

CASP16_TWO-STATE_TABLES

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Supplementary Table S1: 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	4		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	5		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	5	
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	comppharmunibas	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	2		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 S2: 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 S3: 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	1.16	63.11	53.04	TS462.v1.3	TS462.v2.5
TS264	GuijunLab-Human	1.16	55.95	60.07	TS264.v1.6	TS264.v2.2
TS147	Zheng-Multimer	1.16	62.31	53.37	TS147.v1.1	TS147.v2.1
TS148	Guijunlab-Complex	1.15	54.45	60.07	TS148.v2.3	TS148.v1.3
TS481	Vfold	1.12	61.80	50.66	TS481.v1.3	TS481.v2.5
TS167	OpenComplex	1.12	57.07	55.34	TS167.v1.1	TS167.v2.3
TS450	OpenComplex_Server	1.12	57.07	55.34	TS450.v1.1	TS450.v2.3
TS022	Yang	1.12	57.21	54.92	TS022.v1.4	TS022.v2.5
TS052	Yang-Server	1.12	59.50	52.39	TS052.v1.4	TS052.v2.2
TS456	Yang-Multimer	1.11	58.33	52.39	TS456.v1.3	TS456.v2.2
TS204	Zou	1.11	62.17	48.41	TS204.v1.1	TS204.v2.2
TS241	elofsson	1.10	58.57	51.83	TS241.v2.1	TS241.v1.2
TS294	KiharaLab	1.09	59.97	49.44	TS294.v2.5	TS294.v1.3
TS091	Huang-HUST	1.09	54.54	54.63	TS091.v1.2	TS091.v2.5
TS033	Diff	1.09	56.88	51.83	TS033.v2.1	TS033.v1.4
TS262	CoDock	1.08	55.90	52.34	TS262.v1.2	TS262.v2.4
TS212	PIEFold_human	1.08	55.10	52.48	TS212.v2.4	TS212.v1.2
TS375	milliseconds	1.07	59.41	47.57	TS375.v2.4	TS375.v1.3
TS028	NKRNA-s	1.07	51.31	55.38	TS028.v1.2	TS028.v2.5
TS301	GHZ-MAN	1.07	55.95	50.70	TS301.v1.3	TS301.v2.4
TS110	MIEnsembles-Server	1.06	52.25	53.56	TS110.v1.2	TS110.v2.5
TS304	AF3-server	1.05	57.73	46.86	TS304.v1.4	TS304.v2.5
TS051	MULTICOM	1.04	56.65	47.33	TS051.v1.3	TS051.v2.2
TS345	MULTICOM_human	1.04	56.65	47.33	TS345.v1.3	TS345.v2.2
TS319	MULTICOM_LLM	1.04	56.65	47.33	TS319.v1.2	TS319.v2.4
TS331	MULTICOM_AI	1.04	56.65	47.33	TS331.v1.2	TS331.v2.4
TS274	kozakovvajda	1.04	56.32	47.52	TS274.v1.2	TS274.v2.2
TS494	ClusPro	1.04	56.32	47.52	TS494.v1.2	TS494.v2.2
TS231	B-LAB	1.04	56.27	47.33	TS231.v2.4	TS231.v1.4
TS314	GuijunLab-Pathreader	1.04	48.55	55.01	TS314.v2.3	TS314.v1.1
TS286	CSSB_experimental	1.03	56.13	47.33	TS286.v1.5	TS286.v2.4
TS425	MULTICOM_GATE	1.03	55.85	47.33	TS425.v1.1	TS425.v2.1
TS198	colabfold	1.03	56.41	46.16	TS198.v2.2	TS198.v1.2
TS419	CSSB-Human	1.02	55.52	46.77	TS419.v2.4	TS419.v1.3
TS221	CSSB_FAKER	1.02	55.57	46.63	TS221.v2.2	TS221.v1.5
TS369	Bhattacharya	1.02	54.82	47.28	TS369.v1.2	TS369.v2.1
TS019	Zheng-Server	1.02	51.69	50.28	TS019.v1.4	TS019.v2.4
TS475	ptq	1.01	58.43	42.70	TS475.v2.5	TS475.v1.2
TS014	Cool-PSP	1.01	58.57	42.56	TS014.v2.6	TS014.v1.6
TS287	plmfold	1.01	54.07	47.00	TS287.v1.2	TS287.v2.1
TS267	kiharalab_server	1.00	54.68	45.37	TS267.v1.1	TS267.v2.5

