



WARSAW UNIVERSITY OF TECHNOLOGY  
BIOINFORMATICS

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**Structural Analysis of  
Biomolecules Using UCSF  
Chimera**

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## 1 Exercise 1

- **Structure of 7LM9:** Crystal structure of SARS-CoV spike protein receptor-binding domain in complex with a cross-neutralizing antibody CV38-142 Fab isolated from COVID-19 patientRCSB (2024). The structure reveals that CV38-142 binds to a highly conserved cryptic site in the RBD, which is not involved in ACE2 binding. The antibody binds to the site through several interactions, including hydrogen bonds, salt bridges, and van der Waals forces. The structure suggests that CV38-142 could be effective at neutralizing SARS-CoV-2 and SARS-CoV.
- **Protein or Complex:** Spike protein receptor-binding domain in complex with a cross-neutralizing antibody CV38-142 Fab.
- **Experimental Method:** The method used is X-RAY DIFFRACTION
- **Resolution of the model:** The resolution is 1.53 Å
- **Water molecules:** There are 593 molecules of water
- **Ligand:** In my investigation using the UCSF Chimera, I took these steps to highlight the ligand "Select= Structure= ligand" It shows 11 but the actual ligands are located in the area circle in the figure below.

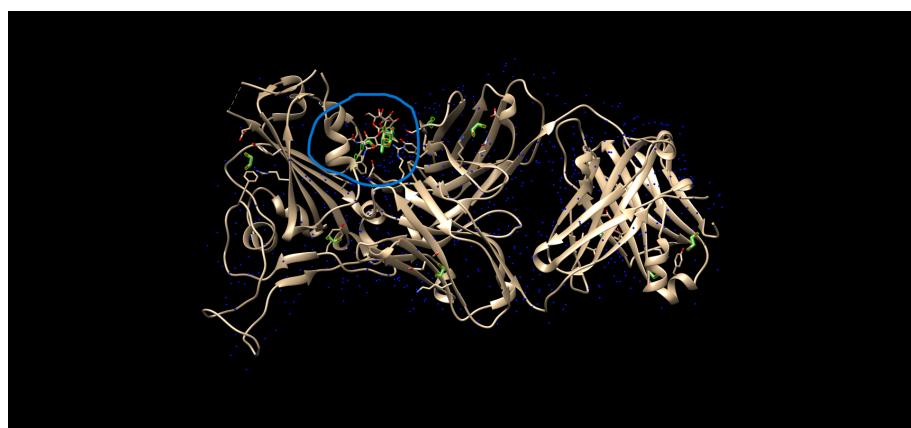


Figure 1: Visualize structure

- **Protein chain and Ligand colored:** I assign the color yellow to the protein chain and red to the ligand as shown below.

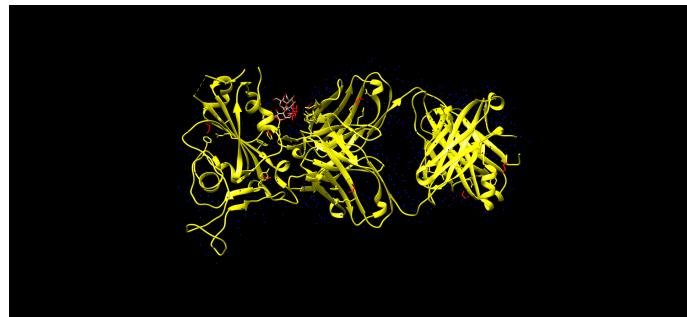


Figure 2: Visualize Protein chain and ligands

- **Helices and Beta sheets (strands):** I assign the color green to the Helices and magenta to the strands as shown below.



Figure 3: Visualize Helices and Beta sheets

- **Surface of the protein chain:** I set the transparency to 75%. The ligand is located at the top right side slope area i.e. the active site. A protein's active site is the area where particular interactions with ligands, substrates, or other molecules take place. Usually, a cleft or pocket on the surface of the protein makes binding and catalysis easier. Comprehending the function of the protein requires an understanding of its active site.

