

# Enhancing Graph Contrastive Learning for Protein Graphs from Perspective of Invariance

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# Background & Motivation

## **Current Limitations:**

- 2D topology-based augmentation ignores biological properties
- 3D structure-based augmentation remains unexplored

## **Core Challenges:**

- How to preserve protein's biological integrity?
- How to design biology-aware graph augmentation strategies?

# Method Overview

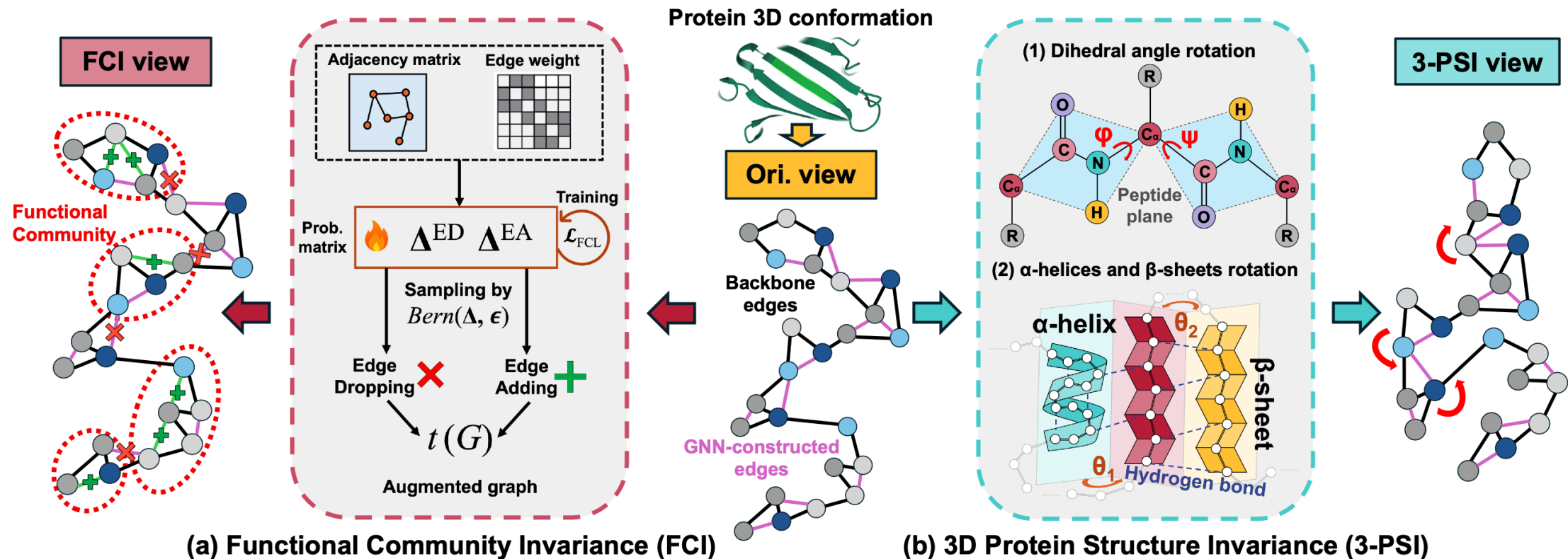
## **Functional Community Invariance (FCI):**

- Preserves topology-driven community structures
- Incorporates residue-level chemical similarity
- Guides edge sampling to maintain functional communities

## **3D Protein Structure Invariance (3-PSI):**

- Dihedral Angle Rotation
- $\alpha$ -helices and  $\beta$ -sheets Rotation
- Retains critical 3D structural information

# Method Overview



# Experiments

Method	EC	GO-BP	GO-MF	GO-CC	FOLD	Reaction
CDConv	0.870	0.450	0.652	0.475	77.0	88.6
CI-GCL	0.870	0.440	0.651	0.453	78.7	86.6
3-PSIDiag + FCI	0.883	0.461	0.662	0.484	80.0	87.8
3-PSIAlpha + FCI	0.885	0.454	0.659	0.477	80.0	89.0

# Conclusion & Impact

## **Key Contributions:**

- First biology-aware protein graph augmentation strategies
- Novel invariance perspective for protein GCL
- Significant performance gains across multiple tasks

## **Broader Impact:**

- Extension to protein-protein interactions
- Application to drug design pipelines