

# CASP16\_DUAL-STATE\_TABLES

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Supplementary Table S1: Results for T1214 Composite Score 1  
dual state

Group	Group_Name	Dual-State_Score	V1_Composite_Score_1	V2_Composite_Score_1	V1_Model
TS204	Zou	161.89	66.94	94.95	TS204.v1.5
TS494	ClusPro	161.70	62.98	98.72	TS494.v1.1
TS274	kozakovvajda	161.70	62.98	98.72	TS274.v1.1
TS059	DeepFold	161.64	67.39	94.25	TS059.v1.6
TS462	Zheng	161.18	86.42	74.76	TS462.v1.6
TS298	ShanghaiTech-human	160.54	89.37	71.17	TS298.v1.4
TS386	ShanghaiTech-Ligand	160.54	89.37	71.17	TS386.v1.4
TS110	MIEnsembles-Server	160.33	84.08	76.25	TS110.v1.2
TS022	Yang	160.13	86.26	73.87	TS022.v1.4
TS040	DELCLAB	160.07	62.72	97.35	TS040.v1.3
TS208	falcon2	159.46	87.66	71.80	TS208.v1.4
TS017	Seder2024hard	159.45	77.75	81.70	TS017.v1.3
TS145	colabfold_baseline	159.45	77.75	81.70	TS145.v1.5
TS419	CSSB-Human	159.37	68.55	90.82	TS419.v1.3
TS221	CSSB-FAKER	159.37	68.55	90.82	TS221.v1.3
TS269	CSSB_server	159.37	68.49	90.88	TS269.v1.3
TS456	Yang-Multimer	159.36	68.48	90.87	TS456.v1.5
TS015	PEZYZFoldings	159.31	91.17	68.14	TS015.v1.5
TS052	Yang-Server	159.24	69.05	90.19	TS052.v1.1
TS286	CSSB_experimental	158.65	65.85	92.80	TS286.v1.2
TS019	Zheng-Server	158.57	79.81	78.76	TS019.v1.1
TS147	Zheng-Multimer	158.47	81.50	76.96	TS147.v1.1
TS262	CoDock	158.46	66.81	91.65	TS262.v1.3
TS314	GuijunLab-Pathreader	158.27	81.13	77.14	TS314.v1.1
TS312	GuijunLab-Assembly	158.27	81.13	77.14	TS312.v1.1
TS393	GuijunLab-QA	158.27	81.13	77.14	TS393.v1.1
TS264	GuijunLab-Human	158.27	81.13	77.14	TS264.v1.1
TS148	Guijunlab-Complex	158.27	81.13	77.14	TS148.v1.5
TS388	DeepFold-server	157.76	82.69	75.08	TS388.v1.4
TS102	Psi-Phi	157.73	81.34	76.39	TS102.v1.1
TS196	HYU_MLLAB	157.72	79.57	78.15	TS196.v1.4
TS311	RAGfold_Prot1	157.66	80.54	77.12	TS311.v1.4
TS235	isyslab-hust	157.57	78.25	79.33	TS235.v1.3
TS167	OpenComplex	157.47	79.46	78.01	TS167.v1.2

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Group	Group_Name	Dual-State_Score	V1_Composite_Score_1	V2_Composite_Score_1	V1_Model
TS450	OpenComplex_Server	157.47	79.46	78.01	TS450_v1_5
TS304	AF3-server	157.37	79.33	78.04	TS304_v1_2
TS241	elofsson	157.37	79.33	78.04	TS241_v1_2
TS464	PocketTracer	157.36	77.38	79.99	TS464_v1_2
TS272	GromihaLab	157.32	77.66	79.66	TS272_v1_3
TS287	plmfold	157.29	81.25	76.04	TS287_v1_1
TS345	MULTICOM_human	157.23	79.25	77.98	TS345_v1_4
TS319	MULTICOM_LLM	157.16	81.15	76.01	TS319_v1_3
TS425	MULTICOM_GATE	157.16	81.15	76.01	TS425_v1_2
TS207	MULTICOM_ligand	157.14	80.33	76.81	TS207_v1_1
TS091	Huang-HUST	157.13	81.57	75.56	TS091_v1_2
TS225	Unknown	157.09	79.86	77.24	TS225_v1_1
TS163	MultiFOLD2	157.09	79.86	77.24	TS163_v1_1
TS164	McGuffin	157.09	79.86	77.24	TS164_v1_1
TS375	milliseconds	157.09	81.32	75.78	TS375_v1_3
TS198	colabfold	156.98	77.92	79.05	TS198_v1_3
TS227	KUMC	156.81	80.86	75.95	TS227_v1_3
TS369	Bhattacharya	156.81	78.81	78.00	TS369_v1_1
TS301	GHZ-MAN	156.72	78.96	77.77	TS301_v1_2
TS267	kiharalab_server	156.72	79.28	77.43	TS267_v1_2
TS293	MRAH	156.69	79.37	77.33	TS293_v1_2
TS079	MRAFold	156.69	79.37	77.33	TS079_v1_1
TS423	ShanghaiTech-server	156.59	81.84	74.76	TS423_v1_1
TS400	OmniFold	156.58	77.54	79.03	TS400_v1_1
TS051	MULTICOM	156.09	78.67	77.42	TS051_v1_1
TS331	MULTICOM_AI	156.09	78.67	77.42	TS331_v1_1
TS014	Cool-PSP	155.27	80.10	75.17	TS014_v1_5
TS465	Wallner	155.20	85.35	69.84	TS465_v1_3
TS475	ptq	155.16	79.41	75.75	TS475_v1_3
TS122	MQA_server	155.00	78.55	76.45	TS122_v1_2
TS284	Unicorn	154.89	78.73	76.15	TS284_v1_2
TS075	GHZ-ISM	154.89	78.73	76.15	TS075_v1_2
TS408	SNU-CHEM-lig	154.02	85.96	68.06	TS408_v1_1
TS055	LCDD-team	153.87	85.68	68.19	TS055_v1_4
TS039	arosko	149.28	65.44	83.85	TS039_v1_3
TS202	test001	148.85	83.44	65.40	TS202_v1_5
TS020	comppharmunibas	148.53	81.19	67.34	TS020_v1_4
TS294	KiharaLab	145.51	80.80	64.72	TS294_v1_3
TS120	Cerebra	144.44	71.99	72.45	TS120_v1_6
TS139	DeepFold-refine	143.55	72.37	71.18	TS139_v1_3
TS461	forlilab	136.22	66.23	69.99	TS461_v1_2
TS275	Seminoles	135.14	69.53	65.61	TS275_v1_1
TS361	Cerebra_server	131.75	62.26	69.48	TS361_v1_1