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Supplementary Table S3 – continued from previous page

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS079	MRAFold	1.00	54.82	44.94	TS079_v1.2	TS079_v2.2
TS293	MRAH	1.00	54.82	44.94	TS293_v1.2	TS293_v2.2
TS489	Fernandez-Recio	1.00	55.48	44.20	TS489_v1.2	TS489_v2.2
TS208	falcon2	0.99	54.54	44.66	TS208_v2.5	TS208_v1.1
TS196	HYU_MLLAB	0.99	53.37	45.37	TS196_v1.5	TS196_v2.5
TS312	GuijunLab-Assembly	0.98	53.84	44.66	TS312_v1.4	TS312_v2.2
TS017	Seder2024hard	0.98	54.35	43.63	TS017_v1.5	TS017_v2.5
TS112	Seder2024easy	0.98	54.35	43.63	TS112_v1.4	TS112_v2.3
TS145	colabfold_baseline	0.98	54.35	43.54	TS145_v1.3	TS145_v2.3
TS465	Wallner	0.97	50.00	47.47	TS465_v1.5	TS465_v2.1
TS235	isyslab-hust	0.97	50.80	45.83	TS235_v1.1	TS235_v2.3
TS311	RAGfold_Prot1	0.97	49.86	46.72	TS311_v1.2	TS311_v2.5
TS163	MultiFOLD2	0.96	53.23	42.79	TS163_v1.5	TS163_v2.2
TS015	PEZYZFoldings	0.96	51.12	44.43	TS015_v2.2	TS015_v1.5
TS298	ShanghaiTech-human	0.95	54.35	40.68	TS298_v1.3	TS298_v2.3
TS284	Unicorn	0.95	44.20	50.70	TS284_v1.3	TS284_v2.4
TS122	MQA_server	0.95	44.20	50.70	TS122_v1.3	TS122_v2.4
TS075	GHZ-ISM	0.95	44.20	50.70	TS075_v1.3	TS075_v2.4
TS164	McGuffin	0.95	48.03	46.72	TS164_v1.1	TS164_v2.2
TS159	406	0.94	49.34	44.94	TS159_v1.1	TS159_v2.1
TS325	405	0.94	49.34	44.94	TS325_v1.1	TS325_v2.1
TS269	CSSB_server	0.93	50.70	42.27	TS269_v1.1	TS269_v2.1
TS059	DeepFold	0.92	46.91	44.62	TS059_v2.3	TS059_v1.3
TS388	DeepFold-server	0.89	44.10	45.13	TS388_v1.3	TS388_v2.3
TS023	FTBiot0119	0.86	45.79	39.84	TS023_v1.3	TS023_v2.4
TS139	DeepFold-refine	0.80	40.59	39.56	TS139_v1.4	TS139_v2.2
TS120	Cerebra	0.76	38.34	37.73	TS120_v1.4	TS120_v2.1
TS361	Cerebra_server	0.66	32.77	33.33	TS361_v1.1	TS361_v2.1

