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BE21B004

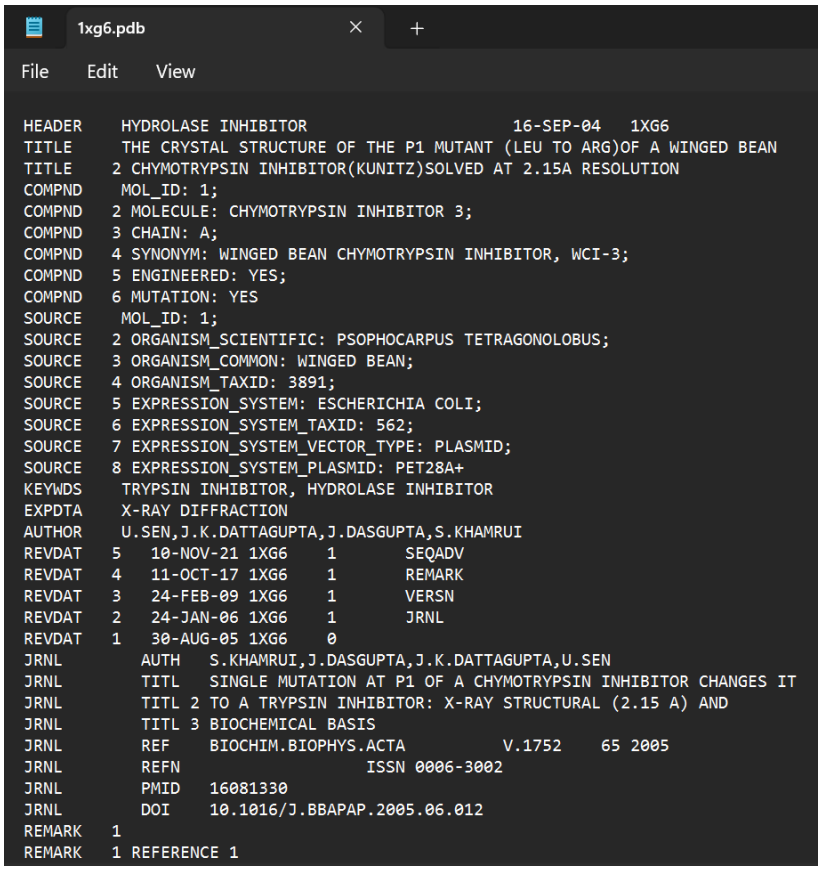
BT5420

Computer Simulations of Biomolecular Systems

Assignment 1 (VMD)

1. The PDB ID of the protein is **1XG6**.

   - The protein corresponding to this PDB ID is a **mutant form of the winged bean chymotrypsin inhibitor 3 (WCI-3)**, which a member of the class of Kunitz-type protease inhibitors.
   - The protein only has one chain, denoted by A, which has 179 residues.
   - According to the authors (https://doi.org/10.1016/j.bbapap.2005.06.012) who provided this structure, the protein has a single Leu65Arg mutation that occurs at the P1 site of the protein.
   - This particular protein has been taken from the plant *Psophocarpus tetragonolobus*, commonly known as the winged bean, and *E. coli* was used as an expression system to obtain the protein.
   - The resolution of the structure provided is 2.15 Å and the structure has 8 missing residues at positions from 179 to 186.



