PRACTICAL 12

Question 1. Get the **PDB** files, **1ALC**, **4LYZ** and **1TIM**

Solution. Below are the images of the PDB search queries to download the PDB files.
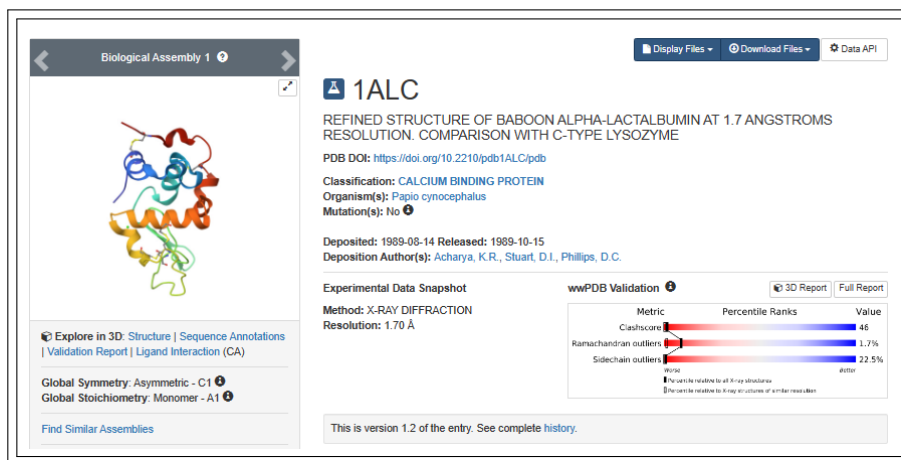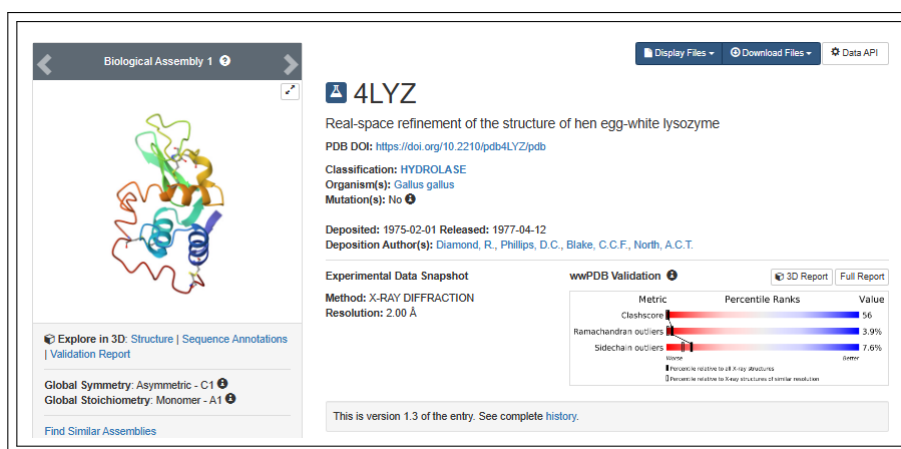

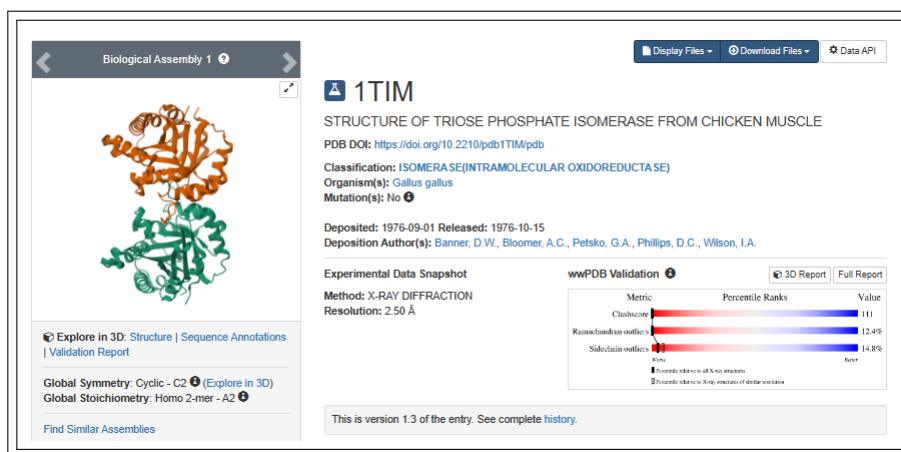FIGURE 1. PDB search: 1ALC

FIGURE 2. PDB search: 4LYZ

FIGURE 3. PDB search: 1TIM

Question 2. Open the file **1TIM** and show in cartoon style (hide line style)

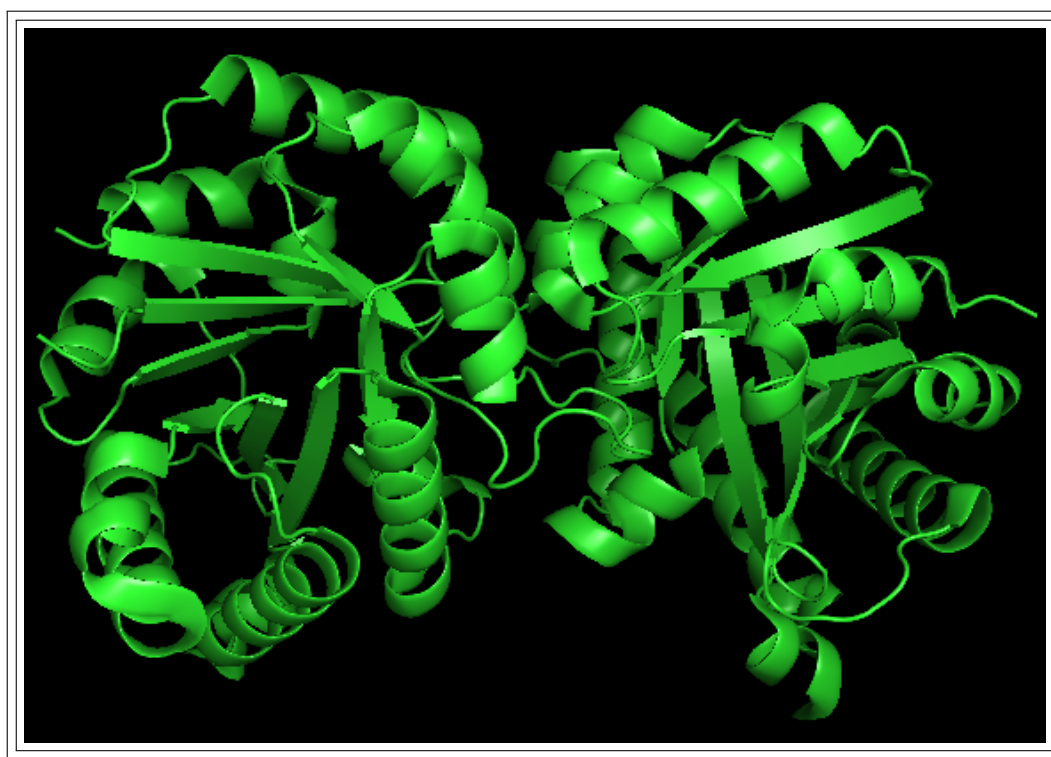**Solution.** The file is opened and selected cartoon style, while hiding line style.

FIGURE 4. 1TIM cartoon style

Question 3. Give different colors to different chains. How many chains are there?

