

FOSSEE Summer Fellowship Report 2023

# 3D Modelling Studies on Proteins of Biological Importance

3D Modelling of Structures  
using Jmol and UCSF Chimera

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Submitted by: -

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# Chapter 1

## Introduction

The project aims at studying the structures of some proteins of biological importance through 3D visualizations using the free and open-source software Jmol and UCSF Chimera. Jmol has a wide application in the visualization of chemical molecules, animations of chemical reactions, crystal structures, and biomolecules.

It allows users to create 3D models of the molecules of their interest and aids in the study of stereochemical aspects, bond lengths, bond angles, etc. It is a powerful educational tool that makes students understand the structures of a molecule. The 3D models made using this application can also be incorporated into websites and blogs. It has a profound use, especially in the visualization of larger molecules which are made up of thousands of atoms. This application helps the user to view the model in a much clearer manner. The provision to rotate and view the molecule from different points provides a better understanding of the studies of the molecule.

UCSF Chimera is a software that is dedicated to the structural studies of biological molecules. The software has provisions to overlap and study the difference between two biomolecules. It also displays the sequence of amino acids in the case of proteins and constructs an isosurface based on the electrostatic potentials of the amino acids present. The software also helps its user to view the Ramachandran plot for protein molecules.

In this project, the Jmol application is used in the construction of webpages on Myoglobin and Hemoglobin, Proteases, and proteins involved in the respiratory transport chain. UCSF Chimera is used to study the difference in the amino acid sequence of normal deoxyhemoglobin and sickle deoxyhemoglobin.

### **The version of Software used:**

Jmol - 16.1.11

UCSF Chimera - 1.17.1

## Chapter 2

# General Description of Proteins

### 2.1 Introduction:

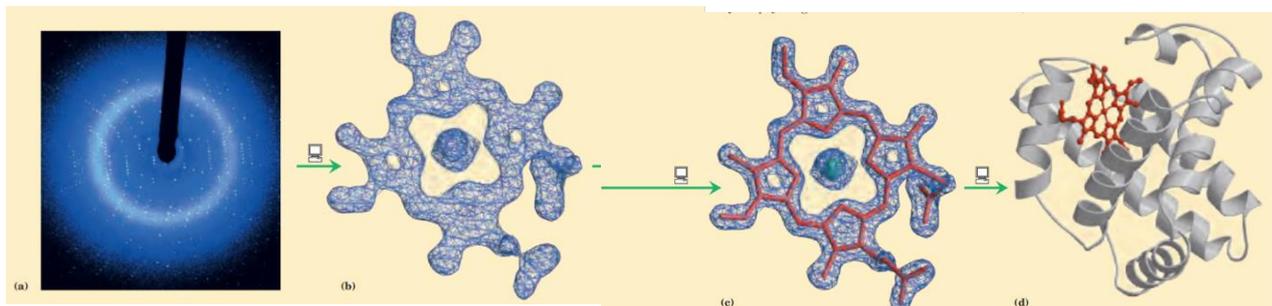
Proteins are the polymers of amino acids linked by amide bonds known as peptide bonds. Proteins play a number of roles as catalysts, structural support, and in the energetics of any organism. They contain more than 100 amino acids and have a mass higher than 10,000 Da.

The proteins can be described into 4 different types of structure – Primary, Secondary, Tertiary, and Quaternary structures.

Among these, the 3D Modelling using the UCSF Chimera and Jmol depicts the secondary and tertiary structure of protein fed.

### 2.2 Determination of protein structures:

About 90% of the structure of proteins present in the protein data bank is determined from the X-Ray diffraction studies done using the protein macro crystals of about 50 $\mu$ m. The diffraction pattern obtained from the X-Ray diffraction is used for electron density mapping and thereby generating the protein model.



Source: Principles of Biochemistry, 4/e © 2006 Pearson Prentice Hall Inc.

Fig 2.1 Depicts the construction of a molecular model from the electron density map obtained using an X-Ray diffraction pattern

## 2.3 Ramachandran Plot:

It is a plot between the phi angle (the angle around the  $-N-C_{\alpha}-$  bond) and the psi angle (the angle between the  $-C_{\alpha}-C-$  bond) of the amino acids present in the protein that are sterically permitted. The plot was developed by the Indian Biochemist, Dr. G. N. Ramachandran in 1963.

The plot had 4 quadrants where the population of amino acids correspond to particular secondary structures based on the steric hindrance. The blank space in the plot denotes non-permissible angles based on their energy levels.

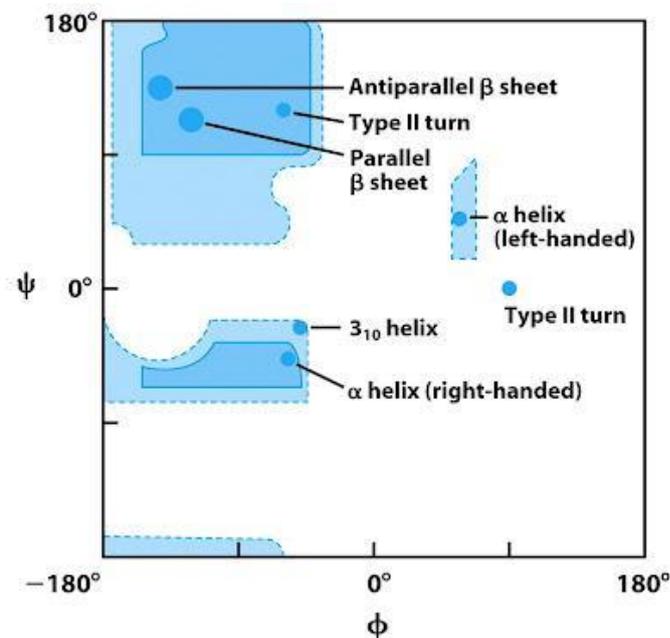


Figure 4-9a Principles of Biochemistry, 4/e  
© 2006 Pearson Prentice Hall, Inc.

Fig 2.2 Ramachandran plot - The values of phi and psi for various allowed secondary structures are represented.

## Chapter 3

# Globins - The Oxygen Binding Proteins

## 3.1 Myoglobin – The Oxygen Storage

Myoglobin is a monomeric heme-containing protein found in almost all mammals. It is used in oxygen storage and is responsible for the red color of muscles due to the presence of Iron as its central metal ion.

