Assignment 1

Question 1

Download a PDB file of your choice and read the remarks sections of the file. Mention the PDB id of the protein and describe your protein in a maximum of 2-3 lines

The protein 1CCV is a Chymotrypsin Inhibitor which has only 1 chain (monomer) - 'A'. It is an NMR solution structure of Apis Mellifera Chymotrypsin Inhibitor(AMCI). This protein has no mutation.
PDB ID 1CCV corresponds to Apis mellifera chymotrypsin/cathepsin G inhibitor-1. This Inhibitor has a structural similarity with Ascaris protease inhibitors. The Molecule has a molecular weight of 5.98kD.

Apis Mellifera - Scientific Name of the Western Honey Bee

Question 2

Is your PDB structure determined by NMR or X-RAY? Which technique can result in resolving hydrogen atoms and provide hydrogen coordinates?

This PDB Structure has been determined by NMR.
NMR is the method used to locate accurately and resolve hydrogen atoms. NMR is used for analyzing the H-bonds interaction.

Question 3

Represent the protein in Licorice and color the protein according to its elements.

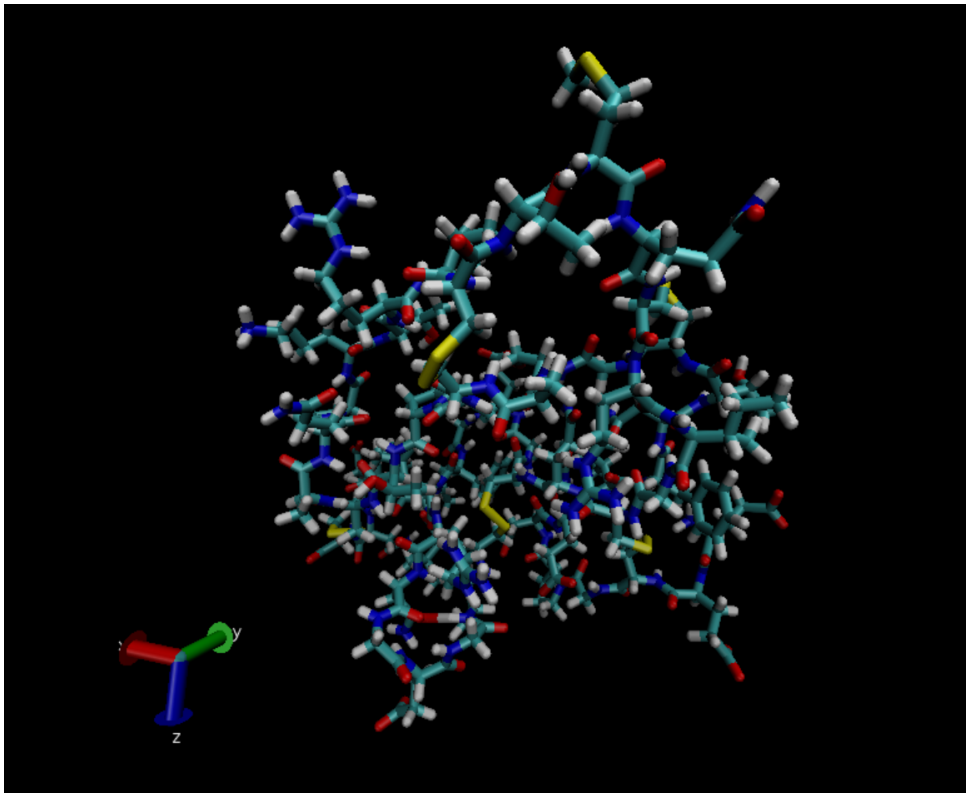

Fig 1: AMCI Protein

Steps : In VMD Application→Graphics→Representation. Select Licorice as Drawing Method and Element as the coloring method and click Apply

Question 4

Does your protein have crystal waters? If yes, represent using VDW.

