Computational Biology Lab

Practical 4

New PDB ID: 2XNI

Reason: The assigned PDB ID does not have any ligand to isolate, and contains only macromolecules. Hence the new PDB ID was assigned to me to perform the given assignment

1. Read the remarks sections of the PDB file and describe your protein.

Protein ID : 2XNI

Information: Protein-ligand complex of a novel macrocyclic HCV NS3 protease inhibitor derived from amino cyclic boronates.

Number of chains in the protein : 4 - "A,B,C,D"

Number of Ligands : 3

Molecular weight : 47.66 kDa

Experimental Details :

EXPERIMENT TYPE   : X-RAY DIFFRACTION

TEMPERATURE   (KELVIN) : 100
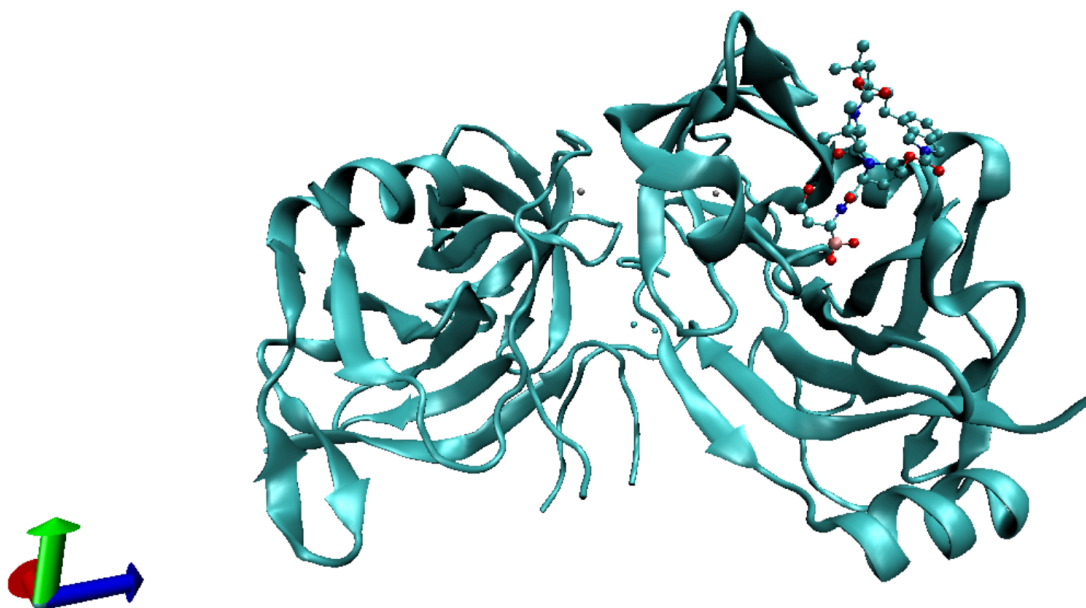
PH   : 6.5

NUMBER OF CRYSTALS USED   : 1

2. Is your PDB structure determined by NMR or X-RAY? What is the resolution?
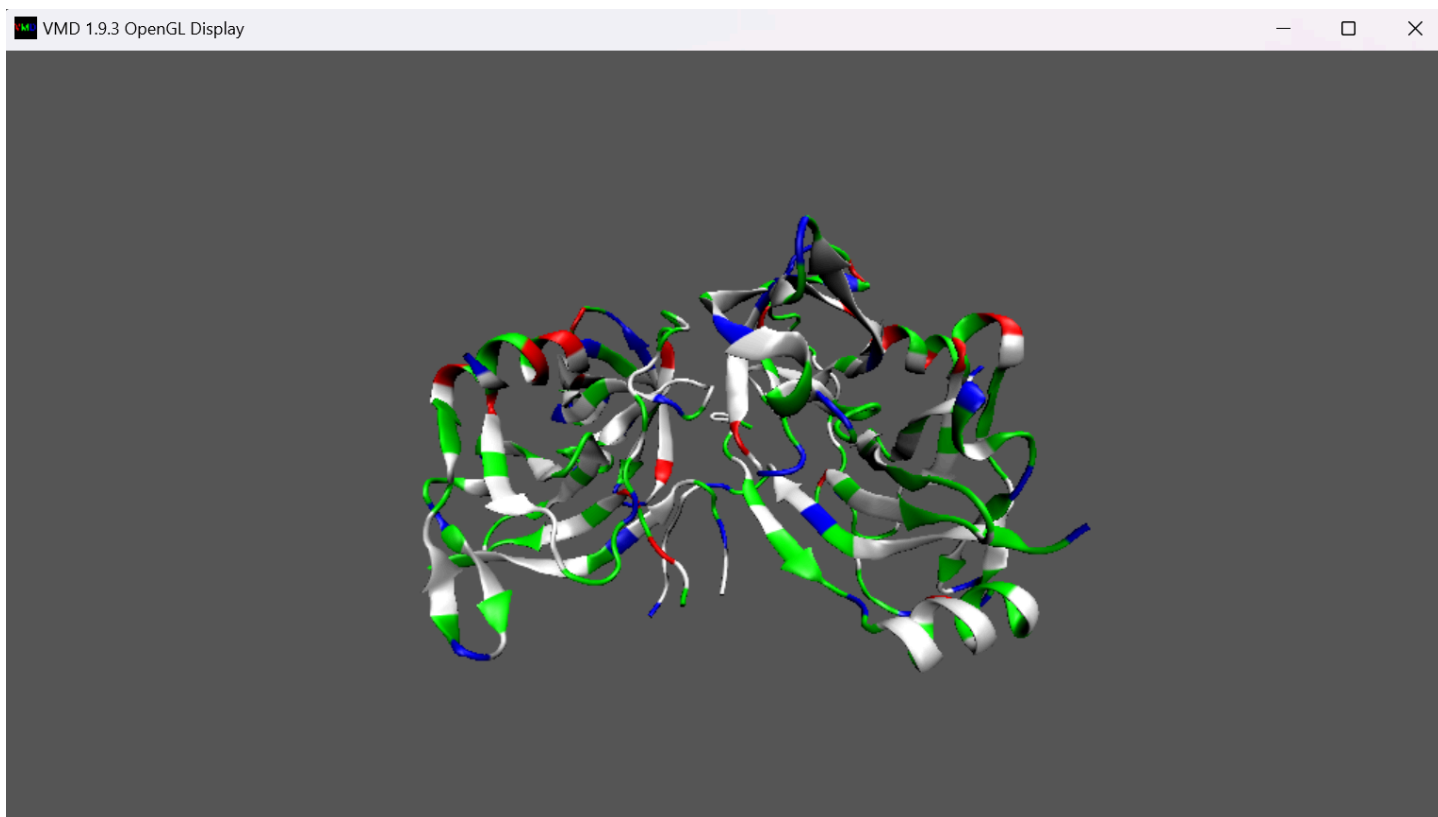
EXPERIMENT TYPE   : X-RAY DIFFRACTION

RESOLUTION.   3.30 ANGSTROMS.

3. In VMD, represent the protein in New Cartoon and ligand/DNA/sugar (non-protein) in CPK.

4. Represent the protein using different colours for different residue types. Change the background to grey and hide the axes.