Myoglobin has two components: -

1. A Polypeptide chain with 153 amino acids
2. Heme – A cyclic tetrapyrrole consisting of four molecules of pyrrole linked by  $\alpha$ -methylene bridges (protoporphyrin IX) to which is bound iron in its ferrous state ( $\text{Fe}^{2+}$ )

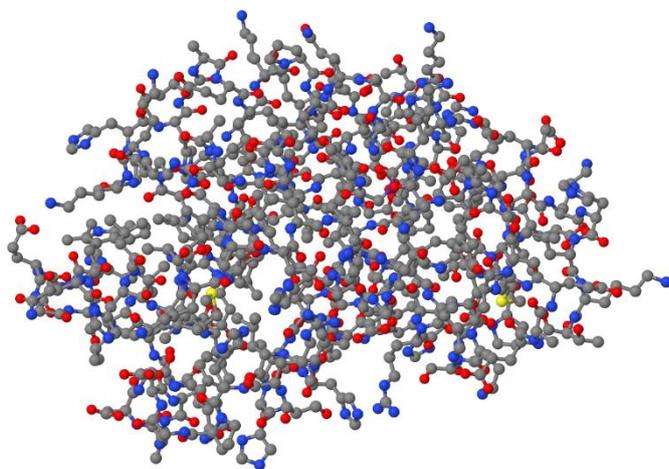


Fig 3.1(a) Polypeptide part of myoglobin

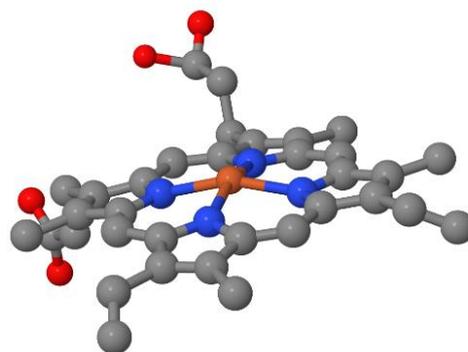


Fig 3.1(b) Heme part of myoglobin

### 3.1.1 Visualisation of oxymyoglobin using Jmol application

PDB Code – 1MBO (Oxymyoglobin)

Link for accessing the PDB file - <https://www.rcsb.org/structure/1mbo>

1. Open Jmol version 16.1.11 using Jmol.jar
2. Go to “File” in the main menu → Click on “Get PDB” → Type 1MBO → Structure of oxymyoglobin gets loaded onto the screen.

3. Open the console by clicking on the “file” in the main menu
4. Type the command `$hide solvent` (to hide the solvent atoms)
5. Right-click and select “style” → Scheme → Choose “trace”
6. Open the console window and the command `$color teal` is written.
7. Give the command `$select HEM` to select the heme part of myoglobin
8. Right-click and choose “style” → “Scheme” → “Ball and stick” which shows the heme ring in a ball and stick fashion.
9. To view the oxygen atoms bound to the heme, Right click and click on “Select” → “Hetero” → “By HETATM” → “Oxygen molecule”

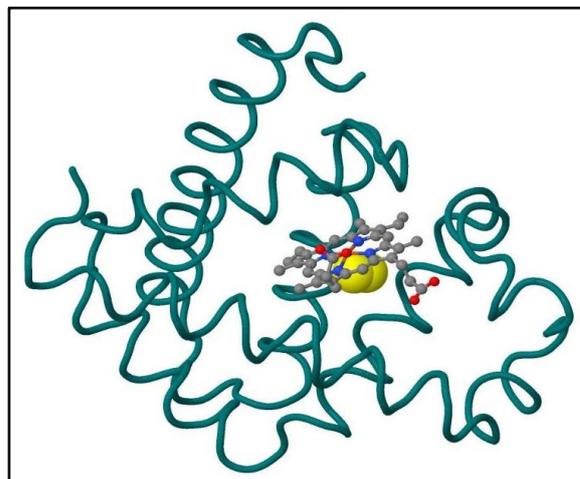


Fig 3.2 Structure of oxymyoglobin molecule

10. Open the console window and type the command `$spacefill; color yellow`, and the oxygen bound to the heme part is shown beside.
11. To Change the background color, Right click and choose “file” → “color” → “Background” → “white”

### 3.1.2 Ramachandran Plot for Oxymyoglobin

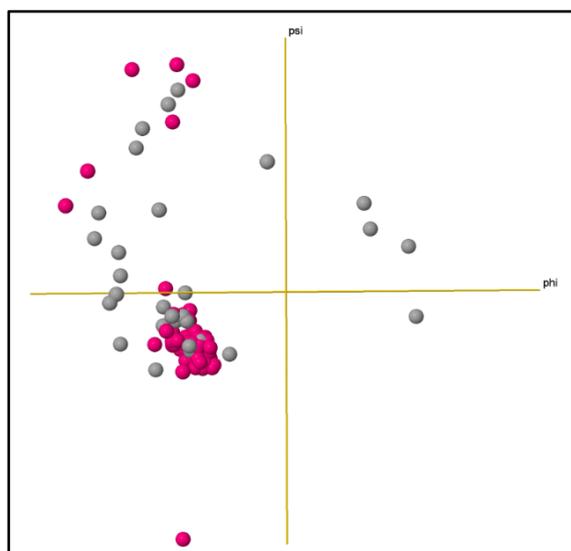


Fig 3.3 Ramachandran plot of oxymyoglobin with 75% of the amino acid residues in the 3rd quadrant.

To obtain the Ramachandran plot for the oxymyoglobin, Open the console window by right-clicking and typing the command

`$rama`



Fig 3.4 Oxymyoglobin molecule made up of 75% right-handed alpha helices corresponding to the plot.

From the Ramachandran plot, it is evident that 75% of the amino acid residues are in right-handed alpha helices as the population in the third quadrant of the population is high.

To view some particular amino acid residue (say the distal histidine[his64] and proximal histidine [hi93]) in the Ramachandran plot, type the command  $\$display$  his64,his93

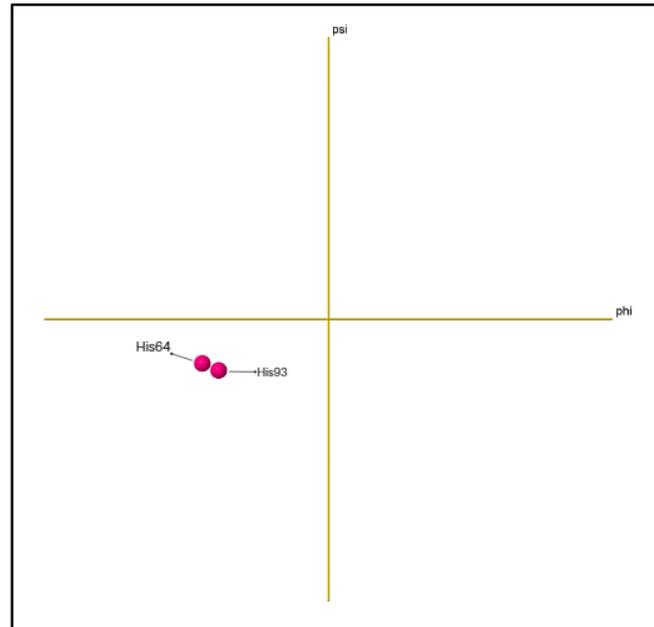


Fig 3.5 The position of the proximal histidine (his93) and the distal histidine (his64) in the Ramachandran plot of oxymyoglobin PDB ID:1MBO

## 3.2 Hemoglobin – The Oxygen Carrier

Hemoglobin is a tetrameric protein that has a vital role in the transport of oxygen from the lungs to the tissues and bringing back carbon-di-oxide and is present in the erythrocytes.

