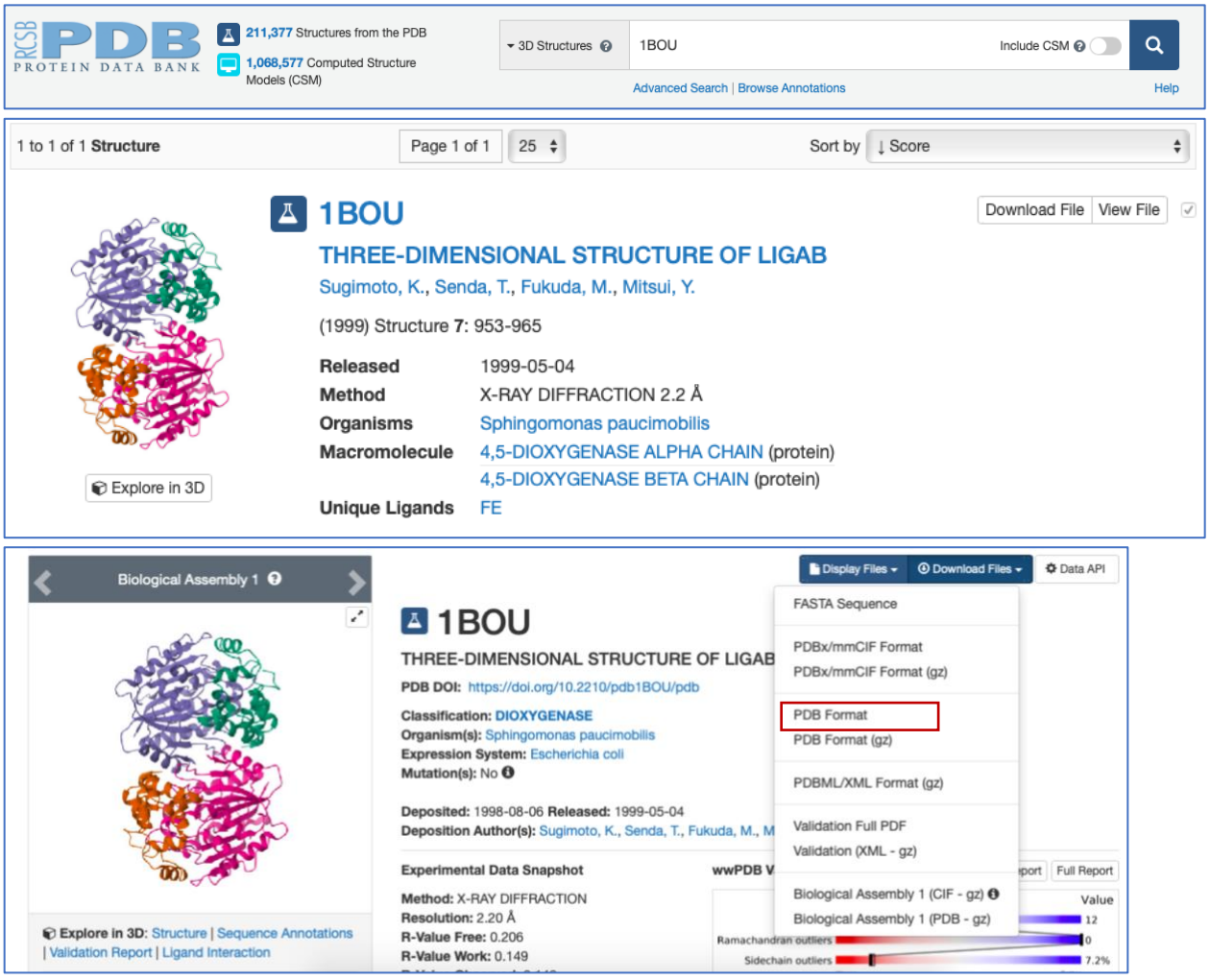
Lab sheet #8
Structure visualization using Jmol

RCSB Protein Data Bank (RCSB PDB) enables breakthroughs in science and education by providing access and tools for exploration, visualization, and analysis of:

1. Experimentally-determined 3D structures from the **Protein Data Bank (PDB)** archive
2. **Computed Structure Models (CSM)** from AlphaFold DB and ModelArchive

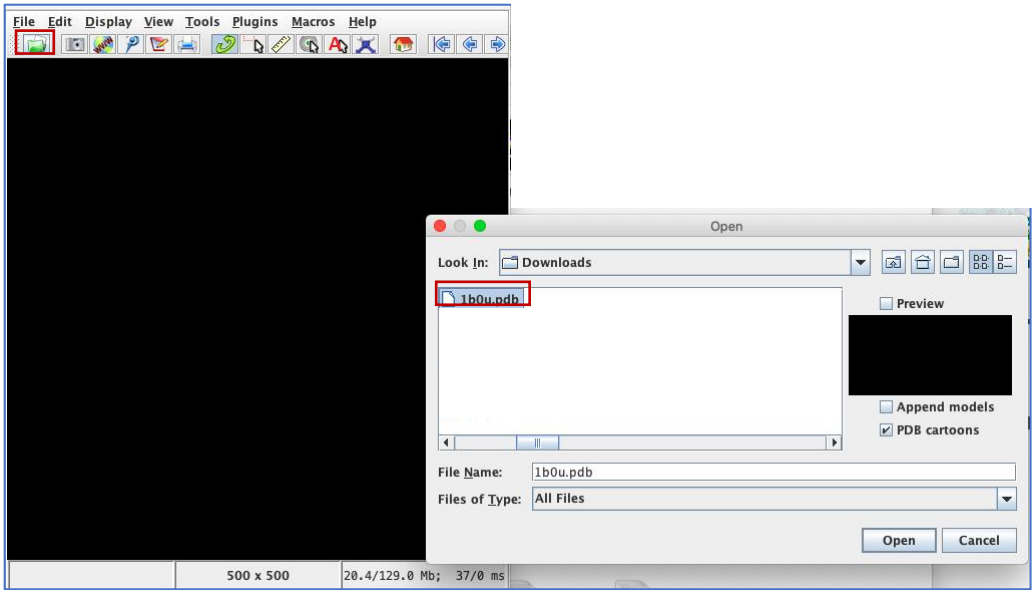
These data can be explored in context of external annotations providing a structural view of biology.

