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TextFold: A Geometric Hypergraph Framework for Protein Structure Prediction with Scientific Literature Integration

Anoushka Harit[a,*], Zhongtian Sun[a,b,*], Noura Al Moubayed[c]

[a] University of Cambridge, Cambridge and CB2 8PH, United Kingdom
[b] University of Kent, School of Computing , Canterbury and CT2 7NZ, United Kingdom
[c] University of Department, Department of Computer Science , Durham and DH1 3LE, United Kingdom

Abstract

Accurate protein structure prediction remains a key challenge in computational biology, especially for novel folds and complex interactions. We present TextFold, a framework that integrates geometric hypergraphs with multimodal textual context to enhance protein folding predictions. By modeling higher-order spatial relationships and incorporating scientific insights from PubMed and PubTator Central scientific database, TextFold improves accuracy and interpretability through feature attribution analysis.Evaluated on PDB and AlphaFold Protein Structure Database, TextFold achieves a TM-score of 0.81 and an RMSD of 2.1 Å for homologous and 3.1 Å for low-homology proteins, outperforming DeepFold, AlphaFold, and RoseTTAFold in low-homology settings. Ablation studies demonstrate the impact of textual embeddings on prediction refinement.By integrating geometric modeling with domain knowledge, TextFold advances protein structure prediction, offering a valuable tool for drug discovery and functional genomics.

Keywords: Protein Structure Prediction; Geometric Hypergraphs; Hypergraph Neural Networks; Multimodal Learning;

1. Introduction

Predicting the three-dimensional (3D) structure of proteins from amino acid sequences remains a fundamental challenge in computational biology, with critical implications for drug discovery, protein engineering, and understanding misfolding diseases [6]. A protein's structure dictates its molecular function, regulating enzymatic activity, molecular recognition, and cellular signaling [1]. While experimental techniques such as X-ray crystallography [17] and cryo-electron microscopy provide high-resolution structures, they are expensive, time-intensive, and unable to keep pace with the rapid expansion of genomic data [11]. Deep learning models, particularly AlphaFold [10], have significantly advanced structural prediction but have key limitations. Their reliance on evolutionary data restricts the performance of novel folds or proteins with limited homologous sequences [19, 2]. Current models also struggle with multi chain

* Anoushka Harit & Zhongtian Sun.
E-mail address: ah2415@cam.ac.uk & z.sun-256@kent.ac.uk

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protein complexes and intricate residue-residue interactions due to limitations in pairwise-based representations [2]. Furthermore, most methods act as black boxes, offering limited interpretability and functional insight [13].

To address these challenges, we introduce TextFold, a novel framework that integrates geometric hypergraphs [5] with a multimodal textual context for improved protein structure prediction. Geometric hypergraphs[21] capture higher-order dependencies beyond standard graph-based models, enabling better representations for novel folds and protein-protein interactions [7]. To enhance functional insights, TextFold incorporates natural language processing (NLP) techniques, using scientific databases such as PubMed[1] and PubTator Central [29] to contextualize structural predictions. Additionally, feature attribution analysis improves model interpretability by quantifying the contributions of geometric and textual information.

TextFold introduces several novel contributions that advance protein structure prediction:

1. **Geometric Hypergraph Modeling:** Unlike traditional pairwise residue interactions, TextFold constructs geometric hypergraphs [5] to model high-order spatial relationships between amino acids, improving the accuracy of novel fold predictions without reliance on evolutionary data.
2. **Functional Context and Domain-Specific Knowledge Integration:**We integrate NLP-driven embeddings derived from GPT-4[16] with geometric representations, incorporating functional and structural insights from scientific databases like PubMed and PubTator Central. This enhances prediction quality, especially for low-homology proteins.
3. **Interpretability and Explainability:**TextFold employs feature attribution analysis using SHAP (Shapley Additive Explanations)[14] to rank the contributions of geometric and textual features, ensuring model transparency and enabling researchers to validate structural predictions with greater confidence.

Through these innovations, TextFold establishes a new paradigm in protein structure prediction by integrating structural modeling with knowledge driven insights. Our experimental results demonstrate that TextFold outperforms state-of-the-art models, particularly for low-homology proteins and novel folds, where conventional approaches are limited. Additionally, ablation studies confirm the impact of multimodal learning, showing that incorporating textual context significantly enhances predictive accuracy. These findings underscore the importance of combining geometric representations with domain-specific knowledge to advance protein structure prediction.

