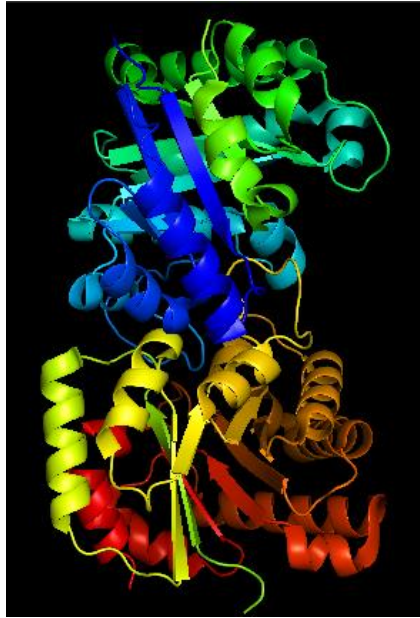# BT3040 – BIOINFORMATICS – Assignment 11
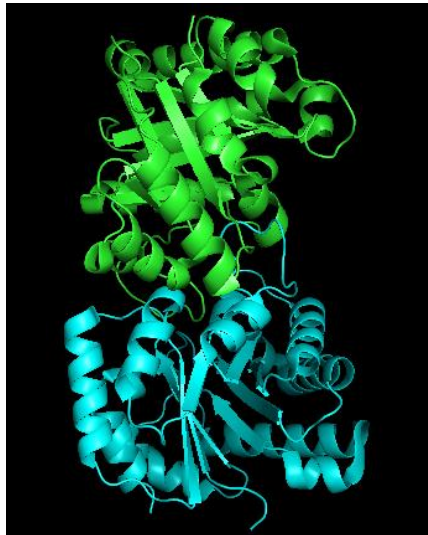
Submitted by Sahana (BE17B038)

Question 1 & 2– Get PDB files and Open the file 1TIM and show in cartoon style (hide line style)

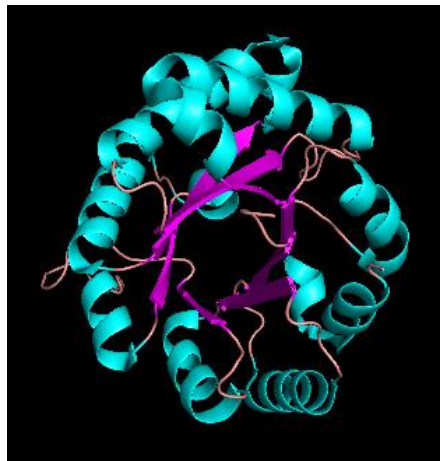**Question 3 -** Give different colors for different chains. How many chains are there?
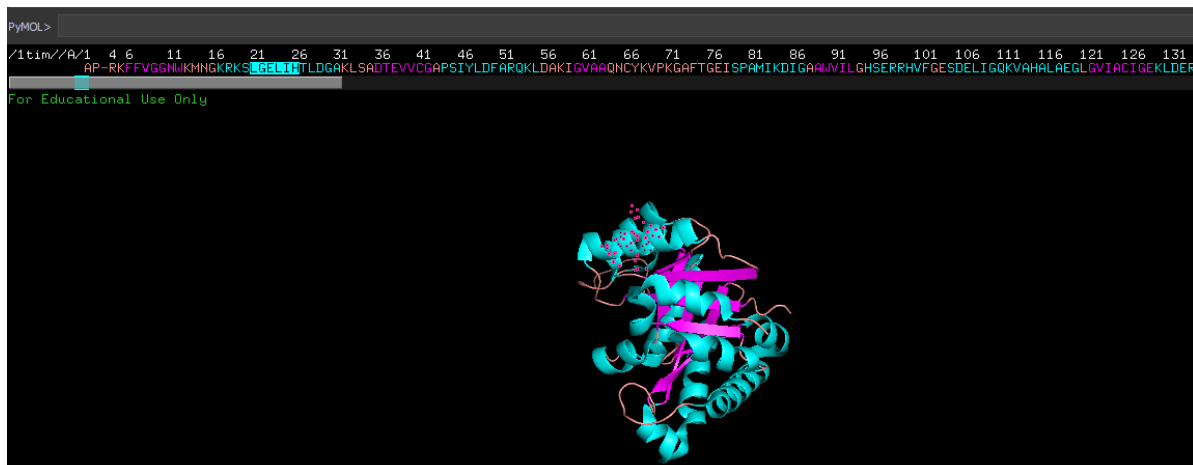
There are 2 chains.