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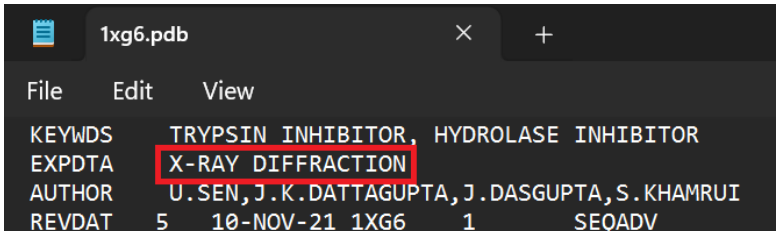
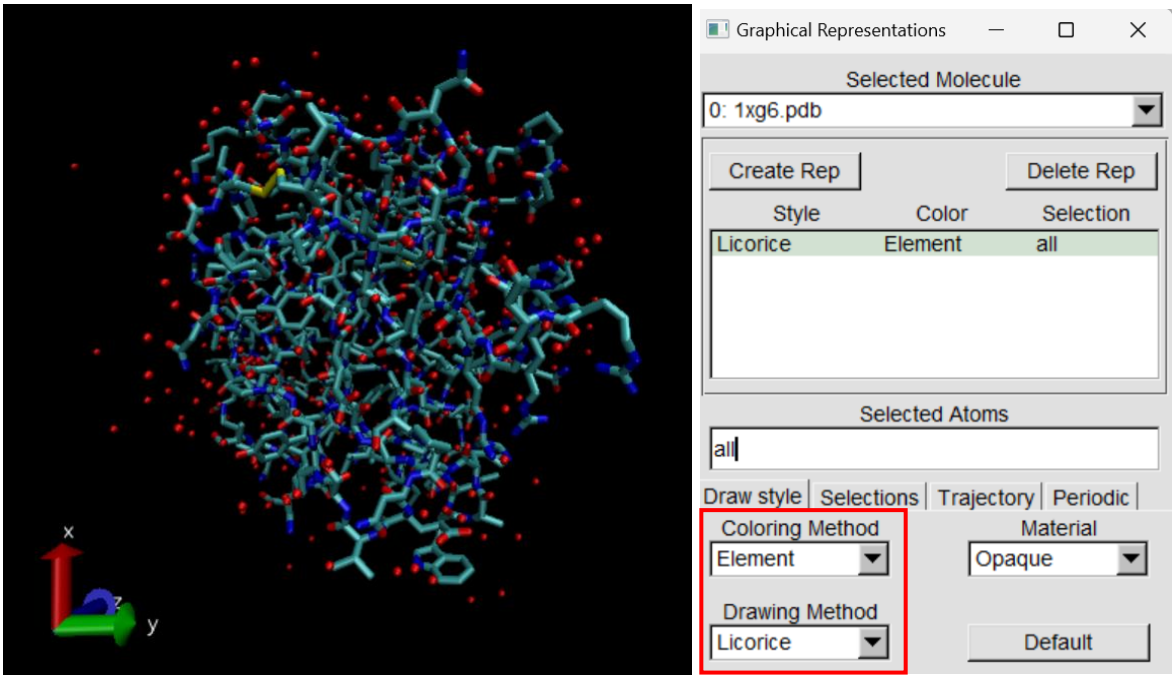
2. The structure of this protein has been determined by X-ray diffraction (XRD) at a resolution of 2.15 Å.



XRD relies on electron scattering to determine the protein's structure. As hydrogen only has one electron, it cannot be resolved by XRD.

However, NMR, particularly 1H NMR, can resolve hydrogen atoms as it works on the basis of chemical shift (difference in resonance frequency) in the local environment of each atom. Also, NMR does not require the protein to be crystallized and can be used to determine structure even when the protein is in solution.

3. The representation of the protein with 'Licorice' as the drawing method and 'Element' as the colouring method is given below.