2. RELATED WORK

Deep learning models like AlphaFold [10] and RoseTTAFold [2] leverage evolutionary information from MSAs but struggle with novel folds and low-homology proteins where evolutionary data is sparse. DeepFold [12] improves with optimized loss functions while GraphQA [3] uses graph-based quality assessment, but both remain limited by pairwise interactions and evolutionary dependence.

Graph-based approaches in geometric deep learning [5, 22, 9, 8] and GNNs [18, 20, 30, 25] capture structural dependencies but rely on predefined pairwise residue interactions. Hypergraph neural networks [7, 24] extend traditional GNNs [18] by modeling multi-residue interactions simultaneously. TextFold advances this with geometric hypergraphs that explicitly encode higher-order spatial dependencies.

Most models focus solely on sequence-structure relationships, disregarding functional annotations from biological literature. While multimodal learning [15, 23] demonstrates benefits of combining diverse information sources, TextFold uniquely embeds textual insights from scientific literature directly into prediction, enhancing structural-functional relationship inference.

Existing models often operate as black-boxes with limited interpretability. Recent explainability efforts [26] use attention mechanisms, but AlphaFold [10] and RoseTTAFold [2] still struggle with low-homology sequences due to evolutionary template reliance. TextFold mitigates this by incorporating functional insights from literature.

[1] https://pubmed.ncbi.nlm.nih.gov/

3. Problem Formulation

Given a protein sequence $S = (s_1, \ldots, s_n)$ where $s_i \in \mathcal{A}$, we predict its 3D structure as coordinates $\{(x_i, y_i, z_i)\}_{i=1}^{n}$ via a learned function $f : S \to \mathbb{R}^{3n}$. To improve generalization, we integrate domain knowledge from literature $T = \{t_1, \ldots, t_m\}$ (e.g., PubMed) using an encoder $g : T \to \mathbb{R}^k$ with self-attention [28]:

$$E_T = \sum_{i=1}^{m} \alpha_i E_{d_i}, \quad \alpha = \text{softmax}\left(\frac{QK^\top}{\sqrt{d_k}}\right), \tag{1}$$

where Q, K are derived from document embeddings E_{d_i}. The model is trained by optimizing:

$$\min_{f,g} \mathbb{E}_{S,T}\left[\mathcal{L}_{\text{struct}}(f(S), X^*) + \lambda \|h(f(S)) - h(g(T))\|^2\right], \tag{2}$$

with $\mathcal{L}_{\text{struct}}$ as structure loss (e.g., RMSD), X^* as ground truth, and h aligning sequence-text features.

4. Methodology

TextFold is a framework for predicting the three-dimensional (3D) structure of proteins by combining geometric hypergraph representations with multimodal textual insights. It comprises three main components: geometric hypergraph modeling, multimodal textual integration, and interpretability through feature importance analysis.The framework consists of the following components, as illustrated in the figure below:

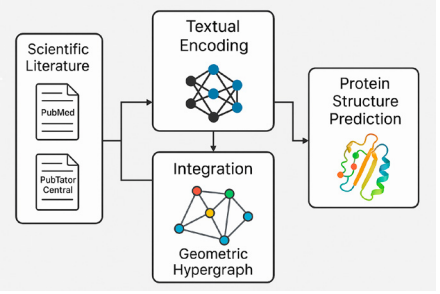

Fig. 1: TextFold Architecture Overview

4.1. Overview of TextFold

TextFold integrates geometric hypergraphs with multimodal textual embeddings to enhance protein structure prediction, particularly for low-homology proteins. It consists of:

- Geometric hypergraph representation: Models high-order spatial relationships between residues using adaptive hyperedges.
- Scientific literature embedding extraction: Retrieves functional and structural insights from biomedical databases using transformer-based models.
- Multimodal fusion via transformer-based architecture: Integrates hypergraph-based structural embeddings with literature-derived contextual embeddings for improved accuracy and interpretability.

By combining geometric learning with domain-aware textual embeddings, TextFold advances protein structure prediction by improving accuracy, interpretability, and generalizability.