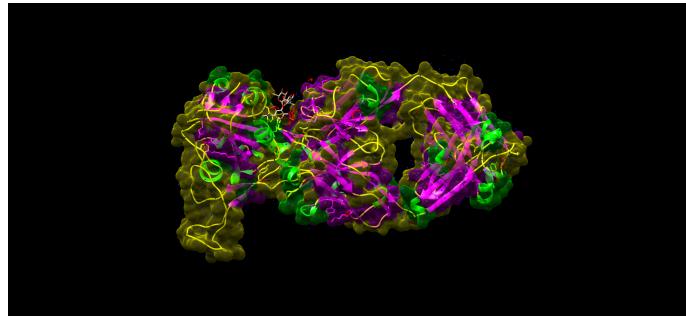


Figure 4: Visualize Helices and Beta sheets

- **Video of the rotating structure:** When attempting to display the video with Chimera, it failed to function. Consequently, I had to resort to using ChimeraX once again. I have attached the session files from both Chimera and ChimeraX for reference.

## 2 Exercise 2

- **Structure of 3LEL:** Structural Insight into the Sequence-Dependence of Nucleosome PositioningRCSB (2024). The structure of 3LEL reveals how the SPE sequence interacts with the histone proteins to stabilize nucleosome positioning. The TA dinucleotides in the SPE sequence are located in minor groove-inward regions of the DNA, where they can contribute to the bending and compression of the minor groove. This structural distortion is thought to be unfavorable for DNA transcription, and it may help to explain why nucleosomes containing SPE sequences are often found in gene-poor regions of the genome.
- **Protein or Complex:** 3LEL is a complex of nucleosome core particles (NCPs) with a synthetic DNA fragment containing a strong positioning element (SPE) sequence.
- **Experimental Method:** The method used is X-RAY DIFFRACTION
- **Resolution of the model:** The resolution is 2.95 Å
- **Chains:** There are 20 chains.

