BT 3040: BIOINFORMATICS

Assignment 12

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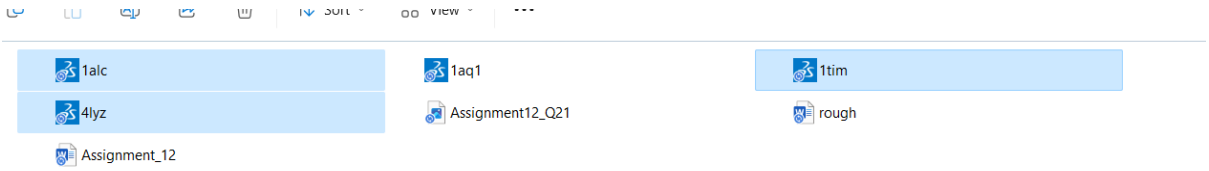
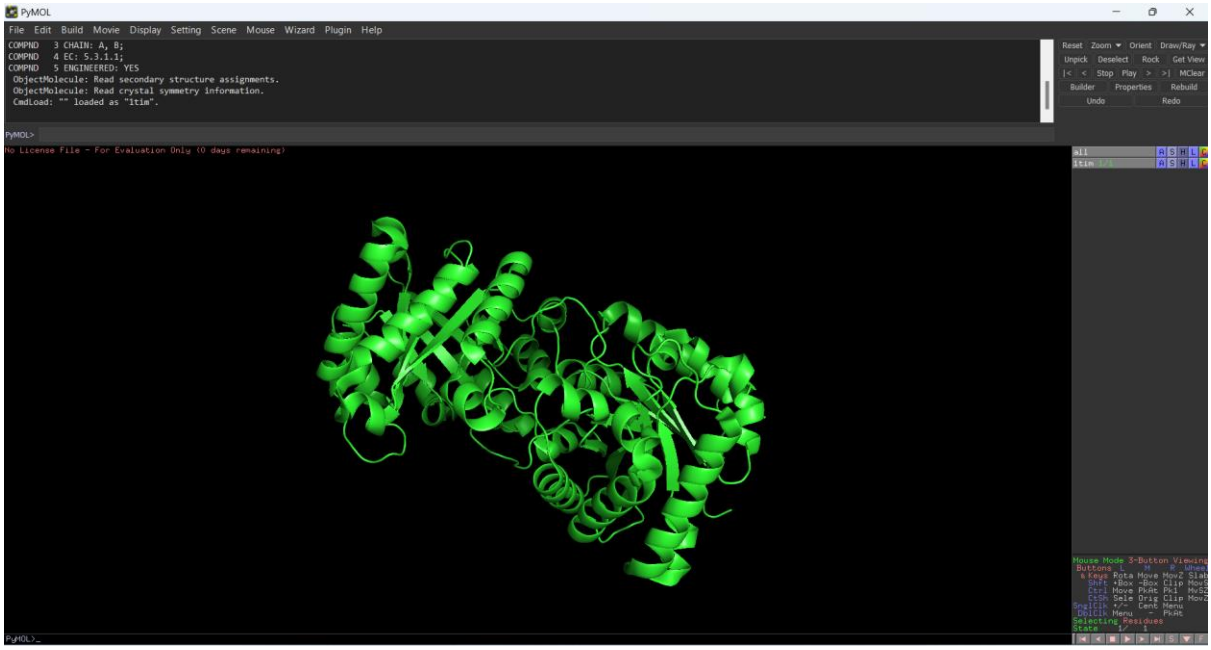
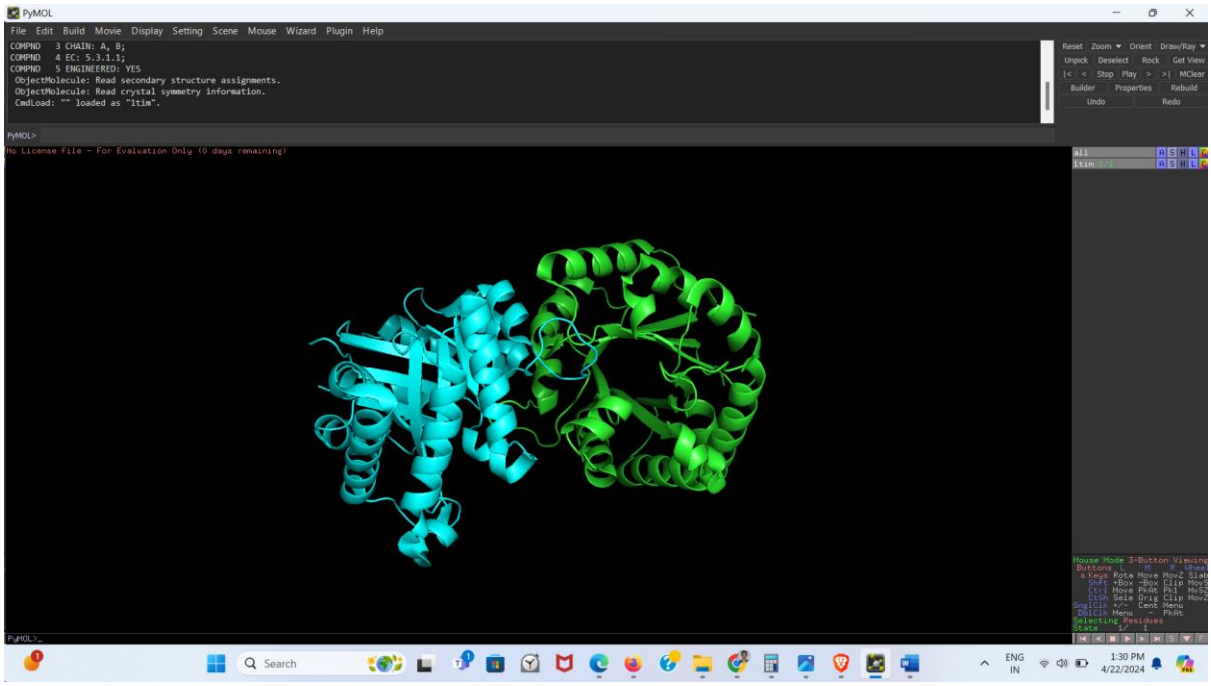
Q1) Get the PDB files, 1ALC, 4LYZ and 1TIM



Q2) Open the file 1TIM and show in cartoon style (hide line style)

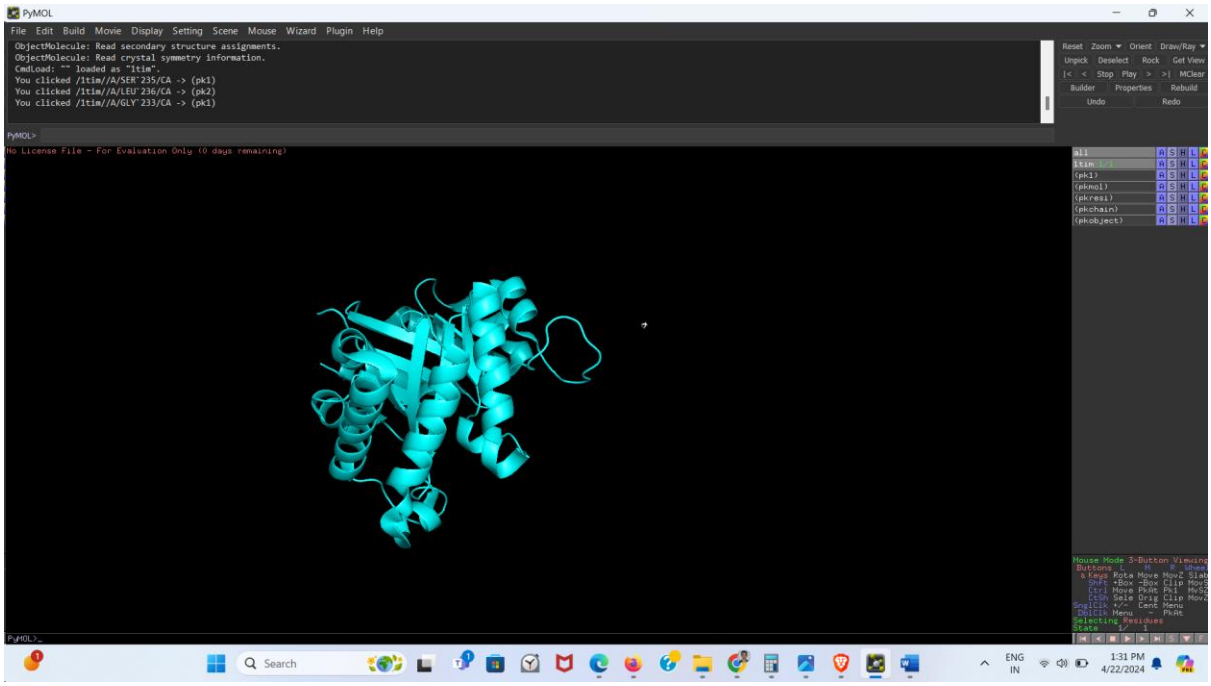


Q3) Give different colours for different chains. How many chains are there?