5. Show all heteroatoms lying within 3.0 Angstrom of your protein in CPK form. List them.

Protein + all hetero atoms

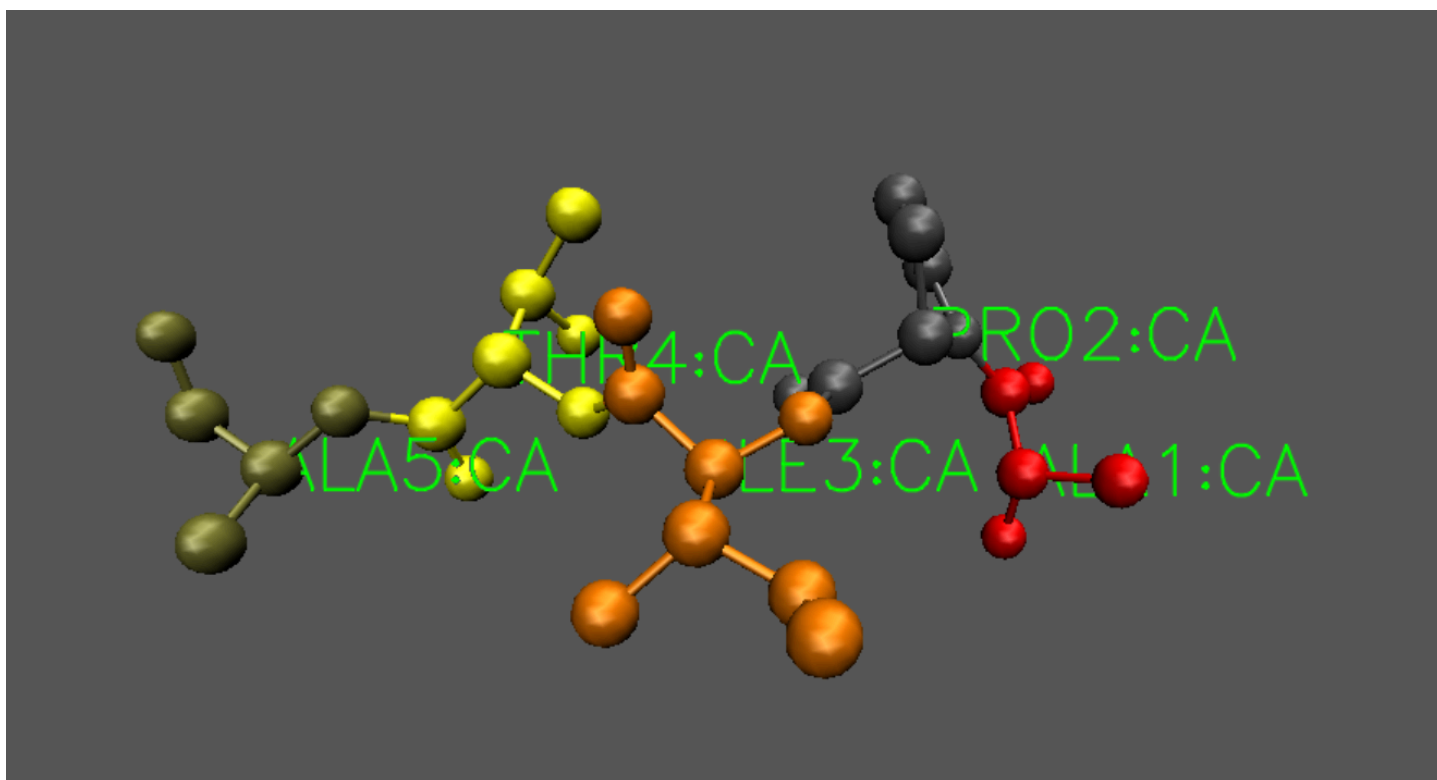Hetero atoms within 3 Angstroms of protein
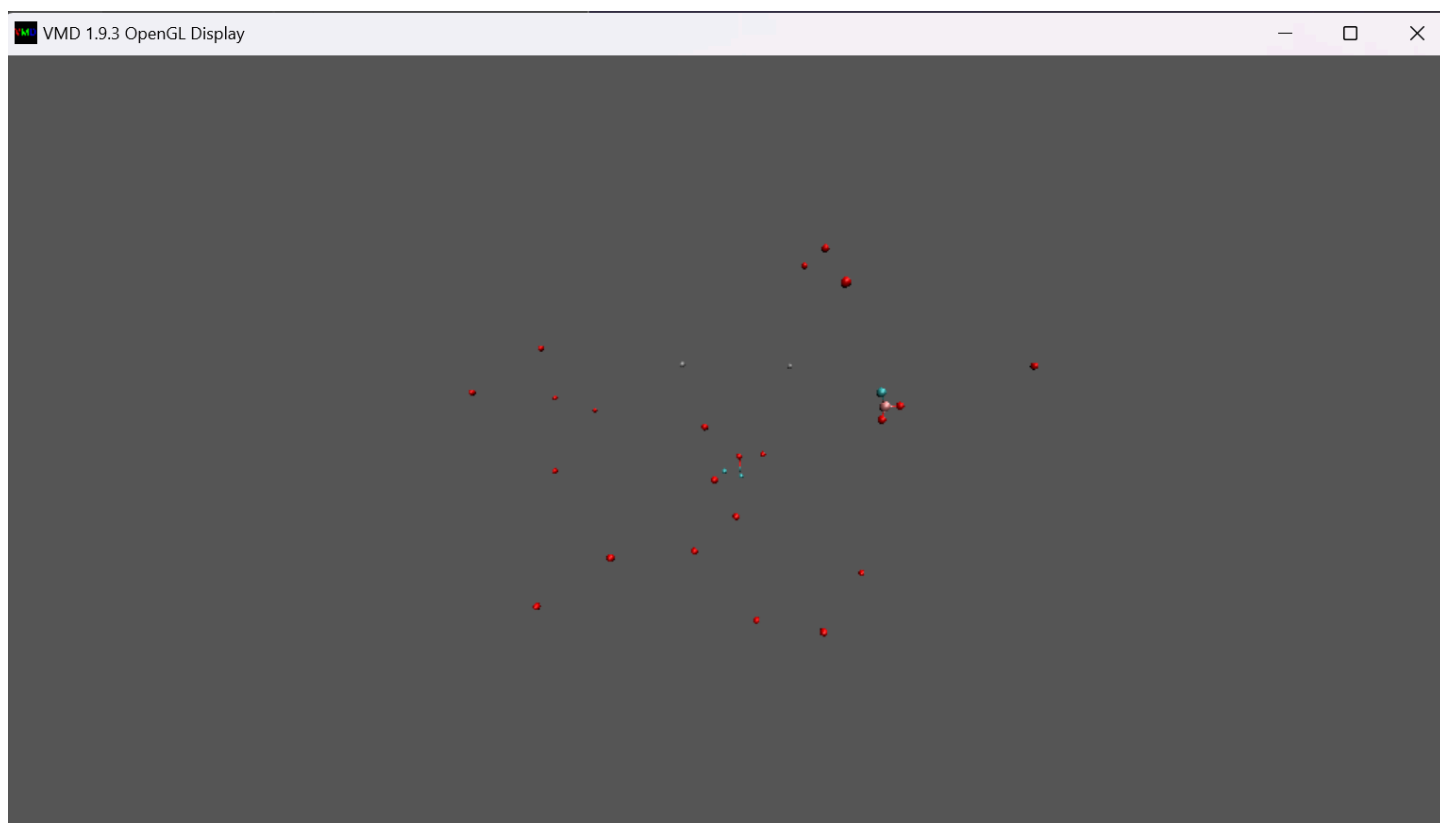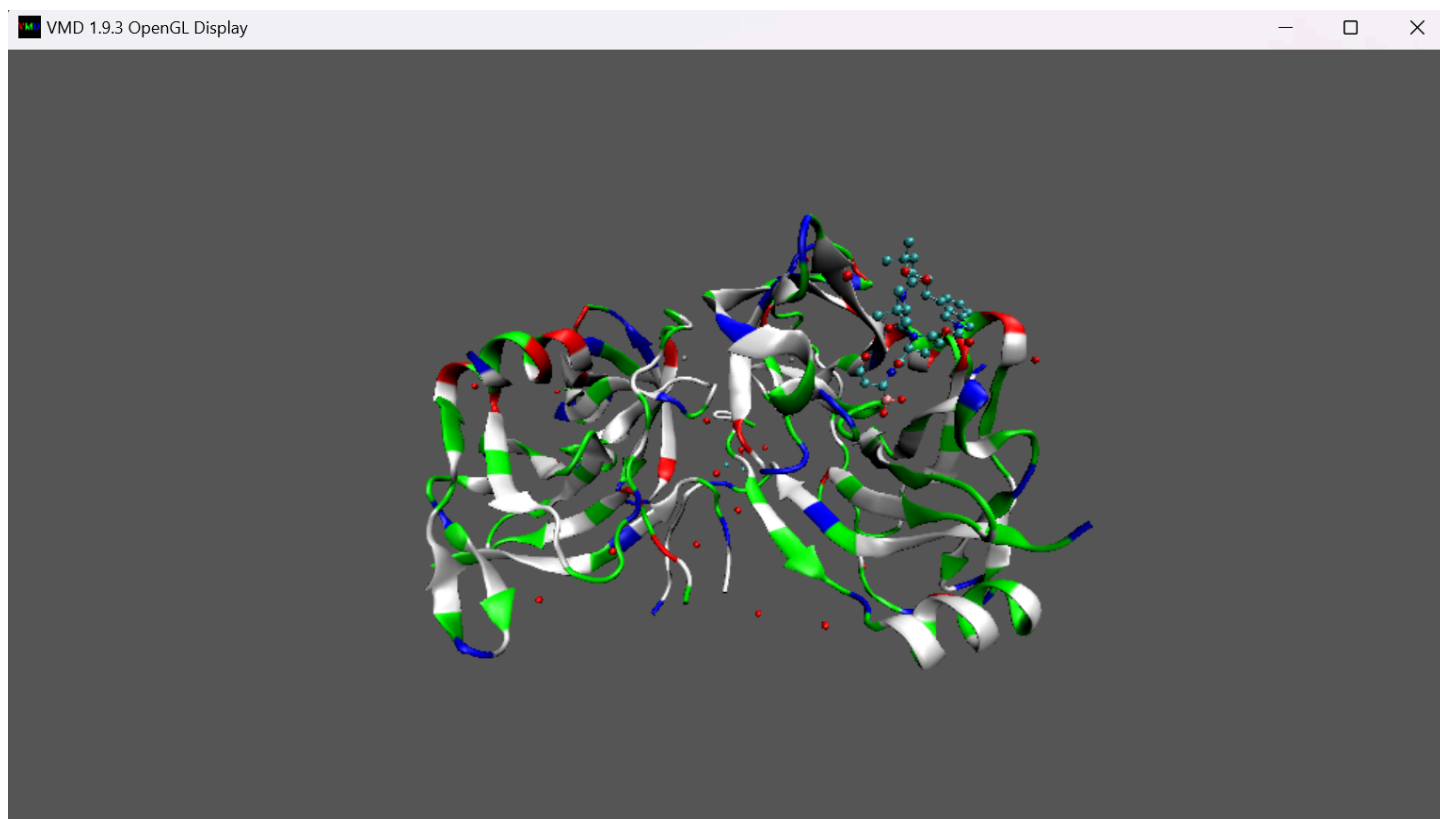