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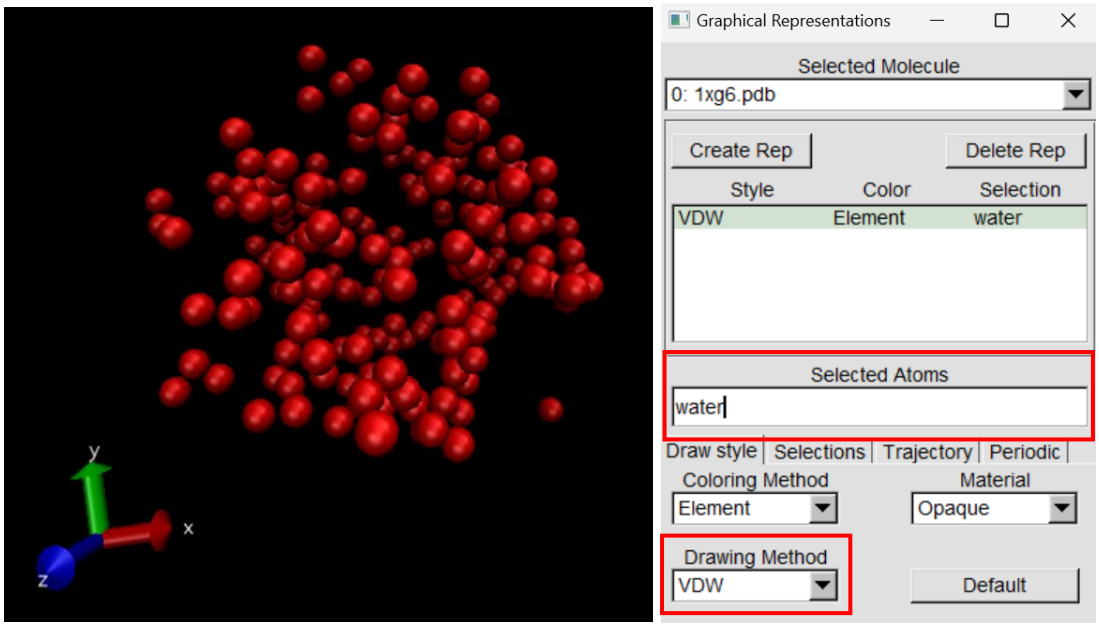
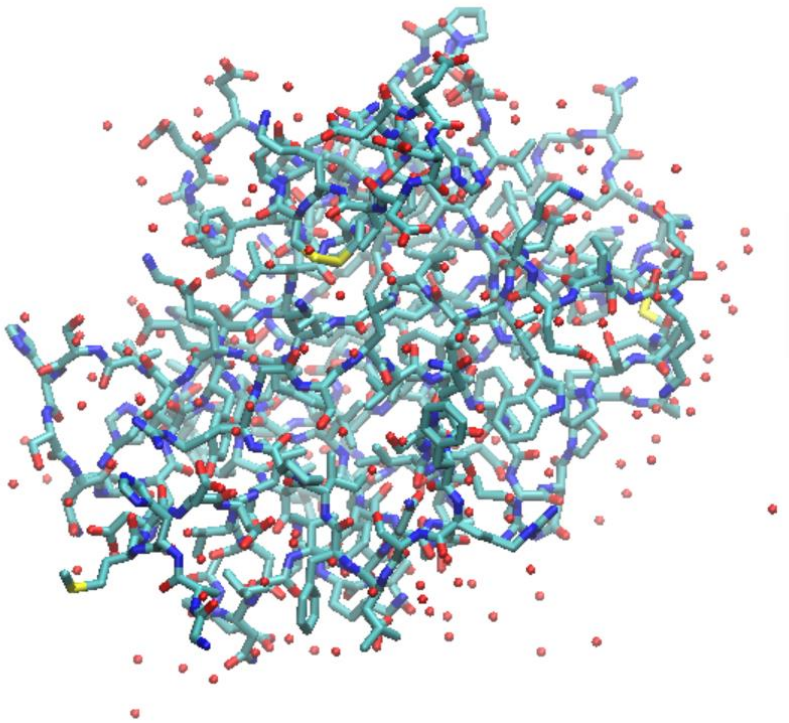
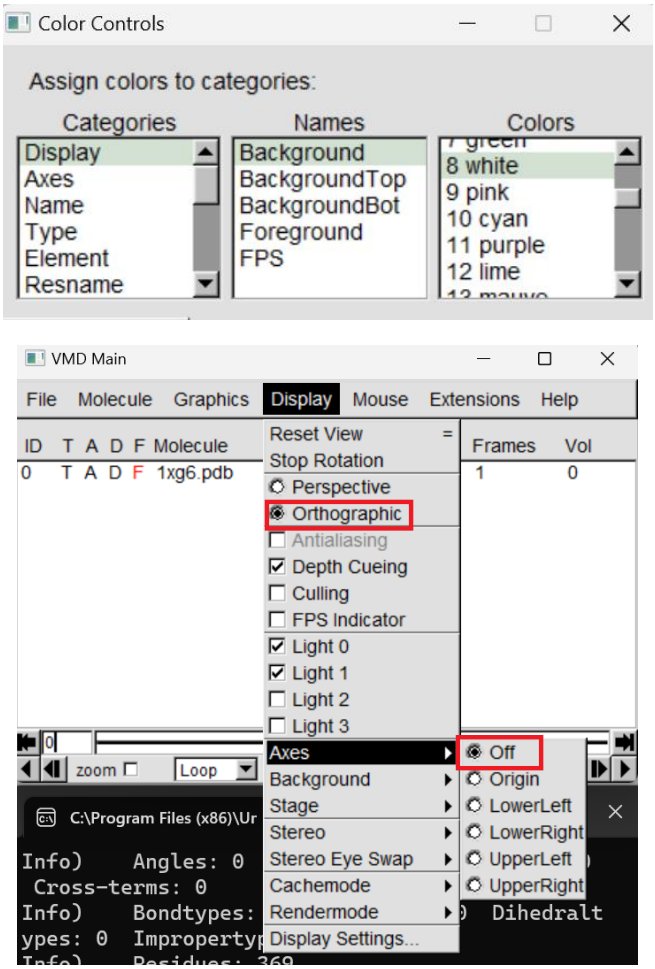
4. The protein structure has 190 crystal waters.