Hemoglobin consists of

- 1) Four Polypeptide chains – Two alpha chains (Chain A and C in PDB codes 1A3N and 1HHO) with 141 amino acid residues in each and two beta chains (Chain B and D in PDB codes 1A3N and 1HHO) with 146 amino acid residues in each.
- 2) Heme group – Protoporphyrin ring bound to iron in its ferrous state ( $Fe^{2+}$ ).

The Hemoglobin permits cooperative interaction in the presence of an oxygen molecule and becomes dimeric. This phenomenon is crucial for its biological action.

### 3.2.1 Viewing the sequence of alpha and beta chains of oxyhemoglobin using UCSF Chimera

PDB Codes: 1HHO (oxyhemoglobin)

Source links: <https://www.rcsb.org/structure/1HHO>

1. Open UCSF Chimera 1.17.1
2. Click “Fetch” → Select “PDB” Database → Enter 1HHO
3. Click on “Favourites” in the main menu and select “Sequence”
4. Choose the chain needed to be sequenced and click show.

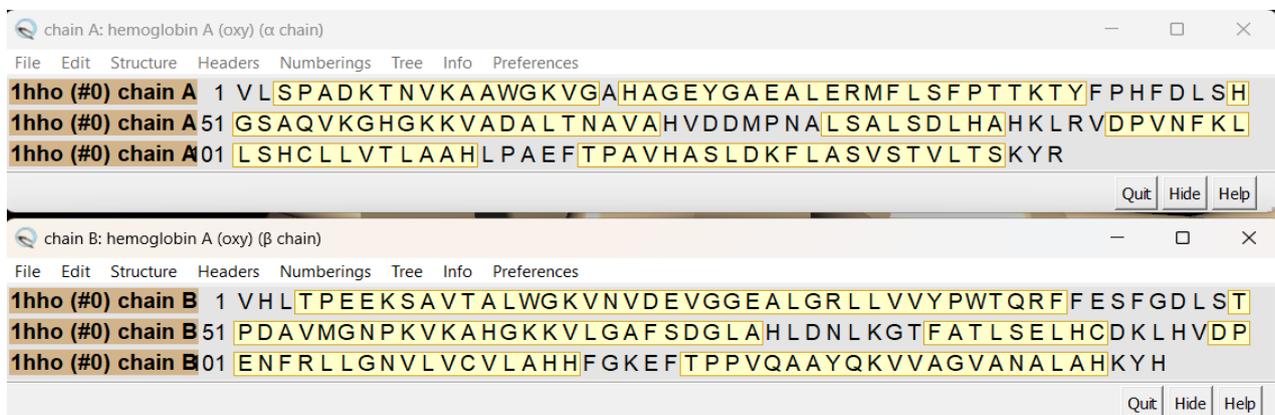


Fig 3.6 Sequence and position of amino acid residues in Chain A and Chain B of oxyhemoglobin

5. The sequence of amino acids appears in one letter code.
6. The sequences highlighted in yellow are those present in the right-handed alpha-helices of the tertiary oxyhemoglobin structure.

### 3.2.2 Conformational changes by oxygenation of deoxyhemoglobin using UCSF Chimera.

1. Open UCSF Chimera 1.17.1
2. Fetch by PDB ID “1A3N” to open deoxyhemoglobin.
3. In the main menu, Click “Tools” → “Structural analysis” → “Metal geometry”
4. A window appears, Click the box “Depict idealized geometry” on the right side of the window.

Metal Geometry			
HEM 142.A FE (1/4)		Next metal	
Coordination Table			
Coordinator	Distance (Å)	Distance RMSD	Best Geometry
HEM 142.A NC	2.02	0.000	N/A
HEM 142.A ND	2.03	0.008	octahedron
HEM 142.A NB	2.04	0.163	trigonal bipyramid
HEM 142.A NA	2.06	0.157	octahedron
HIS 87.A NE2	2.24	0.198	octahedron

Fig 3.7 The window shows the coordination of Iron in the heme part of Chain A with the four nitrogens present inside the heme ring (NA, NB, NC, ND) and the nitrogen on the proximal histidine (his87).

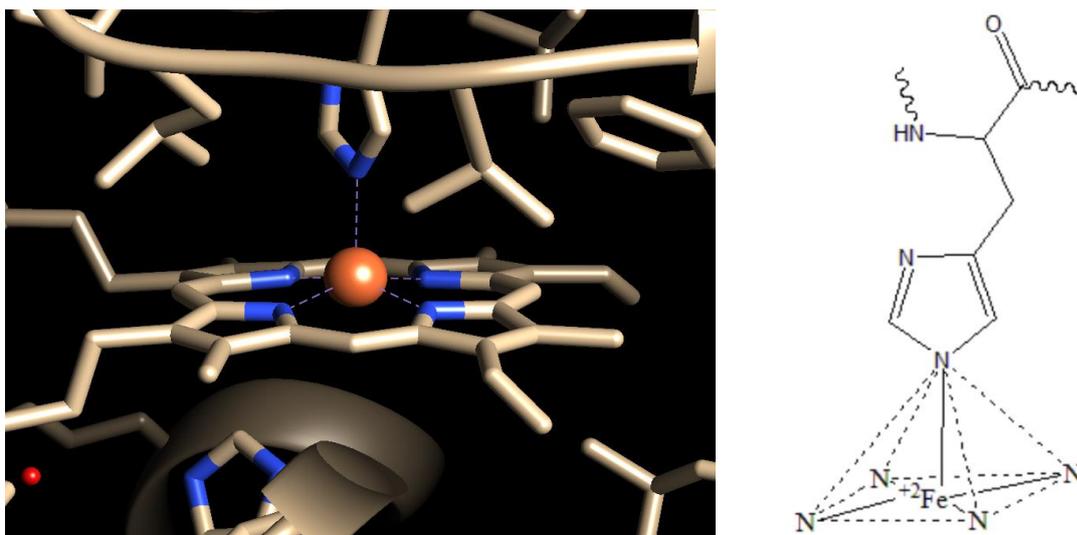


Fig 3.8 Images depicting the square pyramidal geometry of a deoxygenated heme (T-state)

1. To open the oxyhemoglobin, click “File” → “Fetch by ID” → PDB Id “1HHO” is used.
2. Choose “tools” → “Structural analysis” → “Metal Geometry”
3. A window appears, Click the box “Depict idealized geometry” on the right side of the window.

