TS231_v2_1
TS489	Fernandez-Recio	1.29	0.99	0.65	0.64	TS489_v1_1	TS489_v2_1
TS481	Vfold	1.26	0.96	0.60	0.65	TS481_v1_4	TS481_v2_2
TS208	falcon2	1.24	0.81	0.50	0.74	TS208_v1_1	TS208_v2_5
TS286	CSSB_experimental	1.19	0.99	0.59	0.60	TS286_v1_1	TS286_v2_1
TS110	MIEnsembles-Server	1.19	0.93	0.55	0.63	TS110_v1_3	TS110_v2_5
TS028	NKRNA-s	1.16	0.95	0.55	0.61	TS028_v1_4	TS028_v2_4
TS450	OpenComplex_Server	1.07	0.96	0.51	0.56	TS450_v1_1	TS450_v2_2
TS167	OpenComplex	1.07	0.96	0.51	0.56	TS167_v1_1	TS167_v2_2
TS022	Yang	0.38	0.94	0.18	0.20	TS022_v1_4	TS022_v2_5
TS052	Yang-Server	0.38	0.93	0.18	0.20	TS052_v1_3	TS052_v2_5
TS456	Yang-Multimer	0.36	0.98	0.17	0.18	TS456_v1_4	TS456_v2_5
TS494	ClusPro	0.34	0.98	0.17	0.17	TS494_v1_2	TS494_v2_3
TS274	kozakovvajda	0.34	0.98	0.17	0.17	TS274_v1_2	TS274_v2_3
TS014	Cool-PSP	0.32	0.88	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	Balance	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS294	KiharaLab	0.71	0.97	36.90	34.50	TS294_v1_1	TS294_v2_1
TS204	Zou	0.71	0.98	36.40	35.00	TS204_v1_1	TS204_v2_2
TS033	Diff	0.69	0.99	34.30	34.90	TS033_v2_5	TS033_v1_5
TS304	AF3-server	0.69	0.97	35.50	33.70	TS304_v1_3	TS304_v2_3
TS052	Yang-Server	0.69	0.98	33.70	35.40	TS052_v1_4	TS052_v2_4
TS286	CSSB_experimental	0.69	0.98	33.80	35.00	TS286_v2_4	TS286_v1_1
TS481	Vfold	0.67	0.95	35.50	31.80	TS481_v1_3	TS481_v2_1
TS456	Yang-Multimer	0.66	0.93	30.70	35.60	TS456_v1_3	TS456_v2_3
TS241	elofsson	0.66	0.93	30.60	35.10	TS241_v2_5	TS241_v1_1
TS022	Yang	0.66	0.98	33.30	32.30	TS022_v1_4	TS022_v2_4
TS462	Zheng	0.65	0.87	36.70	28.50	TS462_v1_3	TS462_v2_1
TS494	ClusPro	0.65	0.95	30.80	34.10	TS494_v1_2	TS494_v2_1
TS274	kozakovvajda	0.65	0.95	30.80	34.10	TS274_v1_2	TS274_v2_1
TS091	Huang-HUST	0.65	0.95	34.00	30.80	TS091_v1_3	TS091_v2_2
TS323	Yan	0.63	0.95	29.70	32.90	TS323_v1_1	TS323_v2_1
TS167	OpenComplex	0.62	0.98	30.60	31.70	TS167_v1_1	TS167_v2_4
TS450	OpenComplex_Server	0.62	0.98	30.60	31.70	TS450_v1_1	TS450_v2_4
TS028	NKRNA-s	0.61	0.96	31.90	29.40	TS028_v2_5	TS028_v1_2
TS489	Fernandez-Recio	0.61	0.97	31.20	29.40	TS489_v1_2	TS489_v2_2
TS014	Cool-PSP	0.60	0.84	25.30	34.60	TS014_v1_1	TS014_v2_5
TS110	MIEnsembles-Server	0.59	0.95	31.20	28.00	TS110_v2_4	TS110_v1_1
TS159	406	0.59	0.88	26.00	33.00	TS159_v1_1	TS159_v2_1
TS325	405	0.59	0.88	26.00	33.00	TS325_v1_1	TS325_v2_1
TS262	CoDock	0.55	0.77	34.00	21.30	TS262_v1_1	TS262_v2_2
TS231	B-LAB	0.47	0.49	11.70	35.80	TS231_v1_5	TS231_v2_1
TS208	falcon2	0.45	0.51	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	Balance	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS204	Zou	1.33	0.97	0.65	0.68	TS204_v1.5	TS204_v2.5
TS294	KiharaLab	1.32	1.00	0.66	0.66	TS294_v1.1	TS294_v2.3
TS091	Huang-HUST	1.31	0.98	0.66	0.64	TS091_v1.3	TS091_v2.2
TS033	Diff	1.29	1.00	0.65	0.65	TS033_v1.4	TS033_v2.4
TS462	Zheng	1.29	0.97	0.67	0.62	TS462_v1.3	TS462_v2.2
TS241	elofsson	1.28	0.97	0.62	0.66	TS241_v1.3	TS241_v2.1
TS325	405	1.27	0.98	0.62	0.65	TS325_v1.1	TS325_v2.1
TS159	406	1.27	0.98	0.62	0.65	TS159_v1.1	TS159_v2.1
TS110	MIEnsembles-Server	1.27	0.98	0.62	0.65	TS110_v1.4	TS110_v2.3
TS028	NKRNA-s	1.27	0.98	0.62	0.65	TS028_v1.5	TS028_v2.4
TS481	Vfold	1.26	0.99	0.62	0.64	TS481_v1.1	TS481_v2.1
TS304	AF3-server	1.26	0.97	0.61	0.65	TS304_v1.3	TS304_v2.1
TS286	CSSB_experimental	1.26	1.00	0.63	0.63	TS286_v1.1	TS286_v2.1
TS208	falcon2	1.25	0.98	0.61	0.64	TS208_v1.1	TS208_v2.5
TS262	CoDock	1.25	0.99	0.63	0.62	TS262_v1.1	TS262_v2.3
TS231	B-LAB	1.25	0.98	0.61	0.64	TS231_v1.2	TS231_v2.5
TS450	OpenComplex_Server	1.23	1.00	0.62	0.61	TS450_v1.4	TS450_v2.5
TS167	OpenComplex	1.23	1.00	0.62	0.61	TS167_v1.4	TS167_v2.5
TS489	Fernandez-Recio	1.20	0.96	0.62	0.57	TS489_v1.2	TS489_v2.1
TS022	Yang	1.04	0.99	0.53	0.52	TS022_v1.3	TS022_v2.3
TS323	Yan	1.04	1.00	0.52	0.52	TS323_v1.1	TS323_v2.1
TS456	Yang-Multimer	1.04	1.00	0.52	0.52	TS456_v1.1	TS456_v2.5
TS052	Yang-Server	1.03	1.00	0.52	0.52	TS052_v1.1	TS052_v2.5
TS014	Cool-PSP	1.03	0.99	0.52	0.51	TS014_v1.3	TS014_v2.3
TS494	ClusPro	1.00	1.00	0.50	0.50	TS494_v1.2	TS494_v2.3
TS274	kozakovvajda	1.00	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	Balance	V1_GlobDockQ	V2_GlobDockQ	V1_Model	V2_Model
TS294	KiharaLab	0.72	0.96	0.34	0.37	TS294_v1_1	TS294_v2_1
TS033	Diff	0.68	0.94	0.32	0.36	TS033_v1_4	TS033_v2_5
TS462	Zheng	0.66	0.93	0.35	0.31	TS462_v1_3	TS462_v2_3
TS204	Zou	0.66	0.86	0.28	0.38	TS204_v1_2	TS204_v2_2
TS022	Yang	0.64	0.94	0.30	0.34	TS022_v1_4	TS022_v2_5
TS159	406	0.64	0.83	0.27	0.37	TS159_v1_1	TS159_v2_1
TS325	405	0.64	0.83	0.27	0.37	TS325_v1_1	TS325_v2_1
TS052	Yang-Server	0.63	0.93	0.29	0.34	TS052_v1_3	TS052_v2_5
TS304	AF3-server	0.62	0.83	0.26	0.37	TS304_v1_2	TS304_v2_3
TS241	elofsson	0.61	0.83	0.25	0.35	TS241_v1_3	TS241_v2_1
TS091	Huang-HUST	0.60	0.93	0.32	0.28	TS091_v1_3	TS091_v2_2
TS456	Yang-Multimer	0.59	0.98	0.29	0.30	TS456_v1_4	TS456_v2_5
TS262	CoDock	0.58	0.97	0.30	0.28	TS262_v1_1	TS262_v2_3
TS231	B-LAB	0.58	0.79	0.23	0.35	TS231_v1_5	TS231_v2_1
TS489	Fernandez-Recio	0.57	0.98	0.28	0.29	TS489_v1_1	TS489_v2_1
TS494	ClusPro	0.56	0.98	0.28	0.29	TS494_v1_2	TS494_v2_3
TS274	kozakovvajda	0.56	0.98	0.28	0.29	TS274_v1_2	TS274_v2_3
TS481	Vfold	0.56	0.94	0.26	0.30	TS481_v1_4	TS481_v2_2
TS208	falcon2	0.55	0.79	0.22	0.34	TS208_v1_1	TS208_v2_5
TS286	CSSB_experimental	0.53	0.97	0.26	0.27	TS286_v1_1	TS286_v2_1
TS110	MIEnsembles-Server	0.53	0.91	0.24	0.29	TS110_v1_3	TS110_v2_5
TS014	Cool-PSP	0.53	0.88	0.29	0.23	TS014_v1_4	TS014_v2_4
TS028	NKRNA-s	0.52	0.93	0.24	0.28	TS028_v1_4	TS028_v2_4
TS450	OpenComplex_Server	0.48	0.93	0.22	0.25	TS450_v1_4	TS450_v2_2
TS167	OpenComplex	0.48	0.93	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	Balance	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS028	NKRNA-s	1.56	0.98	0.80	0.76	TS028_v2_5	TS028_v1_5
TS462	Zheng	1.55	1.00	0.77	0.78	TS462_v1_1	TS462_v2_1
TS481	Vfold	1.54	0.97	0.74	0.79	TS481_v1_4	TS481_v2_1
TS286	CSSB_experimental	1.52	0.98	0.75	0.77	TS286_v2_5	TS286_v1_3
TS091	Huang-HUST	1.50	0.95	0.71	0.79	TS091_v2_1	TS091_v1_2
TS052	Yang-Server	1.50	0.92	0.69	0.81	TS052_v2_3	TS052_v1_1
TS033	Diff	1.50	0.94	0.71	0.79	TS033_v1_5	TS033_v2_2
TS022	Yang	1.50	0.93	0.70	0.80	TS022_v1_4	TS022_v2_2
TS450	OpenComplex_Server	1.49	0.95	0.79	0.71	TS450_v2_4	TS450_v1_1
TS167	OpenComplex	1.49	0.95	0.79	0.71	TS167_v2_4	TS167_v1_1
TS304	AF3-server	1.49	0.95	0.71	0.78	TS304_v1_4	TS304_v2_5
TS262	CoDock	1.49	0.94	0.80	0.70	TS262_v1_1	TS262_v2_3
TS494	ClusPro	1.46	0.95	0.69	0.77	TS494_v2_2	TS494_v1_3
TS274	kozakovvajda	1.46	0.95	0.69	0.77	TS274_v2_2	TS274_v1_3
TS456	Yang-Multimer	1.46	0.92	0.67	0.78	TS456_v2_3	TS456_v1_1
TS204	Zou	1.45	1.00	0.73	0.73	TS204_v1_1	TS204_v2_1
TS241	elofsson	1.44	0.95	0.69	0.76	TS241_v1_3	TS241_v2_3
TS110	MIEnsembles-Server	1.44	0.91	0.66	0.79	TS110_v1_2	TS110_v2_3
TS294	KiharaLab	1.44	0.99	0.72	0.72	TS294_v1_5	TS294_v2_1
TS369	Bhattacharya	1.40	0.98	0.72	0.69	TS369_v2_5	TS369_v1_2
TS231	B-LAB	1.40	0.97	0.68	0.72	TS231_v1_2	TS231_v2_1
TS208	falcon2	1.37	0.97	0.70	0.67	TS208_v2_5	TS208_v1_1
TS489	Fernandez-Recio	1.37	0.97	0.67	0.70	TS489_v2_2	TS489_v1_2
TS323	Yan	1.33	0.98	0.65	0.68	TS323_v1_1	TS323_v2_1
TS325	405	1.32	0.95	0.63	0.69	TS325_v1_1	TS325_v2_1
TS159	406	1.32	0.95	0.63	0.69	TS159_v1_1	TS159_v2_1
TS014	Cool-PSP	1.31	0.92	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	Balance	V1_BestDockQ	V2_BestDockQ	V1_Model	V2_Model
TS294	KiharaLab	1.53	0.97	0.79	0.74	TS294_v1_4	TS294_v2_3
TS286	CSSB_experimental	1.49	0.99	0.76	0.74	TS286_v1_4	TS286_v2_1
TS110	MIEnsembles-Server	1.47	0.88	0.82	0.65	TS110_v1_1	TS110_v2_4
TS489	Fernandez-Recio	1.34	0.86	0.77	0.57	TS489_v1_5	TS489_v2_4
TS208	falcon2	1.34	0.91	0.73	0.61	TS208_v1_2	TS208_v2_4
TS481	Vfold	1.32	0.84	0.77	0.55	TS481_v1_4	TS481_v2_2
TS325	405	1.27	0.91	0.70	0.58	TS325_v1_2	TS325_v2_2
TS159	406	1.27	0.91	0.70	0.58	TS159_v1_2	TS159_v2_2
TS167	OpenComplex	1.24	0.78	0.76	0.49	TS167_v1_4	TS167_v2_5
TS450	OpenComplex_Server	1.24	0.78	0.76	0.49	TS450_v1_4	TS450_v2_5
TS091	Huang-HUST	1.22	0.92	0.66	0.56	TS091_v1_5	TS091_v2_5
TS262	CoDock	1.21	0.90	0.67	0.54	TS262_v1_5	TS262_v2_4
TS033	Diff	1.20	0.90	0.66	0.54	TS033_v1_3	TS033_v2_3
TS028	NKRNA-s	1.17	0.99	0.59	0.58	TS028_v1_3	TS028_v2_3
TS462	Zheng	1.15	0.98	0.59	0.57	TS462_v1_4	TS462_v2_5
TS231	B-LAB	1.13	0.84	0.65	0.48	TS231_v1_2	TS231_v2_5
TS235	isyslab-hust	0.90	0.98	0.46	0.44	TS235_v1_1	TS235_v2_5
TS272	GromihaLab	0.78	0.87	0.45	0.34	TS272_v1_3	TS272_v2_3
TS241	elofsson	0.68	0.93	0.36	0.32	TS241_v1_3	TS241_v2_3
TS304	AF3-server	0.64	1.00	0.32	0.32	TS304_v1_1	TS304_v2_4
TS014	Cool-PSP	0.27	0.91	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	Balance	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS235	isyslab-hust	0.59	0.98	30.00	28.80	TS235_v2.4	TS235_v1.2
TS462	Zheng	0.59	0.96	30.60	28.20	TS462_v2.2	TS462_v1.4
TS028	NKRNA-s	0.57	0.96	29.80	27.70	TS028_v1.4	TS028_v2.2
TS110	MIEnsembles-Server	0.56	0.95	29.40	26.50	TS110_v1.1	TS110_v2.4
TS481	Vfold	0.54	0.99	27.40	27.00	TS481_v1.4	TS481_v2.5
TS286	CSSB_experimental	0.54	0.98	26.60	27.50	TS286_v1.5	TS286_v2.1
TS262	CoDock	0.54	0.96	28.00	26.00	TS262_v2.2	TS262_v1.4
TS294	KiharaLab	0.53	0.98	25.60	26.90	TS294_v2.2	TS294_v1.1
TS033	Diff	0.51	0.99	25.90	25.40	TS033_v2.1	TS033_v1.3
TS231	B-LAB	0.51	0.90	27.90	23.00	TS231_v2.1	TS231_v1.2
TS091	Huang-HUST	0.51	1.00	25.50	25.30	TS091_v1.2	TS091_v2.2
TS489	Fernandez-Recio	0.51	0.99	25.60	24.90	TS489_v1.3	TS489_v2.5
TS208	falcon2	0.46	0.72	29.70	16.70	TS208_v1.4	TS208_v2.1
TS167	OpenComplex	0.44	0.74	27.90	16.40	TS167_v1.5	TS167_v2.5
TS450	OpenComplex_Server	0.44	0.74	27.90	16.40	TS450_v1.5	TS450_v2.5
TS325	405	0.41	0.76	25.20	15.50	TS325_v1.2	TS325_v2.2
TS159	406	0.41	0.76	25.20	15.50	TS159_v1.2	TS159_v2.2
TS014	Cool-PSP	0.40	0.98	19.40	20.20	TS014_v1.5	TS014_v2.4
TS241	elofsson	0.37	0.98	18.10	18.70	TS241_v2.1	TS241_v1.3
TS304	AF3-server	0.37	0.96	19.20	17.60	TS304_v2.5	TS304_v1.1
TS272	GromihaLab	0.29	1.00	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	Balance	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS286	CSSB_experimental	1.47	1.00	0.73	0.73	TS286_v1.4	TS286_v2.1
TS294	KiharaLab	1.45	0.98	0.74	0.71	TS294_v1.5	TS294_v2.5
TS110	MIEnsembles-Server	1.40	0.96	0.73	0.67	TS110_v1.1	TS110_v2.5
TS489	Fernandez-Recio	1.40	0.97	0.72	0.68	TS489_v1.5	TS489_v2.4
TS208	falcon2	1.40	1.00	0.70	0.70	TS208_v1.1	TS208_v2.5
TS262	CoDock	1.39	0.99	0.70	0.69	TS262_v1.2	TS262_v2.1
TS462	Zheng	1.38	1.00	0.69	0.69	TS462_v1.4	TS462_v2.2
TS028	NKRNA-s	1.38	1.00	0.69	0.69	TS028_v1.3	TS028_v2.3
TS481	Vfold	1.37	0.96	0.71	0.66	TS481_v1.1	TS481_v2.4
TS159	406	1.36	1.00	0.68	0.68	TS159_v1.1	TS159_v2.1
TS325	405	1.35	0.99	0.68	0.67	TS325_v1.1	TS325_v2.2
TS450	OpenComplex_Server	1.35	0.98	0.69	0.66	TS450_v1.1	TS450_v2.5
TS167	OpenComplex	1.35	0.98	0.69	0.66	TS167_v1.1	TS167_v2.5
TS231	B-LAB	1.32	0.97	0.68	0.64	TS231_v1.1	TS231_v2.1
TS091	Huang-HUST	1.31	1.00	0.66	0.65	TS091_v1.5	TS091_v2.5
TS033	Diff	1.30	0.99	0.66	0.65	TS033_v1.4	TS033_v2.4
TS235	isyslab-hust	1.30	1.00	0.65	0.65	TS235_v1.1	TS235_v2.2
TS272	GromihaLab	1.27	1.00	0.64	0.63	TS272_v1.4	TS272_v2.4
TS014	Cool-PSP	1.01	0.99	0.51	0.50	TS014_v1.4	TS014_v2.6
TS241	elofsson	0.74	0.99	0.38	0.36	TS241_v1.2	TS241_v2.3
TS304	AF3-server	0.72	1.00	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	Balance	V1_GlobDockQ	V2_GlobDockQ	V1_Model	V2_Model
TS294	KiharaLab	0.71	0.99	0.36	0.35	TS294_v1.4	TS294_v2.3
TS286	CSSB_experimental	0.69	0.99	0.34	0.35	TS286_v1.4	TS286_v2.1
TS110	MIEnsembles-Server	0.68	0.91	0.37	0.31	TS110_v1.1	TS110_v2.4
TS241	elofsson	0.65	0.98	0.33	0.32	TS241_v1.3	TS241_v2.3
TS235	isyslab-hust	0.64	0.98	0.33	0.32	TS235_v1.1	TS235_v2.5
TS489	Fernandez-Recio	0.62	0.88	0.35	0.27	TS489_v1.5	TS489_v2.4
TS208	falcon2	0.62	0.93	0.33	0.29	TS208_v1.2	TS208_v2.4
TS304	AF3-server	0.61	0.95	0.29	0.32	TS304_v1.1	TS304_v2.4
TS481	Vfold	0.61	0.86	0.35	0.26	TS481_v1.4	TS481_v2.2
TS325	405	0.59	0.93	0.32	0.28	TS325_v1.2	TS325_v2.2
TS159	406	0.59	0.93	0.32	0.28	TS159_v1.2	TS159_v2.2
TS167	OpenComplex	0.58	0.81	0.34	0.23	TS167_v1.4	TS167_v2.5
TS450	OpenComplex_Server	0.58	0.81	0.34	0.23	TS450_v1.4	TS450_v2.5
TS091	Huang-HUST	0.57	0.94	0.30	0.27	TS091_v1.5	TS091_v2.5
TS262	CoDock	0.56	0.92	0.30	0.26	TS262_v1.5	TS262_v2.4
TS033	Diff	0.56	0.92	0.30	0.26	TS033_v1.3	TS033_v2.3
TS028	NKRNA-s	0.54	0.99	0.27	0.28	TS028_v1.3	TS028_v2.3
TS462	Zheng	0.54	0.99	0.27	0.27	TS462_v1.4	TS462_v2.5
TS231	B-LAB	0.52	0.87	0.30	0.23	TS231_v1.2	TS231_v2.5
TS014	Cool-PSP	0.46	0.91	0.25	0.21	TS014_v1.1	TS014_v2.2
TS272	GromihaLab	0.36	0.89	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	Balance	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS294	KiharaLab	1.45	0.88	0.81	0.64	TS294_v1_1	TS294_v2_3
TS462	Zheng	1.41	0.93	0.75	0.66	TS462_v2_3	TS462_v1_1
TS110	MIEnsembles-Server	1.39	0.95	0.73	0.66	TS110_v2_5	TS110_v1_1
TS262	CoDock	1.37	0.92	0.74	0.63	TS262_v1_3	TS262_v2_4
TS028	NKRNA-s	1.37	0.94	0.72	0.64	TS028_v1_5	TS028_v2_1
TS235	isyslab-hust	1.35	1.00	0.67	0.68	TS235_v2_4	TS235_v1_5
TS489	Fernandez-Recio	1.33	0.94	0.71	0.63	TS489_v2_2	TS489_v1_3
TS481	Vfold	1.32	0.98	0.67	0.65	TS481_v1_5	TS481_v2_5
TS204	Zou	1.29	0.99	0.64	0.65	TS204_v2_1	TS204_v1_5
TS208	falcon2	1.27	0.95	0.67	0.60	TS208_v1_4	TS208_v2_1
TS325	405	1.27	0.99	0.64	0.63	TS325_v1_2	TS325_v2_2
TS159	406	1.27	0.99	0.64	0.63	TS159_v1_2	TS159_v2_2
TS286	CSSB_experimental	1.27	0.98	0.65	0.62	TS286_v1_2	TS286_v2_2
TS033	Diff	1.25	0.97	0.65	0.61	TS033_v2_4	TS033_v1_2
TS231	B-LAB	1.25	0.97	0.64	0.60	TS231_v1_2	TS231_v2_1
TS091	Huang-HUST	1.23	0.96	0.64	0.59	TS091_v2_2	TS091_v1_5
TS369	Bhattacharya	1.22	1.00	0.61	0.61	TS369_v2_3	TS369_v1_3
TS167	OpenComplex	1.19	0.96	0.57	0.62	TS167_v2_1	TS167_v1_1
TS450	OpenComplex_Server	1.19	0.96	0.57	0.62	TS450_v2_1	TS450_v1_1
TS014	Cool-PSP	1.06	0.98	0.52	0.54	TS014_v1_5	TS014_v2_4
TS272	GromihaLab	0.77	0.93	0.36	0.41	TS272_v2_1	TS272_v1_3
TS241	elofsson	0.69	0.97	0.35	0.34	TS241_v1_4	TS241_v2_1
TS304	AF3-server	0.66	0.99	0.33	0.33	TS304_v2_4	TS304_v1_1