1. Open Protein Data Bank (**PDB**) website, Search for **1B0U** protein; which is the PDB ID of ATP-binding subunit of the histidine permease from *salmonella typhimurium*.

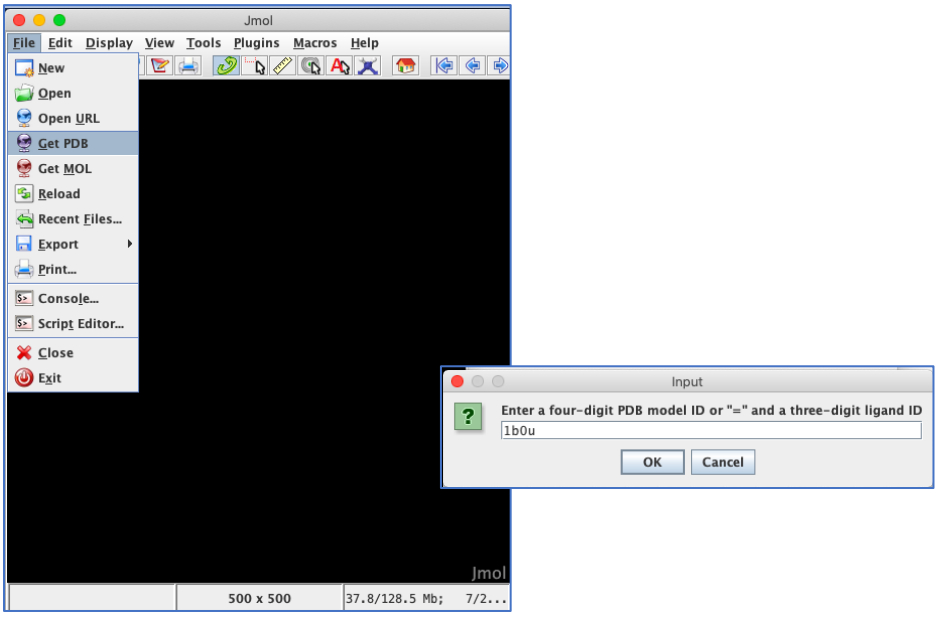


Jmol is a free molecular viewer, used to create and view three dimensional structures of proteins.

