## $CASP16\_TWO\text{-}STATE\_TABLES$

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Supplementary Table S1: Results for T1214 GlobalLDDT Two-State Score

		Table 51: Resul				
Group	Group_Name	Two-State_Score	V1_GlobalLDDT	V2_GlobalLDDT	V1_Model	V2_Model
TS091	Huang-HUST	1.79	0.85	0.94	$TS091_v1_2$	$TS091_v2_1$
TS110	MIEnsembles-Server	1.78	0.85	0.93	$TS110_v1_2$	$TS110_{-}v2_{-}5$
TS147	Zheng-Multimer	1.78	0.85	0.93	$TS147_v1_1$	$TS147_v2_3$
TS462	Zheng	1.78	0.85	0.93	$TS462_v1_1$	$TS462_v2_3$
TS375	milliseconds	1.77	0.85	0.92	TS375_v1_3	$TS375_v2_4$
TS319	MULTICOM_LLM	1.77	0.85	0.92	TS319_v1_3	TS319_v2_4
TS198	colabfold	1.77	0.84	0.93	TS198_v1_5	TS198_v2_1
TS425	MULTICOM_GATE	1.77	0.85	0.91	TS425_v1_2	TS425_v2_4
TS148	Guijunlab-Complex	1.77	0.85	0.92	TS148_v1_5	TS148_v2_2
TS388	DeepFold-server Seder2024hard	1.77	0.86	0.91	TS388_v1_4 TS017_v1_4	TS388_v2_1
TS017 TS145	colabfold_baseline	1.77 $1.77$	$0.84 \\ 0.84$	0.93 0.93	TS145_v1_2	TS017_v2_1 TS145_v2_1
TS015	PEZYFoldings	1.75	0.87	0.93	TS015_v1_5	TS015_v2_1
TS494	ClusPro	1.74	0.75	0.99	TS494_v1_4	TS494_v2_1
TS274	kozakovvajda	1.74	0.75	0.99	TS274_v1_4	TS274_v2_1
TS204	Zou	1.73	0.81	0.93	TS204_v1_5	TS204_v2_3
TS055	LCDD-team	1.72	0.82	0.90	TS055_v1_3	TS055_v2_2
TS039	arosko	1.72	0.75	0.97	TS039_v1_2	TS039_v2_3
TS022	Yang	1.71	0.85	0.86	$TS022_v1_4$	$TS022\_v2\_2$
TS052	Yang-Server	1.70	0.84	0.86	$TS052\_v1\_3$	$TS052_v2_2$
TS456	Yang-Multimer	1.70	0.83	0.86	$TS456_v1_5$	$TS456_v2_4$
TS019	Zheng-Server	1.70	0.85	0.85	$TS019_v1_2$	$TS019_v2_1$
TS040	DELCLAB	1.70	0.75	0.94	$TS040_v1_2$	$TS040_v2_5$
TS059	DeepFold	1.69	0.78	0.91	TS059_v1_5	TS059_v2_6
TS269	CSSB_server	1.69	0.81	0.88	TS269_v1_5	TS269_v2_1
TS221	CSSB_FAKER	1.69	0.81	0.88	TS221_v1_3	TS221_v2_4
TS419	CSSB-Human	1.69	0.81	0.88	TS419_v1_3	TS419_v2_4
TS262	CoDock falcon2	1.69	0.83	0.86	TS262_v1_1	TS262_v2_2
TS208 TS386		1.69	0.86 0.86	0.83 0.82	TS208_v1_4	TS208_v2_1 TS386_v2_5
TS298	ShanghaiTech-Ligand ShanghaiTech-human	1.68 1.68	0.86	0.82	TS386_v1_4 TS298_v1_4	TS298_v2_5
TS267	kiharalab_server	1.68	0.85	0.83	TS267_v1_1	TS267_v2_3
TS465	Wallner	1.68	0.85	0.83	TS465_v1_2	TS465_v2_1
TS393	GuijunLab-QA	1.68	0.85	0.83	TS393_v1_1	TS393_v2_2
TS312	GuijunLab-Assembly	1.68	0.85	0.83	TS312_v1_1	TS312_v2_4
TS314	GuijunLab-PAthreader	1.68	0.85	0.83	TS314_v1_1	TS314_v2_4
TS264	GuijunLab-Human	1.68	0.85	0.83	TS264_v1_1	TS264_v2_6
TS287	plmfold	1.68	0.85	0.83	TS287_v1_2	TS287_v2_4
TS235	isyslab-hust	1.68	0.84	0.83	$TS235_v1_3$	$TS235_v2_2$
TS102	Psi-Phi	1.68	0.85	0.82	$TS102_v1_5$	$TS102_v2_2$
TS207	MULTICOM_ligand	1.67	0.85	0.83	$TS207_v1_2$	$TS207_v2_3$
TS139	DeepFold-refine	1.67	0.76	0.91	TS139_v1_3	TS139_v2_6
TS304	AF3-server	1.67	0.84	0.83	$TS304_v1_4$	$TS304_v2_1$
TS241	elofsson	1.67	0.84	0.83	$TS241_v1_4$	$TS241_v2_1$
TS272	GromihaLab	1.67	0.84	0.83	TS272_v1_3	TS272_v2_2
TS345	MULTICOM_human	1.67	0.85	0.82	TS345_v1_4	TS345_v2_6
TS122	MQA_server	1.67	0.84	0.83	TS122_v1_5	TS122_v2_4
TS311	RAGfold_Prot1	1.67	0.85	0.82	TS311_v1_4	TS311_v2_5
TS464	PocketTracer	1.67	0.84	0.83	TS464_v1_1	TS464_v2_3
TS051	MULTICOM	1.67	0.85	0.82	TS051_v1_1	TS051_v2_6
TS369 $TS227$	Bhattacharya KUMC	1.67 1.67	$0.85 \\ 0.85$	0.82 0.82	TS369_v1_1 TS227_v1_3	TS369_v2_2 TS227_v2_5
TS286	CSSB_experimental	1.67	0.80	0.82	TS286_v1_2	TS286_v2_4
TS301	GHZ-MAN	1.66	0.84	0.82	TS301_v1_2	TS301_v2_4
TS079	MRAFold	1.66	0.85	0.82	TS079_v1_1	TS079_v2_5
TS196	HYU_MLLAB	1.66	0.84	0.82	TS196_v1_3	TS196_v2_4
TS293	MRAH	1.66	0.85	0.81	TS293_v1_2	TS293_v2_1
TS164	McGuffin	1.66	0.84	0.82	TS164_v1_3	TS164_v2_4
TS163	MultiFOLD2	1.66	0.84	0.82	TS163_v1_3	TS163_v2_4
TS423	ShanghaiTech-server	1.66	0.85	0.81	TS423_v1_5	$TS423_v2_4$
TS014	Cool-PSP	1.65	0.84	0.81	TS014_v1_4	$TS014\_v2\_3$
TS331	MULTICOM_AI	1.65	0.85	0.80	$TS331_v1_1$	$TS331\_v2\_5$
TS075	GHZ-ISM	1.65	0.85	0.80	$TS075_v1_1$	$TS075\_v2\_3$
TS284	Unicorn	1.65	0.85	0.80	$TS284\_v1\_1$	$TS284\_v2\_3$
TS408	SNU-CHEM-lig	1.64	0.84	0.81	$TS408\_v1\_3$	$TS408\_v2\_2$
TS475	ptq	1.64	0.83	0.80	TS475_v1_5	TS475_v2_3
TS020	comppharmunibas	1.62	0.77	0.85	TS020_v1_4	TS020_v2_3
TS294	KiharaLab	1.56	0.84	0.72	TS294_v1_2	TS294_v2_3
TS202	test001	1.54	0.81	0.73	TS202_v1_5	TS202_v2_2
TS461	forlilab	1.45	0.71	0.73	TS461_v1_2	TS461_v2_3
TS120	Cerebra	1.35	0.63	0.72	TS120_v1_1	TS120_v2_6
TS361 TS167	Cerebra_server OpenComplex	1.26	0.62	0.64	TS361_v1_4	TS361_v2_1
TS167 $TS450$	OpenComplex_Server	1.24 $1.20$	$0.85 \\ 0.85$	$0.39 \\ 0.35$	TS167_v1_2	TS167_v2_5 TS450_v2_3
	OmniFold				TS450_v1_5	N/A <sup>1</sup>
TS400		0.84	0.84	0.00	TS400_v1_1	$N/A^{1}$ $N/A^{1}$
TS225	Unknown	0.83	0.83	0.00	TS225_v1_1	
TS275	Seminoles	0.69	0.69	0.00	TS275_v1_1 N/A <sup>1</sup>	N/A <sup>1</sup>
TS132	profold2	0.50	0.00	0.50	ın/A	TS132_v2_1