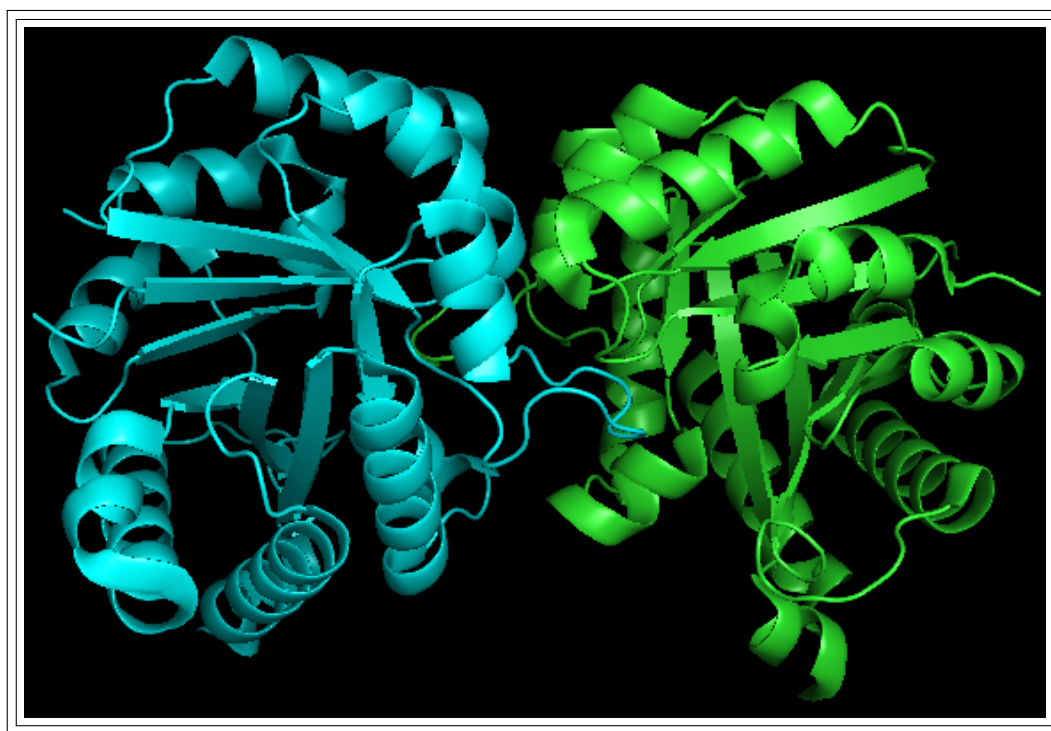**Solution.** The chains have been colored. There are two chains.

FIGURE 5. 1TIM colored chains

Question 4. Remove one chain (right-click on the chain and hide)

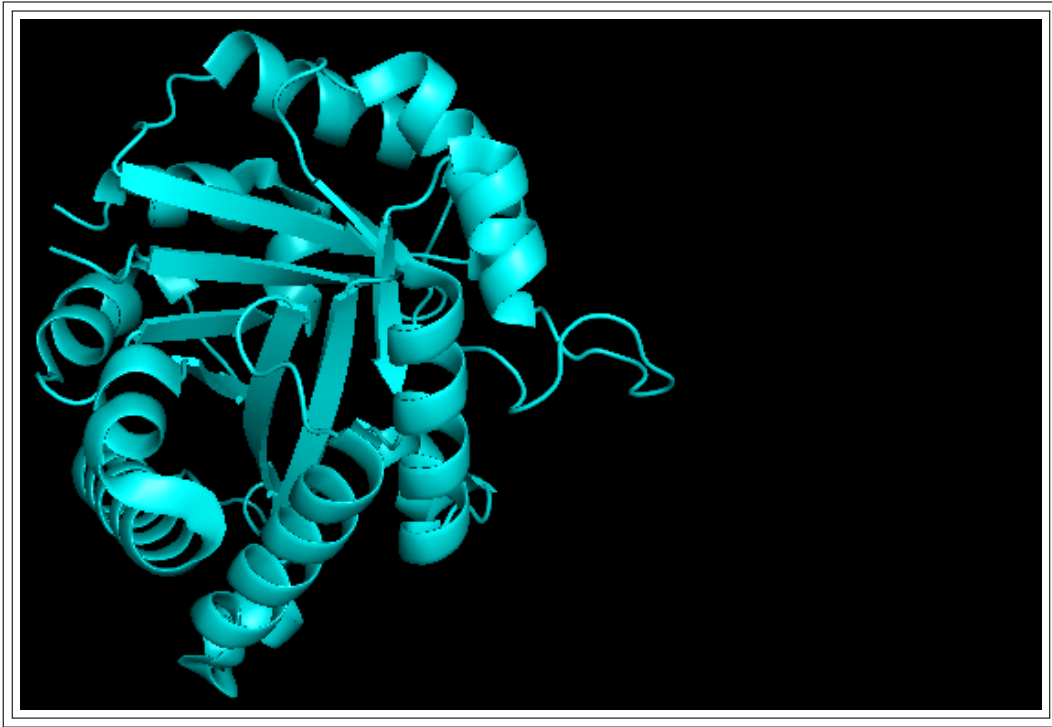**Solution.** The right chain has been removed.

FIGURE 6. 1TIM with one chain removed

Question 5. Identify the secondary structures with different colors

Solution. The chain after coloring secondary structures:
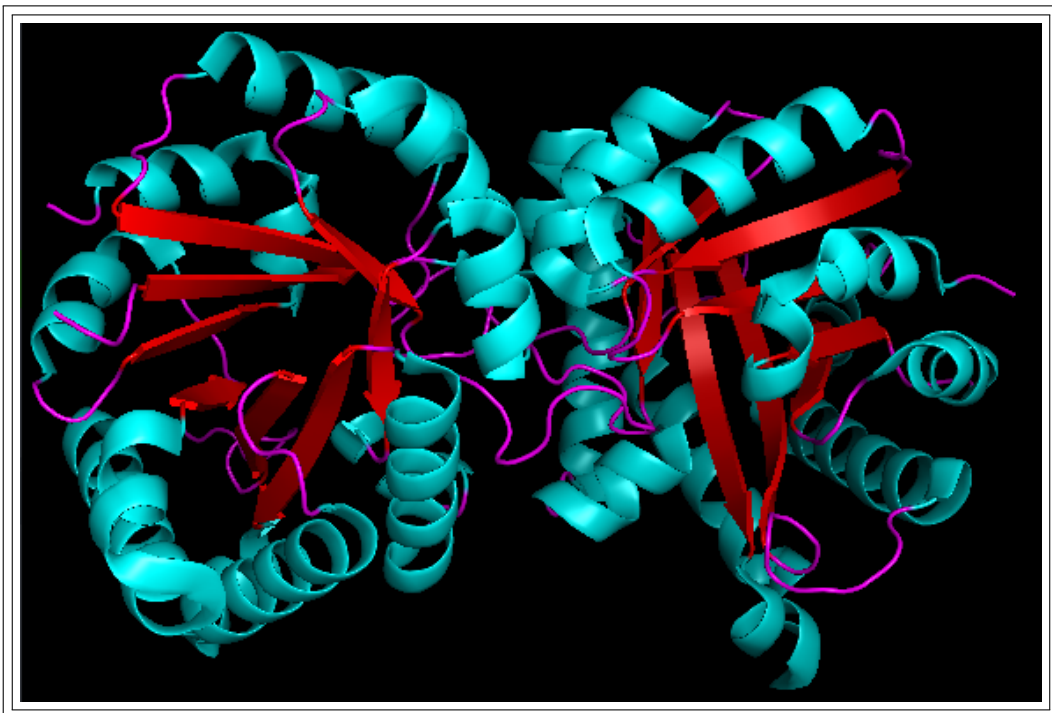Blue: Helix, Red: Sheet, Purple: Loop

