

CASP16_SINGLE-STATE_TABLES

Tiburon Leon Benavides

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

| Group | Group_Name | V1_Composite_Score_1 | V1_Model |
|-------|----------------------|----------------------|------------|
| TS015 | PEZYFoldings | 91.17 | TS015_v1.5 |
| TS298 | ShanghaiTech-human | 89.37 | TS298_v1.4 |
| TS386 | ShanghaiTech-Ligand | 89.37 | TS386_v1.4 |
| TS208 | falcon2 | 87.66 | TS208_v1.4 |
| TS462 | Zheng | 86.42 | TS462_v1.6 |
| TS022 | Yang | 86.26 | TS022_v1.4 |
| TS408 | SNU-CHEM-lig | 85.96 | TS408_v1.1 |
| TS055 | LCDD-team | 85.68 | TS055_v1.4 |
| TS465 | Wallner | 85.35 | TS465_v1.3 |
| TS110 | MIEnsembles-Server | 84.08 | TS110_v1.2 |
| TS202 | test001 | 83.44 | TS202_v1.5 |
| TS388 | DeepFold-server | 82.69 | TS388_v1.4 |
| TS423 | ShanghaiTech-server | 81.84 | TS423_v1.1 |
| TS091 | Huang-HUST | 81.57 | TS091_v1.2 |
| TS147 | Zheng-Multimer | 81.50 | TS147_v1.1 |
| TS102 | Psi-Phi | 81.34 | TS102_v1.1 |
| TS375 | milliseconds | 81.32 | TS375_v1.3 |
| TS287 | plmfold | 81.25 | TS287_v1.1 |
| TS020 | comppharmunibas | 81.19 | TS020_v1.4 |
| TS425 | MULTICOM_GATE | 81.15 | TS425_v1.2 |
| TS319 | MULTICOM_LLM | 81.15 | TS319_v1.3 |
| TS314 | GuijunLab-PAthreader | 81.13 | TS314_v1.1 |
| TS312 | GuijunLab-Assembly | 81.13 | TS312_v1.1 |
| TS393 | GuijunLab-QA | 81.13 | TS393_v1.1 |
| TS264 | GuijunLab-Human | 81.13 | TS264_v1.1 |
| TS148 | Guijunlab-Complex | 81.13 | TS148_v1.5 |
| TS227 | KUMC | 80.86 | TS227_v1.3 |
| TS294 | KiharaLab | 80.80 | TS294_v1.3 |
| TS311 | RAGfold_Prot1 | 80.54 | TS311_v1.4 |
| TS207 | MULTICOM_ligand | 80.33 | TS207_v1.1 |
| TS014 | Cool-PSP | 80.10 | TS014_v1.5 |
| TS164 | McGuffin | 79.86 | TS164_v1.1 |
| TS163 | MultiFOLD2 | 79.86 | TS163_v1.1 |
| TS225 | Unknown | 79.86 | TS225_v1.1 |

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Supplementary Table S1 – continued from previous page

| Group | Group_Name | V1_Composite_Score_1 | V1_Model |
|-------|--------------------|----------------------|------------|
| TS019 | Zheng-Server | 79.81 | TS019_v1_1 |
| TS196 | HYU_MLLAB | 79.57 | TS196_v1_4 |
| TS450 | OpenComplex_Server | 79.46 | TS450_v1_5 |
| TS167 | OpenComplex | 79.46 | TS167_v1_2 |
| TS475 | ptq | 79.41 | TS475_v1_3 |
| TS079 | MRAFold | 79.37 | TS079_v1_1 |
| TS293 | MRAH | 79.37 | TS293_v1_2 |
| TS241 | elofsson | 79.33 | TS241_v1_2 |
| TS304 | AF3-server | 79.33 | TS304_v1_2 |
| TS267 | kiharalab_server | 79.28 | TS267_v1_2 |
| TS345 | MULTICOM_human | 79.25 | TS345_v1_4 |
| TS301 | GHZ-MAN | 78.96 | TS301_v1_2 |
| TS369 | Bhattacharya | 78.81 | TS369_v1_1 |
| TS284 | Unicorn | 78.73 | TS284_v1_2 |
| TS075 | GHZ-ISM | 78.73 | TS075_v1_2 |
| TS331 | MULTICOM_AI | 78.67 | TS331_v1_1 |
| TS051 | MULTICOM | 78.67 | TS051_v1_1 |
| TS122 | MQA_server | 78.55 | TS122_v1_2 |
| TS235 | isyslab-hust | 78.25 | TS235_v1_3 |
| TS198 | colabfold | 77.92 | TS198_v1_3 |
| TS145 | colabfold_baseline | 77.75 | TS145_v1_5 |
| TS017 | Seder2024hard | 77.75 | TS017_v1_3 |
| TS272 | GromihaLab | 77.66 | TS272_v1_3 |
| TS400 | OmniFold | 77.54 | TS400_v1_1 |
| TS464 | PocketTracer | 77.38 | TS464_v1_2 |
| TS139 | DeepFold-refine | 72.37 | TS139_v1_3 |
| TS120 | Cerebra | 71.99 | TS120_v1_6 |
| TS275 | Seminole | 69.53 | TS275_v1_1 |
| TS052 | Yang-Server | 69.05 | TS052_v1_1 |
| TS419 | CSSB-Human | 68.55 | TS419_v1_3 |
| TS221 | CSSB_FAKER | 68.55 | TS221_v1_3 |
| TS269 | CSSB_server | 68.49 | TS269_v1_3 |
| TS456 | Yang-Multimer | 68.48 | TS456_v1_5 |
| TS059 | DeepFold | 67.39 | TS059_v1_6 |
| TS204 | Zou | 66.94 | TS204_v1_5 |
| TS262 | CoDock | 66.81 | TS262_v1_3 |
| TS461 | forlilab | 66.23 | TS461_v1_2 |
| TS286 | CSSB_experimental | 65.85 | TS286_v1_2 |
| TS039 | arosko | 65.44 | TS039_v1_3 |
| TS494 | ClusPro | 62.98 | TS494_v1_1 |
| TS274 | kozakovvajda | 62.98 | TS274_v1_1 |
| TS040 | DELCLAB | 62.72 | TS040_v1_3 |
| TS361 | Cerebra_server | 62.26 | TS361_v1_1 |