 $<sup>^{1}</sup>$  Model either not submitted or not assessed

Supplementary Table S2: Results for M1228 TMscore Two-State Score

Group	Group_Name	$Two\text{-}State\_Score$	$V1\_TMscore$	$V2\_TMscore$	V1_Model	V2_Model
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	$TS481_v2_1$
TS091	Huang-HUST	1.50	0.71	0.79	TS091_v1_3	$TS091_v2_2$
TS033	Diff	1.50	0.71	0.79	TS033_v1_5	$TS033_v2_2$
TS052	Yang-Server	1.50	0.69	0.81	TS052_v1_3	$TS052_v2_5$
TS022	Yang	1.50	0.70	0.80	TS022_v1_4	$TS022\_v2\_2$
TS304	AF3-server	1.49	0.71	0.78	TS304_v1_4	$TS304_v2_5$
TS262	CoDock	1.49	0.80	0.70	$TS262_v1_1$	$TS262_v2_3$
TS456	Yang-Multimer	1.46	0.67	0.78	$TS456_v1_3$	$TS456_v2_5$
TS274	kozakovvajda	1.46	0.69	0.76	$TS274_v1_2$	$TS274_v2_3$
TS494	ClusPro	1.46	0.69	0.76	$TS494_v1_2$	$TS494_v2_3$
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	$TS294_v2_1$
TS028	NKRNA-s	1.44	0.65	0.78	TS028_v1_2	$TS028_v2_4$
TS286	CSSB_experimental	1.42	0.71	0.71	$TS286_v1_5$	$TS286_v2_1$
TS231	B-LAB	1.40	0.68	0.72	$TS231_v1_2$	$TS231_v2_1$
TS489	Fernandez-Recio	1.38	0.69	0.69	TS489_v1_2	$TS489_v2_5$
TS450	OpenComplex_Server	1.37	0.68	0.69	$TS450_v1_1$	$TS450_v2_4$
TS167	OpenComplex	1.37	0.68	0.69	$TS167_v1_1$	$TS167_v2_4$
TS208	falcon2	1.33	0.64	0.69	$TS208_v1_1$	$TS208_v2_5$
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