FIGURE 7. 1TIM with colored side chains

Question 6. Zoom and rotate to get complete views

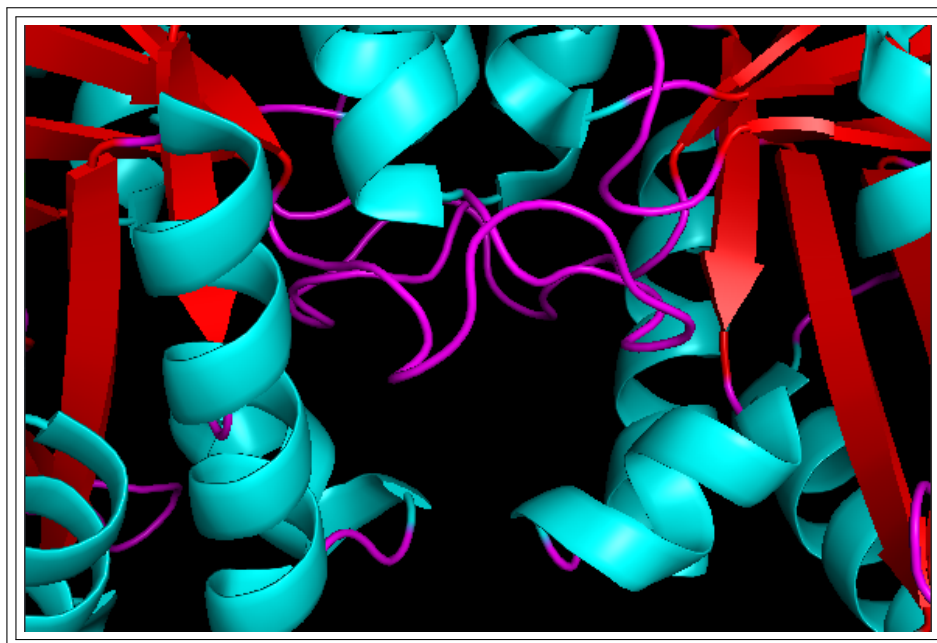**Solution.** The zoomed in picture is shown. Zoomed out is similar to all previous ones.

FIGURE 8. 1TIM zoomed in

Question 7. Show the sequence

Solution. The sequence is displayed

FIGURE 9. 1TIM with sequence

Question 8. Select the residues 21 to 26: **LGELIH**

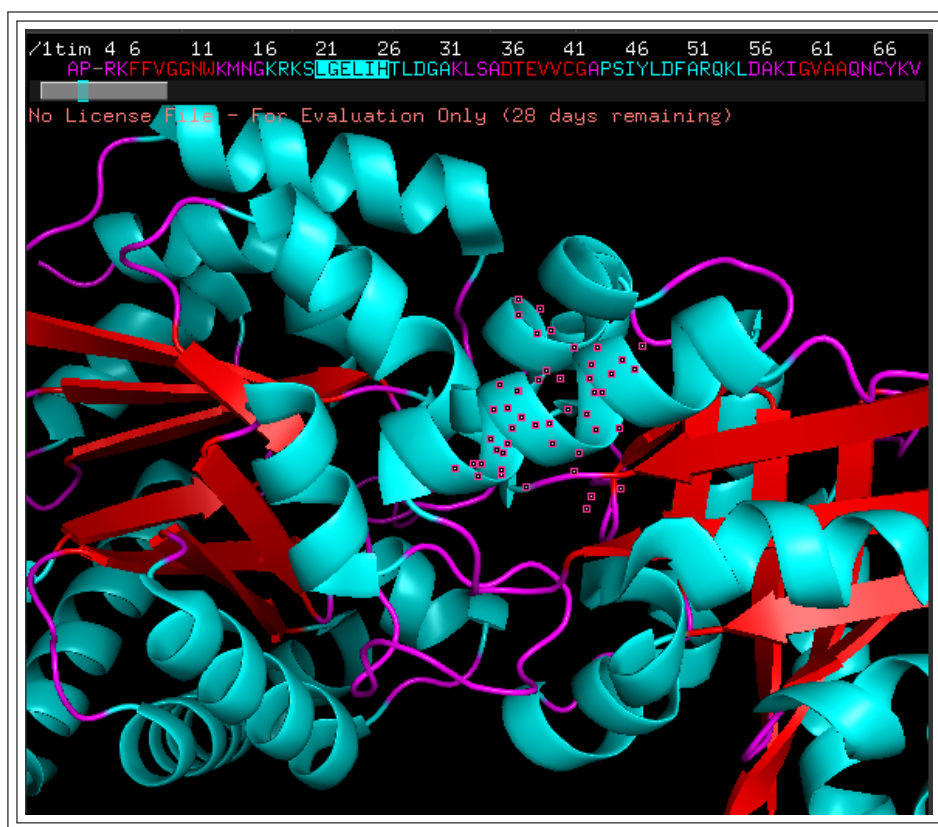**Solution.** The residues given have been selected

FIGURE 10. 1TIM with residues 21-26 selected

Question 9. Hide cartoon diagrams

Solution. The cartoon diagram is hidden, and lines are shown.
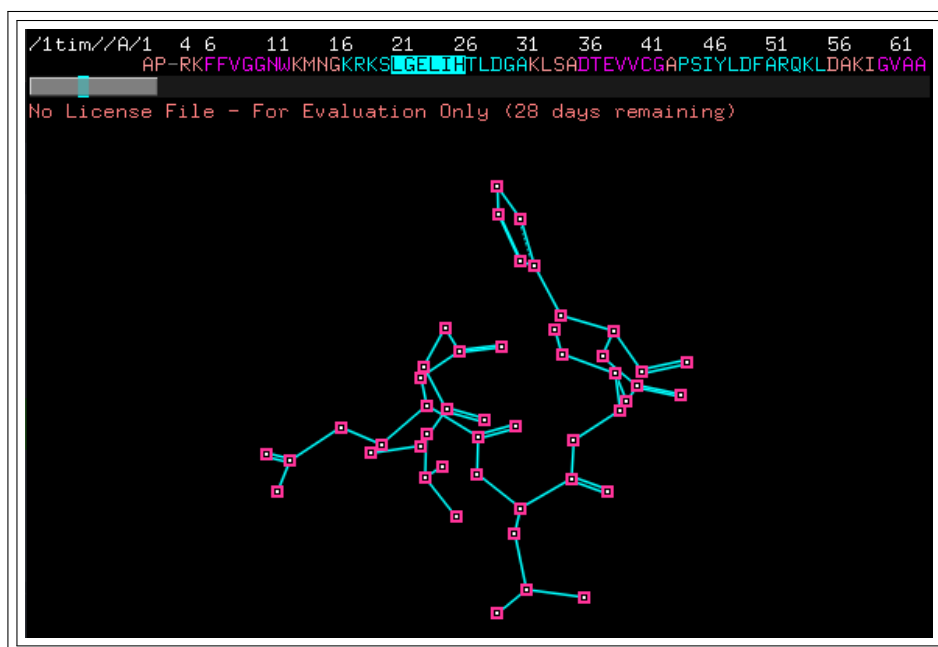