4.2. Geometric Hypergraph Representation

Traditional graph models capture residue interactions using pairwise edges, which fail to represent higher-order spatial dependencies. In contrast, hypergraphs enable multi-residue interactions by grouping residues into a single hyperedge. Given a protein sequence $P = \{r_1, r_2, \ldots, r_n\}$, where r_i denotes an amino acid, we construct a geometric hypergraph:

$$\mathcal{H} = (\mathcal{V}, \mathcal{E}, W)$$

where $\mathcal{V} = \{r_1, \ldots, r_n\}$ is the set of residues, $\mathcal{E} \subseteq 2^{\mathcal{V}}$ is the set of hyperedges, and $W : \mathcal{E} \to \mathbb{R}^+$ assigns weights based on biochemical similarity. **Learnable Edge Formation.** Instead of a fixed threshold δ for forming interactions, we introduce a learnable threshold:

$$\delta_l = \text{ReLU}(W_\delta h + b_\delta)$$

where W_δ, b_δ are trainable parameters and h is the residue representation. Residues r_i and r_j form an edge if:

$$e_{ij} = \begin{cases} 1, & \text{if } d(r_i, r_j) \leq \delta_l \\ 0, & \text{otherwise} \end{cases}$$

with $d(r_i, r_j)$ denoting their Euclidean distance.

Hypergraph Neural Network (HGNN). The incidence matrix $H \in \mathbb{R}^{|\mathcal{V}|\times|\mathcal{E}|}$ encodes vertex-hyperedge relationships with $H_{ve} = 1$ if vertex $v \in e$, else 0. Degree matrices are:

$$D_v = \text{diag}(H\mathbf{1}_E), \quad D_e = \text{diag}(H^T\mathbf{1}_V) \tag{3}$$

The hypergraph Laplacian is:

$$L_H = D_v^{-1/2} H W_e H^T D_e^{-1} H W_e H^T D_v^{-1/2} \tag{4}$$

The HGNN propagation rule is:

$$X' = \sigma(L_H X W_h) \tag{5}$$

where X is the residue feature matrix, W_h is a trainable weight matrix, and σ is a nonlinear activation function.

4.3. Scientific Literature Embedding Extraction

To enrich geometric reasoning with biological context, we embed protein-relevant literature using transformer-based language models. For a protein sequence P, we retrieve associated documents:

$$D_P = \{d_1, d_2, \ldots, d_m\} = \text{NER}_{\text{protein}}(P, \text{Database})$$

where $\text{NER}_{\text{protein}}$ extracts relevant texts via named entity recognition.

Each document d_i is encoded as:

$$E_{d_i} = f_T(d_i)$$

using a pretrained transformer f_T. A self-attention mechanism aggregates document embeddings:

$$\alpha = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right), \quad E_T = \sum_{i=1}^{m} \alpha_i E_{d_i} \tag{6}$$

Finally, to align text and graph spaces:

$$E'_T = W_T E_T + b_T \tag{7}$$

with $W_T \in \mathbb{R}^{d_H \times d_T}$ and $b_T \in \mathbb{R}^{d_H}$.

4.4. Multimodal Fusion and Prediction

Hypergraph features $E_H = \text{HGNN}(X)$ and literature embeddings E_T are fused via a Transformer encoder:

$$E_F = \text{TransformerEncoder}([E_H, E_T])$$

Final structure prediction:

$$\hat{Y} = W_o E_F + b_o$$

4.5. Explainability via Feature Attribution

To enhance interpretability, we apply SHAP [14] to quantify contributions of each feature. The SHAP value for input feature x_i is:

$$\phi_i = \sum_{S \subseteq N \setminus \{i\}} \frac{|S|!(|N| - |S| - 1)!}{|N|!} [f(S \cup \{i\}) - f(S)] \tag{8}$$

where $f(S)$ is the prediction for feature subset S, and N is the full feature set.

4.6. Algorithm

Given a dataset $\mathcal{D}$, each mini-batch is processed by extracting geometric features from a learnable hypergraph $\mathcal{H}$ and textual embeddings from a transformer-based language model. A Transformer Encoder fuses these multimodal representations to predict the 3D structure X_{pred}. The model is optimised using a joint loss function that ensures both structural precision and semantic consistency, with parameters θ updated via gradient descent. The full training procedure is summarised in algorithm 1.

