Proteins structure with UCSF Chimera

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1 Exercise 1

In this section, we will look at the structure of the protein with ID 7E30 in the PDB database. It is a alpha/beta hydrolase. The structure of this protein present Figure1.

(a) Front view.

(b) Side view.

Figure 1: Structure of alpha/beta hydrolase.

1.1 What is the structure?

It is an IV-structure protein because it consists of two protein chains: A and B. Each chain consists of 9 helices and 9 strands. It is seen that there are structures similar to the Rossmann fold.

1.2 Is it a single protein or a complex?

It is a complex protein, because it consists of two subunits - two almost identical chains. Cause the number of subunits is equal two, we can refer to it as dimer.

1.3 What is the experimental method used to solve the structure of this molecule?

The method used to solve the structure is X-RAY Diffraction.

1.4 What is the resolution of the model?

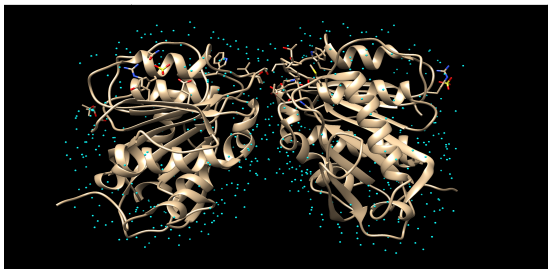
The resolution of the model is 1.56 Å.

1.5 Select and display all water molecules. How many are there? Color them blue.

There are 555 water molecules (see Figure2).

1.6 Find and mark the ligands. How many ligands did you find?

There are 6 ligands.



(a) Protein structure with selected water molecules.

Figure 2: Water molecules

1.7 Color the protein chains and the ligands in different colors.

See Figure3.

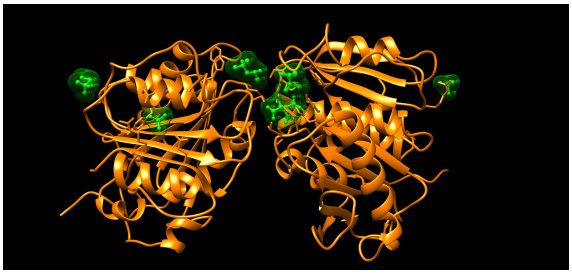


Figure 3: Protein chains and ligands.

1.8 Color all the helices the same color, and the beta sheets (strands) in different color.

See Figure4.

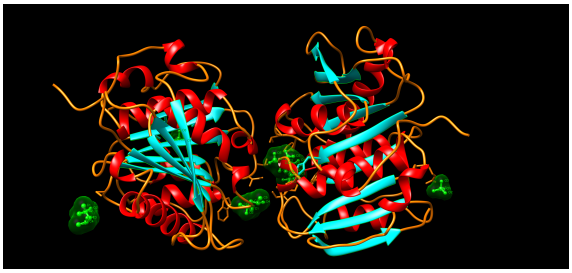


Figure 4: Secondary structures.

1.9 Display the surface of the protein chain (only) and set its transparency to 75%. Where are the ligands located? Explain what is an active site of the protein.

The Figure5 displaying the structure of protein chain and ligands. The active site of a protein is where a substrate molecule binds. Thanks to this connection, a chemical reaction can undergo.

In this molecule, the active site is probably in the center of the protein, between the two chains, where the ligand structures are cumulated.

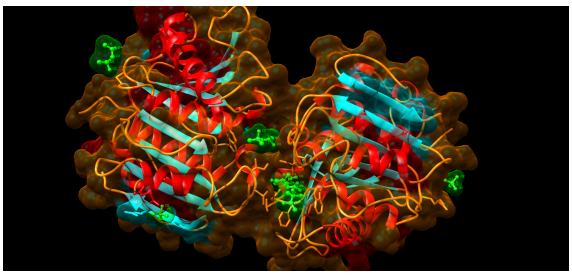


Figure 5: Surface of protein with 75% transparency.

2 Exercise 2

At this time, we will look at the structure of protein with ID 1EQZ in the PDB database. It is a structure of nucleosome core (see Figure6).

(a) Top view.

(b) Front view.

Figure 6: Structure of nucleosome core

2.1 What is this structure?

It is an IV-structure protein because it consists of 10 protein chains (from A to J). Unlike the previous protein, all protein chains are not similar among themselves. However, eight of them show similarity - they are histones. The other two chains that stand out form a DNA strand. Thus, a nucleosome is a unit consisting of 8 histones, on which a DNA strand is wound. It is worth noting that each histone octamer is composed of two copies each of the histone proteins H2A, H2B, H3, and H4. As you can see in the Figure7, histones are structures made mainly of a protein chain coiled in an alpha-helix.

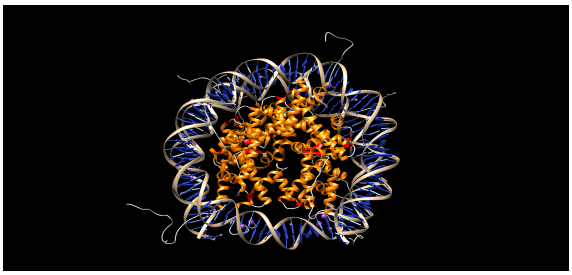


Figure 7: Nucleosome with histones marked (orange - helix part of histones, red - band part of histones).