Supplementary Table S11: Results for R1203 Composite Score 4 Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_Composite_Score_4	V2_Composite_Score_4	V1_Model	V2_Model
TS304	AF3-server	85.08	0.82	50.07	35.01	TS304_v1.3	TS304_v2.2
TS241	elofsson	85.08	0.82	50.07	35.01	TS241_v1.3	TS241_v2.2
TS235	isyslab-hust	83.60	0.89	46.42	37.18	TS235_v1.2	TS235_v2.5
TS435	RNAFOLDX	77.05	0.76	47.74	29.31	TS435_v1.5	TS435_v2.6
TS369	Bhattacharya	73.39	0.90	40.37	33.02	TS369_v1.2	TS369_v2.5
TS006	RNA_Dojo	70.31	0.88	30.80	39.51	TS006_v1.1	TS006_v2.3
TS272	GromihaLab	67.08	0.93	31.19	35.89	TS272_v1.4	TS272_v2.1
TS231	B-LAB	66.58	0.85	28.13	38.45	TS231_v1.1	TS231_v2.5
TS159	406	59.61	0.94	31.73	27.89	TS159_v1.2	TS159_v2.1
TS238	BRIQX	49.74	0.47	11.68	38.06	TS238_v1.2	TS238_v2.5
TS294	KiharaLab	42.72	0.50	10.72	31.99	TS294_v1.4	TS294_v2.1
TS267	kiharalab_server	42.25	0.90	19.02	23.23	TS267_v1.1	TS267_v2.3
TS167	OpenComplex	42.16	0.44	9.21	32.95	TS167_v1.5	TS167_v2.2
TS156	SouthRNA	40.91	0.77	25.12	15.79	TS156_v1.1	TS156_v2.4
TS052	Yang-Server	39.88	1.00	19.93	19.95	TS052_v1.2	TS052_v2.4
TS028	NKRNA-s	36.51	0.66	24.46	12.05	TS028_v1.3	TS028_v2.2
TS165	dfr	35.44	0.63	11.21	24.23	TS165_v1.3	TS165_v2.5
TS400	OmniFold	35.24	0.0	0.00	35.24	N/A ¹	TS400_v2.1
TS110	MIEnsembles-Server	35.06	0.45	7.94	27.12	TS110_v1.2	TS110_v2.5
TS189	LCBio	34.89	0.66	23.45	11.44	TS189_v1.5	TS189_v2.1
TS417	GuangzhouRNA-meta	34.68	0.58	9.97	24.71	TS417_v1.5	TS417_v2.4
TS286	CSSB_experimental	34.08	0.90	18.77	15.31	TS286_v1.1	TS286_v2.3
TS276	FrederickFolding	33.62	0.0	0.00	33.62	N/A ¹	TS276_v2.1
TS317	GuangzhouRNA_AI	33.16	0.55	9.19	23.97	TS317_v1.5	TS317_v2.4
TS448	dNAfold	30.11	0.64	20.49	9.62	TS448_v1.1	TS448_v2.5
TS169	thermomaps	28.57	0.87	12.37	16.20	TS169_v1.5	TS169_v2.2
TS462	Zheng	27.64	0.57	7.94	19.70	TS462_v1.2	TS462_v2.1
TS183	GuangzhouRNA-human	26.84	0.80	16.07	10.77	TS183_v1.5	TS183_v2.2
TS481	Vfold	26.72	0.72	9.62	17.10	TS481_v1.4	TS481_v2.5
TS358	PerezLab_Gators	25.81	0.89	11.55	14.27	TS358_v1.2	TS358_v2.1
TS261	UNRES	25.29	0.76	9.56	15.73	TS261_v1.1	TS261_v2.3
TS338	GeneSilico	25.14	0.85	10.67	14.47	TS338_v1.5	TS338_v2.3
TS456	Yang-Multimer	23.94	0.89	13.31	10.63	TS456_v1.2	TS456_v2.4
TS094	SimRNA-Server	22.53	0.82	13.25	9.28	TS094_v1.2	TS094_v2.3
TS063	RNApolis	22.33	0.91	10.21	12.13	TS063_v1.4	TS063_v2.3
TS450	OpenComplex_Server	18.83	0.94	9.97	8.86	TS450_v1.2	TS450_v2.4
TS298	ShanghaiTech-human	9.18	0.0	9.18	0.00	TS298_v1.1	N/A ¹
TS423	ShanghaiTech-server	9.18	0.0	9.18	0.00	TS423_v1.1	N/A ¹
TS367	AIR	9.14	0.0	0.00	9.14	N/A ¹	TS367_v2.1
TS306	GeneSilicoRNA-server	6.35	0.0	0.00	6.35	N/A ¹	TS306_v2.1
TS208	falcon2	4.34	0.0	4.34	0.00	TS208_v1.1	N/A ¹
TS403	mmagnus	2.86	0.0	0.00	2.86	N/A ¹	TS403_v2.1

¹ Model either not submitted or not assessed

Supplementary Table S12: Results for R1203 GDT TS Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS272	GromihaLab	1.16	0.94	54.85	61.57	TS272_v1.4	TS272_v2.1
TS304	AF3-server	1.15	0.96	55.22	60.26	TS304_v1.4	TS304_v2.2
TS241	elofsson	1.15	0.96	55.22	60.26	TS241_v1.4	TS241_v2.2
TS159	406	1.15	0.88	50.56	64.74	TS159_v1.2	TS159_v2.1
TS369	Bhattacharya	1.11	0.97	53.73	57.46	TS369_v1.5	TS369_v2.3
TS235	isyslab-hust	1.09	0.94	51.31	58.02	TS235_v1.5	TS235_v2.2
TS006	RNA_Dojo	1.09	0.99	53.92	55.22	TS006_v1.3	TS006_v2.1
TS231	B-LAB	1.09	0.84	45.71	63.06	TS231_v1.2	TS231_v2.5
TS238	BRIQX	1.08	0.90	59.52	48.69	TS238_v1.5	TS238_v2.2
TS294	KiharaLab	1.08	0.96	51.68	56.53	TS294_v1.2	TS294_v2.1
TS448	dNAfold	1.08	0.90	48.51	59.33	TS448_v1.3	TS448_v2.4
TS165	dfr	1.07	0.97	52.05	55.41	TS165_v1.3	TS165_v2.4
TS417	GuangzhouRNA-meta	1.07	0.99	52.61	54.10	TS417_v1.5	TS417_v2.3
TS435	RNAFOLDX	1.05	0.85	44.40	60.26	TS435_v1.1	TS435_v2.5
TS317	GuangzhouRNA_AI	1.03	0.99	51.87	50.75	TS317_v1.2	TS317_v2.3
TS183	GuangzhouRNA-human	1.02	0.97	52.80	49.44	TS183_v1.5	TS183_v2.2
TS286	CSSB_experimental	0.99	0.94	46.27	52.42	TS286_v1.3	TS286_v2.2
TS456	Yang-Multimer	0.99	1.00	49.44	49.25	TS456_v1.3	TS456_v2.1
TS338	GeneSilico	0.99	1.00	49.44	49.07	TS338_v1.5	TS338_v2.1
TS063	RNApolis	0.97	1.00	48.69	48.51	TS063_v1.4	TS063_v2.1
TS052	Yang-Server	0.96	0.99	47.95	48.51	TS052_v1.5	TS052_v2.1
TS189	LCBio	0.95	0.96	45.90	49.44	TS189_v1.5	TS189_v2.1
TS267	kiharalab_server	0.93	0.98	45.90	47.58	TS267_v1.4	TS267_v2.5
TS028	NKRNA-s	0.93	0.91	42.35	50.75	TS028_v1.4	TS028_v2.2
TS481	Vfold	0.92	0.95	43.66	47.95	TS481_v1.5	TS481_v2.4
TS167	OpenComplex	0.86	0.79	33.95	52.42	TS167_v1.1	TS167_v2.2
TS156	SoutherRNA	0.83	0.61	25.56	57.84	TS156_v1.4	TS156_v2.1
TS462	Zheng	0.74	0.97	36.19	38.06	TS462_v1.4	TS462_v2.5
TS110	MIEnsembles-Server	0.73	0.95	34.52	38.25	TS110_v1.3	TS110_v2.1
TS276	FrederickFolding	0.59	0.0	0.00	58.95	N/A ¹	TS276_v2.1
TS400	OmniFold	0.58	0.0	0.00	58.40	N/A ¹	TS400_v2.1
TS403	mmagnus	0.50	0.0	50.37	0.00	TS403_v1.1	N/A ¹
TS367	AIR	0.50	0.0	0.00	50.00	N/A ¹	TS367_v2.1
TS306	GeneSilicoRNA-server	0.48	0.0	48.32	0.00	TS306_v1.1	N/A ¹
TS358	PerezLab-Gators	0.47	0.83	27.43	19.59	TS358_v1.3	TS358_v2.4
TS094	SimRNA-Server	0.47	0.90	25.75	21.27	TS094_v1.5	TS094_v2.2
TS208	falcon2	0.42	0.0	42.16	0.00	TS208_v1.1	N/A ¹
TS423	ShanghaiTech-server	0.40	0.0	0.00	39.92	N/A ¹	TS423_v2.1
TS298	ShanghaiTech-human	0.40	0.0	0.00	39.92	N/A ¹	TS298_v2.1
TS169	thermomaps	0.37	0.93	19.59	17.16	TS169_v1.4	TS169_v2.2
TS261	UNRES	0.30	0.92	13.81	16.23	TS261_v1.4	TS261_v2.5
TS450	OpenComplex_Server	0.25	0.99	12.69	12.50	TS450_v1.5	TS450_v2.3