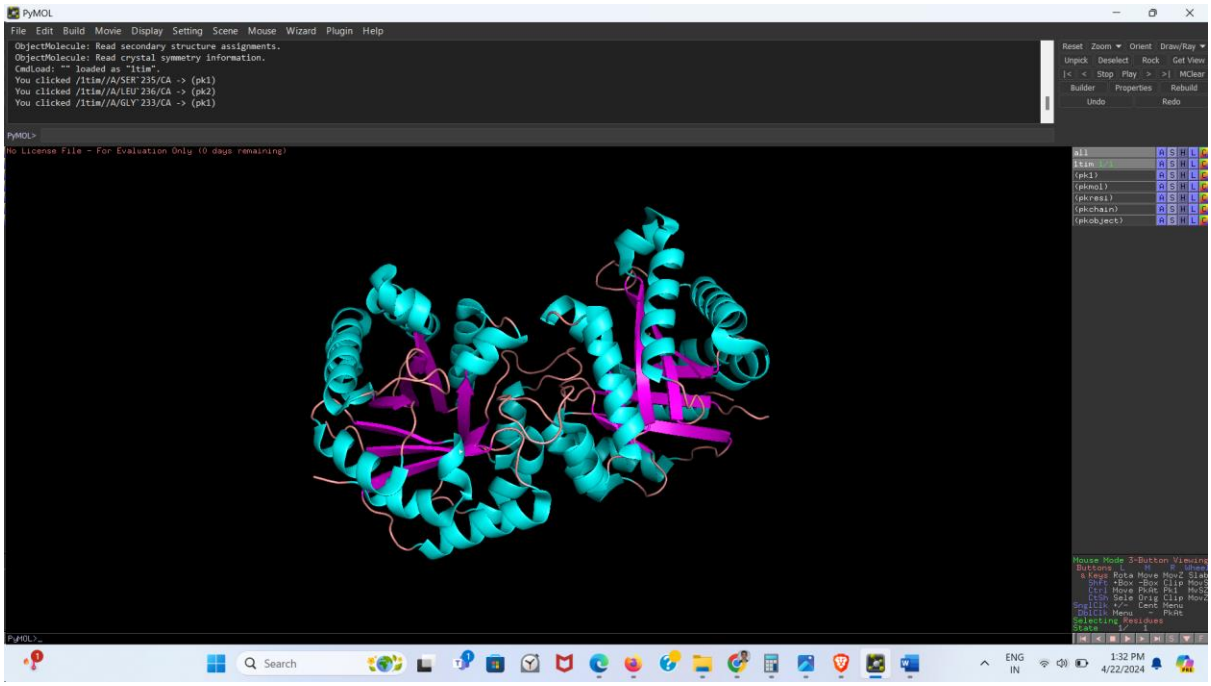
There are **two** chains

Q4) Remove one chain (right click on the chain and hide)