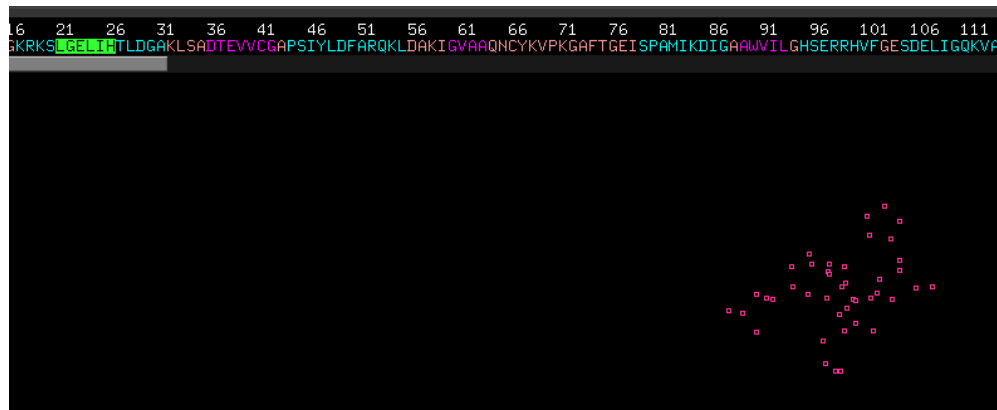**Question 4 -** Remove one chain (right click on the chain and hide)

Question 5 & 6- Identify the secondary structures with different colors and Zoom and rotate to get complete views
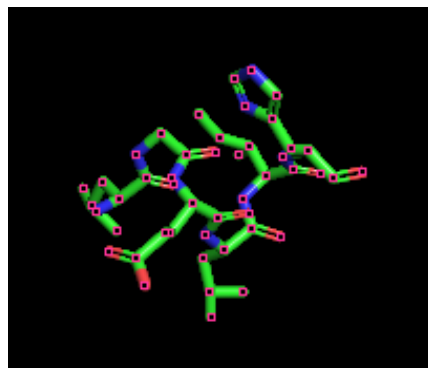

Question 7 & 8- Show the sequence and Select the residues 21 to 26: LGELIH
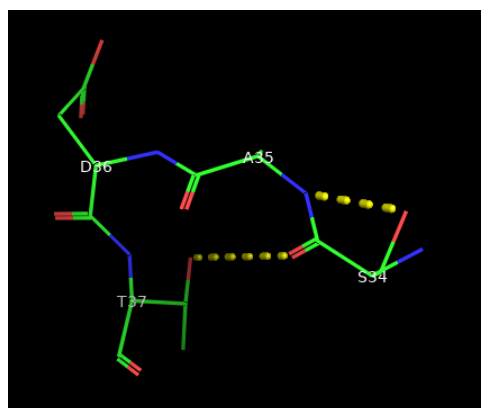
Question 9 - Hide cartoon diagrams

Question 10 - Color the selected residues based on different atoms


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


Salt bridge or an ionic bond is a bond between oppositely charged species. Here, the identified salt bridge is between N atom of Alanine35 and OH in the side chain Serine34.

