MMpred: a distance-assisted multimodal conformation sampling for de novo protein structure prediction

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Abstract

Motivation: The mathematically optimal solution in computational protein folding simulations does not always correspond to the native structure, due to the imperfection of the energy force fields. There is therefore a need to search for more diverse suboptimal solutions in order to identify the states close to the native. We propose a novel multimodal optimization protocol to improve the conformation sampling efficiency and modeling accuracy of de novo protein structure folding simulations.

Results: A distance-assisted multimodal optimization sampling algorithm, MMpred, is proposed for de novo protein structure prediction. The protocol consists of three stages: The first is a modal exploration stage, in which a structural similarity evaluation model DMscore is designed to control the diversity of conformations, generating a population of diverse structures in different low-energy basins. The second is a modal maintaining stage, where an adaptive clustering algorithm MNDcluster is proposed to divide the populations and merge the modal by adjusting the annealing temperature to locate the promising basins. In the last stage of modal exploitation, a greedy search strategy is used to accelerate the convergence of the modal. Distance constraint information is used to construct the conformation scoring model to guide sampling. MMpred is tested on a large set of 320 non-redundant proteins, where MMpred obtains models with TM-score$\geq$0.5 on 268 cases, which is 20.3% higher than that of Rosetta guided with the same set of distance constraints. The results showed that MMpred can help significantly improve the model accuracy of protein assembly simulations through the sampling of multiple promising energy basins with enhanced structural diversity.

Availability: The source code and executable versions are freely available at https://github.com/iobio-zjut/MMpred.

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1 Introduction

As the function of a protein is dependent on its structure, predicting protein structure from its amino acid sequence has been a grand challenge in biology for decades (Abriata *et al.*, 2019; Bradley *et al.*, 2005; Dill and MacCallum, 2012). Protein structure prediction, especially de novo prediction, has made a major breakthrough in recent years, due to the drastic improvement of the accuracy of residue-residue contact and distance prediction (Shrestha *et al.*, 2019). Nevertheless, due to the high dimensionality of protein conformational space, conformation sampling represents still one of the main bottlenecks in de novo protein structure prediction. Monte Carlo (Zhang et al., 2002; Rohl *et al.*, 2004; Gregory *et al.*, 2009; Xu and Zhang 2012), evolutionary algorithm (Zhou *et al.*, 2019; Liu *et al.*, 2019; Peng *et al.*, 2020), multi-objective optimization (Olson and Shehu, 2014), and many other sampling strategies have been proposed to explore the conformational space.

Large-scale conformational sampling is usually based on coarse-grained energy function (Kuhlman *et al.*, 2019; Francois *et al.*, 2011). However, the coarse-grained model also introduces inaccuracy while reducing the search space dimension and improving computational efficiency (Lindorff-Larsen *et al.*, 2011; Lazaridis and Karplus, 2000). As illustrated in **Figure 1**, the lowest energy model (in basin A) does not necessarily correspond to the native structure, and the model in the local basin B of the energy landscape may be closer to it. Therefore, searching only the lowest free energy structure is insufficient, and sampling local minimum solutions with structural diversity in different low energy basins is also important (Park *et al.*, 2018; Rohl *et al.*, 2004; Zhou *et al.*,2019). Rosetta samples a large number of low-energy conformations by running thousands of independent Metropolitan Monte Carlo trajectories in parallel to reveal the local minimum of the energy surface (Raman *et al.*,2008; Zhou and Zhang, 2018). C-QUARK performs a replica-exchange Monte Carlo folding simulation to generate a large number of conformations, which are submitted to SPICKER for clustering, and the model is selected in the most populated clusters instead of the clusters with lowest energy (Zheng *et al.*, 2019; Xu and Zhang, 2012). Memetic evolutionary algorithm has been proposed to sample a diverse ensemble of conformations through genetic operators, which promote the exploration of protein conformational space (Garza-Fabre *et al.*, 2016). These methods alleviate the sampling problem based on inaccurate energy function to a certain extent, but the adaptive determination of cluster number and rapid evaluation of structural similarity need further to be investigated.
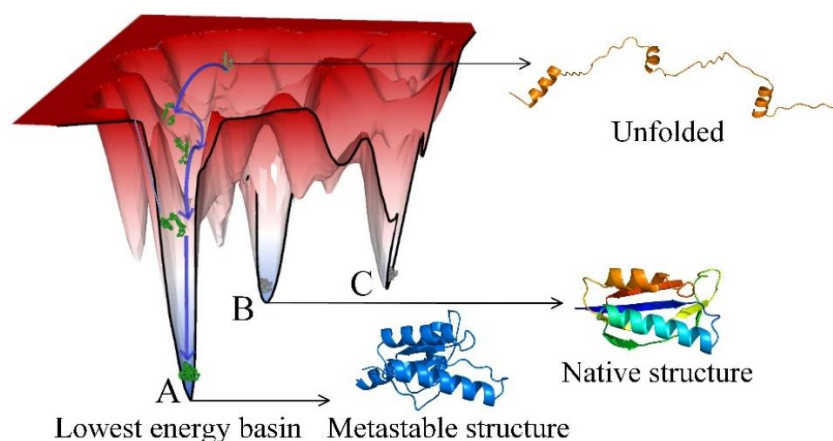

Fig.1. Schematic diagram of protein-folding energy landscape.

To help reshape the energy landscape, inter-residue contact and distance maps have been proposed and shown usefulness for de novo protein structure prediction (Senior *et al*., 2019; Xu and Wang, 2019; Kandathil *et al*., 2019; Li *et al*., 2019). In particular, AlphaFold and RaptorX focused on distance prediction and distance-based protein structure modeling in CASP13. AlphaFold (A7D) constructs the potential energy of the average force from the predicted distance information, which is optimized by the stochastic gradient descent algorithm to generate the structure (Senior *et al*., 2020). RaptorX inputs the predicted distance, secondary structure, and torsion angles predicted by deep convolutional neural networks into the Crystallography and NMR system (CNS) (Brunger et al., 2007) to quickly constructed an accurate 3D model (Xu, 2019; Wang *et al*., 2017). In DMPfold (Gregory *et al*.,2019), the inter-residue distances, hydrogen bonds and torsion angles predicted from DMP are used to generate models with CNS, and a single model is used as additional input to refine the distances and hydrogen bonds. trRosetta introduces inter-residue orientation prediction and uses the predicted orientation and distance to construct constraints for Rosetta-constrained energy minimization protocol in order to generate structure models (Yang *et al*., 2020). However, the predicted contact distance is not sufficiently accurate and has the same defects as the abovementioned energy function (Hou *et al*., 2019).

De novo protein structure prediction based on energy (or distance) -guided conformation sampling is essentially an uncertain optimization problem. Multimodal optimization can discover and maintain multiple feasible solutions (Stoean *et al*., 2010; Sareni *et al*., 1998), which is critical for improving the efficiency of conformational sampling. In this study, a distance-assisted de novo protein structure prediction by multimodal conformation sampling algorithm (MMpred) is proposed. First, the crowding strategy is designed based on the structural similarity evaluation model to explore the conformation space extensively and generate a population of conformations with structural diversity. Then, an adaptive clustering algorithm and a modal merging strategy are used to divide and maintain the modal, respectively. Finally, a greedy search strategy is used to accelerate the convergence of the modal. MMpred can discover and exploit multiple promising low-energy basins to sample a set of diverse structures and ultimately improve structure prediction accuracy.

2 Materials and methods

The pipeline of MMpred is illustrated **Figure 2**. For the query sequence, the fragment library is built by Robetta (http://robetta.bakerlab.org/), and the inter-residue distance is predicted by trRosetta (https://yanglab.nankai.edu.cn/). The initial population is generated by the random fragment assembly. The population goes through three stages of evolution, and finally five prediction models are generated. In the first modal exploration stage, a structural similarity evaluation model, DMscore, is designed to select the conformation that is the most similar to the trial conformation produced by fragment assembly in the population for conformation replacement. In the second modal maintaining stage, an adaptive clustering algorithm, MNDcluster, is proposed to divide the population and then merge the modal by adjusting the annealing temperature to locate promising models. In the final modal exploitation stage, a greedy search strategy is used to accelerate the convergence of the modal. Finally, the modal are sorted according to the average distance score of the conformations in the modal, and the model with the lowest distance score among the top five modals is selected as the final model.
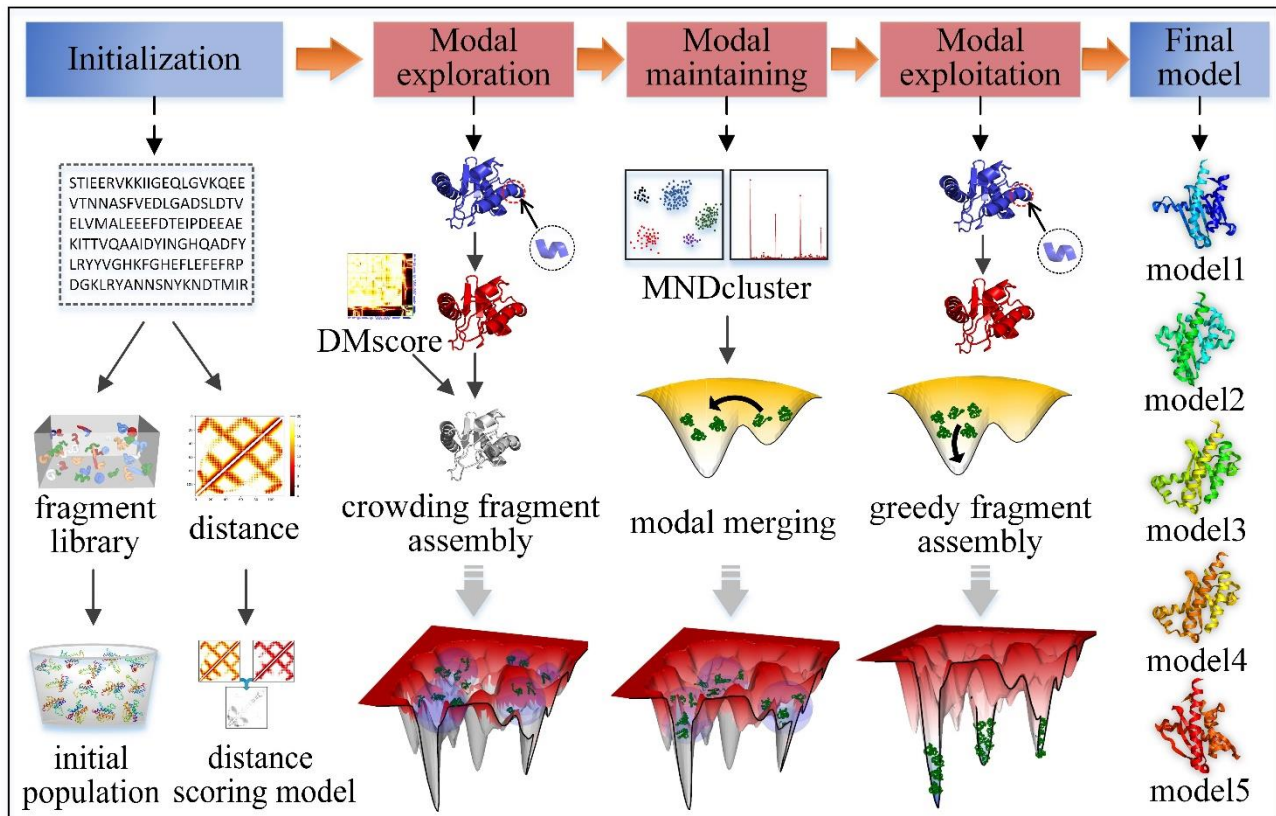
Fig.2. The pipeline of MMpred for multimodal conformation sampling.

2.1 Modal exploration

Maintaining the diversity of the population during the evolution is the key to the multimodal optimization algorithm. The purpose of modal exploration is to generate a conformation population with structural diversity in different low-energy regions through extensive sampling of conformational spaces to obtain a broad view. We use a crowding strategy to maintain population diversity during evolution (De Jong, 1975; Ling *et al*., 2008). Its principle is to replace the most similar conformation in the population with an offspring. However, effective crowding strategies depend on similarity metrics (Thomsen *et al*., 2004). Therefore, we designed a structural similarity evaluation model based on the comparison of residue distance maps (DMscore) to evaluate the structural similarity between two conformations (Simoncini *et al*., 2017; Zhang *et al*., 2004; Cheng *et al*., 2019).

2.1.1 DMscore

DMscore measures the similarity by calculating the difference of Euclidean distance of the corresponding residue pairs in two models, which is defined as follows:

$$\text{DMscore}(a,b) = \frac{1}{L(L-1)}\sum_{i=1}^{L}\sum_{j=1}^{L} K_{i,j} \tag{1}$$

$$K_{i,j} = \frac{1}{1 + \left(\dfrac{d_{i,j}^{a} - d_{i,j}^{b}}{d^{*}}\right)^{2}} \tag{2}$$

where L is the length of the protein structure; $d_{i,j}^{a}$ and $d_{i,j}^{b}$ are the distances between the i th and j th

residues in model a and model b, respectively; and d^* is the normalized scale used to eliminate the inherent dependence of the score on protein size. The value range of $\left(d_{i,j}^a - d_{i,j}^b\right)$ varies with the sequence distance between i and j. So it is unreasonable to set d^* as a constant. We analyzed the relationship between the average Euclidean distance between residues and the length of the protein on the native structure of 500 non-redundant targets with length ranges from 40 to 700. As shown in **Supplementary Figure S1**, the average distance between residues increases logarithmically with increasing protein length. Therefore, d^* is defined as the logarithm of the residue sequence distance, namely:

$$d^* = \log\left(\varepsilon + |i - j|\right), i \neq j \tag{3}$$

where ε is an infinitely small quantity to avoid d^* being zero. The value of DMscore is between (0,1]. The higher value indicates higher similarity between the two models; 1 indicates a perfect match between two models.
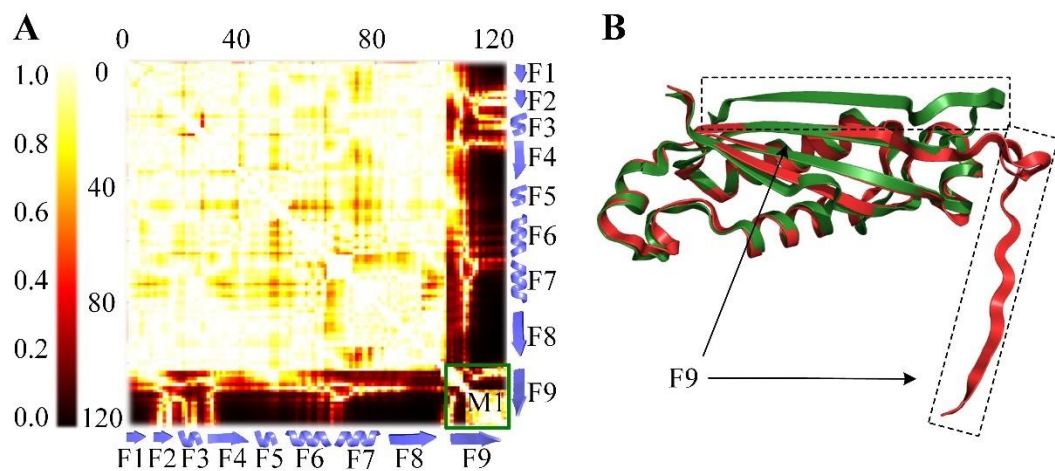
Fig.3. (A) is the comparison of the real distance map of two models, each point represents $K_{i,j}$; (B) is the superposition of the two models. The F1 to F8 of the two models in (B) are well aligned, corresponding to the bright color area (indicating high scores) in the upper left part of (A). F9 deviates from the overall structure significantly. The distance between F9 and other fragments in the two models is significantly different and corresponds to the dark area, which indicates low score. However, the F9 fragments of the two models are very similar. M1 shows a light color in the map, which gives a high score to local fragments.

Without complex structure rotation and translation such as RMSD and TM-score (Zhang et al., 2004), DMscore can quickly evaluate the structural similarity of two conformations by calculating the difference of Euclidian distance of corresponding residual pairs. As shown in **Figure 3**, the comparison of distance maps can well characterize the similarity of two structures. The structural similarity measure which is based on the global rigid body superposition has limitations. The similarity score is dominated by the part with the highest coverage. So, the part with the lowest coverage cannot be matched correctly, leading to artificially unfavorable scores (Hubbard *et al*., 1999; Mariani *et al*., 2013). DMscore not only evaluates the global topology but also considers the local structure differences.

2.1.2 Distance scoring model

The predicted distance constraint is used to construct the distance scoring model, which is used to guide

conformational sampling along with the energy function (Rosetta score3) (Ovchinnikov *et al*., 2018). The principle of the conformation scoring model based on the predicted inter-residue distance, named D_{score}, is the same as DMscore, as shown in **Supplementary Figure S2**. The difference is that D_{score} scores the conformation by calculating the similarity between the real distance map of the conformation and the predicted distance map. D_{score} can be calculated by

$$D_{score} = \sum_{i=1}^{L}\sum_{j=1}^{L} p_{i,j} \frac{\left| d_{i,j} - \bar{d}_{i,j} \right|}{d^*} \tag{4}$$

where $d_{i,j}$ and $\bar{d}_{i,j}$ are the distances between the i th and j th residues in target conformation and predicted distance map, respectively; d^* is a normalized scale calculated by Equation (3). $p_{i,j}$ is the probability of predicted distance. The distance difference is not calculated for the residue pair with no predicted value of distance. A smaller D_{score} indicates the conformation satisfies better the predicted distance constraints.