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Supplementary Table S1 – continued from previous page

| Group | Group_Name | V1_Composite_Score_1 | V1_Model |
|-------|------------|----------------------|------------|
| TS132 | profold2 | 30.97 | TS132_v1_1 |

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

| Group | Group_Name | V1_Composite_Score_2 | V1_Model |
|-------|----------------------|----------------------|------------|
| TS015 | PEZYFoldings | 90.16 | TS015_v1.5 |
| TS298 | ShanghaiTech-human | 88.04 | TS298_v1.4 |
| TS386 | ShanghaiTech-Ligand | 88.04 | TS386_v1.4 |
| TS208 | falcon2 | 86.01 | TS208_v1.4 |
| TS462 | Zheng | 84.51 | TS462_v1.6 |
| TS022 | Yang | 84.28 | TS022_v1.4 |
| TS408 | SNU-CHEM-lig | 83.92 | TS408_v1.1 |
| TS055 | LCDD-team | 83.59 | TS055_v1.5 |
| TS465 | Wallner | 83.15 | TS465_v1.3 |
| TS110 | MIEnsembles-Server | 81.68 | TS110_v1.2 |
| TS202 | test001 | 81.16 | TS202_v1.5 |
| TS388 | DeepFold-server | 79.88 | TS388_v1.4 |
| TS423 | ShanghaiTech-server | 78.89 | TS423_v1.1 |
| TS020 | comp pharmunibas | 78.81 | TS020_v1.4 |
| TS147 | Zheng-Multimer | 78.66 | TS147_v1.1 |
| TS091 | Huang-HUST | 78.62 | TS091_v1.2 |
| TS102 | Psi-Phi | 78.38 | TS102_v1.1 |
| TS375 | milliseconds | 78.31 | TS375_v1.3 |
| TS294 | KiharaLab | 78.29 | TS294_v1.3 |
| TS287 | plmfold | 78.28 | TS287_v1.1 |
| TS264 | GuijunLab-Human | 78.13 | TS264_v1.1 |
| TS393 | GuijunLab-QA | 78.13 | TS393_v1.1 |
| TS148 | Guijunlab-Complex | 78.13 | TS148_v1.5 |
| TS312 | GuijunLab-Assembly | 78.13 | TS312_v1.1 |
| TS314 | GuijunLab-Pathreader | 78.13 | TS314_v1.1 |
| TS319 | MULTICOM.LLM | 78.02 | TS319_v1.3 |
| TS425 | MULTICOM.GATE | 78.02 | TS425_v1.2 |
| TS227 | KUMC | 77.81 | TS227_v1.3 |
| TS311 | RAGfold_Prot1 | 77.44 | TS311_v1.4 |
| TS207 | MULTICOM_ligand | 77.17 | TS207_v1.2 |
| TS014 | Cool-PSP | 76.85 | TS014_v1.5 |
| TS225 | Unknown | 76.67 | TS225_v1.1 |
| TS164 | McGuffin | 76.67 | TS164_v1.1 |
| TS163 | MultiFOLD2 | 76.67 | TS163_v1.1 |
| TS019 | Zheng-Server | 76.56 | TS019_v1.1 |
| TS196 | HYU_MLLAB | 76.32 | TS196_v1.4 |
| TS450 | OpenComplex_Server | 76.09 | TS450_v1.5 |
| TS167 | OpenComplex | 76.09 | TS167_v1.2 |
| TS304 | AF3-server | 76.05 | TS304_v1.2 |
| TS241 | elofsson | 76.05 | TS241_v1.2 |

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Supplementary Table S2 – continued from previous page

