Supplementary Materials

Table S1. Features based on 1D structural feature comparison for QDistance.

Features	Description
surface (SU)	$$SU = \frac{\sum_{i=1}^{L} S_i^{non}}{\sum_{i=1}^{L} S_i}$$ S_i is the exposed area of residue *i* parsed by DSSP (Kabsch and Sander, 1983) and S_i^{non} is the exposed area of nonpolar residue *i*. If residue *i* is polar and S_i^{non} is set to 0.
secondary structure similarity (SS)	$$SS = \frac{SS_{match}}{L}$$ SS_{match}: The number of residues that predicted secondary structure by Spine X (Faraggi, et al., 2012) matches the one derived from the model by DSSP.
secondary structure penalty (SP)	$$SP = 1 - \frac{SS_{mismatch}}{2L}$$ $SS_{mismatch}$: The number of residues that the predicted secondary structure which is alpha-helix or beta-sheet mismatches the one derived from the model by DSSP.
exposed mass (EM)	$$EM = \frac{\sum_{i=1}^{L} M_i^{ex}}{\sum_{i=1}^{L} M_i}$$ M_i^{ex} is the mass of exposed area of residue *i* and M_i is its total mass .
exposed surface (ES)	$$ES = \frac{\sum_{i=1}^{L} S_i^{ex}}{\sum_{i=1}^{L} S_i^{total}}$$ S_i^{ex} is the exposed area of residue i and S_i^{total} is the total area of residue *i*.
solvent accessibility similarity (SA)	$$SA = \frac{SA_{match}}{L}$$ SA_{match}: The number of residues that predicted solvent accessibility by SSpro4 (Cheng, et al., 2005) matches the one derived from the model by DSSP.
Euclidean compact (EC)	$$EC = \frac{\frac{1}{L}\sum_{i,j(i\neq j)}^{L} d_{ij}}{\max(\{d_{ij}\})}$$ d_{ij} is the pairwise Euclidean distance between residue *i* and *j*.

Table S2. Comparison with other top global QA methods on the CASP13 models. The global accuracy is measured based on lDDT.

Method	Diff	Loss	Pearson
MULTICOM_CLUSTER	3.803	7.502	0.854
UOSHAN	4.335	11.122	0.87
QDistance[b]	4.337	11.255	0.863
ModFOLDclust2	5.772	12.121	0.848
ModFoLD7_rank	4.098	8.292	0.836
QDistance[a]	5.127	10.243	0.807
ProQ3D	5.685	9.45	0.734
FaeNNz	6.385	6.181	0.76

a: single-model based; b: multi-models based.

Table S3. Comparison with other top local QA methods on the CASP13 models based on ASEs at different distance cutoffs. The evaluation is on 72 targets that all methods have prediction results.

Methods	d_0=0.5 Å	d_0=1 Å	d_0=2 Å	d_0=4 Å
QDistance[b]	92.116	88.882	87.538	87.646
UOSHAN	94.134	90.266	87.699	86.49
QDistance[a]	93.033	88.599	85.947	85.5
ModFOLDclust2	93.639	88.827	85.516	84.464
Davis-EMAconsensus	93.373	88.113	84.335	83.706
RaptorX-DeepQA	93.261	88.13	84.216	82.992
ModFOLD7	93.591	88.769	84.881	81.88
ModFOLD7_rank	93.591	88.769	84.88	81.88
Pcons	93.206	87.567	82.839	80.858
Pcomb	93.131	87.448	82.569	79.317
Wallner	93.004	86.979	81.631	78.86
ProQ3D	93.012	86.973	81.075	76.58

a: quasi-single-model-based; b: multiple models-based.

Table S4. Comparison of quasi-single model-based QDistance with other top local QA methods on the CAMEO dataset based on Pearson's correlation coefficient (PCC). PCC_r, PCC_m and PCC_t are per-residue, per-model and per-target based PCC, respectively.

Methods	PCC_t	PCC_m	PCC_r
QMEANDisco 3	0.741	0.685	0.881
QDistance	0.712	0.675	0.731
ModFoLD7_IDDT	0.676	0.632	0.779
ProQ3D_LDDT	0.66	0.618	0.758
QMEAN3	0.617	0.57	0.713
ProQ3D	0.525	0.516	0.419
VoroMQA_sw5	0.504	0.457	0.584
VoroMQA_V2	0.479	0.434	0.532
ProQ3	0.438	0.499	0.404
Baseline Potential	0.373	0.312	0.502

Table S5. Impact of the MSA depth (Neff) to the accuracy of the QA predictions on the CASP13 dataset. Neff is measured as the number of sequences in the MSA with less than 90% sequence identity.