2.1.3 Crowding fragment assembly

The crowding fragment assembly is shown in **Supplementary Figure S4**. The trial conformation is obtained by the fragment assembly of the target conformation. The similarity between the trial conformation and each one in the population was calculated by DMscore. In order to improve the success rate of crowding, the top R conformations with the highest DMscore to the trial conformation are selected as the crowded subpopulation. The trial conformation is then attempted sequentially to replace each of the top R conformations starting with the ones with the highest DMscore until the replacement is successful or traverses all conformations in the subpopulation. Conformation replacement is performed by the Metropolis criterion based on energy function and D_{score} sequentially. After successive iterations, a population with diverse structures in different low-energy region is generated.

2.2 Modal maintaining

After obtaining a population with diverse structure distribution, the population will be gradually divided into multiple promising modals in the maintaining stage. Considering the differences in the population distribution of different target proteins, we propose a clustering algorithm to adaptively determine the number of clusters according to the multi-order nearest distance analysis (MNDcluster) (Rodriguez *et al*., 2014). MNDcluster can avoid unreasonable population division caused by a fixed number of clusters. Modal exploration may result in the conformation falling into the unpromising basins. So, we designed a modal merge strategy to merge the unpromising clusters and maintain the promising clusters by adjusting the annealing temperature.

2.2.1 MNDcluster

MNDcluster can obtain the global distribution information of the population by analyzing the distance of multi-order nearest neighbours. The number of clusters is adaptively counted by step information. Then, the K-medoids (Kaufman and Rousseeuw, 2009) algorithm is used to cluster the conformations according to the number of clusters.

The DMscore between conformations in the population is taken as their distance. d_1^i is the first-nearest neighbour distance of the i th conformation in the population, d_2^i is the second-nearest neighbour distance, and so on. These distances satisfy:

$$d_1^i < d_2^i < \cdots < d_{N-1}^i, \forall i = 1, 2, \cdots, N-1. \tag{5}$$

where N is the population size. The mean value and the mean square value of the j th nearest neighbour distances of all conformations are calculated as follows:

$$\overline{d}_j^2 = \frac{1}{N} \sum_{i=1}^{N} \left(d_j^i\right)^2, \forall j = 1, 2, \cdots, N-1. \tag{6}$$

$$\overline{d}_j = \frac{1}{N} \sum_{i=1}^{N} d_j^i, \forall j = 1, 2, \cdots, N-1. \tag{7}$$

The distribution of individuals determines the number of divisible populations. The distribution degree of the population is analyzed by calculating the variance, as follows:

$$S_m^2 = \frac{1}{m} \sum_{j=1}^{m} \left(\overline{d}_j^2 - \left(d_j^i\right)^2\right), \forall j, m = 1, 2, \cdots, N-1. \tag{8}$$

As shown in **Supplementary Figure S3**, the curvature change of variance linearized among individuals in the population is analyzed. The slope of the neighbouring individuals of the same subpopulation varies little. When the slope is calculated from one subpopulation to another, it fluctuates greatly. In the case of multiple populations, all step-jumping information can be captured in this way, and the global distribution of the current population can be obtained. MNDcluster can determine the distribution of the whole population without prior information and then obtain the statistics of the divisible population.

2.2.2 Modal merging

In order to identify the promising modal, a modal evaluation model based on cluster density and cluster size is designed as:

$$M_{score} = \frac{2\log_N X \times \overline{S}_{DMscore}}{\log_N X + \overline{S}_{DMscore}} \tag{9}$$

where N is the population size; X is the cluster size; and $\overline{S}_{DMscore}$ is the average DMscore between conformations in the cluster that reflects the density of the cluster. We define clusters with M_{score} greater than or equal to λ as promising modals.

In the modal maintaining stage, Monte Carlo simulated annealing search and crowding strategy are used to update the modal. The annealing temperature is adjusted to maintain the promising modalities and merge the unpromising modalities. The Monte Carlo simulated annealing search can accept the conformation with increased energy according to the probability. Its dynamic properties enable the conformation to jump out of the energy trap. The conformation update probability can be calculated by:

$$P(\Delta E) = \exp(-\Delta E / kT), kT = \begin{cases} 1, \text{if } M_{score} \geq \lambda \\ 5, \quad \text{otherwith} \end{cases} \tag{10}$$

where ΔE is the energy difference between the target conformation and trial conformation; and kT is the artificial "temperature" (Li and Scheraga, 1987). For promising modal, kT is set to 1. The purpose is to maintain the promising modal and prevent the loss of the modal caused by the deviation of the conformation from the current basin. For the unpromising modal, kT is set to 5. High temperature can increase the

probability of conformation update. Thus, the conformation jumps out of the current basin and enters a promising basin.

The conformational update during the modal maintaining stage is shown in **Supplementary Figure S5**. The DMscore between the trial conformation of the unpromising modal and the centroid of the nearest promising modal is calculated. The two conformations are considered to have similar topologies when DMscore is greater than or equal to 0.5, and the trial conformation is merged into the promising modal.

2.3 Modal exploitation

In the modal exploitation stage, the explored promising modal rapidly converge to the minimum by greedy searching, the flowchart is shown in **Supplementary Figure S6**. The target conformation is randomly selected from the subpopulation. The trial conformation is obtained by fragment assembly of the target. The distance scoring model and energy scoring model are successively used to evaluate the trial conformation. Metropolis criterion is used to determine whether the conformation with the lowest energy or the lowest D_{score} is replaced by trial conformation in the subpopulation. If it failed, the target conformation is passed on to the next generation. The greedy search strategy converges the subpopulations to the minimum of multiple basins, and then, a diverse set of protein conformations is sampled.

3 Results

3.1 Datasets

The benchmark set is constructed according to the SCOPe 2.07 (Fox *et al*., 2014). CD-HIT (Fu *et al*., 2012) is used to cluster the SCOPe dataset with a sequence identity cut-off of 30%, and the representative proteins of each cluster are selected to form 11,198 proteins. The protein is discarded if its length is outside the range of 50-200 residues or contains multiple domains, which result in 2,481 proteins. Finally, 320 proteins are randomly selected as the benchmark set by considering the protein type and length diversity. The detailed information of the benchmark set is shown in **Supplementary Table S1**. In addition, the 24 free modeling (FM) targets of the CASP13 experiment are used to further test the performance of MMpred. The detailed information is shown in Supplementary **Table S2**. The parameters of MMpred are described in **Table 1**.

Table 1. The parameter descriptions in MMpred.

Population size	N	400
Generation of exploration stage	G_a	500
Generation of maintaining stage	G_b	300
Generation of exploitation stage	G_c	800
Crowded subpopulation size (exploration)	R_a	$N/20$
Crowded subpopulation size (maintaining)	R_b	$N/40$
Energy temperature scaling factor	KT	2
D_{score} temperature scaling factor	KT_d	2
M_{score} threshold	λ	0.5
infinitely small quantity	ε	0.001

3.2 Comparison of MMpred and Rosetta-distance

MMpred is compared with distance-constrained Rosetta (Rosetta-distance) on the benchmark set. Both use the same fragment library without homologous structure. For Rosetta-distance, the distance scoring model that is the same as MMPred is used to guide the fragment assembly together with the energy function. 400 independent trajectories are run using Rosetta's ClassicAbinitio protocol with the increase_cycles equal to 1. The central model of the first cluster determined by SPICKER (Zhang and Skolnick, 2004) is considered as the final model.

The predicted results of MMpred and Rosetta-distance on the benchmark set are summarized in **Table 2**, and the detailed results of each protein are presented in **Supplementary Table S1**. The average TM-score of the first model by MMpred (0.629) is 17% higher than that of Rosetta-distance (0.537), and the average RMSD of MMpred (6.63Å) are reduced by 12.8% compared to Rosetta-distance (7.48Å). MMpred and Rosetta-distance obtain models with TM-score≥0.5 on 268 and 203 out of 320 proteins, accounting for 84% and 63% of the total protein, respectively. The significance test results (p-value = 1.09E-45) show that the performance of MMpred is significantly better than that of Rosetta-distance. Since MMpred and Rosetta-distance use the same distance constraint and fragment library, the comparison results reflect the contribution of multimodal optimization to the improvement of prediction accuracy. **Figure 4A** shows the TM-score distribution of the first model predicted by MMpred and Rosetta-distance.

Table 2. The predicted results of MMpred and Rosetta-distance. #TM ≥ 0.5 and #TM ≥ 0.8 are the number of the first model with TM-score ≥ 0.5 and TM-score ≥ 0.8, respectively. The last two columns are the results of the Wilcoxon signed rank test calculated based on the TM-score of the first model.

Method	(first model) TM-score	(first model) RMSD	(best model) TM-score	(best model) RMSD	#TM≥ 0.5	#TM≥ 0.8	p-value	Significance
MMpred	0.629	6.63	0.65	5.81	268	36	NA	NA
Rosetta-distance	0.537	7.48	0.558	6.56	203	10	1.09E-45	+
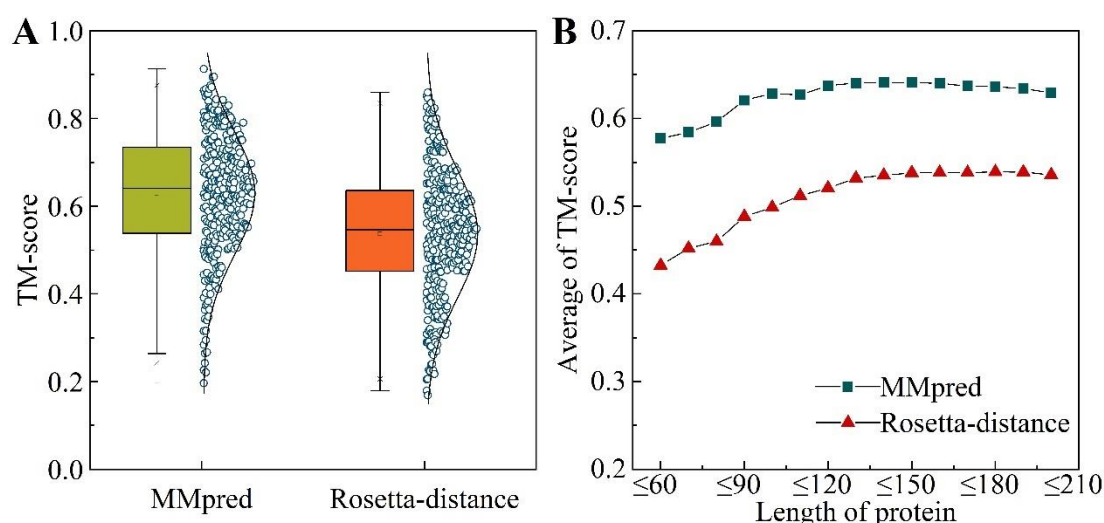
Fig.4. (A)Mean and distribution of TM-score for first model by MMpred and Rosetta-distance. (B)The relationship between the average TM-score of the first model of the benchmark set and the sequence length. The x-axis represents the threshold of sequence length, and the y-axis represents the average TM-score of all predicted models whose sequence length is less than the threshold.

Figure 4B shows the relationship between the TM-score and the sequence length. When the threshold of sequence length is less than or equal to 150, the average TM-score of MMpred gradually increases. The maximum value of 0.641 is reached when the threshold is equal to 150. With the further increase of the threshold value, the average TM-score decreases slightly. Part of the reason for the decreased performance is that the protein conformation space expands exponentially with the increase of sequence length. Therefore, there are more deceptive traps for proteins with larger sequence length, and MMpred needs to generate more conformational samples for the larger-size proteins to explore more promising low-energy basins. **Supplementary Figure S7** shows an example of a protein (PDB ID: 1RZ3_A) with the sequence length of 184. The TM-score of the predicted model increases from 0.463 to 0.607 when the population size increases from 400 to 800 and the generation of modal exploitation increases from 800 to 2000.

3.3 Results of CASP13 test set

MMpred is compared with four CASP server groups, i.e., C-QUARK (Zheng *et al.*, 2019), RaptorX-DeepModeller (Xu and Wang, 2019), BAKER-ROSETTASERVER (Park *et al.*, 2019) and MULTICOM_CLUSTER (Hou *et al.*, 2019) on 24 FM targets of CASP13. The results of these four groups are from the CASP official website (https://predictioncenter.org/download_area/). The detailed results of MMpred and these four methods are shown in **Supplementary Table S2**. MMpred obtains the highest TM-score on 7 targets, while C-QUARK, RaptorX-DeepModeller, BAKER-ROSETTASERVER, and MULTICOM_CLUSTER get the highest TM-score on 5, 8, 3, and 1 protein(s), respectively. MMpred achieves an average TM-score of 0.466 on all targets, which is slightly lower than those of C-QUARK and RaptorX-DeepModeller but higher than those of BAKER-ROSETTASERVER and MULTICOM_CLUSTER. The accuracies of the MMpred models on the three targets (T1005-D1, T0950-D1 and T0969-D1) with a sequence length greater than 300 are relatively low. **Figure 5** shows the relationship between model accuracy and protein size. When the sequence length is less than 300, little difference exists between MMpred and C-QUARK, and RaptorX-Deepmodeller. When the sequence length is less than 150 (with 16 proteins), MMpred achieves an average TM-score of 0.493, which is slightly higher than that by C-QUARK (0.488) and RaptorX-Deepmodeller (0.463).
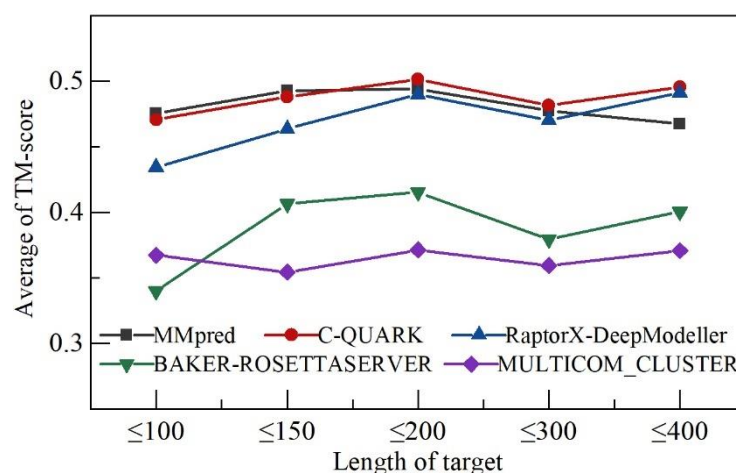
Fig.5. The relationship between the average TM-score of the first model and the sequence length on the 24 FM targets of CASP13. The x-axis represents the threshold of sequence length, and the y-axis represents the average TM-score of all predicted models whose sequence length is less than the threshold.

To further test the prediction performance of MMpred, a comparison with C-QUARK was performed on the 320 benchmark proteins. The result of C-QUARK is predicted by its online server (https://zhanglab.ccmb.med.umich.edu/C-QUARK/). C-QUARK uses multiple contact-maps and performs replica-exchange Monte Carlo for protein folding. The predicted results of MMpred and C-QUARK on the benchmark set are summarized in **Table 3**, and the detailed results of each protein are presented in **Supplementary Table S1**. The average TM-scores of the first model by MMpred and C-QUARK are 0.629 and 0.623, respectively. MMpred and C-QUARK generate models with TM-score$\geq$0.5 on 268 and 256 proteins, accounting for 84% and 80% of the total protein, respectively. The significance test results (*p*-value = 0.723) show that the performance of MMpred is comparable with that of C-QUARK.

Table 3. The predicted results of the first model of MMpred and C-QUARK. #TM $\geq$ 0.5 is the number of the first model with TM-score $\geq$ 0.5. The last two columns are the results of the Wilcoxon signed rank test calculated based on the TM-score of the first model.

Method	TM-score	#TM$\geq$0.5	*p*-value	Significance
MMpred	0.629	268	NA	NA
C-QUARK	0.623	256	0.723	$\approx$

3.4 Component analysis

To examine the effect of the three stages of MMpred on the performance of the algorithm, we construct and compare three different versions of MMpred, MMpred-A_C, MMpred-B_C and MMpred-C. MMpred-A_C includes the modal exploration and the modal exploitation, MMpred-B_C uses the modal maintaining and the modal exploitation, and MMpred-C only contains the modal exploitation. The predicted results of MMpred, MMpred-A_C, MMpred-B_C and MMpred-C on the benchmark set are summarized in **Table 4**, and the detailed results of each protein are presented in **Supplementary Table S3**.

Compared with MMpred-C, the average TM-score of the first model and the best model of MMpred-A_C improved by 11.5% and 11.6%, respectively. This shows that modal exploration is very important. It can discover and develop more potential basins and generate populations with higher structural diversity. The prediction accuracy of MMpred-B_C is only slightly improved compared with MMpred-C. This is due to the lack of effective exploration in the early stage, resulting in the modal maintaining stage cannot play an effective role. This can be reflected in the comparison with MMpred. After adding the exploration stage, the average prediction accuracy increases from 0.541 to 0.629, with an increase of 16.3%. The number of models with TM-score$\geq$0.5 also increases by 71. Compared with MMpred-A_C, the prediction accuracy of MMpred with modal maintaining stage added has also significantly improved. The average prediction accuracy is improved by 5.5%, and the number of models with TM-score$\geq$0.5 is increased by 11.2%. The results of the significance test show that the prediction accuracy of MMpred is significantly better than each of its comparative versions. **Figure 6** visually reflects the comparison between MMpred and each comparison method in the first model and in the best model. MMpred outperforms the individual programs (MMpred-A_C, MMpred-B_C and MMpred-C) in 198, 264 and 274 cases when considering the first models. This data demonstrate again that the importance of the different step of multimodal optimization.