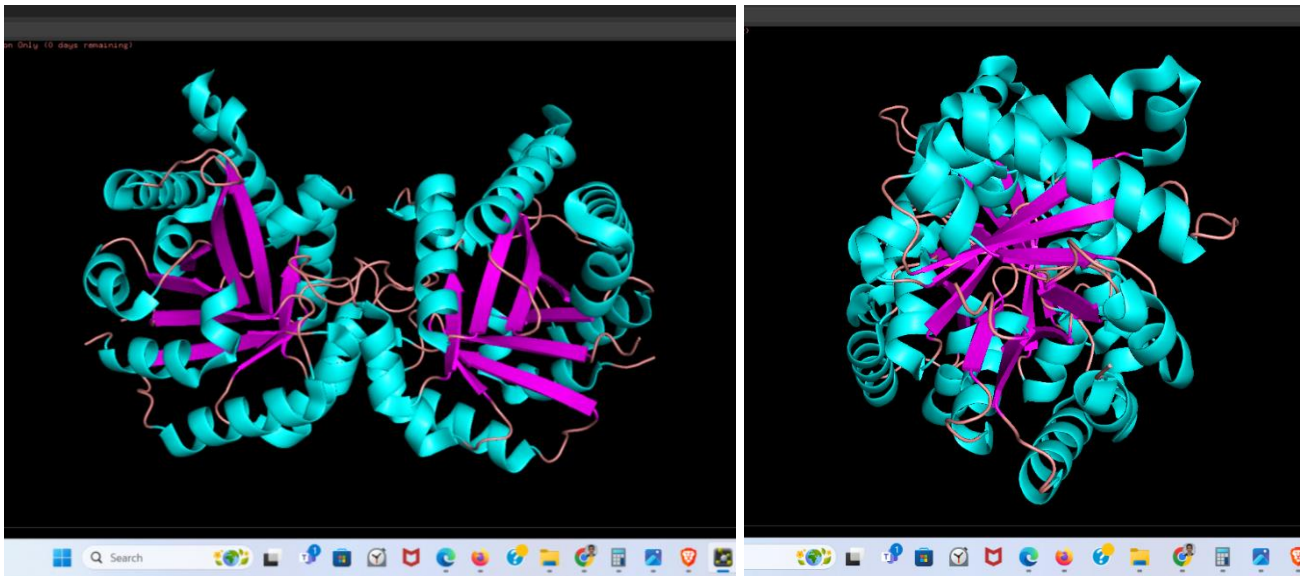
Green Coloured Chain Hidden

Q5) Identify the secondary structures with different colours

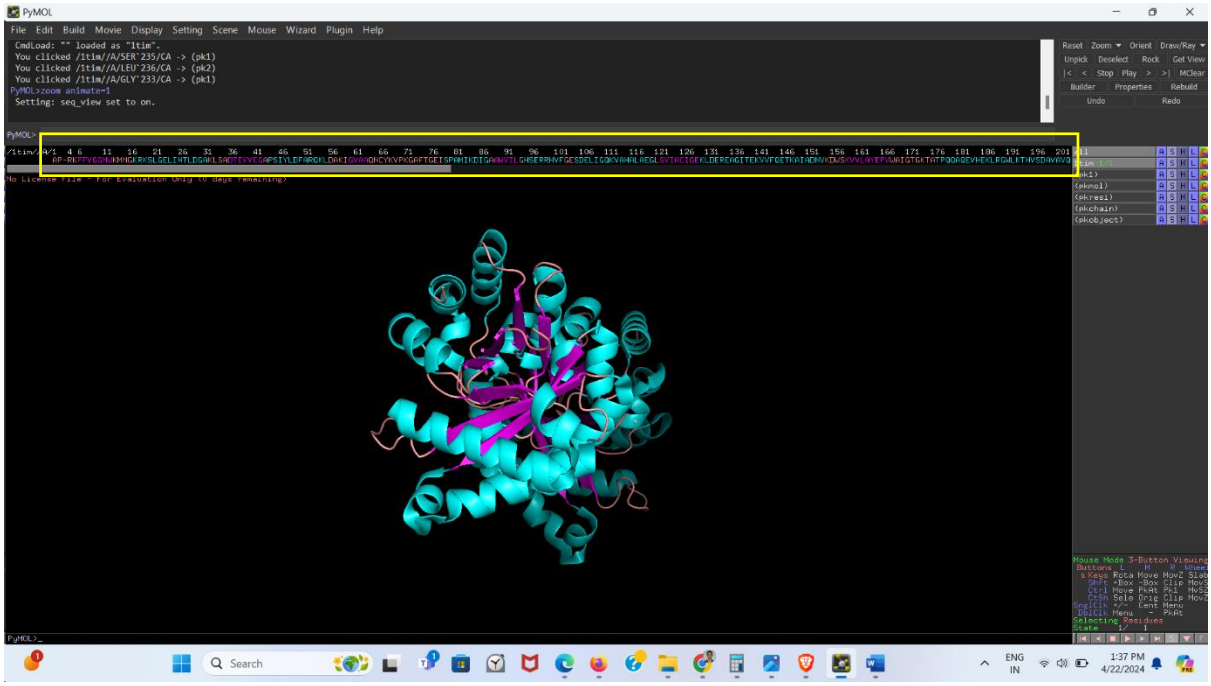


Helix have been represented by Light-Blue, Sheets by Pink and Loops by Orange

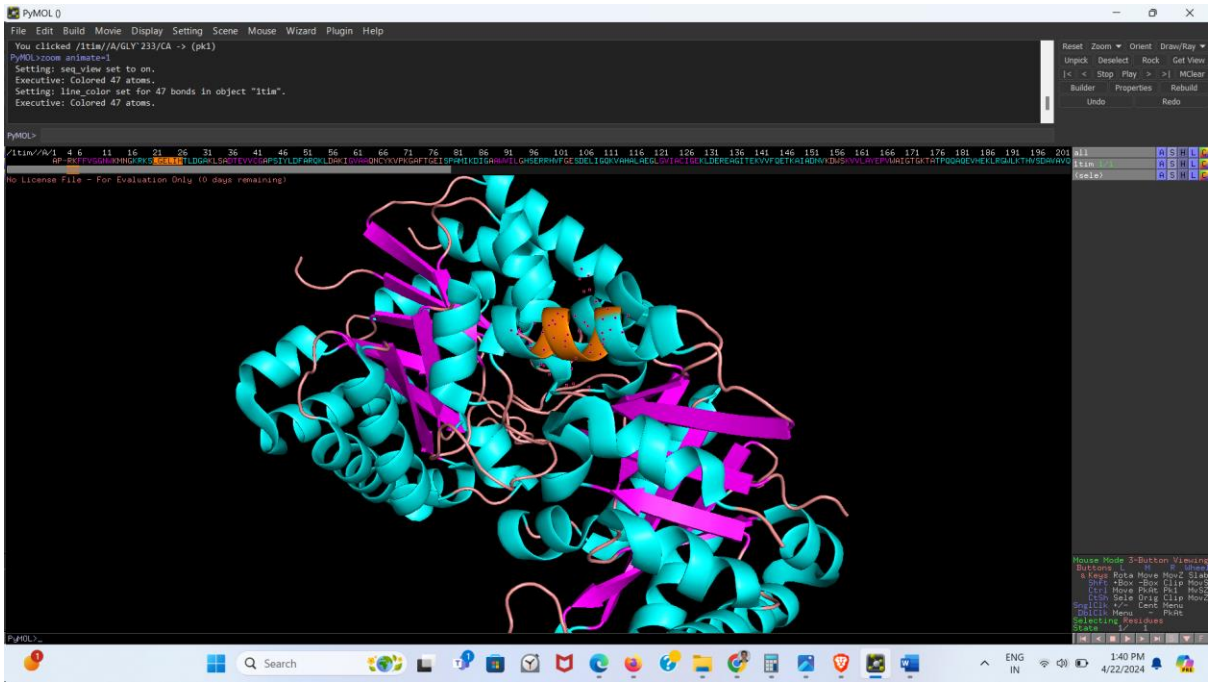
Q6) Zoom and rotate to get complete views