2. Open Jmol program and open the protein sequence file (File➔ Get PDB **OR** file➔ Open)

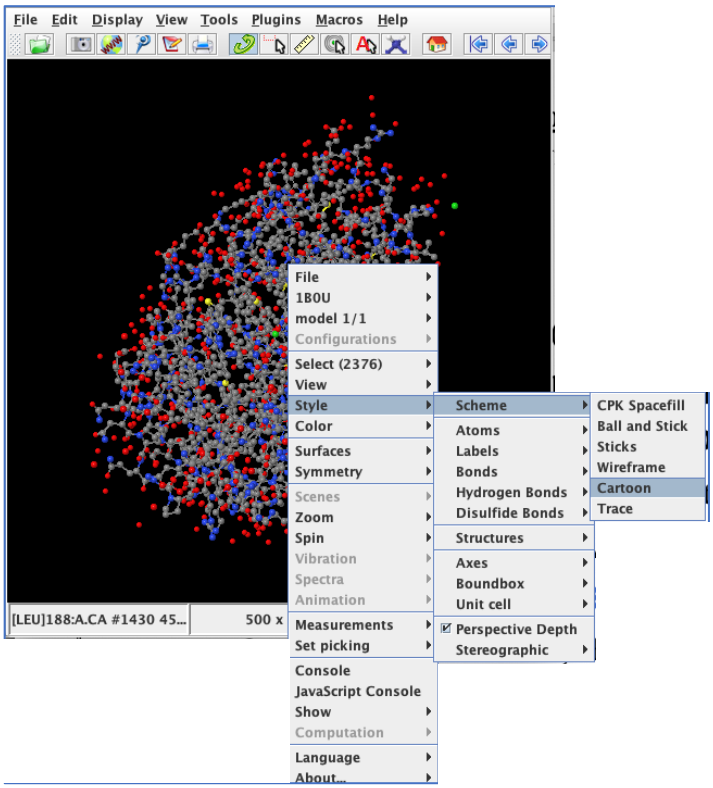


OR



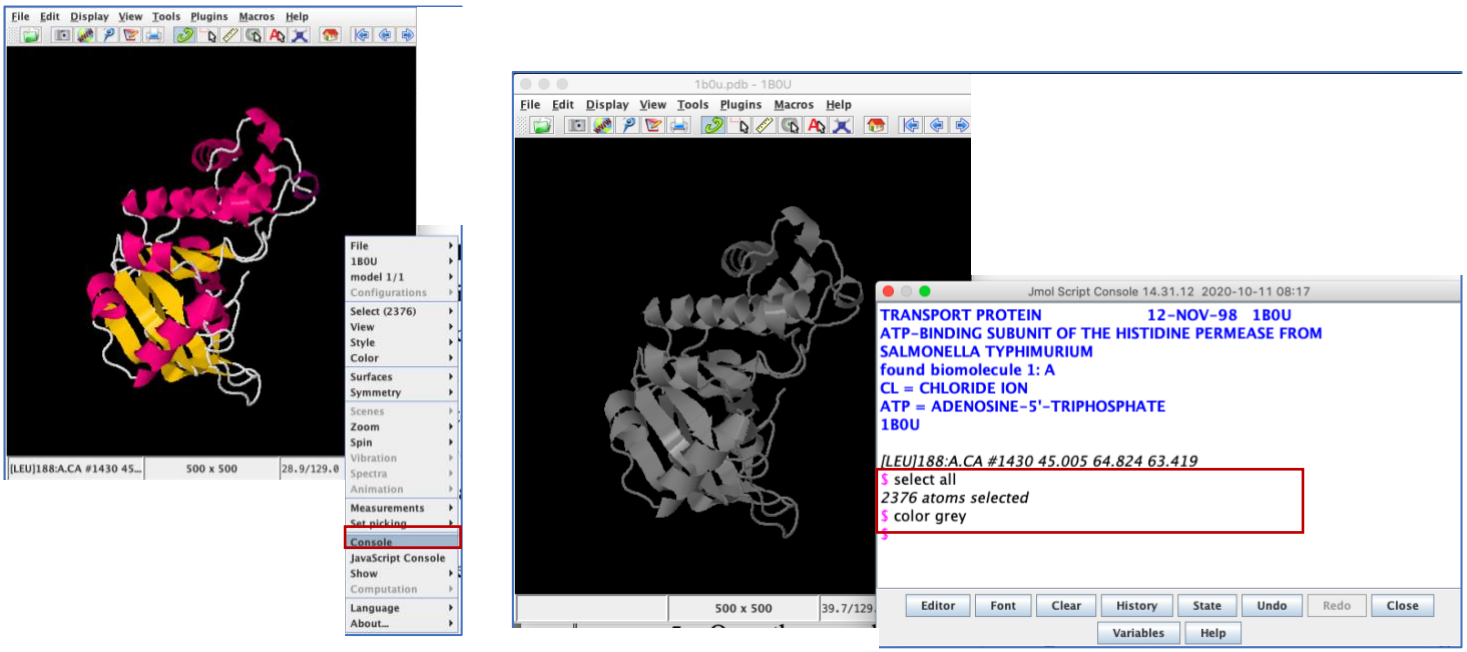
3. Change Style display from Atom style to **<u>Cartoon</u>** scheme style

(Click right ➔ Style➔ Scheme➔ Cartoon).

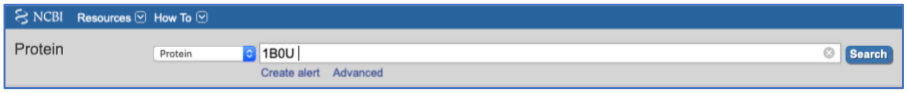


4. Open the console window, change the **color** of the whole structure to **grey**.

(Click right ➔ Console➔ Type: select all➔ Press enter➔ Type: color grey➔ Press enter).



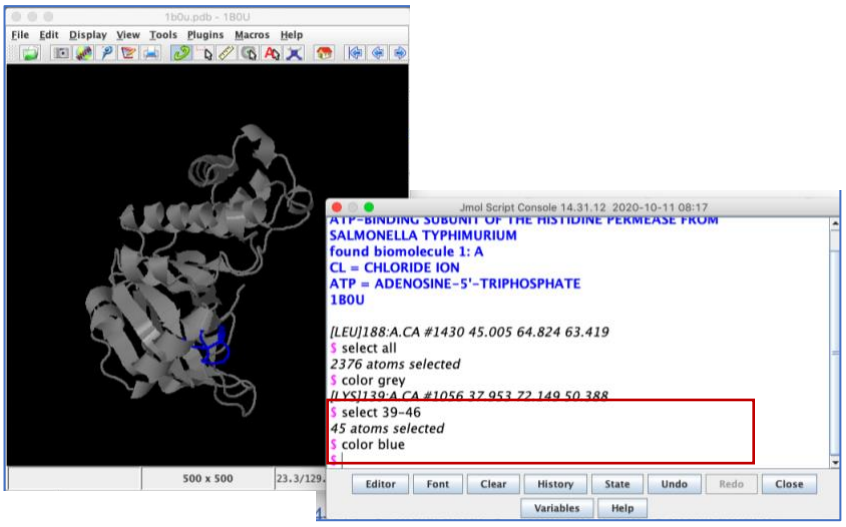
5. Open the protein page in **protein database (NCBI)** to know the different motifs of the protein and their location.



6. Select the **Walker A/P-loop motif** (39-46), and color it by blue.

(Type: select 39-46 ➔ Press enter➔ Type: color blue➔ Press enter).

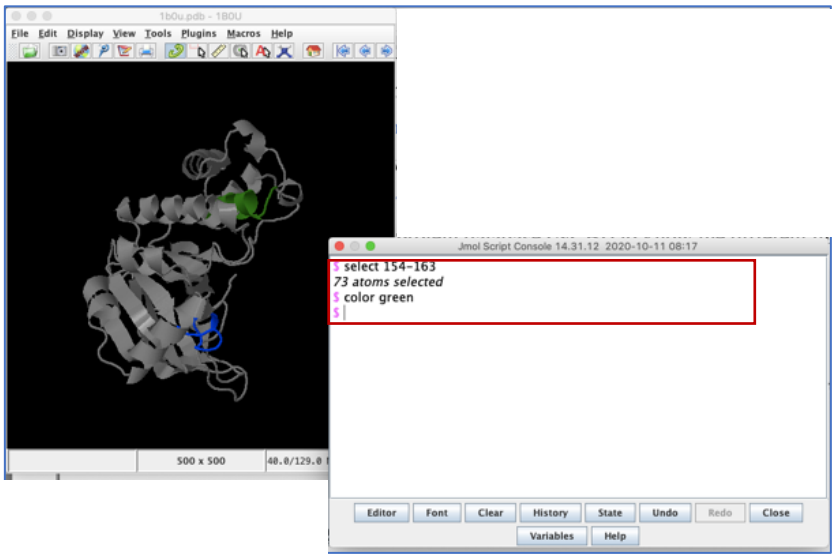
```
Site            39..46
                /site_type="other"
                /note="Walker A/P-loop"
                /db_xref="CDD:213229"
```



