Exp 4. Protein Data Bases, Finding and Viewing

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Introduction

To understand protein's biological function, lots of scientists try to find out the physical structure of proteins. Here are some databases, which collect known protein's structure. So we can get these protein strcture from database conveniently. Here are pdb.org and www.rcsb.org.

Typically, each protein from database contains a PDB text file. PDB file contain recongition information and atoms space positions. PDB file can be visualized and edit by PyMol, which is a open source python package used widely.

We will find and view human hemoglobin structure from database.

Methods

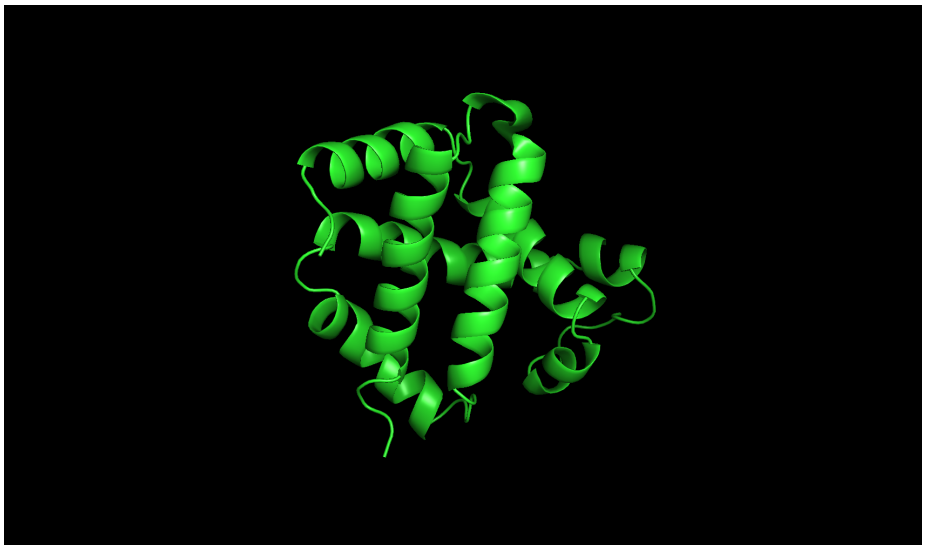
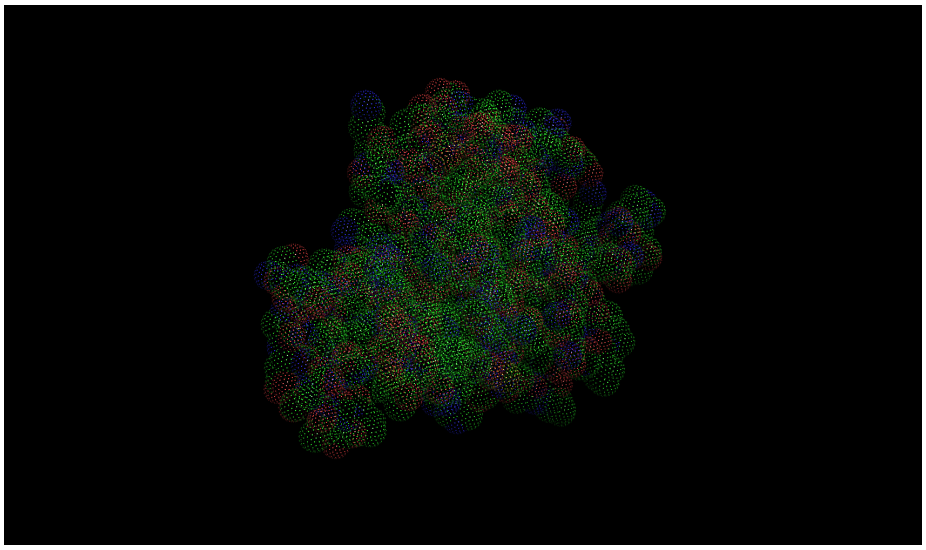
1. Find the PDB ID of human hemoglobin from rcdb.org, whose resolution is higher than 2 A.
2. Download PDB coordinate file and check the detailed information in this file. Find out:

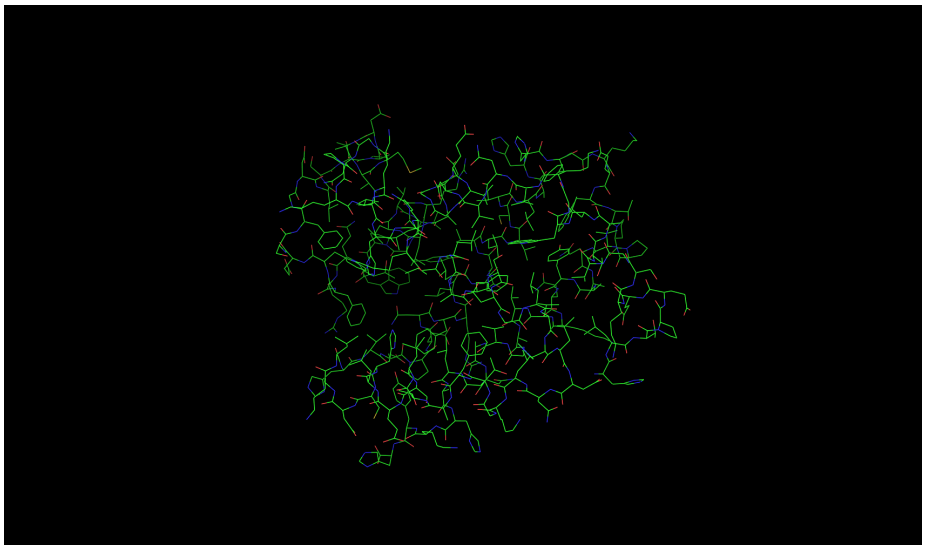
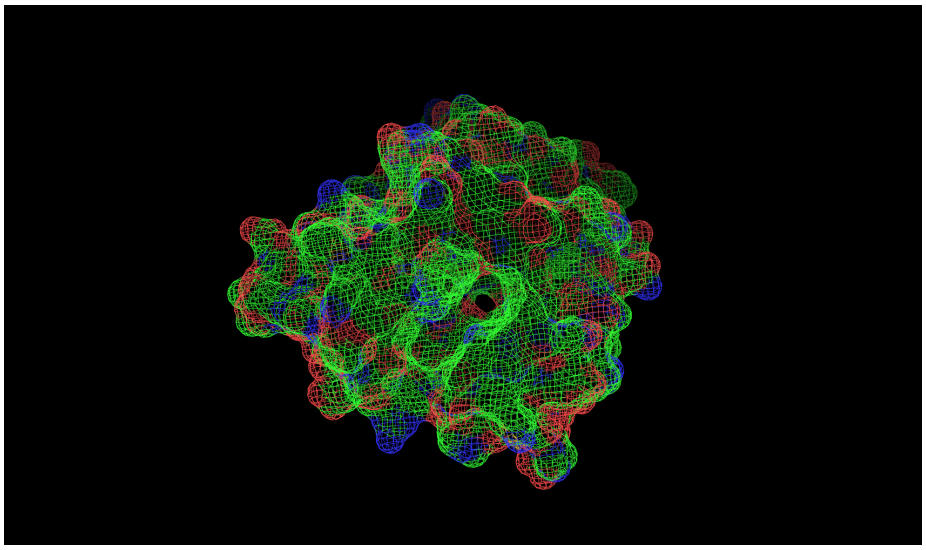
- How many protein chains?
- Which compounds in structures?
- Which residues are missed in the coordinate?

