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Supplemental information

Deep learning geometrical potential for high-accuracy *ab initio* protein structure prediction

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Supporting Figures

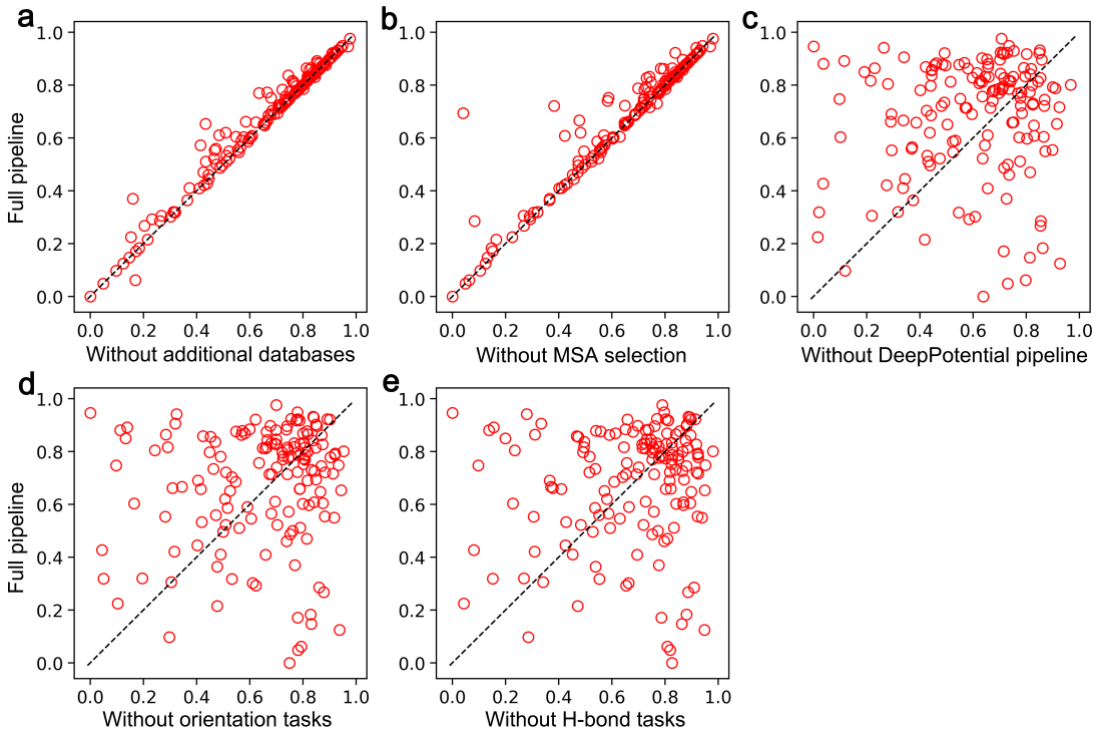

Figure S1. Head-to-head comparisons of Top-*L* contact precision between with and without each component in DeepPotential, related to Figure 2. The success rates for the components, i.e., the proportion of the cases for which the precision of the full pipeline is higher than or equal to that without the corresponding component, are 92.2%, 85.7%, 66.9%, 59.1% and 54.5%, where the components are additional databases, MSA selection, DeepPotential architecture, orientation tasks and H-bond tasks.

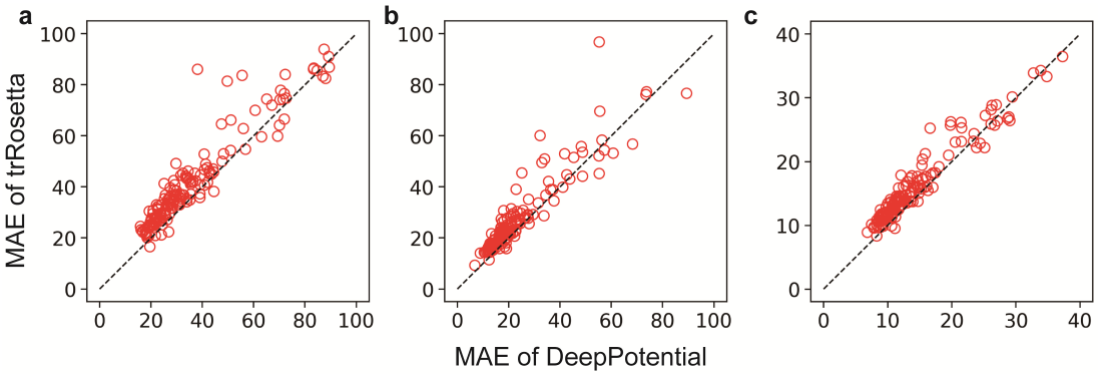

Figure S2. Target-wise head-to-head performance comparison of orientation terms between trRosetta and DeepPotential, related to Table 1. a-c, head-to-head comparison of angle MAE for Ω, Θ and Φangles respectively between trRosetta and DeepPotential.