7. Select the **ABC transporter signature motif** (154-163), and color it to green.

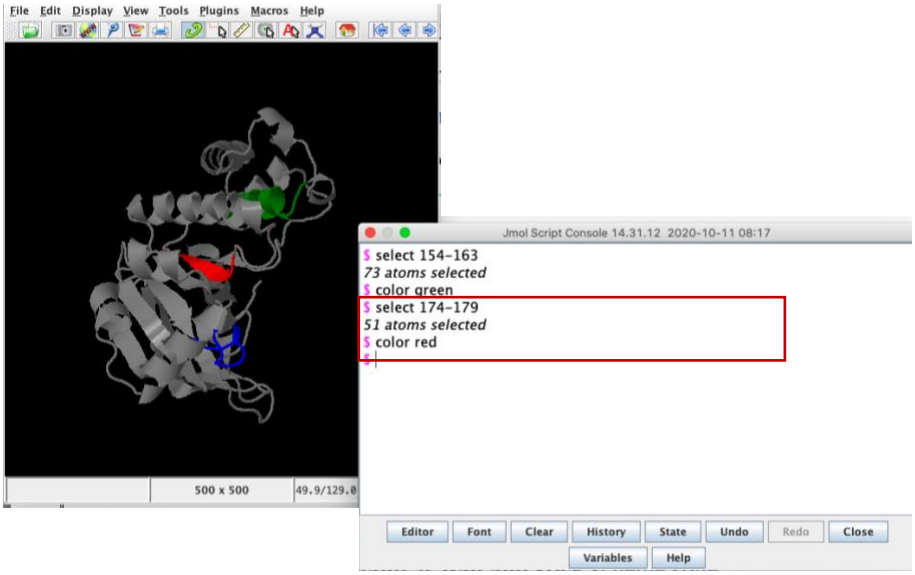
(Type: select 154-163 ➔ Press enter➔ Type: color green ➔ Press enter).

```
Site            154..163
                /site_type="other"
                /note="ABC transporter signature motif"
                /db_xref="CDD:213229"
```



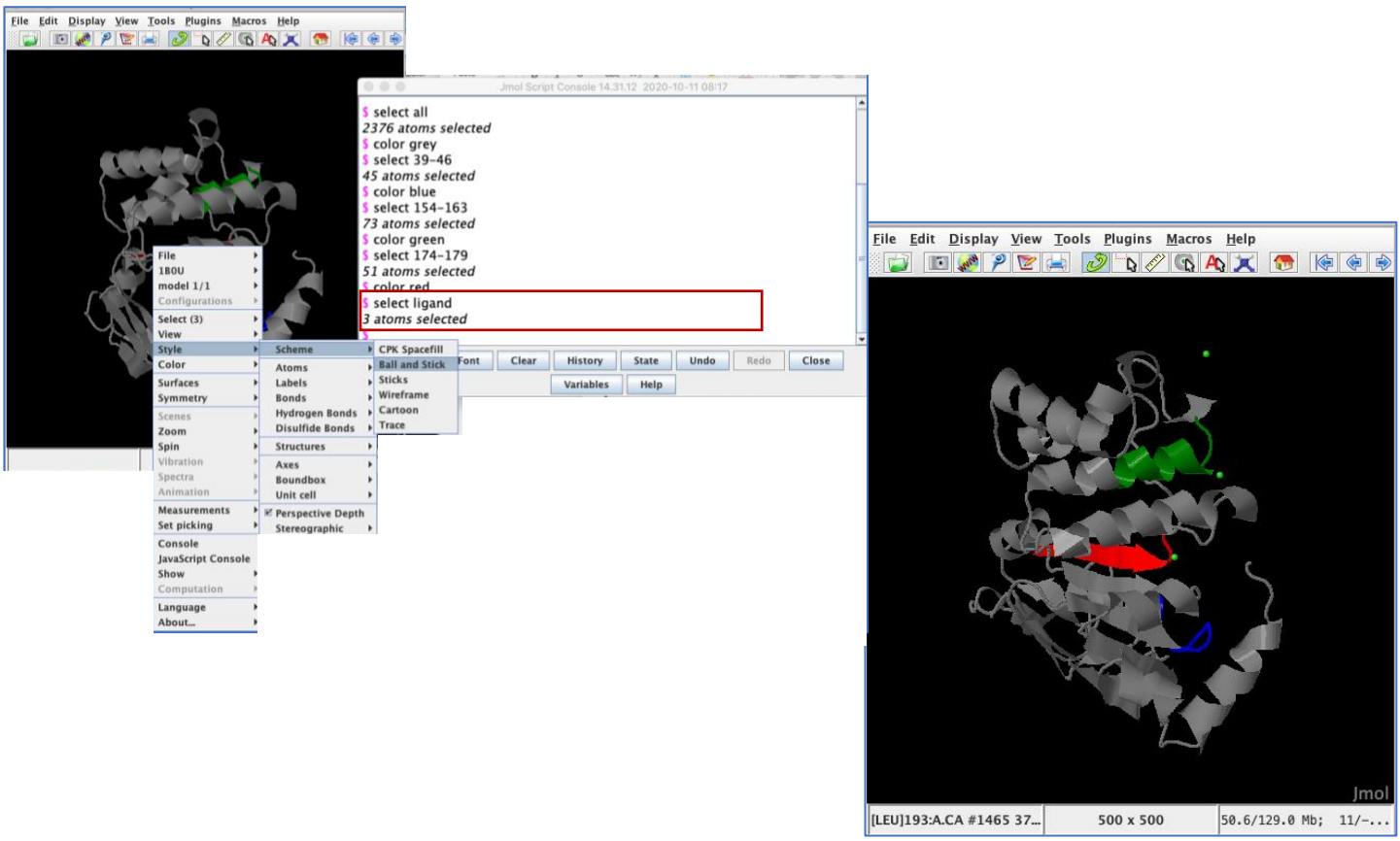
8. Select **Walker B motif** (174-179), and color it red.