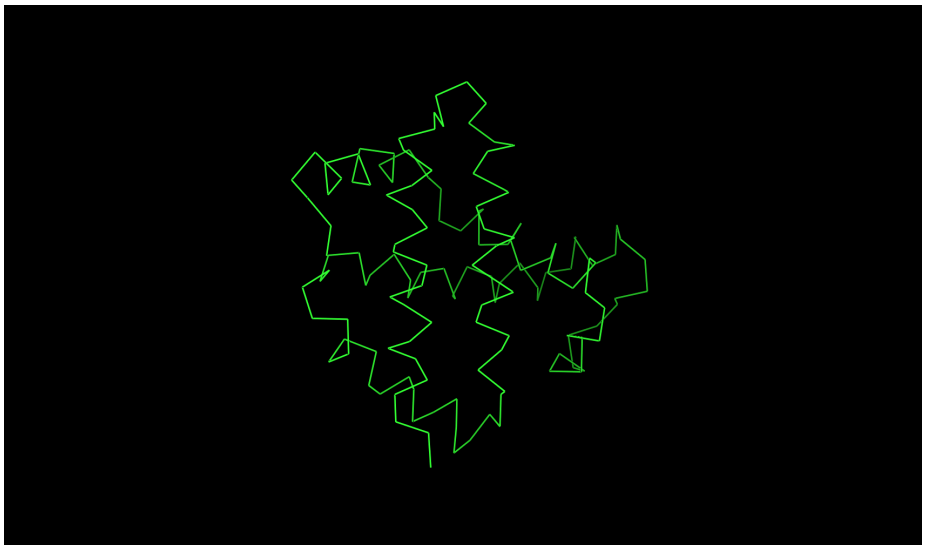
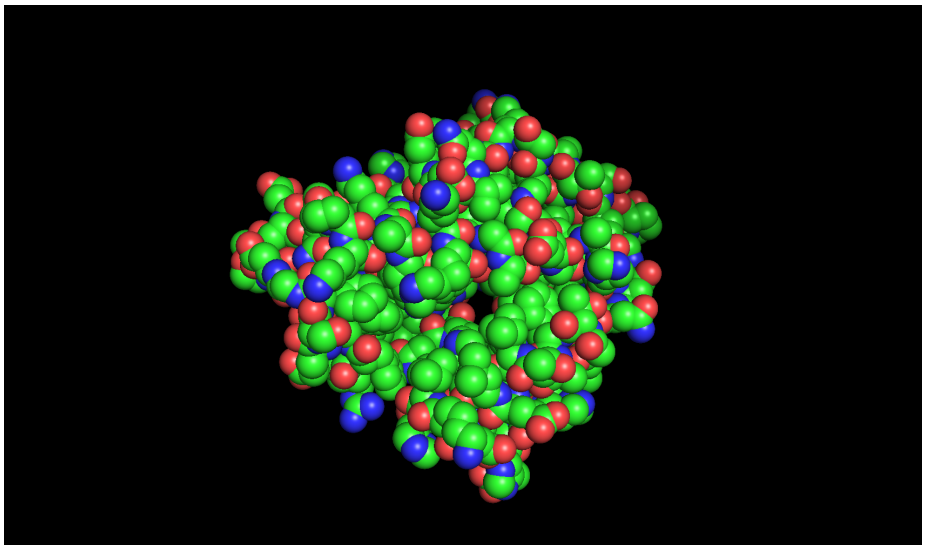
3. Delete the atom positions of chain A, C, D, HOH and HEM. We can get a new coordinate file contained only one beta subunit of hemoglobin (beta-globin).
4. Using PyMol to visualize the beta-globin structures in different viewing. Then save the result as pictures.

