Protein Structure Prediction of Hemoglobin Beta Chain

Task 3 – Bioinformatics Internship (CodeAlpha)

Abstract

Protein structure prediction is essential for understanding the functional and biological properties of proteins. In this task, the three-dimensional structure of the Human Hemoglobin Beta Chain protein was obtained using AlphaFold, a state-of-the-art structure prediction system. The predicted structure was visualized and analyzed using PyMOL. The results reveal a highly stable alpha-helical structure consistent with the known biological role of hemoglobin in oxygen transport.

Introduction

Proteins perform their biological functions through their three-dimensional structures. Understanding protein structure helps in studying protein function, interactions, and disease-associated mutations. Hemoglobin Beta Chain is a crucial component of hemoglobin, responsible for binding and transporting oxygen in vertebrates. Predicting its structure provides insights into its functional regions and structural stability.

Objective

The objectives of this task are:

- To predict the 3D structure of a protein using bioinformatics tools.
- To visualize and analyze the predicted protein structure.
- To understand the structural features related to protein function.

Protein Information

- **Protein Name:** Hemoglobin Subunit Beta
- **Organism:** Homo sapiens (Human)
- **UniProt ID:** P68871
- **Protein Length:** 147 amino acids

Tools and Resources Used

- **AlphaFold Database** – for predicted protein structure

- **PyMOL** – for molecular visualization

- **UniProt** – for protein sequence reference

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Methodology

1. The amino acid sequence of Hemoglobin Beta Chain was obtained from UniProt.

2. The predicted 3D structure was downloaded from the AlphaFold Database in PDB format.

3. The PDB file was loaded into PyMOL.

4. The structure was visualized using cartoon representation.

5. Structural features such as alpha helices and heme-binding regions were analyzed.

6. High-quality images were captured for documentation.

Results

- The predicted structure shows a **globular protein fold**.

- Dominated by **alpha-helical secondary structures**.

- The structure exhibits high confidence scores across most residues.

- The heme-binding pocket is clearly defined.

- No major structural instability was observed.

Discussion

The predicted structure aligns well with the known experimental structure of Hemoglobin Beta Chain. The alpha-helical content and compact folding are essential for oxygen binding and release. High confidence prediction scores indicate the reliability of the AlphaFold model. Structural conservation further supports the evolutionary importance of this protein.

Biological Significance

- Structural integrity is essential for oxygen transport.

- Mutations in the beta chain structure can lead to disorders such as sickle cell anemia.

- Understanding the structure helps in studying disease-related mutations and drug interactions.

Conclusion

Protein structure prediction using AlphaFold successfully provided a reliable 3D model of the Hemoglobin Beta Chain. Visualization and analysis confirmed key structural features necessary for its biological function. This task demonstrates the importance of computational tools in modern bioinformatics research.

References

1. Jumper J et al. Highly accurate protein structure prediction with AlphaFold.

2. UniProt Consortium. UniProt: the universal protein knowledgebase.

3. AlphaFold Protein Structure Database.

4. PyMOL Molecular Graphics System.

Appendix

- Predicted PDB structure file
- PyMOL visualization images
- Sequence reference file