(Type: select 174-179 ➔ Press enter➔ Type: color red ➔ Press enter).

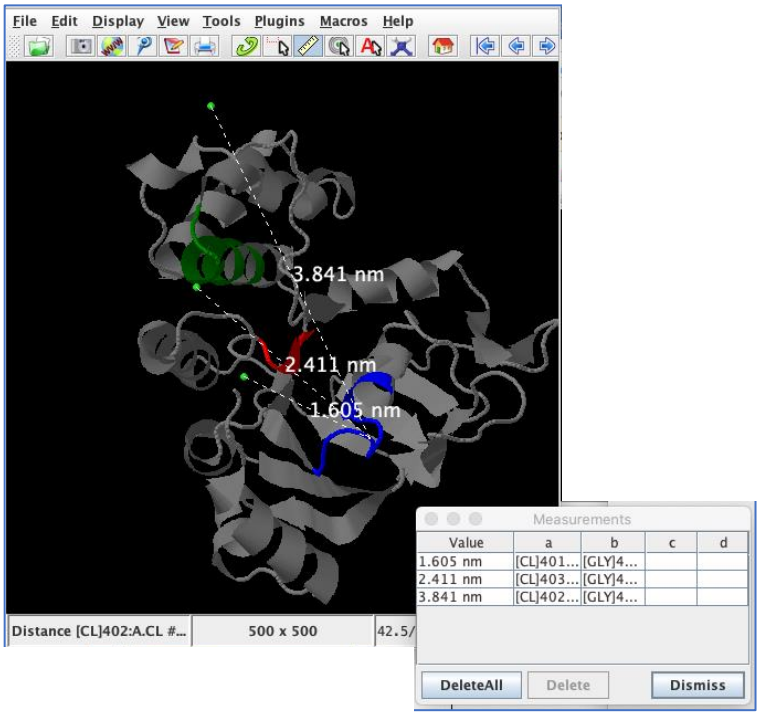


9. Show the ATP **ligand** as **<u>Ball and stick</u>** scheme style.

(Type: select ligand ➔ Press enter ➔ Click right ➔ Style ➔ Scheme➔ Ball and stick).

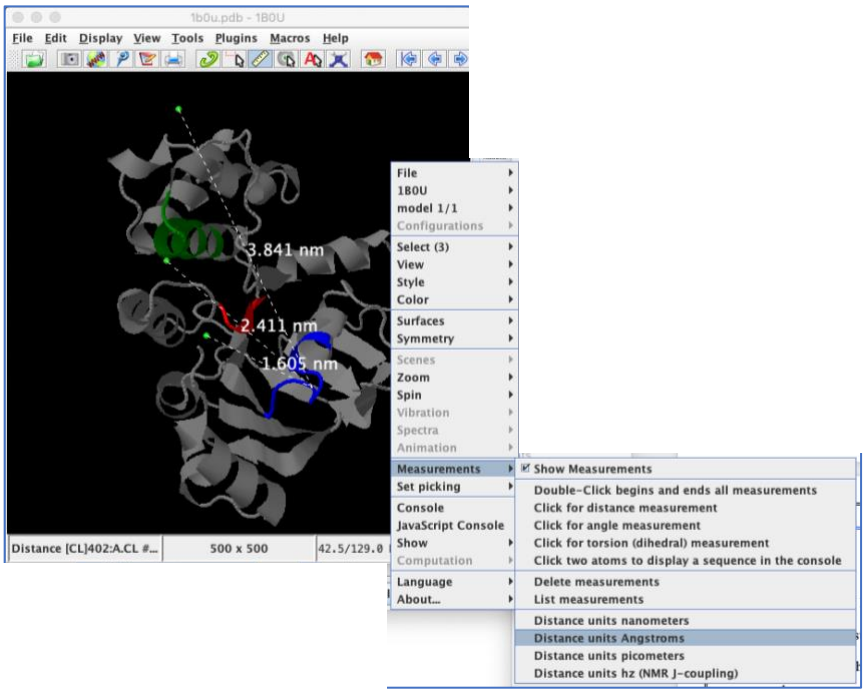


10. Show which one is closest to **Walker A/P-loop motif** and measure the **distance** between them. (Toolbar➔ Click the ruler icon)