Range of log(Neff)	Diff	Loss	Pearson	ASE
0~4	8.971	9.344	0.654	83.642
4~8	6.536	9.085	0.787	85.351
8~12	5.287	9.107	0.774	86.478

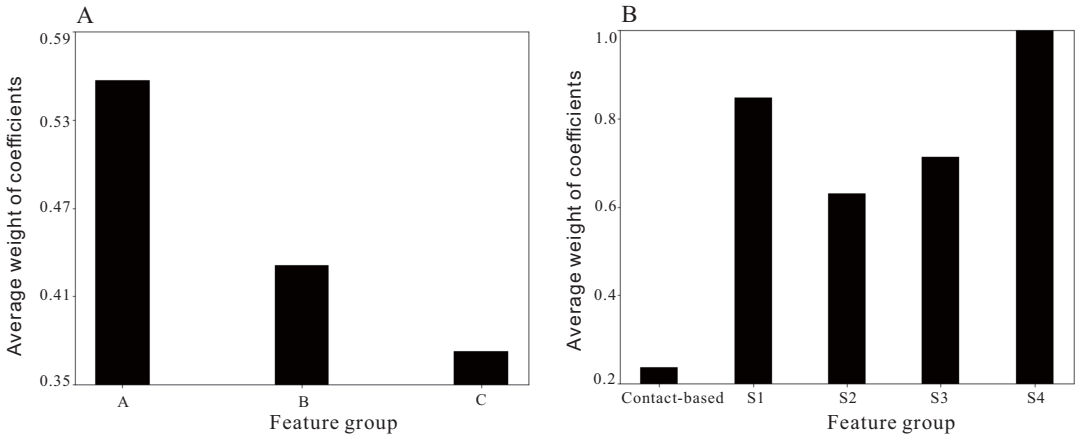

Fig. S1. Contribution of different feature groups measured by the weight of the linear regression coefficients. (A) Weights for the three feature groups in Figure 1c. (B) Weights for the five sub-groups of distance-based features (one from contact-based and four S-scores).

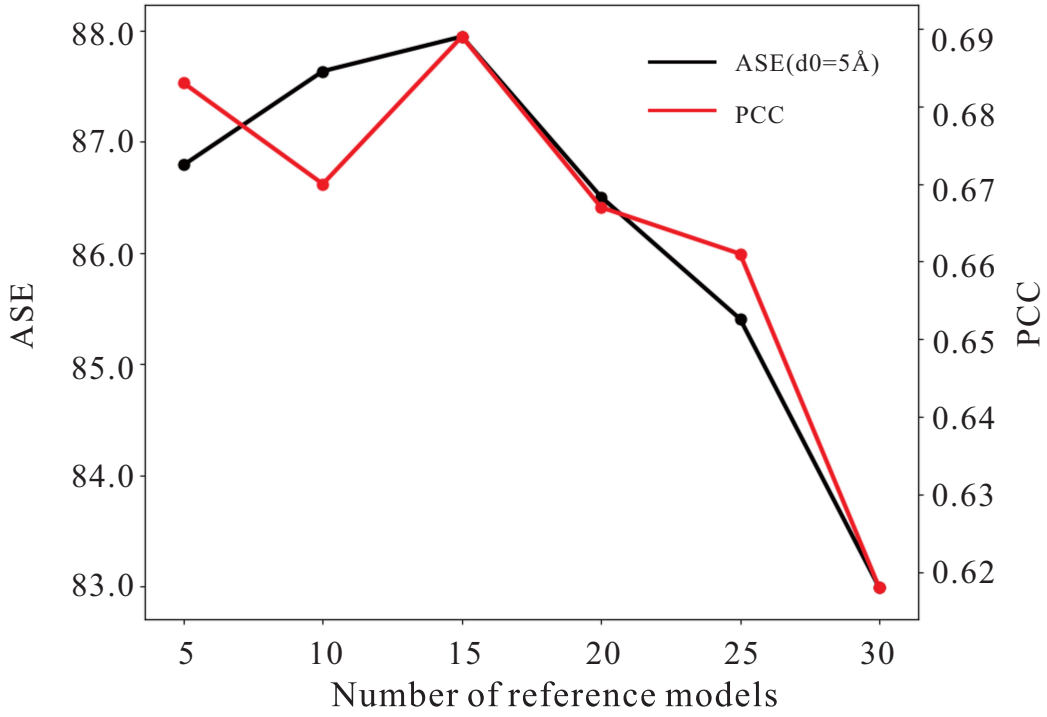

Fig. S2. The relationship between ASE (or PCC) and the number of selected reference models. The dataset consists of models from 60 CASP12 targets.