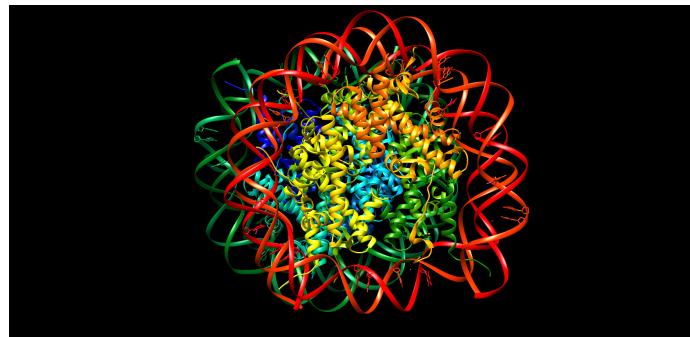


Figure 5: Visualize chains

- **Hydrogen bonds:**

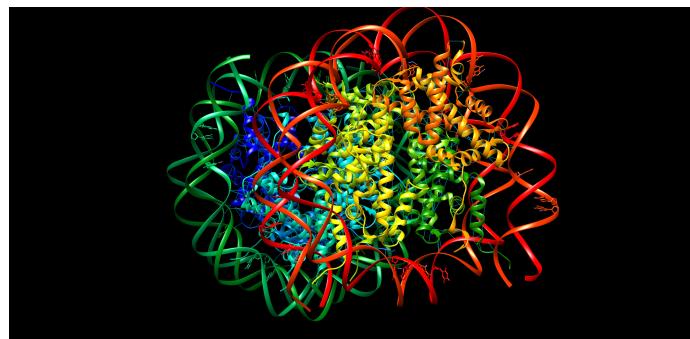


Figure 6: Visualize Hydrogen bonds

- **Nucleic acids:** colored magenta

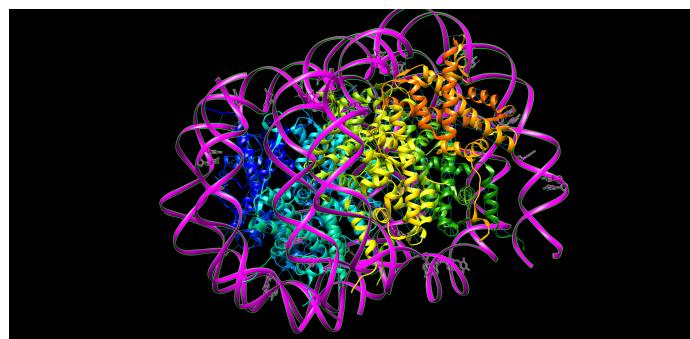


Figure 7: Visualize Nucleic acids

- **Remove all water particles:** colored magenta

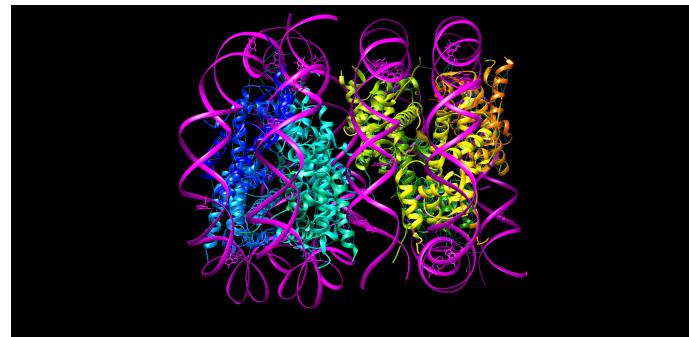


Figure 8: Visualize No water structure

- **Select all the lysines:** There are 1075 atoms, 964 bonds, 6 pseudobonds, 119 lysine residues

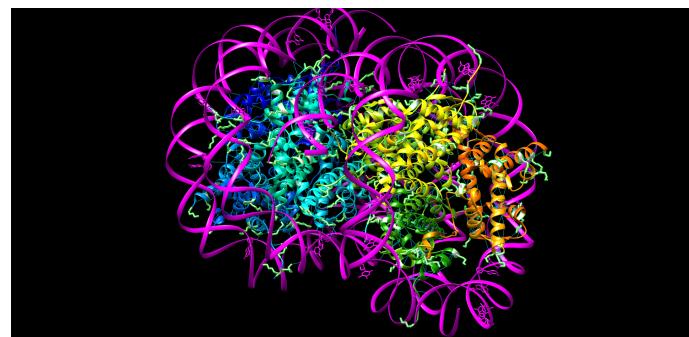


Figure 9: Visualize lysine

- **Display the surface of the DNA:** When attempting to visualize the DNA surface in Chimera, I encountered an error as depicted in the figure below. Subsequently, I exported the scene to Chimera and successfully displayed the DNA surface.

## Structural Analysis of Biomolecules Using UCSF Chimera

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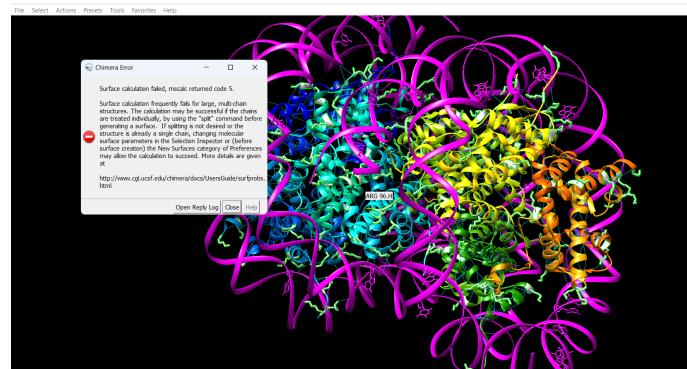


Figure 10: Visualize Error in viewing Surface DNA

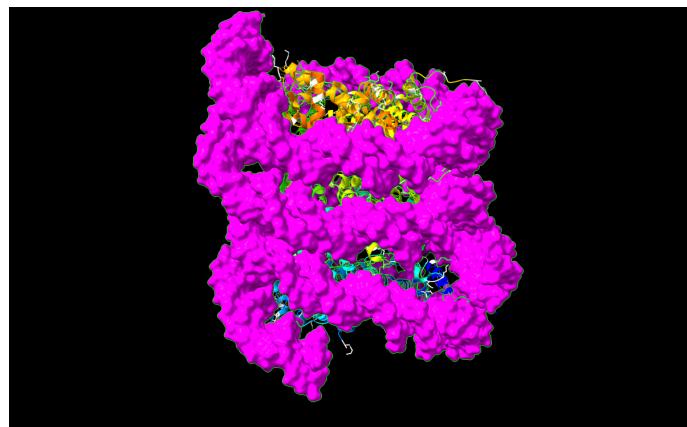


Figure 11: Visualize Surface of DNA

- **Video of the rotating structure:** When attempting to display the video with Chimera, it failed to function. Consequently, I had to resort to using ChimeraX once again. I have attached the session files from both Chimera and ChimeraX for reference.

## References

RCSB (2024), “Protein bank database.” URL <https://www.rcsb.org/>.