¹ Model either not submitted or not assessed

Supplementary Table S13: Results for R1203 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS304	AF3-server	1.65	1.00	0.83	0.82	TS304_v1_1	TS304_v2_3
TS241	elofsson	1.65	1.00	0.83	0.82	TS241_v1_1	TS241_v2_3
TS272	GromihaLab	1.65	1.00	0.82	0.82	TS272_v1_1	TS272_v2_5
TS369	Bhattacharya	1.64	1.00	0.82	0.81	TS369_v1_2	TS369_v2_3
TS235	isyslab-hust	1.63	0.99	0.82	0.81	TS235_v1_5	TS235_v2_2
TS006	RNA_Dojo	1.62	1.00	0.81	0.81	TS006_v1_3	TS006_v2_1
TS159	406	1.60	0.99	0.81	0.79	TS159_v1_2	TS159_v2_1
TS294	KiharaLab	1.60	0.96	0.83	0.77	TS294_v1_1	TS294_v2_2
TS238	BRIQX	1.56	0.95	0.82	0.74	TS238_v1_5	TS238_v2_2
TS183	GuangzhouRNA-human	1.54	1.00	0.77	0.77	TS183_v1_2	TS183_v2_5
TS286	CSSB_experimental	1.52	1.00	0.76	0.76	TS286_v1_1	TS286_v2_2
TS063	RNApolis	1.51	0.99	0.77	0.75	TS063_v1_3	TS063_v2_5
TS481	Vfold	1.50	1.00	0.75	0.75	TS481_v1_3	TS481_v2_4
TS435	RNAFOLDX	1.50	0.91	0.81	0.68	TS435_v1_5	TS435_v2_1
TS165	dfr	1.45	0.98	0.71	0.74	TS165_v1_2	TS165_v2_3
TS417	GuangzhouRNA-meta	1.44	1.00	0.72	0.71	TS417_v1_2	TS417_v2_1
TS231	B-LAB	1.43	0.87	0.81	0.63	TS231_v1_5	TS231_v2_2
TS189	LCBio	1.43	0.99	0.72	0.71	TS189_v1_2	TS189_v2_4
TS338	GeneSilico	1.42	1.00	0.71	0.71	TS338_v1_2	TS338_v2_5
TS456	Yang-Multimer	1.40	0.96	0.73	0.67	TS456_v1_1	TS456_v2_2
TS052	Yang-Server	1.39	0.99	0.70	0.69	TS052_v1_1	TS052_v2_5
TS448	dNAfold	1.38	0.96	0.66	0.72	TS448_v1_1	TS448_v2_5
TS167	OpenComplex	1.38	0.82	0.81	0.56	TS167_v1_2	TS167_v2_3
TS267	kiharalab_server	1.37	0.99	0.68	0.69	TS267_v1_5	TS267_v2_1
TS317	GuangzhouRNA_AI	1.35	0.94	0.63	0.72	TS317_v1_5	TS317_v2_4
TS028	NKRNA-s	1.35	0.96	0.70	0.65	TS028_v1_2	TS028_v2_3
TS450	OpenComplex_Server	1.13	0.99	0.57	0.56	TS450_v1_2	TS450_v2_3
TS462	Zheng	1.13	0.98	0.55	0.57	TS462_v1_4	TS462_v2_1
TS110	MIEnsembles-Server	1.12	0.97	0.55	0.58	TS110_v1_5	TS110_v2_1
TS156	SoutherNA	1.11	0.93	0.59	0.52	TS156_v1_1	TS156_v2_4
TS358	PerezLab_Gators	1.10	0.92	0.51	0.59	TS358_v1_1	TS358_v2_3
TS169	thermomaps	0.85	0.90	0.38	0.47	TS169_v1_5	TS169_v2_4
TS276	FrederickFolding	0.82	0.0	0.82	0.00	TS276_v1_1	N/A ¹
TS400	OmniFold	0.82	0.0	0.82	0.00	TS400_v1_1	N/A ¹
TS261	UNRES	0.78	0.97	0.38	0.40	TS261_v1_1	TS261_v2_3
TS367	AIR	0.63	0.0	0.00	0.63	N/A ¹	TS367_v2_1
TS423	ShanghaiTech-server	0.54	0.0	0.54	0.00	TS423_v1_1	N/A ¹
TS298	ShanghaiTech-human	0.54	0.0	0.54	0.00	TS298_v1_1	N/A ¹
TS403	mmagnus	0.49	0.0	0.00	0.49	N/A ¹	TS403_v2_1
TS208	falcon2	0.39	0.0	0.39	0.00	TS208_v1_1	N/A ¹
TS094	SimRNA-Server	0.20	0.85	0.09	0.12	TS094_v1_3	TS094_v2_5
TS306	GeneSilicoRNA-server	0.01	0.0	0.01	0.00	TS306_v1_1	N/A ¹

¹ Model either not submitted or not assessed

Supplementary Table S14: Results for R1203 TMscore Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS159	406	1.27	0.87	0.56	0.72	TS159_v1_2	TS159_v2_1
TS304	AF3-server	1.23	0.97	0.59	0.63	TS304_v1_1	TS304_v2_2
TS241	elofsson	1.23	0.97	0.59	0.63	TS241_v1_1	TS241_v2_2
TS272	GromihaLab	1.20	0.99	0.59	0.60	TS272_v1_4	TS272_v2_1
TS369	Bhattacharya	1.19	0.99	0.59	0.60	TS369_v1_5	TS369_v2_3
TS238	BRIQX	1.18	0.91	0.64	0.54	TS238_v1_5	TS238_v2_3
TS448	dNAfold	1.17	0.86	0.50	0.67	TS448_v1_3	TS448_v2_4
TS231	B-LAB	1.16	0.92	0.53	0.63	TS231_v1_2	TS231_v2_5
TS006	RNA_Dojo	1.16	1.00	0.58	0.58	TS006_v1_3	TS006_v2_1
TS165	dfr	1.15	0.96	0.56	0.60	TS165_v1_3	TS165_v2_4
TS417	GuangzhouRNA-meta	1.14	0.99	0.56	0.58	TS417_v1_2	TS417_v2_3
TS235	isyslab-hust	1.14	0.95	0.54	0.59	TS235_v1_5	TS235_v2_2
TS294	KiharaLab	1.12	0.95	0.59	0.53	TS294_v1_1	TS294_v2_4
TS317	GuangzhouRNA_AI	1.12	0.98	0.57	0.55	TS317_v1_2	TS317_v2_3
TS435	RNAFOLDX	1.11	0.89	0.50	0.61	TS435_v1_4	TS435_v2_5
TS183	GuangzhouRNA-human	1.10	0.98	0.56	0.54	TS183_v1_2	TS183_v2_3
TS456	Yang-Multimer	1.09	0.98	0.56	0.53	TS456_v1_3	TS456_v2_1
TS063	RNApolis	1.08	0.97	0.56	0.53	TS063_v1_4	TS063_v2_1
TS052	Yang-Server	1.08	0.99	0.54	0.54	TS052_v1_3	TS052_v2_5
TS286	CSSB_experimental	1.06	0.93	0.49	0.57	TS286_v1_4	TS286_v2_3
TS267	kiharalab_server	1.05	0.99	0.52	0.53	TS267_v1_4	TS267_v2_5
TS189	LCBio	1.05	0.94	0.49	0.56	TS189_v1_5	TS189_v2_1
TS028	NKRNA-s	1.02	0.92	0.55	0.47	TS028_v1_2	TS028_v2_4
TS481	Vfold	1.01	0.96	0.48	0.53	TS481_v1_5	TS481_v2_4
TS338	GeneSilico	1.00	0.97	0.49	0.51	TS338_v1_5	TS338_v2_2
TS167	OpenComplex	0.98	0.84	0.41	0.57	TS167_v1_1	TS167_v2_2
TS462	Zheng	0.90	0.98	0.44	0.46	TS462_v1_4	TS462_v2_3
TS110	MIEnsembles-Server	0.89	0.95	0.42	0.47	TS110_v1_3	TS110_v2_1
TS156	SoutheRNA	0.86	0.60	0.26	0.60	TS156_v1_4	TS156_v2_1
TS400	OmniFold	0.65	0.0	0.00	0.65	N/A ¹	TS400_v2_1
TS276	FrederickFolding	0.59	0.0	0.00	0.59	N/A ¹	TS276_v2_1
TS403	mmagnus	0.57	0.0	0.57	0.00	TS403_v1_1	N/A ¹
TS358	PerezLab_Gators	0.56	0.85	0.32	0.24	TS358_v1_3	TS358_v2_2
TS094	SimRNA-Server	0.56	0.92	0.30	0.26	TS094_v1_5	TS094_v2_2
TS306	GeneSilicoRNA-server	0.55	0.0	0.55	0.00	TS306_v1_1	N/A ¹
TS367	AIR	0.55	0.0	0.00	0.55	N/A ¹	TS367_v2_1
TS208	falcon2	0.50	0.0	0.50	0.00	TS208_v1_1	N/A ¹
TS298	ShanghaiTech-human	0.46	0.0	0.00	0.46	N/A ¹	TS298_v2_1
TS423	ShanghaiTech-server	0.46	0.0	0.00	0.46	N/A ¹	TS423_v2_1
TS169	thermomaps	0.42	0.91	0.23	0.19	TS169_v1_4	TS169_v2_2
TS261	UNRES	0.39	0.95	0.18	0.20	TS261_v1_4	TS261_v2_5
TS450	OpenComplex_Server	0.33	0.95	0.15	0.17	TS450_v1_5	TS450_v2_4
TS033	Diff	0.09	0.99	0.04	0.04	TS033_v1_1	TS033_v2_4

¹ Model either not submitted or not assessed

Supplementary Table S15: Results for T1214 Composite Score 4 Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_Composite_Score_4	V2_Composite_Score_4	V1_Model	V2_Model
TS015	PEZyFoldings	189.11	1.00	94.44	94.66	TS015_v1.5	TS015_v2.1
TS462	Zheng	187.90	0.97	91.10	96.79	TS462_v1.6	TS462_v2.3
TS110	MIEnsembles-Server	185.08	0.95	88.23	96.86	TS110_v1.2	TS110_v2.5
TS022	Yang	184.87	0.98	90.16	94.70	TS022_v1.4	TS022_v2.2
TS091	Huang-HUST	183.93	0.93	85.80	98.13	TS091_v1.2	TS091_v2.1
TS388	DeepFold-server	182.94	0.95	86.53	96.41	TS388_v1.4	TS388_v2.1
TS147	Zheng-Multimer	182.75	0.94	85.96	96.79	TS147_v1.1	TS147_v2.3
TS375	milliseconds	182.29	0.94	85.40	96.89	TS375_v1.3	TS375_v2.4
TS319	MULTICOM_LLM	180.79	0.94	85.12	95.67	TS319_v1.3	TS319_v2.4
TS425	MULTICOM_GATE	180.50	0.94	85.12	95.37	TS425_v1.2	TS425_v2.4
TS145	colabfold_baseline	180.33	0.92	83.12	97.21	TS145_v1.5	TS145_v2.1
TS017	Seder2024hard	180.33	0.92	83.12	97.21	TS017_v1.3	TS017_v2.1
TS198	colabfold	179.73	0.92	82.61	97.12	TS198_v1.4	TS198_v2.1
TS148	Guijunlab-Complex	179.36	0.95	85.37	93.99	TS148_v1.5	TS148_v2.2
TS208	falcon2	177.45	0.97	91.66	85.79	TS208_v1.4	TS208_v2.2
TS465	Wallner	175.20	0.98	89.57	85.63	TS465_v1.3	TS465_v2.1
TS408	SNU-CHEM-lig	173.42	0.95	90.61	82.81	TS408_v1.1	TS408_v2.2
TS287	plmfold	172.68	0.99	85.58	87.09	TS287_v1.1	TS287_v2.5
TS369	Bhattacharya	171.54	0.97	83.22	88.32	TS369_v1.1	TS369_v2.5
TS314	GuijunLab-PATHreader	171.11	1.00	85.37	85.74	TS314_v1.1	TS314_v2.5
TS312	GuijunLab-Assembly	171.11	1.00	85.37	85.74	TS312_v1.1	TS312_v2.5
TS393	GuijunLab-QA	171.11	1.00	85.37	85.74	TS393_v1.1	TS393_v2.4
TS264	GuijunLab-Human	170.63	1.00	85.37	85.26	TS264_v1.1	TS264_v2.6
TS386	ShanghaiTech-Ligand	170.07	0.91	93.01	77.06	TS386_v1.4	TS386_v2.5
TS298	ShanghaiTech-human	170.07	0.91	93.01	77.06	TS298_v1.4	TS298_v2.5
TS423	ShanghaiTech-server	169.86	0.99	85.97	83.89	TS423_v1.1	TS423_v2.3
TS163	MultiFOLD2	169.72	1.00	84.58	85.13	TS163_v1.1	TS163_v2.5
TS164	McGuffin	169.72	1.00	84.58	85.13	TS164_v1.1	TS164_v2.5
TS204	Zou	169.38	0.86	72.75	96.63	TS204_v1.3	TS204_v2.5
TS014	Cool-PSP	169.31	1.00	84.85	84.46	TS014_v1.5	TS014_v2.2
TS052	Yang-Server	169.27	0.87	73.95	95.32	TS052_v1.1	TS052_v2.5
TS311	RAGfold_Prot1	169.07	1.00	84.80	84.27	TS311_v1.4	TS311_v2.5
TS267	kiharalab_server	169.01	0.99	83.67	85.34	TS267_v1.2	TS267_v2.3
TS304	AF3-server	168.94	0.99	83.94	85.00	TS304_v1.2	TS304_v2.1
TS241	elofsson	168.94	0.99	83.94	85.00	TS241_v1.2	TS241_v2.1
TS475	ptq	168.75	1.00	84.06	84.70	TS475_v1.3	TS475_v2.5
TS196	HYU_MLLAB	168.73	1.00	84.21	84.52	TS196_v1.4	TS196_v2.1
TS456	Yang-Multimer	168.71	0.87	73.37	95.34	TS456_v1.1	TS456_v2.4
TS269	CSSB_server	168.49	0.88	74.20	94.28	TS269_v1.3	TS269_v2.4
TS419	CSSB-Human	168.46	0.88	74.21	94.25	TS419_v1.3	TS419_v2.5
TS221	CSSB_FAKER	168.46	0.88	74.21	94.25	TS221_v1.3	TS221_v2.5
TS235	isyslab-hust	168.45	0.98	82.62	85.83	TS235_v1.3	TS235_v2.5
TS345	MULTICOM_human	168.44	0.99	83.45	85.00	TS345_v1.4	TS345_v2.1
TS301	GHZ-MAN	168.26	0.99	83.68	84.57	TS301_v1.2	TS301_v2.4
TS055	LCDD-team	168.19	0.93	90.40	77.79	TS055_v1.5	TS055_v2.2
TS051	MULTICOM	168.14	0.99	83.12	85.01	TS051_v1.3	TS051_v2.6
TS122	MQA_server	167.92	0.99	83.13	84.79	TS122_v1.4	TS122_v2.1
TS019	Zheng-Server	167.54	1.00	84.18	83.36	TS019_v1.1	TS019_v2.5
TS227	KUMC	167.41	0.98	85.28	82.13	TS227_v1.3	TS227_v2.5
TS284	Unicorn	167.23	1.00	83.42	83.81	TS284_v1.2	TS284_v2.1
TS075	GHZ-ISM	167.23	1.00	83.42	83.81	TS075_v1.2	TS075_v2.1
TS262	CoDock	166.99	0.86	71.81	95.19	TS262_v1.3	TS262_v2.2
TS102	Psi-Phi	166.85	0.97	85.59	81.26	TS102_v1.2	TS102_v2.1
TS331	MULTICOM_AI	166.71	1.00	83.12	83.59	TS331_v1.3	TS331_v2.5
TS464	PocketTracer	166.62	0.98	81.86	84.76	TS464_v1.4	TS464_v2.1
TS272	GromihaLab	166.56	0.99	82.11	84.45	TS272_v1.1	TS272_v2.3
TS207	MULTICOM_ligand	166.38	0.98	84.68	81.69	TS207_v1.3	TS207_v2.2
TS079	MRAFold	166.20	0.99	83.64	82.57	TS079_v1.5	TS079_v2.2
TS293	MRAH	166.20	0.99	83.63	82.57	TS293_v1.2	TS293_v2.1
TS020	comppharmunibas	161.62	0.85	68.30	93.32	TS020_v1.4	TS020_v2.3
TS139	DeepFold-refine	156.97	0.77	60.63	96.34	TS139_v1.3	TS139_v2.6
TS274	kozakovvajda	149.64	0.68	50.66	98.99	TS274_v1.3	TS274_v2.1
TS494	ClusPro	149.64	0.68	50.66	98.99	TS494_v1.3	TS494_v2.1
TS059	DeepFold	148.71	0.70	52.37	96.34	TS059_v1.1	TS059_v2.6
TS040	DELCLAB	148.42	0.67	49.89	98.53	TS040_v1.5	TS040_v2.3
TS286	CSSB_experimental	147.92	0.70	51.91	96.01	TS286_v1.2	TS286_v2.3
TS294	KiharaLab	139.13	0.79	84.28	54.85	TS294_v1.2	TS294_v2.1
TS039	arosko	137.96	0.77	53.05	84.91	TS039_v1.3	TS039_v2.2
TS202	test001	123.63	0.55	89.38	34.25	TS202_v1.5	TS202_v2.3
TS167	OpenComplex	110.20	0.48	83.59	26.61	TS167_v1.2	TS167_v2.1
TS450	OpenComplex_Server	108.15	0.45	83.59	24.56	TS450_v1.5	TS450_v2.3
TS461	forlilab	106.48	0.69	36.73	69.75	TS461_v1.2	TS461_v2.3
TS120	Cerebra	95.82	0.72	34.59	61.23	TS120_v1.1	TS120_v2.6
TS225	Unknown	84.58	0.0	84.58	0.00	TS225_v1.1	N/A ¹