Q7) Show the sequence

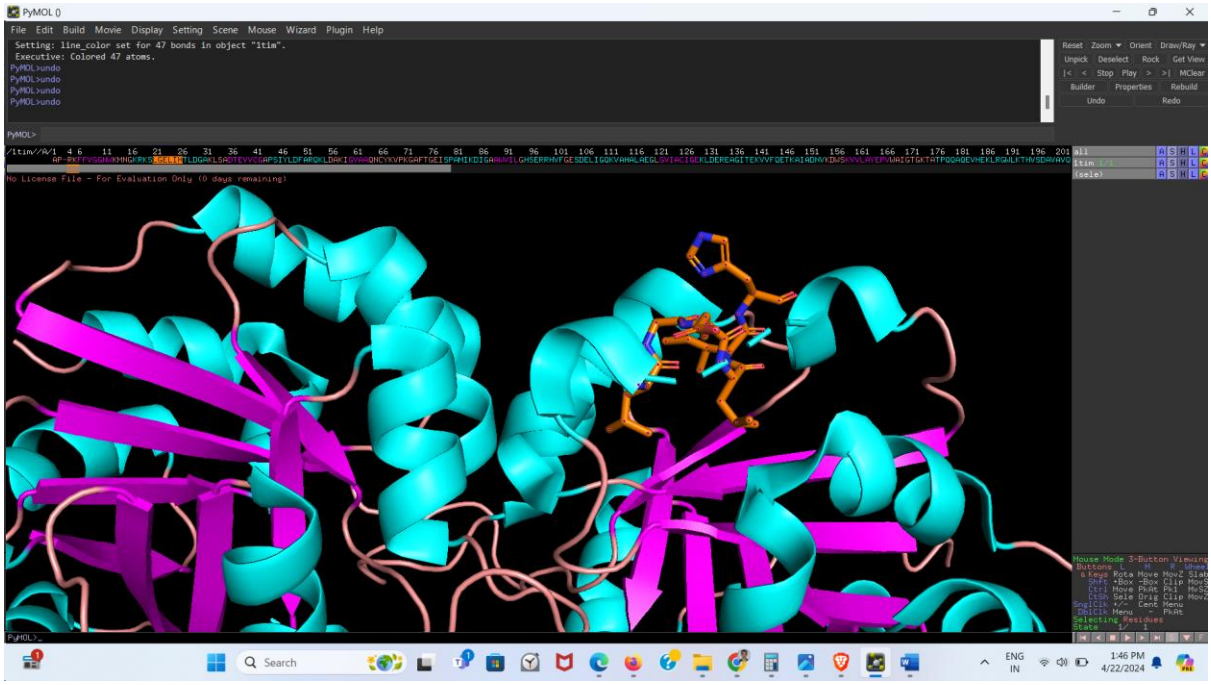


Q8) Select the residues 21 to 26: LGELIH

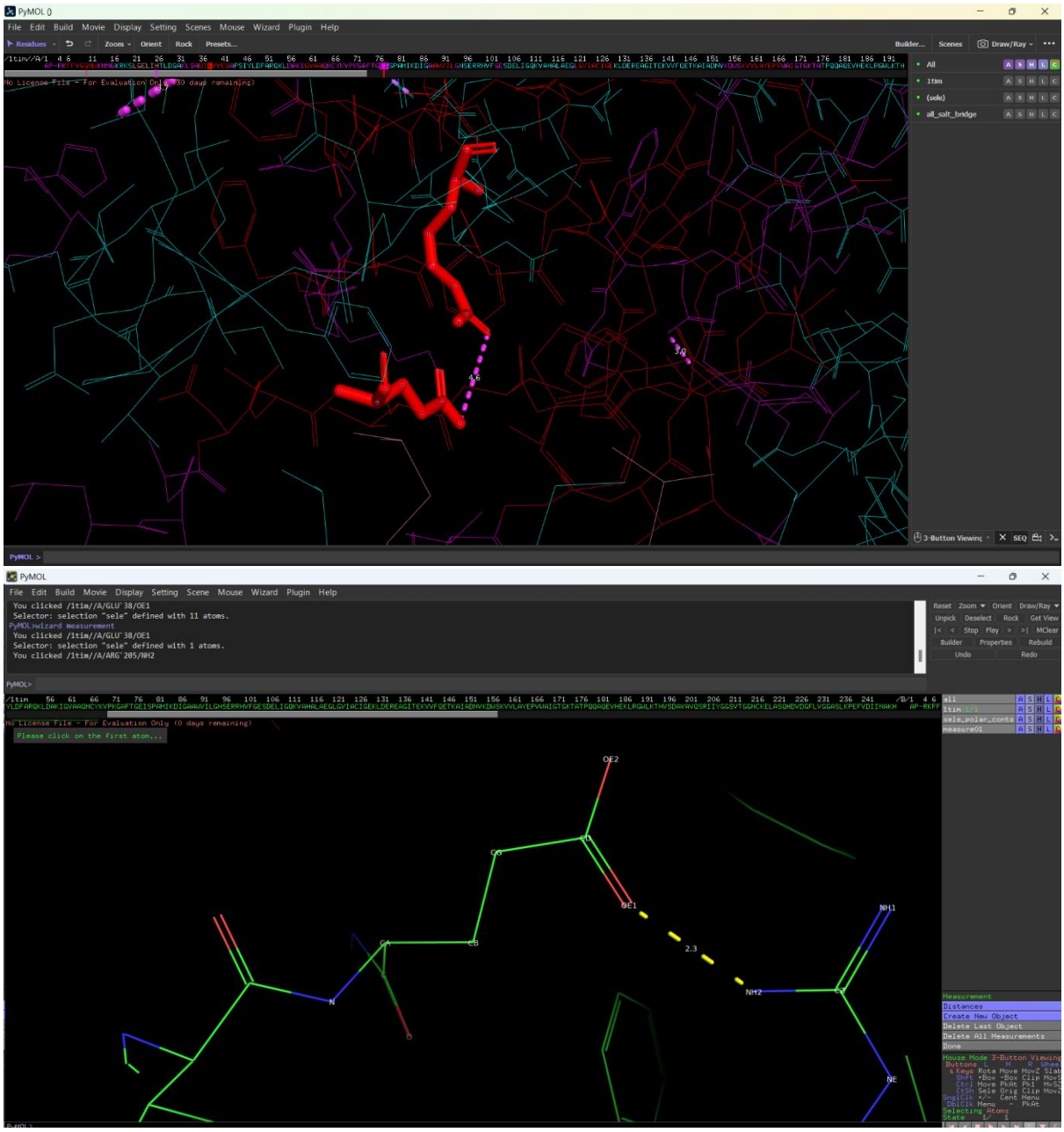


Q9) Hide cartoon diagrams

Q10) Colour the selected residues based on different atoms

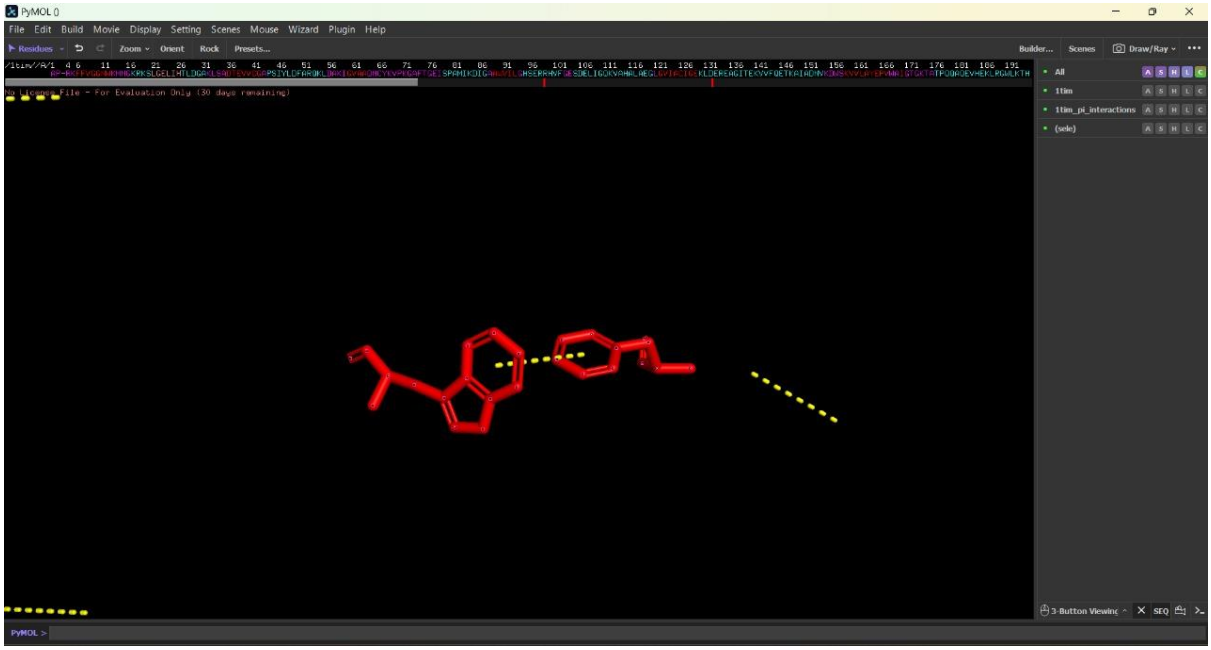


Q11) Identify at least one salt bridge within the protein and list the details of interaction.

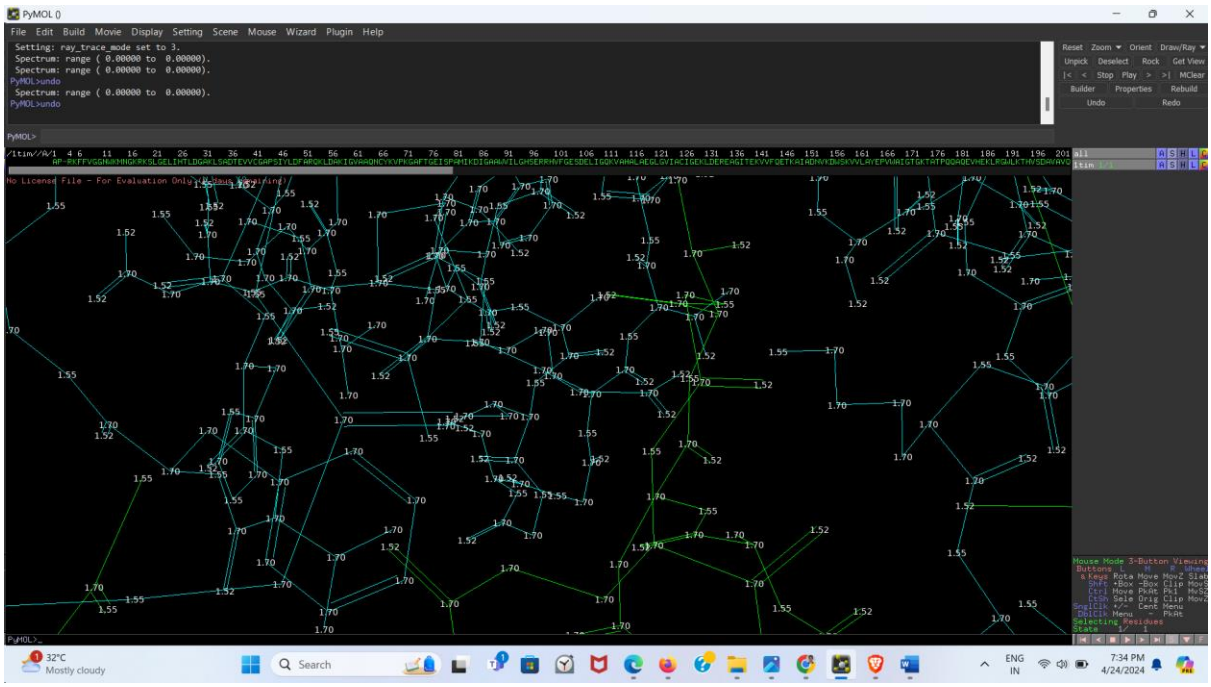


Description: Th interaction is seen between Glutamic Acid (E) at position 36 and Argnine (R) at position 205. The C=O group of Glutamic Acid forms a salt bridge with NH2 group of Arginine. The salt bridge is 2.3 A long.

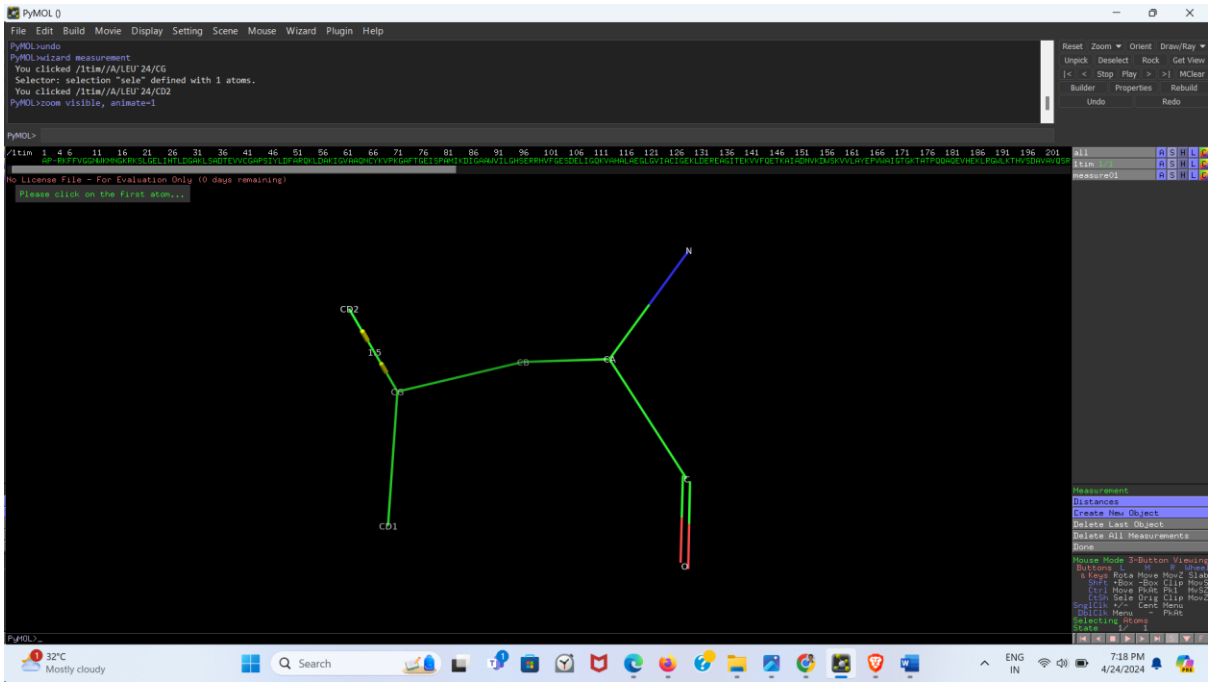
Q12) Identify any hydrophobic interaction / aromatic stacking interaction protein and list the details of interaction.