No, PDB ID 1CCV does not contain crystal waters.
If you try representing water molecules, VMD shows a blank screen

Steps : VMD Application→Graphics→Representation→Selected atoms, type ‘water’. Set Drawing Method as ‘VDW’

Question 5

Change the background color to white, hide the axes and render the image in orthographic mode

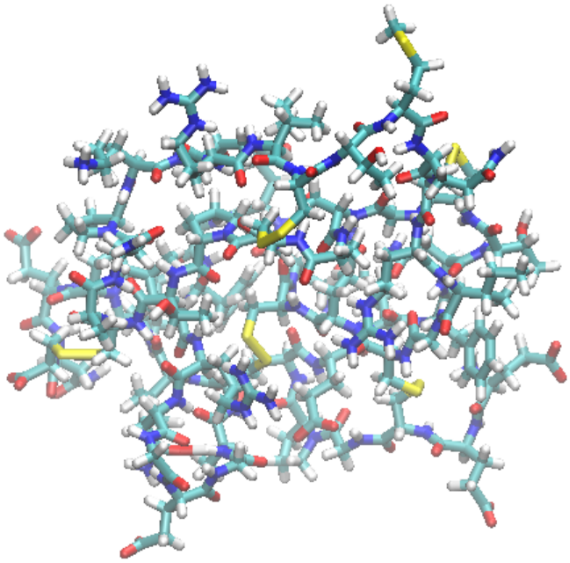

Fig 2: AMCI Protein against a white background

Question 6

Show all hetero atoms (need not include waters) lying within 2.0 Angstrom of your protein in CPK form. List them

Steps : VMD Application→Extensions→TK Console. Type the following command

There are no hetero atoms lying within 2.0 Angstrom of the protein

```
Main console display active (Tcl8.5.6 / Tk8.5.6)
(VMD) 1 % set sel [atomselect top "not water and not protein within 2 of protein
"]
atomselect0
>Main< (VMD) 2 % $sel get {resname index type}
>Main< (VMD) 3 %
```

Fig 3: Code that gives the list of all hetero atoms lying within 2.0 Angstrom of your protein

Question 7

Represent in VDW the first atom of your PDB ID using keyword: index and serial. What do you infer from the observation?

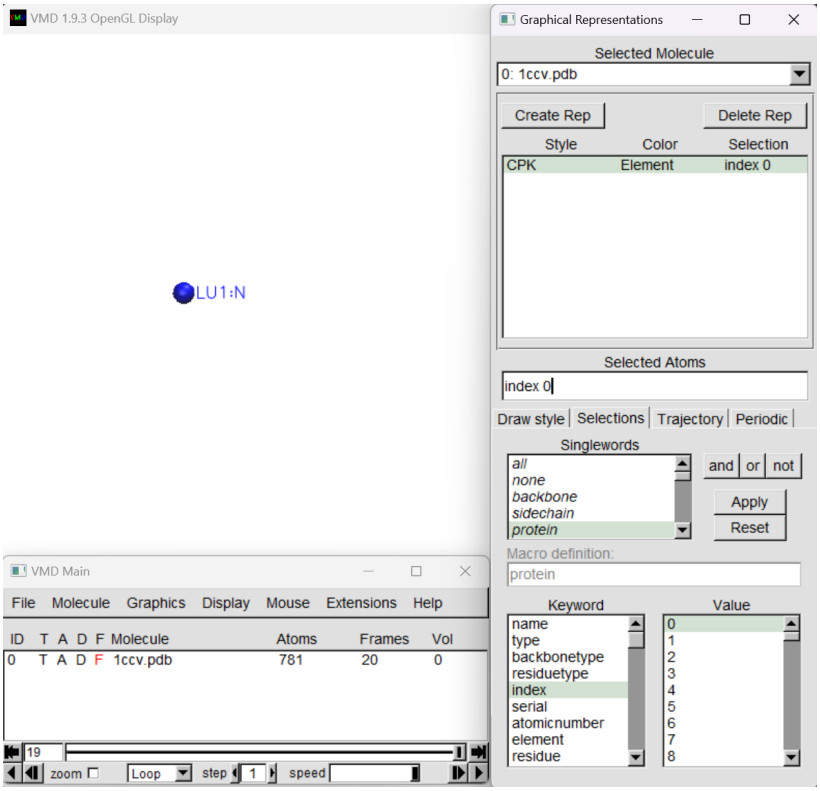

Fig 4: First atom of AMCI

Inference :- The first atom of the protein can be represented by using the index 0 or serial 1

Steps : VMD Application→Graphics→Representation→Selected atoms, type ‘index 0’ or ‘serial 1’.