Question 12 - Identify any hydrophobic interaction / aromatic stacking interaction protein and list the details of interaction.
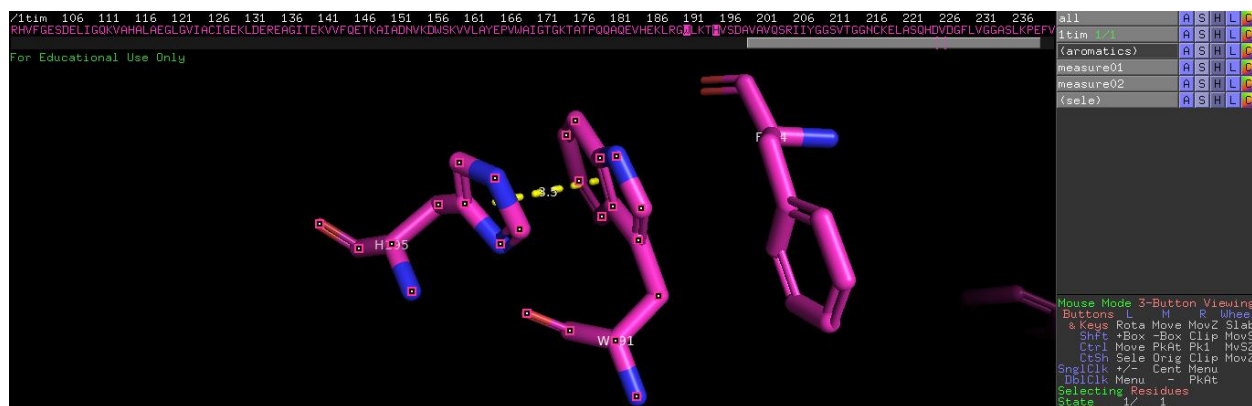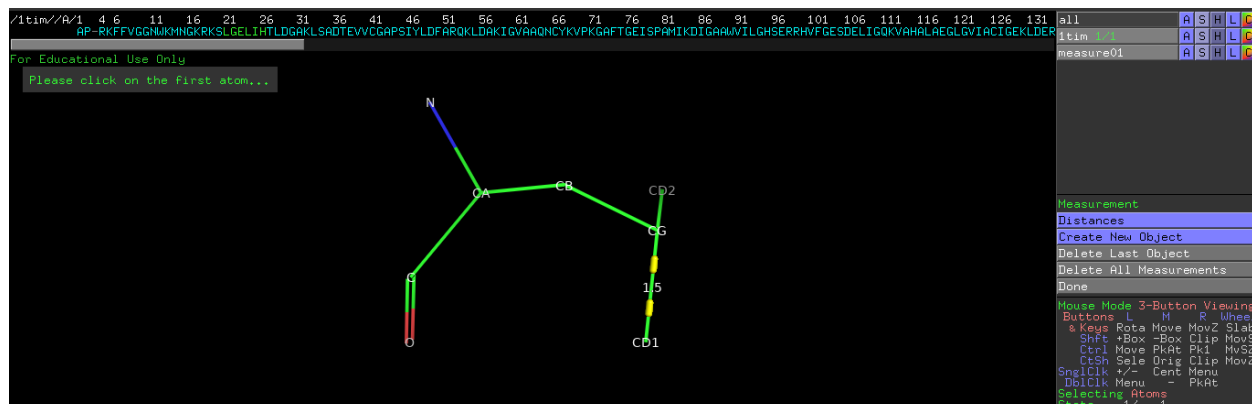
The hydrophobic interaction is between Tryptophan (191) and Histidine (195). The distance between the two rings is 3.5 A^0. This makes the interaction possible.

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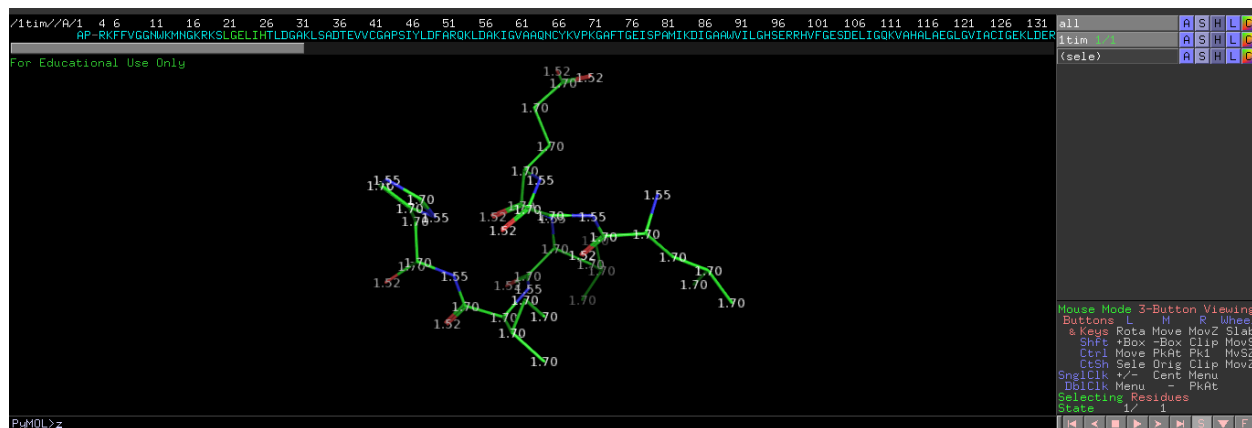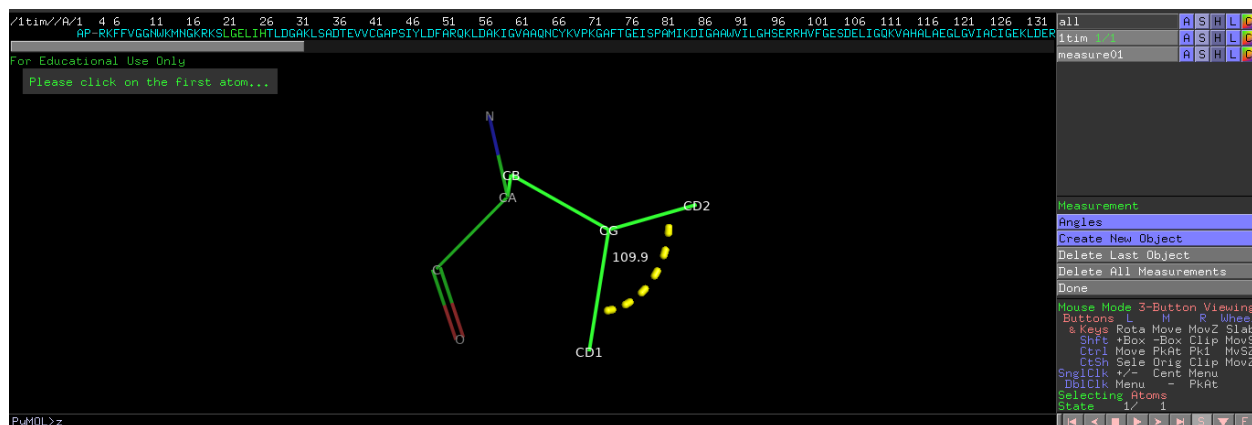