Supplementary Table S16: Results for T1214 GDT TS Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS091	Huang-HUST	194.17	0.97	94.25	99.92	TS091_v1.2	TS091_v2.5
TS388	DeepFold-server	193.81	0.98	95.23	98.58	TS388_v1.4	TS388_v2.1
TS110	MIEnsembles-Server	193.63	0.98	94.67	98.97	TS110_v1.1	TS110_v2.5
TS015	PEZyFoldings	193.26	1.00	96.41	96.86	TS015_v1.2	TS015_v2.1
TS375	milliseconds	193.14	0.98	94.25	98.89	TS375_v1.3	TS375_v2.4
TS319	MULTICOM_LLM	193.02	0.98	94.78	98.24	TS319_v1.3	TS319_v2.4
TS425	MULTICOM_GATE	192.90	0.98	94.78	98.12	TS425_v1.2	TS425_v2.4
TS462	Zheng	192.84	0.97	93.83	99.00	TS462_v1.2	TS462_v2.3
TS147	Zheng-Multimer	192.84	0.97	93.83	99.00	TS147_v1.2	TS147_v2.3
TS198	colabfold	192.42	0.97	93.38	99.04	TS198_v1.5	TS198_v2.1
TS145	colabfold_baseline	192.04	0.97	93.12	98.93	TS145_v1.2	TS145_v2.1
TS017	Seder2024hard	192.04	0.97	93.12	98.93	TS017_v1.4	TS017_v2.1
TS022	Yang	191.98	0.99	95.05	96.93	TS022_v1.4	TS022_v2.3
TS148	Guijunlab-Complex	191.92	0.98	93.87	98.04	TS148_v1.5	TS148_v2.2
TS055	LCDD-team	190.69	0.99	93.99	96.70	TS055_v1.5	TS055_v2.1
TS052	Yang-Server	190.66	0.98	93.50	97.16	TS052_v1.3	TS052_v2.2
TS456	Yang-Multimer	189.79	0.98	92.62	97.16	TS456_v1.3	TS456_v2.4
TS262	CoDock	189.52	0.98	92.44	97.09	TS262_v1.5	TS262_v2.1
TS204	Zou	189.24	0.95	90.32	98.93	TS204_v1.5	TS204_v2.3
TS019	Zheng-Server	188.81	1.00	94.21	94.59	TS019_v1.2	TS019_v2.1
TS465	Wallner	188.80	1.00	94.44	94.36	TS465_v1.4	TS465_v2.1
TS235	isyslab-hust	188.12	1.00	93.87	94.25	TS235_v1.3	TS235_v2.1
TS221	CSSB_FAKER	188.05	0.96	90.55	97.51	TS221_v1.3	TS221_v2.1
TS419	CSSB-Human	188.05	0.96	90.55	97.51	TS419_v1.3	TS419_v2.1
TS267	kiharalab_server	188.01	1.00	93.80	94.21	TS267_v1.1	TS267_v2.3
TS423	ShanghaiTech-server	187.99	0.99	94.78	93.21	TS423_v1.5	TS423_v2.4
TS286	CSSB_experimental	187.99	0.96	89.79	98.20	TS286_v1.4	TS286_v2.1
TS345	MULTICOM_human	187.88	1.00	94.33	93.56	TS345_v1.4	TS345_v2.6
TS208	falcon2	187.81	1.00	94.29	93.52	TS208_v1.4	TS208_v2.2
TS040	DELCLAB	187.78	0.94	87.94	99.85	TS040_v1.2	TS040_v2.3
TS269	CSSB_server	187.75	0.96	90.32	97.43	TS269_v1.1	TS269_v2.2
TS386	ShanghaiTech-Ligand	187.60	0.98	95.27	92.33	TS386_v1.1	TS386_v2.4
TS298	ShanghaiTech-human	187.60	0.98	95.27	92.33	TS298_v1.1	TS298_v2.4
TS311	RAGfold_Prot1	187.54	1.00	94.02	93.52	TS311_v1.2	TS311_v2.3
TS059	DeepFold	187.54	0.95	89.03	98.50	TS059_v1.1	TS059_v2.6
TS051	MULTICOM	187.51	1.00	93.91	93.60	TS051_v1.5	TS051_v2.6
TS079	MRAFold	187.50	1.00	94.21	93.29	TS079_v1.5	TS079_v2.2
TS293	MRAH	187.47	1.00	94.17	93.29	TS293_v1.3	TS293_v2.5
TS393	GuijunLab-QA	187.28	1.00	93.95	93.33	TS393_v1.5	TS393_v2.4
TS312	GuijunLab-Assembly	187.20	1.00	93.87	93.33	TS312_v1.1	TS312_v2.5
TS314	GuijunLab-PATHreader	187.20	1.00	93.87	93.33	TS314_v1.1	TS314_v2.5
TS196	HYU_MLLAB	187.13	1.00	93.46	93.67	TS196_v1.2	TS196_v2.4
TS408	SNU-CHEM-lig	187.12	0.99	94.06	93.06	TS408_v1.1	TS408_v2.2
TS264	GuijunLab-Human	187.09	1.00	93.95	93.14	TS264_v1.3	TS264_v2.2
TS287	plmfold	187.05	1.00	93.53	93.52	TS287_v1.1	TS287_v2.4
TS163	MultiFOLD2	186.87	1.00	93.19	93.67	TS163_v1.3	TS163_v2.5
TS164	McGuffin	186.87	1.00	93.19	93.67	TS164_v1.3	TS164_v2.5
TS102	Psi-Phi	186.86	1.00	93.68	93.17	TS102_v1.3	TS102_v2.2
TS464	PocketTracer	186.82	1.00	93.38	93.44	TS464_v1.2	TS464_v2.1
TS475	ptq	186.82	1.00	93.76	93.06	TS475_v1.3	TS475_v2.1
TS122	MQA_server	186.78	1.00	93.68	93.10	TS122_v1.2	TS122_v2.1
TS301	GHZ-MAN	186.75	1.00	93.38	93.37	TS301_v1.1	TS301_v2.4
TS014	Cool-PSP	186.71	1.00	93.50	93.21	TS014_v1.3	TS014_v2.2
TS494	ClusPro	186.61	0.93	86.61	100.00	TS494_v1.3	TS494_v2.1
TS274	kozakovvajda	186.61	0.93	86.61	100.00	TS274_v1.3	TS274_v2.1
TS272	GromihaLab	186.60	1.00	93.31	93.29	TS272_v1.3	TS272_v2.5
TS227	KUMC	186.55	0.99	93.83	92.72	TS227_v1.1	TS227_v2.4
TS207	MULTICOM_ligand	186.44	1.00	93.42	93.02	TS207_v1.1	TS207_v2.2
TS304	AF3-server	186.21	1.00	93.15	93.06	TS304_v1.4	TS304_v2.3
TS241	elofsson	186.21	1.00	93.15	93.06	TS241_v1.4	TS241_v2.3
TS369	Bhattacharya	186.21	1.00	93.34	92.87	TS369_v1.1	TS369_v2.2
TS331	MULTICOM_AI	185.67	0.99	93.91	91.76	TS331_v1.5	TS331_v2.1
TS284	Unicorn	185.17	0.99	93.76	91.41	TS284_v1.1	TS284_v2.3
TS075	GHZ-ISM	185.17	0.99	93.76	91.41	TS075_v1.1	TS075_v2.3

Supplementary Table S17: Results for T1214 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS091	Huang-HUST	1.79	0.95	0.85	0.94	TS091_v1.2	TS091_v2.1
TS110	MIEnsembles-Server	1.78	0.96	0.85	0.93	TS110_v1.2	TS110_v2.5
TS147	Zheng-Multimer	1.78	0.96	0.85	0.93	TS147_v1.1	TS147_v2.3
TS462	Zheng	1.78	0.96	0.85	0.93	TS462_v1.1	TS462_v2.3
TS375	milliseconds	1.77	0.96	0.85	0.92	TS375_v1.3	TS375_v2.4
TS319	MULTICOM_LLM	1.77	0.96	0.85	0.92	TS319_v1.3	TS319_v2.4
TS198	colabfold	1.77	0.95	0.84	0.93	TS198_v1.5	TS198_v2.1
TS425	MULTICOM_GATE	1.77	0.97	0.85	0.91	TS425_v1.2	TS425_v2.4
TS148	Guijunlab-Complex	1.77	0.96	0.85	0.92	TS148_v1.5	TS148_v2.2
TS388	DeepFold-server	1.77	0.97	0.86	0.91	TS388_v1.4	TS388_v2.1
TS017	Seder2024hard	1.77	0.95	0.84	0.93	TS017_v1.4	TS017_v2.1
TS145	colabfold_baseline	1.77	0.95	0.84	0.93	TS145_v1.2	TS145_v2.1
TS015	PEZYPFoldings	1.75	1.00	0.87	0.88	TS015_v1.5	TS015_v2.1
TS494	ClusPro	1.74	0.86	0.75	0.99	TS494_v1.4	TS494_v2.1
TS274	kozakovvajda	1.74	0.86	0.75	0.99	TS274_v1.4	TS274_v2.1
TS204	Zou	1.73	0.93	0.81	0.93	TS204_v1.5	TS204_v2.3
TS055	LCDD-team	1.72	0.96	0.82	0.90	TS055_v1.3	TS055_v2.2
TS039	arosko	1.72	0.87	0.75	0.97	TS039_v1.2	TS039_v2.3
TS022	Yang	1.71	1.00	0.85	0.86	TS022_v1.4	TS022_v2.2
TS052	Yang-Server	1.70	0.99	0.84	0.86	TS052_v1.3	TS052_v2.2
TS456	Yang-Multimer	1.70	0.98	0.83	0.86	TS456_v1.5	TS456_v2.4
TS019	Zheng-Server	1.70	1.00	0.85	0.85	TS019_v1.2	TS019_v2.1
TS040	DELCLAB	1.70	0.89	0.75	0.94	TS040_v1.2	TS040_v2.5
TS059	DeepFold	1.69	0.93	0.78	0.91	TS059_v1.5	TS059_v2.6
TS269	CSSB_server	1.69	0.96	0.81	0.88	TS269_v1.5	TS269_v2.1
TS221	CSSB_FAKER	1.69	0.96	0.81	0.88	TS221_v1.3	TS221_v2.4
TS419	CSSB-Human	1.69	0.96	0.81	0.88	TS419_v1.3	TS419_v2.4
TS262	CoDock	1.69	0.98	0.83	0.86	TS262_v1.1	TS262_v2.2
TS208	falcon2	1.69	0.98	0.86	0.83	TS208_v1.4	TS208_v2.1
TS386	ShanghaiTech-Ligand	1.68	0.97	0.86	0.82	TS386_v1.4	TS386_v2.5
TS298	ShanghaiTech-human	1.68	0.97	0.86	0.82	TS298_v1.4	TS298_v2.5
TS267	kiharalab_server	1.68	0.99	0.85	0.83	TS267_v1.1	TS267_v2.3
TS465	Wallner	1.68	0.99	0.85	0.83	TS465_v1.2	TS465_v2.1
TS393	GuijunLab-QA	1.68	0.99	0.85	0.83	TS393_v1.1	TS393_v2.2
TS312	GuijunLab-Assembly	1.68	0.99	0.85	0.83	TS312_v1.1	TS312_v2.4
TS314	GuijunLab-PATHreader	1.68	0.99	0.85	0.83	TS314_v1.1	TS314_v2.4
TS264	GuijunLab-Human	1.68	0.99	0.85	0.83	TS264_v1.1	TS264_v2.6
TS287	plmfold	1.68	0.99	0.85	0.83	TS287_v1.2	TS287_v2.4
TS235	isyslab-hust	1.68	0.99	0.84	0.83	TS235_v1.3	TS235_v2.2
TS102	Psi-Phi	1.68	0.98	0.85	0.82	TS102_v1.5	TS102_v2.2
TS207	MULTICOM_ligand	1.67	0.99	0.85	0.83	TS207_v1.2	TS207_v2.3
TS139	DeepFold-refine	1.67	0.91	0.76	0.91	TS139_v1.3	TS139_v2.6
TS304	AF3-server	1.67	0.99	0.84	0.83	TS304_v1.4	TS304_v2.1
TS241	elofsson	1.67	0.99	0.84	0.83	TS241_v1.4	TS241_v2.1
TS272	GromihaLab	1.67	0.99	0.84	0.83	TS272_v1.3	TS272_v2.2
TS345	MULTICOM_human	1.67	0.99	0.85	0.82	TS345_v1.4	TS345_v2.6
TS122	MQA_server	1.67	0.99	0.84	0.83	TS122_v1.5	TS122_v2.4
TS311	RAGfold_Prot1	1.67	0.98	0.85	0.82	TS311_v1.4	TS311_v2.5
TS464	PocketTracer	1.67	0.99	0.84	0.83	TS464_v1.1	TS464_v2.3
TS051	MULTICOM	1.67	0.98	0.85	0.82	TS051_v1.1	TS051_v2.6
TS369	Bhattacharya	1.67	0.98	0.85	0.82	TS369_v1.1	TS369_v2.2
TS227	KUMC	1.67	0.98	0.85	0.82	TS227_v1.3	TS227_v2.5
TS286	CSSB_experimental	1.67	0.96	0.80	0.87	TS286_v1.2	TS286_v2.4
TS301	GHZ-MAN	1.66	0.99	0.84	0.82	TS301_v1.2	TS301_v2.4
TS079	MRAFold	1.66	0.98	0.85	0.82	TS079_v1.1	TS079_v2.5
TS196	HYU_MLLAB	1.66	0.99	0.84	0.82	TS196_v1.3	TS196_v2.4
TS293	MRAH	1.66	0.98	0.85	0.81	TS293_v1.2	TS293_v2.1
TS164	McGuffin	1.66	0.99	0.84	0.82	TS164_v1.3	TS164_v2.4
TS163	MultiFOLD2	1.66	0.99	0.84	0.82	TS163_v1.3	TS163_v2.4
TS423	ShanghaiTech-server	1.66	0.97	0.85	0.81	TS423_v1.5	TS423_v2.4
TS014	Cool-PSP	1.65	0.98	0.84	0.81	TS014_v1.4	TS014_v2.3
TS331	MULTICOM_AI	1.65	0.97	0.85	0.80	TS331_v1.1	TS331_v2.5
TS075	GHZ-ISM	1.65	0.97	0.85	0.80	TS075_v1.1	TS075_v2.3
TS284	Unicorn	1.65	0.97	0.85	0.80	TS284_v1.1	TS284_v2.3
TS408	SNU-CHEM-lig	1.64	0.98	0.84	0.81	TS408_v1.3	TS408_v2.2
TS475	ptq	1.64	0.98	0.83	0.80	TS475_v1.5	TS475_v2.3
TS020	comppharmunibas	1.62	0.95	0.77	0.85	TS020_v1.4	TS020_v2.3
TS294	KiharaLab	1.56	0.93	0.84	0.72	TS294_v1.2	TS294_v2.3
TS202	test001	1.54	0.95	0.81	0.73	TS202_v1.5	TS202_v2.2

Supplementary Table S18: Results for T1228 GDT TS Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS462	Zheng	116.15	0.91	63.11	53.04	TS462_v1.3	TS462_v2.5
TS264	GuijunLab-Human	116.01	0.96	55.95	60.07	TS264_v1.6	TS264_v2.2
TS147	Zheng-Multimer	115.68	0.92	62.31	53.37	TS147_v1.1	TS147_v2.1
TS148	Guijunlab-Complex	114.51	0.95	54.45	60.07	TS148_v2.3	TS148_v1.3
TS481	Vfold	112.45	0.90	61.80	50.66	TS481_v1.3	TS481_v2.5
TS167	OpenComplex	112.41	0.98	57.07	55.34	TS167_v1.1	TS167_v2.3
TS450	OpenComplex_Server	112.41	0.98	57.07	55.34	TS450_v1.1	TS450_v2.3
TS022	Yang	112.13	0.98	57.21	54.92	TS022_v1.4	TS022_v2.5
TS052	Yang-Server	111.89	0.94	59.50	52.39	TS052_v1.4	TS052_v2.2
TS456	Yang-Multimer	110.72	0.95	58.33	52.39	TS456_v1.3	TS456_v2.2
TS204	Zou	110.58	0.88	62.17	48.41	TS204_v1.1	TS204_v2.2
TS241	elofsson	110.39	0.94	58.57	51.83	TS241_v2.1	TS241_v1.2
TS294	KiharaLab	109.41	0.90	59.97	49.44	TS294_v2.5	TS294_v1.2
TS091	Huang-HUST	109.18	1.00	54.54	54.63	TS091_v1.2	TS091_v2.5
TS033	Diff	108.71	0.95	56.88	51.83	TS033_v2.1	TS033_v1.4
TS262	CoDock	108.24	0.97	55.90	52.34	TS262_v1.2	TS262_v2.1
TS212	PIEFold_human	107.58	0.98	55.10	52.48	TS212_v2.4	TS212_v1.2
TS375	milliseconds	106.98	0.89	59.41	47.57	TS375_v2.4	TS375_v1.3
TS028	NKRNA-s	106.69	0.96	51.31	55.38	TS028_v1.2	TS028_v2.5
TS301	GHZ-MAN	106.65	0.95	55.95	50.70	TS301_v1.3	TS301_v2.4
TS110	MIEnsembles-Server	105.81	0.99	52.25	53.56	TS110_v1.2	TS110_v2.5
TS304	AF3-server	104.59	0.90	57.73	46.86	TS304_v1.4	TS304_v2.5
TS331	MULTICOM_AI	103.98	0.91	56.65	47.33	TS331_v1.2	TS331_v2.4
TS319	MULTICOM_LLM	103.98	0.91	56.65	47.33	TS319_v1.2	TS319_v2.4
TS345	MULTICOM_human	103.98	0.91	56.65	47.33	TS345_v1.3	TS345_v2.2
TS051	MULTICOM	103.98	0.91	56.65	47.33	TS051_v1.3	TS051_v2.2
TS274	kozakovvajda	103.84	0.92	56.32	47.52	TS274_v1.2	TS274_v2.2
TS494	ClusPro	103.84	0.92	56.32	47.52	TS494_v1.2	TS494_v2.2
TS231	B-LAB	103.60	0.91	56.27	47.33	TS231_v2.4	TS231_v1.4
TS314	GuijunLab-PATHreader	103.56	0.94	48.55	55.01	TS314_v2.3	TS314_v1.1
TS286	CSSB_experimental	103.46	0.91	56.13	47.33	TS286_v1.5	TS286_v2.4
TS425	MULTICOM_GATE	103.18	0.92	55.85	47.33	TS425_v1.1	TS425_v2.1
TS198	colabfold	102.58	0.90	56.41	46.16	TS198_v2.2	TS198_v1.2
TS419	CSSB-Human	102.29	0.91	55.52	46.77	TS419_v2.4	TS419_v1.3
TS221	CSSB_FAKER	102.20	0.91	55.57	46.63	TS221_v2.2	TS221_v1.5
TS369	Bhattacharya	102.11	0.93	54.82	47.28	TS369_v1.2	TS369_v2.1
TS019	Zheng-Server	101.97	0.99	51.69	50.28	TS019_v1.4	TS019_v2.4
TS475	ptq	101.12	0.84	58.43	42.70	TS475_v2.5	TS475_v1.2
TS014	Cool-PSP	101.12	0.84	58.57	42.56	TS014_v2.6	TS014_v1.6
TS287	plmfold	101.08	0.93	54.07	47.00	TS287_v1.2	TS287_v2.1
TS267	kiharalab_server	100.05	0.91	54.68	45.37	TS267_v1.1	TS267_v2.5
TS079	MRAFold	99.77	0.90	54.82	44.94	TS079_v1.2	TS079_v2.2
TS293	MRAH	99.77	0.90	54.82	44.94	TS293_v1.2	TS293_v2.2
TS489	Fernandez-Recio	99.67	0.89	55.48	44.20	TS489_v1.2	TS489_v2.2
TS208	falcon2	99.20	0.90	54.54	44.66	TS208_v2.5	TS208_v1.1
TS196	HYU_MLLAB	98.74	0.92	53.37	45.37	TS196_v1.5	TS196_v2.5
TS312	GuijunLab-Assembly	98.50	0.91	53.84	44.66	TS312_v1.1	TS312_v2.2
TS112	Seder2024easy	97.99	0.89	54.35	43.63	TS112_v1.4	TS112_v2.3
TS017	Seder2024hard	97.99	0.89	54.35	43.63	TS017_v1.5	TS017_v2.5
TS145	colabfold_baseline	97.89	0.89	54.35	43.54	TS145_v1.3	TS145_v2.3
TS465	Wallner	97.47	0.97	50.00	47.47	TS465_v1.5	TS465_v2.1
TS235	isyslab-hust	96.63	0.95	50.80	45.83	TS235_v1.1	TS235_v2.3
TS311	RAGfold_Prot1	96.58	0.97	49.86	46.72	TS311_v1.2	TS311_v2.5
TS163	MultiFOLD2	96.02	0.89	53.23	42.79	TS163_v1.5	TS163_v2.2
TS015	PEZYFoldings	95.55	0.93	51.12	44.43	TS015_v2.2	TS015_v1.5
TS298	ShanghaiTech-human	95.04	0.86	54.35	40.68	TS298_v1.1	TS298_v2.3
TS284	Unicorn	94.90	0.93	44.20	50.70	TS284_v1.3	TS284_v2.4
TS075	GHZ-ISM	94.90	0.93	44.20	50.70	TS075_v1.3	TS075_v2.4
TS122	MQA_server	94.90	0.93	44.20	50.70	TS122_v1.3	TS122_v2.4
TS164	McGuffin	94.76	0.99	48.03	46.72	TS164_v1.1	TS164_v2.2
TS325	405	94.29	0.95	49.34	44.94	TS325_v1.1	TS325_v2.1
TS159	406	94.29	0.95	49.34	44.94	TS159_v1.1	TS159_v2.1
TS269	CSSB_server	92.98	0.91	50.70	42.27	TS269_v1.1	TS269_v2.1
TS059	DeepFold	91.53	0.97	46.91	44.62	TS059_v2.3	TS059_v1.3