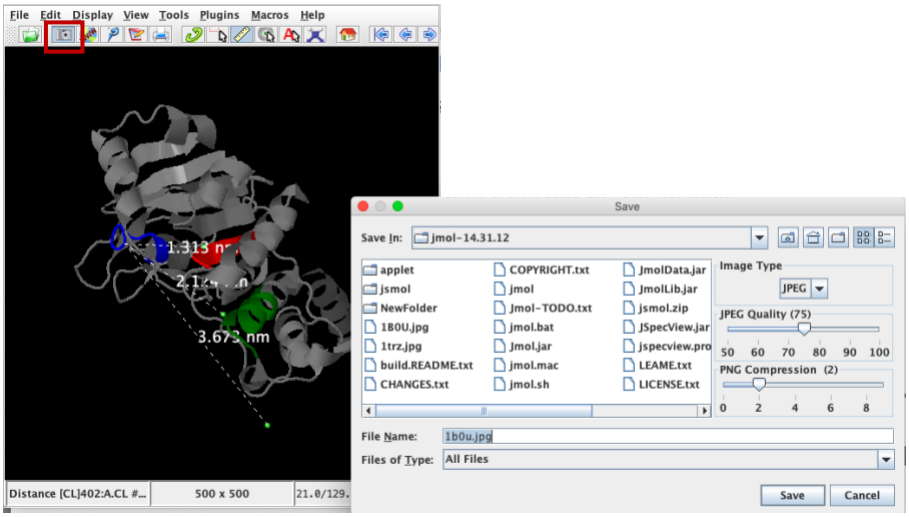


11. Change the measurement unit from **nm to Angstroms**.

(Click right ➔ Measurements➔ Distance unites angstroms)



12. Save the protein structure as a picture. (Toolbar➔ Click the camera icon)



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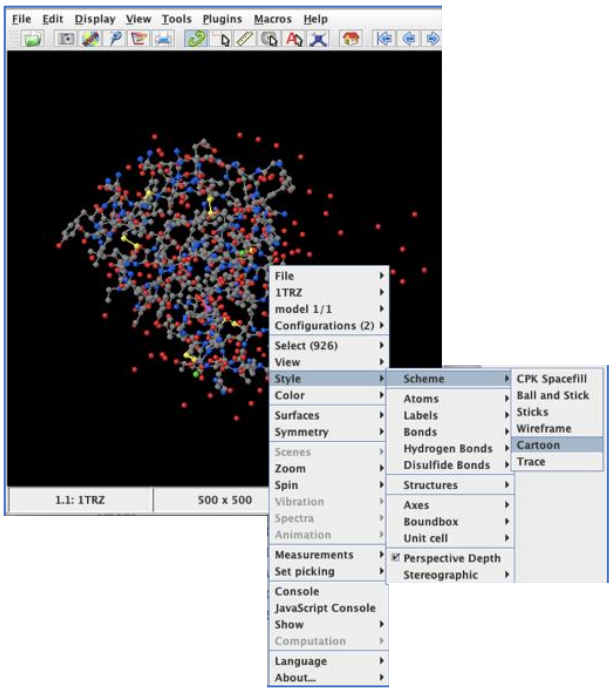
1. Open Protein Data Bank (**PDB**) website, Search for **1TRZ** protein; which is the PDB ID of Human Insulin hexamer.

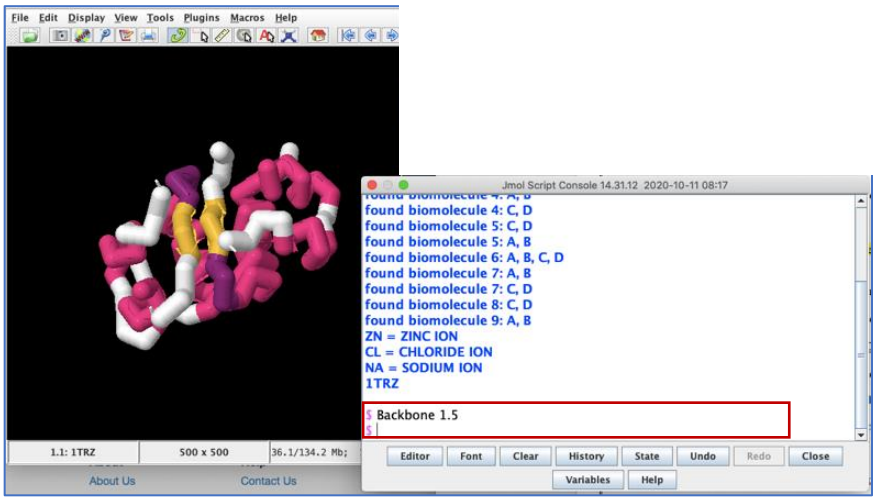
2. Change Style display from Atom style to **<u>Cartoon</u>** scheme style.

(Click right ➔ Style➔ Scheme➔ Cartoon).

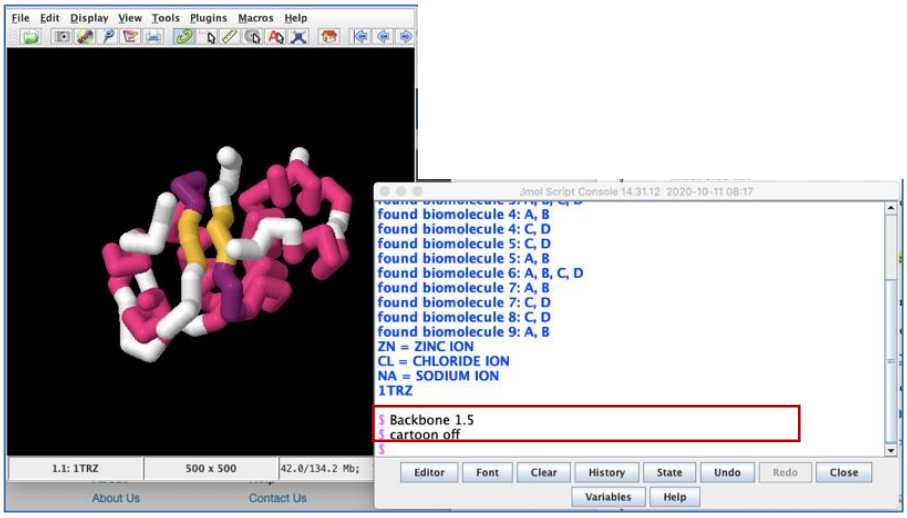


3. Change Style display to **Backbone 1.5** scheme style.

(Click right ➔ Console➔ Type: Backbone 1.5➔ Press enter).