Question 14 - Compute the distance between CG and CD2 in Leu24
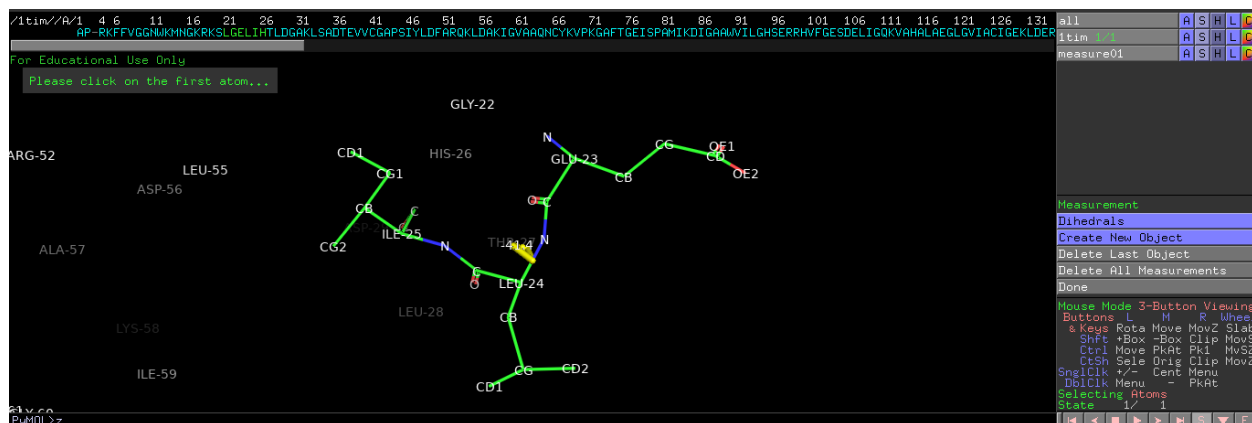

Answer = 1.5 Angstroms

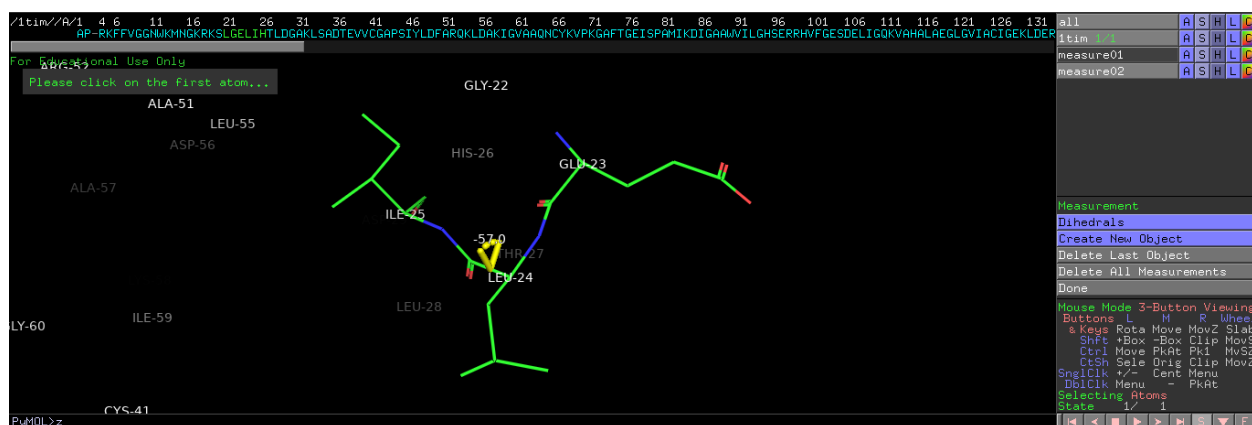**Question 15 -** Compute the angle formed by the atoms CD1, CG and CD2 in Leu24.