	Supplementary	Table 55: Results	3 101 1 1 2 2 0 0	DI ID I WO-	Diate Dedic	
$\operatorname{Group}$	Group_Name	$Two\text{-}State\_Score$	$V1\_GDT\_TS$	$V2\_GDT\_TS$	$V1\_Model$	$V2\_Model$
TS462	Zheng	1.15	0.63	0.52	TS462_v1_3	TS462_v2_5
TS147	Zheng-Multimer	1.15	0.62	0.53	TS147_v1_1	TS147_v2_1
TS264	GuijunLab-Human	1.15	0.56	0.59	TS264_v1_6	TS264_v2_1
TS481	Vfold	1.15	0.62	0.53	TS481_v1_3	TS481_v2_5
TS022	Yang	1.14	0.57	0.57	TS022_v1_4	TS022_v2_5
TS148	Guijunlab-Complex	1.13	0.54	0.59	TS148_v2_3	TS148_v1_4
TS450	OpenComplex_Server	1.13	0.57	0.56	$TS450_v1_1$	$TS450_v2_4$
TS167	OpenComplex	1.13	0.57	0.56	TS167_v1_1	TS167_v2_4
TS052	Yang-Server	1.13	0.59	0.53	TS052_v1_4	TS052_v2_2
TS456	Yang-Multimer	1.11	0.58	0.53	TS456_v1_3	TS456_v2_2
TS241	elofsson	1.11	0.59	0.52	$TS241_v2_1$	$TS241_v1_2$
TS091	Huang-HUST	1.09	0.55	0.54	TS091_v1_2	$TS091_v2_4$
TS204	Zou	1.09	0.62	0.47	$TS204_v1_1$	$TS204_v2_3$
TS262	CoDock	1.09	0.56	0.53	$TS262\_v1\_2$	$TS262_v2_4$
TS375	milliseconds	1.08	0.59	0.49	$TS375_v2_4$	$TS375_v1_5$
TS033	Diff	1.08	0.57	0.51	$TS033_v2_1$	$TS033_v1_4$
TS301	GHZ-MAN	1.08	0.56	0.52	TS301_v1_3	$TS301_v2_4$
TS294	KiharaLab	1.07	0.60	0.48	$TS294_v2_5$	$TS294_v1_4$
TS110	MIEnsembles-Server	1.07	0.52	0.55	$TS110_v1_2$	$TS110_v2_4$
TS028	NKRNA-s	1.07	0.51	0.56	$TS028_v1_2$	$TS028_v2_5$
TS212	PIEFold_human	1.07	0.55	0.52	$TS212\_v2\_4$	$TS212\_v1\_2$
TS345	MULTICOM_human	1.06	0.57	0.49	$TS345_v1_3$	$TS345\_v2\_5$
TS051	MULTICOM	1.06	0.57	0.49	$TS051\_v1\_3$	$TS051\_v2\_5$
TS304	AF3-server	1.05	0.58	0.48	$TS304_v1_4$	$TS304_v2_4$
TS221	CSSB_FAKER	1.04	0.56	0.48	$TS221_v2_2$	$TS221_v1_2$
TS419	CSSB-Human	1.04	0.56	0.48	$TS419_v2_4$	$TS419_v1_2$
TS319	MULTICOM_LLM	1.04	0.57	0.47	$TS319_v1_2$	$TS319_v2_2$
TS331	MULTICOM_AI	1.04	0.57	0.47	$TS331_v1_2$	$TS331_v2_2$
TS274	kozakovvajda	1.04	0.56	0.47	$TS274\_v1\_2$	$TS274_v2_2$
TS494	ClusPro	1.04	0.56	0.47	TS494_v1_2	TS494_v2_2
TS314	GuijunLab-PAthreader		0.49	0.55	TS314_v2_3	TS314_v1_1
TS425	MULTICOM_GATE	1.03	0.56	0.47	TS425_v1_1	TS425_v2_4
TS286	CSSB_experimental	1.03	0.56	0.47	TS286_v1_5	TS286_v2_2
TS231	B-LAB	1.03	0.56	0.46	TS231_v2_4	TS231_v1_2
TS019	Zheng-Server	1.02	0.52	0.51	TS019_v1_4	TS019_v2_1
TS014	Cool-PSP	1.02	0.59	0.44	TS014_v2_6	TS014_v1_5
TS369	Bhattacharya	1.02	0.55	0.47	TS369_v1_2	TS369_v2_1
TS198	colabfold	1.01	0.56	0.45	TS198_v2_2	TS198_v1_2
TS267	kiharalab_server	1.01	0.55	0.46	TS267_v1_1	TS267_v2_4
TS208	falcon2	1.01 1.01	0.55	0.46	TS208_v2_5	TS208_v1_1
TS475 $TS079$	ptq MDAEold	1.01	0.58	$0.42 \\ 0.46$	TS475_v2_5	TS475_v1_1
TS293	MRAFold MRAH	1.01	$0.55 \\ 0.55$	0.46	TS079_v1_2 TS293_v1_2	TS079_v2_2 TS293_v2_2
TS489	Fernandez-Recio	1.00	0.55	0.45	TS489_v1_2	TS489_v2_2
TS465	Wallner	0.99	0.50	0.49	TS465_v1_5	TS465_v2_1
TS287	plmfold	0.99	0.54	0.45	TS287_v1_2	TS287_v2_3
TS159	406	0.98	0.49	0.48	TS159_v1_1	TS159_v2_1
TS325	405	0.98	0.49	0.48	TS325_v1_1	TS325_v2_1
TS312	GuijunLab-Assembly	0.97	0.54	0.44	TS312_v1_4	TS312_v2_2
TS075	GHZ-ISM	0.97	0.43	0.55	TS075_v2_4	TS075_v1_1
TS122	MQA_server	0.97	0.43	0.55	TS122_v2_4	TS122_v1_1
TS284	Unicorn	0.97	0.43	0.55	TS284_v2_4	TS284_v1_1
TS196	HYU_MLLAB	0.97	0.53	0.44	TS196_v1_5	TS196_v2_5
TS145	colabfold_baseline	0.96	0.54	0.42	TS145_v1_3	TS145_v2_3
TS112	Seder2024easy	0.96	0.54	0.42	TS112_v1_4	TS112_v2_3
TS017	Seder2024hard	0.96	0.54	0.42	TS017_v1_5	TS017_v2_5
TS311	RAGfold_Prot1	0.95	0.50	0.46	TS311_v1_2	TS311_v2_1
TS015	PEZYFoldings	0.95	0.51	0.44	$TS015_v2_2$	TS015_v1_5
TS298	ShanghaiTech-human	0.95	0.54	0.41	TS298_v1_3	$TS298_v2_3$
TS163	MultiFOLD2	0.95	0.53	0.42	$TS163\_v1\_5$	$TS163\_v2\_2$
TS235	isyslab-hust	0.94	0.51	0.43	$TS235_v1_1$	$TS235\_v2\_3$
TS164	McGuffin	0.94	0.48	0.46	$TS164_v1_1$	$TS164_v2_3$
TS269	CSSB_server	0.93	0.51	0.42	$TS269_v1_1$	$TS269_v2_1$
TS059	DeepFold	0.90	0.47	0.43	$TS059\_v2\_3$	$TS059\_v1\_3$
TS388	DeepFold-server	0.88	0.45	0.44	$TS388\_v2\_3$	$TS388_v1_3$
TS023	FTBiot0119	0.86	0.46	0.40	$TS023_v1_3$	$TS023\_v2\_4$
TS139	DeepFold-refine	0.79	0.41	0.38	$TS139_v1_4$	$TS139_v2_3$
TS120	Cerebra	0.74	0.38	0.36	$TS120_v1_4$	$TS120_v2_1$
TS361	Cerebra_server	0.65	0.33	0.32	$TS361\_v2\_2$	$TS361_v1_2$

