

Hemoglobin Project – Research Report

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3D Structural Analysis of Human Hemoglobin

Introduction:

Human hemoglobin is a tetrameric protein responsible for transporting oxygen in the blood. It consists of four chains (two alpha and two beta) and contains Heme groups that bind oxygen molecules. Understanding the structural characteristics of hemoglobin is essential for insights into its function and interactions.

Objective:

The goal of this project is to analyze the structural and compositional properties of human hemoglobin using Python and interactive 3D visualization, providing quantitative data and visual insights.

Methodology:

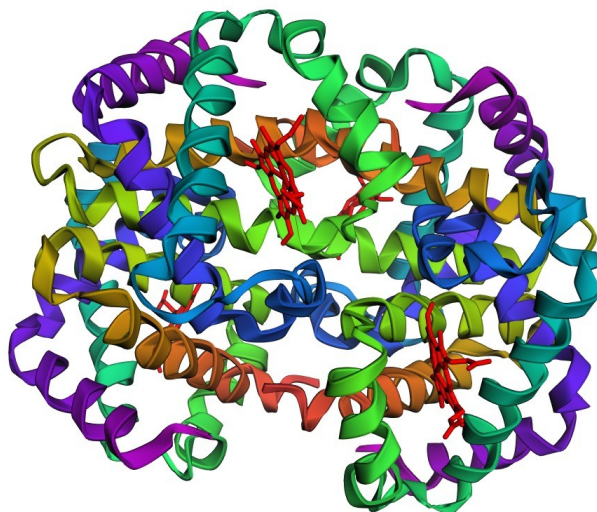
- The PDB file of human hemoglobin (1A3N) was downloaded.
- Chains and amino acid counts were analyzed.
- Structural comparisons between chains were performed using RMSD of C-alpha atoms.
- Amino acid composition (polar, nonpolar, and charged residues) was assessed.
- A 3D interactive model was created using **py3Dmol** and exported as `hemoglobin_3d.html` for exploration.

Results

Chain Lengths (Number of Residues):

Chain	Residues
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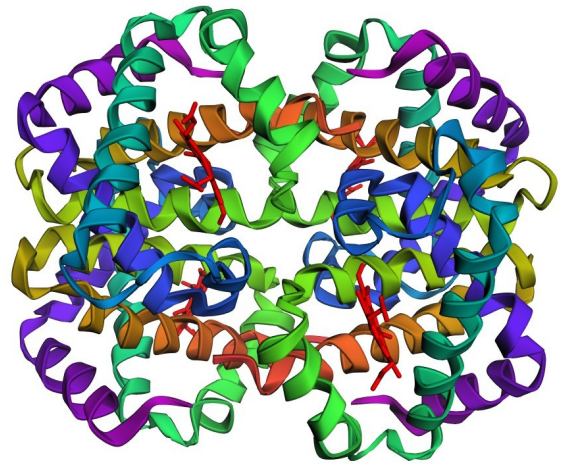
A	265
B	259
C	242
D	261



RMSD Between Chains (C-alpha atoms, Å):

Pair RMSD

A-B	5.94
A-C	0.31
A-D	5.95
B-C	5.95
B-D	0.25
C-D	5.97



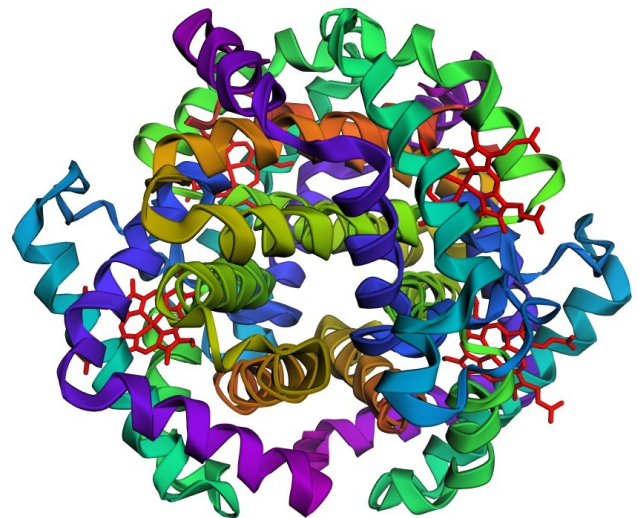
Amino Acid Composition:

Type	Count
Polar	148
Nonpolar	314
Charged	110

3D Visualization:

Three interactive 3D views were captured as screenshots:

Figure	Description
Figure 1	Front view of hemoglobin
Figure 2	Side view highlighting Heme groups
Figure 3	Rotated view showing chain colors



Conclusion / Key Findings

- Human hemoglobin consists of four chains with slightly varying lengths, reflecting structural heterogeneity among subunits.
- RMSD analysis shows two pairs of chains with high structural similarity, while other pairs exhibit larger deviations, indicating distinct conformations.
- Amino acid composition indicates a predominance of nonpolar residues in the protein core for structural stability, with polar and charged residues mostly on the surface for functional interactions.
- The interactive 3D model (`hemoglobin_3d.html`) provides a visual tool for examining chains, Heme groups, and functional regions, useful for education and further research.

Importance of Tables and Results Section

The tables and 3D visualization included in this report serve to provide both quantitative and visual insights into human hemoglobin:

1. **Chain Lengths Table:** Highlights structural differences between protein subunits, serving as a fundamental measurement for the report.
2. **RMSD Table:** Quantifies structural similarities and deviations between chains, offering critical data for structural analysis and interpretation.
3. **Amino Acid Composition Table:** Shows the distribution of residues in the protein's core and surface, supporting functional insights.
4. **3D Visualization:** Visually confirms the position of the chains and heme groups.