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Group	Group_Name	Dual-State_Score	V1_Composite_Score_1	V2_Composite_Score_1	V1_Model
TS132	profold2	64.11	30.97	33.13	TS132_v1_1

Supplementary Table S2: Results for T1214 Composite Score 2  
dual state

Group	Group_Name	Dual-State_Score	V1_Composite_Score_2	V2_Composite_Score_2	V1_Model
TS494	ClusPro	156.48	57.81	98.67	TS494.v1.1
TS274	kozakovvajda	156.48	57.81	98.67	TS274.v1.1
TS059	DeepFold	156.26	62.49	93.77	TS059.v1.6
TS462	Zheng	155.68	84.51	71.17	TS462.v1.6
TS386	ShanghaiTech-Ligand	155.14	88.04	67.10	TS386.v1.4
TS298	ShanghaiTech-human	155.14	88.04	67.10	TS298.v1.4
TS204	Zou	155.13	62.01	93.12	TS204.v1.1
TS040	DELCLAB	155.08	58.05	97.03	TS040.v1.5
TS110	MIEnsembles-Server	154.39	81.68	72.71	TS110.v1.2
TS022	Yang	154.27	84.28	69.99	TS022.v1.4
TS015	PEZYZFoldings	154.11	90.16	63.95	TS015.v1.5
TS208	falcon2	153.77	86.01	67.76	TS208.v1.4
TS456	Yang-Multimer	153.48	63.66	89.82	TS456.v1.5
TS269	CSSB_server	153.44	63.66	89.78	TS269.v1.3
TS221	CSSB_FAKER	153.43	63.71	89.72	TS221.v1.3
TS419	CSSB-Human	153.43	63.71	89.72	TS419.v1.3
TS052	Yang-Server	153.22	64.23	88.98	TS052.v1.1
TS145	colabfold_baseline	153.13	74.24	78.89	TS145.v1.5
TS017	Seder2024hard	153.13	74.24	78.89	TS017.v1.3
TS286	CSSB_experimental	152.85	60.78	92.07	TS286.v1.2
TS262	CoDock	152.70	61.92	90.79	TS262.v1.3
TS147	Zheng-Multimer	152.08	78.66	73.43	TS147.v1.1
TS019	Zheng-Server	152.06	76.56	75.50	TS019.v1.1
TS314	GuijunLab-Pathreader	151.80	78.13	73.67	TS314.v1.1
TS312	GuijunLab-Assembly	151.80	78.13	73.67	TS312.v1.1
TS148	Guijunlab-Complex	151.80	78.13	73.67	TS148.v1.5
TS393	GuijunLab-QA	151.80	78.13	73.67	TS393.v1.1
TS264	GuijunLab-Human	151.80	78.13	73.67	TS264.v1.1
TS388	DeepFold-server	151.20	79.88	71.32	TS388.v1.4
TS102	Psi-Phi	151.17	78.38	72.79	TS102.v1.1
TS196	HYU_MLLAB	151.08	76.32	74.75	TS196.v1.4
TS311	RAGfold_Prot1	151.00	77.44	73.57	TS311.v1.4
TS235	isyslab-hust	150.79	74.66	76.13	TS235.v1.3
TS241	elofsson	150.75	76.05	74.69	TS241.v1.2
TS304	AF3-server	150.75	76.05	74.69	TS304.v1.2
TS167	OpenComplex	150.74	76.09	74.65	TS167.v1.2
TS450	OpenComplex_Server	150.74	76.09	74.65	TS450.v1.5
TS287	plmfold	150.69	78.28	72.41	TS287.v1.1
TS464	PocketTracer	150.64	73.69	76.96	TS464.v1.5
TS272	GromihaLab	150.59	74.03	76.56	TS272.v1.1
TS091	Huang-HUST	150.47	78.62	71.85	TS091.v1.2