Supplementary Table S4: Results for M1239 TMscore Two-State Score

Group	Group_Name	$Two\text{-}State\_Score$	V1_TMscore	$V2\_TMscore$	V1_Model	V2_Model
TS294	KiharaLab	1.45	0.81	0.64	TS294_v1_1	TS294_v2_3
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	1.34	0.67	0.67	$TS235\_v1\_5$	$TS235_v2_4$
TS481	Vfold	1.32	0.67	0.65	TS481_v1_5	$TS481_{v}2_{5}$
TS462	Zheng	1.30	0.67	0.64	$TS462_v1_4$	$TS462_v2_2$
TS110	MIEnsembles-Server	1.28	0.67	0.61	TS110_v1_1	$TS110_v2_5$
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	$TS286_v1_2$	$TS286_v2_2$
TS231	B-LAB	1.25	0.64	0.60	$TS231_v1_2$	$TS231_v2_1$
TS489	Fernandez-Recio	1.25	0.63	0.61	TS489_v1_3	$TS489_v2_4$
TS033	Diff	1.23	0.60	0.62	$TS033_v1_2$	$TS033_v2_2$
TS091	Huang-HUST	1.23	0.64	0.59	$TS091_v1_2$	$TS091_v2_5$
TS450	OpenComplex_Server	1.19	0.62	0.57	$TS450_v1_1$	$TS450_{-}v2_{-}5$
TS167	OpenComplex	1.19	0.62	0.57	$TS167_v1_1$	$TS167_v2_5$
TS014	Cool-PSP	1.06	0.52	0.54	$TS014_v1_5$	$TS014_v2_4$
TS272	GromihaLab	0.76	0.36	0.41	$TS272_v1_1$	$TS272_v2_1$
TS241	elofsson	0.69	0.35	0.34	$TS241_v1_4$	$TS241_v2_1$
TS304	AF3-server	0.66	0.33	0.33	$TS304\_v1\_1$	$TS304\_v2\_4$