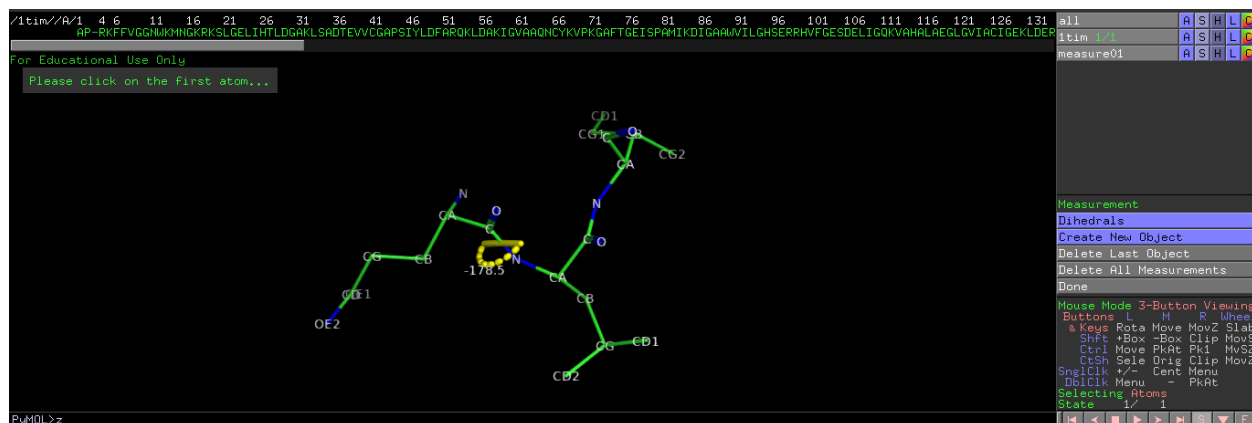**Question 16 -** Compute the dihedral angles of Leu24
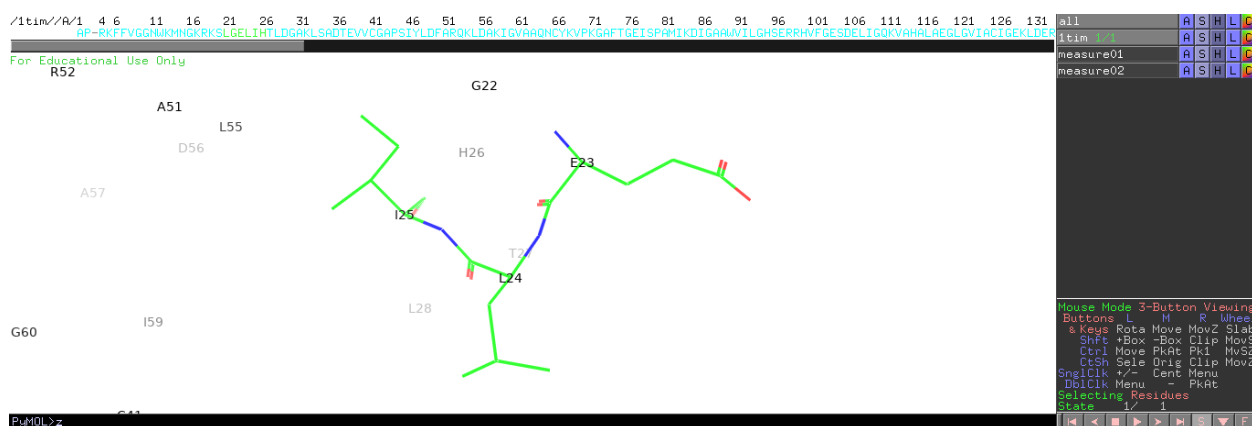
Phi value = -41.4 degrees