| Group | Group_Name | V1_Composite_Score_2 | V1_Model |
|-------|--------------------|----------------------|------------|
| TS475 | ptq | 76.01 | TS475_v1.3 |
| TS293 | MRAH | 76.00 | TS293_v1.2 |
| TS079 | MRAFold | 76.00 | TS079_v1.1 |
| TS267 | kiharalab_server | 75.92 | TS267_v1.2 |
| TS345 | MULTICOM_human | 75.84 | TS345_v1.4 |
| TS301 | GHZ-MAN | 75.56 | TS301_v1.2 |
| TS369 | Bhattacharya | 75.37 | TS369_v1.1 |
| TS284 | Unicorn | 75.26 | TS284_v1.2 |
| TS075 | GHZ-ISM | 75.26 | TS075_v1.2 |
| TS051 | MULTICOM | 75.09 | TS051_v1.1 |
| TS331 | MULTICOM_AI | 75.09 | TS331_v1.1 |
| TS122 | MQA_server | 75.03 | TS122_v1.4 |
| TS235 | isyslab-hust | 74.66 | TS235_v1.3 |
| TS198 | colabfold | 74.33 | TS198_v1.3 |
| TS145 | colabfold_baseline | 74.24 | TS145_v1.5 |
| TS017 | Seder2024hard | 74.24 | TS017_v1.3 |
| TS272 | GromihaLab | 74.03 | TS272_v1.1 |
| TS400 | OmniFold | 73.89 | TS400_v1.1 |
| TS464 | PocketTracer | 73.69 | TS464_v1.5 |
| TS120 | Cerebra | 68.49 | TS120_v1.6 |
| TS139 | DeepFold-refine | 68.36 | TS139_v1.3 |
| TS275 | Seminole | 65.38 | TS275_v1.1 |
| TS052 | Yang-Server | 64.23 | TS052_v1.1 |
| TS419 | CSSB-Human | 63.71 | TS419_v1.3 |
| TS221 | CSSB_FAKER | 63.71 | TS221_v1.3 |
| TS456 | Yang-Multimer | 63.66 | TS456_v1.5 |
| TS269 | CSSB_server | 63.66 | TS269_v1.3 |
| TS059 | DeepFold | 62.49 | TS059_v1.6 |
| TS204 | Zou | 62.01 | TS204_v1.1 |
| TS262 | CoDock | 61.92 | TS262_v1.3 |
| TS461 | forlilab | 61.64 | TS461_v1.2 |
| TS286 | CSSB_experimental | 60.78 | TS286_v1.2 |
| TS039 | arosko | 60.25 | TS039_v1.3 |
| TS040 | DELCLAB | 58.05 | TS040_v1.5 |
| TS361 | Cerebra_server | 58.04 | TS361_v1.1 |
| TS274 | kozakovvajda | 57.81 | TS274_v1.1 |
| TS494 | ClusPro | 57.81 | TS494_v1.1 |
| TS132 | profold2 | 37.74 | TS132_v1.1 |

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

| Group | Group_Name | V1_Composite_Score_3 | V1_Model |
|-------|----------------------|----------------------|------------|
| TS015 | PEZYFoldings | 95.40 | TS015_v1.5 |
| TS386 | ShanghaiTech-Ligand | 94.08 | TS386_v1.4 |
| TS298 | ShanghaiTech-human | 94.08 | TS298_v1.4 |
| TS208 | falcon2 | 92.81 | TS208_v1.4 |
| TS462 | Zheng | 92.29 | TS462_v1.6 |
| TS408 | SNU-CHEM-lig | 91.80 | TS408_v1.1 |
| TS055 | LCDD-team | 91.58 | TS055_v1.3 |
| TS022 | Yang | 91.33 | TS022_v1.4 |
| TS202 | test001 | 90.86 | TS202_v1.5 |
| TS465 | Wallner | 90.74 | TS465_v1.3 |
| TS110 | MIEnsembles-Server | 89.48 | TS110_v1.2 |
| TS388 | DeepFold-server | 87.75 | TS388_v1.4 |
| TS147 | Zheng-Multimer | 87.38 | TS147_v1.1 |
| TS423 | ShanghaiTech-server | 87.25 | TS423_v1.1 |
| TS091 | Huang-HUST | 87.12 | TS091_v1.2 |
| TS287 | plmfold | 86.96 | TS287_v1.1 |
| TS102 | Psi-Phi | 86.95 | TS102_v1.4 |
| TS148 | Guijunlab-Complex | 86.74 | TS148_v1.5 |
| TS264 | GuijunLab-Human | 86.74 | TS264_v1.1 |
| TS314 | GuijunLab-PAthreader | 86.74 | TS314_v1.1 |
| TS393 | GuijunLab-QA | 86.74 | TS393_v1.1 |
| TS312 | GuijunLab-Assembly | 86.74 | TS312_v1.1 |
| TS375 | milliseconds | 86.73 | TS375_v1.3 |
| TS227 | KUMC | 86.67 | TS227_v1.3 |
| TS425 | MULTICOM_GATE | 86.39 | TS425_v1.2 |
| TS319 | MULTICOM.LLM | 86.39 | TS319_v1.3 |
| TS014 | Cool-PSP | 86.23 | TS014_v1.5 |
| TS311 | RAGfold_Prot1 | 86.21 | TS311_v1.4 |
| TS207 | MULTICOM_ligand | 86.09 | TS207_v1.3 |
| TS163 | MultiFOLD2 | 86.06 | TS163_v1.1 |
| TS225 | Unknown | 86.06 | TS225_v1.1 |
| TS164 | McGuffin | 86.06 | TS164_v1.1 |
| TS294 | KiharaLab | 85.78 | TS294_v1.2 |
| TS196 | HYU_MLLAB | 85.70 | TS196_v1.4 |
| TS019 | Zheng-Server | 85.62 | TS019_v1.1 |
| TS304 | AF3-server | 85.46 | TS304_v1.2 |
| TS241 | elofsson | 85.46 | TS241_v1.2 |
| TS475 | ptq | 85.46 | TS475_v1.2 |
| TS301 | GHZ-MAN | 85.17 | TS301_v1.2 |
| TS267 | kiharalab_server | 85.13 | TS267_v1.2 |