Supplementary Table S5: Results for T1239 GDT TS Two-State Score

	Supplementary	Table 55. Results	101 11200 G	DIIDIWO	Diate Deore	
Group	$Group\_Name$	Two-State_Score	$V1\_GDT\_TS$	$V2\_GDT\_TS$	V1_Model	$V2\_Model$
TIC460	71	1.00	0.71	0.40	TIC 4600 0	TIC 4601 1
TS462	Zheng	1.20	0.71	0.49	TS462_v2_2	TS462_v1_1
TS235	isyslab-hust	1.14	0.71	0.43	TS235_v2_4	TS235_v1_1
TS221	CSSB_FAKER	1.14	0.71	0.43	TS221_v2_1	TS221_v1_5
TS419	CSSB-Human	1.14	0.71	0.43	$TS419_v2_1$	TS419_v1_5
TS028	NKRNA-s	1.13	0.71	0.42	$TS028_v2_2$	$TS028\_v1\_2$
TS345	MULTICOM_human	1.13	0.71	0.42	$TS345_v1_4$	$TS345_v2_5$
TS051	MULTICOM	1.13	0.71	0.42	$TS051_v1_4$	$TS051_v2_5$
TS286	CSSB_experimental	1.13	0.70	0.43	$TS286_v2_1$	TS286_v1_2
TS208	falcon2	1.09	0.67	0.42	TS208_v1_4	TS208_v2_4
TS425	MULTICOM_GATE	1.08	0.63	0.44	TS425_v1_2	TS425_v2_4
TS019	Zheng-Server	1.06	0.54	0.52	TS019_v1_5	TS019_v2_5
TS022						
	Yang	1.05	0.61	0.44	TS022_v1_5	TS022_v2_4
TS204	Zou	1.05	0.61	0.44	TS204_v1_5	TS204_v2_2
TS110	MIEnsembles-Server	1.05	0.63	0.42	TS110_v1_1	TS110_v2_2
TS456	Yang-Multimer	1.04	0.60	0.44	TS456_v1_3	TS456_v2_2
TS147	Zheng-Multimer	1.03	0.56	0.47	$TS147_{v1_3}$	$TS147_v2_5$
TS450	OpenComplex_Server	1.03	0.54	0.49	$TS450_v1_5$	$TS450_v2_3$
TS167	OpenComplex	1.03	0.54	0.49	$TS167_v1_5$	TS167_v2_3
TS294	KiharaLab	1.02	0.60	0.42	$TS294_v1_1$	$TS294_v2_2$
TS314	GuijunLab-PAthreader	1.02	0.59	0.43	$TS314_v2_5$	$TS314_v1_2$
TS052	Yang-Server	1.00	0.56	0.44	TS052_v1_5	TS052_v2_2
TS481	Vfold	1.00	0.57	0.43	TS481_v2_5	TS481_v1_2
TS091	Huang-HUST	0.99	$0.57 \\ 0.52$	0.43	TS091_v1_5	TS091_v2_3
TS319	MULTICOM_LLM	0.99	0.56	0.43	TS319_v1_2	TS319_v2_5
TS262	CoDock	0.98	0.58	0.41	TS262_v1_2	TS262_v2_5
TS033	Diff	0.98	0.54	0.44	TS033_v2_2	TS033_v1_1
TS331	MULTICOM_AI	0.98	0.56	0.42	$TS331_v1_2$	$TS331_v2_2$
TS325	405	0.97	0.55	0.42	$TS325_v1_2$	$TS325_v2_2$
TS159	406	0.97	0.55	0.42	$TS159_v1_2$	$TS159_v2_2$
TS369	Bhattacharya	0.97	0.54	0.43	$TS369_v1_4$	$TS369_v2_4$
TS489	Fernandez-Recio	0.97	0.55	0.42	TS489_v1_3	$TS489_v2_4$
TS298	ShanghaiTech-human	0.96	0.62	0.34	$TS298_v1_1$	$TS298_v2_1$
TS212	PIEFold_human	0.96	0.55	0.41	TS212_v2_1	TS212_v1_3
TS241	elofsson	0.95	0.54	0.41	TS241_v1_1	TS241_v2_5
TS231	B-LAB	0.94	0.54	0.40	TS231_v2_1	TS231_v1_2
TS304	AF3-server	0.94	0.51	0.43	TS304_v2_5	TS304_v1_2
TS465	Wallner	0.93	0.48	0.45	TS465_v1_4	TS465_v2_2