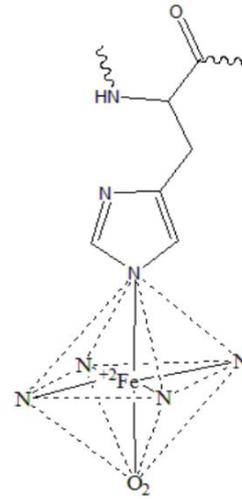
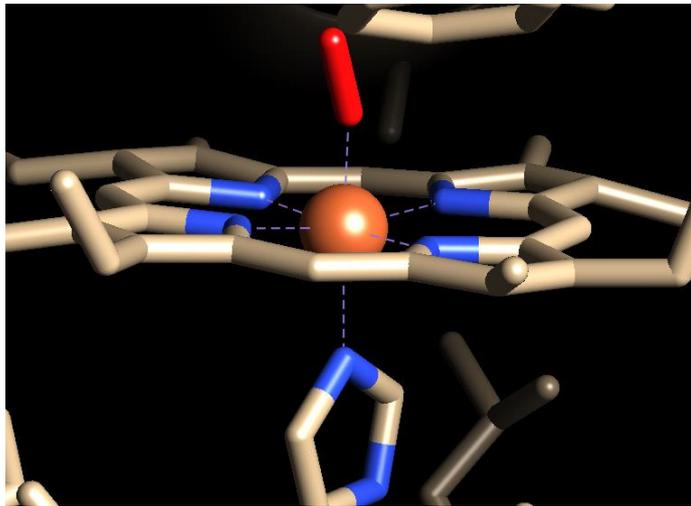


Fig 3.9 Images depicting the octahedral geometry of oxygenated heme (R-State)

Metal Geometry

HEM 143.A FE (1/2)

Coordination Table

Coordinator	Distance (Å)	Distance RMSD	Best Geometry
OXY 150.A O1	1.66	0.000	N/A
HEM 143.A ND	1.93	0.194	tetrahedral
HIS 87.A NE2	1.94	0.509	tetrahedral
HEM 143.A NC	1.95	0.485	tetrahedral
HEM 143.A NA	2.02		N/A
HEM 143.A NB	2.04		N/A

Fig 3.10 The window shows the coordination of iron with the four nitrogens in the heme ring, one nitrogen in the proximal histidine, and with the oxygen molecule.

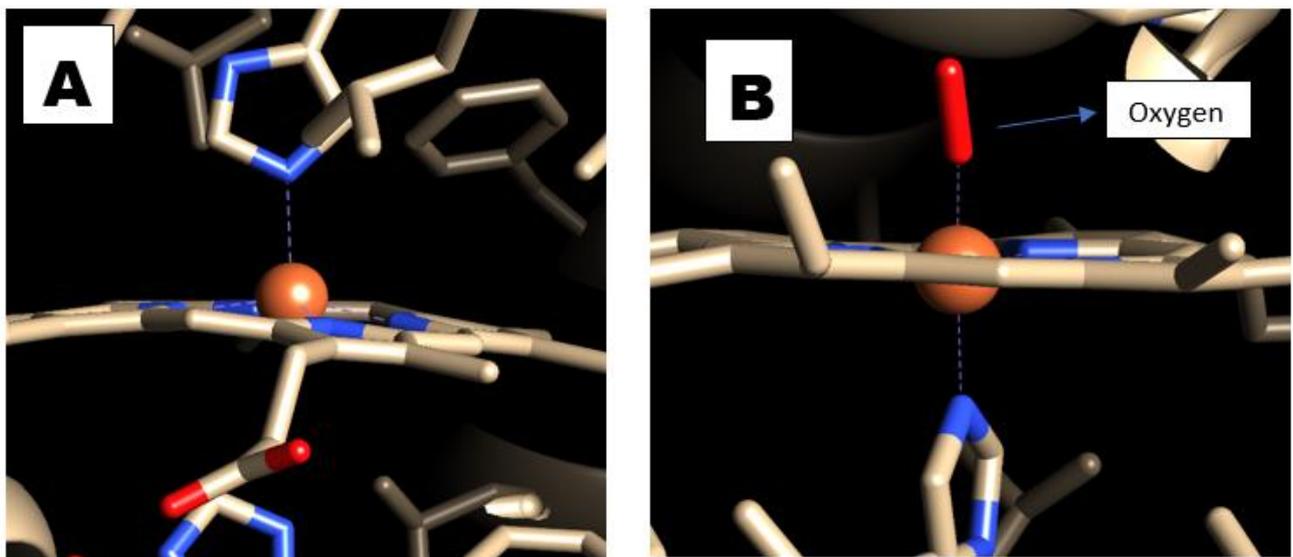


Fig 3.11 A and B depict the movement of the iron atom into the plane of the heme ring on oxygenation.

### 3.2.3 Measuring the distance of distal histidine from the iron atom in the oxyhemoglobin and deoxyhemoglobin using the Jmol application.

1. Open Jmol using Jmol.jar
  2. Get PDB 1A3N by clicking on the file in the main menu.
  3. Open the console and write the command `$delete solvent`
  4. Right-click and select “style” → Scheme → Choose “trace”
  5. To choose only one beta chain (say Chain B), Open the console window and give the command `$hide :a,:c,:d`
  6. To color write the command `$color darkslateblue`
  7. In the console write `$select HEM`
  8. Right-click and choose “style” → “Scheme” → “Ball and stick”
  9. In the console window, give the command `$select his63:B, his92:B`
  10. Right-click and choose “style” → “Scheme” → “Ball and stick”. This shows the proximal and distal histidines in chain B.
  11. To measure the distance between the Nitrogen atom in the distal histidine and the iron atom, Right click and choose “measurements” → “Distance using angstroms”.
  12. Now zoom in near the heme part and drag a line between the iron atom and his63:b.NE2
  13. The distance is found to be **4.22Å**
  14. To save the file, right-click → file → save → Save script with state.
  15. Similarly, the distance between the iron atom and his63:b.NE2 is found for oxyhemoglobin by loading the PDB Code 1HHO.
  16. Additionally, write the command `$select oxy; spacefill; color mediumvioletred` to view the bound oxygen.
  17. The distance is found to be **4.19Å**
  18. To turn on the label, Write the command `$select his63:b.ne2; label on`
- From the above two values it could be concluded that in the presence of the dioxygen molecule, the distance between the distal histidine and iron atom is reduced by **0.03Å**.