   We can select only these water molecules and represent them with 'VDW' as the drawing method.

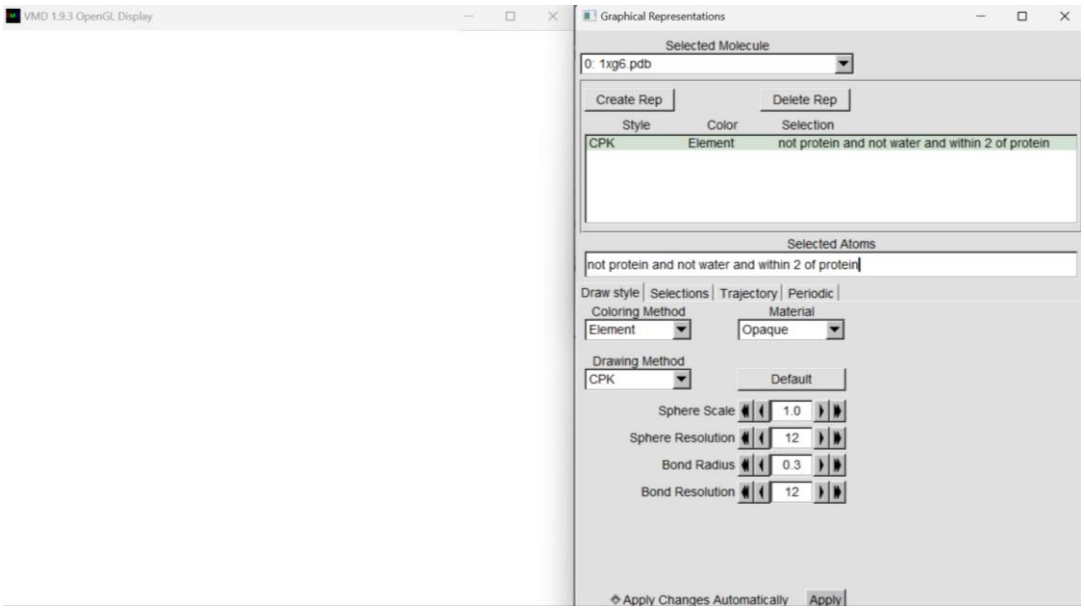


5. After changing the background to white, removing the axes, and switching from 'Perspective' to 'Orthographic' mode, we get the below representation.