FIGURE 11. 1TIM with lines diagram

Question 10. Color the selected residues based on different atoms

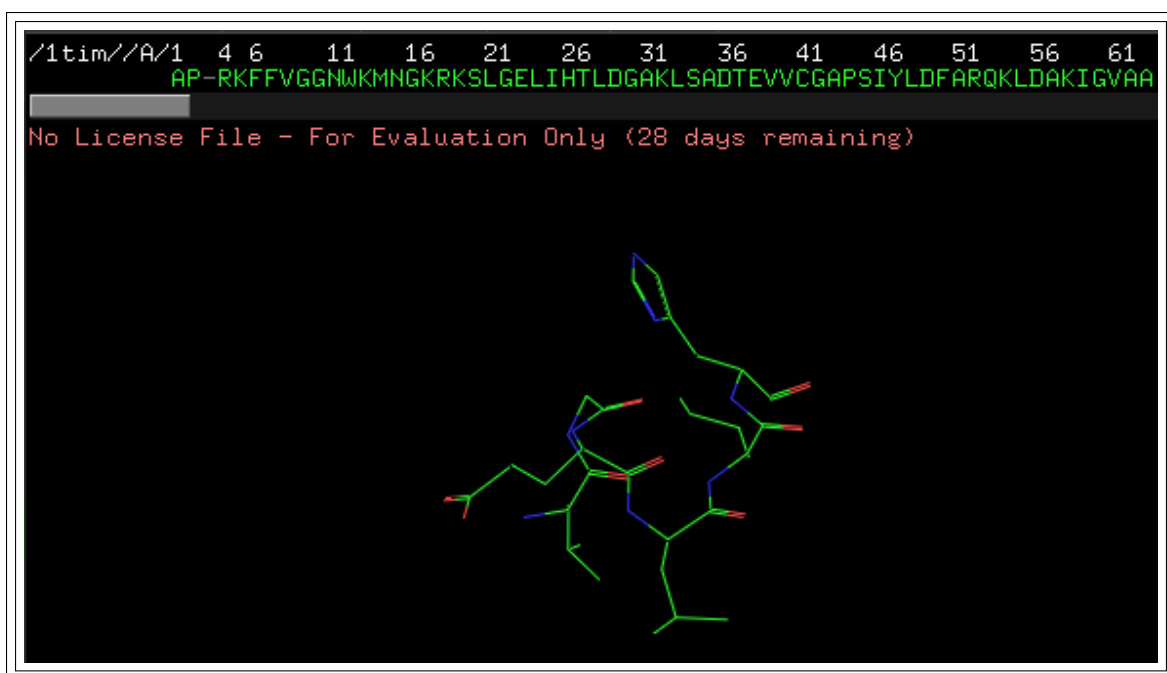**Solution.** The selected residue **LGELIH** has been colored

FIGURE 12. 1TIM with colored residues

Question 11. Identify at least one salt bridge within the protein and list the details of inter-action.

Solution. The salt bridges have been identified. One salt bridge is **E38-R205: 2.3A**
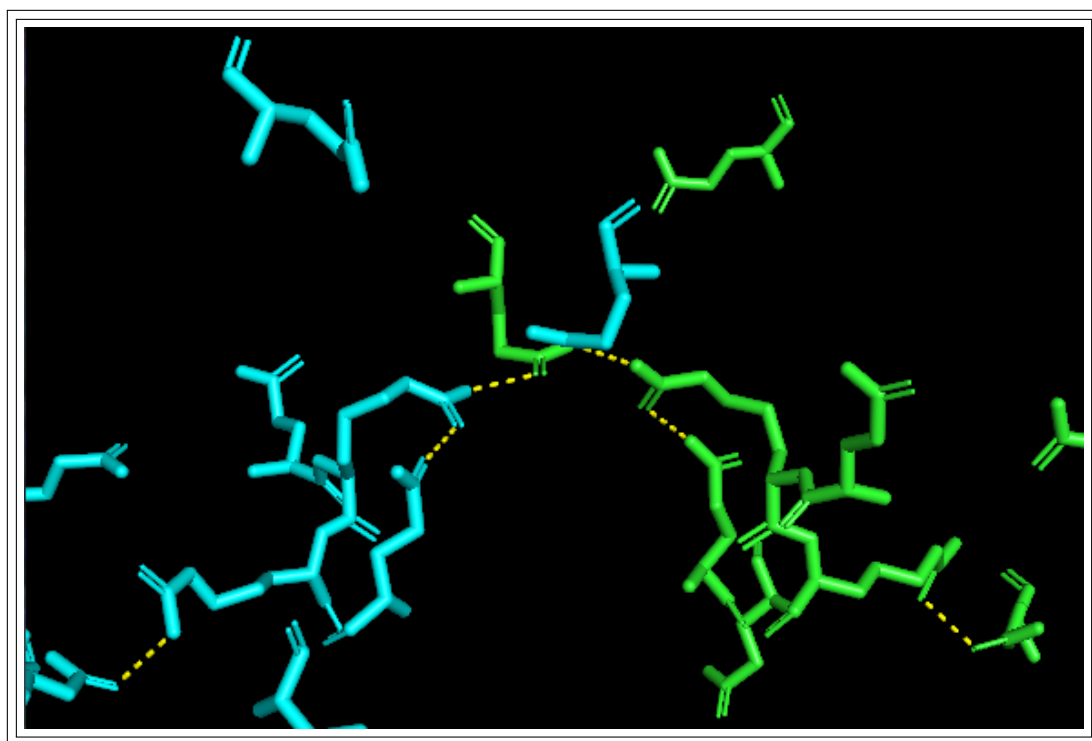

FIGURE 13. 1TIM with salt bridges

Question 12. Identify any hydrophobic interaction / aromatic stacking interaction protein and list the details of the interaction.

Solution. The aromatic stacking interaction has been identified.
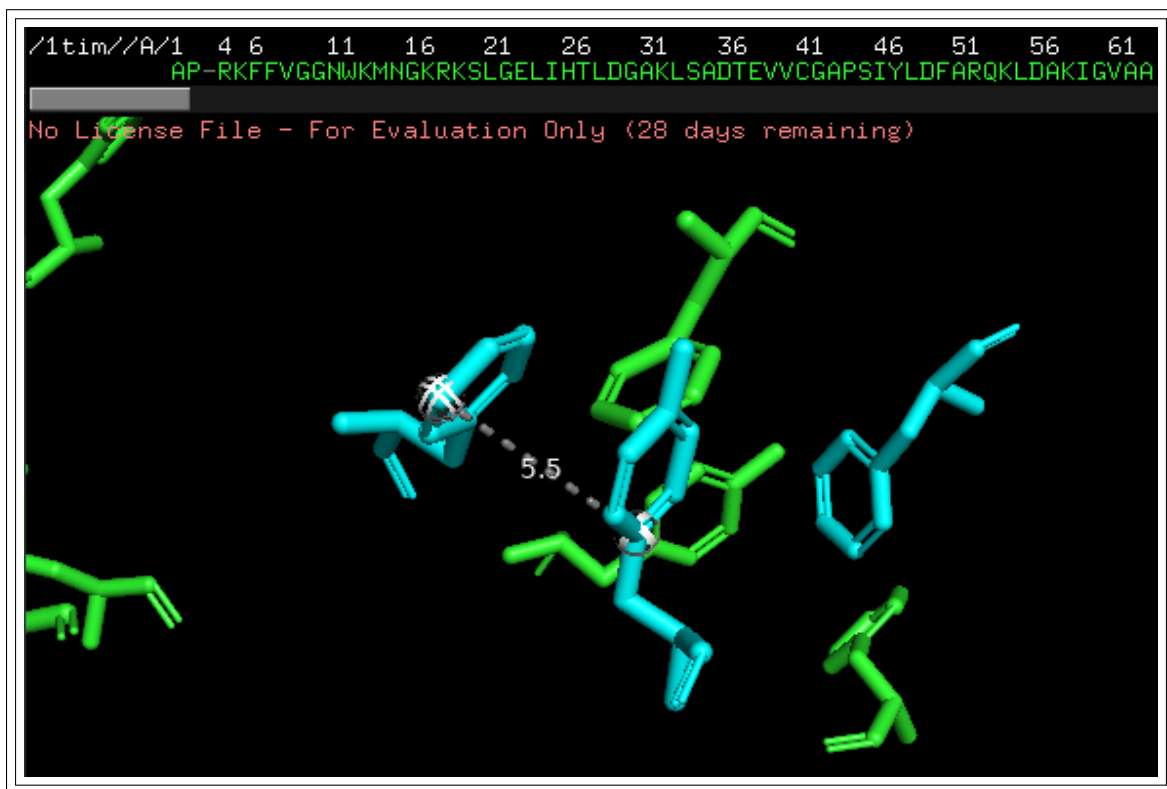