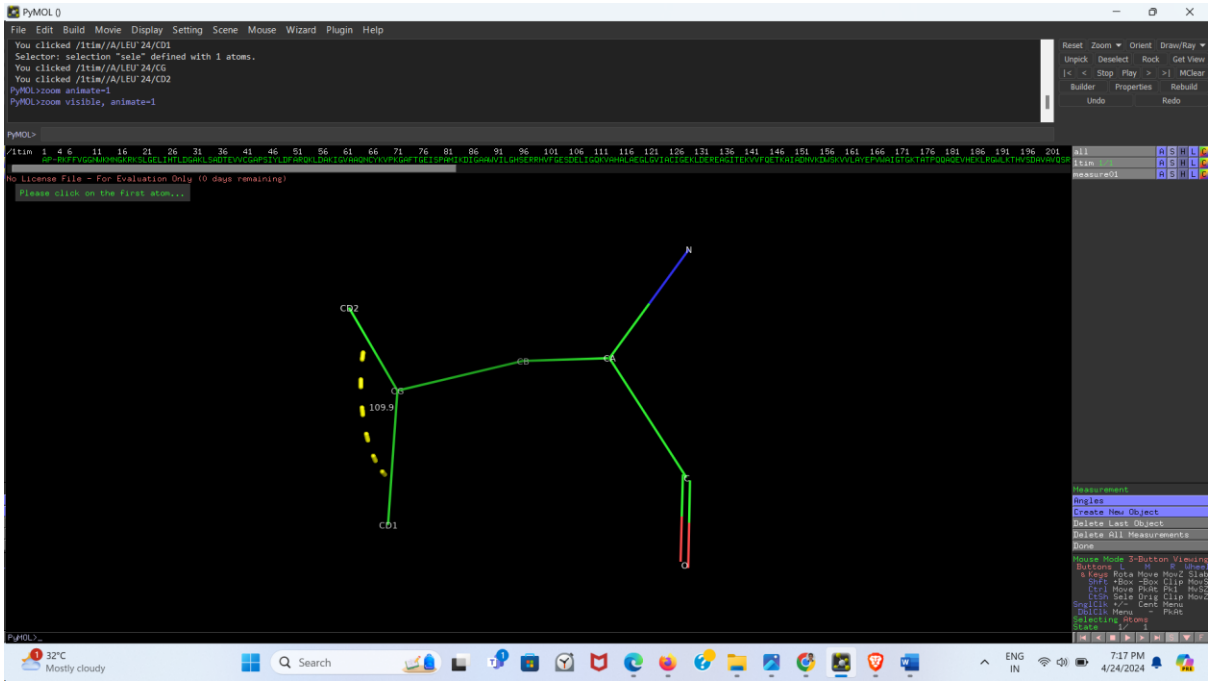
Q13) Label the residues using the atom name and show their van der Waal radii.



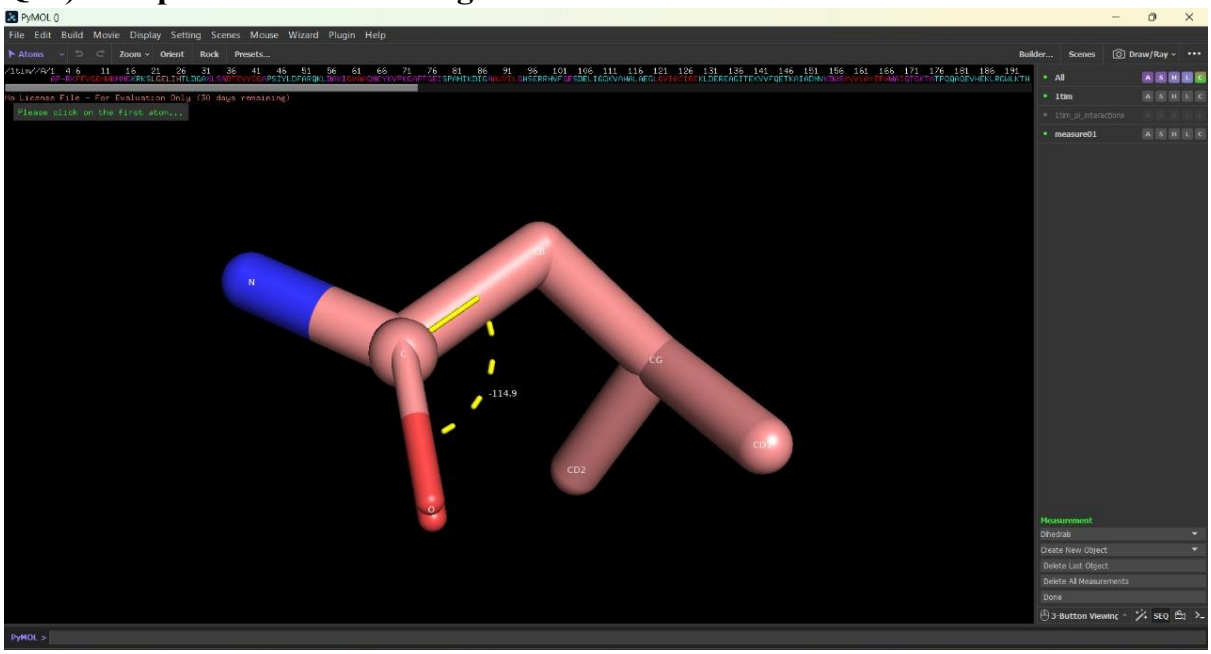
Q14) Compute the distance between CG and CD2 in Leu24



Q15) Compute the angle formed by the atoms CD1, CG and CD2 in Leu24.