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Group	Group_Name	Dual-State_Score	V1_Composite_Score.2	V2_Composite_Score.2	V1_Model
TS122	MQA_server	150.47	75.03	75.44	TS122_v1.4
TS207	MULTICOM_ligand	150.44	77.17	73.26	TS207_v1.2
TS319	MULTICOM_LLM	150.43	78.02	72.41	TS319_v1.3
TS425	MULTICOM_GATE	150.43	78.02	72.41	TS425_v1.2
TS163	MultiFOLD2	150.43	76.67	73.76	TS163_v1.1
TS164	McGuffin	150.43	76.67	73.76	TS164_v1.1
TS225	Unknown	150.43	76.67	73.76	TS225_v1.1
TS375	milliseconds	150.42	78.31	72.11	TS375_v1.3
TS345	MULTICOM_human	150.40	75.84	74.56	TS345_v1.4
TS198	colabfold	150.18	74.33	75.84	TS198_v1.3
TS227	KUMC	150.14	77.81	72.33	TS227_v1.3
TS369	Bhattacharya	150.00	75.37	74.63	TS369_v1.1
TS301	GHZ-MAN	149.95	75.56	74.39	TS301_v1.2
TS267	kiharalab_server	149.88	75.92	73.95	TS267_v1.2
TS079	MRAFold	149.79	76.00	73.79	TS079_v1.1
TS293	MRAH	149.79	76.00	73.79	TS293_v1.2
TS423	ShanghaiTech-server	149.78	78.89	70.89	TS423_v1.1
TS400	OmniFold	149.71	73.89	75.82	TS400_v1.1
TS331	MULTICOM_AI	149.16	75.09	74.07	TS331_v1.1
TS051	MULTICOM	149.16	75.09	74.07	TS051_v1.1
TS465	Wallner	148.76	83.15	65.61	TS465_v1.3
TS014	Cool-PSP	148.41	76.85	71.55	TS014_v1.5
TS284	Unicorn	147.97	75.26	72.71	TS284_v1.2
TS075	GHZ-ISM	147.97	75.26	72.71	TS075_v1.2
TS475	ptq	147.93	76.01	71.92	TS475_v1.3
TS408	SNU-CHEM-lig	147.87	83.92	63.95	TS408_v1.1
TS055	LCDD-team	147.69	83.59	64.11	TS055_v1.5
TS202	test001	142.40	81.16	61.24	TS202_v1.5
TS020	comp pharmunibas	141.97	78.81	63.17	TS020_v1.4
TS039	arosko	141.24	60.25	80.99	TS039_v1.3
TS294	KiharaLab	138.27	78.29	59.98	TS294_v1.3
TS120	Cerebra	137.37	68.49	68.88	TS120_v1.6
TS139	DeepFold-refine	135.49	68.36	67.13	TS139_v1.3
TS461	forlilab	127.61	61.64	65.97	TS461_v1.2
TS275	Seminoles	126.47	65.38	61.08	TS275_v1.1
TS361	Cerebra_server	124.46	58.04	66.42	TS361_v1.1
TS132	profold2	78.01	37.74	40.27	TS132_v1.1

Supplementary Table S3: Results for T1214 Composite Score 3  
dual state

Group	Group_Name	Dual-State_Score	V1_Composite_Score_3	V2_Composite_Score_3	V1_Model
TS298	ShanghaiTech-human	172.93	94.08	78.85	TS298_v1.4
TS386	ShanghaiTech-Ligand	172.93	94.08	78.85	TS386_v1.4
TS204	Zou	172.75	75.40	97.35	TS204_v1.5
TS139	DeepFold-refine	172.73	75.62	97.11	TS139_v1.6
TS059	DeepFold	172.73	75.62	97.11	TS059_v1.6
TS462	Zheng	172.32	92.29	80.03	TS462_v1.6
TS015	PEZYZFoldings	172.26	95.40	76.86	TS015_v1.5
TS208	falcon2	172.17	92.81	79.36	TS208_v1.4
TS110	MIEnsembles-Server	171.90	89.48	82.42	TS110_v1.2
TS022	Yang	171.70	91.33	80.38	TS022_v1.4
TS269	CSSB_server	171.47	76.64	94.83	TS269_v1.3
TS221	CSSB_FAKER	171.42	76.63	94.78	TS221_v1.3
TS419	CSSB-Human	171.42	76.63	94.78	TS419_v1.3
TS456	Yang-Multimer	171.13	75.87	95.26	TS456_v1.1
TS052	Yang-Server	170.99	76.28	94.71	TS052_v1.1
TS020	comp pharmunibas	170.93	76.56	94.36	TS020_v1.3
TS262	CoDock	170.61	74.54	96.08	TS262_v1.3
TS264	GuijunLab-Human	170.55	86.74	83.80	TS264_v1.1
TS148	Guijunlab-Complex	170.55	86.74	83.80	TS148_v1.5
TS312	GuijunLab-Assembly	170.55	86.74	83.80	TS312_v1.1
TS314	GuijunLab-Pathreader	170.55	86.74	83.80	TS314_v1.1
TS393	GuijunLab-QA	170.55	86.74	83.80	TS393_v1.1
TS388	DeepFold-server	170.46	87.75	82.71	TS388_v1.4
TS017	Seder2024hard	170.45	84.76	85.69	TS017_v1.3
TS145	colabfold_baseline	170.45	84.76	85.69	TS145_v1.5
TS198	colabfold	170.45	84.29	86.16	TS198_v1.4
TS147	Zheng-Multimer	170.42	87.38	83.03	TS147_v1.1
TS196	HYU_MLLAB	170.32	85.70	84.62	TS196_v1.4
TS225	Unknown	170.18	86.06	84.12	TS225_v1.1
TS164	McGuffin	170.18	86.06	84.12	TS164_v1.1
TS163	MultiFOLD2	170.18	86.06	84.12	TS163_v1.1
TS019	Zheng-Server	170.17	85.62	84.56	TS019_v1.1
TS304	AF3-server	170.16	85.46	84.70	TS304_v1.2
TS241	elofsson	170.16	85.46	84.70	TS241_v1.2
TS091	Huang-HUST	170.08	87.12	82.95	TS091_v1.2
TS311	RAGfold_Prot1	170.08	86.21	83.87	TS311_v1.4
TS227	KUMC	170.06	86.67	83.40	TS227_v1.3
TS102	Psi-Phi	170.06	86.95	83.11	TS102_v1.4
TS375	milliseconds	170.00	86.73	83.27	TS375_v1.3
TS287	plmfold	169.99	86.96	83.03	TS287_v1.1
TS235	isyslab-hust	169.95	84.11	85.85	TS235_v1.3

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Supplementary Table S3 – continued from previous page

