Protein structure

heavy-atom coordinates
(optional histidine-state assignments)

Local surface encoder

residue descriptors +
≤24 candidate water positions

Residue graph

two edge-gated layers
≤24 Cα neighbors within 12 Å

Residue embedding

16 features per residue

optional export

- Fdewet
- PC1
- PC2
- PC3

four prediction heads

predictions averaged over three independently trained networks

A Local surface encoding

for each candidate water position

8 nearby atoms

19 descriptors per atom

Shared atom encoder

MLP: 19 → 16 → 16

Pool the 8 atoms

concatenate mean and max (32)
project to 24 features

Solvent-space geometry

11 descriptors per position

Shared geometry encoder

MLP: 11 → 24 → 24

24 features

combined probe vector (24)

Pool candidate positions

mean (24) and max (24)
concatenate → 48 features

Residue descriptors (35)

identity (20), SASA (10), terminal flags (2),
protonated histidine (1), solvent shell (2)

Residue representation (16)

linear projection: 35 → 16

Surface representation (16)

linear projection: 48 → 16

initial residue embedding (16)

B Local graph refinement

apply the entire block twice · separate weights

Neighbor state (16)

linear projection: 16 → 16

Edge geometry (20)

MLP + sigmoid → 16 gates

gate neighbor message (16)
feature-wise multiplication

mean over neighbors (16)

Own state (16)

current residue features

Concatenate

own state and mean message → 32

learned update: MLP 32 → 16 → 16

retain own state

residual addition

LayerNorm: within each residue

updated residue embedding (16)