FIGURE 14. 1TIM aromatic stacking interactions

The interaction is **TYR47-PHE50**. The interaction distance is 5.2 A as seen in the diagram below.
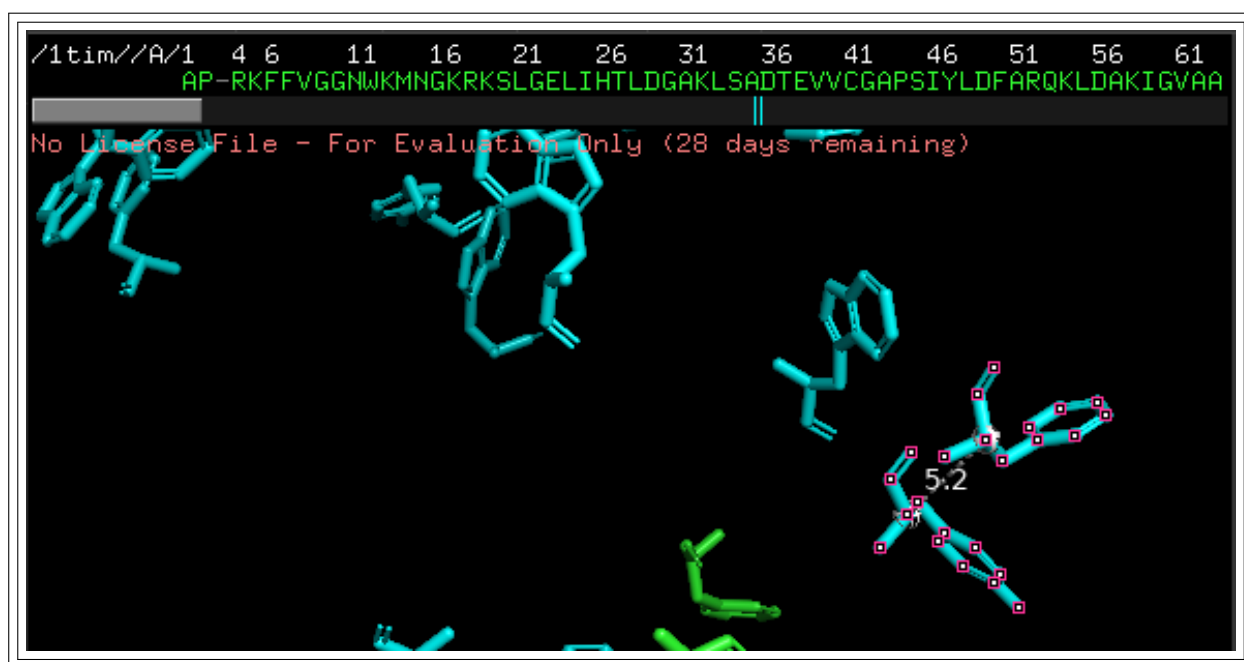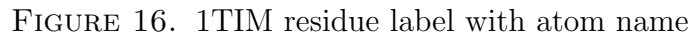

FIGURE 15. 1TIM aromatic stacking interactions dist method

Question 13. Label the residues using the atom name and show their van der Waal radii.

Solution. The labels of residues with atom name and van der Waal radii is given below:

FIGURE 16. 1TIM residue label with atom name

FIGURE 17. 1TIM residue label with van der Waal radii

Question 14. Compute the distance between CG and CD2 in Leu24

Solution. The distance is found to be **1.5A**.

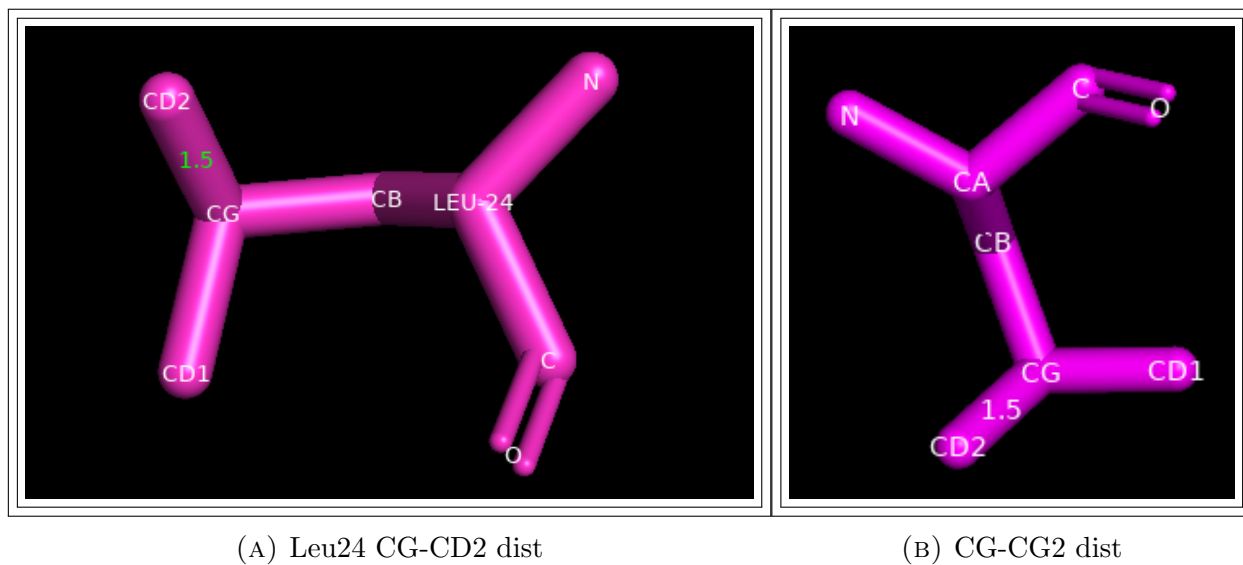(A) Leu24 CG-CD2 dist   (B) CG-CG2 dist

FIGURE 18. The distance between CG and CD2 in Leu24

Question 15. Compute the angle formed by the atoms CD1, CG and CD2 in Leu24.

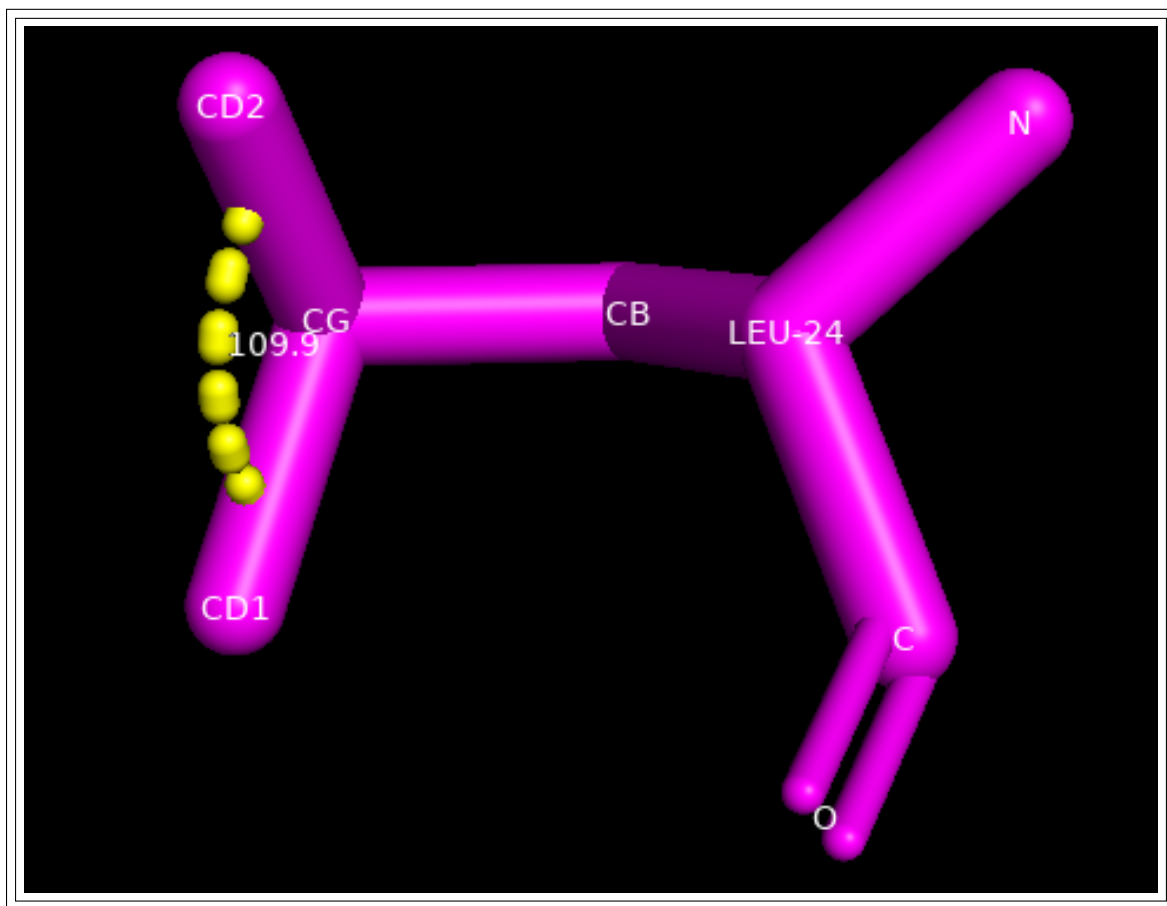**Solution.** The angle formed by the atoms CD1, CG and CD2 in Leu24 is found to be **109.9°**.