Table 4. The predicted results of the first model of MMpred, MMpred-A_C, MMpred-B_C and MMpred-C. #TM ≥ 0.5 is the number of the first model with TM-score ≥ 0.5. The last two columns are the results of the Wilcoxon signed rank test calculated based on the TM-score of the first model.

Method	TM-score	#TM $\geqslant 0.5$	p-value	Significance
MMpred	0.629	268	NA	NA
MMpred-A_C	0.596	197	1.13E-11	+
MMpred-B_C	0.541	241	3.94E-41	+
MMpred-C	0.534	189	3.13E-42	+
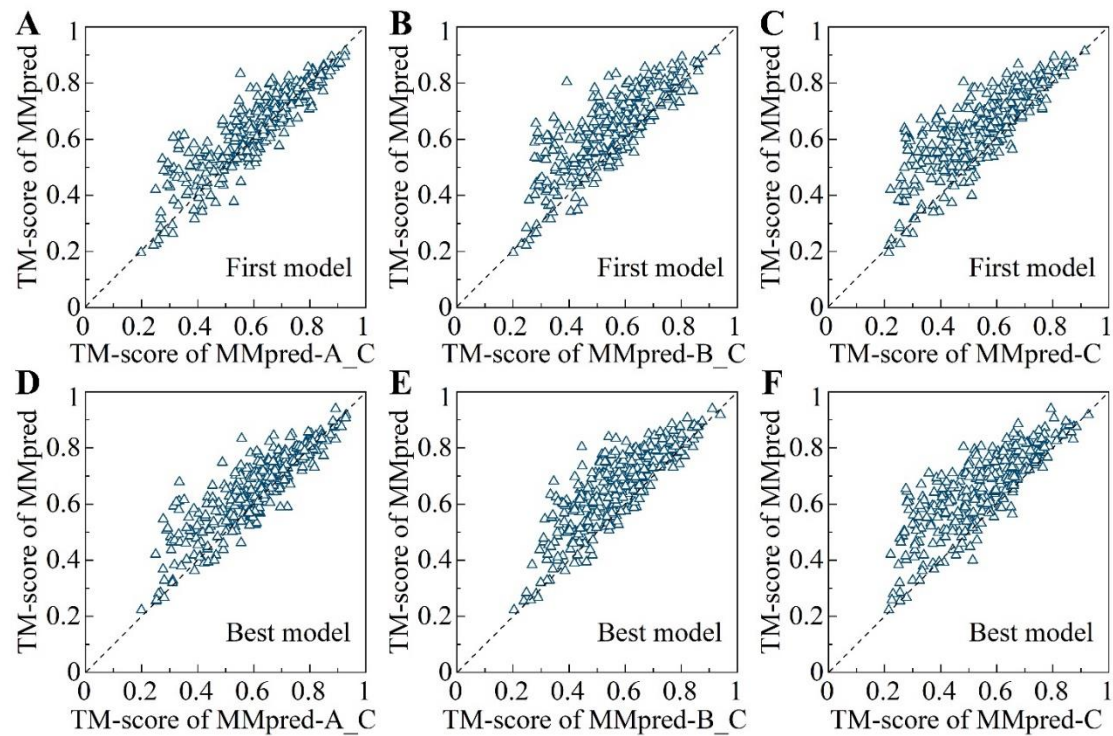
Fig.6. The comparison of MMpred with MMpred-A_C, MMpred-B_C, and MMpred-C. (A-C) are the TM-score of the predicted first model between MMpred and MMpred-A_C, MMpred-B_C, and MMpred-C, respectively. (D-F) are the TM-score of the predicted best model of between MMpred and MMpred-A_C, MMpred-B_C, and MMpred-C, respectively.
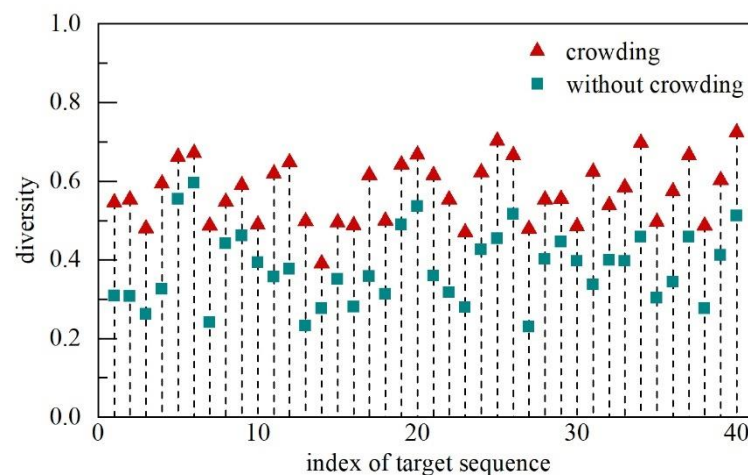
Fig.7. Comparison of population diversity between the method using crowding strategy and that without crowding strategy in the modal exploration stage.

In order to verify the role of the crowding strategy in the modal exploration stage, 40 proteins were randomly selected from the benchmark set for analysis. We respectively calculated the diversity of the population obtained by using the crowding strategy and by the method without crowding strategy in the modal exploration stage. The results are shown in **Figure 7**. The diversity of the population is characterized by the average value of the DMscore of any two individuals in the population. A lower DMscore indicates a greater population diversity. The results indicate that the use of crowding strategy in all proteins can better maintain the diversity of the population.

3.5 Experimental analysis of DMscore

DMscore is tested on 20 targets of CASP13, each containing the first model predicted by all the server groups. For each target, we calculated the DMscore between the first model predicted by all groups and its native structure and analyzed its correlation with GDT_TS. Then, we compared it with TM-score. The comparison results of all proteins are shown in **Supplementary Figure S8**. The DMscore and GDT_TS have a strong correlation on the predicted models by different groups, especially for the model with DMscore≥0.5. The characteristic of DMscore is that it can quickly evaluate the similarity between models without rotation and translation, and it focuses on topological structure matching. **Figure 8** shows an example of T0954-D1. For the 78th model ranked by GDT_TS, the TM-score is 0.31, but DMscore is 0.74. By observing the 75th to 78th models and the native structure, the topological structure of the 75th to 77th models is disordered, and the topological structure of the 78th model is more similar to the native structure and may be better.
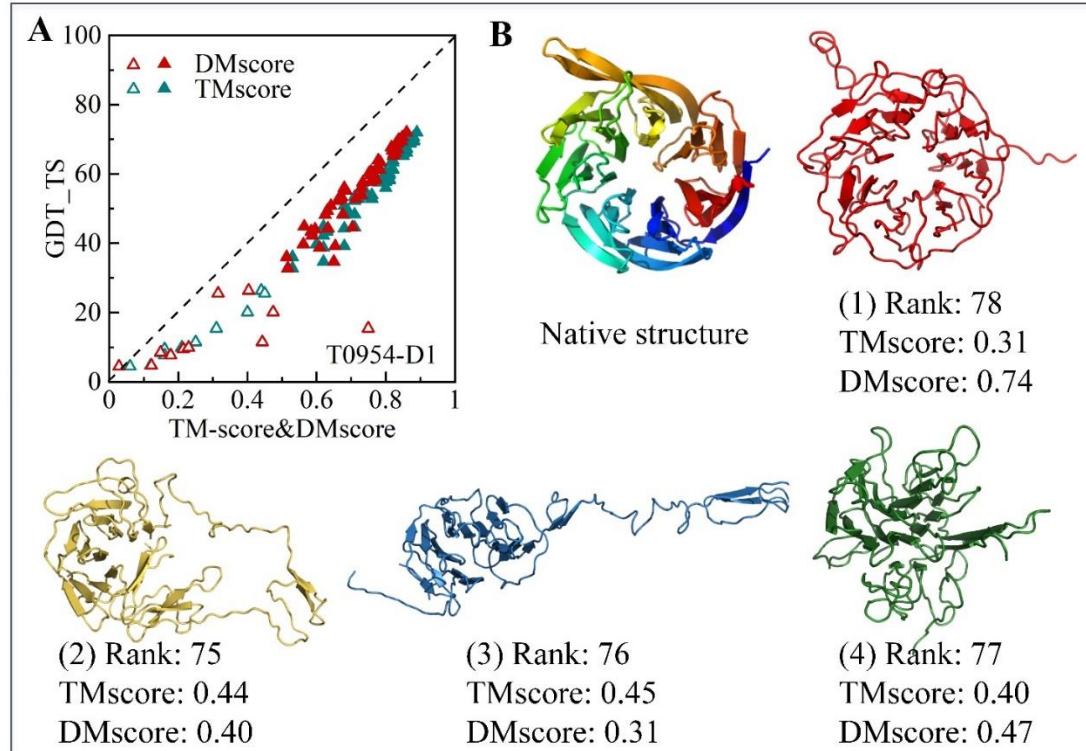
Fig.8. Example of DMscore analysis of CASP13 target T0954-D1. (A) Comparison of the relationship among DMscore, TM-score and CDT_TS of the first model predicted by all groups. The model with DMscore or TM-score greater than or equal to 0.5 is represented as a solid triangle, and the 78th model ranked by GDT_TS is marked. (B) The native structure and the structure of the 75th to 78th models.

3.6 Case studies

Figure 9 shows the RMSD-energy scatter diagram of the sampling process conformations of Rosetta-distance, MMpred-C and MMpred and the comparison of the predicted first model with the native structure. The RMSD of the conformations sampled by Rosetta-distance are all greater than 3Å. Although the last generation conformations are diverse, the RMSD of most conformations is between 5 and12 Å. The final model clustered by SPICKER is 5.86Å. The RMSD of the conformations sampled by MMpred-C are all greater than 5 Å, and the conformations in the last generation population are concentrated. In contrast, MMpred can sample conformations with an RMSD less than 2 Å, and the conformations in the last generation of population are sampled in different basins. MMpred not only sampled the same low-energy basin (black arrow in **Figure 9C**) as that sampled by Rosetta-distance and MMpred-C, but also explored a more promising basin (yellow arrow in **Figure 9C**). The accuracy of the first model predicted by MMpred (RMSD = 2.93Å, TM-score = 0.80) is also significantly better than that of Rosetta-distance (RMSD = 5.86Å, TM-score = 0.61) and MMpred-C (RMSD = 5.95Å, TM-score = 0.56). This case shows that MMpred with multimodal optimization can effectively maintain the diversity of the population, explore more potential conformations of low-energy basins, and ultimately improve the accuracy of the prediction model.
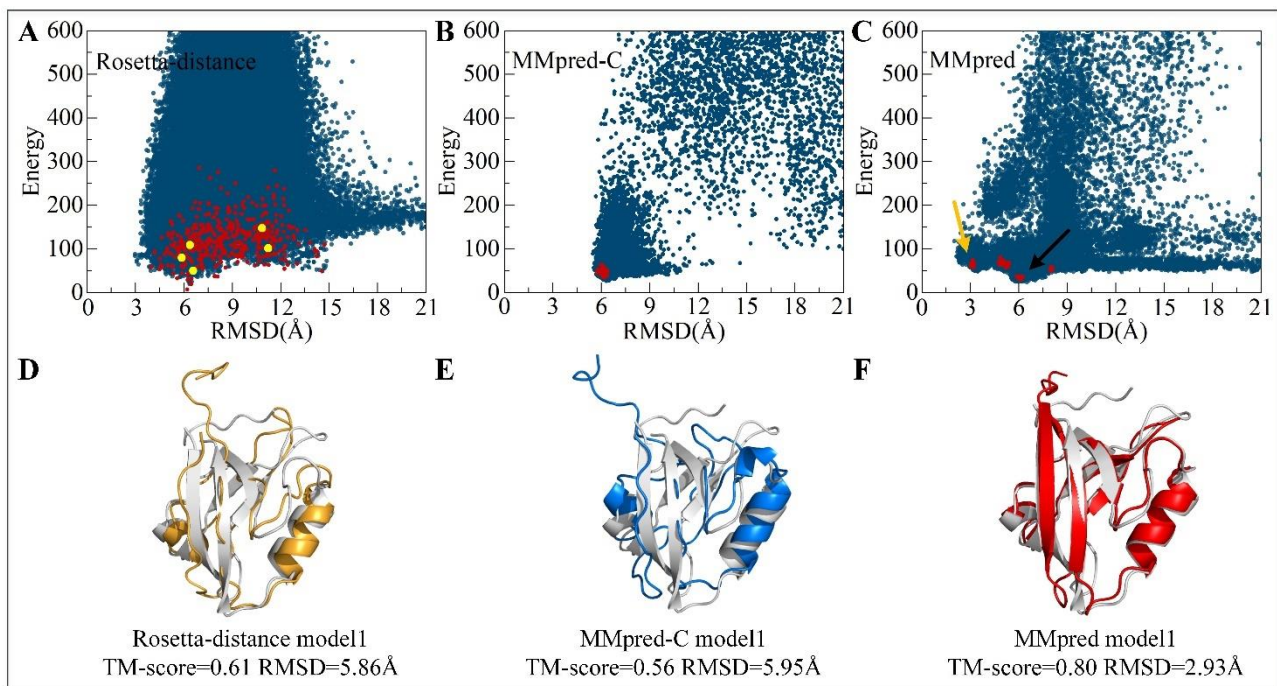
Fig.9. Example of comparing Rosetta-distance, MMpred-C and MMpred on the target 4Q2Q_A. (A), (B) and (C) are the RMSD-energy scatter diagram of process conformations. The process conformations is marked in blue, the last generation conformations is marked in red. The yellow points in (A) are the final five models of Rosetta-distance determined by SPICKER clustering. (D), (E) and (F) show the comparison of the predicted first model with the native structure (gray).

4 Conclusion

A distance-assisted multimodal optimization sampling algorithm, MMpred, is proposed. MMpred consists of three stages. In the first modal exploration stage, a structural similarity evaluation model DMscore is designed to control the diversity of conformations and generate the population with structural diversity. In the second modal maintaining stage, an adaptive clustering algorithm MNDcluster is proposed to divide the population, and then merge the modal by adjusting the annealing temperature. In the final modal exploitation

stage, a greedy search strategy is used to accelerate the convergence of the modal. In addition, a distance scoring model based on the predicted distance constraint is used to guide conformational sampling together with the energy function. MMpred was compared with Rosetta-distance using distance constraint on 320 benchmark proteins. MMpred obtains models with TM-score≥0.5 on 268 benchmark proteins, accounting for 84% of the total, which is better than Rosetta-distance. The comparison of MMpred and Rosetta-distance reflects the contribution of multimodal optimization to improving prediction accuracy. Furthermore, MMpred is tested on 24 FM targets of CASP13 and the result is comparable with the four state-of-the-art CASP13 server groups.

It is important to note that the multimodal optimization strategy in MMpred is an independent protocol proposed for improving conformational sampling of protein folding simulations. Although as an illustrative example, it has been applied to the Rosetta platform in this study, the MMpred protocol can be used for improving the sampling and model accuracy on other advanced folding simulation programs, such as C-QUARK, or combine the modeling advantages of both platforms of Rosetta and C-QUARK. In addition, combining molecular dynamics and intelligent optimization is expected to further refine model. Integrating the local abstract convex underestimation (Zhou and Zhang, 2017; Zhou et al., 2016) into the modal exploration is a good direction to improve the efficiency of the algorithm. Studies along these lines is under progress.