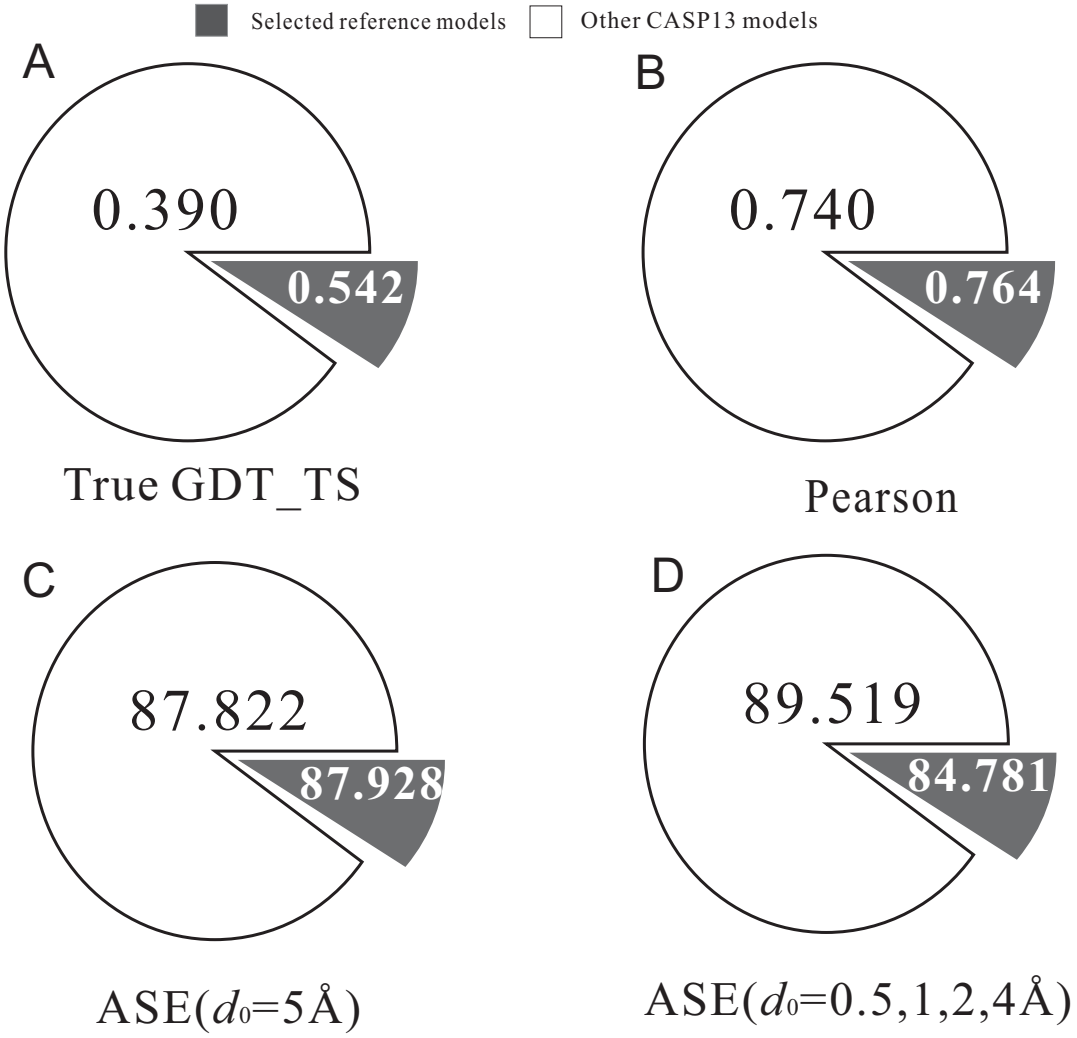

Fig. S3. Comparison on selected reference models and other models. A, true GDT_TS score of the models. B, Pearson's correlation coefficient between the predicted and real local QA scores. C, ASE for the predicted local distance deviation at distance cutoff d_0=5 Å. D, Average ASE for the predicted local distance deviation at four distance cutoffs (d_0=0.5, 1, 2, 4 Å).

References

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