Group	Group_Name	Dual-State_Score	V1_Composite_Score_3	V2_Composite_Score_3	V1_Model
TS122	MQA_server	169.95	84.65	85.30	TS122_v1_4
TS425	MULTICOM_GATE	169.86	86.39	83.47	TS425_v1_2
TS319	MULTICOM_LLM	169.86	86.39	83.47	TS319_v1_3
TS464	PocketTracer	169.77	83.44	86.33	TS464_v1_1
TS301	GHZ-MAN	169.74	85.17	84.56	TS301_v1_2
TS272	GromihaLab	169.71	83.67	86.04	TS272_v1_1
TS294	KiharaLab	169.63	85.78	83.85	TS294_v1_2
TS167	OpenComplex	169.60	85.00	84.59	TS167_v1_2
TS450	OpenComplex_Server	169.60	85.00	84.59	TS450_v1_5
TS207	MULTICOM_ligand	169.59	86.09	83.50	TS207_v1_3
TS423	ShanghaiTech-server	169.48	87.25	82.23	TS423_v1_1
TS345	MULTICOM_human	169.48	84.87	84.61	TS345_v1_4
TS369	Bhattacharya	169.40	84.70	84.70	TS369_v1_1
TS400	OmniFold	169.30	83.80	85.50	TS400_v1_1
TS267	kiharalab_server	169.19	85.13	84.07	TS267_v1_2
TS079	MRAFold	169.11	85.06	84.04	TS079_v1_1
TS293	MRAH	169.11	85.06	84.04	TS293_v1_2
TS040	DELCLAB	152.62	53.84	98.77	TS040_v1_5
TS274	kozakovvajda	152.29	53.91	98.38	TS274_v1_3
TS494	ClusPro	152.29	53.91	98.38	TS494_v1_3
TS286	CSSB_experimental	151.54	54.69	96.85	TS286_v1_4
TS465	Wallner	149.56	90.74	58.83	TS465_v1_3
TS014	Cool-PSP	149.50	86.23	63.27	TS014_v1_5
TS408	SNU-CHEM-lig	149.08	91.80	57.28	TS408_v1_1
TS075	GHZ-ISM	149.00	84.89	64.12	TS075_v1_2
TS284	Unicorn	149.00	84.89	64.12	TS284_v1_2
TS055	LCDD-team	148.98	91.58	57.40	TS055_v1_3
TS331	MULTICOM_AI	148.96	84.56	64.40	TS331_v1_3
TS051	MULTICOM	148.96	84.56	64.40	TS051_v1_3
TS475	ptq	148.62	85.46	63.16	TS475_v1_2
TS202	test001	147.80	90.86	56.94	TS202_v1_5
TS039	arosko	141.65	55.81	85.85	TS039_v1_3
TS120	Cerebra	127.10	63.21	63.89	TS120_v1_6
TS275	Seminoles	82.36	42.73	39.64	TS275_v1_1
TS461	forlilab	82.14	39.80	42.33	TS461_v1_2
TS361	Cerebra_server	63.99	18.76	45.22	TS361_v1_1
TS132	profold2	20.83	9.66	11.17	TS132_v1_1

Supplementary Table S4: Results for T1214 Composite Score 4  
dual state

Group	Group_Name	Dual-State_Score	V1_Composite_Score_4	V2_Composite_Score_4	V1_Model
TS204	Zou	169.39	72.76	96.63	TS204_v1.5
TS139	DeepFold-refine	169.36	73.02	96.34	TS139_v1.6
TS059	DeepFold	169.36	73.02	96.34	TS059_v1.6
TS386	ShanghaiTech-Ligand	169.36	93.01	76.34	TS386_v1.4
TS298	ShanghaiTech-human	169.36	93.01	76.34	TS298_v1.4
TS462	Zheng	168.96	91.10	77.85	TS462_v1.6
TS110	MIEnsembles-Server	168.72	88.23	80.50	TS110_v1.2
TS208	falcon2	168.61	91.66	76.95	TS208_v1.4
TS022	Yang	168.42	90.16	78.25	TS022_v1.4
TS015	PEZYFoldings	168.29	94.44	73.84	TS015_v1.5
TS269	CSSB_server	168.08	74.20	93.88	TS269_v1.3
TS221	CSSB_FAKER	168.04	74.21	93.83	TS221_v1.3
TS419	CSSB-Human	168.04	74.21	93.83	TS419_v1.3
TS052	Yang-Server	167.66	73.95	93.71	TS052_v1.1
TS456	Yang-Multimer	167.62	73.37	94.25	TS456_v1.1
TS020	comppharmunibas	167.48	74.16	93.32	TS020_v1.3
TS198	colabfold	167.41	82.61	84.80	TS198_v1.4
TS145	colabfold_baseline	167.40	83.12	84.28	TS145_v1.5
TS017	Seder2024hard	167.40	83.12	84.28	TS017_v1.3
TS148	Guijunlab-Complex	167.38	85.37	82.01	TS148_v1.5
TS312	GuijunLab-Assembly	167.38	85.37	82.01	TS312_v1.1
TS264	GuijunLab-Human	167.38	85.37	82.01	TS264_v1.1
TS314	GuijunLab-Pathreader	167.38	85.37	82.01	TS314_v1.1
TS393	GuijunLab-QA	167.38	85.37	82.01	TS393_v1.1
TS388	DeepFold-server	167.26	86.53	80.73	TS388_v1.4
TS147	Zheng-Multimer	167.21	85.96	81.25	TS147_v1.1
TS196	HYU_MLLAB	167.17	84.21	82.96	TS196_v1.4
TS019	Zheng-Server	167.10	84.18	82.92	TS019_v1.1
TS311	RAGfold_Prot1	166.93	84.80	82.13	TS311_v1.4
TS241	elofsson	166.93	83.94	82.99	TS241_v1.2
TS304	AF3-server	166.93	83.94	82.99	TS304_v1.2
TS225	Unknown	166.93	84.58	82.35	TS225_v1.1
TS164	McGuffin	166.93	84.58	82.35	TS164_v1.1
TS163	MultiFOLD2	166.93	84.58	82.35	TS163_v1.1
TS262	CoDock	166.91	71.81	95.10	TS262_v1.3
TS235	isyslab-hust	166.89	82.62	84.27	TS235_v1.3
TS102	Psi-Phi	166.85	85.59	81.26	TS102_v1.5
TS091	Huang-HUST	166.84	85.80	81.03	TS091_v1.2
TS227	KUMC	166.76	85.28	81.48	TS227_v1.3
TS375	milliseconds	166.76	85.40	81.36	TS375_v1.3
TS287	plmfold	166.72	85.58	81.14	TS287_v1.1