Supplementary Table S19: Results for T1228 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS314	GuijunLab-PAthreader	1.51	0.98	0.77	0.74	TS314.v1.4	TS314.v2.5
TS028	NKRNA-s	1.51	0.99	0.77	0.75	TS028.v1.5	TS028.v2.4
TS110	MIEnsembles-Server	1.51	0.99	0.77	0.75	TS110.v1.3	TS110.v2.3
TS051	MULTICOM	1.51	0.98	0.77	0.74	TS051.v1.1	TS051.v2.3
TS345	MULTICOM.human	1.51	0.98	0.77	0.74	TS345.v1.1	TS345.v2.3
TS331	MULTICOM_AI	1.51	0.98	0.77	0.74	TS331.v1.1	TS331.v2.2
TS319	MULTICOM.LLM	1.51	0.98	0.77	0.74	TS319.v1.1	TS319.v2.2
TS147	Zheng-Multimer	1.51	0.98	0.77	0.74	TS147.v2.4	TS147.v1.5
TS425	MULTICOM.GATE	1.50	0.97	0.77	0.73	TS425.v2.4	TS425.v1.4
TS462	Zheng	1.50	0.97	0.77	0.73	TS462.v2.2	TS462.v1.2
TS022	Yang	1.50	0.98	0.77	0.74	TS022.v1.3	TS022.v2.5
TS204	Zou	1.50	0.98	0.76	0.74	TS204.v1.4	TS204.v2.5
TS075	GHZ-ISM	1.50	0.98	0.76	0.74	TS075.v1.2	TS075.v2.4
TS122	MQA_server	1.50	0.98	0.76	0.74	TS122.v1.2	TS122.v2.4
TS284	Unicorn	1.50	0.98	0.76	0.74	TS284.v1.2	TS284.v2.4
TS145	colabfold_baseline	1.50	0.98	0.77	0.73	TS145.v1.3	TS145.v2.3
TS450	OpenComplex_Server	1.50	0.98	0.76	0.73	TS450.v1.1	TS450.v2.5
TS167	OpenComplex	1.50	0.98	0.76	0.73	TS167.v1.1	TS167.v2.5
TS198	colabfold	1.50	0.98	0.77	0.73	TS198.v1.3	TS198.v2.2
TS475	ptq	1.50	0.98	0.76	0.73	TS475.v1.5	TS475.v2.4
TS017	Seder2024hard	1.50	0.98	0.77	0.73	TS017.v1.4	TS017.v2.2
TS301	GHZ-MAN	1.49	0.99	0.76	0.74	TS301.v1.3	TS301.v2.4
TS325	405	1.49	0.98	0.76	0.73	TS325.v1.1	TS325.v2.1
TS159	406	1.49	0.98	0.76	0.73	TS159.v1.1	TS159.v2.1
TS456	Yang-Multimer	1.49	0.98	0.76	0.73	TS456.v1.1	TS456.v2.2
TS231	B-LAB	1.49	0.98	0.76	0.73	TS231.v2.4	TS231.v1.1
TS033	Diff	1.49	0.98	0.76	0.73	TS033.v2.1	TS033.v1.4
TS164	McGuffin	1.49	0.98	0.76	0.73	TS164.v2.5	TS164.v1.2
TS148	Guijunlab-Complex	1.49	0.99	0.76	0.74	TS148.v2.2	TS148.v1.2
TS298	ShanghaiTech-human	1.49	0.97	0.77	0.73	TS298.v1.3	TS298.v2.3
TS465	Wallner	1.49	0.98	0.76	0.73	TS465.v1.1	TS465.v2.4
TS052	Yang-Server	1.49	0.98	0.76	0.73	TS052.v1.1	TS052.v2.2
TS294	KiharaLab	1.49	0.97	0.76	0.73	TS294.v2.4	TS294.v1.4
TS375	milliseconds	1.49	0.97	0.76	0.73	TS375.v2.4	TS375.v1.2
TS264	GuijunLab-Human	1.49	0.97	0.76	0.73	TS264.v2.4	TS264.v1.6
TS196	HYU_MLLAB	1.49	0.98	0.76	0.73	TS196.v1.2	TS196.v2.4
TS241	elofsson	1.49	0.98	0.76	0.73	TS241.v2.1	TS241.v1.2
TS489	Fernandez-Recio	1.49	0.97	0.77	0.72	TS489.v1.2	TS489.v2.2
TS019	Zheng-Server	1.49	0.98	0.76	0.73	TS019.v1.4	TS019.v2.4
TS369	Bhattacharya	1.49	0.98	0.76	0.73	TS369.v1.1	TS369.v2.1
TS269	CSSB_server	1.49	0.98	0.76	0.73	TS269.v1.1	TS269.v2.1
TS481	Vfold	1.49	0.98	0.76	0.73	TS481.v2.1	TS481.v1.4
TS287	plmfold	1.49	0.98	0.76	0.73	TS287.v1.4	TS287.v2.3
TS312	GuijunLab-Assembly	1.49	0.98	0.76	0.73	TS312.v2.5	TS312.v1.1
TS208	falcon2	1.49	0.97	0.76	0.72	TS208.v2.5	TS208.v1.1
TS235	isyslab-hust	1.49	0.98	0.76	0.73	TS235.v1.2	TS235.v2.2
TS267	kiharalab_server	1.49	0.97	0.76	0.72	TS267.v2.3	TS267.v1.3
TS015	PEZYZFoldings	1.48	0.98	0.76	0.72	TS015.v1.5	TS015.v2.2
TS304	AF3-server	1.48	0.98	0.76	0.72	TS304.v2.1	TS304.v1.3
TS388	DeepFold-server	1.48	0.99	0.75	0.73	TS388.v1.3	TS388.v2.3
TS023	FTBiot0119	1.48	0.98	0.76	0.73	TS023.v1.3	TS023.v2.4
TS014	Cool-PSP	1.48	0.98	0.76	0.72	TS014.v1.5	TS014.v2.5
TS059	DeepFold	1.48	0.99	0.75	0.73	TS059.v1.4	TS059.v2.4
TS091	Huang-HUST	1.48	0.98	0.75	0.73	TS091.v1.3	TS091.v2.4
TS419	CSSB-Human	1.47	0.98	0.75	0.72	TS419.v2.3	TS419.v1.2
TS079	MRAFold	1.47	0.98	0.76	0.72	TS079.v1.1	TS079.v2.1
TS221	CSSB.FAKER	1.47	0.98	0.75	0.72	TS221.v2.4	TS221.v1.2
TS311	RAGfold_Prot1	1.47	0.99	0.75	0.73	TS311.v1.4	TS311.v2.5
TS163	MultiFOLD2	1.47	0.98	0.75	0.72	TS163.v1.1	TS163.v2.2
TS293	MRAH	1.47	0.97	0.75	0.72	TS293.v1.4	TS293.v2.4
TS112	Seder2024easy	1.47	0.97	0.75	0.71	TS112.v1.1	TS112.v2.2
TS286	CSSB_experimental	1.47	0.98	0.75	0.72	TS286.v2.3	TS286.v1.4
TS262	CoDock	1.46	0.98	0.74	0.71	TS262.v1.4	TS262.v2.2
TS274	kozakovvajda	1.45	0.98	0.74	0.71	TS274.v1.1	TS274.v2.3
TS494	ClusPro	1.45	0.98	0.74	0.71	TS494.v1.1	TS494.v2.3
TS139	DeepFold-refine	1.45	0.97	0.75	0.70	TS139.v1.6	TS139.v2.6
TS212	PIEFold_human	1.37	0.98	0.70	0.67	TS212.v2.5	TS212.v1.2
TS120	Cerebra	1.28	0.98	0.65	0.63	TS120.v2.5	TS120.v1.2
TS361	Cerebra_server	1.27	0.98	0.65	0.62	TS361.v1.2	TS361.v2.1

Supplementary Table S20: Results for T1228 TMscore Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS264	GuijunLab-Human	1.61	0.98	0.78	0.82	TS264_v1_6	TS264_v2_1
TS148	Guijunlab-Complex	1.59	0.96	0.77	0.83	TS148_v2_3	TS148_v1_2
TS147	Zheng-Multimer	1.55	0.93	0.83	0.72	TS147_v1_1	TS147_v2_1
TS167	OpenComplex	1.55	0.97	0.80	0.75	TS167_v1_1	TS167_v2_3
TS450	OpenComplex_Server	1.55	0.97	0.80	0.75	TS450_v1_1	TS450_v2_3
TS022	Yang	1.55	0.99	0.78	0.76	TS022_v1_3	TS022_v2_5
TS481	Vfold	1.54	0.93	0.82	0.71	TS481_v1_3	TS481_v2_5
TS462	Zheng	1.53	0.92	0.83	0.70	TS462_v1_3	TS462_v2_5
TS091	Huang-HUST	1.51	0.98	0.77	0.74	TS091_v1_3	TS091_v2_5
TS241	elofsson	1.51	0.95	0.79	0.71	TS241_v2_1	TS241_v1_2
TS456	Yang-Multimer	1.50	0.94	0.80	0.70	TS456_v1_3	TS456_v2_2
TS052	Yang-Server	1.50	0.94	0.79	0.70	TS052_v1_4	TS052_v2_2
TS033	Diff	1.48	0.92	0.80	0.68	TS033_v2_1	TS033_v1_4
TS262	CoDock	1.48	0.96	0.77	0.71	TS262_v1_2	TS262_v2_1
TS028	NKRNA-s	1.47	0.97	0.72	0.76	TS028_v1_2	TS028_v2_4
TS212	PIEFold_human	1.47	0.96	0.77	0.71	TS212_v2_3	TS212_v1_2
TS110	MIEnsembles-Server	1.47	1.00	0.73	0.74	TS110_v1_2	TS110_v2_3
TS314	GuijunLab-PATHreader	1.46	0.95	0.69	0.77	TS314_v2_3	TS314_v1_1
TS019	Zheng-Server	1.41	0.97	0.73	0.68	TS019_v1_4	TS019_v2_3
TS204	Zou	1.39	0.81	0.83	0.56	TS204_v1_1	TS204_v2_2
TS301	GHZ-MAN	1.38	0.97	0.72	0.67	TS301_v1_3	TS301_v2_5
TS294	KiharaLab	1.38	0.81	0.82	0.56	TS294_v2_5	TS294_v1_1
TS375	milliseconds	1.38	0.82	0.81	0.56	TS375_v2_4	TS375_v1_2
TS345	MULTICOM_human	1.36	0.82	0.80	0.56	TS345_v1_3	TS345_v2_5
TS051	MULTICOM	1.36	0.82	0.80	0.56	TS051_v1_3	TS051_v2_5
TS274	kozakovvajda	1.36	0.82	0.80	0.56	TS274_v1_1	TS274_v2_2
TS494	ClusPro	1.36	0.82	0.80	0.56	TS494_v1_1	TS494_v2_2
TS331	MULTICOM_AI	1.36	0.82	0.80	0.56	TS331_v1_2	TS331_v2_1
TS319	MULTICOM_LLM	1.36	0.82	0.80	0.56	TS319_v1_2	TS319_v2_1
TS231	B-LAB	1.35	0.82	0.79	0.56	TS231_v2_2	TS231_v1_4
TS425	MULTICOM_GATE	1.35	0.82	0.79	0.56	TS425_v1_1	TS425_v2_2
TS419	CSSB-Human	1.35	0.83	0.79	0.56	TS419_v1_1	TS419_v2_2
TS198	colabfold	1.34	0.83	0.78	0.56	TS198_v1_2	TS198_v2_2
TS221	CSSB_FAKER	1.34	0.83	0.78	0.56	TS221_v1_1	TS221_v2_1
TS014	Cool-PSP	1.34	0.82	0.79	0.55	TS014_v2_5	TS014_v1_5
TS286	CSSB_experimental	1.34	0.83	0.78	0.56	TS286_v1_1	TS286_v2_4
TS489	Fernandez-Recio	1.34	0.82	0.79	0.55	TS489_v1_2	TS489_v2_5
TS287	plmfold	1.34	0.86	0.76	0.58	TS287_v1_2	TS287_v2_1
TS235	isyslab-hust	1.33	0.91	0.72	0.61	TS235_v1_1	TS235_v2_3
TS304	AF3-server	1.33	0.84	0.77	0.56	TS304_v2_2	TS304_v1_4
TS312	GuijunLab-Assembly	1.33	0.85	0.76	0.56	TS312_v1_5	TS312_v2_2
TS293	MRAH	1.32	0.85	0.76	0.56	TS293_v1_2	TS293_v2_2
TS079	MRAFold	1.32	0.85	0.76	0.56	TS079_v1_2	TS079_v2_2
TS267	kiharalab_server	1.32	0.86	0.76	0.57	TS267_v1_1	TS267_v2_5
TS369	Bhattacharya	1.32	0.85	0.76	0.56	TS369_v1_2	TS369_v2_1
TS208	falcon2	1.32	0.84	0.76	0.55	TS208_v2_5	TS208_v1_1
TS112	Seder2024easy	1.31	0.84	0.76	0.55	TS112_v1_4	TS112_v2_3
TS017	Seder2024hard	1.31	0.84	0.76	0.55	TS017_v1_5	TS017_v2_5
TS145	colabfold_baseline	1.31	0.84	0.76	0.55	TS145_v1_3	TS145_v2_3
TS015	PEZyFoldings	1.31	0.86	0.74	0.56	TS015_v2_2	TS015_v1_3
TS163	MultiFOLD2	1.30	0.83	0.76	0.54	TS163_v1_5	TS163_v2_2
TS269	CSSB_server	1.29	0.84	0.75	0.54	TS269_v1_1	TS269_v2_1
TS465	Wallner	1.28	0.90	0.71	0.58	TS465_v1_3	TS465_v2_1
TS298	ShanghaiTech-human	1.28	0.81	0.76	0.52	TS298_v1_3	TS298_v2_3
TS475	ptq	1.27	0.85	0.73	0.54	TS475_v2_5	TS475_v1_2
TS325	405	1.27	0.87	0.71	0.55	TS325_v1_1	TS325_v2_1
TS159	406	1.27	0.87	0.71	0.55	TS159_v1_1	TS159_v2_1
TS196	HYU_MLLAB	1.26	0.88	0.70	0.56	TS196_v1_5	TS196_v2_5
TS164	McGuffin	1.25	0.92	0.67	0.58	TS164_v1_1	TS164_v2_2
TS075	GHZ-ISM	1.23	0.88	0.54	0.69	TS075_v2_4	TS075_v1_3
TS122	MQA_server	1.23	0.88	0.54	0.69	TS122_v2_4	TS122_v1_3
TS284	Unicorn	1.23	0.88	0.54	0.69	TS284_v2_4	TS284_v1_3
TS059	DeepFold	1.21	0.99	0.61	0.60	TS059_v1_5	TS059_v2_4
TS023	FTBiot0119	1.19	0.89	0.66	0.53	TS023_v1_1	TS023_v2_1