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| Group | Group_Name | V1_Composite_Score_3 | V1_Model |
|-------|--------------------|----------------------|------------|
| TS293 | MRAH | 85.06 | TS293_v1_2 |
| TS079 | MRAFold | 85.06 | TS079_v1_1 |
| TS167 | OpenComplex | 85.00 | TS167_v1_2 |
| TS450 | OpenComplex_Server | 85.00 | TS450_v1_5 |
| TS284 | Unicorn | 84.89 | TS284_v1_2 |
| TS075 | GHZ-ISM | 84.89 | TS075_v1_2 |
| TS345 | MULTICOM_human | 84.87 | TS345_v1_4 |
| TS017 | Seder2024hard | 84.76 | TS017_v1_3 |
| TS145 | colabfold_baseline | 84.76 | TS145_v1_5 |
| TS369 | Bhattacharya | 84.70 | TS369_v1_1 |
| TS122 | MQA_server | 84.65 | TS122_v1_4 |
| TS331 | MULTICOM_AI | 84.56 | TS331_v1_3 |
| TS051 | MULTICOM | 84.56 | TS051_v1_3 |
| TS198 | colabfold | 84.29 | TS198_v1_4 |
| TS235 | isyslab-hust | 84.11 | TS235_v1_3 |
| TS400 | OmniFold | 83.80 | TS400_v1_1 |
| TS272 | GromihaLab | 83.67 | TS272_v1_1 |
| TS464 | PocketTracer | 83.44 | TS464_v1_1 |
| TS269 | CSSB_server | 76.64 | TS269_v1_3 |
| TS221 | CSSB_FAKER | 76.63 | TS221_v1_3 |
| TS419 | CSSB-Human | 76.63 | TS419_v1_3 |
| TS020 | comp pharmunibas | 76.56 | TS020_v1_3 |
| TS052 | Yang-Server | 76.28 | TS052_v1_1 |
| TS456 | Yang-Multimer | 75.87 | TS456_v1_1 |
| TS139 | DeepFold-refine | 75.62 | TS139_v1_6 |
| TS059 | DeepFold | 75.62 | TS059_v1_6 |
| TS204 | Zou | 75.40 | TS204_v1_5 |
| TS262 | CoDock | 74.54 | TS262_v1_3 |
| TS120 | Cerebra | 63.21 | TS120_v1_6 |
| TS039 | arosko | 55.81 | TS039_v1_3 |
| TS286 | CSSB_experimental | 54.69 | TS286_v1_4 |
| TS494 | ClusPro | 53.91 | TS494_v1_3 |
| TS274 | kozakovvajda | 53.91 | TS274_v1_3 |
| TS040 | DELCLAB | 53.84 | TS040_v1_5 |
| TS275 | Seminole | 42.73 | TS275_v1_1 |
| TS461 | forlilab | 39.80 | TS461_v1_2 |
| TS361 | Cerebra_server | 18.76 | TS361_v1_1 |
| TS132 | profold2 | 9.66 | TS132_v1_1 |

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

| Group | Group_Name | V1_Composite_Score_4 | V1_Model |
|-------|----------------------|----------------------|------------|
| TS015 | PEZYFoldings | 94.44 | TS015_v1.5 |
| TS298 | ShanghaiTech-human | 93.01 | TS298_v1.4 |
| TS386 | ShanghaiTech-Ligand | 93.01 | TS386_v1.4 |
| TS208 | falcon2 | 91.66 | TS208_v1.4 |
| TS462 | Zheng | 91.10 | TS462_v1.6 |
| TS408 | SNU-CHEM-lig | 90.61 | TS408_v1.1 |
| TS055 | LCDD-team | 90.40 | TS055_v1.4 |
| TS022 | Yang | 90.16 | TS022_v1.4 |
| TS465 | Wallner | 89.57 | TS465_v1.3 |
| TS202 | test001 | 89.38 | TS202_v1.5 |
| TS110 | MIEnsembles-Server | 88.23 | TS110_v1.2 |
| TS388 | DeepFold-server | 86.53 | TS388_v1.4 |
| TS423 | ShanghaiTech-server | 85.97 | TS423_v1.1 |
| TS147 | Zheng-Multimer | 85.96 | TS147_v1.1 |
| TS091 | Huang-HUST | 85.80 | TS091_v1.2 |
| TS102 | Psi-Phi | 85.59 | TS102_v1.5 |
| TS287 | plmfold | 85.58 | TS287_v1.1 |
| TS375 | milliseconds | 85.40 | TS375_v1.3 |
| TS393 | GuijunLab-QA | 85.37 | TS393_v1.1 |
| TS148 | Guijunlab-Complex | 85.37 | TS148_v1.5 |
| TS264 | GuijunLab-Human | 85.37 | TS264_v1.1 |
| TS314 | GuijunLab-PATHreader | 85.37 | TS314_v1.1 |
| TS312 | GuijunLab-Assembly | 85.37 | TS312_v1.1 |
| TS227 | KUMC | 85.28 | TS227_v1.3 |
| TS425 | MULTICOM_GATE | 85.12 | TS425_v1.2 |
| TS319 | MULTICOM.LLM | 85.12 | TS319_v1.3 |
| TS014 | Cool-PSP | 84.85 | TS014_v1.5 |
| TS311 | RAGfold_Prot1 | 84.80 | TS311_v1.4 |
| TS207 | MULTICOM_ligand | 84.68 | TS207_v1.2 |
| TS225 | Unknown | 84.58 | TS225_v1.1 |
| TS164 | McGuffin | 84.58 | TS164_v1.1 |
| TS163 | MultiFOLD2 | 84.58 | TS163_v1.1 |
| TS294 | KiharaLab | 84.28 | TS294_v1.2 |
| TS196 | HYU_MLLAB | 84.21 | TS196_v1.4 |
| TS019 | Zheng-Server | 84.18 | TS019_v1.1 |
| TS475 | ptq | 84.06 | TS475_v1.3 |
| TS304 | AF3-server | 83.94 | TS304_v1.2 |
| TS241 | elofsson | 83.94 | TS241_v1.2 |
| TS301 | GHZ-MAN | 83.68 | TS301_v1.2 |
| TS267 | kiharalab_server | 83.67 | TS267_v1.2 |