Funding

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MMpred: a distance-assisted multimodal conformation sampling for de novo protein structure prediction

Supplementary Information
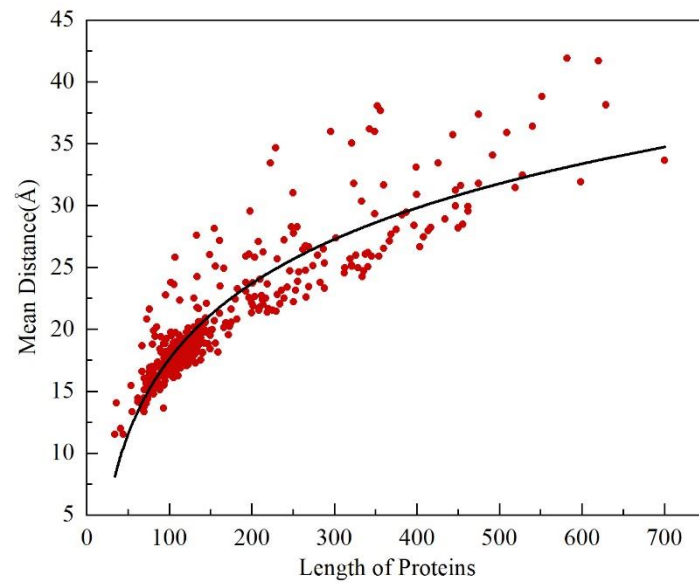
Figure S1: The relationship between the protein size and the mean Euclidean distance of inter-residues of the protein structure. We experimented with 500 native structures with a length of 40 to 700. The average distance between residues increases logarithmically as the length of the protein increases.
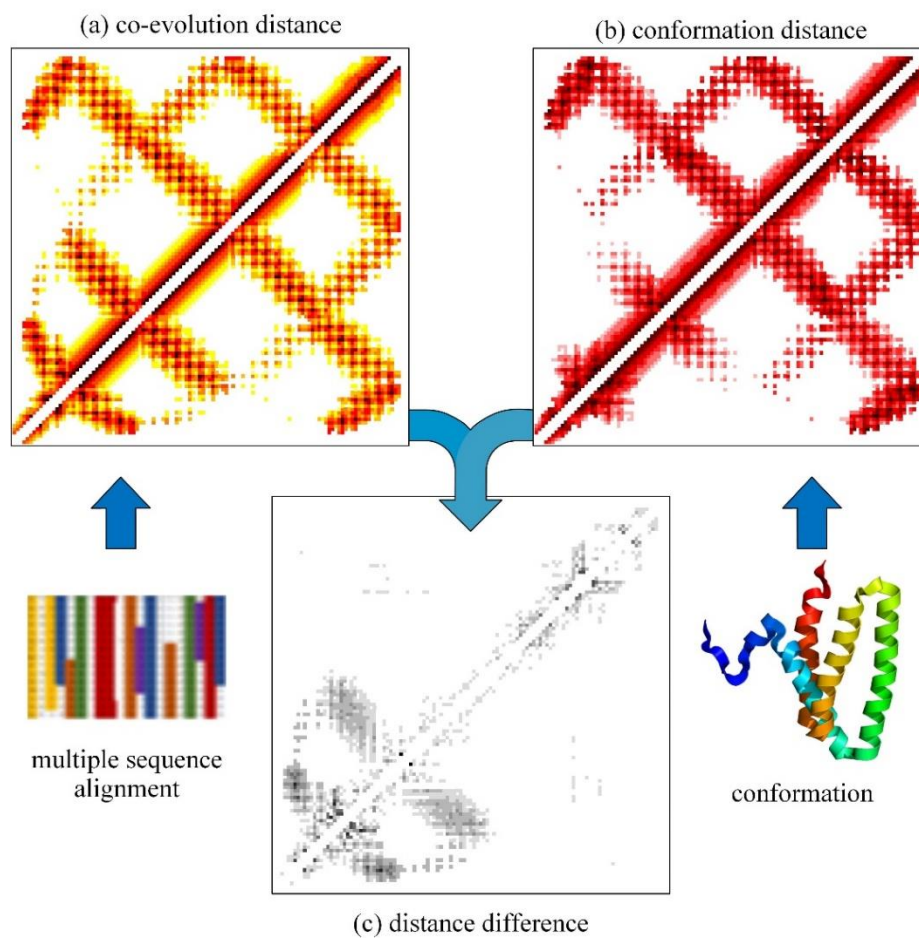
Figure S2: (a) is the inter-residue distance map predicted, (b) is the inter-residue distance map of sampled conformation, and (c) is the distance difference map after the superposition of (a) and (b).
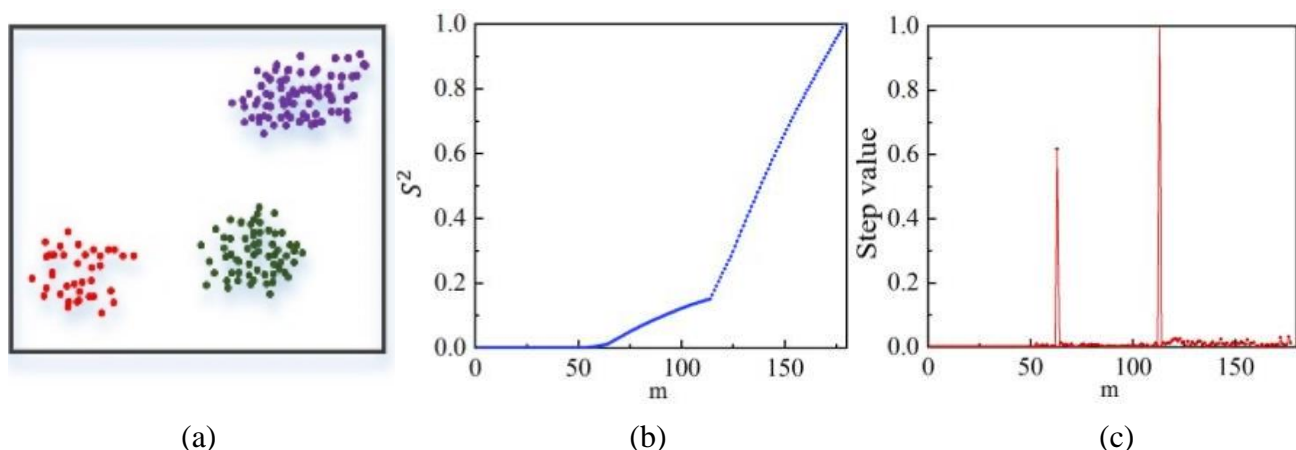
Figure S3: Schematic of MNDcluster. (a) Population distribution. (b) The relationship between the number of nearest neighbours and the variance. (c) Slope change of nearest neighbours values.
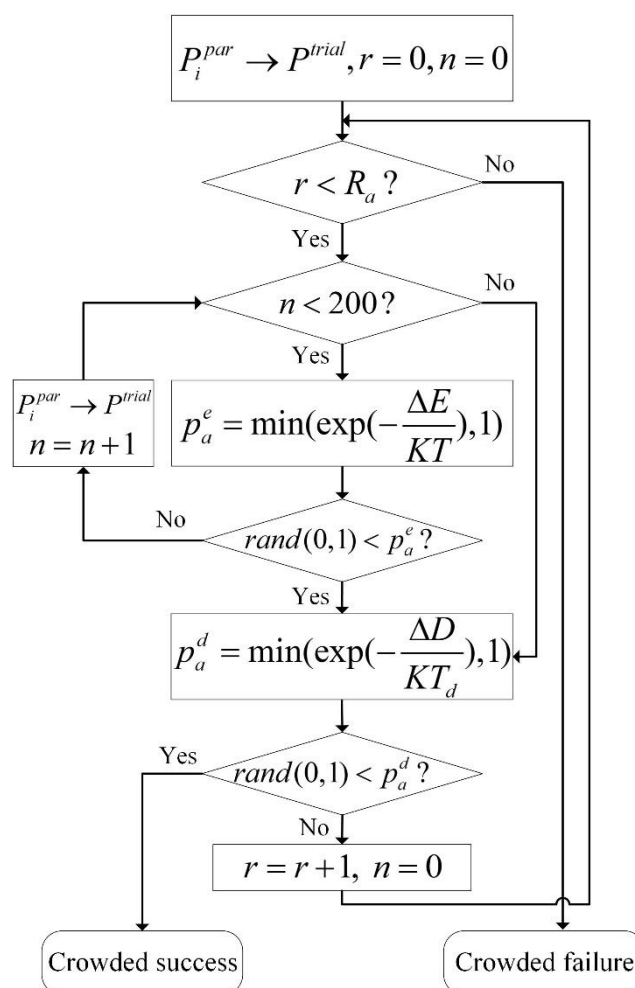
Figure S4: Flowchart of crowding fragment assembly in modal exploration stage. Where $\Delta E = E^{trial} - E^{par}$, $\Delta D = D^{trial} - D^{similar}$, $D^{similar}$ is the distance score of the conformation with the most similar conformation to trial conformation in the population; R_a is crowding subpopulation size; KT and KT_d are the temperature scaling factor.

Trial conformation are produced by piecework assembly，The conformation is received according to the p_a^e based on the energy score. If received fails, fragment assembly is performed again, up to 200 times. And then conformation is crowded according to the p_a^d based on the distance score. Perform the iterating operation in sequence with the top R most similar conformations until the crowding is successful.
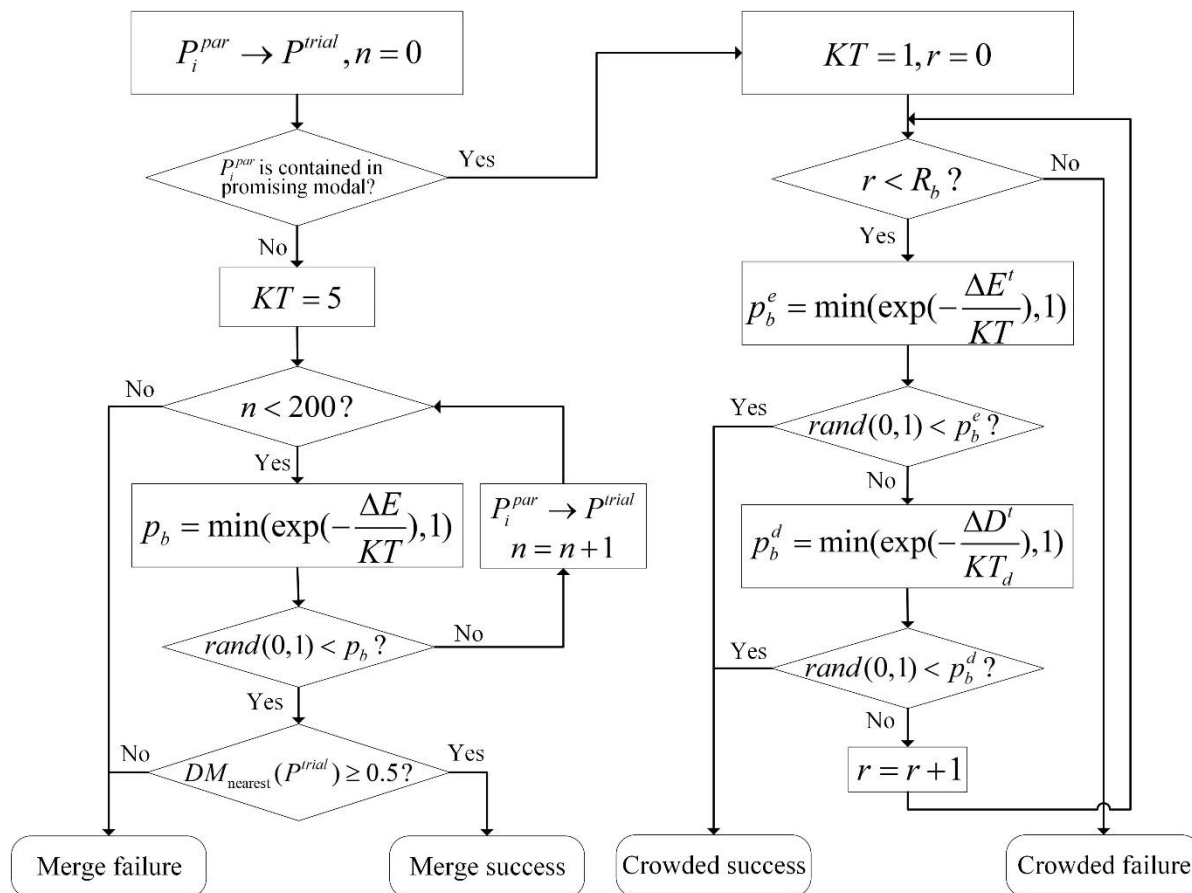
Figure S5: Flowchart of conformation update strategy in modal maintaining stage. Where $\Delta E = E^{trial} - E^{par}$, $\Delta E^t = E^{trial} - E^{similar}$, $\Delta D = D^{trial} - D^{similar}$, $D^{similar}$ is the distance score of the conformation with the most similar conformation to trial conformation in the population; R_b is crowding subpopulation size;

If the conformation contained in the promising modal, the temperature is raised. After successful acceptance according to P_b, the DMscore between the trial conformation of the unpromising modal and the centroid of the nearest promising modal was calculated. When DMscore is greater than or equal to 0.5, the conformations will merge into the promising modal. If the conformation contained in the unpromising modal, then the temperature is reduced. Metropolis criterion is used to determine whether the target conformation is crowded by trial conformation.

$$P_i^{par} \rightarrow P^{trial}$$

$$p_c^d = \min(\exp(-\frac{\Delta D}{KT_d}),1)$$

$rand(0,1) < p_c^d$? —Yes / No

$$p_c^e = \min(\exp(-\frac{\Delta E}{KT}),1)$$

$rand(0,1) < p_c^e$? —Yes / No

Receive   Reject
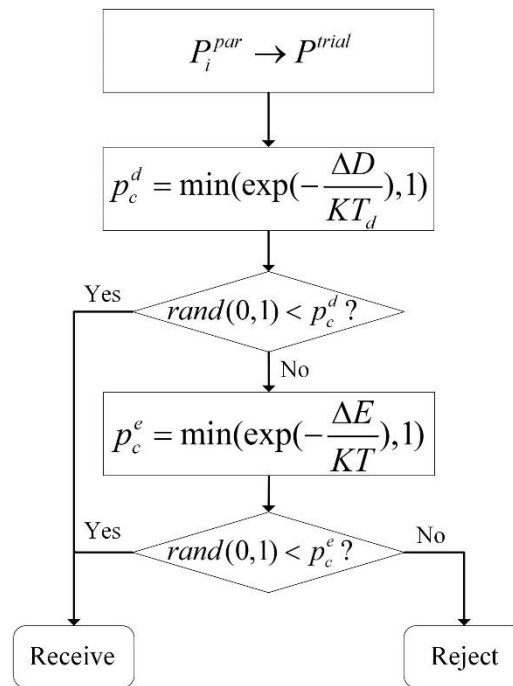
Figure S6: Flowchart of greedy fragment assembly in modal exploitation stage. Where $\Delta D = D^{trial} - D^{min}, \Delta E = E^{trial} - E^{min}, D^{min}$ is the lowest distance score and E^{min} is the lowest energy score in the population.

(a)TM-score=0.463   (b)TM-score=0.607
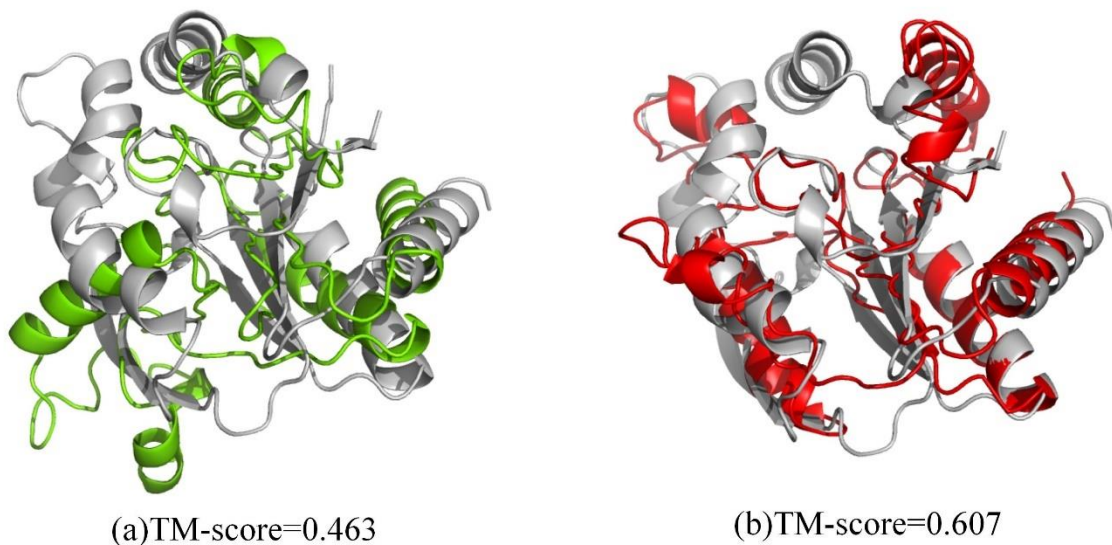
Figure S7: (a) is the predicted result of MMpred with a population size of 400 and generation of modal exploitation of 800. (b) is the predicted result of MMpred with a population size of 800 and generation of modal exploitation of 2000.