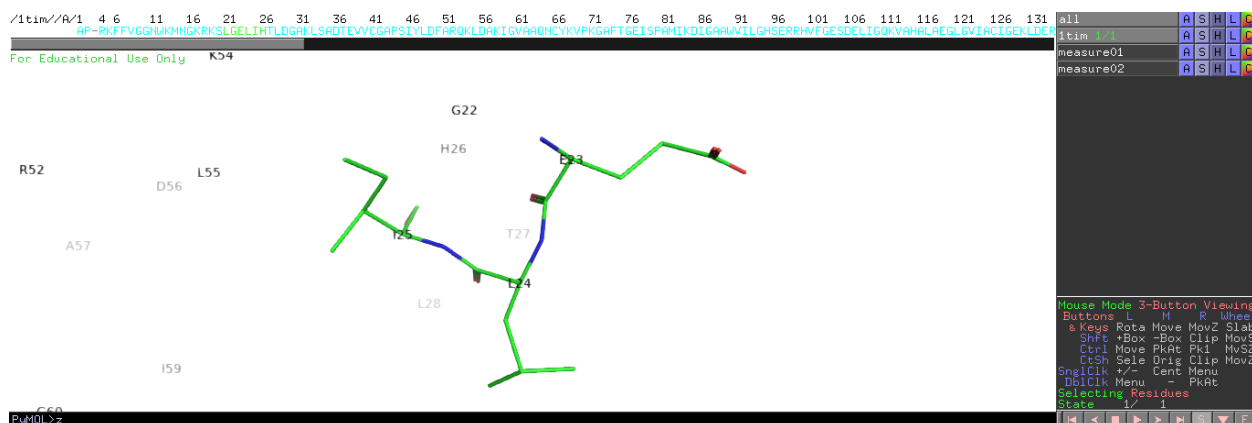Psi value = -57.0 degrees

Omega value = -178.5 degrees

Question 17 - Change background white

Question 18 - Make high quality picture (use ray)

Display -> Quality -> Maximum quality

Question 19 - Show B-factors to see flexible and rigid regions (color by spectrum, b-factor)
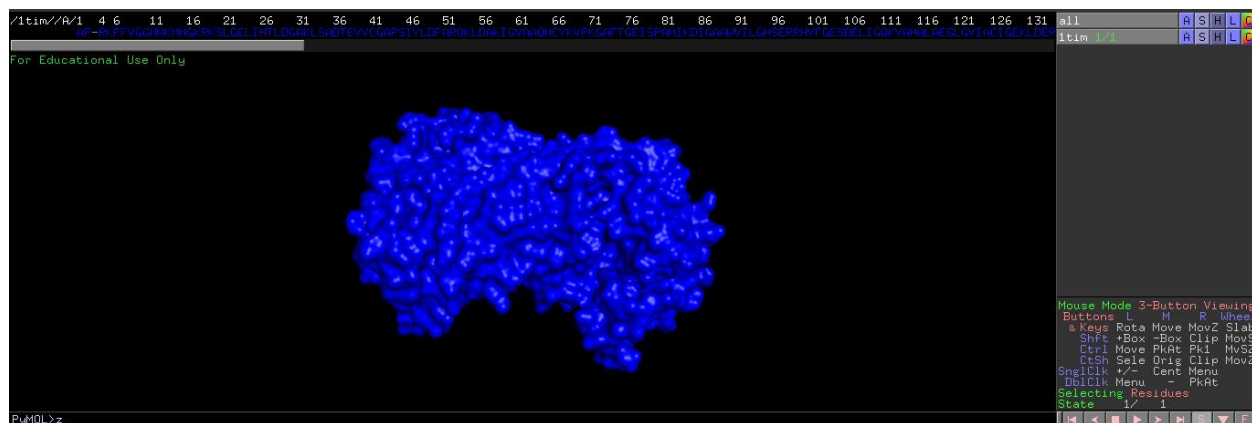
Question 20 - Compute the electrostatic potential (A -> generate -> vacuum statistics -> protein contact potential) (screenshot is shown)