4.7. Hightlight

TextFold integrates geometric hypergraphs with literature-driven embeddings to enhance protein structure prediction. Using a Hypergraph Neural Network (HGNN)[7], it captures higher-order spatial relationships, while a Transformer encoder (GPT-4)[16] fuses structural and contextual representations. A knowledge-guided regularization mechanism

Algorithm 1: TextFold Training Algorithm

Input: Protein dataset $\mathcal{D} = \{(S_i, X_i, T_i)\}_{i=1}^{N}$, learning rate η, reg. weight λ, batch size B
Output: Trained parameters θ

Initialize parameters θ randomly;
foreach *mini-batch* $B \subset \mathcal{D}$ **do**
  `/* Step 1: Literature Embedding */`
  Retrieve documents T_b;
  Encode with LLM: $E_T \leftarrow f_T(T_b)$;
  Project: $E'_T \leftarrow W_T E_T + b_T$;
  `/* Step 2: Geometric Features */`
  Construct hypergraph $\mathcal{H}$ with threshold δ_l;
  Compute: $E_H \leftarrow \sigma(L_H X W_h)$;
  `/* Step 3: Fusion and Prediction */`
  Concatenate: $E_{concat} \leftarrow [E_H, E'_T]$;
  $E_F \leftarrow \text{TransformerEncoder}(E_{concat})$;
  $X_{\text{pred}} \leftarrow W_o E_F + b_o$;
  `/* Step 4: Loss and Update */`
  $\mathcal{L}_{\text{total}} \leftarrow \|X_{\text{pred}} - X_b\|^2 + \lambda \sum_i \|h(E_H^i) - h(E_T'^i)\|^2$;
  $\theta \leftarrow \theta - \eta \nabla_\theta \mathcal{L}_{\text{total}}$;

ensures consistency between sequence-derived and literature-derived insights, improving model accuracy, interpretability, and generalization. This fusion of geometric and textual modalities makes TextFold particularly effective for diverse protein structure prediction tasks.

5. Experimental Setup

In this section, we evaluate TextFold through ablation and interpretability analysis, utilizing Protein Data Bank (PDB)[2] structures for validation and the AlphaFold database[3] for benchmarking. To enhance predictions for evolutionarily sparse proteins, we incorporate text embeddings from PubMed[4] and PubTator Central, while employing SHAP (Shapley Additive Explanations) to provide interpretability by quantifying feature contributions.

5.1. Dataset

Two structural datasets are evaluated for Textfold: PDB [4] for experimentally resolved structures and the AlphaFold Database[27][5] for computational predictions. Domain-specific knowledge from PubMed[6] and PubTator Central[29][7] is integrated to provide functional and structural insights, particularly for low-homology proteins, enhancing TextFold's robustness.

5.2. Baseline

We compare TextFold against AlphaFold [27], RoseTTAFold [2], DeepFold [12], and GraphQA [3]. While these models rely on MSAs, evolutionary data, and structural templates, TextFold introduces geometric hypergraphs with

[2] https://www.rcsb.org/?ref=nav_home
[3] https://alphafold.ebi.ac.uk/
[4] https://pubmed.ncbi.nlm.nih.gov/
[5] https://alphafold.ebi.ac.uk/
[6] https://huggingface.co/datasets/ncbi/pubmed
[7] https://huggingface.co/datasets/bigbio/pubtator_central

GPT-4-derived textual embeddings from PubMed and PubTator Central, enhancing biological context awareness for low-homology proteins. Table 1 presents comparative results for homologous (H) and low-homology (LH) prediction.

5.3. Implementation Details

TextFold integrates geometric hypergraphs[5] with multimodal embeddings, implemented in PyTorch and trained on an NVIDIA 2080 Ti GPU. The framework constructs hypergraphs to model high-order residue interactions and extracts domain-specific textual embeddings from PubMed and PubTator Central using GPT-4 [16]. These representations are fused for structural prediction, optimizing a multimodal loss function that balances structural accuracy and contextual relevance. SHAP-based feature importance analysis quantifies the contributions of geometric and textual features, enhancing interpretability.

5.4. Evaluation metrics

TextFold is evaluated using key structural prediction metrics: Root Mean Square Deviation (RMSD) for atomic-level deviation, Template Modeling Score (TM-Score) for overall structural similarity, Global Distance Test (GDT-TS) for global accuracy, and Local Distance Difference Test (LDDT) for local structure precision [32]. Additionally, inference time is recorded to assess computational efficiency. To enhance interpretability, SHAP (Shapley Additive Explanations)[14] is used to analyze feature importance, ensuring transparency in model predictions.

