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Supplementary information

The trRosetta server for fast and accurate protein structure prediction

Supplementary Information

Supplementary Table 1 | List of 31 CASP13 free modeling (FM) domains. A target is defined as a FM target if it lacks homologous templates in PDB.

T0950-D1	T0975-D1	T0990-D3	T1022s1-D1
T0953s2-D2	T0980s1-D1	T0991-D1	
T0953s2-D3	T0981-D2	T0998-D1	
T0957s1-D1	T0986s2-D1	T1000-D2	
T0957s2-D1	T0987-D1	T1001-D1	
T0960-D2	T0987-D2	T1010-D1	
T0963-D2	T0989-D1	T1015s1-D1	
T0968s1-D1	T0989-D2	T1017s2-D1	
T0968s2-D1	T0990-D1	T1021s3-D1	
T0969-D1	T0990-D2	T1021s3-D2	

Supplementary Table 2 | List of 131 CAMEO hard targets. According to CAMEO (https://www.cameo3d.org/cameong_help/3d/), hard targets are those with an average lDDT < 50 over the models from the participating servers.

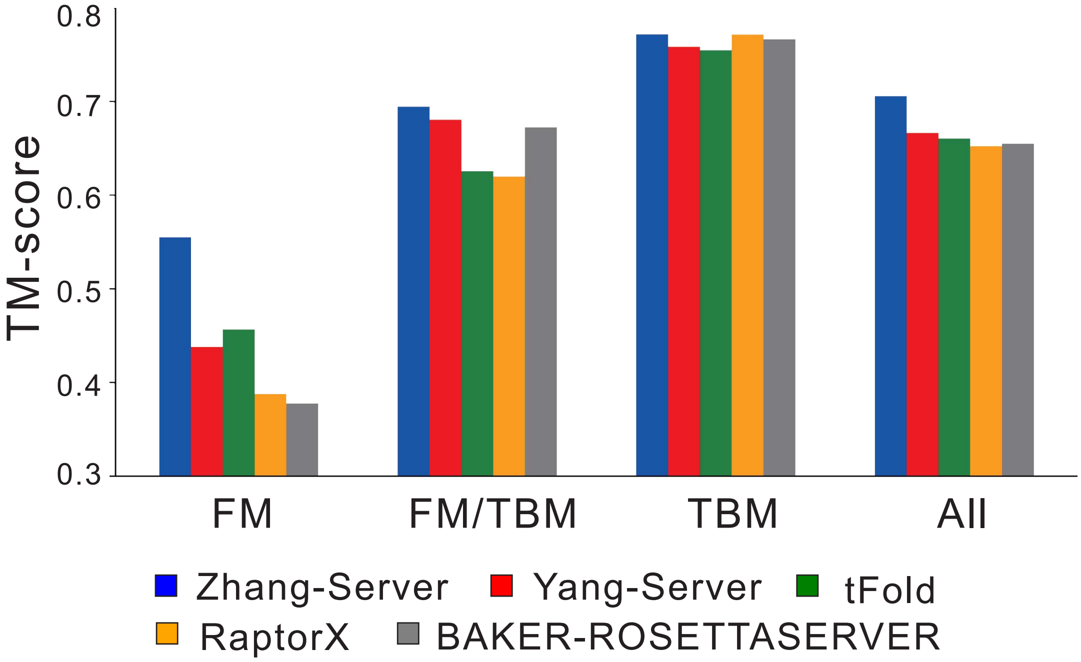
5OD1_A	6A5G_B	6CZT_A	6GHO_B
5OD9_B	6A68_A	6D0I_C	6GMA_F
5OQK_A	6A83_A	6D0I_D	6GMS_A
5OVM_A	6A9J_B	6D2S_A	6GW7_A
5W5P_A	6A9W_A	6D7Y_A	6H2X_A
5WB4_H	6AAY_A	6D7Y_B	6H6N_B
5XJO_E	6AE1_B	6D97_D	6HC2_X
5XKJ_F	6AE8_D	6D9F_B	6HPV_A
5XKN_F	6AE9_B	6D9M_A	6I1R_B
5Y08_A	6AEF_A	6DAN_D	6I9H_A
5YA6_B	6AGH_B	6DFL_A	6IAI_D
5YRQ_E	6AGJ_B	6DGN_B	6IEH_A
5YVQ_A	6AHQ_T	6DII_L	6N0T_A
5YVQ_B	6AIT_F	6DKA_I	6N8P_A
5Z2H_B	6AJJ_A	6DKM_G	6NU4_A
5Z2I_D	6AKJ_B	6DLC_A	6NX4_A
5Z34_A	6BEA_A	6DLO_A	6OHZ_A
5Z36_A	6BS5_A	6DRF_A	
5Z3F_A	6BS5_B	6DTD_A	
5Z3K_B	6BWH_C	6E0K_A	
5Z6D_B	6BXS_C	6E0M_A	
5Z7C_A	6BXW_A	6E3C_C	
5Z8B_B	6BZJ_A	6E9B_D	
5Z9T_B	6BZK_A	6E9O_A	
5ZB2_A	6BZT_D	6EAZ_B	
5ZER_B	6CB6_A	6EDB_B	
5ZKE_A	6CCI_A	6EGC_A	
5ZKH_B	6CGO_B	6FCG_F	
5ZKT_B	6CK1_D	6FTO_C	
5ZME_A	6CMK_A	6FXD_B	
5ZNS_A	6CP8_B	6G1H_A	
5ZOR_A	6CP8_D	6G3B_B	
5ZT0_J	6CP9_G	6G70_B	
5ZT7_B	6CP9_H	6G7G_A	
5ZX9_A	6CPU_A	6G7O_A	
5ZYO_D	6CSV_D	6G8Y_A	
6A2W_A	6CUL_H	6GCJ_A	
6A5F_B	6CZ6_D	6GDJ_B	