Supplementary Table S21: Results for T1239 GDT TS Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS462	Zheng	119.79	0.82	70.81	48.98	TS462_v2.2	TS462_v1.1
TS235	isyslab-hust	114.17	0.75	71.31	42.85	TS235_v2.4	TS235_v1.1
TS419	CSSB-Human	114.04	0.75	71.10	42.94	TS419_v2.1	TS419_v1.5
TS221	CSSB_FAKER	114.04	0.75	71.10	42.94	TS221_v2.1	TS221_v1.5
TS028	NKRNA-s	113.49	0.74	71.36	42.13	TS028_v2.2	TS028_v1.2
TS345	MULTICOM_human	113.32	0.74	71.23	42.09	TS345_v1.4	TS345_v2.5
TS051	MULTICOM	113.32	0.74	71.23	42.09	TS051_v1.4	TS051_v2.5
TS286	CSSB_experimental	112.64	0.76	69.87	42.77	TS286_v2.1	TS286_v1.2
TS208	falcon2	108.53	0.77	66.99	41.54	TS208_v1.4	TS208_v2.4
TS425	MULTICOM_GATE	107.68	0.83	63.22	44.46	TS425_v1.2	TS425_v2.4
TS019	Zheng-Server	106.22	0.98	54.02	52.20	TS019_v1.5	TS019_v2.5
TS022	Yang	105.14	0.84	60.72	44.42	TS022_v1.5	TS022_v2.4
TS204	Zou	104.76	0.83	61.23	43.53	TS204_v1.5	TS204_v2.2
TS110	MIEnsembles-Server	104.72	0.80	63.01	41.71	TS110_v1.1	TS110_v2.2
TS456	Yang-Multimer	104.50	0.85	60.21	44.29	TS456_v1.3	TS456_v2.2
TS147	Zheng-Multimer	103.35	0.91	56.27	47.08	TS147_v1.3	TS147_v2.5
TS167	OpenComplex	102.59	0.95	54.07	48.52	TS167_v1.5	TS167_v2.3
TS450	OpenComplex_Server	102.59	0.95	54.07	48.52	TS450_v1.5	TS450_v2.3
TS294	KiharaLab	101.71	0.83	59.58	42.13	TS294_v1.1	TS294_v2.2
TS314	GuijunLab-PAthreader	101.54	0.84	58.77	42.77	TS314_v2.5	TS314_v1.2
TS052	Yang-Server	100.05	0.88	55.93	44.12	TS052_v1.5	TS052_v2.2
TS481	Vfold	99.67	0.86	56.57	43.10	TS481_v2.5	TS481_v1.2
TS091	Huang-HUST	99.24	0.95	52.08	47.17	TS091_v1.5	TS091_v2.3
TS319	MULTICOM_LLM	98.53	0.87	55.64	42.89	TS319_v1.2	TS319_v2.5
TS262	CoDock	98.36	0.83	57.63	40.74	TS262_v1.2	TS262_v2.1
TS033	Diff	97.93	0.90	53.94	43.99	TS033_v2.2	TS033_v1.1
TS331	MULTICOM_AI	97.73	0.86	55.64	42.09	TS331_v1.2	TS331_v2.2
TS325	405	97.47	0.87	55.21	42.26	TS325_v1.2	TS325_v2.2
TS159	406	97.47	0.87	55.21	42.26	TS159_v1.2	TS159_v2.2
TS369	Bhattacharya	97.17	0.89	54.07	43.10	TS369_v1.4	TS369_v2.4
TS489	Fernandez-Recio	96.71	0.86	54.96	41.75	TS489_v1.3	TS489_v2.4
TS298	ShanghaiTech-human	96.00	0.71	61.74	34.26	TS298_v1.1	TS298_v2.1
TS212	PIEFold_human	95.91	0.85	55.21	40.69	TS212_v2.1	TS212_v1.3
TS241	elofsson	95.14	0.86	54.32	40.82	TS241_v1.1	TS241_v2.5
TS231	B-LAB	94.34	0.85	54.07	40.27	TS231_v2.1	TS231_v1.2
TS304	AF3-server	94.04	0.92	50.89	43.15	TS304_v2.5	TS304_v1.2
TS465	Wallner	92.97	0.96	48.14	44.84	TS465_v1.4	TS465_v2.2
TS358	PerezLab_Gators	92.78	0.82	54.96	37.82	TS358_v2.2	TS358_v1.4
TS293	MRAH	91.92	0.91	49.91	42.01	TS293_v1.2	TS293_v2.3
TS079	MRAFold	91.92	0.91	49.91	42.01	TS079_v1.2	TS079_v2.3
TS272	GromihaLab	91.33	0.90	50.09	41.24	TS272_v1.1	TS272_v2.1
TS423	ShanghaiTech-server	91.08	0.86	51.91	39.17	TS423_v2.4	TS423_v1.1
TS267	kiharalab_server	89.30	0.88	50.00	39.30	TS267_v1.1	TS267_v2.4
TS148	Guijunlab-Complex	88.53	0.89	48.94	39.59	TS148_v2.5	TS148_v1.4
TS287	plmfold	88.49	0.89	49.32	39.17	TS287_v1.3	TS287_v2.4
TS198	colabfold	88.11	0.86	50.34	37.77	TS198_v1.2	TS198_v2.1
TS375	milliseconds	87.73	0.92	47.16	40.57	TS375_v2.3	TS375_v1.4
TS112	Seder2024easy	86.88	0.89	48.09	38.79	TS112_v1.4	TS112_v2.5
TS014	Cool-PSP	86.84	0.86	49.49	37.35	TS014_v2.3	TS014_v1.3
TS301	GHZ-MAN	86.84	0.93	46.65	40.19	TS301_v2.4	TS301_v1.1
TS163	MultiFOLD2	86.72	0.88	48.39	38.33	TS163_v1.3	TS163_v2.3
TS040	DELCLAB	86.50	0.89	48.09	38.41	TS040_v1.3	TS040_v2.3
TS145	colabfold_baseline	86.46	0.90	47.67	38.79	TS145_v1.2	TS145_v2.1
TS023	FTBiot0119	86.46	0.90	47.67	38.79	TS023_v1.2	TS023_v2.1
TS264	GuijunLab-Human	86.20	0.90	47.54	38.66	TS264_v2.2	TS264_v1.5
TS312	GuijunLab-Assembly	85.86	0.92	46.27	39.59	TS312_v2.4	TS312_v1.4
TS122	MQA_server	85.78	0.91	46.65	39.13	TS122_v1.3	TS122_v2.2
TS139	DeepFold-refine	84.76	0.92	45.93	38.83	TS139_v1.6	TS139_v2.6
TS059	DeepFold	84.76	0.92	45.93	38.83	TS059_v1.6	TS059_v2.6
TS017	Seder2024hard	84.52	0.86	48.05	36.46	TS017_v1.5	TS017_v2.4
TS397	smg_ulaval	84.13	0.93	45.00	39.13	TS397_v1.1	TS397_v2.1
TS164	McGuffin	83.83	0.92	45.47	38.37	TS164_v2.2	TS164_v1.3
TS015	PEZYPfoldings	83.79	0.93	45.00	38.79	TS015_v1.4	TS015_v2.1
TS196	HYU_MLLAB	78.41	0.99	38.94	39.47	TS196_v1.2	TS196_v2.2

Supplementary Table S22: Results for T1239 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS028	NKRNA-s	1.67	0.98	0.82	0.85	TS028_v1.4	TS028_v2.1
TS208	falcon2	1.66	0.97	0.81	0.85	TS208_v1.4	TS208_v2.4
TS051	MULTICOM	1.66	0.98	0.81	0.85	TS051_v1.3	TS051_v2.2
TS345	MULTICOM_human	1.66	0.98	0.81	0.85	TS345_v1.1	TS345_v2.2
TS425	MULTICOM_GATE	1.65	0.98	0.81	0.85	TS425_v1.2	TS425_v2.1
TS456	Yang-Multimer	1.65	0.98	0.81	0.84	TS456_v1.3	TS456_v2.4
TS462	Zheng	1.65	0.98	0.81	0.84	TS462_v1.4	TS462_v2.2
TS235	isyslab-hust	1.65	0.98	0.81	0.84	TS235_v2.4	TS235_v1.2
TS110	MIEnsembles-Server	1.65	0.97	0.80	0.85	TS110_v2.5	TS110_v1.2
TS019	Zheng-Server	1.64	0.96	0.79	0.85	TS019_v1.1	TS019_v2.5
TS489	Fernandez-Recio	1.64	0.97	0.79	0.85	TS489_v1.3	TS489_v2.5
TS331	MULTICOM_AI	1.64	0.97	0.80	0.85	TS331_v1.2	TS331_v2.1
TS319	MULTICOM_LLM	1.64	0.97	0.80	0.85	TS319_v1.2	TS319_v2.1
TS022	Yang	1.64	0.97	0.80	0.84	TS022_v1.5	TS022_v2.1
TS052	Yang-Server	1.64	0.97	0.79	0.84	TS052_v1.1	TS052_v2.4
TS419	CSSB-Human	1.63	0.97	0.80	0.84	TS419_v1.2	TS419_v2.2
TS221	CSSB_FAKER	1.63	0.97	0.80	0.84	TS221_v1.2	TS221_v2.2
TS314	GuijunLab-PATHreader	1.63	0.97	0.79	0.84	TS314_v1.5	TS314_v2.5
TS294	KiharaLab	1.63	0.97	0.79	0.84	TS294_v2.1	TS294_v1.4
TS325	405	1.63	0.97	0.79	0.84	TS325_v2.2	TS325_v1.1
TS159	406	1.63	0.97	0.79	0.84	TS159_v1.2	TS159_v2.1
TS481	Vfold	1.63	0.97	0.79	0.84	TS481_v1.4	TS481_v2.4
TS272	GromihaLab	1.61	0.97	0.78	0.83	TS272_v1.3	TS272_v2.4
TS262	CoDock	1.61	0.97	0.78	0.83	TS262_v1.2	TS262_v2.5
TS147	Zheng-Multimer	1.60	0.94	0.76	0.85	TS147_v2.4	TS147_v1.1
TS286	CSSB_experimental	1.60	0.96	0.77	0.83	TS286_v1.4	TS286_v2.1
TS241	elofsson	1.60	0.94	0.75	0.85	TS241_v2.3	TS241_v1.2
TS204	Zou	1.58	0.95	0.75	0.83	TS204_v2.1	TS204_v1.5
TS298	ShanghaiTech-human	1.57	0.94	0.74	0.83	TS298_v2.1	TS298_v1.1
TS167	OpenComplex	1.57	0.94	0.74	0.83	TS167_v1.1	TS167_v2.5
TS450	OpenComplex_Server	1.57	0.94	0.74	0.83	TS450_v1.1	TS450_v2.5
TS304	AF3-server	1.54	0.96	0.74	0.81	TS304_v1.1	TS304_v2.2
TS033	Diff	1.54	0.95	0.73	0.81	TS033_v1.1	TS033_v2.4
TS231	B-LAB	1.54	0.96	0.74	0.80	TS231_v1.2	TS231_v2.5
TS091	Huang-HUST	1.52	0.97	0.74	0.78	TS091_v1.4	TS091_v2.4
TS264	GuijunLab-Human	1.51	0.96	0.72	0.79	TS264_v2.6	TS264_v1.5
TS198	colabfold	1.50	0.95	0.72	0.79	TS198_v1.5	TS198_v2.4
TS023	FTBiot0119	1.50	0.95	0.71	0.79	TS023_v1.5	TS023_v2.4
TS145	colabfold_baseline	1.50	0.95	0.71	0.79	TS145_v1.2	TS145_v2.4
TS164	McGuffin	1.50	0.97	0.73	0.78	TS164_v1.5	TS164_v2.5
TS017	Seder2024hard	1.50	0.95	0.71	0.79	TS017_v1.1	TS017_v2.5
TS358	PerezLab_Gators	1.50	0.95	0.71	0.78	TS358_v1.5	TS358_v2.1
TS369	Bhattacharya	1.50	0.97	0.72	0.77	TS369_v1.4	TS369_v2.1
TS148	Guijunlab-Complex	1.49	0.95	0.71	0.78	TS148_v2.5	TS148_v1.3
TS312	GuijunLab-Assembly	1.49	0.95	0.71	0.78	TS312_v2.5	TS312_v1.3
TS287	plmfold	1.49	0.96	0.71	0.77	TS287_v2.4	TS287_v1.5
TS163	MultiFOLD2	1.49	0.96	0.71	0.78	TS163_v1.3	TS163_v2.5
TS112	Seder2024easy	1.48	0.94	0.70	0.79	TS112_v1.2	TS112_v2.1
TS301	GHZ-MAN	1.48	0.96	0.71	0.77	TS301_v2.5	TS301_v1.4
TS375	milliseconds	1.48	0.96	0.71	0.77	TS375_v2.3	TS375_v1.2
TS397	smg_ulaval	1.47	0.96	0.71	0.77	TS397_v1.1	TS397_v2.1
TS122	MQA_server	1.47	0.96	0.71	0.76	TS122_v1.4	TS122_v2.2
TS423	ShanghaiTech-server	1.44	0.95	0.68	0.76	TS423_v2.3	TS423_v1.2
TS465	Wallner	1.43	0.94	0.68	0.75	TS465_v1.3	TS465_v2.2
TS212	PIEFold_human	1.43	0.92	0.66	0.77	TS212_v1.3	TS212_v2.1
TS267	kiharalab_server	1.42	0.96	0.68	0.74	TS267_v1.5	TS267_v2.4
TS388	DeepFold-server	1.41	0.92	0.65	0.76	TS388_v1.2	TS388_v2.3
TS014	Cool-PSP	1.41	0.96	0.68	0.73	TS014_v2.6	TS014_v1.1
TS059	DeepFold	1.41	0.95	0.67	0.74	TS059_v1.6	TS059_v2.3
TS293	MRAH	1.39	0.97	0.67	0.72	TS293_v1.3	TS293_v2.3
TS079	MRAFold	1.39	0.97	0.67	0.72	TS079_v1.3	TS079_v2.3
TS139	DeepFold-refine	1.39	0.96	0.67	0.72	TS139_v1.6	TS139_v2.6
TS040	DELCLAB	1.34	0.96	0.65	0.70	TS040_v1.2	TS040_v2.3
TS015	PEZYFoldings	1.34	0.96	0.65	0.70	TS015_v2.6	TS015_v1.6
TS196	HYU_MLLAB	1.27	0.95	0.60	0.66	TS196_v1.1	TS196_v2.3
TS351	digiwiser-ensemble	1.23	0.96	0.59	0.64	TS351_v1.1	TS351_v2.1
TS120	Cerebra	1.12	0.97	0.54	0.58	TS120_v1.4	TS120_v2.3
TS475	ptq	0.77	0.0	0.00	0.77	N/A ¹	TS475_v2.5
TS262	CSSB	0.73	0.0	0.00	0.73	N/A ¹	TS262_v2.3