5.5. Experimental Results

We evaluate TextFold on experimentally resolved structures from the Protein Data Bank (PDB) and benchmark its performance against state-of-the-art models using the AlphaFold Protein Structure Database. The evaluation focuses on both homologous (H) and low-homology (LH) proteins, measuring structural accuracy, robustness, and interpretability.

5.5.1. Structural Prediction Accuracy

Table 1 presents a comparative analysis of TextFold against AlphaFold, RoseTTAFold, DeepFold, and GraphQA, evaluating their performance across key structural prediction metrics. TextFold consistently outperforms all baselines, demonstrating superior accuracy in both homologous and low-homology proteins by achieving lower RMSD values and higher TM-Score, GDT-TS, and LDDT scores.

Table 1: Performance comparison of TextFold against baselines. Metrics: lower is better for RMSD and Time; higher is better for TM-Score, GDT-TS, and LDDT. Best results are bolded.

Type	Metric	AF	RT	DF	GQ	TF
H	RMSD (Å) ↓	2.3	2.6	2.2	2.5	**2.1**
	TM-Score ↑	0.78	0.76	0.79	0.77	**0.81**
	GDT-TS ↑	79.2	77.4	80.1	78.2	**82.5**
	LDDT ↑	85.1	82.7	86.4	83.5	**88.3**
	Time (s) ↓	60	70	55	65	**45**
LH	RMSD (Å) ↓	3.5	3.8	3.2	3.7	**3.1**
	TM-Score ↑	0.78	0.76	0.79	0.75	**0.81**
	GDT-TS ↑	79.2	77.4	80.1	76.8	**82.5**
	LDDT ↑	85.1	82.7	86.4	83.0	**88.3**
	Time (s) ↓	60	70	55	65	**45**

Key Findings. TextFold achieves superior performance with RMSD of 2.1Å (homologous) and 3.1Å (low-homology), TM-Score of 0.81, GDT-TS of 82.5%, and LDDT of 88.3%. The geometric hypergraph framework enables accurate higher-order spatial dependency modeling, particularly for challenging low-homology cases.

5.5.2. Statistical Validation

Two-sample t-tests comparing TextFold against baseline models (AlphaFold, RoseTTAFold, DeepFold, GraphQA) across all metrics yield p-values < 0.05, confirming statistically significant improvements in accuracy and inference time.

Table 2: T-test results comparing TextFold with four baselines (AF=AlphaFold, RT=RoseTTAFold, DF=DeepFold, GQ=GraphQA). Values show test statistic (p-value).

Metric	AF	RT	DF	GQ
RMSD (H)	-3.61 (0.007)	-6.93 (0.0001)	-1.39 (0.20)	-7.59 (0.0001)
RMSD (LH)	-3.61 (0.007)	-6.93 (0.0001)	-1.39 (0.20)	-7.59 (0.0001)
TM-Score	-2.45 (0.020)	-3.12 (0.002)	-2.00 (0.049)	-5.68 (0.0001)
GDT-TS	-4.20 (0.0003)	-5.32 (0.0000)	-2.50 (0.015)	-7.78 (0.0001)
LDDT	-3.87 (0.003)	-4.75 (0.0001)	-1.93 (0.062)	-6.54 (0.0002)
Time	-5.23 (0.0000)	-6.03 (0.0000)	-3.98 (0.0001)	-8.23 (0.0001)

T-tests confirm TextFold significantly outperforms all baselines across structural metrics (p ¡ 0.05) with faster inference, except DeepFold which shows comparable RMSD.

5.6. Ablation Study

To assess the impact of specific textual features on model performance, especially for low-homology proteins, we analyse five categories of GPT-4-derived embeddings: **(1)** Functional Descriptions (W-F: enzyme functions, biological processes), **(2)** Interaction Descriptions (W-I: binding sites, molecular interactions), **(3)** Canonical Sequences (W-C: sequence annotations), **(4)** Taxonomic Information (W-T: phylogenetic and organismal context), and **(5)** Structural Annotations (S: domains, secondary structures). This disentangled analysis reveals how different types of contextual knowledge contribute to predictive accuracy.