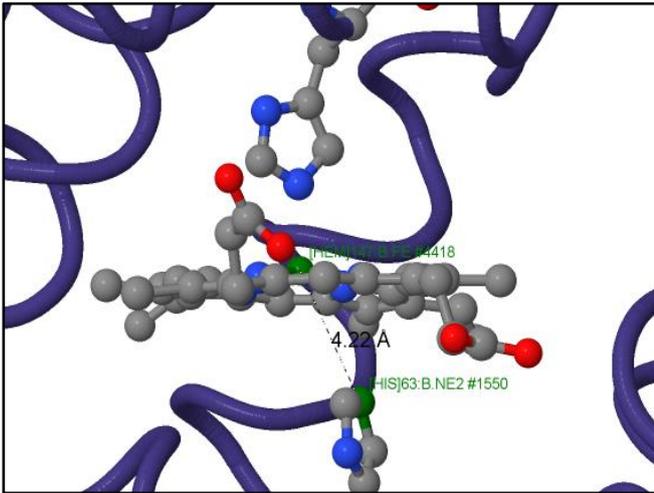


Fig 3.12 The image shows the distance between the iron and distal histidine as 4.22Å in deoxyhemoglobin.

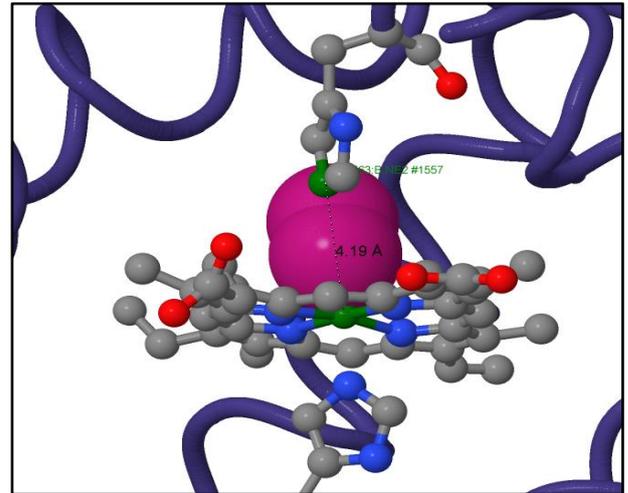


Fig 3.13 The image shows the distance between iron and distal histidine as 4.19Å in oxyhemoglobin.

### 3.3 Sickle Cell Anemia

Sickle-cell anemia is an autosomal recessive genetic disorder that arises due to a point mutation in the Hb Gene of Chromosome 11. The polar glutamic acid present in the 6<sup>th</sup> position of the beta chain of hemoglobin is negatively charged at pH=7.4 (at Blood pH) and is replaced with non-polar valine residue in the condition of sickle cell anemia. The presence of non-polar valine residue forms a hydrophobic “sticky patch”.

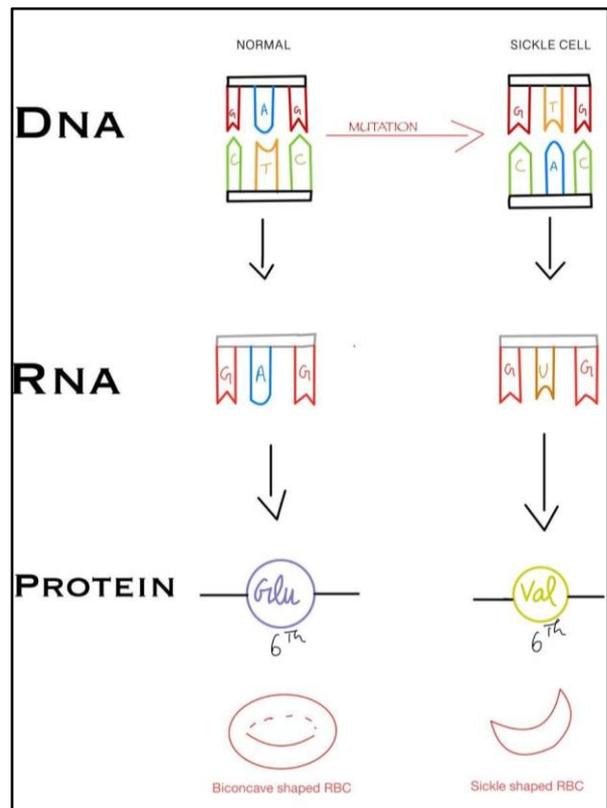


Fig 3.14 Mutation resulting in sickle cell anemia

A person with sickle cell anemia has a large number of immature erythrocytes that are sickle-shaped. Both the normal Hb and Sickle Hb contain a complementary sticky patch on their surfaces that is exposed only in the deoxygenated, R state. Thus, at low PO<sub>2</sub>, deoxyHbS can polymerize to form long, insoluble fibers.

PDB Code: 2HBS (Sickle Hemoglobin)

Link to access the PDB File: <https://www.rcsb.org/structure/2HBS>

### 3.3.1 Overlapping the deoxyhemoglobin and sickle deoxyhemoglobin using UCSF Chimera

1. Open Chimera 1.17.1
2. Fetch by PDB ID 2HBS
3. In the main menu, select “Favourites” → “Command line”
4. In the command line type the following commands, `delete solvent, delete :a delete :c delete :d delete :e delete :f delete :g delete :h`
5. The Chain B of deoxy sickle hemoglobin is visible on screen
6. Type the command `open 1a3n` to load the structure of Normal deoxyhemoglobin.
7. In the command line type the command, `delete solvent, delete :a delete :c delete :d`
8. Go to “tools” in the main menu → “Structure comparison” → “Matchmaker” → A pop-up window appears, select the Normal deoxyhemoglobin (1a3n) as reference structure and click “apply”.