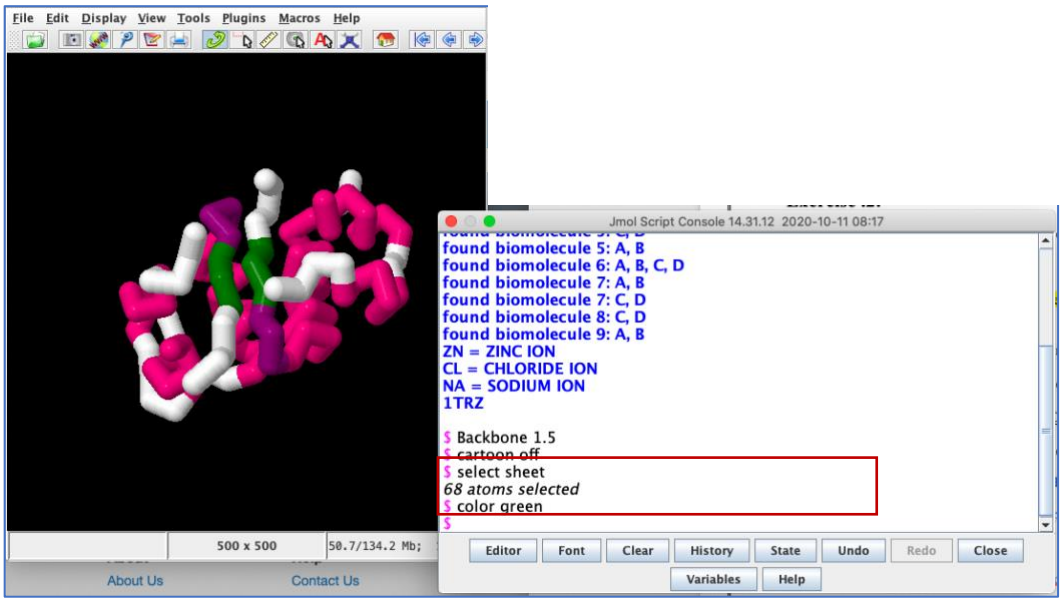


4. Turn cartoon style off. (Type: cartoon off➔ Press enter)



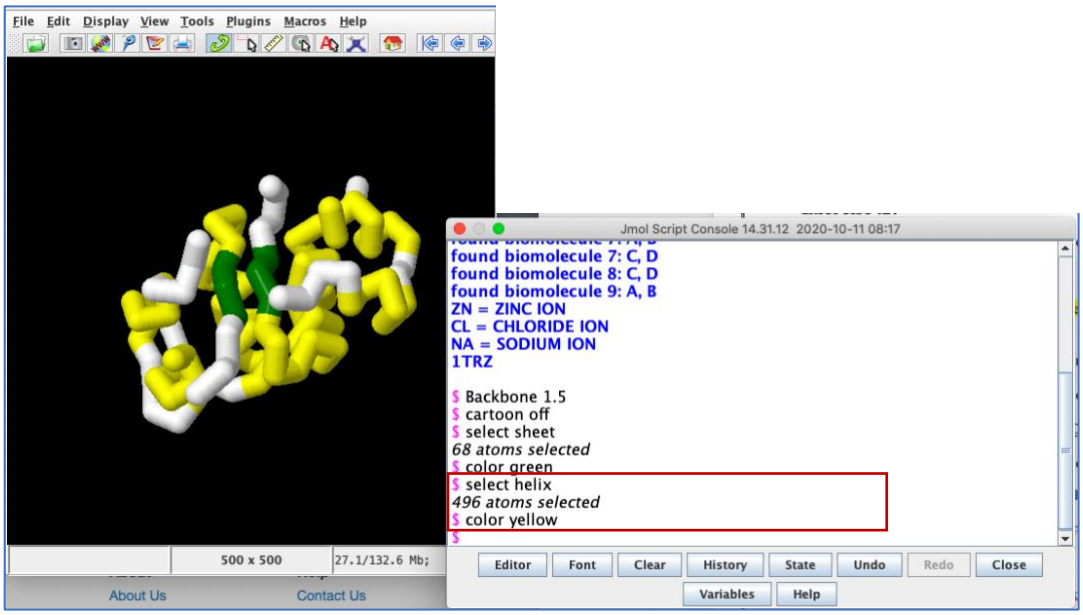
5. Select sheets and color it green.

(Type: select sheets ➔ Press enter➔ Type: color green ➔ Press enter)