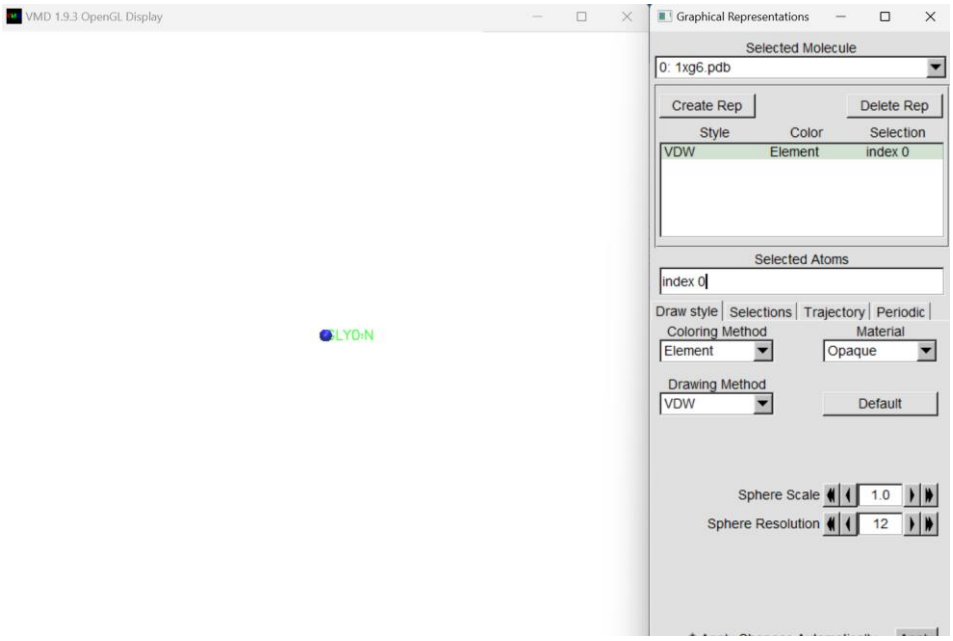


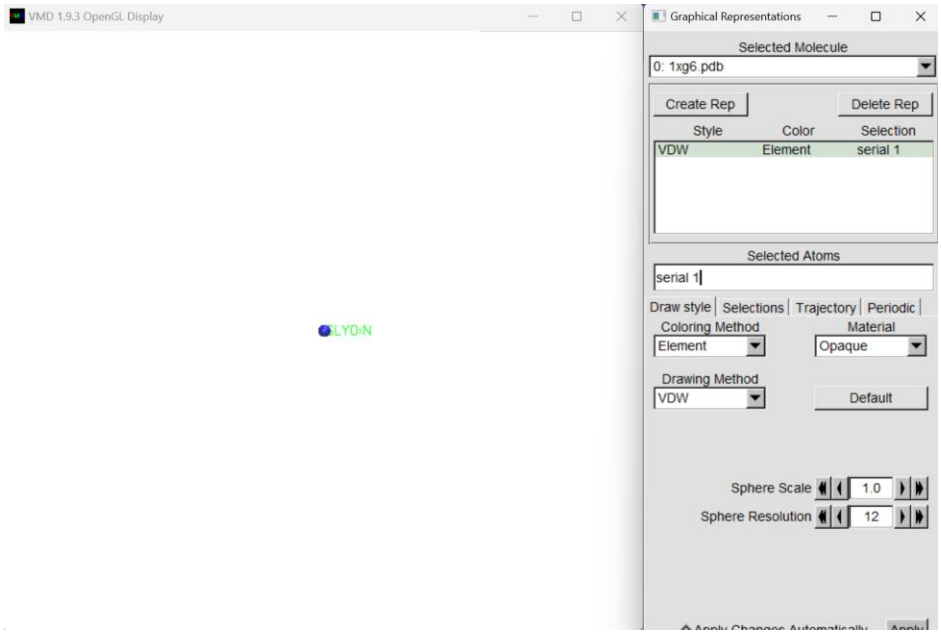


6. There are no non-water hetero atoms lying within 2 Å of the protein.

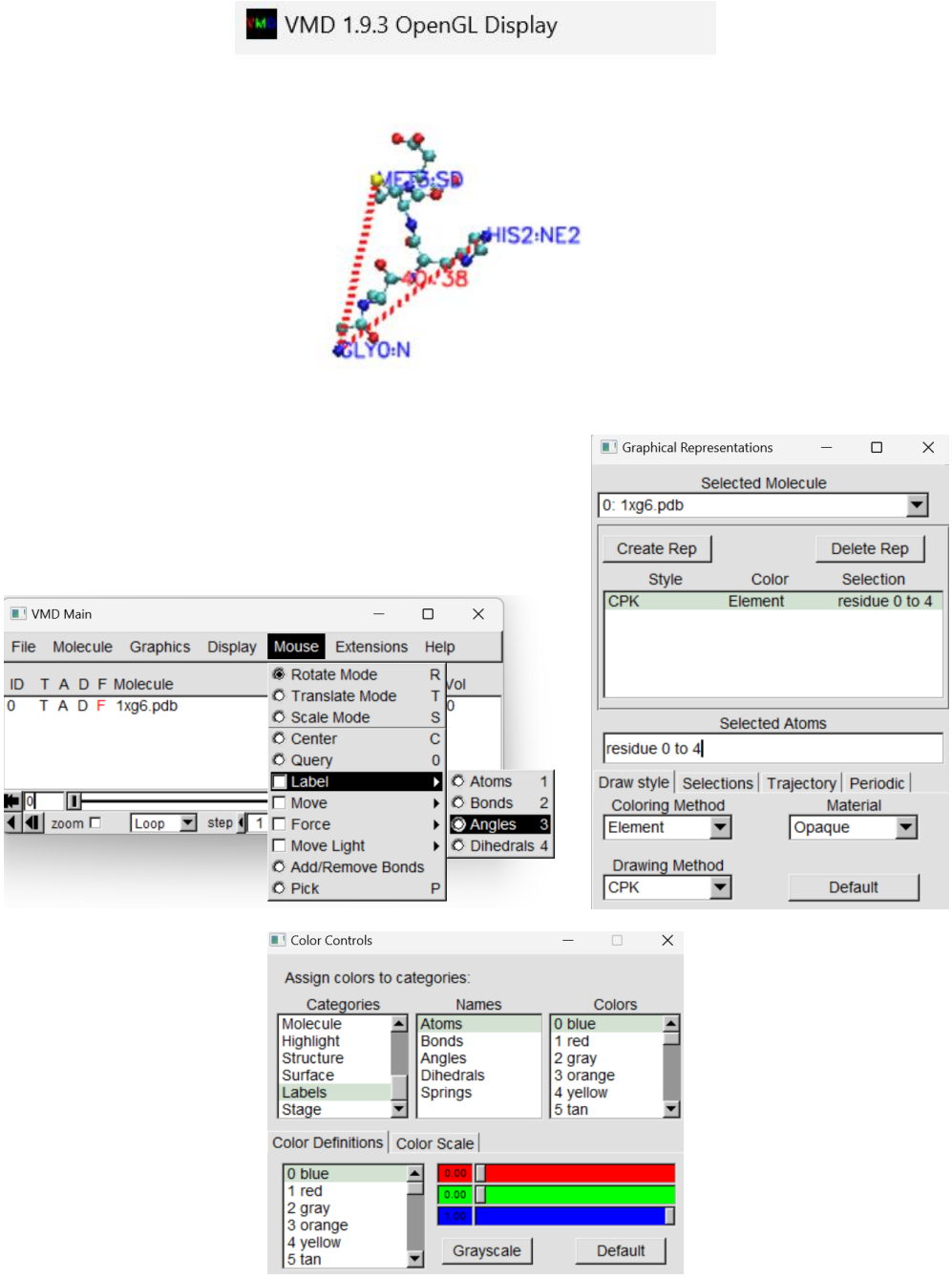


7. To represent the first atom using the keyword ‘index’, we have to provide the atom number as 0. However, if we are using the keyword ‘serial’ we have to provide the atom number as 1 in order to represent the same atom.





8. The first 5 residues of the protein are displayed with ‘CPK’ as the drawing method. 3 atoms were randomly selected and the angle between them was found using the ‘Label’ option. The atom and angle labels were coloured as required.



9. The same PDB file is loaded twice. The ‘F’ flag for one of the molecules is turned off. The mouse is changed to ‘Translate’ mode to move the unfrozen molecule. We set the colouring method for both molecules as ‘ColorID’ in order to show them in different colours.