Supplementary Table S4: 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 S5: 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	1.20	70.81	48.98	TS462.v2.2	TS462.v1.1
TS235	isyslab-hust	1.14	71.31	42.85	TS235.v2.4	TS235.v1.1
TS221	CSSB_FAKER	1.14	71.10	42.94	TS221.v2.1	TS221.v1.5
TS419	CSSB-Human	1.14	71.10	42.94	TS419.v2.1	TS419.v1.5
TS028	NKRNA-s	1.13	71.36	42.13	TS028.v2.2	TS028.v1.2
TS345	MULTICOM_human	1.13	71.23	42.09	TS345.v1.4	TS345.v2.5
TS051	MULTICOM	1.13	71.23	42.09	TS051.v1.4	TS051.v2.5
TS286	CSSB_experimental	1.13	69.87	42.77	TS286.v2.1	TS286.v1.2
TS208	falcon2	1.09	66.99	41.54	TS208.v1.4	TS208.v2.4
TS425	MULTICOM_GATE	1.08	63.22	44.46	TS425.v1.2	TS425.v2.4
TS019	Zheng-Server	1.06	54.02	52.20	TS019.v1.5	TS019.v2.5
TS022	Yang	1.05	60.72	44.42	TS022.v1.5	TS022.v2.4
TS204	Zou	1.05	61.23	43.53	TS204.v1.5	TS204.v2.2
TS110	MIEnsembles-Server	1.05	63.01	41.71	TS110.v1.1	TS110.v2.2
TS456	Yang-Multimer	1.04	60.21	44.29	TS456.v1.3	TS456.v2.2
TS147	Zheng-Multimer	1.03	56.27	47.08	TS147.v1.3	TS147.v2.5
TS450	OpenComplex_Server	1.03	54.07	48.52	TS450.v1.5	TS450.v2.3
TS167	OpenComplex	1.03	54.07	48.52	TS167.v1.5	TS167.v2.3
TS294	KiharaLab	1.02	59.58	42.13	TS294.v1.1	TS294.v2.2
TS314	GuijunLab-Pathreader	1.02	58.77	42.77	TS314.v2.5	TS314.v1.2
TS052	Yang-Server	1.00	55.93	44.12	TS052.v1.5	TS052.v2.2
TS481	Vfold	1.00	56.57	43.10	TS481.v2.5	TS481.v1.2
TS091	Huang-HUST	0.99	52.08	47.17	TS091.v1.5	TS091.v2.3
TS319	MULTICOM_LLM	0.99	55.64	42.89	TS319.v1.2	TS319.v2.5
TS262	CoDock	0.98	57.63	40.74	TS262.v1.2	TS262.v2.5
TS033	Diff	0.98	53.94	43.99	TS033.v2.2	TS033.v1.1
TS331	MULTICOM_AI	0.98	55.64	42.09	TS331.v1.2	TS331.v2.2
TS325	405	0.97	55.21	42.26	TS325.v1.2	TS325.v2.2
TS159	406	0.97	55.21	42.26	TS159.v1.2	TS159.v2.2
TS369	Bhattacharya	0.97	54.07	43.10	TS369.v1.4	TS369.v2.4
TS489	Fernandez-Recio	0.97	54.96	41.75	TS489.v1.3	TS489.v2.4
TS298	ShanghaiTech-human	0.96	61.74	34.26	TS298.v1.1	TS298.v2.1
TS212	PIEFold_human	0.96	55.21	40.69	TS212.v2.1	TS212.v1.3
TS241	elofsson	0.95	54.32	40.82	TS241.v1.1	TS241.v2.5
TS231	B-LAB	0.94	54.07	40.27	TS231.v2.1	TS231.v1.2
TS304	AF3-server	0.94	50.89	43.15	TS304.v2.5	TS304.v1.2
TS465	Wallner	0.93	48.14	44.84	TS465.v1.4	TS465.v2.2
TS358	PerezLab_Gators	0.93	54.96	37.82	TS358.v2.2	TS358.v1.4
TS079	MRAFold	0.92	49.91	42.01	TS079.v1.2	TS079.v2.3
TS293	MRAH	0.92	49.91	42.01	TS293.v1.2	TS293.v2.3
TS272	GromihaLab	0.91	50.09	41.24	TS272.v1.3	TS272.v2.4