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Supplementary Table S4 – continued from previous page

Group	Group_Name	Dual-State_Score	V1_Composite_Score_4	V2_Composite_Score_4	V1_Model
TS122	MQA_server	166.72	83.13	83.59	TS122_v1_4
TS425	MULTICOM_GATE	166.68	85.12	81.56	TS425_v1_2
TS319	MULTICOM_LLM	166.68	85.12	81.56	TS319_v1_3
TS464	PocketTracer	166.62	81.86	84.76	TS464_v1_5
TS272	GromihaLab	166.56	82.11	84.45	TS272_v1_1
TS301	GHZ-MAN	166.50	83.68	82.81	TS301_v1_2
TS167	OpenComplex	166.47	83.59	82.88	TS167_v1_2
TS450	OpenComplex_Server	166.47	83.59	82.88	TS450_v1_5
TS345	MULTICOM_human	166.39	83.45	82.95	TS345_v1_4
TS207	MULTICOM_ligand	166.38	84.68	81.69	TS207_v1_2
TS294	KiharaLab	166.31	84.28	82.03	TS294_v1_2
TS423	ShanghaiTech-server	166.25	85.97	80.28	TS423_v1_1
TS369	Bhattacharya	166.21	83.22	82.99	TS369_v1_1
TS400	OmniFold	166.11	82.22	83.88	TS400_v1_1
TS079	MRAFold	166.06	83.64	82.42	TS079_v1_5
TS267	kiharalab_server	166.01	83.67	82.34	TS267_v1_2
TS293	MRAH	165.97	83.63	82.34	TS293_v1_2
TS475	ptq	165.20	84.06	81.14	TS475_v1_3
TS494	ClusPro	148.73	50.66	98.07	TS494_v1_3
TS274	kozakovvajda	148.73	50.66	98.07	TS274_v1_3
TS040	DELCLAB	148.69	50.16	98.53	TS040_v1_3
TS286	CSSB_experimental	147.77	51.91	95.86	TS286_v1_2
TS014	Cool-PSP	146.05	84.85	61.20	TS014_v1_5
TS465	Wallner	145.75	89.57	56.18	TS465_v1_3
TS051	MULTICOM	145.61	83.12	62.49	TS051_v1_3
TS331	MULTICOM_AI	145.61	83.12	62.49	TS331_v1_3
TS075	GHZ-ISM	145.52	83.42	62.10	TS075_v1_2
TS284	Unicorn	145.52	83.42	62.10	TS284_v1_2
TS408	SNU-CHEM-lig	144.80	90.61	54.19	TS408_v1_1
TS055	LCDD-team	144.70	90.40	54.30	TS055_v1_4
TS202	test001	142.73	89.38	53.35	TS202_v1_5
TS039	arosko	137.95	53.05	84.90	TS039_v1_3
TS120	Cerebra	121.64	60.41	61.23	TS120_v1_6
TS275	Seminoles	76.33	39.95	36.38	TS275_v1_1
TS461	forlilab	76.27	36.73	39.55	TS461_v1_2
TS361	Cerebra_server	76.16	34.59	41.57	TS361_v1_1
TS132	profold2	22.53	10.44	12.09	TS132_v1_1

Supplementary Table S5: Results for T1214 GDT TS dual state

Group	Group_Name	Dual-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model
TS052	Yang-Server	190.08	93.50	96.59	TS052.v1.3
TS456	Yang-Multimer	189.52	92.62	96.89	TS456.v1.3
TS262	CoDock	189.48	92.44	97.05	TS262.v1.5
TS059	DeepFold	189.43	90.92	98.50	TS059.v1.6
TS139	DeepFold-refine	189.43	90.92	98.50	TS139.v1.6
TS204	Zou	189.24	90.32	98.93	TS204.v1.3
TS022	Yang	189.18	95.05	94.13	TS022.v1.4
TS110	MIEnsembles-Server	188.88	94.67	94.21	TS110.v1.1
TS020	comppharmunibas	188.53	92.13	96.40	TS020.v1.3
TS286	CSSB_experimental	187.91	89.79	98.12	TS286.v1.4
TS221	CSSB_FAKER	187.75	90.55	97.20	TS221.v1.3
TS419	CSSB-Human	187.75	90.55	97.20	TS419.v1.3
TS345	MULTICOM_human	187.66	94.33	93.33	TS345.v1.4
TS450	OpenComplex_Server	187.65	94.44	93.21	TS450.v1.5
TS167	OpenComplex	187.65	94.44	93.21	TS167.v1.2
TS269	CSSB_server	187.60	90.32	97.28	TS269.v1.3
TS386	ShanghaiTech-Ligand	187.56	95.27	92.29	TS386.v1.1
TS298	ShanghaiTech-human	187.56	95.27	92.29	TS298.v1.1
TS040	DELCLAB	187.55	87.94	99.62	TS040.v1.2
TS293	MRAH	187.47	94.17	93.29	TS293.v1.5
TS423	ShanghaiTech-server	187.46	94.78	92.68	TS423.v1.5
TS079	MRAFold	187.43	94.21	93.21	TS079.v1.5
TS311	RAGfold_Prot1	187.39	94.02	93.37	TS311.v1.2
TS235	isyslab-hust	187.35	93.87	93.48	TS235.v1.3
TS267	kiharalab_server	187.12	93.80	93.33	TS267.v1.1
TS312	GuijunLab-Assembly	186.97	93.87	93.10	TS312.v1.1
TS314	GuijunLab-PAthreader	186.97	93.87	93.10	TS314.v1.1
TS148	Guijunlab-Complex	186.97	93.87	93.10	TS148.v1.5
TS196	HYU_MLLAB	186.94	93.46	93.48	TS196.v1.2
TS393	GuijunLab-QA	186.93	93.95	92.98	TS393.v1.5
TS264	GuijunLab-Human	186.93	93.95	92.98	TS264.v1.3
TS014	Cool-PSP	186.90	93.50	93.41	TS014.v1.3
TS102	Psi-Phi	186.86	93.68	93.17	TS102.v1.2
TS145	colabfold_baseline	186.83	93.12	93.71	TS145.v1.2
TS017	Seder2024hard	186.83	93.12	93.71	TS017.v1.4
TS164	McGuffin	186.83	93.19	93.64	TS164.v1.3
TS163	MultiFOLD2	186.83	93.19	93.64	TS163.v1.3
TS464	PocketTracer	186.82	93.38	93.44	TS464.v1.5
TS388	DeepFold-server	186.72	95.23	91.49	TS388.v1.4
TS319	MULTICOM_LLM	186.69	94.78	91.91	TS319.v1.3
TS425	MULTICOM_GATE	186.69	94.78	91.91	TS425.v1.2