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Supplementary Table S4 – continued from previous page

| Group | Group_Name | V1_Composite_Score_4 | V1_Model |
|-------|--------------------|----------------------|------------|
| TS079 | MRAFold | 83.64 | TS079_v1.5 |
| TS293 | MRAH | 83.63 | TS293_v1.2 |
| TS167 | OpenComplex | 83.59 | TS167_v1.2 |
| TS450 | OpenComplex_Server | 83.59 | TS450_v1.5 |
| TS345 | MULTICOM_human | 83.45 | TS345_v1.4 |
| TS284 | Unicorn | 83.42 | TS284_v1.2 |
| TS075 | GHZ-ISM | 83.42 | TS075_v1.2 |
| TS369 | Bhattacharya | 83.22 | TS369_v1.1 |
| TS122 | MQA_server | 83.13 | TS122_v1.4 |
| TS051 | MULTICOM | 83.12 | TS051_v1.3 |
| TS331 | MULTICOM_AI | 83.12 | TS331_v1.3 |
| TS145 | colabfold_baseline | 83.12 | TS145_v1.5 |
| TS017 | Seder2024hard | 83.12 | TS017_v1.3 |
| TS235 | isyslab-hust | 82.62 | TS235_v1.3 |
| TS198 | colabfold | 82.61 | TS198_v1.4 |
| TS400 | OmniFold | 82.22 | TS400_v1.1 |
| TS272 | GromihaLab | 82.11 | TS272_v1.1 |
| TS464 | PocketTracer | 81.86 | TS464_v1.5 |
| TS221 | CSSB_FAKER | 74.21 | TS221_v1.3 |
| TS419 | CSSB-Human | 74.21 | TS419_v1.3 |
| TS269 | CSSB_server | 74.20 | TS269_v1.3 |
| TS020 | compopharmunibas | 74.16 | TS020_v1.3 |
| TS052 | Yang-Server | 73.95 | TS052_v1.1 |
| TS456 | Yang-Multimer | 73.37 | TS456_v1.1 |
| TS059 | DeepFold | 73.02 | TS059_v1.6 |
| TS139 | DeepFold-refine | 73.02 | TS139_v1.6 |
| TS204 | Zou | 72.76 | TS204_v1.5 |
| TS262 | CoDock | 71.81 | TS262_v1.3 |
| TS120 | Cerebra | 60.41 | TS120_v1.6 |
| TS039 | arosko | 53.05 | TS039_v1.3 |
| TS286 | CSSB_experimental | 51.91 | TS286_v1.2 |
| TS274 | kozakovvajda | 50.66 | TS274_v1.3 |
| TS494 | ClusPro | 50.66 | TS494_v1.3 |
| TS040 | DELCLAB | 50.16 | TS040_v1.3 |
| TS275 | Seminole | 39.95 | TS275_v1.1 |
| TS461 | forlilab | 36.73 | TS461_v1.2 |
| TS361 | Cerebra_server | 34.59 | TS361_v1.1 |
| TS132 | profold2 | 10.44 | TS132_v1.1 |

Supplementary Table S5: Results for T1214 GDT TS single state

| Group | Group_Name | V1_GDT_TS | V1_Model |
|-------|----------------------|-----------|------------|
| TS015 | PEZYFoldings | 96.41 | TS015_v1.2 |
| TS298 | ShanghaiTech-human | 95.27 | TS298_v1.1 |
| TS386 | ShanghaiTech-Ligand | 95.27 | TS386_v1.1 |
| TS388 | DeepFold-server | 95.23 | TS388_v1.4 |
| TS022 | Yang | 95.05 | TS022_v1.4 |
| TS319 | MULTICOM_LLM | 94.78 | TS319_v1.3 |
| TS423 | ShanghaiTech-server | 94.78 | TS423_v1.5 |
| TS425 | MULTICOM_GATE | 94.78 | TS425_v1.2 |
| TS110 | MIEnsembles-Server | 94.67 | TS110_v1.1 |
| TS465 | Wallner | 94.44 | TS465_v1.4 |
| TS167 | OpenComplex | 94.44 | TS167_v1.2 |
| TS450 | OpenComplex_Server | 94.44 | TS450_v1.5 |
| TS345 | MULTICOM_human | 94.33 | TS345_v1.4 |
| TS208 | falcon2 | 94.29 | TS208_v1.4 |
| TS091 | Huang-HUST | 94.25 | TS091_v1.2 |
| TS375 | milliseconds | 94.25 | TS375_v1.3 |
| TS019 | Zheng-Server | 94.21 | TS019_v1.2 |
| TS079 | MRAFold | 94.21 | TS079_v1.5 |
| TS293 | MRAH | 94.17 | TS293_v1.5 |
| TS408 | SNU-CHEM-lig | 94.06 | TS408_v1.1 |
| TS311 | RAGfold_Prot1 | 94.02 | TS311_v1.2 |
| TS055 | LCDD-team | 93.99 | TS055_v1.3 |
| TS264 | GuijunLab-Human | 93.95 | TS264_v1.3 |
| TS393 | GuijunLab-QA | 93.95 | TS393_v1.5 |
| TS051 | MULTICOM | 93.91 | TS051_v1.5 |
| TS331 | MULTICOM_AI | 93.91 | TS331_v1.5 |
| TS312 | GuijunLab-Assembly | 93.87 | TS312_v1.1 |
| TS314 | GuijunLab-PATHreader | 93.87 | TS314_v1.1 |
| TS148 | Guijunlab-Complex | 93.87 | TS148_v1.5 |
| TS235 | isyslab-hust | 93.87 | TS235_v1.3 |
| TS227 | KUMC | 93.83 | TS227_v1.5 |
| TS147 | Zheng-Multimer | 93.83 | TS147_v1.2 |
| TS462 | Zheng | 93.83 | TS462_v1.2 |
| TS267 | kiharalab_server | 93.80 | TS267_v1.1 |
| TS284 | Unicorn | 93.76 | TS284_v1.1 |
| TS475 | ptq | 93.76 | TS475_v1.3 |
| TS075 | GHZ-ISM | 93.76 | TS075_v1.1 |
| TS102 | Psi-Phi | 93.68 | TS102_v1.2 |
| TS122 | MQA_server | 93.68 | TS122_v1.2 |
| TS287 | plmfold | 93.53 | TS287_v1.1 |
| TS014 | Cool-PSP | 93.50 | TS014_v1.3 |