Supplementary Table 3 | List of 96 CASP14 domains. TBM: template-based modeling; FM/TBM: free modeling/template-based modeling; FM: free modeling. The classification is given by the assessors, which depends on whether good templates could be found or not at the time of the experiment.

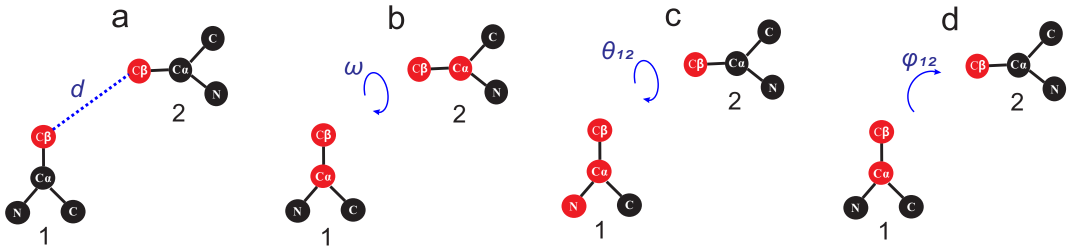
TBM		**TBM/FM**	**FM**
T1024-D1	T1084-D1	T1035-D1	T1027-D1
T1024-D2	T1085-D1	T1038-D2	T1029-D1
T1025-D1	T1085-D3	T1046s1-D1	T1031-D1
T1026-D1	T1086-D1	T1047s2-D1	T1033-D1
T1028-D1	T1086-D2	T1047s2-D3	T1037-D1
T1030-D1	T1087-D1	T1052-D3	T1038-D1
T1030-D2	T1089-D1	T1053-D1	T1039-D1
T1032-D1	T1091-D1	T1053-D2	T1040-D1
T1034-D1	T1091-D2	T1055-D1	T1041-D1
T1036s1-D1	T1091-D3	T1058-D1	T1042-D1
T1045s1-D1	T1091-D4	T1061-D1	T1043-D1
T1045s2-D1	T1092-D1	T1065s2-D1	T1047s1-D1
T1046s2-D1	T1092-D2	T1080-D1	T1049-D1
T1047s2-D2	T1093-D2	T1082-D1	T1061-D2
T1050-D1	T1094-D1	T1085-D2	T1064-D1
T1050-D2	T1095-D1		T1070-D1
T1050-D3	T1099-D1		T1074-D1
T1052-D1	T1100-D1		T1090-D1
T1052-D2	T1100-D2		T1093-D1
T1054-D1	T1101-D1		T1093-D3
T1056-D1	T1101-D2		T1094-D2
T1057-D1			T1096-D1
T1058-D2			T1096-D2
T1060s2-D1			
T1060s3-D1			
T1061-D3			
T1065s1-D1			
T1067-D1			
T1068-D1			
T1070-D2			
T1070-D3			
T1070-D4			
T1073-D1			
T1076-D1			
T1078-D1			
T1079-D1			
T1083-D1			

Supplementary Table 4 | List of 161 CAMEO targets. According to CAMEO, the difficulty of a target is based on average lDDT over the models from the participating servers (average lDDT ≥ 75 for easy, 50 ≤ average lDDT<75 for medium, average lDDT < 50 for hard).

