Supporting Information

Supporting Figures

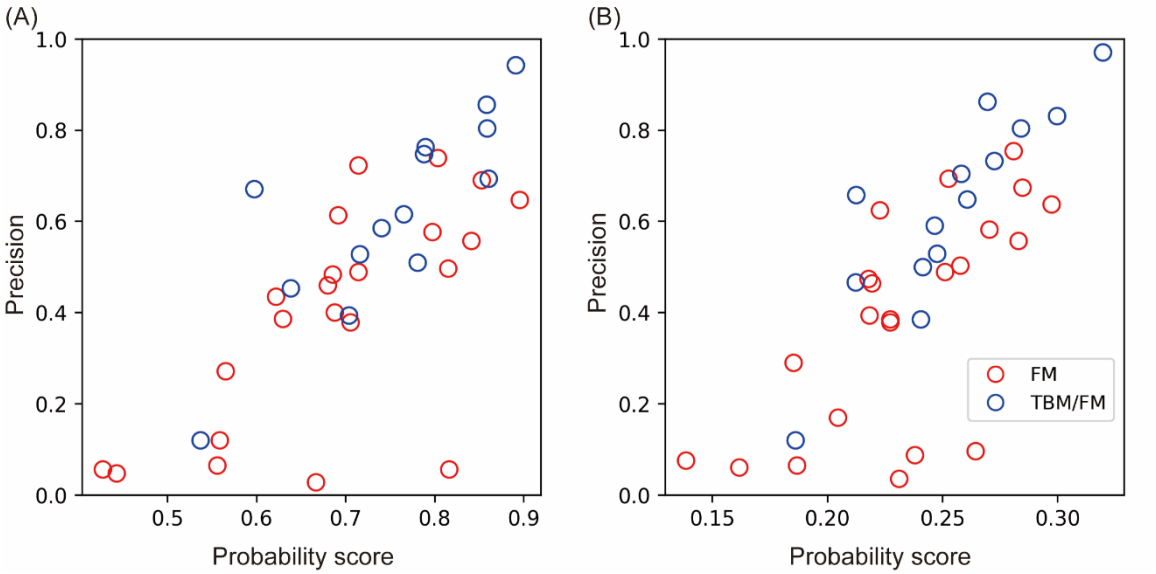

Figure S1. Correlation between mean predicted cumulative probability under d_{th} Å of the top 10*L all-range contacts (confidence score for MSA selection) and their long-range Top-L precision. (A) Group 010, d_{th}=12. (B) Group 024, d_{th}=8.

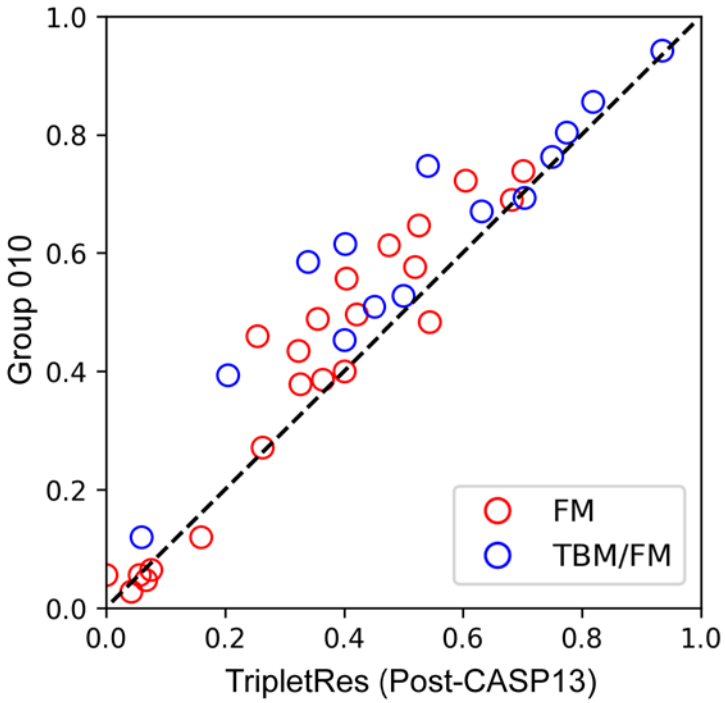

Figure S2. Head-to-head comparison of long-range Top-*L* precision between our pipeline in CASP14 and TripletRes (Post-CASP13). The two methods used the same training set and input MSAs.