DMscore experimental results
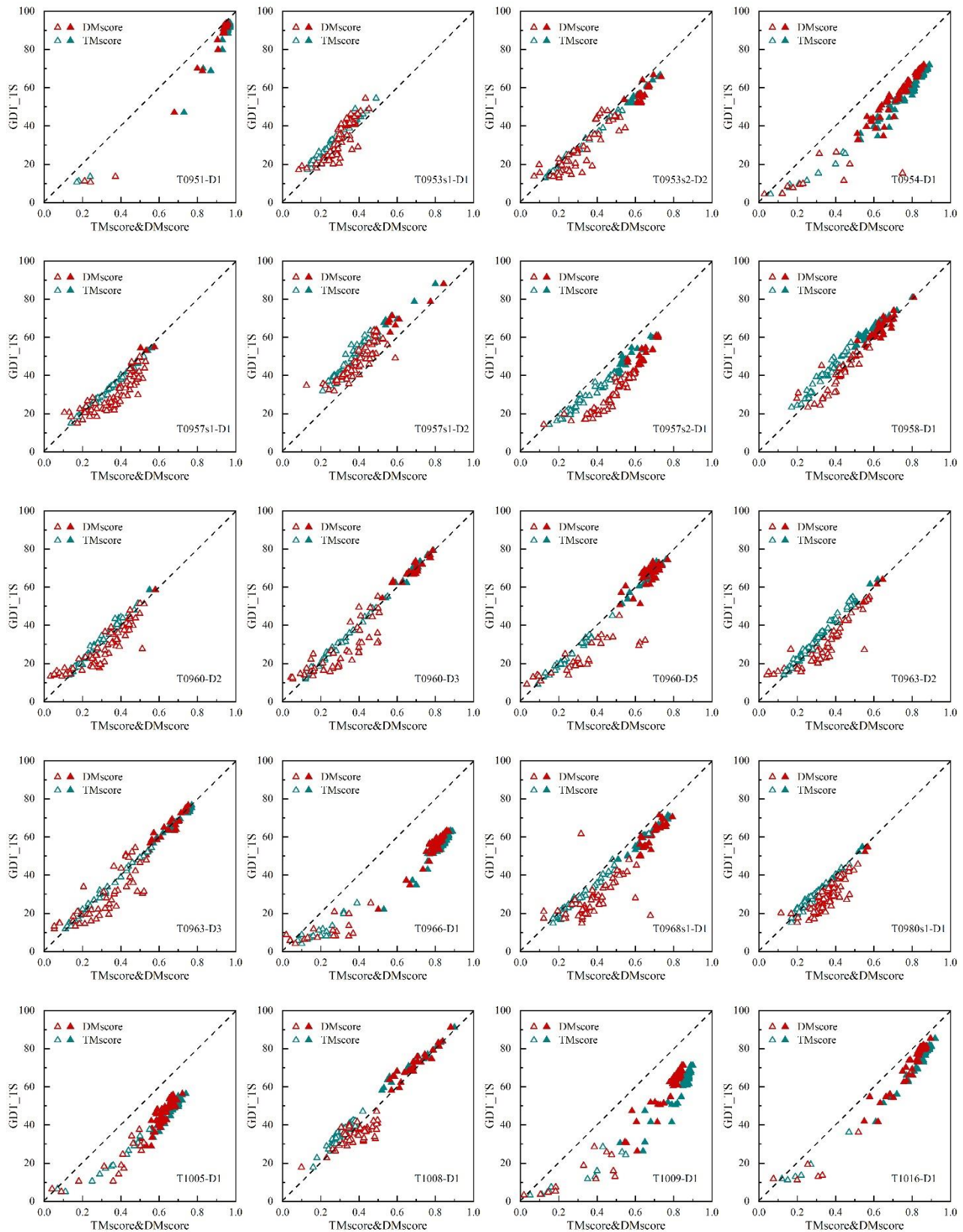
Figure S8: The relationship between GDT_TS and DMscore/TM-score. DMscore tested on 20 targets of CASP13, each containing the first model predicted by all the groups. Red triangle represents DMscore, blue triangle represents TM-score; Solid triangle means that DMscore and TM-score are both greater than or equal to 0.5.

Table S1: Prediction results (TM-score) of MMpred, Rosetta-distance and C-QUARK for 320 benchmark proteins.

No.	PDB	Type	Size	MMpred		Rosetta-distance		C-QUARK	
				First model	Best model	First model	Best model	First model	Best model
1	1FAQ_A	β	52	0.596	0.634	0.185	0.273	0.402	0.425
2	1JEI_A	α	53	0.628	0.637	0.581	0.581	0.610	0.619
3	1NKZ_A	α	53	0.571	0.587	0.289	0.357	0.417	0.424
4	1AUU_A	β	55	0.599	0.652	0.437	0.437	0.692	0.692
5	1FCA_A	α/β	55	0.814	0.845	0.690	0.753	0.675	0.675
6	2UUX_A	α/β	55	0.678	0.682	0.186	0.267	0.355	0.464
7	1H9E_A	α	56	0.504	0.536	0.492	0.492	0.521	0.568
8	1H9F_A	α	57	0.565	0.568	0.542	0.542	0.595	0.597
9	1LR1_B	α	57	0.498	0.507	0.482	0.520	0.434	0.437
10	1DL6_A	β	58	0.392	0.392	0.383	0.411	0.369	0.374
11	1E53_A	α/β	59	0.620	0.620	0.470	0.547	0.516	0.516
12	1FEX_A	α	59	0.645	0.662	0.568	0.568	0.587	0.592
13	1UG4_A	β	60	0.589	0.625	0.320	0.320	0.440	0.440
14	1VYX_A	α/β	60	0.444	0.486	0.270	0.270	0.433	0.450
15	3P8B_A	α/β	60	0.518	0.666	0.296	0.296	0.669	0.669
16	1F43_A	α	61	0.563	0.576	0.560	0.587	0.559	0.576
17	1L2P_A	α	61	0.864	0.939	0.300	0.326	0.458	0.490
18	4MLF_D	β	61	0.284	0.284	0.206	0.226	0.247	0.248
19	1BE3_J	α	62	0.544	0.605	0.365	0.365	0.271	0.287
20	1BGY_J	α	62	0.540	0.567	0.400	0.400	0.270	0.292
21	1TYG_B	α/β	65	0.797	0.823	0.632	0.648	0.803	0.818
22	1DTV_A	α/β	67	0.226	0.255	0.204	0.204	0.362	0.428
23	2JP3_A	α	67	0.364	0.389	0.342	0.348	0.257	0.257
24	1CHC_A	α/β	68	0.489	0.501	0.290	0.381	0.504	0.545
25	1J9I_A	α/β	68	0.623	0.623	0.462	0.493	0.632	0.655
26	1TAF_A	α	68	0.859	0.874	0.533	0.576	0.513	0.530
27	1DWM_A	α/β	69	0.688	0.688	0.565	0.565	0.643	0.653
28	1L6H_A	α	69	0.516	0.519	0.508	0.508	0.413	0.416
29	1W1W_E	α/β	70	0.805	0.834	0.807	0.807	0.813	0.813
30	2CMX_A	α/β	70	0.709	0.760	0.605	0.638	0.596	0.704
31	1LDD_A	α/β	71	0.850	0.862	0.354	0.669	0.708	0.732
32	1K73_1	α/β	73	0.642	0.682	0.468	0.468	0.447	0.469
33	1KN6_A	α/β	73	0.575	0.594	0.512	0.512	0.591	0.591
34	1PIH_A	α/β	73	0.558	0.604	0.288	0.288	0.519	0.564
35	2HI3_A	α	73	0.641	0.643	0.654	0.673	0.695	0.704
36	1ABT_A	α/β	74	0.484	0.484	0.373	0.417	0.496	0.496
37	1HHV_A	α/β	74	0.598	0.605	0.439	0.439	0.628	0.628
38	2V85_A	α/β	74	0.430	0.464	0.284	0.325	0.275	0.346
39	3CX5_F	α	74	0.788	0.788	0.501	0.517	0.709	0.735
40	3MQK_C	β	75	0.805	0.850	0.539	0.539	0.754	0.756
41	4M75_F	α/β	75	0.742	0.742	0.574	0.574	0.719	0.724
42	1DP7_P	α/β	76	0.745	0.770	0.489	0.531	0.744	0.748
43	1EKZ_A	α/β	76	0.674	0.693	0.591	0.664	0.690	0.693
44	1VCC_A	α/β	77	0.557	0.559	0.517	0.517	0.552	0.594
45	1K1Z_A	β	78	0.519	0.541	0.503	0.503	0.602	0.624
46	1PFS_A	β	78	0.530	0.547	0.327	0.383	0.538	0.567
47	4V2O_A	α	78	0.773	0.804	0.592	0.592	0.545	0.545
48	1A91_A	α	79	0.506	0.540	0.562	0.562	0.475	0.503
49	1KP6_A	α/β	79	0.242	0.280	0.293	0.293	0.330	0.351
50	2ZMZ_B	α/β	79	0.713	0.729	0.497	0.563	0.456	0.611

No.	PDB	Type	Size	MMpred		Rosetta-distance		C-QUARK	
				First model	Best model	First model	Best model	First model	Best model
51	1B4R_A	β	80	0.650	0.717	0.553	0.553	0.718	0.756
52	1PZW_A	α/β	80	0.717	0.762	0.287	0.335	0.523	0.533
53	1R6R_A	α	80	0.531	0.531	0.323	0.406	0.385	0.397
54	4LMS_A	α/β	80	0.402	0.402	0.269	0.269	0.346	0.346
55	1D8B_A	α	81	0.732	0.744	0.684	0.684	0.659	0.690
56	1EZV_G	α/β	81	0.374	0.418	0.371	0.397	0.324	0.324
57	1F9P_A	α/β	81	0.593	0.599	0.548	0.569	0.611	0.629
58	1GGS_A	α/β	81	0.681	0.695	0.589	0.625	0.659	0.679
59	1U84_A	α	81	0.840	0.848	0.633	0.701	0.800	0.828
60	4ASW_C	α/β	81	0.726	0.778	0.534	0.534	0.710	0.721
61	1CF7_B	α/β	82	0.718	0.776	0.520	0.520	0.684	0.689
62	1LFU_P	α	82	0.589	0.590	0.593	0.613	0.567	0.567
63	1WMH_B	α/β	82	0.782	0.795	0.459	0.495	0.733	0.783
64	2ODM_B	α	83	0.826	0.832	0.780	0.795	0.682	0.731
65	2AQ0_A	α	84	0.644	0.651	0.627	0.646	0.630	0.644
66	2GBJ_B	α/β	84	0.749	0.754	0.551	0.623	0.779	0.804
67	1IS7_K	α/β	85	0.643	0.643	0.417	0.417	0.484	0.484
68	5T17_A	α/β	85	0.753	0.753	0.729	0.729	0.724	0.753
69	1CXZ_B	α	86	0.867	0.886	0.708	0.708	0.797	0.850
70	1NOE_A	α/β	86	0.611	0.611	0.271	0.302	0.515	0.515
71	2J6Z_A	α	86	0.720	0.739	0.413	0.586	0.666	0.674
72	4OW1_A	α/β	86	0.738	0.741	0.564	0.564	0.657	0.712
73	1C9F_A	α/β	87	0.578	0.589	0.552	0.572	0.601	0.616
74	1GVP_A	α/β	87	0.671	0.671	0.479	0.479	0.595	0.595
75	1RHX_A	α/β	87	0.580	0.595	0.511	0.511	0.568	0.584
76	3X15_A	α	87	0.498	0.498	0.261	0.261	0.445	0.458
77	4GDK_A	α/β	88	0.671	0.694	0.505	0.505	0.696	0.746
78	4J20_A	α/β	88	0.704	0.743	0.558	0.558	0.553	0.592
79	1H8E_H	α/β	89	0.657	0.657	0.519	0.519	0.775	0.809
80	1HBX_E	α/β	89	0.516	0.527	0.523	0.523	0.414	0.451
81	5IZB_A	α/β	89	0.565	0.565	0.441	0.441	0.557	0.584
82	1JR5_A	α	90	0.522	0.572	0.349	0.446	0.345	0.461
83	4Q2Q_A	α/β	90	0.801	0.801	0.612	0.612	0.703	0.803
84	4MMG_A	α/β	91	0.823	0.840	0.633	0.633	0.727	0.763
85	5L38_A	α/β	91	0.825	0.843	0.664	0.667	0.856	0.856
86	1IUY_A	α/β	92	0.689	0.697	0.458	0.458	0.677	0.677
87	2BYK_D	α	92	0.856	0.876	0.575	0.655	0.570	0.600
88	4Q2O_A	α/β	92	0.665	0.665	0.615	0.615	0.776	0.798
89	5O2V_A	α/β	92	0.747	0.747	0.590	0.626	0.775	0.794
90	1J8I_A	α/β	93	0.538	0.555	0.539	0.571	0.568	0.579
91	3X0G_A	α	93	0.533	0.533	0.322	0.445	0.559	0.603
92	1G2R_A	α/β	94	0.811	0.819	0.655	0.655	0.771	0.787
93	1PD6_A	β	94	0.598	0.634	0.607	0.607	0.662	0.662
94	2ICT_A	α	94	0.744	0.763	0.707	0.712	0.750	0.765
95	1I35_A	α/β	95	0.573	0.573	0.457	0.457	0.439	0.482
96	1IM3_D	α/β	95	0.264	0.328	0.219	0.298	0.278	0.282
97	5TMF_E	α/β	95	0.553	0.567	0.388	0.388	0.505	0.505
98	3N9U_C	α/β	96	0.731	0.736	0.586	0.640	0.758	0.770
99	1JO0_A	α/β	97	0.820	0.852	0.415	0.599	0.806	0.839
100	2LWP_A	α/β	97	0.501	0.557	0.458	0.486	0.541	0.552

No.	PDB	Type	Size	MMpred		Rosetta-distance		C-QUARK	
				First model	Best model	First model	Best model	First model	Best model
101	3SDL_B	α	97	0.315	0.329	0.351	0.351	0.295	0.327
102	1FRD_A	α/β	98	0.705	0.727	0.565	0.572	0.704	0.785
103	1JMT_A	α/β	98	0.752	0.752	0.578	0.578	0.701	0.716
104	2ACY_A	α/β	98	0.657	0.670	0.589	0.599	0.859	0.863
105	1MWQ_A	α/β	99	0.674	0.674	0.599	0.599	0.576	0.583
106	2NCM_A	β	99	0.834	0.834	0.616	0.616	0.861	0.861
107	2NDP_A	α/β	99	0.480	0.520	0.441	0.477	0.416	0.416
108	1F2R_I	α/β	100	0.627	0.643	0.431	0.549	0.643	0.646
109	1KA8_A	α/β	100	0.560	0.601	0.340	0.505	0.470	0.504
110	1PSR_A	α/β	100	0.752	0.752	0.604	0.604	0.660	0.733
111	1SMP_I	α/β	100	0.700	0.700	0.340	0.411	0.694	0.694
112	4IOS_A	α/β	100	0.549	0.593	0.431	0.431	0.460	0.558
113	1FJG_F	α/β	101	0.721	0.726	0.618	0.618	0.809	0.809
114	1TUL_A	α/β	102	0.378	0.505	0.260	0.328	0.460	0.528
115	2K9X_A	α/β	102	0.536	0.536	0.487	0.487	0.621	0.655
116	1F93_A	α/β	103	0.779	0.790	0.681	0.689	0.860	0.860
117	1IUJ_B	α/β	103	0.730	0.762	0.706	0.708	0.706	0.736
118	4ESB_A	α/β	103	0.844	0.844	0.762	0.762	0.687	0.704
119	1E3Y_A	α	104	0.713	0.731	0.618	0.618	0.685	0.690
120	1FMB_A	α/β	104	0.528	0.599	0.352	0.402	0.633	0.637
121	3N1G_C	α/β	104	0.642	0.658	0.620	0.627	0.818	0.818
122	4UIJ_A	α/β	104	0.759	0.795	0.618	0.618	0.766	0.788
123	5TUV_B	α/β	104	0.343	0.394	0.423	0.423	0.388	0.388
124	1ABV_A	α	105	0.795	0.812	0.755	0.755	0.758	0.794
125	1CDB_A	β	105	0.625	0.625	0.541	0.541	0.665	0.665
126	1JIW_I	α/β	105	0.539	0.539	0.462	0.464	0.662	0.662
127	1KPT_A	α/β	105	0.623	0.667	0.326	0.326	0.619	0.638
128	1A6L_A	α/β	106	0.658	0.684	0.503	0.503	0.360	0.520
129	1ID2_A	α/β	106	0.566	0.679	0.499	0.499	0.656	0.675
130	1S7Z_A	α	106	0.554	0.588	0.576	0.576	0.686	0.736
131	4RUV_A	α/β	106	0.857	0.857	0.832	0.844	0.850	0.854
132	1KX5_D	α	107	0.708	0.775	0.524	0.530	0.477	0.497
133	1ROW_A	α/β	107	0.549	0.600	0.471	0.471	0.677	0.688
134	1V74_A	α/β	107	0.727	0.727	0.539	0.540	0.596	0.644
135	2BSE_A	α/β	107	0.448	0.462	0.295	0.329	0.306	0.344
136	1MFQ_C	α	108	0.637	0.644	0.608	0.611	0.583	0.603
137	1S7O_C	α	108	0.574	0.574	0.511	0.644	0.679	0.679
138	1TZ0_A	α/β	108	0.545	0.618	0.527	0.527	0.650	0.658
139	1K3S_A	α/β	109	0.616	0.690	0.496	0.518	0.299	0.453
140	1VD0_A	α/β	109	0.433	0.479	0.220	0.303	0.599	0.610
141	2CWP_A	α/β	109	0.659	0.736	0.507	0.507	0.725	0.725
142	2NAZ_A	α/β	109	0.661	0.698	0.618	0.654	0.747	0.747
143	1BJX_A	α/β	110	0.786	0.786	0.598	0.599	0.741	0.785
144	1I85_A	β	110	0.598	0.628	0.641	0.641	0.605	0.632
145	1QFW_B	β	110	0.383	0.383	0.330	0.332	0.372	0.395
146	2D0P_B	α/β	110	0.683	0.752	0.659	0.659	0.747	0.747
147	3W1Z_D	α/β	110	0.569	0.624	0.530	0.554	0.597	0.636
148	1EM8_D	α/β	112	0.649	0.712	0.499	0.499	0.568	0.579
149	1JLI_A	α	112	0.365	0.378	0.205	0.260	0.336	0.466
150	1NZE_A	α	112	0.867	0.878	0.826	0.826	0.869	0.875