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Supplementary Table S5 – continued from previous page

| Group | Group_Name | V1_GDT_TS | V1_Model |
|-------|--------------------|-----------|------------|
| TS052 | Yang-Server | 93.50 | TS052.v1.3 |
| TS196 | HYU_MLLAB | 93.46 | TS196.v1.2 |
| TS207 | MULTICOM_ligand | 93.42 | TS207.v1.1 |
| TS301 | GHZ-MAN | 93.38 | TS301.v1.1 |
| TS198 | colabfold | 93.38 | TS198.v1.5 |
| TS464 | PocketTracer | 93.38 | TS464.v1.5 |
| TS369 | Bhattacharya | 93.34 | TS369.v1.1 |
| TS272 | GromihaLab | 93.31 | TS272.v1.3 |
| TS164 | McGuffin | 93.19 | TS164.v1.3 |
| TS163 | MultiFOLD2 | 93.19 | TS163.v1.3 |
| TS304 | AF3-server | 93.15 | TS304.v1.4 |
| TS241 | elofsson | 93.15 | TS241.v1.4 |
| TS145 | colabfold_baseline | 93.12 | TS145.v1.2 |
| TS017 | Seder2024hard | 93.12 | TS017.v1.4 |
| TS225 | Unknown | 92.93 | TS225.v1.1 |
| TS400 | OmniFold | 92.85 | TS400.v1.1 |
| TS456 | Yang-Multimer | 92.62 | TS456.v1.3 |
| TS262 | CoDock | 92.44 | TS262.v1.5 |
| TS294 | KiharaLab | 92.32 | TS294.v1.2 |
| TS020 | comppharmunibas | 92.13 | TS020.v1.3 |
| TS139 | DeepFold-refine | 90.92 | TS139.v1.6 |
| TS059 | DeepFold | 90.92 | TS059.v1.6 |
| TS221 | CSSB_FAKER | 90.55 | TS221.v1.3 |
| TS419 | CSSB-Human | 90.55 | TS419.v1.3 |
| TS204 | Zou | 90.32 | TS204.v1.3 |
| TS269 | CSSB_server | 90.32 | TS269.v1.3 |
| TS286 | CSSB_experimental | 89.79 | TS286.v1.4 |
| TS202 | test001 | 89.56 | TS202.v1.5 |
| TS040 | DELCLAB | 87.94 | TS040.v1.2 |
| TS039 | arosko | 87.03 | TS039.v1.1 |
| TS494 | ClusPro | 86.65 | TS494.v1.1 |
| TS274 | kozakovvajda | 86.65 | TS274.v1.1 |
| TS120 | Cerebra | 85.70 | TS120.v1.6 |
| TS275 | Seminole | 78.71 | TS275.v1.1 |
| TS461 | forlilab | 76.74 | TS461.v1.3 |
| TS361 | Cerebra_server | 76.55 | TS361.v1.3 |
| TS132 | profold2 | 54.50 | TS132.v1.1 |