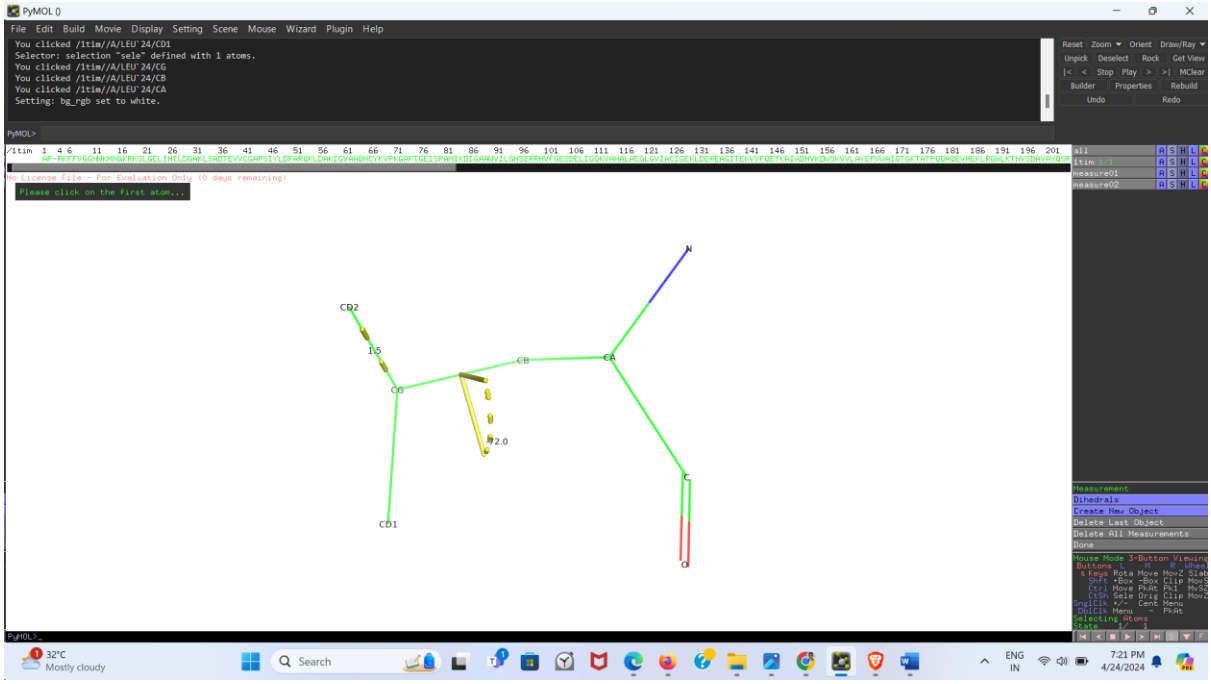


Q16) Compute the dihedral angles of Leu24

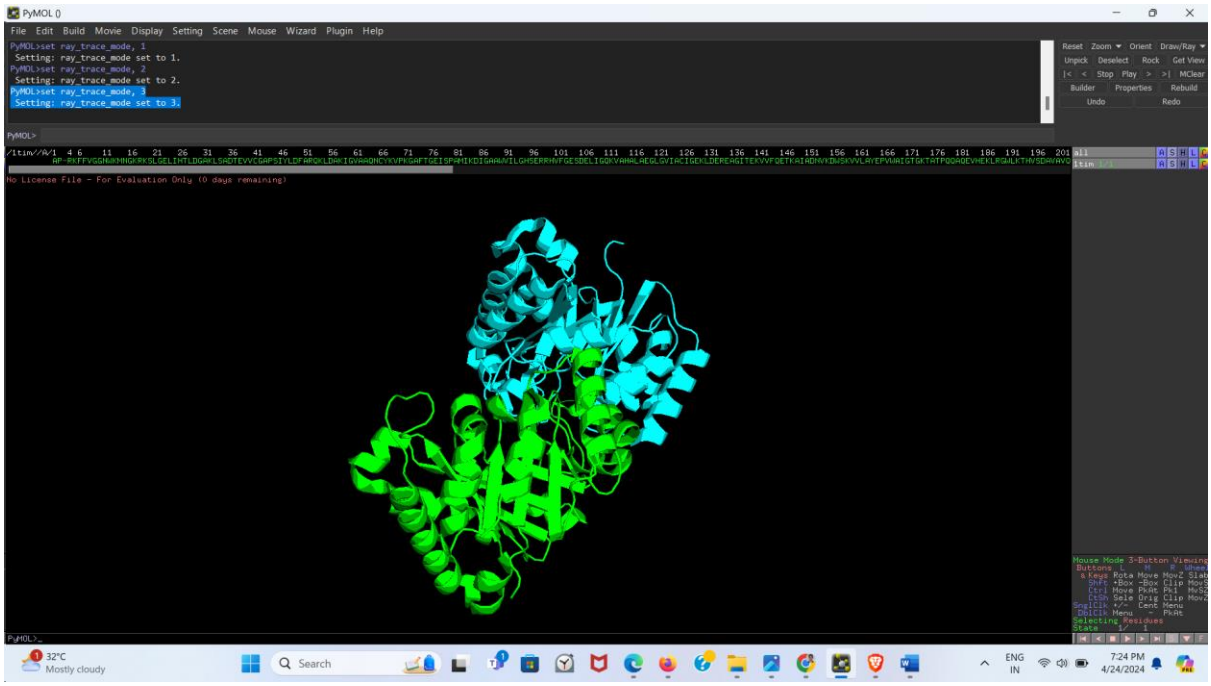


Dihedral Angle: -114.9

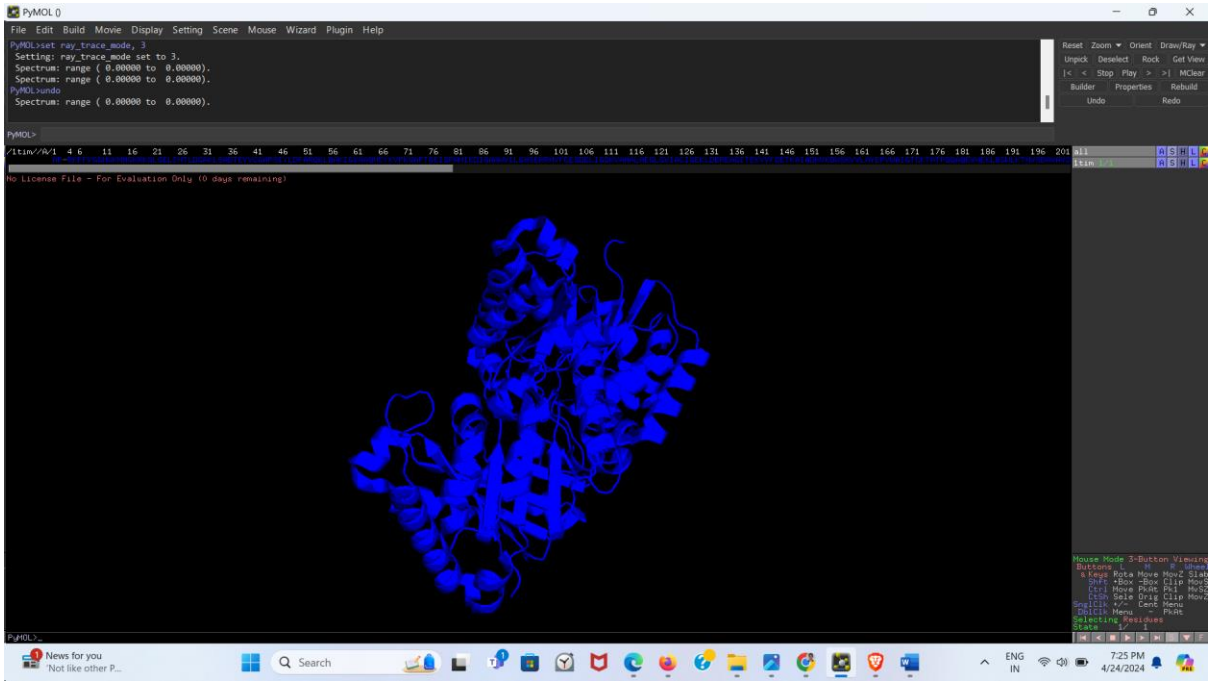
Q17) Change the background to white.



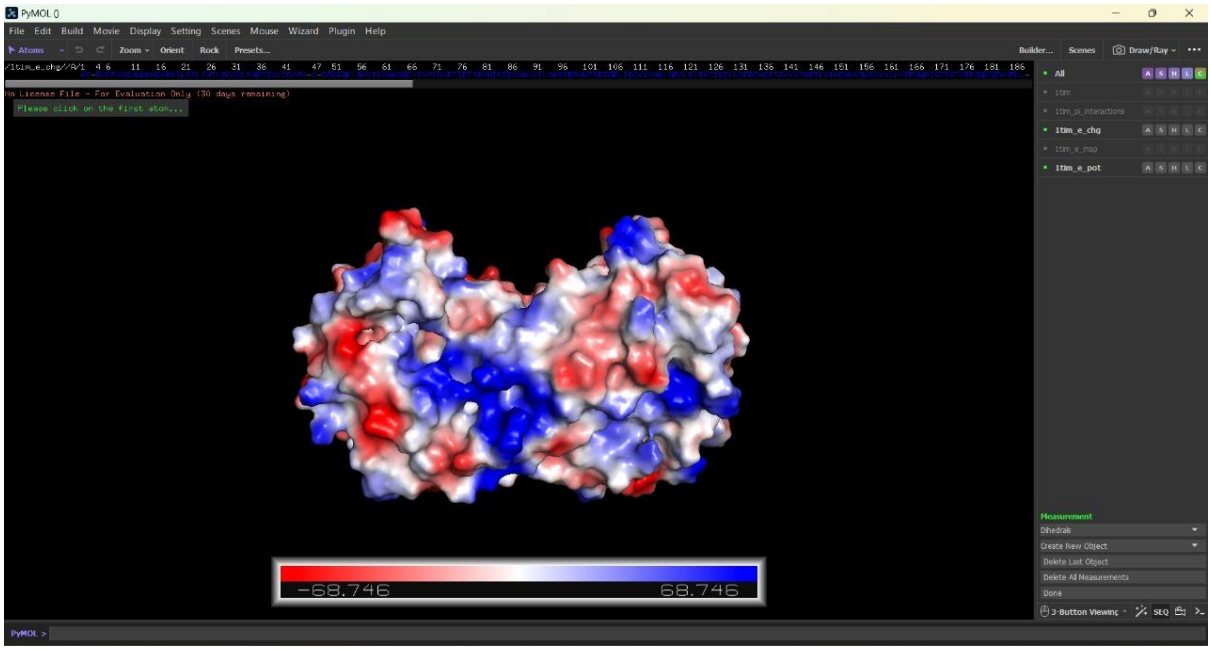
Q18) Make high quality picture (use ray)



Q19) Show B-factors to see flexible and rigid regions (color by spectrum, b-factor)



Q20) Compute the electrostatic potential (A -> generate -> vacuum statistics -> protein contact potential)