No.	PDB	Type	Size	MMpred		Rosetta-distance		C-QUARK	
				First model	Best model	First model	Best model	First model	Best model
151	1N3G_A	α/β	113	0.692	0.699	0.654	0.654	0.753	0.753
152	1SAU_A	α/β	114	0.678	0.705	0.355	0.475	0.672	0.787
153	2APN_A	α/β	114	0.615	0.615	0.461	0.501	0.666	0.666
154	5WSE_A	α/β	114	0.654	0.711	0.636	0.636	0.667	0.688
155	3EOD_A	α/β	115	0.817	0.820	0.681	0.727	0.795	0.827
156	3LQV_B	α/β	115	0.640	0.645	0.498	0.508	0.613	0.647
157	1FC3_A	α	116	0.819	0.828	0.671	0.671	0.772	0.804
158	1FHT_A	α/β	116	0.624	0.624	0.545	0.572	0.663	0.677
159	2RLD_C	α	116	0.876	0.883	0.793	0.819	0.825	0.868
160	1D6T_A	α/β	117	0.619	0.694	0.477	0.574	0.705	0.717
161	1ELW_A	α	117	0.913	0.918	0.880	0.950	0.870	0.894
162	1WJ8_A	α	117	0.872	0.875	0.758	0.758	0.839	0.861
163	1A7D_A	α	118	0.789	0.791	0.641	0.641	0.760	0.791
164	1HCD_A	α/β	118	0.626	0.626	0.323	0.372	0.671	0.724
165	2Q2H_A	α/β	118	0.498	0.593	0.455	0.471	0.664	0.681
166	1JJ2_S	α/β	119	0.669	0.727	0.435	0.435	0.437	0.453
167	1MAI_A	α/β	119	0.611	0.703	0.535	0.535	0.705	0.708
168	1OFT_A	α/β	119	0.799	0.799	0.704	0.704	0.776	0.776
169	1ORY_A	α	119	0.783	0.783	0.722	0.722	0.731	0.736
170	1VKE_E	α	119	0.790	0.790	0.619	0.645	0.642	0.642
171	2CZV_D	α/β	119	0.681	0.710	0.372	0.378	0.670	0.734
172	2GJ3_A	α/β	119	0.802	0.802	0.663	0.663	0.833	0.838
173	2LKP_A	α/β	119	0.594	0.607	0.586	0.586	0.561	0.567
174	2PI2_F	α/β	119	0.782	0.782	0.486	0.486	0.743	0.745
175	3G20_B	α/β	119	0.570	0.570	0.454	0.454	0.618	0.618
176	1DUN_A	α/β	120	0.609	0.609	0.419	0.447	0.764	0.786
177	1JPY_Y	α/β	120	0.414	0.415	0.401	0.401	0.472	0.472
178	2H8E_A	α/β	120	0.614	0.614	0.390	0.390	0.628	0.679
179	1BUO_A	α/β	121	0.804	0.804	0.478	0.479	0.791	0.791
180	2QZJ_A	α/β	121	0.895	0.895	0.800	0.852	0.923	0.923
181	1NR3_A	α/β	122	0.316	0.362	0.292	0.361	0.272	0.294
182	2EWC_B	α/β	122	0.684	0.701	0.594	0.615	0.746	0.760
183	2WCW_B	α/β	122	0.714	0.759	0.634	0.634	0.749	0.759
184	3QU3_A	α/β	122	0.552	0.552	0.472	0.472	0.508	0.587
185	5O8G_A	α/β	122	0.641	0.710	0.534	0.563	0.772	0.772
186	1L3G_A	α/β	123	0.531	0.583	0.513	0.538	0.557	0.557
187	1QMA_A	α/β	123	0.653	0.749	0.640	0.640	0.893	0.893
188	4GF3_A	α/β	123	0.577	0.637	0.574	0.574	0.658	0.658
189	1BGF_A	α/β	124	0.801	0.816	0.362	0.449	0.608	0.633
190	1FSP_A	α/β	124	0.843	0.847	0.816	0.858	0.843	0.846
191	1OOF_A	α/β	124	0.731	0.770	0.628	0.628	0.756	0.794
192	1F98_A	α/β	125	0.662	0.711	0.530	0.538	0.658	0.678
193	1FR0_A	α	125	0.741	0.767	0.723	0.728	0.699	0.708
194	1HKQ_A	α/β	125	0.623	0.688	0.645	0.645	0.610	0.633
195	2L74_A	α/β	125	0.712	0.712	0.525	0.555	0.646	0.701
196	2P7L_A	α/β	125	0.709	0.750	0.574	0.574	0.654	0.685
197	2RD5_D	α/β	126	0.502	0.502	0.450	0.476	0.530	0.554
198	3BDB_A	α/β	126	0.505	0.525	0.605	0.605	0.670	0.670
199	3CG4_A	α/β	126	0.802	0.807	0.776	0.776	0.845	0.845
200	3CX5_G	α	126	0.709	0.709	0.440	0.440	0.544	0.544

No.	PDB	Type	Size	MMpred		Rosetta-distance		C-QUARK	
				First model	Best model	First model	Best model	First model	Best model
201	5CJ3_B	α/β	126	0.690	0.729	0.499	0.499	0.627	0.666
202	1B8Q_A	α/β	127	0.436	0.437	0.244	0.268	0.506	0.521
203	1DBF_A	α/β	127	0.661	0.661	0.553	0.553	0.639	0.648
204	1UFB_A	α	127	0.788	0.788	0.751	0.751	0.801	0.801
205	2A9U_B	α	127	0.783	0.794	0.664	0.664	0.719	0.738
206	3I9V_7	α/β	127	0.538	0.538	0.451	0.451	0.423	0.610
207	1DOI_A	α/β	128	0.499	0.499	0.339	0.339	0.520	0.537
208	1GPQ_B	α/β	128	0.640	0.641	0.470	0.470	0.664	0.680
209	1PXW_A	α/β	128	0.655	0.720	0.536	0.536	0.757	0.776
210	4I60_A	α/β	128	0.564	0.564	0.511	0.531	0.753	0.753
211	4JGX_B	α/β	128	0.676	0.719	0.666	0.666	0.647	0.657
212	1AHK_A	β	129	0.483	0.483	0.552	0.552	0.512	0.581
213	2QVG_A	α/β	129	0.794	0.821	0.795	0.795	0.810	0.810
214	2XGY_A	α	129	0.624	0.632	0.543	0.543	0.436	0.589
215	1AX8_A	α/β	130	0.576	0.589	0.456	0.471	0.428	0.563
216	1GQA_A	α/β	130	0.763	0.791	0.738	0.738	0.756	0.796
217	2HYB_A	α/β	130	0.618	0.625	0.616	0.616	0.772	0.772
218	4B0M_A	α/β	131	0.554	0.605	0.434	0.495	0.510	0.510
219	1B4U_A	α	132	0.616	0.619	0.642	0.642	0.592	0.611
220	3CAE_A	α/β	132	0.508	0.508	0.328	0.328	0.471	0.471
221	4CXT_A	α/β	132	0.703	0.703	0.457	0.516	0.706	0.706
222	1DCF_A	α/β	133	0.822	0.823	0.763	0.763	0.823	0.823
223	1OA8_D	α/β	133	0.295	0.320	0.241	0.261	0.276	0.309
224	1Y14_A	α	133	0.442	0.571	0.410	0.445	0.508	0.554
225	4LE0_B	α/β	133	0.895	0.907	0.800	0.870	0.914	0.914
226	4Z6J_A	β	133	0.488	0.507	0.276	0.486	0.643	0.643
227	1PMS_A	α/β	135	0.533	0.568	0.544	0.544	0.614	0.614
228	1S56_B	α/β	135	0.751	0.759	0.712	0.712	0.724	0.758
229	1OJG_A	α/β	136	0.624	0.624	0.599	0.599	0.633	0.633
230	1SVJ_A	α/β	136	0.750	0.756	0.639	0.639	0.757	0.765
231	1TWU_A	α/β	137	0.738	0.738	0.585	0.585	0.606	0.606
232	1FJG_H	α/β	138	0.712	0.740	0.470	0.470	0.782	0.782
233	3UE6_E	α/β	138	0.685	0.690	0.572	0.582	0.797	0.797
234	1LNW_C	α/β	139	0.812	0.826	0.769	0.769	0.663	0.752
235	4AIH_A	α/β	139	0.772	0.772	0.652	0.666	0.643	0.682
236	1KQ6_A	α/β	140	0.699	0.712	0.571	0.571	0.722	0.727
237	1NPB_A	α/β	140	0.592	0.649	0.554	0.554	0.485	0.567
238	1OZ9_A	α/β	141	0.677	0.700	0.600	0.621	0.807	0.807
239	1R5T_A	α/β	141	0.691	0.711	0.625	0.625	0.739	0.739
240	2FA5_B	α/β	142	0.714	0.730	0.658	0.687	0.625	0.648
241	2HQ7_B	α/β	142	0.697	0.697	0.664	0.664	0.712	0.712
242	1HKX_E	α/β	143	0.471	0.471	0.509	0.509	0.657	0.712
243	1HL6_D	α/β	143	0.486	0.574	0.270	0.315	0.540	0.668
244	1S3J_A	α/β	143	0.770	0.787	0.804	0.804	0.752	0.752
245	2F22_B	α/β	143	0.671	0.685	0.566	0.566	0.737	0.771
246	4KA0_A	α/β	143	0.798	0.804	0.708	0.708	0.849	0.849
247	5L8R_D	α/β	143	0.435	0.464	0.287	0.318	0.360	0.428
248	1KSX_A	α/β	144	0.652	0.697	0.537	0.537	0.730	0.730
249	1LE2_A	α	144	0.267	0.267	0.299	0.380	0.357	0.457
250	1A3A_C	α/β	146	0.607	0.643	0.493	0.555	0.758	0.758

No.	PDB	Type	Size	MMpred		Rosetta-distance		C-QUARK	
				First model	Best model	First model	Best model	First model	Best model
251	1K5D_B	α/β	146	0.583	0.583	0.512	0.531	0.618	0.688
252	1LZW_B	α/β	146	0.807	0.807	0.704	0.704	0.815	0.820
253	1HBG_A	α	147	0.830	0.833	0.780	0.780	0.840	0.858
254	3E6M_E	α/β	147	0.730	0.731	0.665	0.665	0.618	0.678
255	3PD2_A	α/β	147	0.622	0.622	0.533	0.533	0.723	0.723
256	4GQY_A	α/β	147	0.664	0.664	0.591	0.591	0.742	0.742
257	1UNG_D	α	149	0.683	0.718	0.493	0.493	0.503	0.638
258	1GME_A	α/β	150	0.528	0.528	0.250	0.375	0.478	0.485
259	1F1E_A	α/β	151	0.667	0.667	0.374	0.432	0.476	0.551
260	2H30_A	α/β	151	0.661	0.706	0.651	0.666	0.713	0.718
261	2PYB_A	α	151	0.755	0.791	0.731	0.731	0.858	0.869
262	1NTV_A	α/β	152	0.614	0.614	0.545	0.545	0.695	0.695
263	2NS9_B	α/β	152	0.783	0.788	0.636	0.636	0.718	0.819
264	3GMX_A	α/β	153	0.437	0.437	0.265	0.265	0.340	0.349
265	2GKC_A	α/β	155	0.459	0.459	0.555	0.555	0.617	0.617
266	5JTM_A	α/β	155	0.580	0.580	0.366	0.443	0.580	0.594
267	3ALU_A	α/β	157	0.400	0.400	0.472	0.472	0.630	0.630
268	1OX7_A	α/β	158	0.655	0.655	0.477	0.477	0.792	0.809
269	1USL_C	α/β	158	0.756	0.775	0.671	0.671	0.775	0.790
270	2KBW_A	α	160	0.722	0.756	0.583	0.659	0.693	0.725
271	3F8L_A	α/β	162	0.628	0.654	0.504	0.541	0.863	0.868
272	1C03_A	α/β	163	0.645	0.645	0.515	0.542	0.679	0.700
273	3H05_B	α/β	163	0.605	0.605	0.442	0.442	0.723	0.764
274	4NBI_A	α/β	163	0.503	0.503	0.524	0.524	0.683	0.704
275	1FW9_A	α/β	164	0.552	0.552	0.432	0.447	0.607	0.634
276	2AEN_A	α/β	164	0.421	0.421	0.313	0.313	0.261	0.396
277	1C41_A	α/β	165	0.696	0.696	0.706	0.706	0.712	0.712
278	1F3Y_A	α/β	165	0.340	0.368	0.433	0.433	0.513	0.548
279	1S2D_A	α/β	165	0.642	0.695	0.602	0.605	0.721	0.721
280	2LRB_A	α/β	165	0.607	0.607	0.585	0.585	0.679	0.679
281	3V1O_A	α/β	165	0.595	0.595	0.510	0.510	0.662	0.662
282	1PGV_A	α/β	167	0.782	0.806	0.584	0.592	0.788	0.788
283	2FKB_C	α/β	167	0.522	0.522	0.482	0.493	0.635	0.635
284	1AP7_A	α	168	0.775	0.787	0.590	0.590	0.736	0.736
285	2C4W_A	α/β	168	0.636	0.649	0.661	0.661	0.723	0.723
286	2O70_F	α	168	0.750	0.774	0.607	0.607	0.782	0.782
287	2WGP_A	α/β	168	0.762	0.769	0.662	0.668	0.835	0.844
288	3M1N_B	α/β	168	0.433	0.439	0.371	0.385	0.492	0.501
289	1XJA_C	α/β	169	0.643	0.654	0.549	0.570	0.691	0.697
290	1YG2_A	α/β	169	0.445	0.623	0.393	0.448	0.438	0.451
291	1QZG_A	α/β	170	0.561	0.561	0.387	0.387	0.687	0.687
292	1NF6_F	α/β	171	0.806	0.806	0.703	0.718	0.815	0.842
293	1NQZ_A	α/β	171	0.605	0.607	0.452	0.523	0.677	0.677
294	5IAO_A	α/β	171	0.491	0.493	0.470	0.548	0.690	0.696
295	6AQ3_B	α/β	171	0.558	0.569	0.489	0.493	0.508	0.593
296	1KOH_D	α/β	172	0.752	0.752	0.597	0.597	0.544	0.553
297	1TEO_A	α/β	173	0.554	0.554	0.545	0.545	0.647	0.647
298	2A5Y_A	α	173	0.698	0.723	0.550	0.550	0.623	0.719
299	1AK6_A	α/β	174	0.514	0.514	0.507	0.507	0.630	0.630
300	1QFT_A	α/β	175	0.506	0.506	0.534	0.562	0.689	0.689

No.	PDB	Type	Size	MMpred		Rosetta-distance		C-QUARK	
				First model	Best model	First model	Best model	First model	Best model
301	2L5P_A	α/β	175	0.632	0.632	0.595	0.595	0.658	0.676
302	2C2F_A	α/β	178	0.802	0.802	0.747	0.758	0.802	0.802
303	1NGL_A	α/β	179	0.552	0.552	0.526	0.557	0.602	0.602
304	3IAM_2	α/β	179	0.530	0.616	0.345	0.382	0.509	0.511
305	2Z3B_A	α/β	180	0.751	0.751	0.443	0.443	0.661	0.661
306	1Y1X_A	α/β	182	0.667	0.667	0.738	0.738	0.629	0.648
307	1RZ3_A	α/β	184	0.463	0.515	0.516	0.597	0.604	0.604
308	1WLQ_C	α/β	185	0.629	0.648	0.501	0.501	0.576	0.593
309	1TJF_B	α/β	186	0.791	0.791	0.726	0.746	0.772	0.782
310	3O61_A	α/β	187	0.348	0.418	0.407	0.434	0.567	0.567
311	1TLJ_A	α/β	189	0.536	0.536	0.527	0.527	0.470	0.554
312	1DTP_A	α/β	190	0.222	0.258	0.160	0.188	0.223	0.314
313	1F15_C	α/β	191	0.197	0.222	0.149	0.162	0.215	0.273
314	1GXD_C	α/β	192	0.455	0.455	0.197	0.255	0.427	0.484
315	1VCY_A	α/β	193	0.464	0.464	0.351	0.355	0.322	0.411
316	2VUL_A	α/β	193	0.411	0.411	0.393	0.398	0.424	0.645
317	4ZBY_A	α/β	194	0.657	0.657	0.591	0.591	0.794	0.794
318	1IOO_A	α/β	196	0.447	0.447	0.404	0.404	0.530	0.574
319	5EKT_A	α/β	196	0.461	0.461	0.525	0.528	0.690	0.713
320	4K1F_A	α/β	198	0.535	0.601	0.529	0.572	0.785	0.785

Table S2: Prediction results (TM-score) of MMpred, C-QUARK, RaptorX-DeepModeller, BAKER-ROSETTASERVER and MULTICOM_ CLUSTER for 24 free modeling (FM) targets of CASP13.