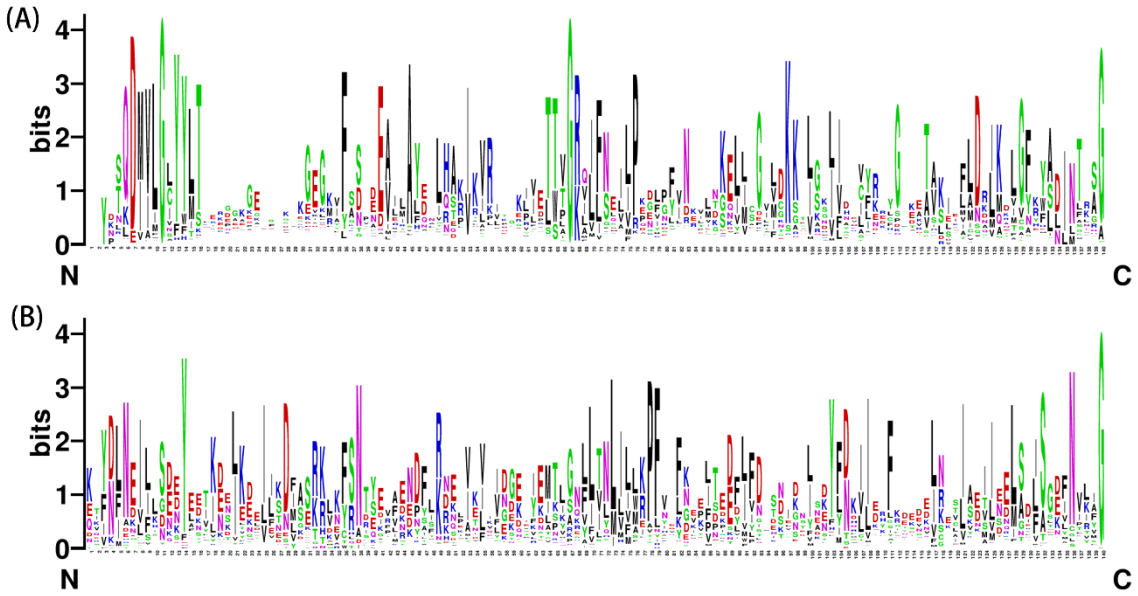

Figure S3. MSA consensus visualization of T1093-D1. (A) MSA collected by full-length sequence. (B) MSA collected by domain sequence.

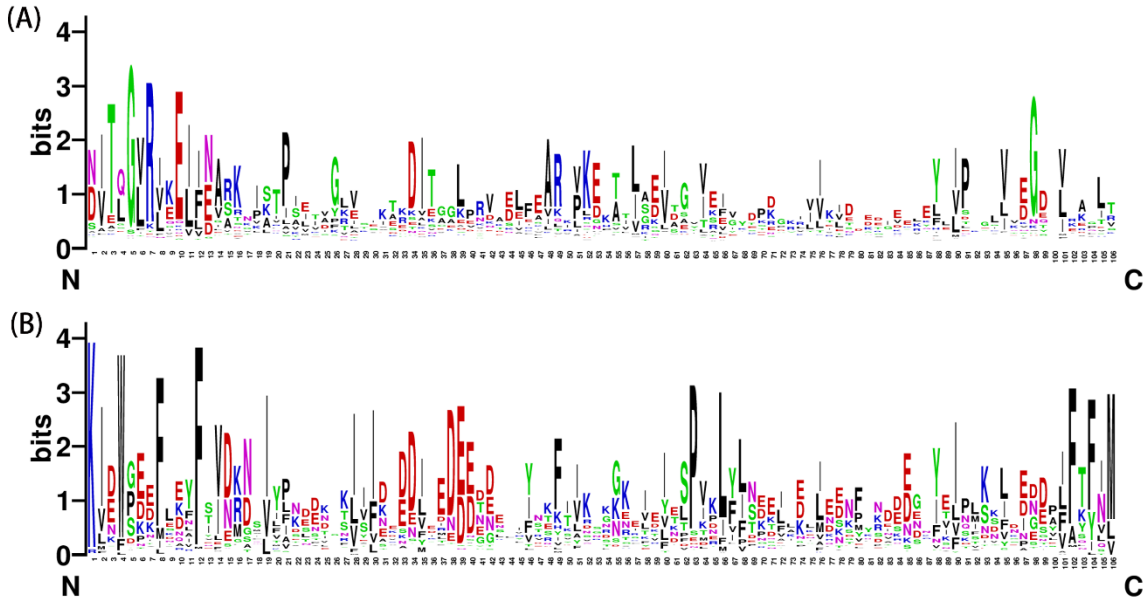

Figure S4. MSA consensus visualization of T1093-D3. (A) MSA collected by full-length sequence. (B) MSA collected by domain sequence.