Supplementary Table S6: Results for T1214 GlobalLDDT single state

| Group | Group_Name | V1_gLDDT | V1_Model |
|-------|----------------------|----------|------------|
| TS015 | PEZYZFoldings | 0.87 | TS015_v1.5 |
| TS298 | ShanghaiTech-human | 0.86 | TS298_v1.4 |
| TS386 | ShanghaiTech-Ligand | 0.86 | TS386_v1.4 |
| TS208 | falcon2 | 0.86 | TS208_v1.4 |
| TS388 | DeepFold-server | 0.86 | TS388_v1.4 |
| TS022 | Yang | 0.85 | TS022_v1.4 |
| TS319 | MULTICOM_LLM | 0.85 | TS319_v1.3 |
| TS425 | MULTICOM_GATE | 0.85 | TS425_v1.2 |
| TS375 | milliseconds | 0.85 | TS375_v1.3 |
| TS465 | Wallner | 0.85 | TS465_v1.2 |
| TS423 | ShanghaiTech-server | 0.85 | TS423_v1.5 |
| TS102 | Psi-Phi | 0.85 | TS102_v1.5 |
| TS019 | Zheng-Server | 0.85 | TS019_v1.2 |
| TS110 | MIEnsembles-Server | 0.85 | TS110_v1.2 |
| TS462 | Zheng | 0.85 | TS462_v1.1 |
| TS147 | Zheng-Multimer | 0.85 | TS147_v1.1 |
| TS264 | GuijunLab-Human | 0.85 | TS264_v1.1 |
| TS148 | Guijunlab-Complex | 0.85 | TS148_v1.5 |
| TS393 | GuijunLab-QA | 0.85 | TS393_v1.1 |
| TS312 | GuijunLab-Assembly | 0.85 | TS312_v1.1 |
| TS314 | GuijunLab-PATHreader | 0.85 | TS314_v1.1 |
| TS287 | plmfold | 0.85 | TS287_v1.2 |
| TS167 | OpenComplex | 0.85 | TS167_v1.2 |
| TS450 | OpenComplex_Server | 0.85 | TS450_v1.5 |
| TS284 | Unicorn | 0.85 | TS284_v1.1 |
| TS207 | MULTICOM_ligand | 0.85 | TS207_v1.2 |
| TS075 | GHZ-ISM | 0.85 | TS075_v1.1 |
| TS227 | KUMC | 0.85 | TS227_v1.3 |
| TS267 | kiharalab_server | 0.85 | TS267_v1.1 |
| TS311 | RAGfold_Prot1 | 0.85 | TS311_v1.4 |
| TS331 | MULTICOM_AI | 0.85 | TS331_v1.1 |
| TS051 | MULTICOM | 0.85 | TS051_v1.1 |
| TS345 | MULTICOM_human | 0.85 | TS345_v1.4 |
| TS369 | Bhattacharya | 0.85 | TS369_v1.1 |
| TS091 | Huang-HUST | 0.85 | TS091_v1.2 |
| TS293 | MRAH | 0.85 | TS293_v1.2 |
| TS079 | MRAFold | 0.85 | TS079_v1.1 |
| TS272 | GromihaLab | 0.84 | TS272_v1.3 |
| TS304 | AF3-server | 0.84 | TS304_v1.4 |
| TS241 | elofsson | 0.84 | TS241_v1.4 |
| TS122 | MQA_server | 0.84 | TS122_v1.5 |

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Supplementary Table S6 – continued from previous page

| Group | Group_Name | V1_gLDDT | V1_Model |
|-------|--------------------|----------|------------|
| TS235 | isyslab-hust | 0.84 | TS235_v1.3 |
| TS464 | PocketTracer | 0.84 | TS464_v1.1 |
| TS198 | colabfold | 0.84 | TS198_v1.5 |
| TS014 | Cool-PSP | 0.84 | TS014_v1.4 |
| TS301 | GHZ-MAN | 0.84 | TS301_v1.2 |
| TS052 | Yang-Server | 0.84 | TS052_v1.3 |
| TS196 | HYU_MLLAB | 0.84 | TS196_v1.3 |
| TS400 | OmniFold | 0.84 | TS400_v1.1 |
| TS163 | MultiFOLD2 | 0.84 | TS163_v1.3 |
| TS164 | McGuffin | 0.84 | TS164_v1.3 |
| TS408 | SNU-CHEM-lig | 0.84 | TS408_v1.3 |
| TS145 | colabfold_baseline | 0.84 | TS145_v1.2 |
| TS017 | Seder2024hard | 0.84 | TS017_v1.4 |
| TS294 | KiharaLab | 0.84 | TS294_v1.2 |
| TS225 | Unknown | 0.83 | TS225_v1.1 |
| TS456 | Yang-Multimer | 0.83 | TS456_v1.5 |
| TS475 | ptq | 0.83 | TS475_v1.5 |
| TS262 | CoDock | 0.83 | TS262_v1.1 |
| TS055 | LCDD-team | 0.82 | TS055_v1.3 |
| TS020 | comppharmunibas | 0.82 | TS020_v1.3 |
| TS269 | CSSB_server | 0.81 | TS269_v1.5 |
| TS419 | CSSB-Human | 0.81 | TS419_v1.3 |
| TS221 | CSSB_FAKER | 0.81 | TS221_v1.3 |
| TS139 | DeepFold-refine | 0.81 | TS139_v1.6 |
| TS059 | DeepFold | 0.81 | TS059_v1.6 |
| TS202 | test001 | 0.81 | TS202_v1.5 |
| TS204 | Zou | 0.81 | TS204_v1.5 |
| TS286 | CSSB_experimental | 0.80 | TS286_v1.2 |
| TS040 | DELCLAB | 0.75 | TS040_v1.5 |
| TS494 | ClusPro | 0.75 | TS494_v1.1 |
| TS274 | kozakovvajda | 0.75 | TS274_v1.1 |
| TS039 | arosko | 0.75 | TS039_v1.3 |
| TS120 | Cerebra | 0.72 | TS120_v1.6 |
| TS461 | forlilab | 0.71 | TS461_v1.2 |
| TS275 | Seminoles | 0.69 | TS275_v1.1 |
| TS361 | Cerebra_server | 0.63 | TS361_v1.1 |
| TS132 | profold2 | 0.48 | TS132_v1.1 |