TS358	PerezLab_Gators	0.93	0.55	0.38	TS358_v2_2	TS358_v1_4
TS079	MRAFold	0.92	0.50	0.42	$TS079_v1_2$	$TS079_v2_3$
TS293	MRAH	0.92	0.50	0.42	$TS293_v1_2$	TS293_v2_3
TS272	GromihaLab	0.91	0.50	0.41	$TS272_v1_3$	$TS272_v2_4$
TS423	ShanghaiTech-server	0.91	0.52	0.39	$TS423_v2_4$	TS423_v1_1
TS267	kiharalab_server	0.89	0.50	0.39	$TS267_v1_1$	$TS267_v2_4$
TS148	Guijunlab-Complex	0.89	0.49	0.40	$TS148_v2_5$	TS148_v1_4
TS287	plmfold	0.88	0.49	0.39	TS287_v1_3	$TS287_v2_4$
TS198	colabfold	0.88	0.50	0.38	TS198_v1_2	TS198_v2_1
TS375	milliseconds	0.88	0.47	0.41	TS375_v2_3	TS375_v1_4
	Seder2024easy					
TS112		0.87	0.48	0.39	TS112_v1_4	TS112_v2_5
TS014	Cool-PSP	0.87	0.49	0.37	TS014_v2_3	TS014_v1_3
TS301	GHZ-MAN	0.87	0.47	0.40	TS301_v2_4	TS301_v1_1
TS163	MultiFOLD2	0.87	0.48	0.38	TS163_v1_3	TS163_v2_3
TS040	DELCLAB	0.86	0.48	0.38	$TS040_v1_3$	$TS040_v2_3$
TS023	FTBiot0119	0.86	0.48	0.39	$TS023\_v1\_2$	$TS023_v2_1$
TS145	$colabfold\_baseline$	0.86	0.48	0.39	$TS145_v1_2$	$TS145_v2_1$
TS264	GuijunLab-Human	0.86	0.48	0.39	$TS264_v2_2$	$TS264_v1_5$
TS312	GuijunLab-Assembly	0.86	0.46	0.40	TS312_v2_4	TS312_v1_4
TS122	MQA_server	0.86	0.47	0.39	TS122_v1_3	TS122_v2_2
TS059	DeepFold	0.85	0.46	0.39	TS059_v1_6	TS059_v2_6
TS139	DeepFold-refine		0.46	0.39	TS139_v1_6	TS139_v2_6
		0.85				
TS017	Seder2024hard	0.85	0.48	0.36	TS017_v1_5	TS017_v2_4
TS397	smg_ulaval	0.84	0.45	0.39	TS397_v1_1	TS397_v2_1
TS164	McGuffin	0.84	0.45	0.38	TS164_v2_2	TS164_v1_3
TS015	PEZYFoldings	0.84	0.45	0.39	$TS015_v1_4$	TS015_v2_1
TS196	$HYU\_MLLAB$	0.78	0.39	0.39	$TS196_v1_2$	$TS196_v2_2$
TS388	DeepFold-server	0.76	0.38	0.38	TS388_v1_3	$TS388_v2_2$
TS120	Cerebra	0.61	0.31	0.30	$TS120_v1_3$	$TS120_v2_2$
TS475	ptq	0.49	0.49	0.00	TS475_v2_1	$N/A^1$
TS351	digiwiser-ensemble	0.49	0.24	0.24	TS351_v1_1	TS351_v2_1
			0.24			N/A <sup>1</sup>
TS269	_	0.40		0.00	$TS269_v2_4$	1N / A.
	CSSB_server	0.48				27/41
TS075	CSSB_server GHZ-ISM	0.47	0.47	0.00	$TS075\_v2\_4$	$N/A^1$
TS075 $TS284$	CSSB_server					$N/A^1$ $N/A^1$
	CSSB_server GHZ-ISM	0.47	0.47	0.00	$TS075\_v2\_4$	$N/A^1$ $N/A^1$ $N/A^1$
TS284 TS311	CSSB_server GHZ-ISM Unicorn RAGfold_Prot1	$0.47 \\ 0.47 \\ 0.42$	$0.47 \\ 0.47 \\ 0.42$	0.00 0.00 0.00	TS075_v2_4 TS284_v2_4 TS311_v1_1	$N/A^1$ $N/A^1$ $N/A^1$
TS284	CSSB_server GHZ-ISM Unicorn	$0.47 \\ 0.47$	$0.47 \\ 0.47$	0.00 0.00	$TS075_{-}v2_{-}4$ $TS284_{-}v2_{-}4$	$N/A^1$ $N/A^1$