Supplementary Table S23: Results for T1239 TMscore Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS462	Zheng	1.58	0.85	0.91	0.67	TS462_v2_2	TS462_v1_1
TS019	Zheng-Server	1.54	0.99	0.76	0.77	TS019_v1_1	TS019_v2_5
TS425	MULTICOM_GATE	1.52	0.84	0.88	0.64	TS425_v1_2	TS425_v2_4
TS481	Vfold	1.47	0.89	0.81	0.65	TS481_v1_5	TS481_v2_4
TS147	Zheng-Multimer	1.44	0.89	0.80	0.64	TS147_v1_3	TS147_v2_5
TS221	CSSB_FAKER	1.43	0.72	0.91	0.52	TS221_v2_1	TS221_v1_4
TS419	CSSB-Human	1.43	0.72	0.91	0.52	TS419_v2_1	TS419_v1_4
TS028	NKRNA-s	1.43	0.71	0.92	0.51	TS028_v2_2	TS028_v1_4
TS051	MULTICOM	1.43	0.71	0.92	0.51	TS051_v1_4	TS051_v2_4
TS345	MULTICOM_human	1.43	0.71	0.92	0.51	TS345_v1_4	TS345_v2_4
TS286	CSSB_experimental	1.42	0.73	0.91	0.52	TS286_v2_1	TS286_v1_5
TS235	isyslab-hust	1.42	0.72	0.91	0.51	TS235_v2_4	TS235_v1_1
TS208	falcon2	1.40	0.71	0.90	0.50	TS208_v1_4	TS208_v2_4
TS204	Zou	1.39	0.74	0.87	0.52	TS204_v1_5	TS204_v2_2
TS456	Yang-Multimer	1.38	0.75	0.86	0.52	TS456_v1_3	TS456_v2_2
TS450	OpenComplex_Server	1.38	0.95	0.72	0.65	TS450_v1_1	TS450_v2_4
TS167	OpenComplex	1.38	0.95	0.72	0.65	TS167_v1_1	TS167_v2_4
TS110	MIEnsembles-Server	1.36	0.75	0.85	0.51	TS110_v1_1	TS110_v2_2
TS022	Yang	1.34	0.78	0.82	0.52	TS022_v1_5	TS022_v2_4
TS298	ShanghaiTech-human	1.34	0.70	0.87	0.47	TS298_v1_1	TS298_v2_1
TS052	Yang-Server	1.34	0.79	0.81	0.53	TS052_v1_5	TS052_v2_3
TS294	KiharaLab	1.34	0.76	0.83	0.51	TS294_v1_1	TS294_v2_2
TS262	CoDock	1.34	0.75	0.83	0.50	TS262_v1_2	TS262_v2_2
TS033	Diff	1.33	0.94	0.70	0.62	TS033_v2_2	TS033_v1_1
TS091	Huang-HUST	1.32	0.92	0.71	0.61	TS091_v1_5	TS091_v2_3
TS314	GuijunLab-PATHreader	1.32	0.76	0.82	0.51	TS314_v2_5	TS314_v1_5
TS319	MULTICOM_LLM	1.32	0.77	0.81	0.51	TS319_v1_2	TS319_v2_5
TS331	MULTICOM_AI	1.32	0.77	0.81	0.51	TS331_v1_2	TS331_v2_5
TS159	406	1.31	0.78	0.80	0.51	TS159_v1_2	TS159_v2_2
TS325	405	1.31	0.78	0.80	0.51	TS325_v1_2	TS325_v2_2
TS212	PIEFold_human	1.30	0.77	0.80	0.50	TS212_v2_1	TS212_v1_4
TS465	Wallner	1.30	0.98	0.66	0.63	TS465_v1_4	TS465_v2_2
TS489	Fernandez-Recio	1.28	0.78	0.78	0.50	TS489_v1_3	TS489_v2_4
TS241	elofsson	1.27	0.81	0.76	0.51	TS241_v1_4	TS241_v2_5
TS423	ShanghaiTech-server	1.23	0.83	0.72	0.51	TS423_v1_4	TS423_v2_5
TS369	Bhattacharya	1.22	0.83	0.71	0.51	TS369_v1_3	TS369_v2_4
TS231	B-LAB	1.21	0.83	0.71	0.50	TS231_v2_1	TS231_v1_2
TS358	PerezLab_Gators	1.21	0.81	0.72	0.49	TS358_v2_2	TS358_v1_4
TS272	GromihaLab	1.21	0.83	0.70	0.50	TS272_v1_1	TS272_v2_1
TS040	DELCLAB	1.21	0.84	0.70	0.51	TS040_v1_3	TS040_v2_3
TS112	Seder2024easy	1.20	0.85	0.69	0.51	TS112_v1_4	TS112_v2_4
TS017	Seder2024hard	1.20	0.85	0.69	0.51	TS017_v1_1	TS017_v2_4
TS145	colabfold_baseline	1.20	0.85	0.69	0.51	TS145_v1_2	TS145_v2_3
TS079	MRAFold	1.20	0.88	0.67	0.53	TS079_v1_2	TS079_v2_3
TS293	MRAH	1.20	0.88	0.67	0.53	TS293_v1_2	TS293_v2_3
TS023	FTBiot0119	1.20	0.85	0.69	0.51	TS023_v1_2	TS023_v2_3
TS304	AF3-server	1.20	0.87	0.67	0.52	TS304_v2_4	TS304_v1_2
TS198	colabfold	1.19	0.83	0.70	0.49	TS198_v1_2	TS198_v2_1
TS148	Guijunlab-Complex	1.19	0.84	0.69	0.50	TS148_v2_5	TS148_v1_3
TS059	DeepFold	1.19	0.88	0.67	0.52	TS059_v1_6	TS059_v2_3
TS014	Cool-PSP	1.19	0.83	0.69	0.50	TS014_v2_3	TS014_v1_5
TS163	MultiFOLD2	1.19	0.84	0.69	0.50	TS163_v1_2	TS163_v2_3
TS139	DeepFold-refine	1.18	0.87	0.67	0.52	TS139_v1_6	TS139_v2_2
TS375	milliseconds	1.18	0.85	0.68	0.50	TS375_v1_3	TS375_v2_3
TS301	GHZ-MAN	1.16	0.88	0.65	0.51	TS301_v2_4	TS301_v1_1
TS312	GuijunLab-Assembly	1.16	0.87	0.66	0.50	TS312_v2_4	TS312_v1_3
TS264	GuijunLab-Human	1.16	0.87	0.65	0.50	TS264_v2_2	TS264_v1_5
TS267	kiharalab_server	1.16	0.86	0.66	0.50	TS267_v1_1	TS267_v2_4
TS122	MQA_server	1.15	0.87	0.65	0.50	TS122_v1_3	TS122_v2_3
TS287	plmfold	1.15	0.89	0.64	0.51	TS287_v1_3	TS287_v2_4
TS015	PEZYPFoldings	1.14	0.91	0.62	0.52	TS015_v2_3	TS015_v1_4
TS164	McGuffin	1.14	0.88	0.64	0.50	TS164_v2_2	TS164_v1_2
TS397	smg-ulaval	1.12	0.90	0.61	0.50	TS397_v2_1	TS397_v1_1
TS196	HYU_MLLAB	1.08	0.96	0.52	0.56	TS196_v1_2	TS196_v2_3

Supplementary Table S24: Results for T1249 AvgDockQ Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_AvgDockQ	V2_AvgDockQ	V1_Model	V2_Model
TS393	GuijunLab-QA	0.97	0.98	0.47	0.50	TS393.v1.3o	TS393.v2.6o
TS304	AF3-server	0.94	0.91	0.43	0.51	TS304.v1.2o	TS304.v2.1o
TS314	GuijunLab-Pathreader	0.88	0.83	0.37	0.52	TS314.v1.2o	TS314.v2.1o
TS345	MULTICOM_human	0.87	0.43	0.69	0.19	TS345.v2.4o	TS345.v1.5o
TS397	smg_ulaval	0.87	0.49	0.65	0.21	TS397.v2.1o	TS397.v1.1o
TS015	PEZYZFoldings	0.86	0.34	0.71	0.14	TS015.v1.2o	TS015.v2.1o
TS456	Yang-Multimer	0.81	0.38	0.65	0.15	TS456.v1.2o	TS456.v2.2o
TS051	MULTICOM	0.79	0.46	0.61	0.18	TS051.v1.6o	TS051.v2.5o
TS293	MRAH	0.78	0.40	0.62	0.16	TS293.v1.2o	TS293.v2.5o
TS079	MRAFold	0.78	0.40	0.62	0.16	TS079.v1.2o	TS079.v2.5o
TS014	Cool-PSP	0.77	0.32	0.65	0.12	TS014.v1.1o	TS014.v2.1o
TS322	XGroup	0.76	0.70	0.49	0.26	TS322.v1.4o	TS322.v2.1o
TS219	XGroup-Server	0.76	0.70	0.49	0.26	TS219.v1.4o	TS219.v2.1o
TS465	Wallner	0.73	0.40	0.58	0.15	TS465.v1.1o	TS465.v2.3o
TS241	elofsson	0.73	0.50	0.55	0.18	TS241.v2.5o	TS241.v1.1o
TS052	Yang-Server	0.72	0.72	0.46	0.26	TS052.v1.3o	TS052.v2.1o
TS091	Huang-HUST	0.71	0.63	0.49	0.23	TS091.v2.5o	TS091.v1.1o
TS462	Zheng	0.71	0.73	0.45	0.26	TS462.v2.1o	TS462.v1.6o
TS290	Pierce	0.71	0.70	0.46	0.25	TS290.v1.5o	TS290.v2.4o
TS167	OpenComplex	0.70	0.62	0.48	0.22	TS167.v2.2o	TS167.v1.5o
TS450	OpenComplex_Server	0.70	0.62	0.48	0.22	TS450.v2.2o	TS450.v1.5o
TS008	HADDOCK	0.70	0.69	0.46	0.24	TS008.v1.1o	TS008.v2.5o
TS059	DeepFold	0.68	0.62	0.47	0.21	TS059.v2.3o	TS059.v1.5o
TS369	Bhattacharya	0.66	0.66	0.44	0.22	TS369.v1.3o	TS369.v2.2o
TS022	Yang	0.64	0.57	0.46	0.18	TS022.v1.5o	TS022.v2.1o
TS425	MULTICOM_GATE	0.64	0.57	0.46	0.18	TS425.v2.3o	TS425.v1.4o
TS331	MULTICOM_AI	0.64	0.57	0.46	0.18	TS331.v2.3o	TS331.v1.4o
TS319	MULTICOM_LLM	0.64	0.57	0.46	0.18	TS319.v2.3o	TS319.v1.4o
TS301	GHZ-MAN	0.64	0.44	0.50	0.14	TS301.v1.4o	TS301.v2.1o
TS267	kiharalab_server	0.64	0.48	0.48	0.15	TS267.v1.2o	TS267.v2.5o
TS375	milliseconds	0.64	0.57	0.45	0.18	TS375.v2.1o	TS375.v1.4o
TS423	ShanghaiTech-server	0.63	0.46	0.49	0.14	TS423.v1.2o	TS423.v2.2o
TS294	KiharaLab	0.62	0.53	0.46	0.17	TS294.v2.4o	TS294.v1.5o
TS204	Zou	0.62	0.37	0.51	0.11	TS204.v2.5o	TS204.v1.1o
TS145	colabfold_baseline	0.62	0.78	0.38	0.24	TS145.v1.2o	TS145.v2.5o
TS380	mialab_prediction	0.62	0.78	0.38	0.24	TS380.v1.4o	TS380.v2.5o
TS311	RAGfold_Prot1	0.62	0.47	0.47	0.14	TS311.v1.2o	TS311.v2.1o
TS148	Guijunlab-Complex	0.62	0.11	0.58	0.03	TS148.v2.2o	TS148.v1.3o
TS264	GuijunLab-Human	0.61	0.09	0.58	0.03	TS264.v2.2o	TS264.v1.4o
TS312	GuijunLab-Assembly	0.61	0.09	0.58	0.03	TS312.v2.2o	TS312.v1.4o
TS287	plmfold	0.60	0.41	0.47	0.12	TS287.v2.2o	TS287.v1.5o
TS198	colabfold	0.60	0.70	0.39	0.21	TS198.v2.2o	TS198.v1.3o
TS122	MQA_server	0.59	0.08	0.57	0.02	TS122.v2.2o	TS122.v1.3o
TS075	GHZ-ISM	0.59	0.08	0.57	0.02	TS075.v2.1o	TS075.v1.2o
TS475	ptq	0.59	0.08	0.57	0.02	TS475.v2.1o	TS475.v1.2o
TS284	Unicorn	0.59	0.08	0.57	0.02	TS284.v2.1o	TS284.v1.2o
TS031	MassiveFold	0.56	0.49	0.42	0.14	TS031.v2.4o	TS031.v1.5o
TS163	MultiFOLD2	0.55	0.69	0.36	0.19	TS163.v1.3o	TS163.v2.5o
TS494	ClusPro	0.55	0.72	0.35	0.20	TS494.v1.4o	TS494.v2.4o
TS261	UNRES	0.55	0.94	0.29	0.26	TS261.v1.1o	TS261.v2.1o
TS187	Ayush	0.53	0.63	0.36	0.17	TS187.v2.1o	TS187.v1.1o
TS274	kozakovvajda	0.52	0.59	0.36	0.15	TS274.v2.1o	TS274.v1.5o
TS272	GromihaLab	0.52	0.22	0.06	0.46	TS272.v2.1o	TS272.v1.2o
TS164	McGuffin	0.52	0.47	0.39	0.12	TS164.v2.5o	TS164.v1.4o
TS028	NKRNA-s	0.49	0.13	0.46	0.03	TS028.v2.1o	TS028.v1.4o
TS208	falcon2	0.48	0.44	0.37	0.10	TS208.v2.4o	TS208.v1.5o
TS110	MIEnsembles-Server	0.48	0.11	0.45	0.03	TS110.v2.1o	TS110.v1.4o
TS147	Zheng-Multimer	0.48	0.11	0.45	0.03	TS147.v2.1o	TS147.v1.3o
TS117	Vakser	0.41	0.09	0.02	0.39	TS117.v1.2o	TS117.v2.3o
TS040	DELCLAB	0.39	0.0	0.39	0.00	TS040.v2.3o	N/A ¹
TS419	CSSB-Human	0.39	0.64	0.26	0.12	TS419.v1.3o	TS419.v2.1o
TS221	CSSB_FAKER	0.39	0.64	0.26	0.12	TS221.v1.3o	TS221.v2.1o
TS286	CSSB_experimental	0.39	0.64	0.26	0.12	TS286.v1.3o	TS286.v2.1o
TS323	Yan	0.33	0.14	0.31	0.02	TS323.v2.1o	TS323.v1.1o
TS262	CoDock	0.33	0.52	0.24	0.09	TS262.v2.5o	TS262.v1.1o
TS489	Fernandez-Recio	0.20	0.51	0.15	0.05	TS489.v1.1o	TS489.v2.5o
TS196	HYU_MLLAB	0.07	0.42	0.01	0.05	TS196.v1.3o	TS196.v2.5o
TS114	COAST	0.04	0.08	0.08	0.01	TS114.v1.5o	TS114.v2.1o

Supplementary Table S25: Results for T1249 GDT TS Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS393	GuijunLab-QA	1.51	0.95	79.50	71.70	TS393_v1.2	TS393_v2.6
TS304	AF3-server	1.46	0.97	70.80	75.00	TS304_v1.2	TS304_v2.1
TS059	DeepFold	1.44	0.82	84.80	59.00	TS059_v2.3	TS059_v1.5
TS345	MULTICOM_human	1.42	0.76	88.00	53.60	TS345_v2.4	TS345_v1.2
TS052	Yang-Server	1.41	0.83	82.50	58.30	TS052_v1.3	TS052_v2.1
TS079	MRAFold	1.40	0.76	86.40	53.20	TS079_v2.1	TS079_v1.4
TS091	Huang-HUST	1.40	0.87	78.80	60.80	TS091_v2.1	TS091_v1.1
TS293	MRAH	1.40	0.76	86.40	53.20	TS293_v2.1	TS293_v1.4
TS314	GuijunLab-PATHreader	1.39	0.89	61.60	77.60	TS314_v1.2	TS314_v2.1
TS015	PEZyFoldings	1.39	0.75	86.60	52.20	TS015_v1.2	TS015_v2.5
TS456	Yang-Multimer	1.38	0.74	87.30	51.00	TS456_v1.1	TS456_v2.2
TS397	smg-ulaval	1.38	0.81	82.40	55.70	TS397_v2.1	TS397_v1.1
TS241	elofsson	1.38	0.85	79.10	58.40	TS241_v1.3	TS241_v2.4
TS014	Cool-PSP	1.37	0.75	85.60	51.30	TS014_v1.1	TS014_v2.1
TS375	milliseconds	1.37	0.83	79.90	56.90	TS375_v1.3	TS375_v2.2
TS423	ShanghaiTech-server	1.37	0.76	84.60	52.20	TS423_v1.2	TS423_v2.4
TS008	HADDOCK	1.37	0.86	78.00	58.70	TS008_v1.4	TS008_v2.5
TS290	Pierce	1.36	0.79	82.70	53.80	TS290_v2.3	TS290_v1.5
TS462	Zheng	1.36	0.85	78.30	58.10	TS462_v2.3	TS462_v1.6
TS167	OpenComplex	1.36	0.86	77.60	58.60	TS167_v2.2	TS167_v1.5
TS294	KiharaLab	1.36	0.77	84.10	52.10	TS294_v2.4	TS294_v1.4
TS267	kiharalab_server	1.36	0.78	83.20	53.00	TS267_v2.3	TS267_v1.1
TS450	OpenComplex_Server	1.36	0.86	77.60	58.60	TS450_v2.2	TS450_v1.5
TS145	colabfold_baseline	1.36	0.95	71.50	64.40	TS145_v1.2	TS145_v2.5
TS380	mialab_prediction	1.36	0.95	71.50	64.40	TS380_v1.4	TS380_v2.5
TS198	colabfold	1.36	0.89	75.20	60.60	TS198_v1.2	TS198_v2.3
TS301	GHZ-MAN	1.35	0.76	83.90	51.50	TS301_v1.2	TS301_v2.1
TS031	MassiveFold	1.35	0.78	82.60	52.30	TS031_v2.3	TS031_v1.5
TS022	Yang	1.35	0.78	82.50	52.20	TS022_v1.3	TS022_v2.5
TS051	MULTICOM	1.34	0.80	80.50	53.60	TS051_v1.6	TS051_v2.2
TS311	RAGfold_Prot1	1.31	0.82	77.20	53.90	TS311_v1.2	TS311_v2.1
TS163	MultiFOLD2	1.30	0.91	71.20	59.30	TS163_v1.3	TS163_v2.5
TS319	MULTICOM_LLM	1.30	0.80	77.90	52.30	TS319_v2.3	TS319_v1.5
TS425	MULTICOM_GATE	1.30	0.80	77.90	52.30	TS425_v2.3	TS425_v1.5
TS331	MULTICOM_AI	1.30	0.80	77.90	52.30	TS331_v2.3	TS331_v1.5
TS219	XGroup-Server	1.30	0.89	71.90	58.20	TS219_v1.3	TS219_v2.4
TS322	XGroup	1.30	0.89	71.90	58.20	TS322_v1.3	TS322_v2.4
TS204	Zou	1.30	0.71	84.00	46.00	TS204_v2.4	TS204_v1.2
TS369	Bhattacharya	1.29	0.84	74.90	54.40	TS369_v1.3	TS369_v2.2
TS187	Ayush	1.26	0.88	70.80	55.20	TS187_v1.1	TS187_v2.1
TS494	ClusPro	1.26	0.92	67.90	58.00	TS494_v1.3	TS494_v2.4
TS261	UNRES	1.22	0.96	58.30	63.40	TS261_v2.4	TS261_v1.5
TS465	Wallner	1.20	0.74	75.30	44.20	TS465_v1.1	TS465_v2.3
TS287	plmfold	1.19	0.82	70.50	48.50	TS287_v2.1	TS287_v1.5
TS274	kozakovvajda	1.18	0.86	67.50	50.80	TS274_v2.1	TS274_v1.4
TS264	GuijunLab-Human	1.18	0.53	86.40	31.10	TS264_v2.2	TS264_v1.3
TS312	GuijunLab-Assembly	1.18	0.53	86.40	31.10	TS312_v2.2	TS312_v1.3
TS148	Guijunlab-Complex	1.17	0.52	86.40	30.50	TS148_v2.2	TS148_v1.4
TS164	McGuffin	1.15	0.81	68.30	46.20	TS164_v2.5	TS164_v1.4
TS208	falcon2	1.13	0.82	66.70	46.20	TS208_v2.4	TS208_v1.5
TS110	MIEnsembles-Server	1.09	0.57	78.30	31.00	TS110_v2.4	TS110_v1.4
TS028	NKRNA-s	1.09	0.56	78.80	30.50	TS028_v2.1	TS028_v1.1
TS147	Zheng-Multimer	1.09	0.57	78.30	31.00	TS147_v2.3	TS147_v1.4
TS075	GHZ-ISM	1.05	0.59	74.00	30.70	TS075_v2.2	TS075_v1.1
TS122	MQA_server	1.05	0.59	74.00	30.70	TS122_v2.3	TS122_v1.1
TS284	Unicorn	1.05	0.59	74.00	30.70	TS284_v2.2	TS284_v1.1
TS475	ptq	1.05	0.59	74.00	30.70	TS475_v2.2	TS475_v1.1
TS272	GromihaLab	1.04	0.69	35.90	68.40	TS272_v2.1	TS272_v1.2
TS286	CSSB_experimental	0.97	0.89	53.90	43.10	TS286_v2.1	TS286_v1.1
TS221	CSSB_FAKER	0.97	0.89	53.90	43.10	TS221_v2.1	TS221_v1.1
TS419	CSSB-Human	0.97	0.89	53.90	43.10	TS419_v2.1	TS419_v1.1
TS117	Vakser	0.77	0.41	15.70	61.30	TS117_v1.2	TS117_v2.4
TS323	Yan	0.76	0.42	59.60	16.00	TS323_v2.1	TS323_v1.1
TS262	CoDock	0.75	0.87	42.40	32.60	TS262_v2.1	TS262_v1.2