Question 8

Represent the first 5 residues in CPK. Find the angle between any three non-consecutive atoms and display the angle value in red and atom labels in blue.

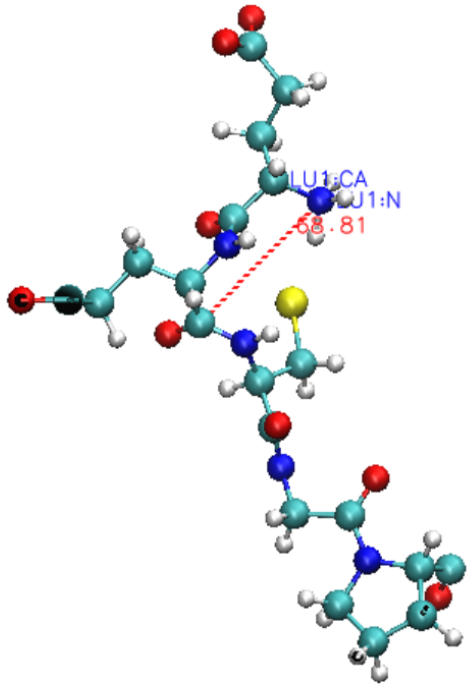

Fig 5: First 5 residues of protein AMCI

Steps : VMD Application→Graphics→Representation→Selected Atoms, type ‘residue 0 to 4’, to get the first 5 residues of the protein.
Select ‘3’ on the keyboard and choose three non-consecutive Atoms. This will display the angle enclosed within these three atoms
For setting angle color . VMD Application→Graphics→Colors→Set categories as ‘label’ and choose ‘Angles’ and select ‘1 red’ in the color panel for the angles.
Follow similarly for the atom label color as well.

Question 9

Load the same PDB twice and place them next to each other in different colors.

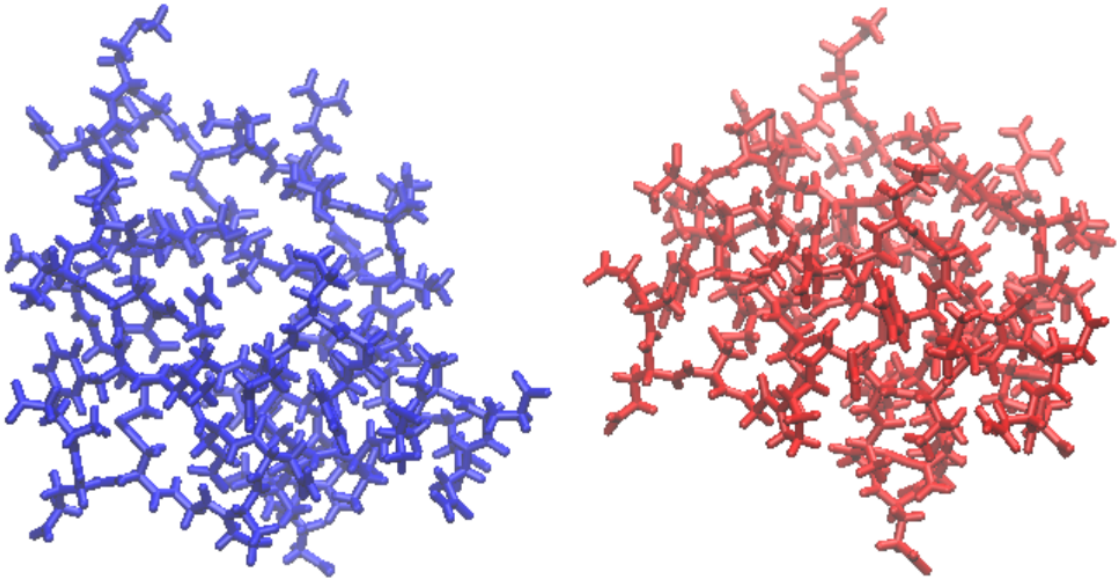

Fig 6: 2 Molecules of AMCI next to each other

Steps : Load the first molecule. Move it to the required position. Set color mode based on color ID. Next Fix the molecule by choosing 'Toggle Fixed' under the 'Molecule' Panel, in the VMD Application.