 $<sup>^{1}</sup>$  Model either not submitted or not assessed

Supplementary Table S6: Results for T1249 AvgDockQ Two-State Score

	Supplementary	Table So: Resul	ts 101 11249 A	rgDockQ Iwo	<i>y</i> -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	PEZYFoldings	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_50
TS079	MRAFold Cool-PSP	0.78	$0.62 \\ 0.65$	$0.16 \\ 0.12$	TS079_v1_2o TS014_v1_1o	TS079_v2_50 TS014_v2_10
TS014 TS322	XGroup	0.77 0.76	0.49	0.12	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 TS301	MULTICOM_LLM GHZ-MAN	$0.64 \\ 0.64$	$0.46 \\ 0.50$	$0.18 \\ 0.14$	TS319_v2_3o TS301_v1_4o	TS319_v1_4o
TS267	kiharalab_server	0.64	0.48	0.14	TS267_v1_2o	TS301_v2_1o 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
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 MassiveFold	0.59	0.57	0.02	TS284_v2_1o	TS284_v1_2o
TS031 TS163	MultiFOLD2	0.56 0.55	$0.42 \\ 0.36$	$0.14 \\ 0.19$	TS031_v2_4o TS163_v1_3o	TS031_v1_5o TS163_v2_5o
TS494	ClusPro	0.55	0.35	0.19	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_50
TS196	HYU_MLLAB	0.07	0.01	0.05	TS196_v1_3o	TS196_v2_50
TS114 TS337	COAST APOLLO	0.04 0.03	$0.02 \\ 0.02$	$0.01 \\ 0.02$	TS114_v1_5o TS337_v1_1o	TS114_v2_1o TS337_v2_4o
TS139	DeepFold-refine	0.03	0.02	0.02	TS139_v1_4o	TS139_v2_3o
TS300	ARC	0.03	0.01	0.02	TS300_v1_2o	TS300_v2_2o
TS085	Bates	0.03	0.01	0.01	TS085_v1_5o	TS085_v2_4o
TS023	FTBiot0119	0.03	0.01	0.01	TS023_v1_3o	TS023_v2_1o
		0.02	0.01	0.01		