Supplementary Table S7: Results for T1214 TMscore single state

| Group | Group_Name | V1_TMscore | V1_Model |
|-------|----------------------|------------|------------|
| TS015 | PEZYFoldings | 0.99 | TS015_v1.2 |
| TS298 | ShanghaiTech-human | 0.99 | TS298_v1.1 |
| TS386 | ShanghaiTech-Ligand | 0.99 | TS386_v1.1 |
| TS208 | falcon2 | 0.99 | TS208_v1.4 |
| TS465 | Wallner | 0.99 | TS465_v1.3 |
| TS022 | Yang | 0.99 | TS022_v1.4 |
| TS408 | SNU-CHEM-lig | 0.99 | TS408_v1.1 |
| TS055 | LCDD-team | 0.99 | TS055_v1.3 |
| TS388 | DeepFold-server | 0.99 | TS388_v1.4 |
| TS462 | Zheng | 0.99 | TS462_v1.6 |
| TS319 | MULTICOM.LLM | 0.99 | TS319_v1.3 |
| TS425 | MULTICOM.GATE | 0.99 | TS425_v1.2 |
| TS423 | ShanghaiTech-server | 0.99 | TS423_v1.1 |
| TS110 | MIEnsembles-Server | 0.99 | TS110_v1.2 |
| TS375 | milliseconds | 0.99 | TS375_v1.3 |
| TS091 | Huang-HUST | 0.99 | TS091_v1.2 |
| TS019 | Zheng-Server | 0.99 | TS019_v1.2 |
| TS311 | RAGfold.Prot1 | 0.99 | TS311_v1.1 |
| TS102 | Psi-Phi | 0.99 | TS102_v1.1 |
| TS287 | plmfold | 0.99 | TS287_v1.2 |
| TS227 | KUMC | 0.99 | TS227_v1.2 |
| TS393 | GuijunLab-QA | 0.99 | TS393_v1.1 |
| TS475 | ptq | 0.99 | TS475_v1.3 |
| TS312 | GuijunLab-Assembly | 0.99 | TS312_v1.1 |
| TS314 | GuijunLab-Pathreader | 0.99 | TS314_v1.1 |
| TS148 | Guijunlab-Complex | 0.99 | TS148_v1.5 |
| TS264 | GuijunLab-Human | 0.99 | TS264_v1.1 |
| TS284 | Unicorn | 0.99 | TS284_v1.3 |
| TS075 | GHZ-ISM | 0.99 | TS075_v1.3 |
| TS122 | MQA_server | 0.99 | TS122_v1.2 |
| TS167 | OpenComplex | 0.99 | TS167_v1.2 |
| TS450 | OpenComplex_Server | 0.99 | TS450_v1.5 |
| TS051 | MULTICOM | 0.99 | TS051_v1.1 |
| TS079 | MRAFold | 0.99 | TS079_v1.5 |
| TS345 | MULTICOM_human | 0.99 | TS345_v1.4 |
| TS331 | MULTICOM.AI | 0.99 | TS331_v1.1 |
| TS014 | Cool-PSP | 0.99 | TS014_v1.4 |
| TS147 | Zheng-Multimer | 0.99 | TS147_v1.4 |
| TS293 | MRAH | 0.99 | TS293_v1.3 |
| TS207 | MULTICOM_ligand | 0.99 | TS207_v1.3 |
| TS267 | kiharalab_server | 0.99 | TS267_v1.1 |

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Supplementary Table S7 – continued from previous page

| Group | Group_Name | V1_TMscore | V1_Model |
|-------|--------------------|------------|------------|
| TS235 | isyslab-hust | 0.99 | TS235_v1.3 |
| TS164 | McGuffin | 0.98 | TS164_v1.1 |
| TS163 | MultiFOLD2 | 0.98 | TS163_v1.1 |
| TS369 | Bhattacharya | 0.98 | TS369_v1.1 |
| TS196 | HYU_MLLAB | 0.98 | TS196_v1.2 |
| TS225 | Unknown | 0.98 | TS225_v1.1 |
| TS301 | GHZ-MAN | 0.98 | TS301_v1.2 |
| TS304 | AF3-server | 0.98 | TS304_v1.2 |
| TS241 | elofsson | 0.98 | TS241_v1.2 |
| TS272 | GromihaLab | 0.98 | TS272_v1.4 |
| TS202 | test001 | 0.98 | TS202_v1.5 |
| TS198 | colabfold | 0.98 | TS198_v1.5 |
| TS464 | PocketTracer | 0.98 | TS464_v1.3 |
| TS400 | OmniFold | 0.98 | TS400_v1.1 |
| TS017 | Seder2024hard | 0.98 | TS017_v1.4 |
| TS145 | colabfold_baseline | 0.98 | TS145_v1.2 |
| TS294 | KiharaLab | 0.98 | TS294_v1.2 |
| TS020 | comppharmunibas | 0.98 | TS020_v1.4 |
| TS052 | Yang-Server | 0.98 | TS052_v1.1 |
| TS456 | Yang-Multimer | 0.98 | TS456_v1.5 |
| TS221 | CSSB_FAKER | 0.97 | TS221_v1.3 |
| TS419 | CSSB-Human | 0.97 | TS419_v1.3 |
| TS269 | CSSB_server | 0.97 | TS269_v1.3 |
| TS059 | DeepFold | 0.97 | TS059_v1.6 |
| TS139 | DeepFold-refine | 0.97 | TS139_v1.6 |
| TS262 | CoDock | 0.97 | TS262_v1.5 |
| TS204 | Zou | 0.97 | TS204_v1.3 |
| TS286 | CSSB_experimental | 0.97 | TS286_v1.2 |
| TS120 | Cerebra | 0.97 | TS120_v1.6 |
| TS275 | Seminole | 0.96 | TS275_v1.1 |
| TS040 | DELCLAB | 0.96 | TS040_v1.3 |
| TS461 | forlilab | 0.96 | TS461_v1.2 |
| TS039 | arosko | 0.96 | TS039_v1.1 |
| TS494 | ClusPro | 0.95 | TS494_v1.3 |
| TS274 | kozakovvajda | 0.95 | TS274_v1.3 |
| TS361 | Cerebra_server | 0.95 | TS361_v1.1 |
| TS132 | profold2 | 0.80 | TS132_v1.1 |