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Supplementary Table S5 – continued from previous page

Group	Group_Name	Dual-State_Score	V1_GDT_TS	V2_GDT_TS	V1_Model
TS494	ClusPro	186.65	86.65	100.00	TS494.v1.1
TS274	kozakovvajda	186.65	86.65	100.00	TS274.v1.1
TS272	GromihaLab	186.60	93.31	93.29	TS272.v1.3
TS227	KUMC	186.55	93.83	92.72	TS227.v1.5
TS015	PEZYZFoldings	186.51	96.41	90.11	TS015.v1.2
TS208	falcon2	186.50	94.29	92.22	TS208.v1.4
TS207	MULTICOM_ligand	186.44	93.42	93.02	TS207.v1.1
TS475	ptq	186.40	93.76	92.64	TS475.v1.3
TS198	colabfold	186.33	93.38	92.94	TS198.v1.5
TS400	OmniFold	186.29	92.85	93.44	TS400.v1.1
TS369	Bhattacharya	186.21	93.34	92.87	TS369.v1.1
TS301	GHZ-MAN	186.13	93.38	92.75	TS301.v1.1
TS091	Huang-HUST	186.04	94.25	91.79	TS091.v1.2
TS375	milliseconds	185.93	94.25	91.68	TS375.v1.3
TS287	plmfold	185.90	93.53	92.37	TS287.v1.1
TS331	MULTICOM_AI	185.90	93.91	91.99	TS331.v1.5
TS051	MULTICOM	185.90	93.91	91.99	TS051.v1.5
TS465	Wallner	185.89	94.44	91.45	TS465.v1.4
TS304	AF3-server	185.75	93.15	92.60	TS304.v1.4
TS241	elofsson	185.75	93.15	92.60	TS241.v1.4
TS225	Unknown	185.68	92.93	92.75	TS225.v1.1
TS462	Zheng	185.17	93.83	91.33	TS462.v1.2
TS147	Zheng-Multimer	185.17	93.83	91.33	TS147.v1.2
TS019	Zheng-Server	185.13	94.21	90.91	TS019.v1.2
TS122	MQA_server	185.09	93.68	91.41	TS122.v1.2
TS039	arosko	184.92	87.03	97.89	TS039.v1.1
TS294	KiharaLab	184.69	92.32	92.37	TS294.v1.2
TS075	GHZ-ISM	184.63	93.76	90.87	TS075.v1.1
TS284	Unicorn	184.63	93.76	90.87	TS284.v1.1
TS408	SNU-CHEM-lig	184.51	94.06	90.45	TS408.v1.1
TS055	LCDD-team	184.36	93.99	90.38	TS055.v1.3
TS202	test001	173.11	89.56	83.55	TS202.v1.5
TS120	Cerebra	169.33	85.70	83.63	TS120.v1.6
TS461	forlilab	161.25	76.74	84.51	TS461.v1.3
TS275	Seminoles	157.20	78.71	78.49	TS275.v1.1
TS361	Cerebra_server	152.51	76.55	75.96	TS361.v1.3
TS132	profold2	109.41	54.50	54.91	TS132.v1.1