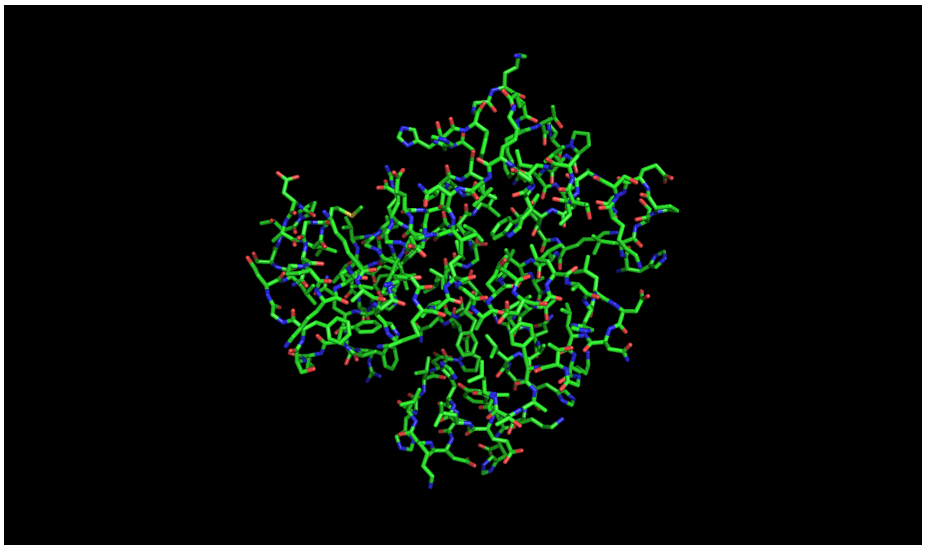
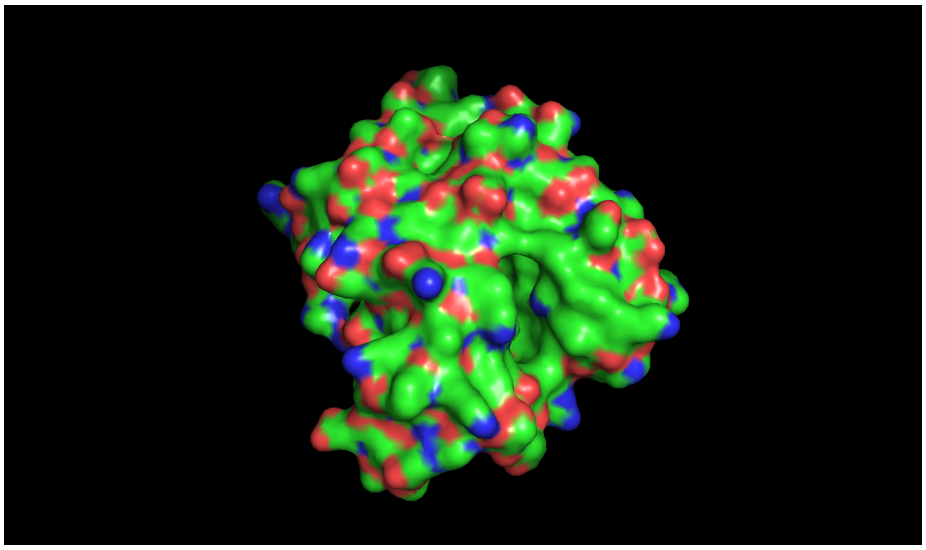
Results

1. The Human Hemoglobin PDB ID is 1A3N. 1A3N's resolution is 1.80 angstroms, has 574 residues, related in 4/29/1998.
2. 1A3N has 4 chains, 2 alpha chains and 2 beta chains. Each chain contains one cofactor, called HEM PROTOPORPHYRIN IX CONTAINING FE . 450 water molecules is around hemoglobin. The first amino acid VAL in chain D is missed.
3. The file name is 1A3N_beta.pdb
4. Visual pictures

Mode	Picture
Carton View	
Dots View	

Mode	Picture
Line View	
Mesh View	

Mode	Picture
Ribon View	
Spheres View	

Mode	Picture
Sticks View	
Surface View	

Conclusion

PyMOL is a big and interactive draft paper for studying structure biology.