Question 21 - Save the image in PNG format

File -> Export image as -> PNG -> Save PNG as

Question 22 - Open the files 1ALC and 4LYZ

Question 23 & 24 & 25- Align the structures and Compute RMSD and Save the aligned protein structures.
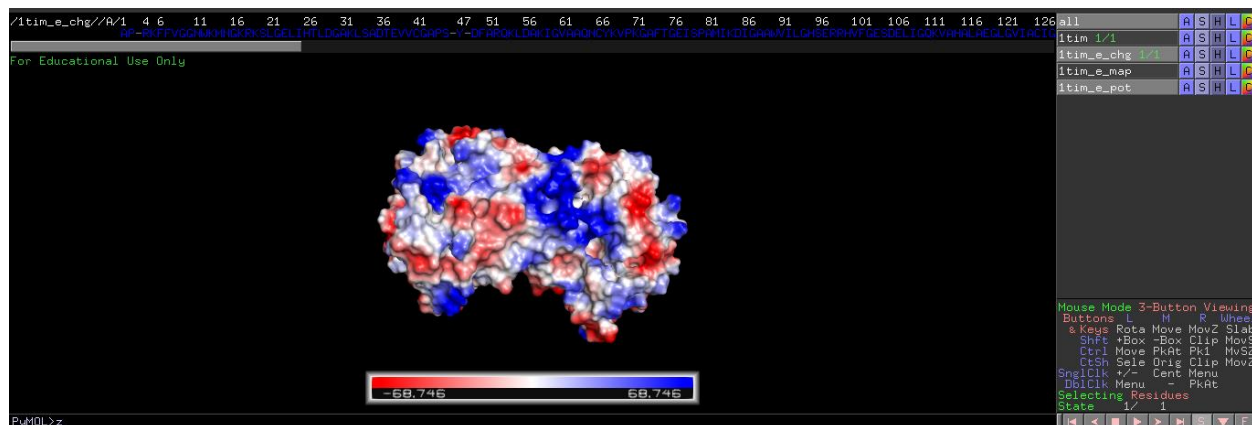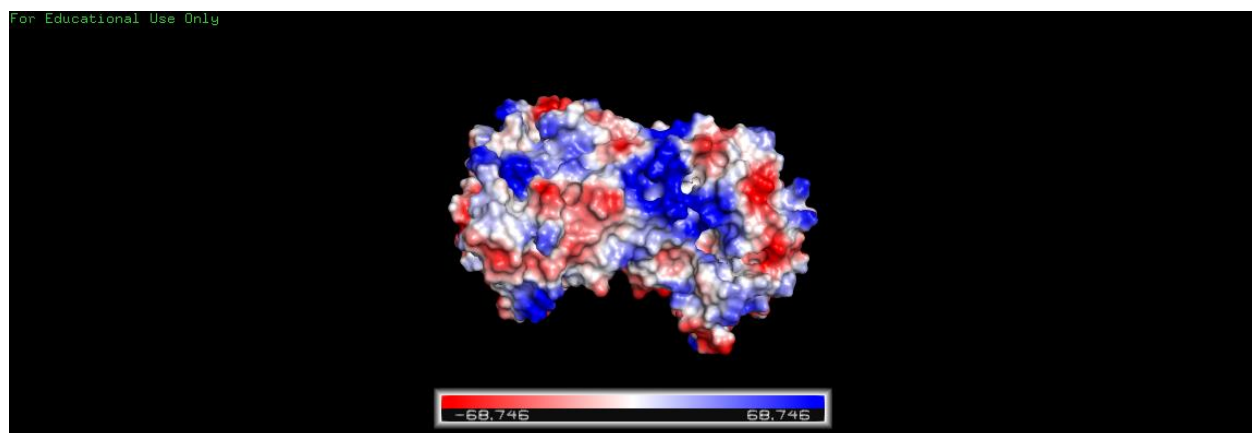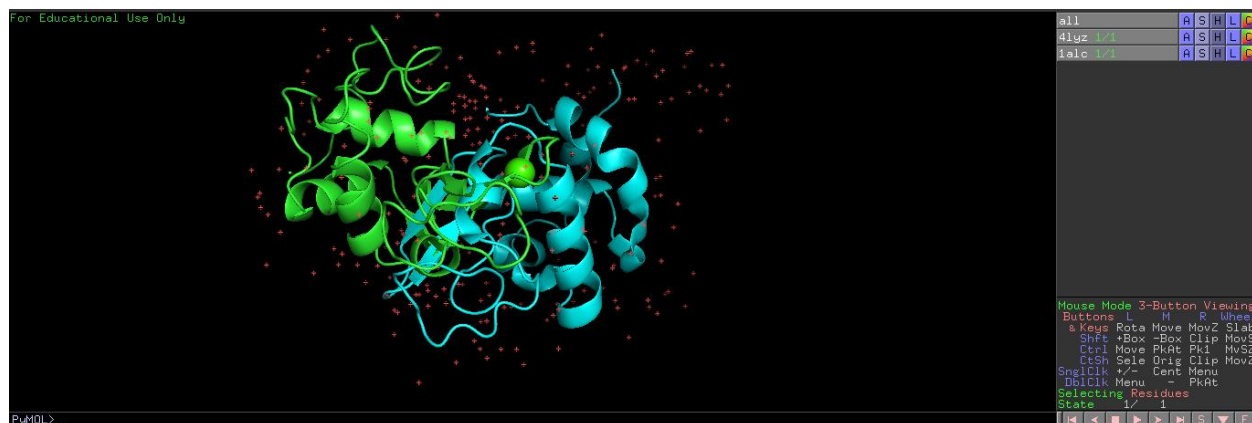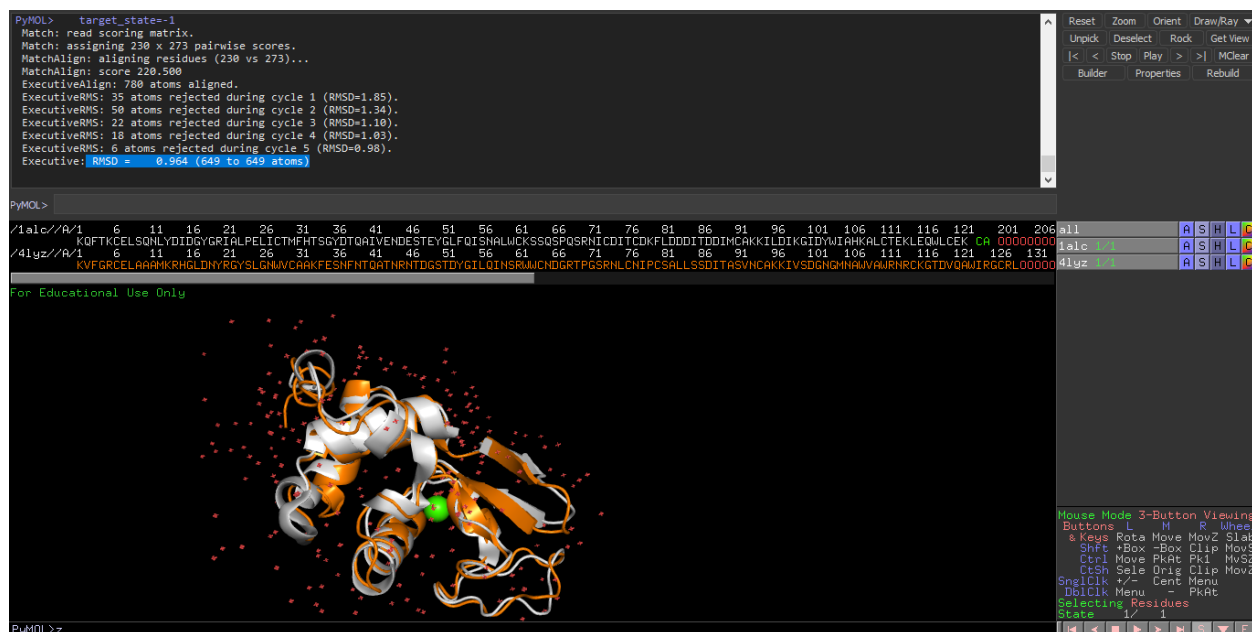