Supplementary Table S6: Results for T1214 GlobalLDDT dual state

Group	Group_Name	Dual-State_Score	V1_gLDDT	V2_gLDDT	V1_Model
TS274	kozakovvajda	1.74	0.75	0.99	TS274_v1.1
TS494	ClusPro	1.74	0.75	0.99	TS494_v1.1
TS204	Zou	1.73	0.81	0.93	TS204_v1.5
TS059	DeepFold	1.72	0.81	0.91	TS059_v1.6
TS139	DeepFold-refine	1.72	0.81	0.91	TS139_v1.6
TS039	arosko	1.72	0.75	0.97	TS039_v1.3
TS040	DELCLAB	1.70	0.75	0.94	TS040_v1.5
TS052	Yang-Server	1.70	0.84	0.86	TS052_v1.3
TS110	MIEnsembles-Server	1.69	0.85	0.84	TS110_v1.2
TS022	Yang	1.69	0.85	0.84	TS022_v1.4
TS456	Yang-Multimer	1.69	0.83	0.86	TS456_v1.5
TS462	Zheng	1.69	0.85	0.84	TS462_v1.1
TS147	Zheng-Multimer	1.69	0.85	0.84	TS147_v1.1
TS221	CSSB_FAKER	1.69	0.81	0.88	TS221_v1.3
TS419	CSSB-Human	1.69	0.81	0.88	TS419_v1.3
TS269	CSSB_server	1.69	0.81	0.87	TS269_v1.5
TS262	CoDock	1.69	0.83	0.86	TS262_v1.1
TS386	ShanghaiTech-Ligand	1.68	0.86	0.82	TS386_v1.4
TS298	ShanghaiTech-human	1.68	0.86	0.82	TS298_v1.4
TS015	PEZYZFoldings	1.68	0.87	0.80	TS015_v1.5
TS208	falcon2	1.68	0.86	0.82	TS208_v1.4
TS102	Psi-Phi	1.68	0.85	0.82	TS102_v1.5
TS264	GuijunLab-Human	1.67	0.85	0.83	TS264_v1.1
TS148	Guijunlab-Complex	1.67	0.85	0.83	TS148_v1.5
TS393	GuijunLab-QA	1.67	0.85	0.83	TS393_v1.1
TS312	GuijunLab-Assembly	1.67	0.85	0.83	TS312_v1.1
TS314	GuijunLab-PATHreader	1.67	0.85	0.83	TS314_v1.1
TS207	MULTICOM_ligand	1.67	0.85	0.83	TS207_v1.2
TS450	OpenComplex_Server	1.67	0.85	0.82	TS450_v1.5
TS167	OpenComplex	1.67	0.85	0.82	TS167_v1.2
TS272	GromihaLab	1.67	0.84	0.83	TS272_v1.3
TS287	plmfold	1.67	0.85	0.82	TS287_v1.2
TS122	MQA_server	1.67	0.84	0.83	TS122_v1.5
TS267	kiharalab_server	1.67	0.85	0.82	TS267_v1.1
TS020	comppharmunibas	1.67	0.82	0.85	TS020_v1.3
TS241	elofsson	1.67	0.84	0.82	TS241_v1.4
TS304	AF3-server	1.67	0.84	0.82	TS304_v1.4
TS464	PocketTracer	1.67	0.84	0.83	TS464_v1.1
TS369	Bhattacharya	1.67	0.85	0.82	TS369_v1.1
TS345	MULTICOM_human	1.67	0.85	0.82	TS345_v1.4
TS286	CSSB_experimental	1.66	0.80	0.87	TS286_v1.2

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Supplementary Table S6 – continued from previous page

Group	Group_Name	Dual-State_Score	V1_gLDDT	V2_gLDDT	V1_Model
TS311	RAGfold_Prot1	1.66	0.85	0.82	TS311_v1.4
TS293	MRAH	1.66	0.85	0.82	TS293_v1.2
TS079	MRAFold	1.66	0.85	0.82	TS079_v1.1
TS400	OmniFold	1.66	0.84	0.82	TS400_v1.1
TS235	isyslab-hust	1.66	0.84	0.82	TS235_v1.3
TS301	GHZ-MAN	1.66	0.84	0.82	TS301_v1.2
TS388	DeepFold-server	1.66	0.86	0.80	TS388_v1.4
TS425	MULTICOM_GATE	1.66	0.85	0.80	TS425_v1.2
TS375	milliseconds	1.66	0.85	0.80	TS375_v1.3
TS319	MULTICOM_LLM	1.66	0.85	0.80	TS319_v1.3
TS423	ShanghaiTech-server	1.66	0.85	0.81	TS423_v1.5
TS091	Huang-HUST	1.65	0.85	0.81	TS091_v1.2
TS227	KUMC	1.65	0.85	0.81	TS227_v1.3
TS164	McGuffin	1.65	0.84	0.82	TS164_v1.3
TS163	MultiFOLD2	1.65	0.84	0.82	TS163_v1.3
TS145	colabfold_baseline	1.65	0.84	0.82	TS145_v1.2
TS017	Seder2024hard	1.65	0.84	0.82	TS017_v1.4
TS196	HYU_MLLAB	1.65	0.84	0.82	TS196_v1.3
TS225	Unknown	1.65	0.83	0.82	TS225_v1.1
TS051	MULTICOM	1.65	0.85	0.80	TS051_v1.1
TS331	MULTICOM_AI	1.65	0.85	0.80	TS331_v1.1
TS198	colabfold	1.65	0.84	0.81	TS198_v1.5
TS475	ptq	1.65	0.83	0.82	TS475_v1.5
TS019	Zheng-Server	1.65	0.85	0.80	TS019_v1.2
TS284	Unicorn	1.65	0.85	0.80	TS284_v1.1
TS075	GHZ-ISM	1.65	0.85	0.80	TS075_v1.1
TS294	KiharaLab	1.65	0.84	0.81	TS294_v1.2
TS408	SNU-CHEM-lig	1.65	0.84	0.81	TS408_v1.3
TS465	Wallner	1.64	0.85	0.79	TS465_v1.2
TS014	Cool-PSP	1.63	0.84	0.79	TS014_v1.4
TS055	LCDD-team	1.62	0.82	0.79	TS055_v1.3
TS202	test001	1.57	0.81	0.77	TS202_v1.5
TS120	Cerebra	1.45	0.72	0.72	TS120_v1.6
TS461	forlilab	1.44	0.71	0.72	TS461_v1.2
TS275	Seminoles	1.37	0.69	0.68	TS275_v1.1
TS361	Cerebra_server	1.27	0.63	0.64	TS361_v1.1
TS132	profold2	0.98	0.48	0.50	TS132_v1.1