Q21) Save the image in PNG format

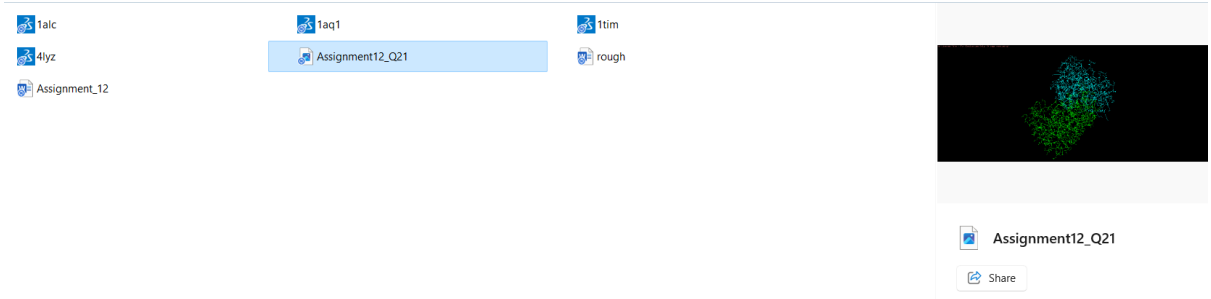
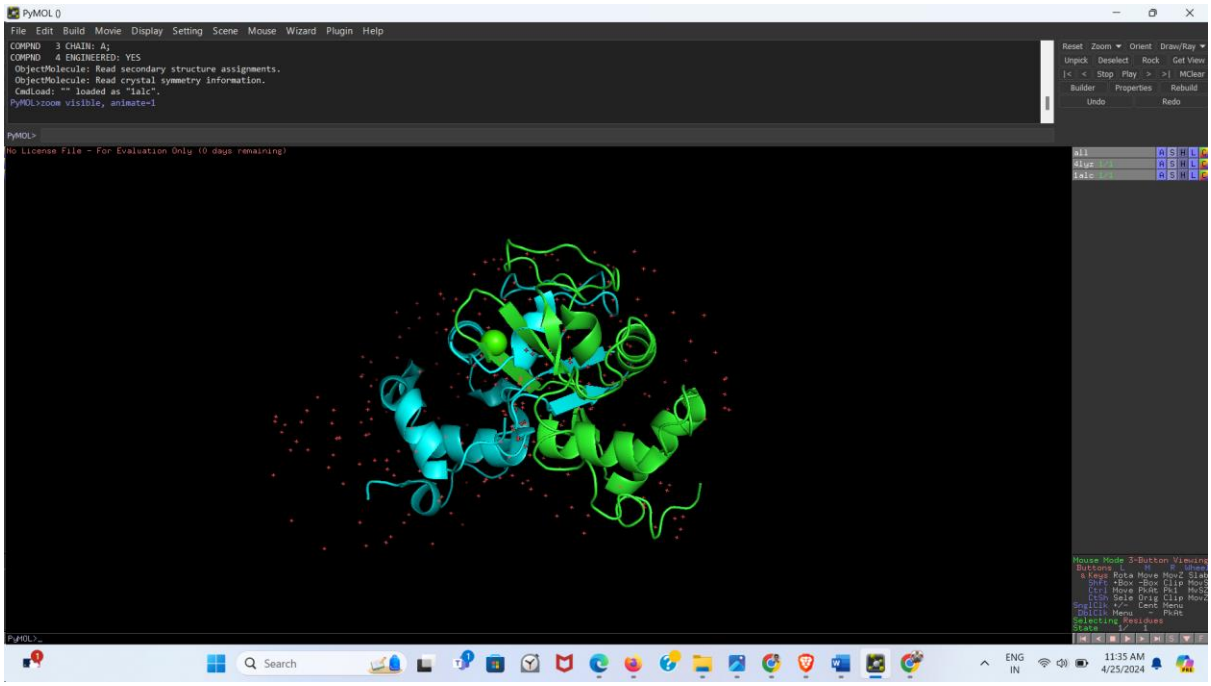
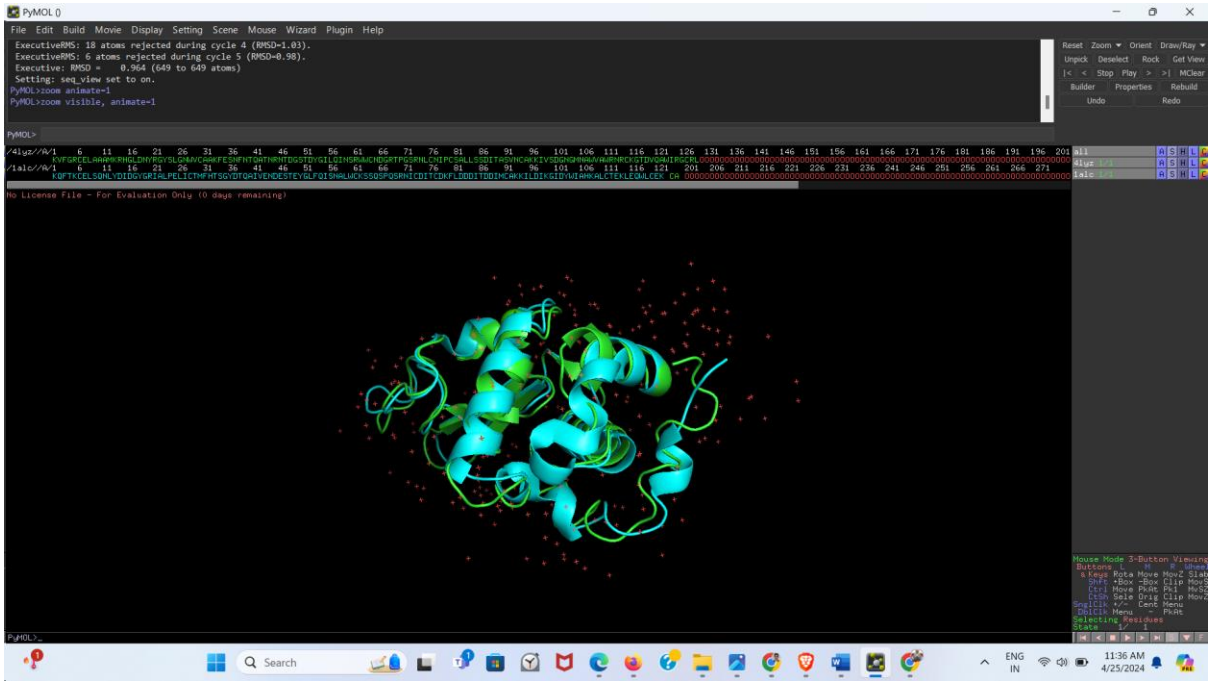


Image saved with file name ‘Assignment12_Q21.png’

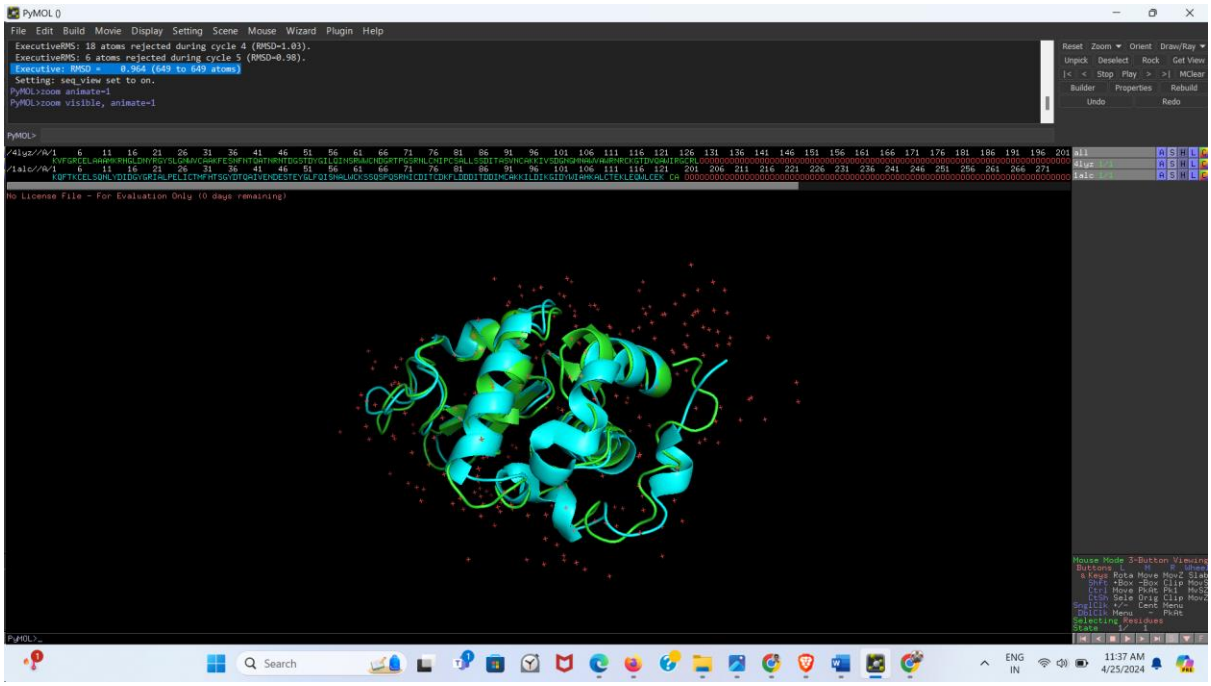
Q22) Open the files 1ALC and 4LYZ



Q23) Align the structures

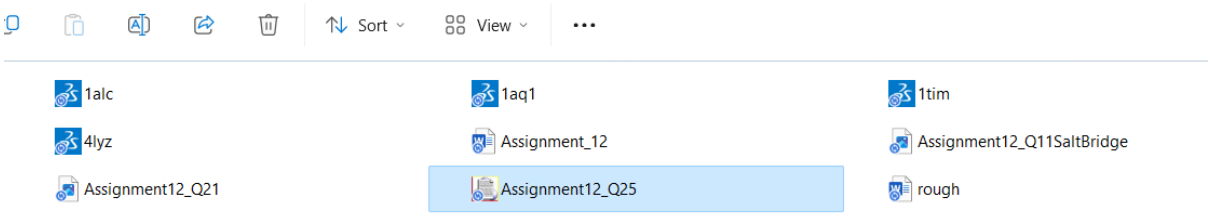


Q24) Compute RMSD.