FIGURE 19. Angle formed by CD1, CG and CD2 in Leu24

Question 16. Compute the dihedral angles of Leu24
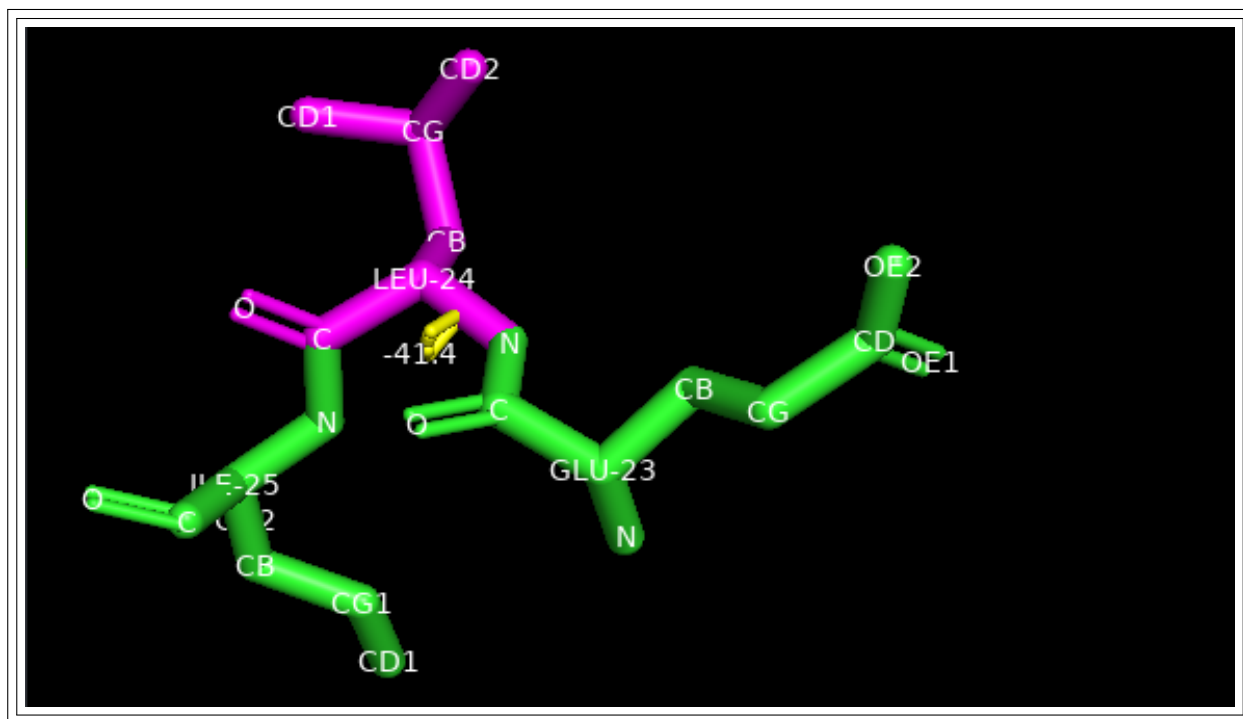
Solution. The dihedral angles are:
ϕ:**-41.4°**.