No.	PDB	Size	MMpred	C-QUARK	RaptorX-Deep Modeller	BAKER-ROSETTAS ERVER	MULTICOM _ CLUSTER
1	T0955-D1	41	0.67	0.73	0.59	\	0.77
2	T0953s2-D1	44	0.32	0.36	0.18	0.33	0.20
3	T0953s1-D1	67	0.38	0.40	0.28	0.19	0.38
4	T0990-D1	76	0.44	0.58	0.40	0.37	0.36
5	T0958-D1	77	0.73	0.55	0.66	0.53	0.55
6	T1008-D1	77	0.70	0.35	0.28	0.56	0.38
7	T0963-D2	82	0.43	0.46	0.48	0.36	0.28
8	T0960-D2	84	0.42	0.44	0.49	0.28	0.38
9	T0970-D1	85	0.54	0.51	0.54	0.40	0.33
10	T0953s2-D3	93	0.16	0.35	0.29	0.19	0.14
11	T1021s3-D2	97	0.42	0.45	0.59	0.19	0.27
12	T0980s1-D1	104	0.45	0.54	0.37	0.41	0.25
13	T0957s1-D1	108	0.42	0.40	0.37	0.42	0.31
14	T0953s2-D2	111	0.50	0.48	0.69	0.47	0.22
15	T0968s2-D1	115	0.60	0.65	0.59	0.66	0.42
16	T0968s1-D1	118	0.69	0.56	0.62	0.74	0.43
17	T0957s2-D1	155	0.70	0.53	0.65	0.48	0.51
18	T1022s1-D1	156	0.37	0.55	0.58	0.40	0.38
19	T1021s3-D1	166	0.43	0.64	0.66	0.50	0.50
20	T0990-D3	213	0.25	0.22	0.22	0.23	0.24
21	T0990-D2	231	0.40	0.37	0.35	0.26	0.25
22	T1005-D1	326	0.43	0.70	0.70	0.70	0.69
23	T0950-D1	342	0.41	0.44	0.56	0.46	0.22
24	T0969-D1	354	0.33	0.64	0.65	0.49	0.44

Table S3: Prediction results (TM-score) of MMpred, MMpred-A_C, MMpred-B_C and MMpred-C for 320 benchmark proteins.

No.	PDB	MMpred		MMpred-A_C		MMpred-B_C		MMpred-C	
		First model	Best model	First model	Best model	First model	Best model	First model	Best model
1	1FAQ_A	0.596	0.634	0.551	0.560	0.324	0.334	0.415	0.416
2	1JEI_A	0.628	0.637	0.611	0.616	0.609	0.609	0.591	0.593
3	1NKZ_A	0.571	0.587	0.573	0.610	0.608	0.608	0.553	0.554
4	1AUU_A	0.599	0.652	0.590	0.590	0.403	0.439	0.619	0.619
5	1FCA_A	0.814	0.845	0.667	0.671	0.654	0.732	0.684	0.684
6	2UUX_A	0.678	0.682	0.545	0.546	0.345	0.345	0.386	0.388
7	1H9E_A	0.504	0.536	0.520	0.520	0.556	0.556	0.508	0.512
8	1H9F_A	0.565	0.568	0.624	0.624	0.526	0.537	0.490	0.502
9	1LR1_B	0.498	0.507	0.488	0.508	0.542	0.542	0.489	0.531
10	1DL6_A	0.392	0.392	0.404	0.404	0.423	0.431	0.412	0.412
11	1E53_A	0.620	0.620	0.627	0.628	0.440	0.464	0.574	0.575
12	1FEX_A	0.645	0.662	0.658	0.658	0.650	0.650	0.643	0.645
13	1UG4_A	0.589	0.625	0.435	0.435	0.277	0.354	0.435	0.435
14	1VYX_A	0.444	0.486	0.360	0.372	0.284	0.359	0.262	0.265
15	3P8B_A	0.518	0.666	0.453	0.453	0.471	0.471	0.412	0.439
16	1F43_A	0.563	0.576	0.589	0.595	0.588	0.603	0.557	0.560
17	1L2P_A	0.864	0.939	0.850	0.892	0.786	0.911	0.793	0.793
18	4MLF_D	0.284	0.284	0.267	0.268	0.248	0.248	0.255	0.255
19	1BE3_J	0.544	0.605	0.448	0.462	0.450	0.471	0.397	0.404
20	1BGY_J	0.540	0.567	0.404	0.404	0.452	0.483	0.399	0.399
21	1TYG_B	0.797	0.823	0.656	0.656	0.604	0.604	0.716	0.717
22	1DTV_A	0.226	0.255	0.252	0.252	0.231	0.239	0.256	0.256
23	2JP3_A	0.364	0.389	0.417	0.424	0.326	0.419	0.373	0.373
24	1CHC_A	0.489	0.501	0.493	0.501	0.351	0.372	0.466	0.466
25	1J9I_A	0.623	0.623	0.615	0.620	0.589	0.589	0.619	0.624
26	1TAF_A	0.859	0.874	0.850	0.888	0.805	0.838	0.755	0.772
27	1DWM_A	0.688	0.688	0.695	0.695	0.584	0.618	0.673	0.674
28	1L6H_A	0.516	0.519	0.530	0.534	0.518	0.524	0.505	0.512
29	1W1W_E	0.805	0.834	0.780	0.793	0.768	0.795	0.764	0.766
30	2CMX_A	0.709	0.760	0.715	0.720	0.589	0.629	0.618	0.653
31	1LDD_A	0.850	0.862	0.810	0.839	0.771	0.771	0.750	0.750
32	1K73_1	0.642	0.682	0.654	0.654	0.540	0.545	0.467	0.469
33	1KN6_A	0.575	0.594	0.566	0.567	0.469	0.551	0.568	0.568
34	1PIH_A	0.558	0.604	0.475	0.476	0.375	0.375	0.343	0.344
35	2HI3_A	0.641	0.643	0.659	0.667	0.649	0.666	0.649	0.657
36	1ABT_A	0.484	0.484	0.296	0.303	0.369	0.430	0.474	0.475
37	1HHV_A	0.598	0.605	0.614	0.620	0.500	0.500	0.490	0.490
38	2V85_A	0.430	0.464	0.302	0.305	0.309	0.309	0.323	0.323
39	3CX5_F	0.788	0.788	0.675	0.690	0.673	0.673	0.593	0.604
40	3MQK_C	0.805	0.850	0.736	0.736	0.684	0.684	0.766	0.769
41	4M75_F	0.742	0.742	0.717	0.717	0.601	0.618	0.650	0.650
42	1DP7_P	0.745	0.770	0.763	0.765	0.642	0.672	0.600	0.620
43	1EKZ_A	0.674	0.693	0.719	0.720	0.661	0.661	0.653	0.653
44	1VCC_A	0.557	0.559	0.582	0.587	0.513	0.569	0.480	0.480
45	1K1Z_A	0.519	0.541	0.582	0.582	0.535	0.535	0.523	0.524
46	1PFS_A	0.530	0.547	0.274	0.277	0.314	0.314	0.459	0.459
47	4V2O_A	0.773	0.804	0.725	0.748	0.842	0.842	0.659	0.662
48	1A91_A	0.506	0.540	0.508	0.508	0.541	0.541	0.504	0.531
49	1KP6_A	0.242	0.280	0.260	0.260	0.257	0.282	0.224	0.230
50	2ZMZ_B	0.713	0.729	0.688	0.689	0.587	0.589	0.663	0.664

No.	PDB	MMpred		MMpred-A_C		MMpred-B_C		MMpred-C	
		First model	Best model	First model	Best model	First model	Best model	First model	Best model
51	1B4R_A	0.650	0.717	0.549	0.549	0.538	0.538	0.489	0.489
52	1PZW_A	0.717	0.762	0.652	0.652	0.594	0.594	0.600	0.612
53	1R6R_A	0.531	0.531	0.485	0.487	0.537	0.537	0.540	0.545
54	4LMS_A	0.402	0.402	0.359	0.361	0.278	0.321	0.278	0.278
55	1D8B_A	0.732	0.744	0.803	0.810	0.794	0.794	0.750	0.756
56	1EZV_G	0.374	0.418	0.464	0.466	0.449	0.483	0.440	0.455
57	1F9P_A	0.593	0.599	0.598	0.604	0.625	0.625	0.608	0.608
58	1GGS_A	0.681	0.695	0.701	0.702	0.689	0.698	0.675	0.676
59	1U84_A	0.840	0.848	0.840	0.843	0.802	0.802	0.810	0.810
60	4ASW_C	0.726	0.778	0.616	0.620	0.517	0.517	0.657	0.663
61	1CF7_B	0.718	0.776	0.688	0.688	0.605	0.664	0.600	0.600
62	1LFU_P	0.589	0.590	0.635	0.721	0.598	0.640	0.604	0.612
63	1WMH_B	0.782	0.795	0.687	0.689	0.631	0.631	0.514	0.521
64	2ODM_B	0.826	0.832	0.866	0.892	0.817	0.845	0.840	0.873
65	2AQ0_A	0.644	0.651	0.649	0.672	0.659	0.664	0.633	0.633
66	2GBJ_B	0.749	0.754	0.679	0.687	0.486	0.509	0.706	0.707
67	1IS7_K	0.643	0.643	0.678	0.681	0.400	0.470	0.422	0.422
68	5T17_A	0.753	0.753	0.754	0.754	0.736	0.736	0.654	0.657
69	1CXZ_B	0.867	0.886	0.885	0.890	0.767	0.767	0.677	0.677
70	1NOE_A	0.611	0.611	0.332	0.334	0.328	0.393	0.287	0.287
71	2J6Z_A	0.720	0.739	0.683	0.693	0.728	0.728	0.715	0.741
72	4OW1_A	0.738	0.741	0.622	0.622	0.582	0.582	0.585	0.586
73	1C9F_A	0.578	0.589	0.559	0.573	0.581	0.632	0.650	0.651
74	1GVP_A	0.671	0.671	0.578	0.580	0.576	0.576	0.330	0.331
75	1RHX_A	0.580	0.595	0.614	0.614	0.557	0.557	0.369	0.371
76	3X15_A	0.498	0.498	0.410	0.410	0.351	0.358	0.390	0.391
77	4GDK_A	0.671	0.694	0.680	0.680	0.555	0.555	0.385	0.385
78	4J20_A	0.704	0.743	0.672	0.677	0.576	0.576	0.557	0.571
79	1H8E_H	0.657	0.657	0.643	0.644	0.550	0.550	0.441	0.441
80	1HBX_E	0.516	0.527	0.605	0.606	0.577	0.577	0.519	0.519
81	5IZB_A	0.565	0.565	0.515	0.515	0.477	0.477	0.419	0.420
82	1JR5_A	0.522	0.572	0.525	0.525	0.391	0.437	0.388	0.392
83	4Q2Q_A	0.801	0.801	0.709	0.709	0.626	0.626	0.563	0.563
84	4MMG_A	0.823	0.840	0.725	0.730	0.541	0.541	0.672	0.672
85	5L38_A	0.825	0.843	0.846	0.846	0.722	0.722	0.731	0.732
86	1IUY_A	0.689	0.697	0.586	0.586	0.552	0.555	0.557	0.560
87	2BYK_D	0.856	0.876	0.888	0.889	0.670	0.796	0.826	0.875
88	4Q2O_A	0.665	0.665	0.693	0.693	0.690	0.690	0.653	0.653
89	5O2V_A	0.747	0.747	0.740	0.740	0.640	0.697	0.736	0.736
90	1J8I_A	0.538	0.555	0.592	0.592	0.553	0.555	0.588	0.590
91	3X0G_A	0.533	0.533	0.610	0.610	0.433	0.468	0.337	0.364
92	1G2R_A	0.811	0.819	0.786	0.795	0.687	0.687	0.710	0.710
93	1PD6_A	0.598	0.634	0.602	0.612	0.573	0.573	0.540	0.541
94	2ICT_A	0.744	0.763	0.766	0.767	0.765	0.765	0.739	0.739
95	1I35_A	0.573	0.573	0.617	0.617	0.562	0.562	0.575	0.577
96	1IM3_D	0.264	0.328	0.311	0.311	0.271	0.331	0.300	0.300
97	5TMF_E	0.553	0.567	0.564	0.564	0.483	0.483	0.463	0.464
98	3N9U_C	0.731	0.736	0.665	0.668	0.589	0.614	0.578	0.580
99	1JO0_A	0.820	0.852	0.800	0.804	0.681	0.744	0.660	0.660
100	2LWP_A	0.501	0.557	0.520	0.520	0.496	0.496	0.465	0.465

No.	PDB	MMpred		MMpred-A_C		MMpred-B_C		MMpred-C	
		First model	Best model	First model	Best model	First model	Best model	First model	Best model
101	3SDL_B	0.315	0.329	0.269	0.281	0.322	0.322	0.305	0.325
102	1FRD_A	0.705	0.727	0.562	0.586	0.603	0.603	0.532	0.569
103	1JMT_A	0.752	0.752	0.614	0.615	0.580	0.584	0.696	0.706
104	2ACY_A	0.657	0.670	0.729	0.731	0.623	0.623	0.604	0.615
105	1MWQ_A	0.674	0.674	0.623	0.623	0.652	0.652	0.642	0.662
106	2NCM_A	0.834	0.834	0.553	0.557	0.567	0.567	0.636	0.636
107	2NDP_A	0.480	0.520	0.430	0.446	0.445	0.470	0.440	0.444
108	1F2R_I	0.627	0.643	0.641	0.674	0.545	0.589	0.587	0.589
109	1KA8_A	0.560	0.601	0.548	0.548	0.570	0.570	0.550	0.550
110	1PSR_A	0.752	0.752	0.643	0.650	0.649	0.649	0.601	0.608
111	1SMP_I	0.700	0.700	0.607	0.607	0.512	0.512	0.604	0.605
112	4IOS_A	0.549	0.593	0.516	0.516	0.486	0.486	0.374	0.378
113	1FJG_F	0.721	0.726	0.668	0.676	0.630	0.643	0.583	0.584
114	1TUL_A	0.378	0.505	0.529	0.537	0.318	0.422	0.270	0.270
115	2K9X_A	0.536	0.536	0.404	0.406	0.439	0.455	0.450	0.450
116	1F93_A	0.779	0.790	0.774	0.774	0.768	0.768	0.735	0.735
117	1IUJ_B	0.730	0.762	0.754	0.756	0.675	0.685	0.733	0.734
118	4ESB_A	0.844	0.844	0.811	0.822	0.705	0.705	0.783	0.830
119	1E3Y_A	0.713	0.731	0.702	0.707	0.691	0.710	0.686	0.706
120	1FMB_A	0.528	0.599	0.516	0.517	0.456	0.456	0.342	0.342
121	3N1G_C	0.642	0.658	0.517	0.517	0.445	0.445	0.426	0.465
122	4UIJ_A	0.759	0.795	0.756	0.760	0.644	0.653	0.738	0.744
123	5TUV_B	0.343	0.394	0.417	0.437	0.406	0.462	0.394	0.394
124	1ABV_A	0.795	0.812	0.798	0.800	0.814	0.814	0.778	0.781
125	1CDB_A	0.625	0.625	0.553	0.557	0.439	0.439	0.417	0.418
126	1JIW_I	0.539	0.539	0.501	0.502	0.571	0.571	0.500	0.500
127	1KPT_A	0.623	0.667	0.617	0.619	0.288	0.433	0.425	0.427
128	1A6L_A	0.658	0.684	0.694	0.695	0.557	0.557	0.613	0.613
129	1ID2_A	0.566	0.679	0.331	0.335	0.523	0.523	0.419	0.421
130	1S7Z_A	0.554	0.588	0.612	0.620	0.631	0.631	0.608	0.617
131	4RUV_A	0.857	0.857	0.794	0.795	0.725	0.725	0.865	0.866
132	1KX5_D	0.708	0.775	0.798	0.798	0.632	0.643	0.762	0.773
133	1ROW_A	0.549	0.600	0.432	0.433	0.483	0.483	0.401	0.401
134	1V74_A	0.727	0.727	0.675	0.679	0.595	0.595	0.635	0.639
135	2BSE_A	0.448	0.462	0.554	0.555	0.371	0.410	0.398	0.400
136	1MFQ_C	0.637	0.644	0.650	0.656	0.644	0.644	0.595	0.595
137	1S7O_C	0.574	0.574	0.599	0.604	0.571	0.585	0.541	0.548
138	1TZ0_A	0.545	0.618	0.564	0.577	0.561	0.561	0.540	0.541
139	1K3S_A	0.616	0.690	0.588	0.590	0.480	0.480	0.525	0.527
140	1VD0_A	0.433	0.479	0.395	0.395	0.278	0.309	0.255	0.255
141	2CWP_A	0.659	0.736	0.636	0.636	0.447	0.447	0.599	0.599
142	2NAZ_A	0.661	0.698	0.667	0.675	0.657	0.662	0.569	0.571
143	1BJX_A	0.786	0.786	0.732	0.734	0.656	0.656	0.664	0.667
144	1I85_A	0.598	0.628	0.512	0.513	0.442	0.462	0.289	0.289
145	1QFW_B	0.383	0.383	0.315	0.317	0.258	0.268	0.249	0.250
146	2D0P_B	0.683	0.752	0.713	0.713	0.703	0.703	0.589	0.592
147	3W1Z_D	0.569	0.624	0.595	0.595	0.558	0.558	0.546	0.546
148	1EM8_D	0.649	0.712	0.597	0.602	0.521	0.521	0.527	0.527
149	1JLI_A	0.365	0.378	0.331	0.342	0.335	0.377	0.332	0.337
150	1NZE_A	0.867	0.878	0.902	0.907	0.861	0.861	0.844	0.846