Since there are a lot of non protein molecules for this PDB ID, we label and list a few of them and they are shown and listed below
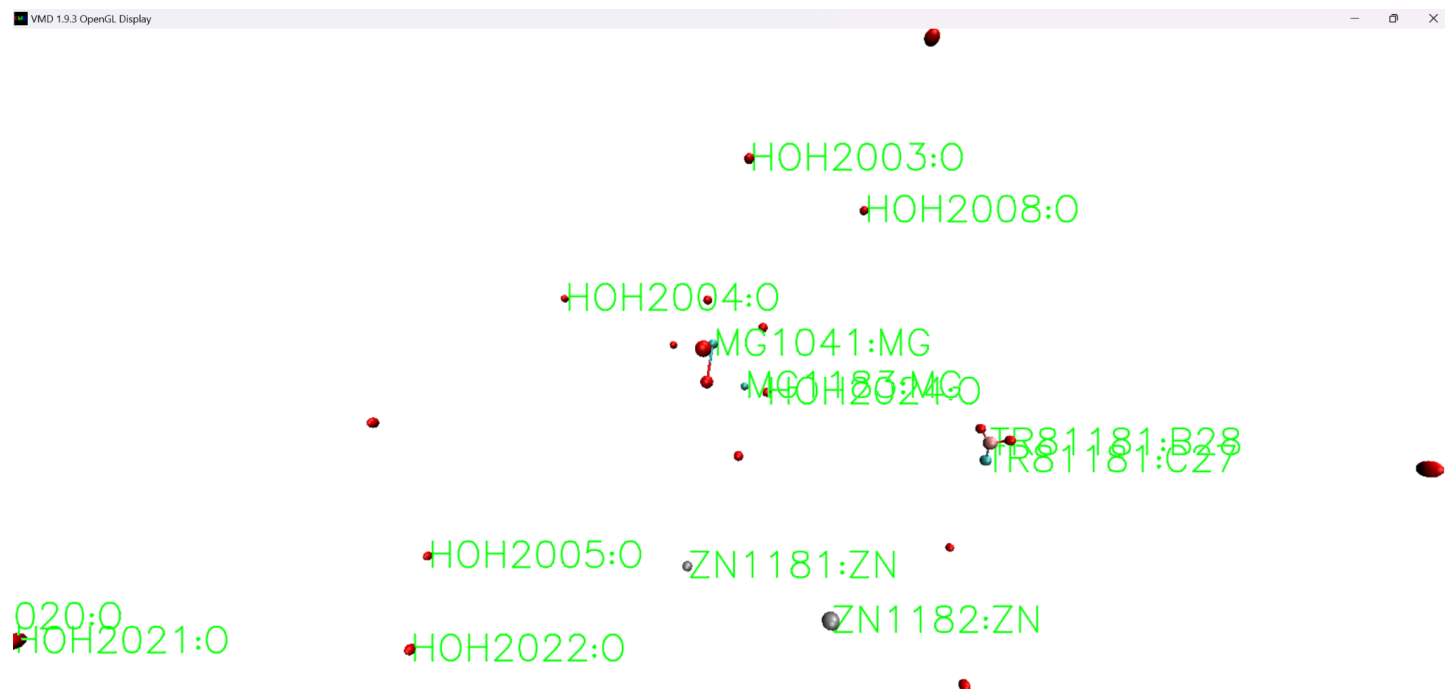
ZN1181:ZN
HOH2004:O
HOH2003:O
ZN1181:ZN
ZN1182:ZN
TR81181:B2
TR81181:C2
MG1183:MG