FIGURE 20. ϕ angle

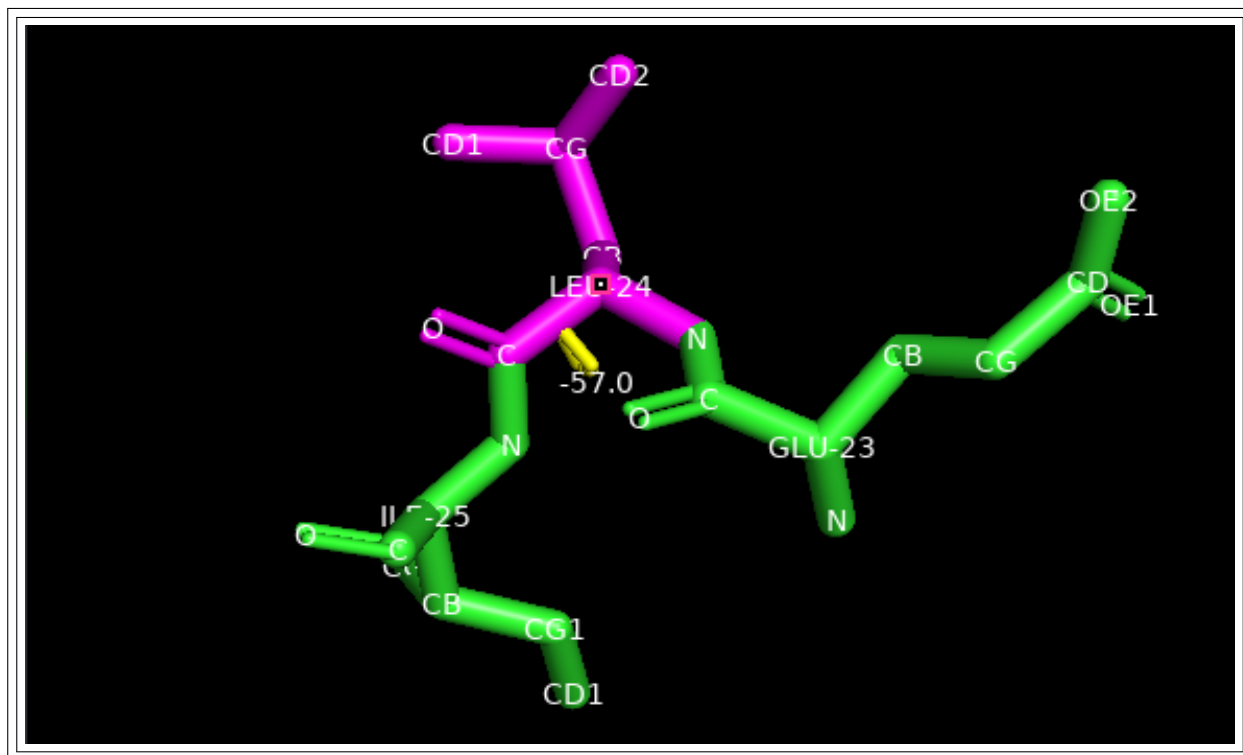ψ:**-51.0°**

FIGURE 21. ψ angle

Question 17. Change background white

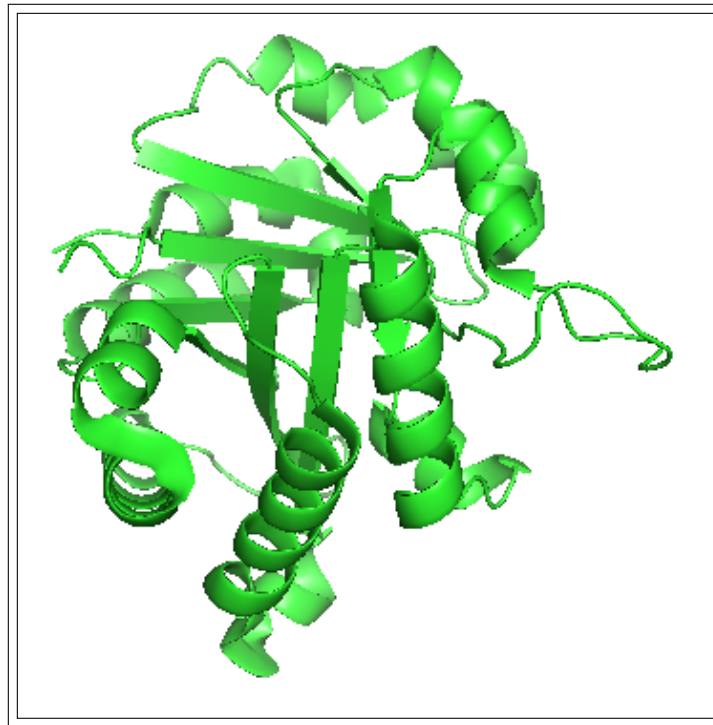**Solution.** The background has been whitened.

FIGURE 22. Background whitened

Question 18. Make high quality picture (use ray)

Solution. The high quality picture is obtained below:

FIGURE 23. High quality picture using **ray**

Question 19. Show B-factors to see flexible and rigid regions (color by spectrum, b-factor)

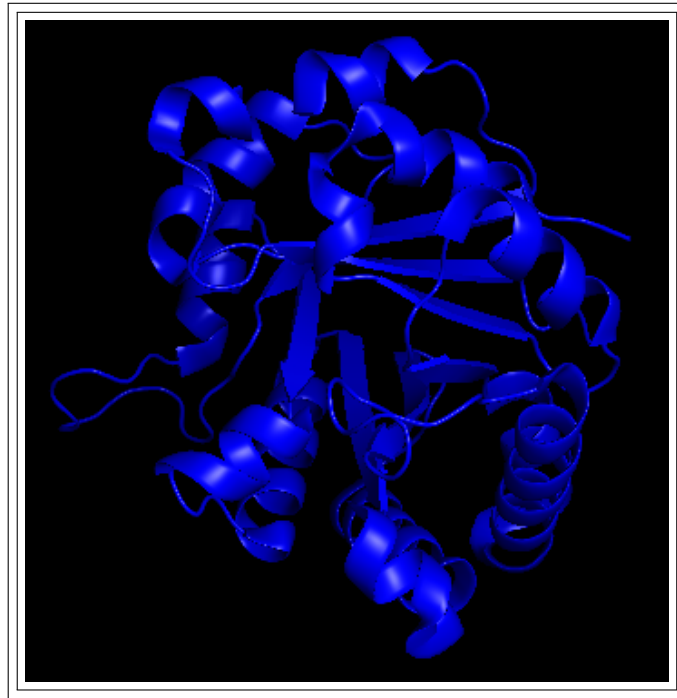**Solution.** Entirety is blue color, implying rigidity.

FIGURE 24. B factors to see flexible and rigid regions

Question 20. Compute the electrostatic potential (A ->generate ->vacuum statistics ->protein contact potential)

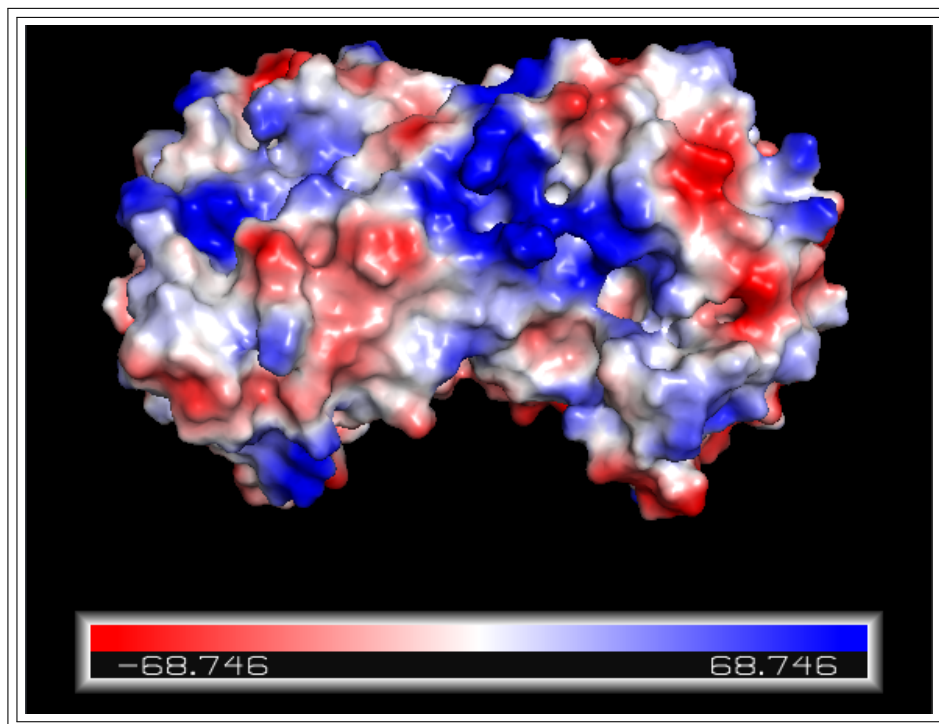**Solution.** Below is the electrostatic potential for the chain:

FIGURE 25. Electrostatic potential

Question 21. Save the image in PNG format

Solution. The link to the saved image is Electrostatic_Potential_1TIM

Question 22. Open the files 1ALC and 4LYZ

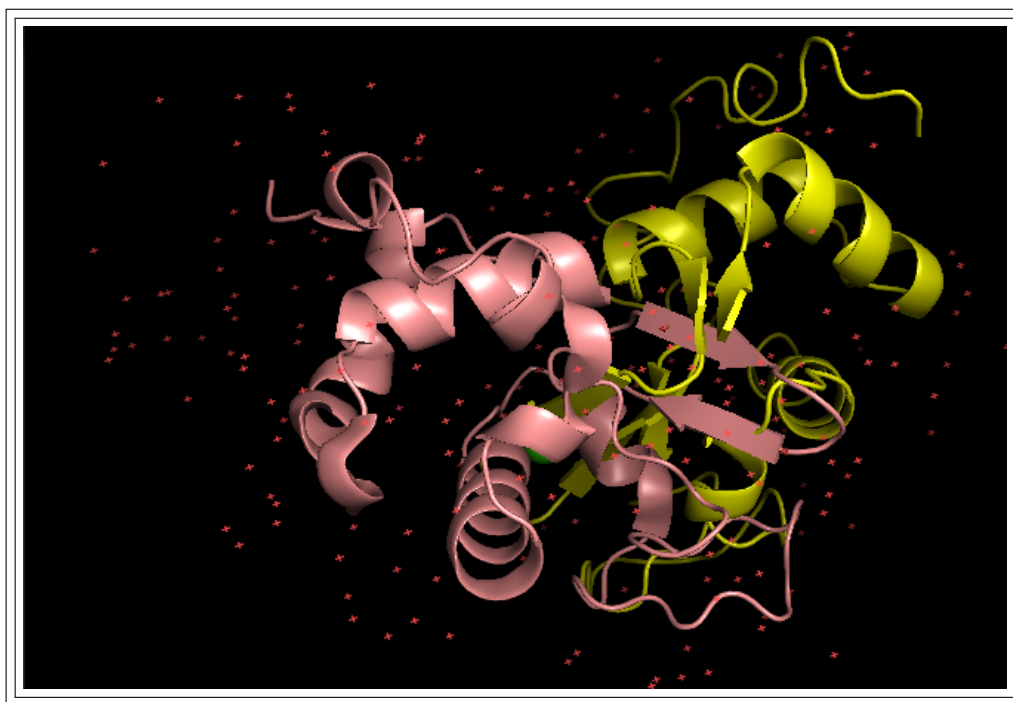**Solution.** Both the PDB files have been opened and the image is below:

FIGURE 26. PDB files of 1ALC and 4LYZ

Question 23. Align the structures
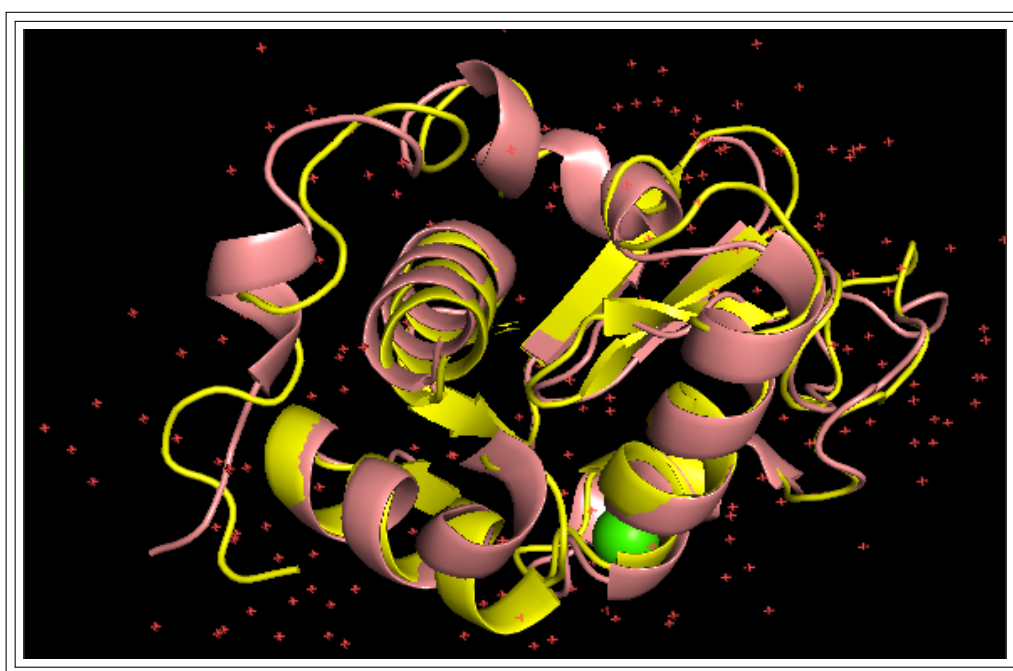
Solution. The aligned structure is shown below:

FIGURE 27. Aligned PDB files of 1ALC and 4LYZ

Question 24. Compute rmsd

Solution. The RMSD for the given aligned sequences is **0.964**

FIGURE 28. RMSD for aligned PDB files of 1ALC and 4LYZ

Question 25. Save the aligned protein structures

Solution. The link to the saved image is Aligned_1ALC_4LYZ

Question 26. Download a protein structure with ligand(s). Identify the ligand and select residues within 4 Å. Show any one type of interaction between them.

Solution. 19 residues are present within 4A. The images for above are shown below:

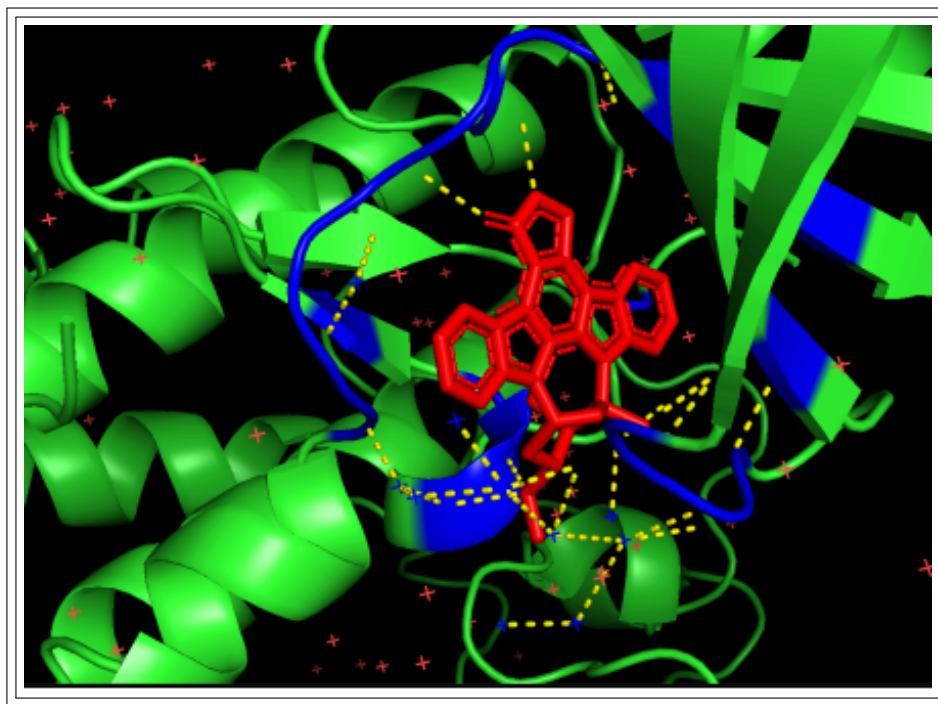FIGURE 29. PDB of AQ1

FIGURE 30. Ligand in AQ1

FIGURE 31. AQ1 polar contacts

Question 27. Mutate any one of the active site residues and describe the change in the interaction with the ligand before and after the mutation.

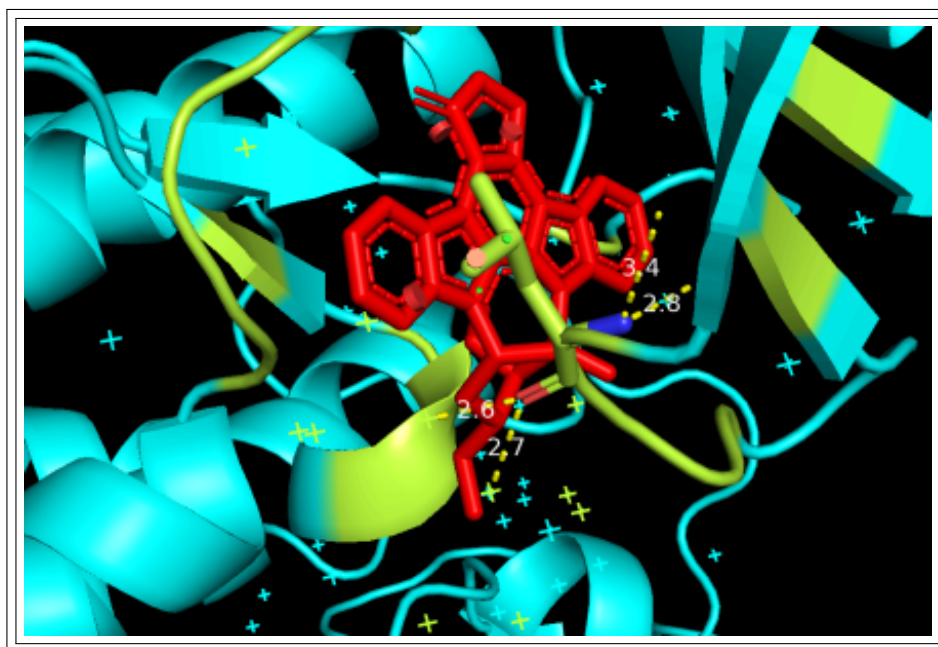**Solution.** Below is the image after mutation of an active site. The mutation is:
I10 ->L10

FIGURE 32. Mutation I10 ->L10