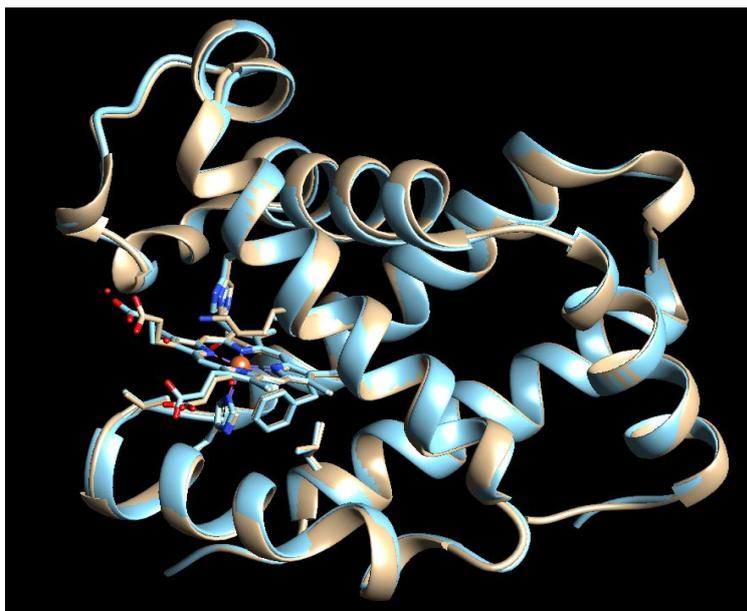


Fig 3.15 The image depicts the overlapping of Chain B of Normal deoxyhemoglobin and Sickle deoxyhemoglobin.

9. Now to see the change in the sequence, click “Tools” in the main menu → “Structure comparison” → “Match” → “Align”
10. Select both the chains in the pop-up window and click “apply”
11. A window showing the sequence and position of amino acids appears.
12. From this, it is evident that there is a change in only one amino acid at position 6.
13. Select E in the 6<sup>th</sup> position of 1a3n (Normal Hb) on the pop-up window and in the menu “Actions” → “color” → “hot pink”
14. Similarly, select V in the 6<sup>th</sup> position of 2hbs (Sickle Hb) and in the menu “Actions” → “color” → “yellow”

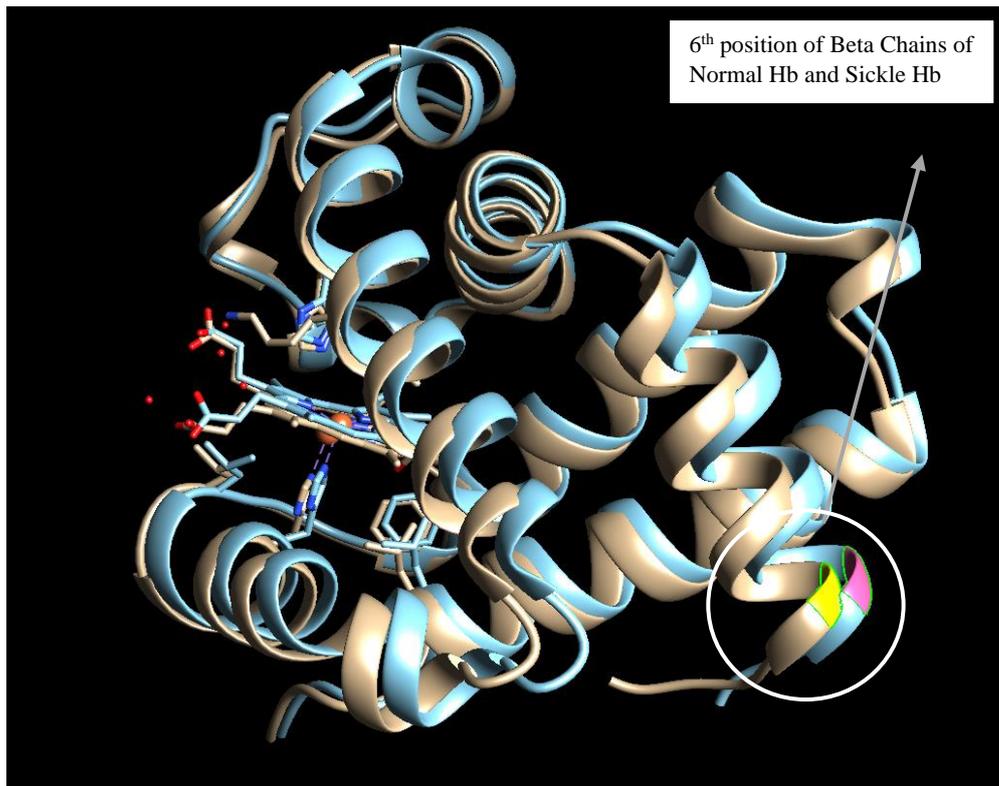


Fig 3.16 The Valine residue in the 6<sup>th</sup> position of Sickle Hemoglobin (highlighted yellow) and the glutamic acid residue in the 6<sup>th</sup> position of Normal Hemoglobin (highlighted pink)

Match of 2hbs, chain B and 1a3n, chain B		1	11	21	31	41				
RMSD: ca										
2hbs, chain B	1	V	HLTP	VEKS	AVTALW	GKVN	VDEVGGEALG	RLLVVYPWTQ	RF	FFESFGDLS
1a3n, chain B	1	V	HLTP	EKS	AVTALW	GKVN	VDEVGGEALG	RLLVVYPWTQ	RF	FFESFGDLS
RMSD: ca										
2hbs, chain B	50	TPDAVMGNPK	VKAHGKKV	LVG	AFSDGLAHL	LD	NLKGTFATLS	ELHCDK	KLHVD	
1a3n, chain B	50	TPDAVMGNPK	VKAHGKKV	LVG	AFSDGLAHL	LD	NLKGTFATLS	ELHCDK	KLHVD	
RMSD: ca										
2hbs, chain B	100	PENFRLLGNV	LVCVLAH	HF	G	KEFTPPVQAA	YQKVVAGVAN	ALAH	KYH	
1a3n, chain B	100	PENFRLLGNV	LVCVLAH	HF	G	KEFTPPVQAA	YQKVVAGVAN	ALAH	KYH	

Fig 3.17 Sequences of Chain B of Normal Hemoglobin and Sickle Hemoglobin

## Chapter 4

# Construction of Jmol integrated webpage in Windows machine

1. Download the code files from  
<https://spokentutorial.org/watch/Jmol+Application/Editing+the+JSmol+Integrated+Web+Page/English/>
2. Extract the Editing-the-JSmol-Integrated-Web-Page-Codefiles folder
3. Move the jspage folder to the desktop
4. Download the latest version of Jmol from  
<https://jmol.sourceforge.net/download/>
5. Extract the Jmol folder and move the Jmol-version no. folder to the jspage folder
6. Install the latest Visual C++ Studio available on the link  
[https://aka.ms/vs/17/release/VC\\_redist.x64.exe](https://aka.ms/vs/17/release/VC_redist.x64.exe)
7. Install the Apache lounge from  
<https://www.apachelounge.com/download/VS17/binaries/httpd-2.4.57-win64-VS17.zip>
8. Unzip the contents of httpd-2.4.57-win64-VS17
9. Move the Apache24 file to the local disk C
10. Move VC\_redist.x64.exe from the downloads to the Apache24 folder in the local disk C.
11. Open the file explorer options, click on “view” and unbox the “hide extensions for known file extensions”. Click Apply and then click ok.
12. Run the command prompt as administrator by left-clicking

### 13. Installation of Apache:

```
c:\Windows\system32>cd ..
```

```
c:\Windows>cd ..
```

```
c:\>cd Apache24
```

```
c:\Apache24\bin>httpd.exe -k install
```

```
c:\Apache24\bin>httpd.exe -k start
```

*“Allow access” if a Windows Defender firewall pop-up window opens.*

### To Check the service has started:

Open the web browser and search <http://localhost/>

A message “It works” appears on the window.