Easy	Medium			Hard
6KBW_A	6I1M_A	6OZ2_H	6WW3_A	6KAW_A
6KDD_A	6K9N_A	6OZ3_H	6WW4_B	6L82_A
6KFS_A	6KA2_B	6OZ3_L	6XGP_B	6LBR_A
6KM9_B	6KBH_A	6PMH_A	6XMI_F	6LBT_B
6KR5_B	6KCO_A	6PMU_B	6XNU_A	6LCC_A
6KUI_B	6KFW_A	6QJZ_A	6XS4_A	6LHY_A
6KV3_B	6KG8_A	6R16_J	6Y4R_B	6NWX_B
6L2I_A	6KG9_A	6S5F_A	6Y93_B	6OHG_A
6L5D_B	6KGC_B	6SDU_A	6YF5_A	6OV6_A
6LPA_A	6KHU_A	6SER_A	6YUC_G	6POO_A
6M0D_A	6KMH_D	6SHD_A	6YWN_A	6PQT_A
6M1J_A	6KNA_A	6SIF_A	6Z46_B	6PSH_A
6Q1I_B	6KOG_A	6SL7_A	6Z4A_A	6PSK_T
6QPN_A	6KPD_B	6SLM_A	6Z4U_A	6PXE_F
6QPO_A	6KQ9_A	6SM7_B	6ZHK_A	6RMO_I
6SAR_A	6KRA_A	6SNR_A	6ZLZ_B	6RY0_A
6SJD_A	6KRX_A	6SP0_A	6ZRV_B	6S0R_B
6SKX_A	6KSA_B	6SUI_A	7BUT_A	6SBP_A
6SME_B	6KTH_A	6SUM_A	7BWN_D	6SE1_A
6UKA_A	6KTQ_A	6T3H_A	7C2G_G	6T6H_A
6URA_A	6KWS_A	6TDD_A	7C2P_A	6TAZ_B
6W5G_A	6KYB_B	6TPK_A	7C9O_A	6TO6_A
6XD8_A	6KYT_F	6TZN_A	7JID_A	6U08_A
6XDK_D	6L08_A	6U4K_A	7JJK_A	6U08_F
6XGS_A	6L2L_A	6UCD_A	7JNN_A	6U8T_B
6XMY_A	6L4B_A	6UIO_A		6WT9_A
6YPB_A	6LB8_C	6UY9_A		6YJ1_A
6ZHI_B	6LBJ_B	6V97_B		7BQ9_B
7BUM_A	6LBK_A	6VAX_B		7BW1_A
7CDV_A	6LCJ_A	6VCF_B		7JH5_A
7JWK_C	6LFA_A	6VEE_A		7JN6_A
	6LL9_A	6VGA_A		
	6LLW_A	6VHI_A		
	6LS9_A	6VZQ_D		
	6LUG_B	6W90_A		
	6M4P_A	6WHB_A		
	6ON4_A	6WP7_D		



Supplementary Figure 1 | A zoomed-in view of Figure2a. To better illustrate the scale of difference, we draw the average TM-score of five representative server groups on CASP14 domains with a truncated y-axis.



Supplementary Figure 2 | Definition of the inter-residue geometries. For residues 1 and 2, the relative positions of the backbone atoms can be defined by one distance (*d*) and five orientations (3 dihedral angles ω, θ_{12}, θ_{21} and 2 planar angles φ_{12}, φ_{21}). **a,** The distance between residues 1 and 2, which is defined as the space between their C_β atoms (C_α for Glycine). **b,** The ω angle, i.e., the dihedral angle formed by the C_α^1-C_β^1-C_β^2 and C_β^1-C_β^2-C_α^2 planes. Here C_α^1 refers the C_α atom of residue 1 and other notations have similar meanings. **c,** The θ_{12} angle, which is the dihedral angle formed by the N^1-C_α^1-C_β^1 and C_α^1-C_β^1-C_β^2 planes. **d,** The φ_{12} angle, which is the planar angle formed by C_α^1-C_β^1 and C_β^1-C_β^2 lines.