Supplementary file 1: Representative 1D and 2D properties

The 1D properties of residues are features along one dimensional protein sequence. Generally speaking, solvent accessibility (SA), secondary structure (SS), backbone torsion angles (BTA), residue depth (RD) are classified to 1D properties. The 2D properties are relationships between amino acid residues of proteins, such as residue-residue contacts. More recently, residue contact number called half-sphere exposure (HSE) is proposed and it is also a 2D property. The descriptions of these 1D and 2D properties are shown in Table S1.

Table S1. Representative 1D and 2D properties

1D property[a]		
Note	Description	Refs
SA	SA is the surface area of a biomolecule that is accessible to a solvent.	1, 2
SS	Protein secondary structures, including α-helix, β-strand and coil.	3
BTA	Backbone torsion angles, including as phi and psi angles.	4
RD	Residue depth, which describes the depth of a residue from the protein surface.	5
2D property[b]		
CN	Residue contact between all amino acids of a protein structure.	6
HSE	Orientation-dependent residue contact number called half-sphere exposure (HSE).	7-9

[a]1D properties are features of each residues along one dimensional protein sequence.

[b]2D properties describe the relationship between amino acid residues of proteins.

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Supplementary file 2: The optimal parameters for Net1 and Net2 for residue depth prediction

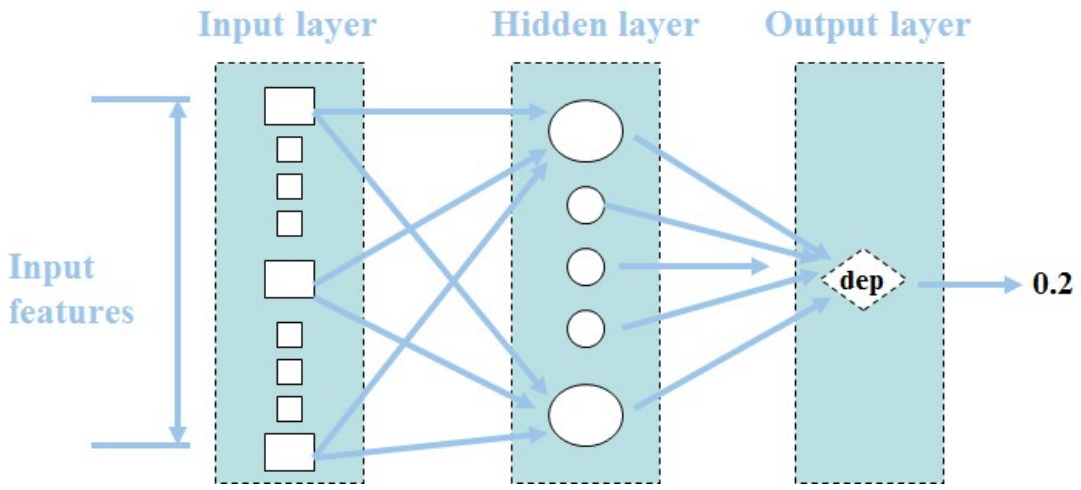

Figure S1. The architecture of the neural network for residue depth prediction

As shown in Figure S1, neural networks for both Net1 and Net2 were designed with an input layer, a hidden layer and an output layer. The output layer contains only one single node, which represents the predicted residue depth score (e.g. 0.2). A fragment profile of 2n +1 residues surrounding the central residue whose depth is to be predicted (i.e. the window size is equal to 2n+1) is extracted from sequence profiles. The lengths of the input features for PSSM, PSFM, MTX, SP, L1, SS, RSA, rp and CS are 20, 20, 20, 20, 1, 1, 1, 1 and 1, respectively. Grid search algorithm is used to optimize the performance and the window sizes of Net1 and Net2 were set as 15. Therefore, the number of input nodes (i.e. input dimensions) for both Net1 and Net2 are 15*(20+20+1+1+1+1+1). The learning rate and momentum were set as 0.001 and 0.85, respectively. The input nodes for the hidden layers of Net1 and Net2 were set as 150 and 250, respectively. The sigmoid activation function is used as

$$f(x) = \frac{1}{1+e^{-x}} \tag{S1}$$

where x is the input value and $f(x)$ is the output value. The output value of the sigmoid activiation lies in the range of [0, 1]. Both Net1 and Net2 were intensively trained on the training dataset (i.e. PDB_TRAIN6675) until the prediction performance can't be improved any longer. The SCOPe_TEST1073 dataset is an indepdent dataset to benchmark the methods.