14. To edit the path, open httpd.conf file in the conf folder of Apache24

using Notepad.

15. Edit line number 236 as <Directory "C:/Users/Dell/Desktop/jspage"> and save.

16. Make a copy of the example.html and rename it as xyz.html

17. To edit the html file, open it in the notepad, Edit the title in line 12, and specify the Jmol version number in lines 13 and 14.

18. Edit the topic in line number 49.

19. The structures saved in the .pdb or .spt format can be loaded by editing line numbers 59, 80, and 99.

20. The description for structures 1,2 and 3 can be added by editing Lines 122, 128, and 134 respectively.

21. Edit the file names in lines 121, 127, and 133 with respective structure files.

22. Open the constructed web page in the browser by typing in the search bar  
jspage/xyz.html

**Note:** Opening by double-clicking on the edited HTML file may not open up the .mol files and it is preferred to open by the above-said way.

Link to the webpage constructed for globins

[https://drive.google.com/drive/folders/18c131Hh2RPAVugc3Q14gjpCHJQxAa9YY?usp=drive\\_link](https://drive.google.com/drive/folders/18c131Hh2RPAVugc3Q14gjpCHJQxAa9YY?usp=drive_link)

# Chapter 5

## Active site interactions in Chymotrypsin

### 5.1 Introduction

Chymotrypsin is a serine protease that is present in the digestive systems of many organisms. It is a vital component in the pancreatic juice. Chymotrypsin is activated from its inactive zymogen (chymotrypsinogen) form by the enzyme trypsin. Inhibitors for this enzyme are synthesized and used to study its active site and ligand-enzyme interactions.

A large number of chymotrypsin-inhibitor complexes are crystallized and their structures are analyzed.



Fig 5.1 Chymotrypsin - trifluoromethyl ketone inhibitor complex. (PDB ID - 7GCH)



Fig 5.2 Chymotrypsin - Eglin C inhibitor complex. (PDB ID - 4H4F)

There are certain inhibitors that bind to the enzymes irreversibly, such inhibitors are called suicide inactivators. Amino acids with key catalytic functions in the active site can sometimes be identified by determining which residue is covalently linked to an inhibitor after the enzyme is inactivated.

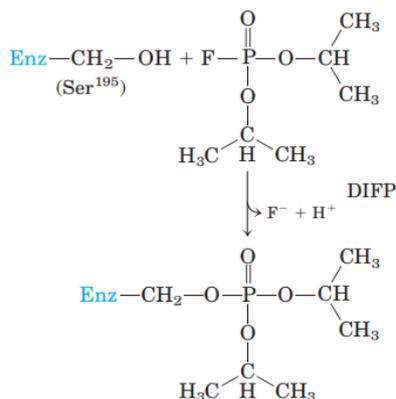


Fig 5.3 The reaction of chymotrypsin with diisopropylfluorophosphate (DIFP) irreversibly inhibits the enzyme. This has led to the conclusion that Ser195 is the key active-site Ser residue in chymotrypsin.

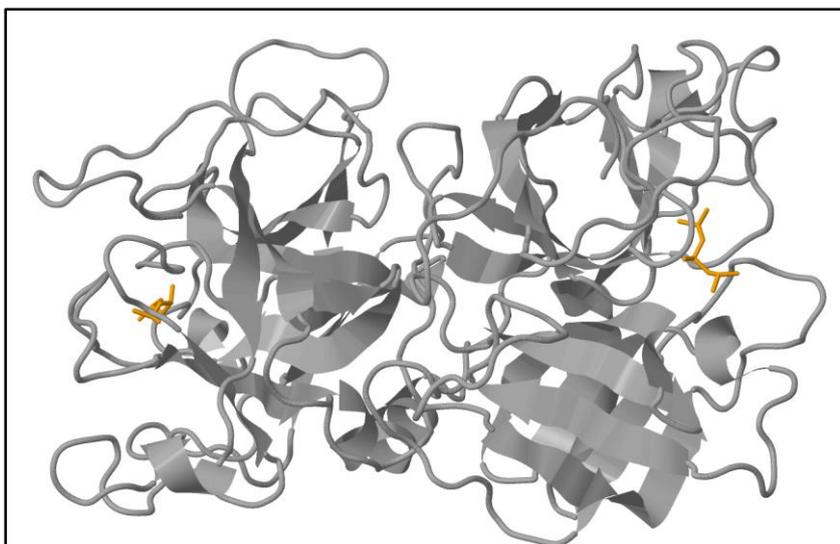
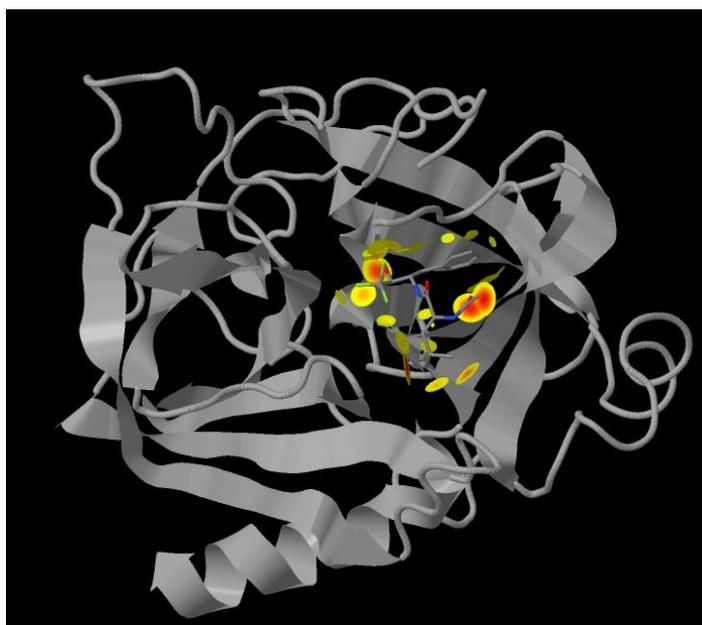