6. Label the first five amino acid residues of your protein. List them.

ALA5:CA
THR4:CA
ILE3:CA
PRO2:CA
ALA1:CA

## 7. Write a line about the different molecule status flags [T A D F].

T - Top : implies currently selected molecule,

A - Active : molecule is available for display and manipulation,

D - Displayed : determines whether the molecule is visible in the graphical window

F - Fixed : locks the molecule's position

8. Display the Ramachandran plot for your protein using in-built function. Name any two residues that lie in the disallowed region of the plot.
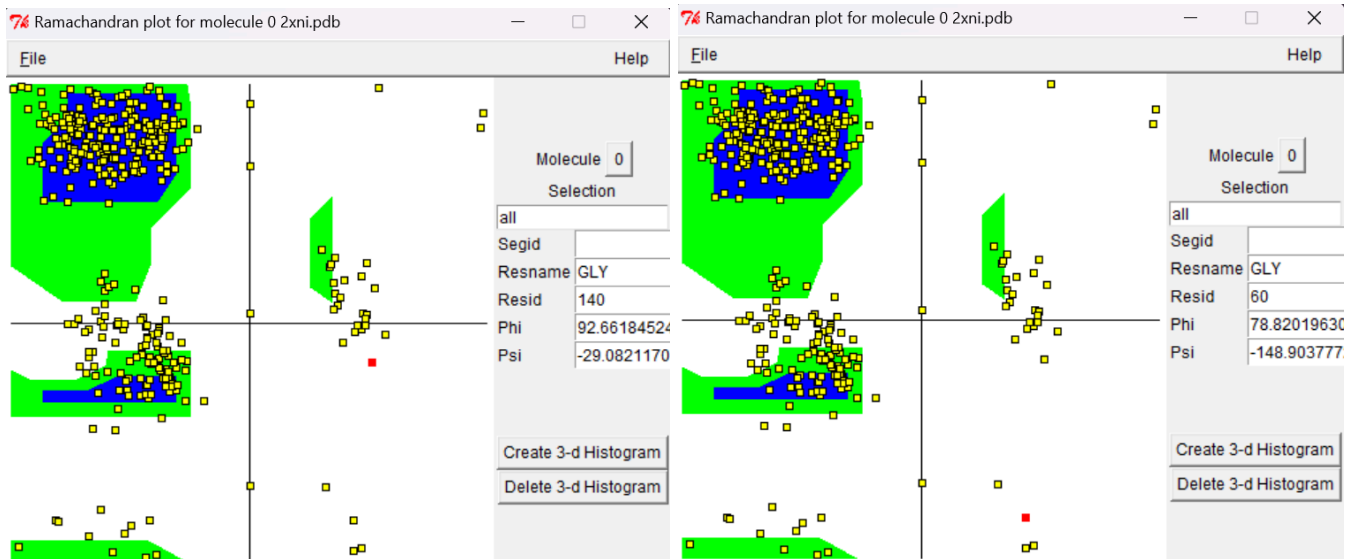
GLY 140

GLY 60

Are the two residues in the disallowed region

9. Find out from the sequence viewer about the secondary structure of your protein. Is there any occurrence of H (helix) in the secondary structure? If yes, mention which residues contribute towards those structures.

From the sequence viewer we see that there are several residues that contribute to the helix secondary structure.
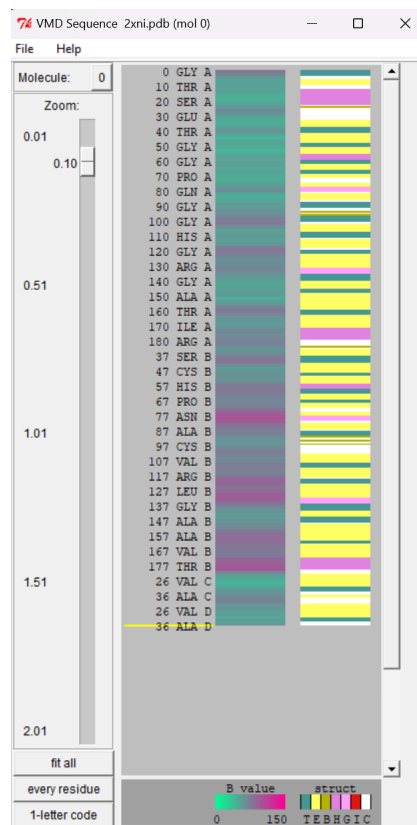
The residues that contribute to the same are shown below as seen from the sequence viewer:

56 TYR A	56 TYR B
57 HIS A	57 HIS B
58 GLY A	58 GLY B
59 ALA A	59 ALA B
172 VAL A	172 VAL B
172 GLU A	172 GLU B
174 ASN A	174 ASN B
175 LEU A	175 LEU B
176 GLU A	176 GLU B
177 THR A	177 THR B
178 THR A	178 THR B
179 MET A	179 MET B

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