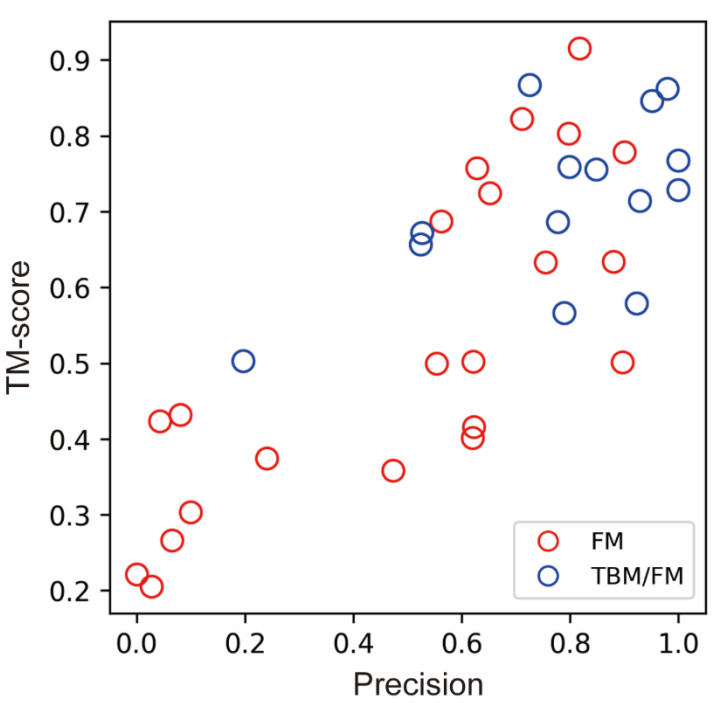

Figure S5. The TM-score vs. precision of long-range Top-*L*/2 contact prediction on FM and FM/TBM targets.

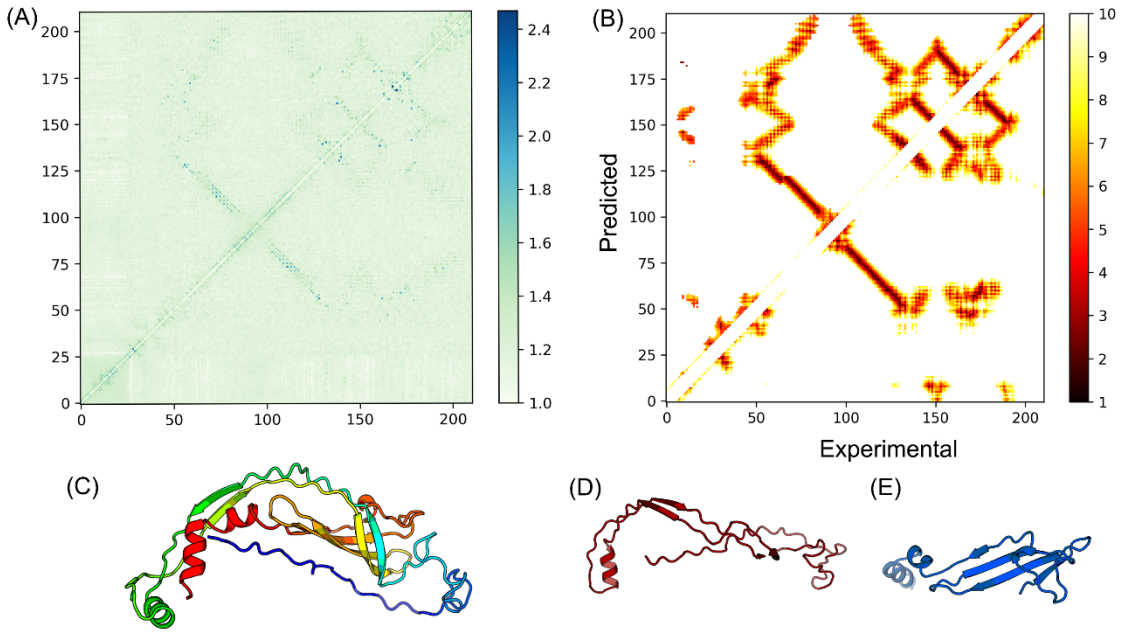

Figure S6. An illustrative example of CASP14 domain T1047s-D1. (A) Residue-wise coupling score map by direct coupling analysis based on Potts model. (B) Comparison of predicted discrete distance map by DeepPotential and the discrete distance map of the experimental structure. The distance bins are defined according to the CASP format. (C) Predicted structure of T1047s-D1. (D) The predicted structure of the beta-sheet region. (E) The predicted structure of the region near the C-terminal.

Supporting Tables

Table S1. Average Precision, Recall and F1-score of long-range Top-*N* distance prediction for DeepPotential's two Groups in CASP14 with standard error in brackets.

Index	Group	FM				TBM/FM			
		L/2	L	2L	5L	L/2	L	2L	5L
Precision	010	0.312 (0.049)	0.285 (0.042)	0.297 (0.044)	0.240 (0.034)	0.515 (0.049)	0.476 (0.041)	0.449 (0.031)	0.390 (0.032)
	024	0.292 (0.042)	0.308 (0.044)	0.288 (0.041)	0.242 (0.036)	0.553 (0.052)	0.538 (0.048)	0.463 (0.032)	0.414 (0.036)
Recall	010	0.321 (0.044)	0.282 (0.036)	0.274 (0.035)	0.215 (0.027)	0.479 (0.045)	0.435 (0.036)	0.389 (0.033)	0.333 (0.032)
	024	0.305 (0.035)	0.303 (0.037)	0.271 (0.034)	0.225 (0.029)	0.518 (0.045)	0.503 (0.042)	0.408 (0.033)	0.360 (0.035)
F1-score	010	0.297 (0.045)	0.272 (0.039)	0.270 (0.039)	0.210 (0.030)	0.472 (0.047)	0.431 (0.040)	0.394 (0.035)	0.338 (0.034)
	024	0.278 (0.038)	0.289 (0.041)	0.264 (0.037)	0.218 (0.032)	0.511 (0.048)	0.500 (0.046)	0.413 (0.034)	0.366 (0.037)