2.2 Is it a single protein or a complex?

It is a complex protein as before. We can say that it is an octamer with DNA strand.

2.3 What is the experimental method used to solve the structure of this molecule?

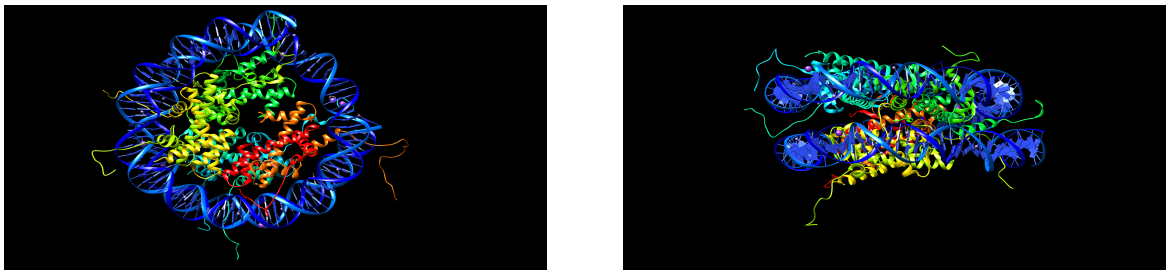
The method use to solve the structure is X-RAY Diffraction.

2.4 What is the resolution of the model?

The resolution of the model is 2.50 Å.

2.5 How many chains does this protein have? Color each of them a different color with Rainbow.

The protein - histone is, as we said before, an octamer, which means it's composed of 8 subunits (chains). The protein - histone is, as we said earlier, an octamer, which means that it consists of 8 subunits (chains). Moreover, there are two additional chains that come from the DNA strand. (Figure8 present chains colored with rainbow colors).



(a) Top view.

(b) Front view.

Figure 8: Chains colored with rainbow palette.

2.6 Display all hydrogen bonds in a protein.

In Figure9 we display hydorgen bonds with light blue color.

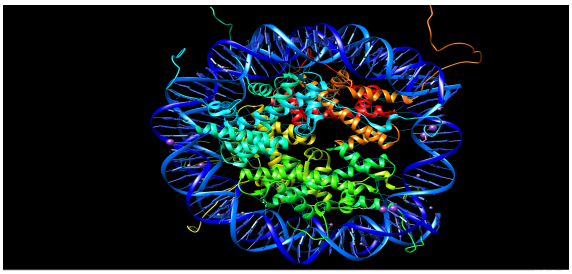


Figure 9: Protein structure with hydrogen bonds.

2.7 Color all nucleic acids in different colors.

Here we color nucleic acids in DNA strand. Adenine with red, cytosine with yellow, guanine with blue, thymine with green (see Figure10)

2.8 Remove all water particles.

See Figure11.

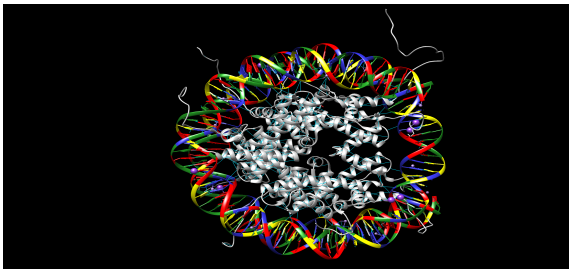


Figure 10: Protein structure with colored nucleic acids.

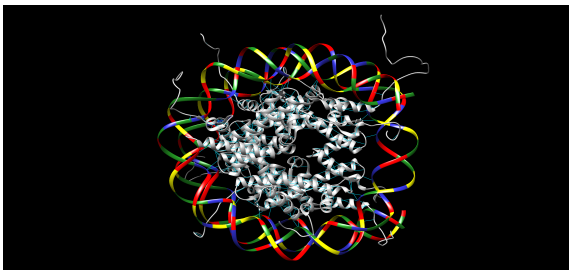


Figure 11: Protein structure without water particles.

2.9 Select all the lysines (how many?), color them white and display the side chains.

In Figure12 there is the protein structere with lysine colored. There are 93 lysine parts.

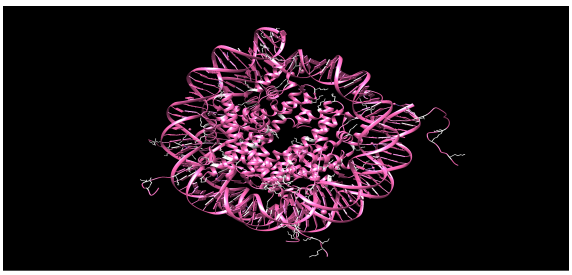


Figure 12: Protein structure with selected lysines.

2.10 Display the surface of the DNA.

Figure13 present the DNA surface only.

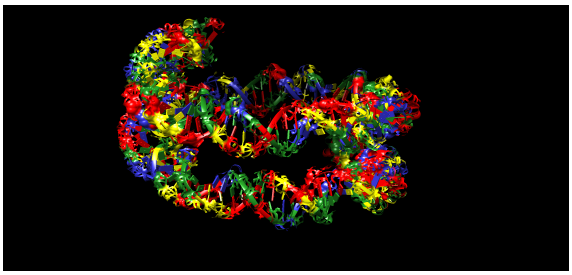


Figure 13: Surface of DNA.