Load the new molecule and follow the above steps, choose a different color for differentiation

Question 10

Display the contact map of protein. What do you interpret from the graph?

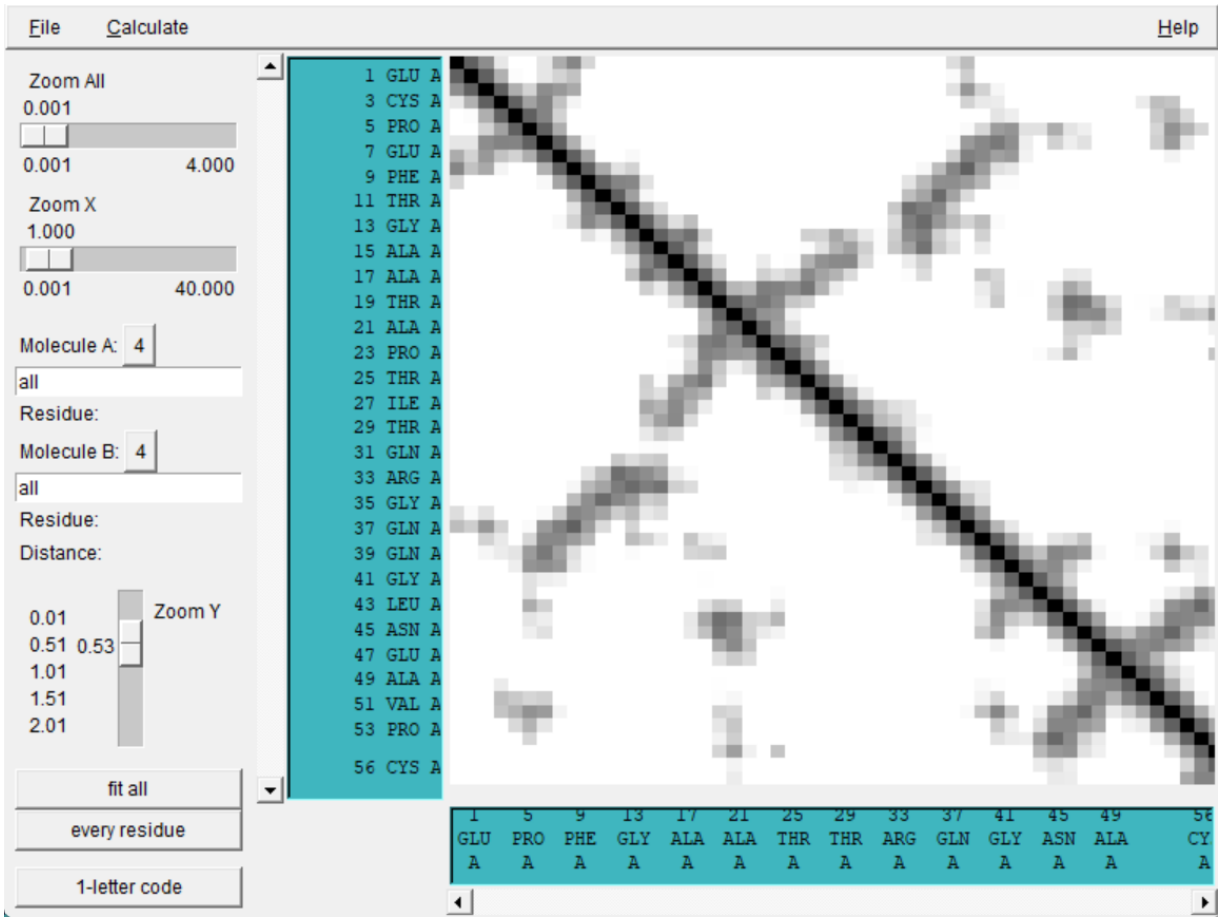

Fig 7: Contact Map of the protein AMCI

Inference : -

1)Alpha Helix is observed with short range contacts i.e, strips that are very close to the main diagonal.

2)Beta Sheets are infered with lower long-range contacts. Anti-parallel beta sheets appear as cross dr diagonal lines

3)Other long range contacts imply loops or turns. Breaks in the main diagonal of the contact map imply loops

Steps : VMD Application →Extensions→Analysis→Contact map. Once the new file opens, click on Calculate→Cal. Res-res Dists.

****