Supplementary Table S7: Results for T1214 TMscore dual state

Group	Group_Name	Dual-State_Score	V1_TMscore	V2_TMscore	V1_Model
TS462	Zheng	1.97	0.99	0.98	TS462_v1.6
TS110	MIEnsembles-Server	1.97	0.99	0.98	TS110_v1.2
TS235	isyslab-hust	1.97	0.99	0.98	TS235_v1.3
TS204	Zou	1.97	0.97	1.00	TS204_v1.3
TS059	DeepFold	1.97	0.97	1.00	TS059_v1.6
TS139	DeepFold-refine	1.97	0.97	1.00	TS139_v1.6
TS345	MULTICOM_human	1.97	0.99	0.98	TS345_v1.4
TS022	Yang	1.97	0.99	0.98	TS022_v1.4
TS052	Yang-Server	1.97	0.98	0.99	TS052_v1.1
TS079	MRAFold	1.97	0.99	0.98	TS079_v1.5
TS293	MRAH	1.97	0.99	0.98	TS293_v1.3
TS450	OpenComplex_Server	1.97	0.99	0.98	TS450_v1.5
TS167	OpenComplex	1.97	0.99	0.98	TS167_v1.2
TS017	Seder2024hard	1.97	0.98	0.98	TS017_v1.4
TS145	colabfold_baseline	1.97	0.98	0.98	TS145_v1.2
TS456	Yang-Multimer	1.97	0.98	0.99	TS456_v1.5
TS272	GromihaLab	1.97	0.98	0.98	TS272_v1.4
TS267	kiharalab_server	1.97	0.99	0.98	TS267_v1.1
TS464	PocketTracer	1.97	0.98	0.98	TS464_v1.3
TS393	GuijunLab-QA	1.97	0.99	0.98	TS393_v1.1
TS148	Guijunlab-Complex	1.97	0.99	0.98	TS148_v1.5
TS196	HYU_MLLAB	1.97	0.98	0.98	TS196_v1.2
TS264	GuijunLab-Human	1.97	0.99	0.98	TS264_v1.1
TS314	GuijunLab-PAthreader	1.97	0.99	0.98	TS314_v1.1
TS475	ptq	1.97	0.99	0.98	TS475_v1.3
TS312	GuijunLab-Assembly	1.97	0.99	0.98	TS312_v1.1
TS102	Psi-Phi	1.97	0.99	0.98	TS102_v1.1
TS319	MULTICOM_LLM	1.97	0.99	0.98	TS319_v1.3
TS221	CSSB_FAKER	1.97	0.97	0.99	TS221_v1.3
TS425	MULTICOM_GATE	1.97	0.99	0.98	TS425_v1.2
TS419	CSSB-Human	1.97	0.97	0.99	TS419_v1.3
TS198	colabfold	1.97	0.98	0.98	TS198_v1.5
TS388	DeepFold-server	1.97	0.99	0.98	TS388_v1.4
TS269	CSSB_server	1.97	0.97	0.99	TS269_v1.3
TS369	Bhattacharya	1.97	0.98	0.98	TS369_v1.1
TS287	plmfold	1.97	0.99	0.98	TS287_v1.2
TS207	MULTICOM_ligand	1.97	0.99	0.98	TS207_v1.3
TS400	OmniFold	1.97	0.98	0.98	TS400_v1.1
TS423	ShanghaiTech-server	1.97	0.99	0.98	TS423_v1.1
TS241	elofsson	1.97	0.98	0.98	TS241_v1.2
TS304	AF3-server	1.97	0.98	0.98	TS304_v1.2

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Supplementary Table S7 – continued from previous page

Group	Group_Name	Dual-State_Score	V1_TMscore	V2_TMscore	V1_Model
TS375	milliseconds	1.97	0.99	0.98	TS375_v1.3
TS091	Huang-HUST	1.97	0.99	0.98	TS091_v1.2
TS225	Unknown	1.97	0.98	0.98	TS225_v1.1
TS164	McGuffin	1.97	0.98	0.98	TS164_v1.1
TS301	GHZ-MAN	1.97	0.98	0.98	TS301_v1.2
TS163	MultiFOLD2	1.97	0.98	0.98	TS163_v1.1
TS331	MULTICOM_AI	1.97	0.99	0.98	TS331_v1.1
TS051	MULTICOM	1.97	0.99	0.98	TS051_v1.1
TS386	ShanghaiTech-Ligand	1.97	0.99	0.98	TS386_v1.1
TS298	ShanghaiTech-human	1.97	0.99	0.98	TS298_v1.1
TS286	CSSB_experimental	1.97	0.97	0.99	TS286_v1.2
TS227	KUMC	1.97	0.99	0.98	TS227_v1.2
TS019	Zheng-Server	1.97	0.99	0.98	TS019_v1.2
TS262	CoDock	1.97	0.97	0.99	TS262_v1.5
TS075	GHZ-ISM	1.97	0.99	0.98	TS075_v1.3
TS284	Unicorn	1.97	0.99	0.98	TS284_v1.3
TS122	MQA_server	1.97	0.99	0.98	TS122_v1.2
TS147	Zheng-Multimer	1.97	0.99	0.98	TS147_v1.4
TS208	falcon2	1.96	0.99	0.98	TS208_v1.4
TS311	RAGfold_Prot1	1.96	0.99	0.98	TS311_v1.1
TS014	Cool-PSP	1.96	0.99	0.98	TS014_v1.4
TS040	DELCLAB	1.96	0.96	1.00	TS040_v1.3
TS294	KiharaLab	1.96	0.98	0.98	TS294_v1.2
TS015	PEZYZFoldings	1.96	0.99	0.97	TS015_v1.2
TS465	Wallner	1.96	0.99	0.97	TS465_v1.3
TS408	SNU-CHEM-lig	1.96	0.99	0.97	TS408_v1.1
TS055	LCDD-team	1.96	0.99	0.97	TS055_v1.3
TS494	ClusPro	1.95	0.95	1.00	TS494_v1.3
TS274	kozakovvajda	1.95	0.95	1.00	TS274_v1.3
TS039	arosko	1.95	0.96	0.99	TS039_v1.1
TS202	test001	1.94	0.98	0.96	TS202_v1.5
TS020	comppharmunibas	1.94	0.98	0.96	TS020_v1.4
TS120	Cerebra	1.94	0.97	0.97	TS120_v1.6
TS461	forlilab	1.92	0.96	0.96	TS461_v1.2
TS275	Seminoles	1.92	0.96	0.96	TS275_v1.1
TS361	Cerebra_server	1.90	0.95	0.95	TS361_v1.1
TS132	profold2	1.60	0.80	0.80	TS132_v1.1