Supplementary Table S26: Results for T1249 GlobalLDDT Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS304	AF3-server	1.60	0.99	0.79	0.81	TS304.v1.2o	TS304.v2.1o
TS393	GuijunLab-QA	1.57	0.99	0.78	0.79	TS393.v1.6o	TS393.v2.6o
TS462	Zheng	1.57	0.99	0.79	0.78	TS462.v1.6o	TS462.v2.6o
TS314	GuijunLab-Pathreader	1.56	0.97	0.76	0.81	TS314.v1.2o	TS314.v2.1o
TS241	elofsson	1.55	0.98	0.79	0.76	TS241.v2.5o	TS241.v1.3o
TS015	PEZyFoldings	1.55	0.96	0.81	0.74	TS015.v1.2o	TS015.v2.1o
TS345	MULTICOM_human	1.55	0.98	0.79	0.76	TS345.v1.5o	TS345.v2.5o
TS272	GromihaLab	1.55	0.96	0.74	0.80	TS272.v2.1o	TS272.v1.2o
TS375	milliseconds	1.55	0.98	0.79	0.76	TS375.v1.3o	TS375.v2.2o
TS284	Unicorn	1.54	0.97	0.80	0.75	TS284.v2.1o	TS284.v1.4o
TS475	ptq	1.54	0.97	0.80	0.75	TS475.v2.1o	TS475.v1.4o
TS075	GHZ-ISM	1.54	0.97	0.80	0.75	TS075.v2.1o	TS075.v1.4o
TS110	MIEnsembles-Server	1.54	0.98	0.79	0.76	TS110.v2.5o	TS110.v1.3o
TS122	MQA_server	1.54	0.97	0.80	0.75	TS122.v2.2o	TS122.v1.5o
TS052	Yang-Server	1.54	0.99	0.78	0.76	TS052.v1.1o	TS052.v2.1o
TS051	MULTICOM	1.54	0.98	0.79	0.76	TS051.v1.3o	TS051.v2.5o
TS290	Pierce	1.54	0.98	0.78	0.76	TS290.v1.5o	TS290.v2.1o
TS319	MULTICOM_LLM	1.54	0.99	0.78	0.76	TS319.v1.4o	TS319.v2.2o
TS425	MULTICOM_GATE	1.54	0.99	0.78	0.76	TS425.v1.4o	TS425.v2.2o
TS331	MULTICOM_AI	1.54	0.99	0.78	0.76	TS331.v1.4o	TS331.v2.2o
TS028	NKRNA-s	1.54	0.98	0.79	0.76	TS028.v2.4o	TS028.v1.2o
TS287	plmfold	1.54	0.97	0.79	0.75	TS287.v2.1o	TS287.v1.4o
TS147	Zheng-Multimer	1.54	0.98	0.79	0.76	TS147.v2.3o	TS147.v1.1o
TS397	smg_ulaval	1.54	0.97	0.79	0.75	TS397.v2.1o	TS397.v1.1o
TS167	OpenComplex	1.54	0.98	0.78	0.76	TS167.v2.2o	TS167.v1.5o
TS450	OpenComplex_Server	1.54	0.98	0.78	0.76	TS450.v2.2o	TS450.v1.5o
TS293	MRAH	1.54	0.96	0.80	0.74	TS293.v1.2o	TS293.v2.5o
TS079	MRAFold	1.54	0.96	0.80	0.74	TS079.v1.2o	TS079.v2.5o
TS369	Bhattacharya	1.54	0.99	0.78	0.76	TS369.v1.3o	TS369.v2.2o
TS456	Yang-Multimer	1.53	0.97	0.79	0.74	TS456.v1.2o	TS456.v2.5o
TS312	GuijunLab-Assembly	1.53	0.99	0.77	0.76	TS312.v2.1o	TS312.v1.5o
TS264	GuijunLab-Human	1.53	0.99	0.77	0.76	TS264.v2.1o	TS264.v1.5o
TS294	KiharaLab	1.53	0.97	0.79	0.75	TS294.v2.3o	TS294.v1.1o
TS022	Yang	1.53	0.98	0.78	0.75	TS022.v1.5o	TS022.v2.1o
TS091	Huang-HUST	1.53	0.99	0.77	0.76	TS091.v2.4o	TS091.v1.1o
TS148	Guijunlab-Complex	1.52	0.98	0.77	0.75	TS148.v2.1o	TS148.v1.1o
TS204	Zou	1.52	0.97	0.78	0.74	TS204.v2.3o	TS204.v1.3o
TS008	HADDOCK	1.52	0.99	0.77	0.75	TS008.v1.4o	TS008.v2.5o
TS059	DeepFold	1.52	0.98	0.77	0.74	TS059.v1.1o	TS059.v2.6o
TS267	kiharalab_server	1.51	0.97	0.78	0.73	TS267.v2.3o	TS267.v1.3o
TS145	colabfold_baseline	1.51	1.00	0.76	0.76	TS145.v1.1o	TS145.v2.5o
TS164	McGuffin	1.51	0.98	0.77	0.74	TS164.v2.5o	TS164.v1.2o
TS380	mialab_prediction	1.51	1.00	0.76	0.76	TS380.v1.3o	TS380.v2.5o
TS311	RAGfold_Prot1	1.51	0.99	0.76	0.75	TS311.v1.3o	TS311.v2.1o
TS198	colabfold	1.51	0.99	0.76	0.75	TS198.v2.2o	TS198.v1.3o
TS301	GHZ-MAN	1.51	0.98	0.77	0.74	TS301.v2.1o	TS301.v1.3o
TS014	Cool-PSP	1.51	0.94	0.80	0.71	TS014.v1.1o	TS014.v2.1o
TS208	falcon2	1.51	0.99	0.76	0.74	TS208.v2.4o	TS208.v1.5o
TS163	MultiFOLD2	1.50	0.99	0.76	0.74	TS163.v1.3o	TS163.v2.3o
TS494	ClusPro	1.49	1.00	0.75	0.74	TS494.v1.2o	TS494.v2.5o
TS187	Ayush	1.49	0.99	0.75	0.74	TS187.v1.1o	TS187.v2.1o
TS322	XGroup	1.48	1.00	0.74	0.74	TS322.v1.4o	TS322.v2.1o
TS219	XGroup-Server	1.48	1.00	0.74	0.74	TS219.v1.4o	TS219.v2.1o
TS274	kozakovvajda	1.48	0.99	0.75	0.73	TS274.v2.1o	TS274.v1.5o
TS423	ShanghaiTech-server	1.47	0.98	0.75	0.72	TS423.v2.2o	TS423.v1.4o
TS031	MassiveFold	1.47	0.97	0.75	0.71	TS031.v2.5o	TS031.v1.5o
TS261	UNRES	1.44	1.00	0.72	0.72	TS261.v1.3o	TS261.v2.1o
TS465	Wallner	1.43	0.97	0.74	0.69	TS465.v1.1o	TS465.v2.3o
TS262	CoDock	1.32	0.92	0.61	0.72	TS262.v2.2o	TS262.v1.5o
TS323	Yan	1.24	0.79	0.76	0.49	TS323.v2.1o	TS323.v1.1o
TS419	CSSB-Human	1.22	0.94	0.65	0.57	TS419.v1.1o	TS419.v2.1o
TS221	CSSB_FAKER	1.22	0.94	0.65	0.57	TS221.v1.1o	TS221.v2.1o
TS286	CSSB_experimental	1.22	0.94	0.65	0.57	TS286.v1.1o	TS286.v2.1o
TS489	Fernandez-Recio	1.08	0.98	0.55	0.53	TS489.v1.3o	TS489.v2.3o
TS117	Vakser	1.07	0.78	0.65	0.42	TS117.v2.2o	TS117.v1.2o
TS196	HYU_MLLAB	1.07	0.96	0.51	0.56	TS196.v2.3o	TS196.v1.1o
TS085	Bates	0.98	0.88	0.43	0.55	TS085.v1.5o	TS085.v2.5o
TS040	DELCLAB	0.72	0.0	0.72	0.00	TS040.v2.3o	N/A ¹
TS139	DeepFold-refine	0.65	0.77	0.25	0.40	TS139.v2.4o	TS139.v1.5o
TS114	COAST	0.36	0.99	0.18	0.18	TS114.v1.4o	TS114.v2.4o

Supplementary Table S27: Results for T1249 TMscore Two-State Score

Group	Group_Name	Two-State_Score	Balance	V1_TMscore	V2_TMscore	V1_Model	V2_Model
TS304	AF3-server	1.91	0.99	0.95	0.97	TS304_v1.2o	TS304_v2.1o
TS393	GuijunLab-QA	1.91	1.00	0.96	0.95	TS393_v1.2o	TS393_v2.6o
TS314	GuijunLab-PATHreader	1.90	0.98	0.94	0.96	TS314_v1.2o	TS314_v2.1o
TS145	colabfold_baseline	1.88	0.99	0.95	0.93	TS145_v2.1o	TS145_v1.5o
TS380	mialab_prediction	1.88	0.99	0.95	0.93	TS380_v2.3o	TS380_v1.5o
TS091	Huang-HUST	1.88	0.98	0.96	0.92	TS091_v2.4o	TS091_v1.1o
TS052	Yang-Server	1.88	0.97	0.96	0.91	TS052_v1.3o	TS052_v2.1o
TS059	DeepFold	1.87	0.97	0.96	0.91	TS059_v2.3o	TS059_v1.5o
TS198	colabfold	1.87	0.98	0.95	0.92	TS198_v1.2o	TS198_v2.3o
TS450	OpenComplex_Server	1.87	0.97	0.96	0.91	TS450_v2.2o	TS450_v1.5o
TS167	OpenComplex	1.87	0.97	0.96	0.91	TS167_v2.2o	TS167_v1.5o
TS462	Zheng	1.87	0.97	0.96	0.91	TS462_v2.3o	TS462_v1.6o
TS008	HADDOCK	1.87	0.97	0.96	0.91	TS008_v2.1o	TS008_v1.5o
TS345	MULTICOM_human	1.86	0.95	0.98	0.89	TS345_v2.4o	TS345_v1.2o
TS322	XGroup	1.86	0.99	0.94	0.92	TS322_v1.3o	TS322_v2.4o
TS219	XGroup-Server	1.86	0.99	0.94	0.92	TS219_v1.3o	TS219_v2.4o
TS015	PEZyFoldings	1.86	0.95	0.98	0.88	TS015_v1.2o	TS015_v2.3o
TS293	MRAH	1.86	0.95	0.98	0.88	TS293_v1.2o	TS293_v2.5o
TS079	MRAFold	1.86	0.95	0.98	0.88	TS079_v1.2o	TS079_v2.5o
TS163	MultiFOLD2	1.86	0.98	0.95	0.91	TS163_v1.3o	TS163_v2.5o
TS311	RAGfold_Prot1	1.86	0.96	0.97	0.89	TS311_v1.2o	TS311_v2.1o
TS375	milliseconds	1.86	0.97	0.96	0.90	TS375_v1.3o	TS375_v2.2o
TS290	Pierce	1.86	0.96	0.96	0.89	TS290_v2.2o	TS290_v1.5o
TS494	ClusPro	1.85	0.98	0.94	0.91	TS494_v1.4o	TS494_v2.4o
TS397	smg-ulaval	1.85	0.96	0.97	0.88	TS397_v2.1o	TS397_v1.1o
TS456	Yang-Multimer	1.85	0.94	0.98	0.87	TS456_v1.2o	TS456_v2.2o
TS051	MULTICOM	1.85	0.96	0.96	0.89	TS051_v1.6o	TS051_v2.2o
TS241	elofsson	1.85	0.96	0.96	0.89	TS241_v2.1o	TS241_v1.1o
TS369	Bhattacharya	1.85	0.97	0.95	0.90	TS369_v1.3o	TS369_v2.2o
TS267	kiharalab_server	1.85	0.96	0.96	0.88	TS267_v2.3o	TS267_v1.1o
TS022	Yang	1.85	0.96	0.96	0.88	TS022_v1.3o	TS022_v2.5o
TS294	KiharaLab	1.85	0.96	0.96	0.88	TS294_v2.4o	TS294_v1.5o
TS187	Ayush	1.84	0.97	0.95	0.90	TS187_v1.1o	TS187_v2.1o
TS014	Cool-PSP	1.84	0.94	0.98	0.87	TS014_v1.1o	TS014_v2.1o
TS423	ShanghaiTech-server	1.84	0.95	0.97	0.88	TS423_v1.2o	TS423_v2.4o
TS319	MULTICOM_LLM	1.84	0.96	0.96	0.88	TS319_v2.3o	TS319_v1.5o
TS425	MULTICOM_GATE	1.84	0.96	0.96	0.88	TS425_v2.3o	TS425_v1.5o
TS331	MULTICOM_AI	1.84	0.96	0.96	0.88	TS331_v2.3o	TS331_v1.5o
TS301	GHZ-MAN	1.84	0.95	0.97	0.87	TS301_v1.5o	TS301_v2.1o
TS261	UNRES	1.84	0.99	0.91	0.93	TS261_v1.1o	TS261_v2.5o
TS031	MassiveFold	1.84	0.95	0.96	0.87	TS031_v2.5o	TS031_v1.5o
TS274	kozakovvajda	1.82	0.97	0.94	0.88	TS274_v2.1o	TS274_v1.4o
TS287	plmfold	1.82	0.96	0.95	0.87	TS287_v2.1o	TS287_v1.5o
TS204	Zou	1.81	0.93	0.96	0.84	TS204_v2.3o	TS204_v1.2o
TS465	Wallner	1.80	0.94	0.95	0.84	TS465_v1.1o	TS465_v2.3o
TS164	McGuffin	1.79	0.94	0.94	0.84	TS164_v2.5o	TS164_v1.4o
TS208	falcon2	1.78	0.94	0.94	0.83	TS208_v2.4o	TS208_v1.5o
TS286	CSSB_experimental	1.68	0.98	0.86	0.82	TS286_v1.3o	TS286_v2.3o
TS419	CSSB-Human	1.68	0.98	0.86	0.82	TS419_v1.3o	TS419_v2.3o
TS221	CSSB_FAKER	1.68	0.98	0.86	0.82	TS221_v1.3o	TS221_v2.3o
TS272	GromihaLab	1.63	0.84	0.69	0.94	TS272_v2.1o	TS272_v1.2o
TS262	CoDock	1.56	0.95	0.82	0.74	TS262_v2.1o	TS262_v1.1o
TS122	MQA_server	1.41	0.65	0.95	0.46	TS122_v2.2o	TS122_v1.2o
TS475	ptq	1.41	0.65	0.95	0.46	TS475_v2.1o	TS475_v1.5o
TS075	GHZ-ISM	1.41	0.65	0.95	0.46	TS075_v2.1o	TS075_v1.5o
TS284	Unicorn	1.41	0.65	0.95	0.46	TS284_v2.1o	TS284_v1.5o
TS264	GuijunLab-Human	1.40	0.62	0.97	0.43	TS264_v2.2o	TS264_v1.6o
TS110	MIEnsembles-Server	1.40	0.63	0.96	0.44	TS110_v2.5o	TS110_v1.4o
TS312	GuijunLab-Assembly	1.36	0.57	0.97	0.39	TS312_v2.2o	TS312_v1.1o
TS148	Guijunlab-Complex	1.36	0.57	0.97	0.39	TS148_v2.2o	TS148_v1.3o
TS147	Zheng-Multimer	1.35	0.58	0.96	0.39	TS147_v2.3o	TS147_v1.4o
TS028	NKRNA-s	1.34	0.57	0.96	0.38	TS028_v2.1o	TS028_v1.1o
TS117	Vakser	1.30	0.57	0.37	0.93	TS117_v1.2o	TS117_v2.4o
TS323	Yan	1.23	0.52	0.92	0.32	TS323_v2.1o	TS323_v1.1o
TS489	Fernandez-Recio	1.21	0.77	0.74	0.46	TS489_v1.1o	TS489_v2.5o