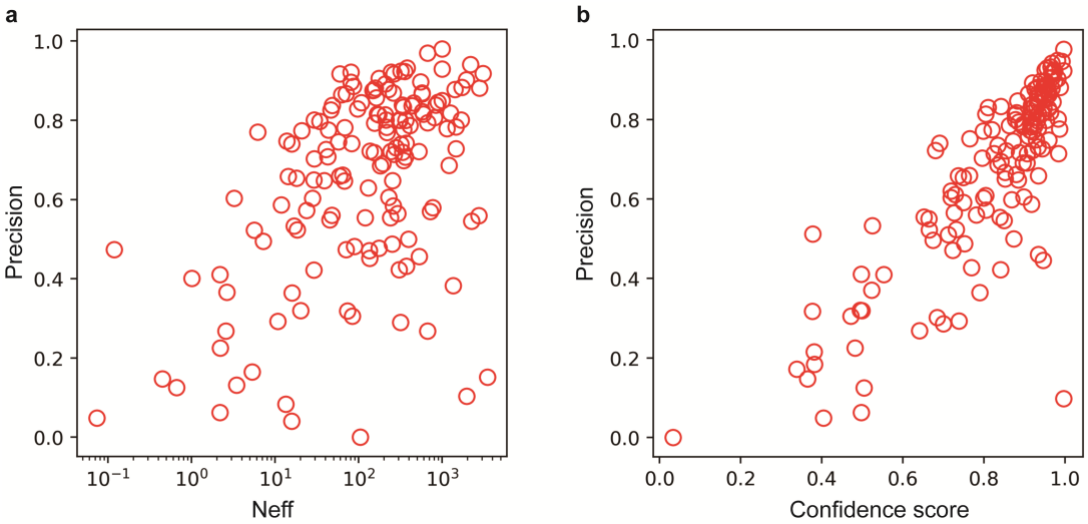

Figure S3. Correlation between Top-*L* contact precision and (a) Neff and (b) Confidence score, related to Figure 2.

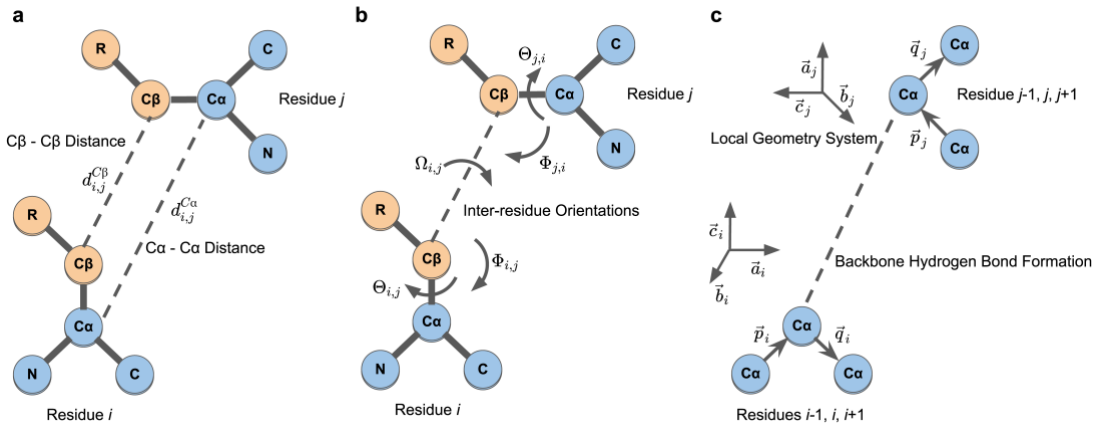

Figure S4. Geometrical prediction terms of DeepPotential, related to the STAR Methods. **a,** Cα/Cβ distances. **b,** inter-residue orientation angles. **c,** backbone hydrogen bond terms.