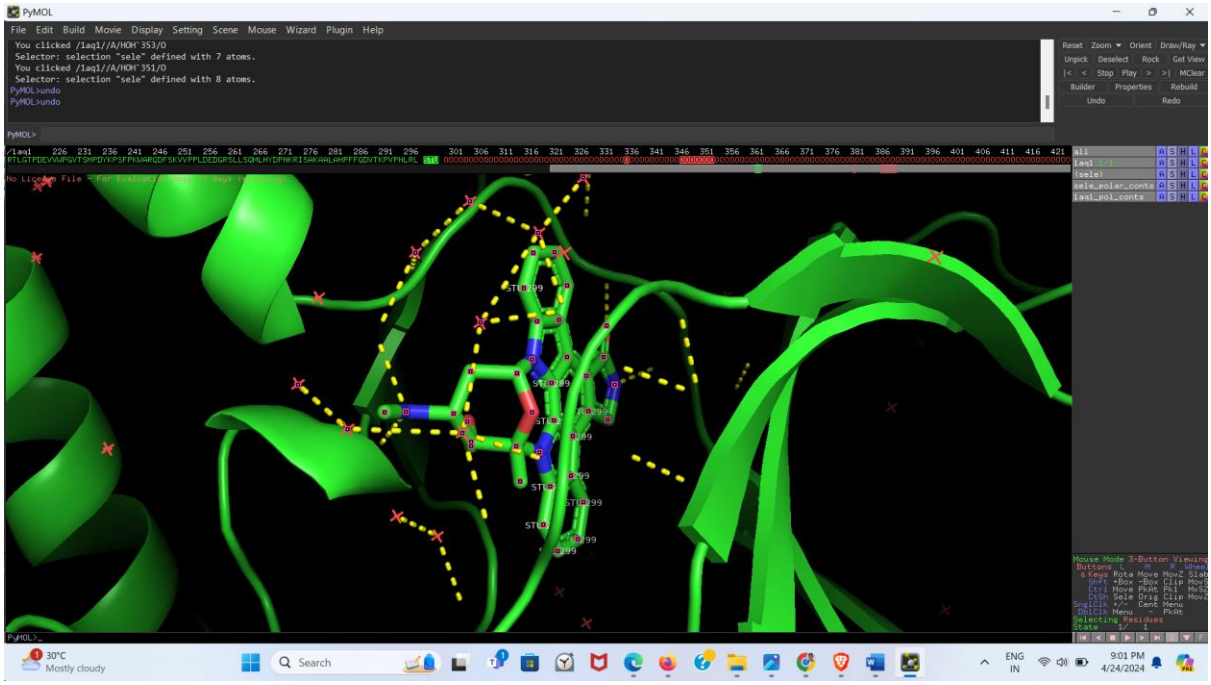
RMSD = 0.946

Q25) Save the aligned protein structure



File saved as ‘Assignment12_Q25’

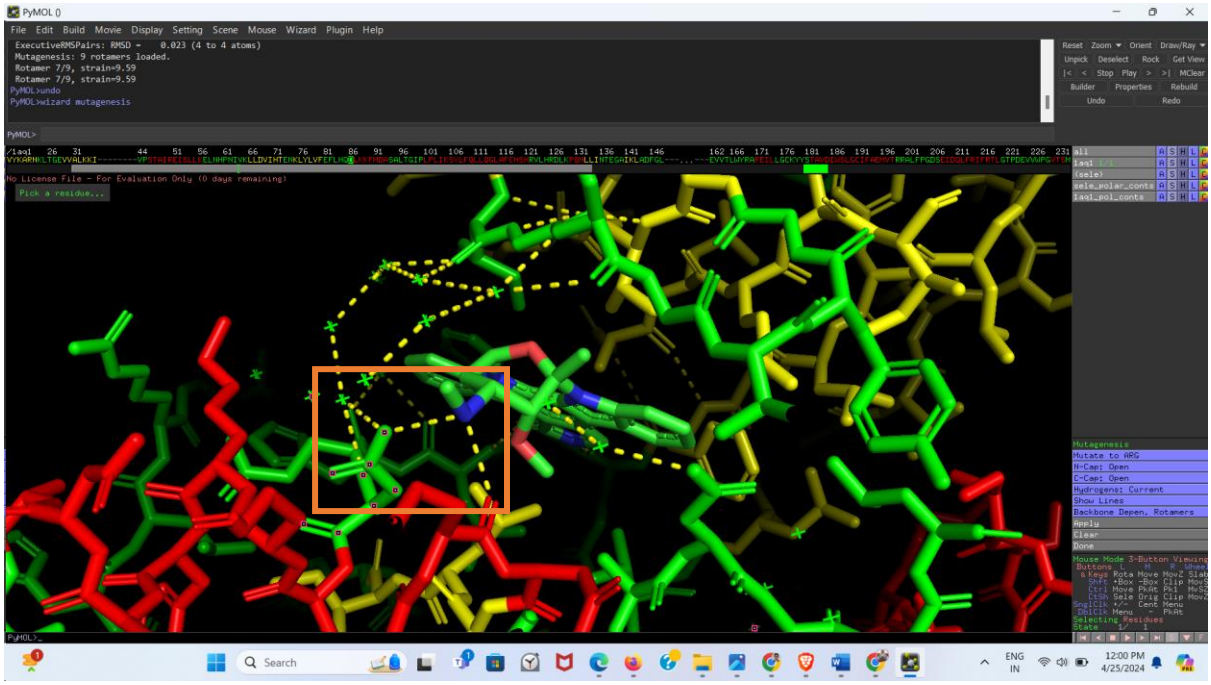
Q26) Download a protein structure with ligand(s). Identify the ligand and select residues within 3.5Å. Show any one type of interaction between them.



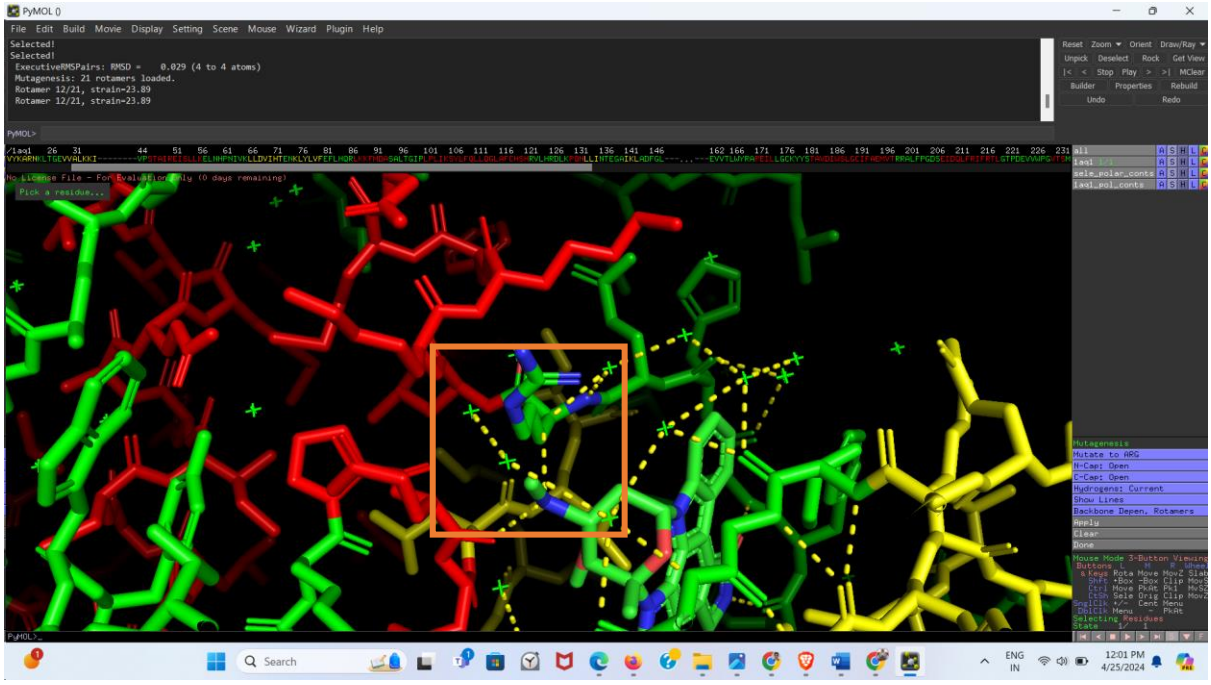
The yellow lines represent polar interactions.

Q27) Mutate any one of the active site residues and describe the change in the interaction with the ligand before and after mutation.

Before:



After:



Description: Aspartic Acid (D) was changed to Arginine (R), thus replacing a negative charge with positive charge. The interaction of protein-ligand at that residue is lost. Earlier the interaction, was between positively charged 'N' of ligand and 'O^{-}' of Aspartic Acid. Now there is no interaction, in fact repulsion between positively charged 'N' of both the groups