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Supplementary Table S5 – continued from previous page

Group	Group_Name	Two-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model	V2_Model
TS423	ShanghaiTech-server	0.91	51.91	39.17	TS423_v2.4	TS423_v1.1
TS267	kiharalab_server	0.89	50.00	39.30	TS267_v1.1	TS267_v2.4
TS148	Guijunlab-Complex	0.89	48.94	39.59	TS148_v2.5	TS148_v1.4
TS287	plmfold	0.88	49.32	39.17	TS287_v1.3	TS287_v2.4
TS198	colabfold	0.88	50.34	37.77	TS198_v1.2	TS198_v2.1
TS375	milliseconds	0.88	47.16	40.57	TS375_v2.3	TS375_v1.4
TS112	Seder2024easy	0.87	48.09	38.79	TS112_v1.4	TS112_v2.5
TS014	Cool-PSP	0.87	49.49	37.35	TS014_v2.3	TS014_v1.3
TS301	GHZ-MAN	0.87	46.65	40.19	TS301_v2.4	TS301_v1.1
TS163	MultiFOLD2	0.87	48.39	38.33	TS163_v1.3	TS163_v2.3
TS040	DELCLAB	0.86	48.09	38.41	TS040_v1.3	TS040_v2.3
TS023	FTBiot0119	0.86	47.67	38.79	TS023_v1.2	TS023_v2.1
TS145	colabfold_baseline	0.86	47.67	38.79	TS145_v1.2	TS145_v2.1
TS264	GuijunLab-Human	0.86	47.54	38.66	TS264_v2.2	TS264_v1.5
TS312	GuijunLab-Assembly	0.86	46.27	39.59	TS312_v2.4	TS312_v1.4
TS122	MQA_server	0.86	46.65	39.13	TS122_v1.3	TS122_v2.2
TS059	DeepFold	0.85	45.93	38.83	TS059_v1.6	TS059_v2.6
TS139	DeepFold-refine	0.85	45.93	38.83	TS139_v1.6	TS139_v2.6
TS017	Seder2024hard	0.85	48.05	36.46	TS017_v1.5	TS017_v2.4
TS397	smg_ulaval	0.84	45.00	39.13	TS397_v1.1	TS397_v2.1
TS164	McGuffin	0.84	45.47	38.37	TS164_v2.2	TS164_v1.3
TS015	PEZYFoldings	0.84	45.00	38.79	TS015_v1.4	TS015_v2.1
TS196	HYU_MLLAB	0.78	38.94	39.47	TS196_v1.2	TS196_v2.2
TS388	DeepFold-server	0.76	37.92	37.99	TS388_v1.3	TS388_v2.2
TS120	Cerebra	0.61	31.48	29.95	TS120_v1.3	TS120_v2.2
TS475	ptq	0.49	49.20	0.00	TS475_v2.1	N/A ¹
TS351	digiwiser-ensemble	0.49	24.45	24.28	TS351_v1.1	TS351_v2.1
TS269	CSSB_server	0.48	48.18	0.00	TS269_v2.4	N/A ¹
TS075	GHZ-ISM	0.47	46.65	0.00	TS075_v2.4	N/A ¹
TS284	Unicorn	0.47	46.65	0.00	TS284_v2.4	N/A ¹
TS311	RAGfold_Prot1	0.42	42.25	0.00	TS311_v1.1	N/A ¹
TS361	Cerebra_server	0.31	31.40	0.00	TS361_v1.2	N/A ¹
TS105	PFSC-PFVM	0.04	4.20	0.00	TS105_v1.3	N/A ¹

¹ Model either not submitted or not assessed

Supplementary Table S6: 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 S6 – 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 S7: 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
TS241	elofsson	85.08	50.07	35.01	TS241.v1.3	TS241.v2.2
TS304	AF3-server	85.08	50.07	35.01	TS304.v1.3	TS304.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