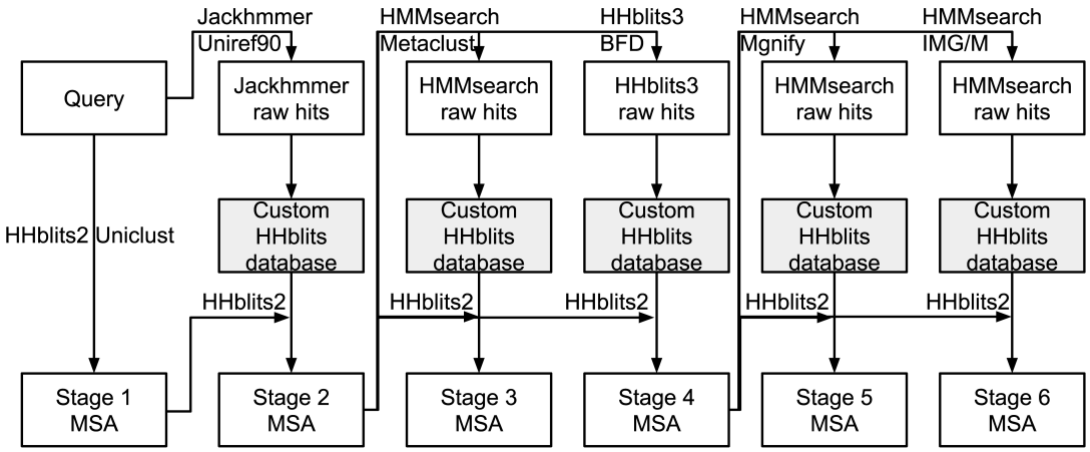

Figure S5. The progressive pipeline to construct candidate MSAs from whole- and meta-genome sequence databases, related to STAR Methods.

Supporting Tables

Table S1. Performance comparison between DeepPotential and the control methods in the blind CASP14 experiment, related to Figure 2. All the predictions of methods are downloaded from the CASP14 website. The bold fonts highlight the highest precision and lowest MAE in the corresponding category.

Methods	Contact precision (*p*-value)			Distance MAE (*p*-value)		
	$L/5$	$L/2$	L	L	$2 \times L$	$5 \times L$
RaptorX	0.454 (1.3e-02)	0.376 (9.7e-02)	0.282 (2.1e-01)	3.628 (3.4e-03)	3.927 (3.8e-01)	4.470 (3.9e-02)
CopulaNet	0.518 (4.2e-04)	0.393 (2.6e-03)	0.296 (1.4e-01)	3.199 (4.7e-03)	3.491 (4.0e-02)	3.919 (1.6e-01)
trRosettaX	0.538 (4.1e-02)	0.445 (6.6e-03)	0.334 (6.0e-04)	3.492 (6.8e-03)	3.563 (5.4e-02)	4.012 (2.8e-04)
DeepPotential	**0.638**	**0.544**	**0.396**	**2.786**	**2.891**	**3.098**

Table S2. The performance of MSA selection indexes with different confidence thresholds for RosettaFold and AlphaFold2, related to the STAR Methods. 'CS' stands for confidence score. Bold fonts highlight the best performance in each category.

Confidence threshold	AlphaFold2		RosettaFold	
	Neff	CS	Neff	CS
0% ($N_{targets}$=79)	0.806	**0.812**	0.765	**0.770**
1% ($N_{targets}$=38)	0.758	**0.765**	0.696	**0.712**
2% ($N_{targets}$=22)	0.701	**0.724**	0.672	**0.665**
3% ($N_{targets}$=16)	0.666	**0.690**	0.622	**0.633**
4% ($N_{targets}$=11)	0.561	**0.596**	0.520	**0.534**

Table S3. Performance comparison of *ab initio* protein structure prediction between DeepPotential and trRosetta2, RosettaFold and AlphaFold2 on 22 CASP14 FM targets, related to Table 1. 'Correct Folds' represents the number of proteins with TM-scores $\geqslant 0.5$.

Methods	TM-score	RMSD	Correct Folds
AlphaFold2	0.728	6.846	17
RosettaFold	0.606	8.319	13
RosettaFold (e2e)	0.590	9.232	13
trRosetta2	0.559	9.590	13
DeepPotential	0.575	9.161	13