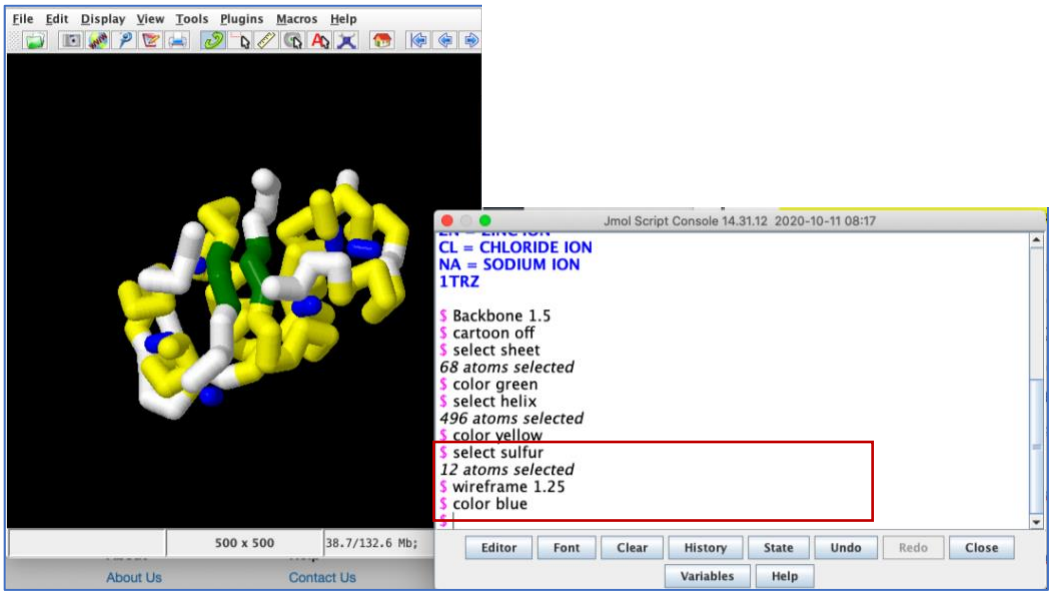
6. Select helix and color yellow.

(Type: select helix ➔ Press enter➔ Type: color yellow➔ Press enter)

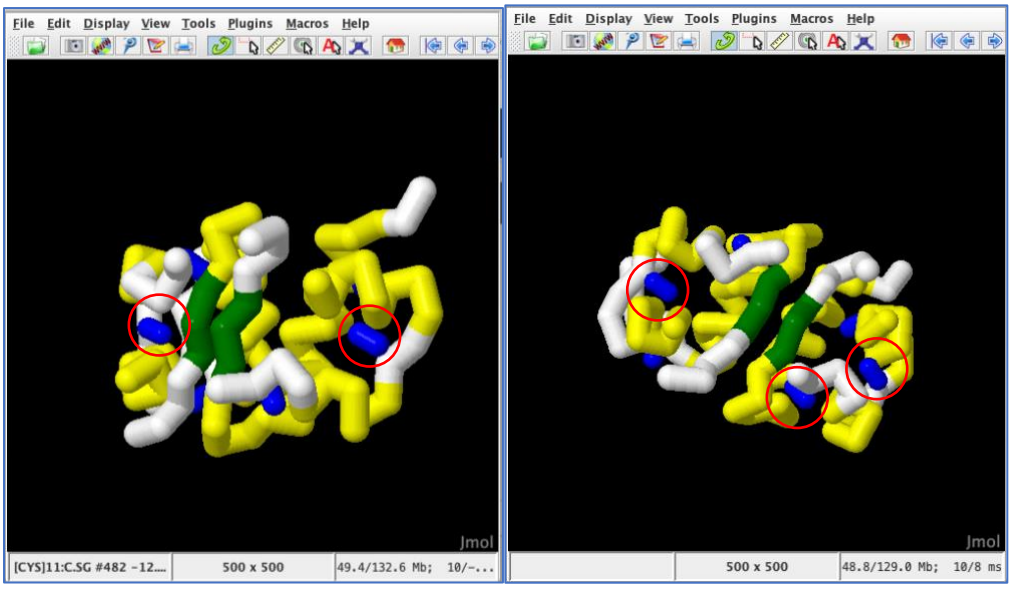


7. Show cysteins (Sulfur) that forms disulphide bridges "showing how the polypeptides hold together through S-S bonds". Change to wireframe 1.25 and color them blue.

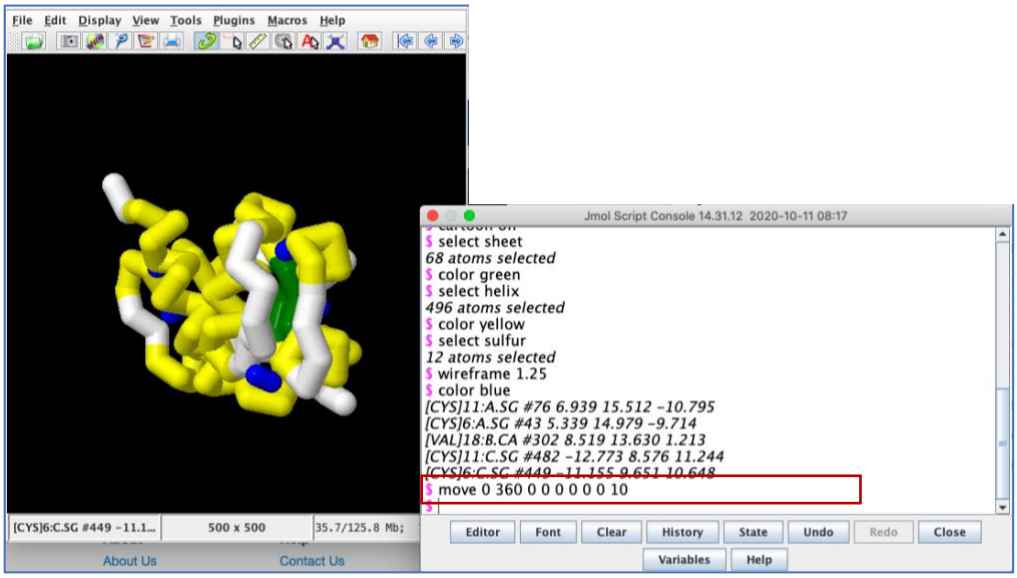
(Type: select sulfur ➔ Press enter➔ Type: wireframe 1.25➔Press enter➔Type: color blue).



8. Show for each disulphide bridge the position of each Cys and the chain involved.



9. Move the structure 360º. (Type: move 0 360 0 0 0 0 0 0 10 ➔ Press enter)



10. Save the protein structure.