No.	PDB	MMpred		MMpred-A_C		MMpred-B_C		MMpred-C	
		First model	Best model	First model	Best model	First model	Best model	First model	Best model
151	1N3G_A	0.692	0.699	0.675	0.678	0.606	0.616	0.663	0.663
152	1SAU_A	0.678	0.705	0.691	0.691	0.572	0.652	0.659	0.663
153	2APN_A	0.615	0.615	0.352	0.352	0.573	0.573	0.417	0.417
154	5WSE_A	0.654	0.711	0.637	0.637	0.576	0.576	0.441	0.441
155	3EOD_A	0.817	0.820	0.790	0.790	0.760	0.760	0.708	0.709
156	3LQV_B	0.640	0.645	0.573	0.573	0.478	0.499	0.271	0.280
157	1FC3_A	0.819	0.828	0.820	0.828	0.776	0.776	0.761	0.762
158	1FHT_A	0.624	0.624	0.602	0.604	0.497	0.497	0.561	0.561
159	2RLD_C	0.876	0.883	0.901	0.903	0.847	0.847	0.856	0.859
160	1D6T_A	0.619	0.694	0.661	0.661	0.596	0.596	0.630	0.633
161	1ELW_A	0.913	0.918	0.926	0.930	0.921	0.939	0.914	0.927
162	1WJ8_A	0.872	0.875	0.910	0.913	0.858	0.858	0.873	0.883
163	1A7D_A	0.789	0.791	0.824	0.824	0.760	0.760	0.751	0.751
164	1HCD_A	0.626	0.626	0.555	0.563	0.467	0.467	0.336	0.336
165	2Q2H_A	0.498	0.593	0.315	0.315	0.403	0.417	0.406	0.407
166	1JJ2_S	0.669	0.727	0.570	0.576	0.542	0.542	0.571	0.571
167	1MAI_A	0.611	0.703	0.533	0.536	0.508	0.508	0.473	0.476
168	1OFT_A	0.799	0.799	0.749	0.753	0.662	0.717	0.646	0.648
169	1ORY_A	0.783	0.783	0.799	0.800	0.779	0.784	0.768	0.768
170	1VKE_E	0.790	0.790	0.711	0.711	0.749	0.749	0.675	0.678
171	2CZV_D	0.681	0.710	0.695	0.695	0.626	0.626	0.581	0.581
172	2GJ3_A	0.802	0.802	0.660	0.671	0.639	0.639	0.584	0.585
173	2LKP_A	0.594	0.607	0.644	0.646	0.584	0.634	0.570	0.577
174	2PI2_F	0.782	0.782	0.588	0.588	0.491	0.528	0.522	0.524
175	3G20_B	0.570	0.570	0.564	0.580	0.506	0.545	0.502	0.516
176	1DUN_A	0.609	0.609	0.612	0.616	0.361	0.361	0.438	0.438
177	1JPY_Y	0.414	0.415	0.367	0.409	0.317	0.377	0.272	0.275
178	2H8E_A	0.614	0.614	0.562	0.562	0.564	0.564	0.418	0.440
179	1BUO_A	0.804	0.804	0.769	0.769	0.392	0.445	0.482	0.482
180	2QZJ_A	0.895	0.895	0.878	0.883	0.875	0.875	0.847	0.847
181	1NR3_A	0.316	0.362	0.389	0.389	0.334	0.386	0.309	0.334
182	2EWC_B	0.684	0.701	0.720	0.723	0.512	0.593	0.641	0.647
183	2WCW_B	0.714	0.759	0.715	0.715	0.612	0.612	0.568	0.569
184	3QU3_A	0.552	0.552	0.596	0.597	0.477	0.477	0.438	0.441
185	5O8G_A	0.641	0.710	0.640	0.643	0.525	0.525	0.354	0.358
186	1L3G_A	0.531	0.583	0.489	0.490	0.521	0.521	0.475	0.480
187	1QMA_A	0.653	0.749	0.488	0.488	0.534	0.534	0.561	0.561
188	4GF3_A	0.577	0.637	0.562	0.564	0.571	0.571	0.405	0.406
189	1BGF_A	0.801	0.816	0.787	0.787	0.759	0.759	0.702	0.706
190	1FSP_A	0.843	0.847	0.874	0.874	0.860	0.860	0.833	0.835
191	1OOF_A	0.731	0.770	0.757	0.763	0.614	0.680	0.717	0.735
192	1F98_A	0.662	0.711	0.635	0.636	0.490	0.507	0.606	0.610
193	1FR0_A	0.741	0.767	0.775	0.780	0.756	0.756	0.776	0.781
194	1HKQ_A	0.623	0.688	0.708	0.711	0.599	0.640	0.640	0.640
195	2L74_A	0.712	0.712	0.611	0.611	0.495	0.495	0.487	0.489
196	2P7L_A	0.709	0.750	0.625	0.625	0.511	0.511	0.499	0.502
197	2RD5_D	0.502	0.502	0.523	0.524	0.431	0.431	0.488	0.488
198	3BDB_A	0.505	0.525	0.585	0.585	0.399	0.405	0.285	0.311
199	3CG4_A	0.802	0.807	0.844	0.846	0.777	0.777	0.782	0.787
200	3CX5_G	0.709	0.709	0.678	0.713	0.508	0.508	0.460	0.490

No.	PDB	MMpred		MMpred-A_C		MMpred-B_C		MMpred-C	
		First model	Best model	First model	Best model	First model	Best model	First model	Best model
201	5CJ3_B	0.690	0.729	0.702	0.722	0.699	0.699	0.652	0.652
202	1B8Q_A	0.436	0.437	0.492	0.492	0.439	0.475	0.442	0.444
203	1DBF_A	0.661	0.661	0.627	0.628	0.564	0.564	0.538	0.538
204	1UFB_A	0.788	0.788	0.772	0.772	0.715	0.717	0.747	0.747
205	2A9U_B	0.783	0.794	0.786	0.812	0.746	0.767	0.754	0.754
206	3I9V_7	0.538	0.538	0.555	0.555	0.468	0.468	0.490	0.492
207	1DOI_A	0.499	0.499	0.418	0.418	0.393	0.393	0.271	0.271
208	1GPQ_B	0.640	0.641	0.631	0.632	0.457	0.541	0.377	0.377
209	1PXW_A	0.655	0.720	0.660	0.676	0.616	0.616	0.583	0.583
210	4I60_A	0.564	0.564	0.514	0.519	0.553	0.553	0.656	0.656
211	4JGX_B	0.676	0.719	0.757	0.772	0.642	0.673	0.690	0.695
212	1AHK_A	0.483	0.483	0.471	0.471	0.448	0.448	0.417	0.417
213	2QVG_A	0.794	0.821	0.801	0.802	0.822	0.822	0.744	0.745
214	2XGY_A	0.624	0.632	0.634	0.641	0.495	0.566	0.471	0.479
215	1AX8_A	0.576	0.589	0.691	0.695	0.471	0.510	0.480	0.487
216	1GQA_A	0.763	0.791	0.680	0.688	0.566	0.617	0.728	0.733
217	2HYB_A	0.618	0.625	0.553	0.565	0.498	0.498	0.405	0.405
218	4B0M_A	0.554	0.605	0.556	0.573	0.482	0.482	0.428	0.429
219	1B4U_A	0.616	0.619	0.635	0.640	0.651	0.651	0.614	0.624
220	3CAE_A	0.508	0.508	0.442	0.442	0.463	0.477	0.410	0.411
221	4CXT_A	0.703	0.703	0.552	0.553	0.519	0.519	0.401	0.403
222	1DCF_A	0.822	0.823	0.808	0.811	0.763	0.763	0.689	0.689
223	1OA8_D	0.295	0.320	0.310	0.310	0.284	0.299	0.253	0.254
224	1Y14_A	0.442	0.571	0.479	0.480	0.488	0.499	0.445	0.461
225	4LE0_B	0.895	0.907	0.925	0.928	0.803	0.822	0.804	0.804
226	4Z6J_A	0.488	0.507	0.280	0.289	0.399	0.399	0.412	0.421
227	1PMS_A	0.533	0.568	0.580	0.581	0.286	0.383	0.411	0.417
228	1S56_B	0.751	0.759	0.773	0.774	0.746	0.746	0.739	0.739
229	1OJG_A	0.624	0.624	0.555	0.558	0.592	0.592	0.462	0.477
230	1SVJ_A	0.750	0.756	0.652	0.655	0.580	0.580	0.732	0.740
231	1TWU_A	0.738	0.738	0.548	0.554	0.510	0.564	0.499	0.499
232	1FJG_H	0.712	0.740	0.713	0.716	0.539	0.582	0.539	0.539
233	3UE6_E	0.685	0.690	0.661	0.672	0.524	0.566	0.581	0.584
234	1LNW_C	0.812	0.826	0.831	0.859	0.741	0.763	0.801	0.814
235	4AIH_A	0.772	0.772	0.848	0.849	0.682	0.813	0.618	0.623
236	1KQ6_A	0.699	0.712	0.623	0.623	0.527	0.578	0.547	0.547
237	1NPB_A	0.592	0.649	0.534	0.539	0.630	0.630	0.597	0.597
238	1OZ9_A	0.677	0.700	0.672	0.703	0.658	0.658	0.656	0.656
239	1R5T_A	0.691	0.711	0.532	0.534	0.482	0.482	0.562	0.570
240	2FA5_B	0.714	0.730	0.808	0.817	0.771	0.771	0.762	0.764
241	2HQ7_B	0.697	0.697	0.614	0.617	0.509	0.509	0.656	0.663
242	1HKX_E	0.471	0.471	0.318	0.318	0.485	0.485	0.524	0.530
243	1HL6_D	0.486	0.574	0.458	0.465	0.414	0.414	0.365	0.365
244	1S3J_A	0.770	0.787	0.749	0.773	0.798	0.798	0.733	0.741
245	2F22_B	0.671	0.685	0.705	0.709	0.596	0.596	0.526	0.539
246	4KA0_A	0.798	0.804	0.793	0.794	0.692	0.692	0.624	0.630
247	5L8R_D	0.435	0.464	0.412	0.412	0.348	0.348	0.270	0.311
248	1KSX_A	0.652	0.697	0.585	0.601	0.362	0.421	0.501	0.503
249	1LE2_A	0.267	0.267	0.281	0.281	0.283	0.289	0.278	0.278
250	1A3A_C	0.607	0.643	0.546	0.554	0.447	0.525	0.460	0.480

No.	PDB	MMpred		MMpred-A_C		MMpred-B_C		MMpred-C	
		First model	Best model	First model	Best model	First model	Best model	First model	Best model
251	1K5D_B	0.583	0.583	0.387	0.387	0.462	0.462	0.332	0.332
252	1LZW_B	0.807	0.807	0.753	0.754	0.614	0.667	0.668	0.668
253	1HBG_A	0.830	0.833	0.840	0.843	0.685	0.733	0.758	0.760
254	3E6M_E	0.730	0.731	0.761	0.775	0.725	0.725	0.651	0.655
255	3PD2_A	0.622	0.622	0.557	0.562	0.540	0.540	0.545	0.549
256	4GQY_A	0.664	0.664	0.539	0.539	0.601	0.601	0.650	0.652
257	1UNG_D	0.683	0.718	0.631	0.633	0.627	0.627	0.691	0.701
258	1GME_A	0.528	0.528	0.458	0.458	0.318	0.364	0.299	0.301
259	1F1E_A	0.667	0.667	0.490	0.495	0.568	0.568	0.445	0.446
260	2H30_A	0.661	0.706	0.657	0.657	0.535	0.535	0.594	0.594
261	2PYB_A	0.755	0.791	0.712	0.712	0.670	0.709	0.752	0.754
262	1NTV_A	0.614	0.614	0.513	0.520	0.322	0.391	0.334	0.341
263	2NS9_B	0.783	0.788	0.610	0.611	0.644	0.644	0.618	0.620
264	3GMX_A	0.437	0.437	0.292	0.306	0.292	0.295	0.307	0.308
265	2GKC_A	0.459	0.459	0.489	0.492	0.455	0.455	0.367	0.372
266	5JTM_A	0.580	0.580	0.333	0.333	0.348	0.420	0.283	0.286
267	3ALU_A	0.400	0.400	0.447	0.460	0.359	0.359	0.511	0.515
268	1OX7_A	0.655	0.655	0.655	0.693	0.558	0.558	0.406	0.406
269	1USL_C	0.756	0.775	0.789	0.798	0.551	0.551	0.684	0.693
270	2KBW_A	0.722	0.756	0.735	0.737	0.594	0.594	0.630	0.630
271	3F8L_A	0.628	0.654	0.501	0.501	0.435	0.544	0.275	0.276
272	1C03_A	0.645	0.645	0.643	0.643	0.656	0.656	0.534	0.543
273	3H05_B	0.605	0.605	0.658	0.658	0.434	0.453	0.539	0.545
274	4NBI_A	0.503	0.503	0.376	0.376	0.415	0.451	0.439	0.442
275	1FW9_A	0.552	0.552	0.408	0.427	0.316	0.338	0.348	0.350
276	2AEN_A	0.421	0.421	0.250	0.250	0.323	0.323	0.221	0.222
277	1C41_A	0.696	0.696	0.648	0.649	0.637	0.637	0.541	0.541
278	1F3Y_A	0.340	0.368	0.269	0.277	0.342	0.342	0.374	0.376
279	1S2D_A	0.642	0.695	0.664	0.664	0.589	0.589	0.579	0.580
280	2LRB_A	0.607	0.607	0.313	0.324	0.506	0.506	0.278	0.280
281	3V1O_A	0.595	0.595	0.533	0.533	0.294	0.387	0.292	0.326
282	1PGV_A	0.782	0.806	0.757	0.762	0.692	0.692	0.544	0.544
283	2FKB_C	0.522	0.522	0.392	0.399	0.546	0.546	0.352	0.366
284	1AP7_A	0.775	0.787	0.715	0.716	0.565	0.565	0.606	0.624
285	2C4W_A	0.636	0.649	0.590	0.591	0.579	0.579	0.511	0.511
286	2O70_F	0.750	0.774	0.710	0.710	0.587	0.591	0.508	0.529
287	2WGP_A	0.762	0.769	0.736	0.781	0.636	0.636	0.564	0.572
288	3M1N_B	0.433	0.439	0.431	0.435	0.405	0.405	0.449	0.465
289	1XJA_C	0.643	0.654	0.627	0.628	0.556	0.556	0.635	0.657
290	1YG2_A	0.445	0.623	0.434	0.454	0.428	0.441	0.483	0.491
291	1QZG_A	0.561	0.561	0.428	0.428	0.342	0.342	0.282	0.303
292	1NF6_F	0.806	0.806	0.796	0.802	0.779	0.779	0.762	0.767
293	1NQZ_A	0.605	0.607	0.533	0.542	0.485	0.485	0.276	0.282
294	5IAO_A	0.491	0.493	0.333	0.333	0.383	0.433	0.327	0.327
295	6AQ3_B	0.558	0.569	0.577	0.584	0.552	0.552	0.569	0.571
296	1KOH_D	0.752	0.752	0.742	0.744	0.624	0.624	0.666	0.675
297	1TEO_A	0.554	0.554	0.508	0.529	0.495	0.535	0.318	0.320
298	2A5Y_A	0.698	0.723	0.702	0.705	0.668	0.668	0.717	0.717
299	1AK6_A	0.514	0.514	0.294	0.294	0.420	0.440	0.330	0.330
300	1QFT_A	0.506	0.506	0.372	0.373	0.377	0.402	0.313	0.313

No.	PDB	MMpred		MMpred-A_C		MMpred-B_C		MMpred-C	
		First model	Best model	First model	Best model	First model	Best model	First model	Best model
301	2L5P_A	0.632	0.632	0.634	0.635	0.370	0.443	0.515	0.518
302	2C2F_A	0.802	0.802	0.771	0.771	0.667	0.671	0.763	0.770
303	1NGL_A	0.552	0.552	0.368	0.368	0.449	0.490	0.389	0.389
304	3IAM_2	0.530	0.616	0.540	0.553	0.415	0.438	0.487	0.522
305	2Z3B_A	0.751	0.751	0.644	0.669	0.504	0.528	0.592	0.592
306	1Y1X_A	0.667	0.667	0.652	0.670	0.631	0.651	0.634	0.661
307	1RZ3_A	0.463	0.515	0.361	0.361	0.498	0.498	0.514	0.515
308	1WLQ_C	0.629	0.648	0.539	0.540	0.505	0.525	0.492	0.492
309	1TJF_B	0.791	0.791	0.781	0.782	0.739	0.739	0.716	0.720
310	3O61_A	0.348	0.418	0.387	0.387	0.430	0.430	0.331	0.340
311	1TLJ_A	0.536	0.536	0.441	0.457	0.370	0.383	0.452	0.453
312	1DTP_A	0.222	0.258	0.243	0.254	0.247	0.263	0.216	0.226
313	1F15_C	0.197	0.222	0.198	0.200	0.201	0.204	0.215	0.215
314	1GXD_C	0.455	0.455	0.401	0.401	0.295	0.327	0.308	0.308
315	1VCY_A	0.464	0.464	0.327	0.337	0.303	0.437	0.258	0.258
316	2VUL_A	0.411	0.411	0.407	0.407	0.345	0.360	0.306	0.306
317	4ZBY_A	0.657	0.657	0.656	0.660	0.282	0.467	0.543	0.550
318	1IOO_A	0.447	0.447	0.415	0.436	0.321	0.336	0.503	0.505
319	5EKT_A	0.461	0.461	0.348	0.358	0.408	0.415	0.441	0.476
320	4K1F_A	0.535	0.601	0.443	0.453	0.277	0.380	0.566	0.566