 $<sup>^{1}</sup>$  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
TS159	406	78.65	31.27	47.39	TS159_v1_2	TS159_v2_1
TS272	GromihaLab	67.74	31.85	35.89	TS272_v1_4	$TS272_v2_1$
TS231	B-LAB	66.14	9.84	56.30	TS231_v1_2	TS231_v2_5
TS235	isyslab-hust	64.72	30.77	33.95	TS235_v1_2	$TS235_v2_5$
TS369	Bhattacharya	64.58	32.05	32.53	TS369_v1_5	TS369_v2_3
TS304	AF3-server	64.20	31.63	32.57	TS304_v1_1	$TS304_v2_2$
TS241	elofsson	64.20	31.63	32.57	TS241_v1_1	$TS241_v2_2$
TS006	RNA_Dojo	64.02	31.40	32.61	TS006_v1_3	$TS006_v2_1$
TS238	BRIQX	43.98	33.27	10.71	TS238_v1_5	TS238_v2_3
TS294	KiharaLab	42.91	31.63	11.28	TS294_v1_1	TS294_v2_2
TS435	RNAFOLDX	42.09	31.51	10.57	TS435_v1_5	TS435_v2_3
TS167	OpenComplex	40.87	8.25	32.61	TS167_v1_3	$TS167_v2_2$
TS400	OmniFold	32.89	0.00	32.89	$N/A^1$	$TS400_v2_1$
TS276	FrederickFolding	31.82	0.00	31.82	$N/A^1$	TS276_v2_1
TS286	CSSB_experimental	24.40	11.11	13.29	TS286_v1_3	TS286_v2_2
TS165	dfr	22.76	11.07	11.69	TS165_v1_3	$TS165_v2_1$
TS063	RNApolis	21.91	11.00	10.91	TS063_v1_3	$TS063_v2_1$
TS481	Vfold	21.86	10.40	11.47	TS481_v1_5	$TS481_v2_4$
TS189	LCBio	21.83	9.95	11.88	TS189_v1_3	$TS189_v2_1$
TS338	GeneSilico	21.79	11.53	10.26	TS338_v1_5	$TS338_v2_1$
TS156	SoutheRNA	21.63	8.91	12.72	TS156_v1_5	$TS156_v2_1$
TS183	GuangzhouRNA-human	21.33	10.19	11.14	TS183_v1_5	TS183_v2_2
TS317	GuangzhouRNA_AI	21.17	9.62	11.55	TS317_v1_5	$TS317_v2_4$
TS456	Yang-Multimer	20.86	10.04	10.82	TS456_v1_1	$TS456_v2_4$
TS417	GuangzhouRNA-meta	20.81	9.98	10.83	TS417_v1_2	$TS417_v2_5$
TS052	Yang-Server	19.66	10.16	9.49	$TS052_v1_1$	$TS052_v2_5$
TS267	kiharalab_server	18.53	9.29	9.23	TS267_v1_4	$TS267_v2_5$
TS261	UNRES	18.48	7.55	10.93	$TS261_v1_1$	$TS261_v2_3$
TS028	NKRNA-s	17.52	9.63	7.89	TS028_v1_3	$TS028_v2_1$
TS358	PerezLab_Gators	17.35	8.09	9.26	TS358_v1_4	$TS358_v2_1$
TS448	dNAfold	17.33	9.24	8.08	TS448_v1_5	$TS448_v2_1$
TS450	OpenComplex_Server	16.77	8.27	8.50	$TS450_v1_1$	$TS450_v2_2$
TS110	MIEnsembles-Server	16.58	7.88	8.70	TS110_v1_3	TS110_v2_1
TS462	Zheng	16.12	7.92	8.21	TS462_v1_3	$TS462_v2_5$
TS169	thermomaps	15.26	7.03	8.23	TS169_v1_3	$TS169_v2_4$
TS367	AIR	7.78	0.00	7.78	$N/A^1$	$TS367_v2_1$
TS403	mmagnus	3.65	3.65	0.00	TS403_v1_1	$N/A^1$
TS298	Shanghai Tech-human	3.64	3.64	0.00	TS298_v1_1	$N/A^1$
TS423	ShanghaiTech-server	3.64	3.64	0.00	TS423_v1_1	$N/A^1$
TS094	SimRNA-Server	3.43	2.35	1.07	TS094_v1_5	TS094_v2_3
TS208	falcon2	3.13	3.13	0.00	TS208_v1_1	$N/A^1$
TS306	GeneSilicoRNA-server	0.02	0.02	0.00	TS306_v1_1	N/A <sup>1</sup>
TS033	Diff	0.00	0.00	0.00	TS033_v1_1	TS033_v2_4

 $<sup>^{1}</sup>$  Model either not submitted or not assessed