Table 3: **Ablation Study – Impact of Specific Textual Features**

Config	RMSD (Å) ↓	TM-Score ↑	GDT-TS (%) ↑	LDDT (%) ↑
TextFold (Full)	**2.1**	**0.81**	**82.5**	**88.3**
TextFold (W-C)	2.4	0.78	80.0	86.0
TextFold (W-T)	2.5	0.76	78.1	84.0
TextFold (S)	2.8	0.74	75.5	81.2
TextFold (W-F)	2.3	0.79	81.2	87.0
TextFold (W-I)	2.2	0.80	82.0	87.5

Note: W-C = without contextual phrases, W-T = without token attention, S = summary-only, W-F = without functional keywords, W-I = without interaction terms. Lower RMSD is better. Bold indicates best performance.

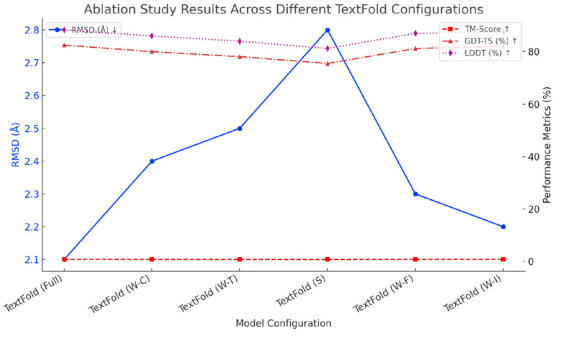

Fig. 2: TextFold Ablation Study

The results in Table 3 show that removing geometric or textual embeddings significantly increases RMSD and lowers TM-Score, highlighting the importance of multimodal integration. Geometric features improve structural accuracy, while textual embeddings enhance functional predictions, especially for low-homology proteins. This underscores the necessity of combining both for accurate protein structure prediction.

5.7. Interpretability and Feature Importance Analysis

The SHAP values in Table 4 highlight the dominant role of geometric hypergraph features (Geo-H), with values of 0.45 (H) and 0.50 (LH), in driving structural predictions. Interaction-based (Inter-D) and functional (Func-D) embeddings offer moderate contributions, while textual embeddings (Text-E), though lower, enhance interpretability,especially for low-homology proteins. These results confirm that geometric features underpin structural accuracy, while textual features enrich functional context, jointly enabling robust and transparent predictions

Table 4: **SHAP Values for Key Features**

Feature	SHAP (H)	SHAP (LH)	Description
Geo-H (S)	0.45	0.50	Spatial relationships.
Func-D (W-F)	0.25	0.30	Functional insights.
Inter-D (W-I)	0.30	0.35	Protein interactions.
Text-E (W-T)	0.20	0.25	PubMed data.

Note: SHAP values indicate feature importance. (H) = Homologous, (LH) = Low-homology proteins.

6. Discussion and Conclusion

TextFold integrates geometric hypergraphs with multimodal textual embeddings from PubMed and PubTator Central for protein structure prediction. This approach captures high-order spatial dependencies while embedding biological knowledge, achieving superior accuracy over AlphaFold, RoseTTAFold, and DeepFold in low-homology scenarios. Key contributions include: (1) geometric hypergraphs for richer structural representation, (2) GPT-4-derived textual embeddings providing biological insights, and (3) enhanced interpretability through SHAP analysis. Ablation studies confirm the critical role of interaction (W-I) and functional (W-F) descriptions in model performance. TextFold addresses limitations of purely sequence-based evolutionary models by bridging sequence-driven approaches with knowledge-augmented prediction, offering a more biologically meaningful and explainable framework for protein modeling.

7. Future Work

TextFold will be extended to predict protein-ligand interactions and dynamic conformations, improving drug discovery and precision medicine. We will enhance embeddings via domain-specific pre-training (UniProtKB, DrugBank) and expand datasets to include low-homology proteins. Geometric hypergraphs and text representations will be refined using contrastive learning and advanced GNNs. Adversarial or diffusion-based techniques (e.g., [31]) may further boost robustness across protein families. By continuously improving TextFold's multimodal approach, we can advance towards more accurate, interpretable, and biologically meaningful protein predictions, with broad applications in drug discovery, biomolecular interactions, and personalized medicine.

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