RMSD of 1ALC and 4LYZ = 0.964 (649 to 649 atoms)

Question 26 – Download a protein structure with ligand(s). Identify the ligand and select residues within 3.5Å. Show any one type of interaction between them.

Protein – 1MBO

Action -> Preset -> Ligand sites -> Sticks (This will result in ligand being in sticks and everything else in cartoon representation. It will also show the interactions that are less than 3.5 A^0 in length.

Show -> Labels (Will show the dimension of each interaction.

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

Position 64 is initially Histidine.

It makes 2 ionic contacts with oxygen atoms (ligand) and 2 hydrogen bonds with HOH(341) and HOH(223).

The ligand O2 has the following interactions – One H bond with a nearby water molecule and 2 H bonds with Histidine 64.

H64 is now mutated to Alanine 64.

The surrounding interaction changes to the following
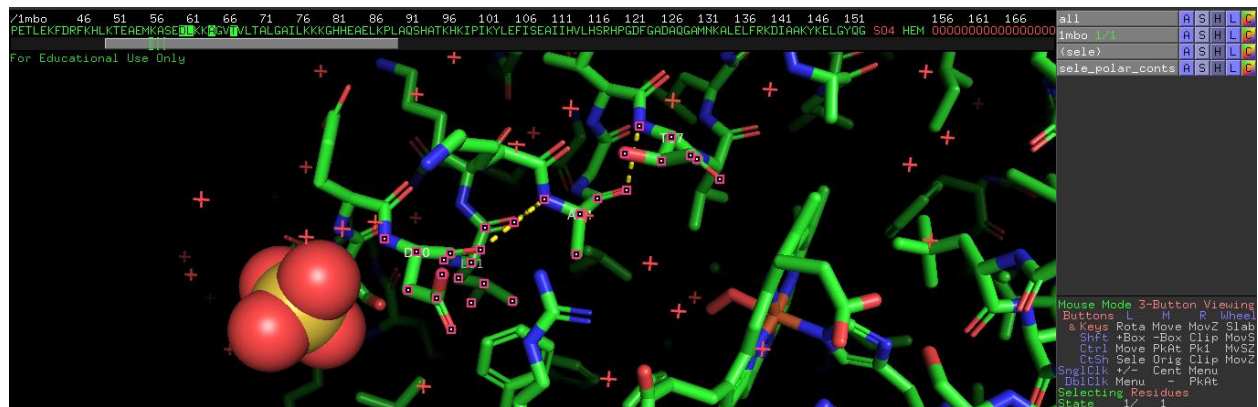
We notice that there are no interactions of Alanine with the oxygen atoms anymore. Also, the ligand O_2's interactions also get restricted to only 1 H bond with a neighbouring water molecule.