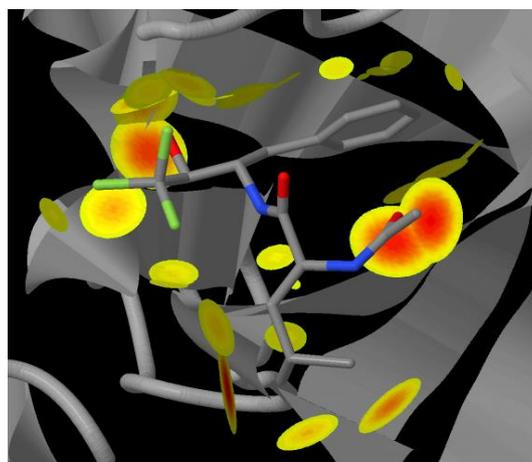
Fig 5.4 Chymotrypsin with diisopropylfluorophosphate (DIFP) inhibitor (PDB ID 1DFP)

## 5.2 Study of contacts of the enzyme-inhibitor complex using Jmol.

1. Open Jmol using Jmol.jar
2. Get PDB 7GCH by clicking the file option in the main menu.
3. The Structure of Chymotrypsin-trifluoromethyl complex appears on the screen.
4. Right click → Style → Scheme → Cartoon
5. Open the console and type the command `$color grey` to change color.
6. Again, type the command `$select ligand; wireframe; color cpk`
7. The command `$contact{ligand}` to view the points of contact of the inhibitor with the enzyme's active site.



(a)



(b)

Fig 5.5 (a) and (b) denote the interaction of trifluoromethyl ketone with chymotrypsin. (PDB ID -7GCH)

## 5.3 Viewing the hydrophobic pockets in Chymotrypsin using Jmol.

1. Open Jmol using Jmol.jar
2. Get PDB 7GCH from the file option in the main menu.
3. Right-click → “Style” → “Scheme” → “trace”
4. In the console window, type the command `$color grey`
5. Give the command `$select ligand; wireframe; color cpk` to view the inhibitor.
6. In the console, `$isosurface select{protein}only pocket cavity vdw` command is written to view the hydrophobic pockets present in the enzyme chymotrypsin.
7. The inhibitor bound to a deep hydrophobic cleft of the enzyme is also seen.

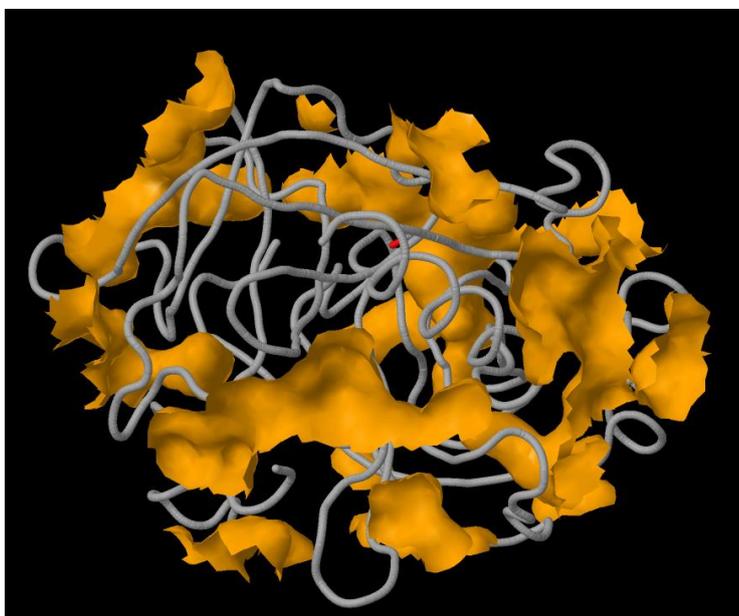
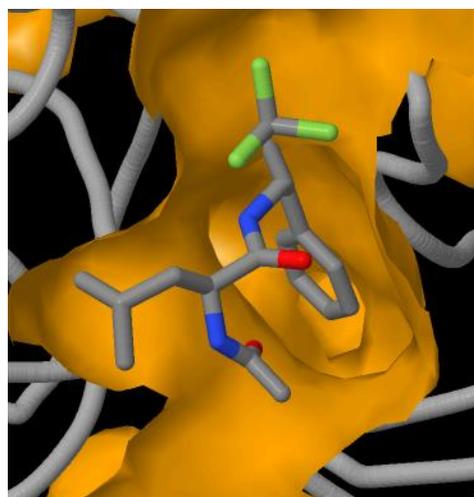


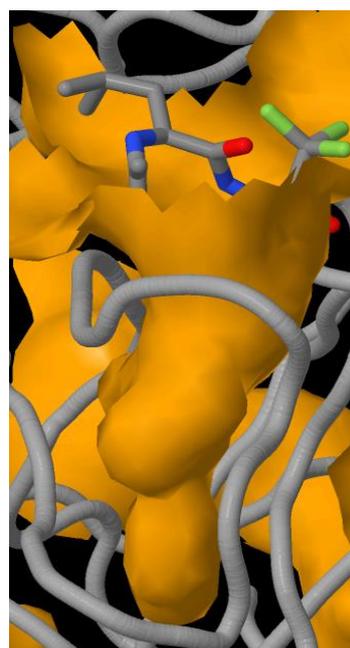
Fig 5.6

The hydrophobic pockets present in the enzyme chymotrypsin (PDB ID 7GCH)

Fig 5.7 shows the hydrophobic pocket where the inhibitor trifluoromethyl ketone binds to chymotrypsin. (a) top view and (b) side view of the hydrophobic pocket.



5.7 (a)



5.7 (b)

## Conclusion:

In this project, Jmol and UCSF Chimera software were used to study the secondary and tertiary structures of Globular proteins such as Hemoglobin, myoglobin and Hydrolases such as Chymotrypsin and trypsin. Ramachandran plot for the proteins is also plotted. The sequencing and position of amino acids is determined using UCSF Chimera. The software is also used to visualize the geometry of the central atom. Jmol is one of the excellent tools to visualize the hydrophobic pockets present in the enzyme. The points of contact of the ligand-enzyme complex can be viewed using the script commands. Both Jmol and UCSF Chimera are powerful tools in the structural studies of proteins; they could be employed by teachers for interactive learning sessions for a deep understanding of concepts

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