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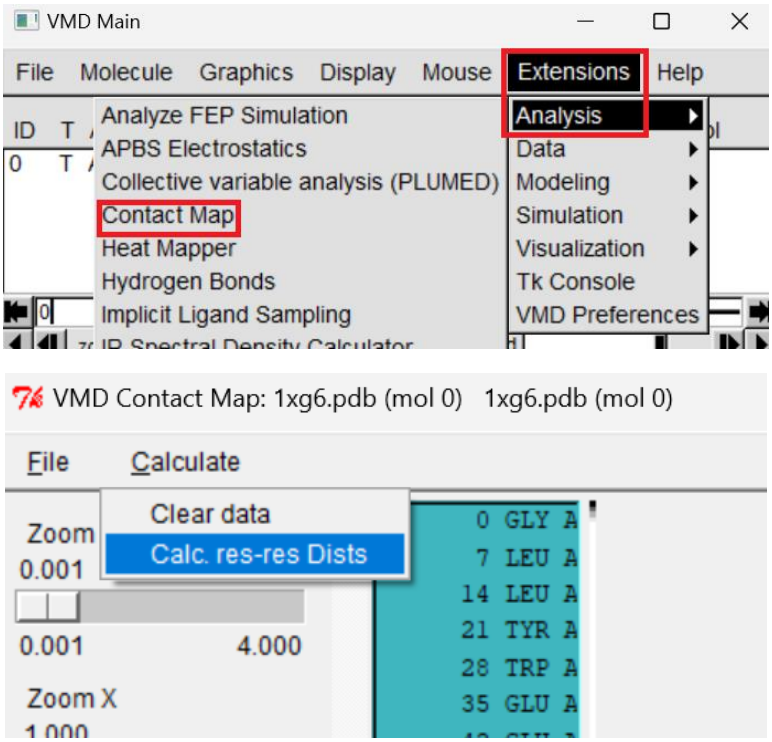
10. The contact map of the protein can be found by using the 'Contact Map' analysis tool and calculating the pairwise distance between residues of the protein.



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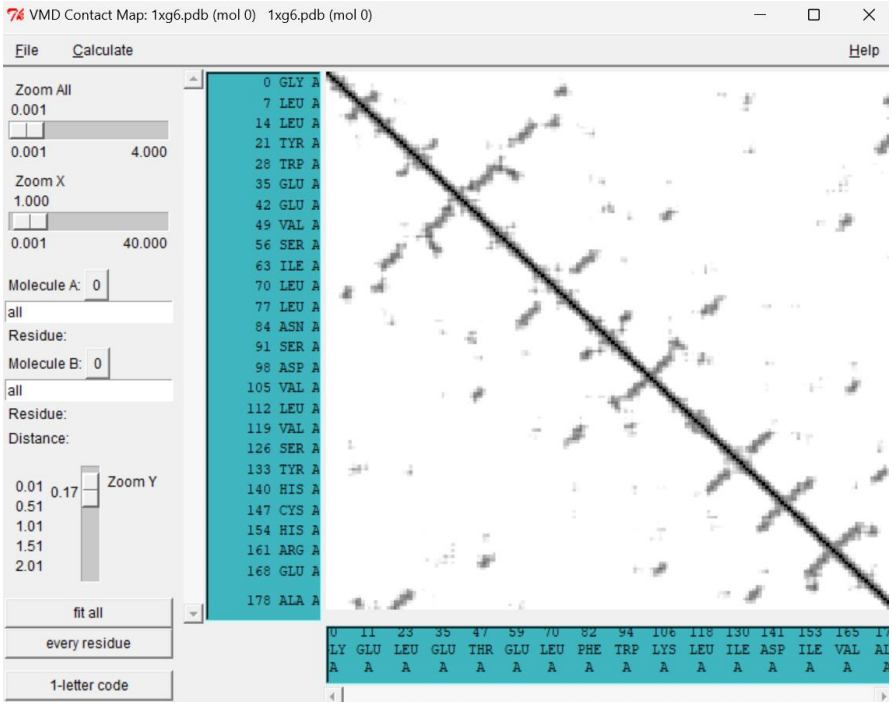

In the contact map of this protein, we can see many off-diagonal interactions. This shows that residues that are far away from each other interact in the tertiary structure of the protein for stabilization. Neighbouring residues can form secondary structures like alpha helices (which appear along the main diagonal) and beta sheets (which appear orthogonal to the main diagonal).