

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 **1BOU** protein; which is the PDB ID of ATP-binding subunit of the histidine permease from *salmonella typhimurium*.

RCSB PDB PROTEIN DATA BANK

211,377 Structures from the PDB

4,068,577 Computed Structure Models (CSM)

3D Structures 1BOU

Include CSM

Advanced Search | Browse Annotations

1 to 1 of 1 Structure

Page 1 of 1 25

Sort by Score

1BOU

THREE-DIMENSIONAL STRUCTURE OF LIGAB

Sugimoto, K., Senda, T., Fukuda, M., Mitsui, Y.

(1999) Structure 7: 953-965

Released 1999-05-04

Method X-RAY DIFFRACTION 2.2 Å

Organisms *Sphingomonas paucimobillis*

Macromolecule 4,5-DIOXYGENASE ALPHA CHAIN (protein)
4,5-DIOXYGENASE BETA CHAIN (protein)

Unique Ligands FE

Download File View File

Explore in 3D

Biological Assembly 1

1BOU

THREE-DIMENSIONAL STRUCTURE OF LIGAB

PDB DOI: <https://doi.org/10.2210/pdb1BOU/pdb>

Classification: DIOXYGENASE

Organism(s): *Sphingomonas paucimobillis*

Expression System: *Escherichia coli*

Mutation(s): No

Deposited: 1998-08-06 **Released:** 1999-05-04

Deposition Author(s): Sugimoto, K., Senda, T., Fukuda, M., Mitsui, Y.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 2.20 Å

R-Value Free: 0.206

R-Value Work: 0.149

Display Files Download Files Data API

FASTA Sequence

PDBx/mmCIF Format

PDBx/mmCIF Format (gz)

PDB Format

PDB Format (gz)

PDBML/XML Format (gz)

Validation Full PDF

Validation (XML - gz)

Biological Assembly 1 (CIF - gz)

Biological Assembly 1 (PDB - gz)

Report Full Report

Value

12

0

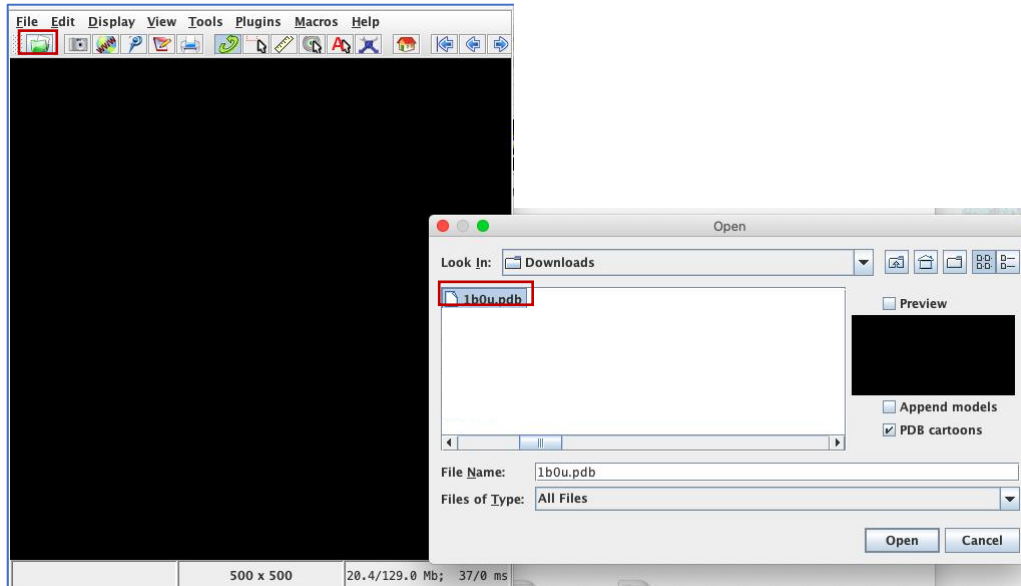
Ramachandran outliers

Sidechain outliers

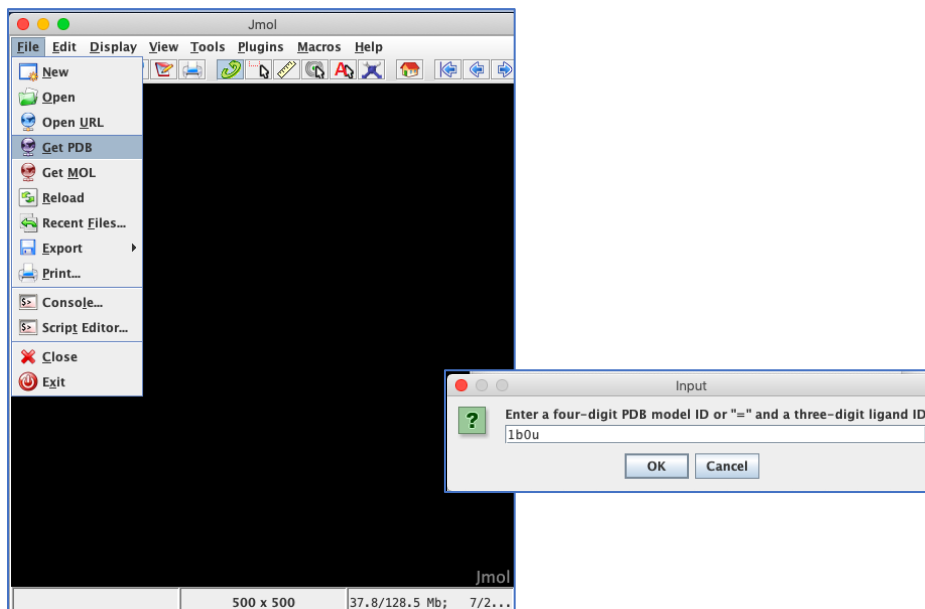
7.2%

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)

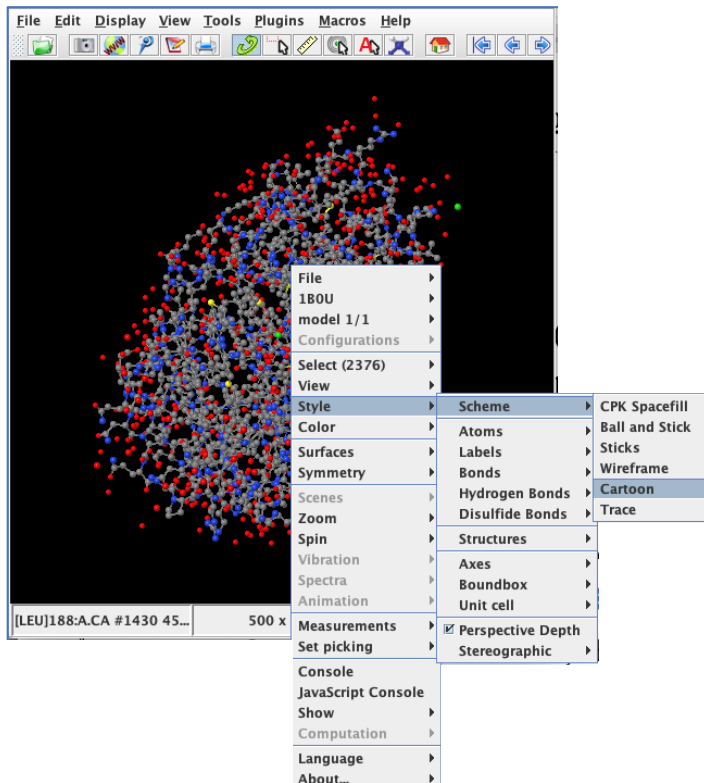


OR



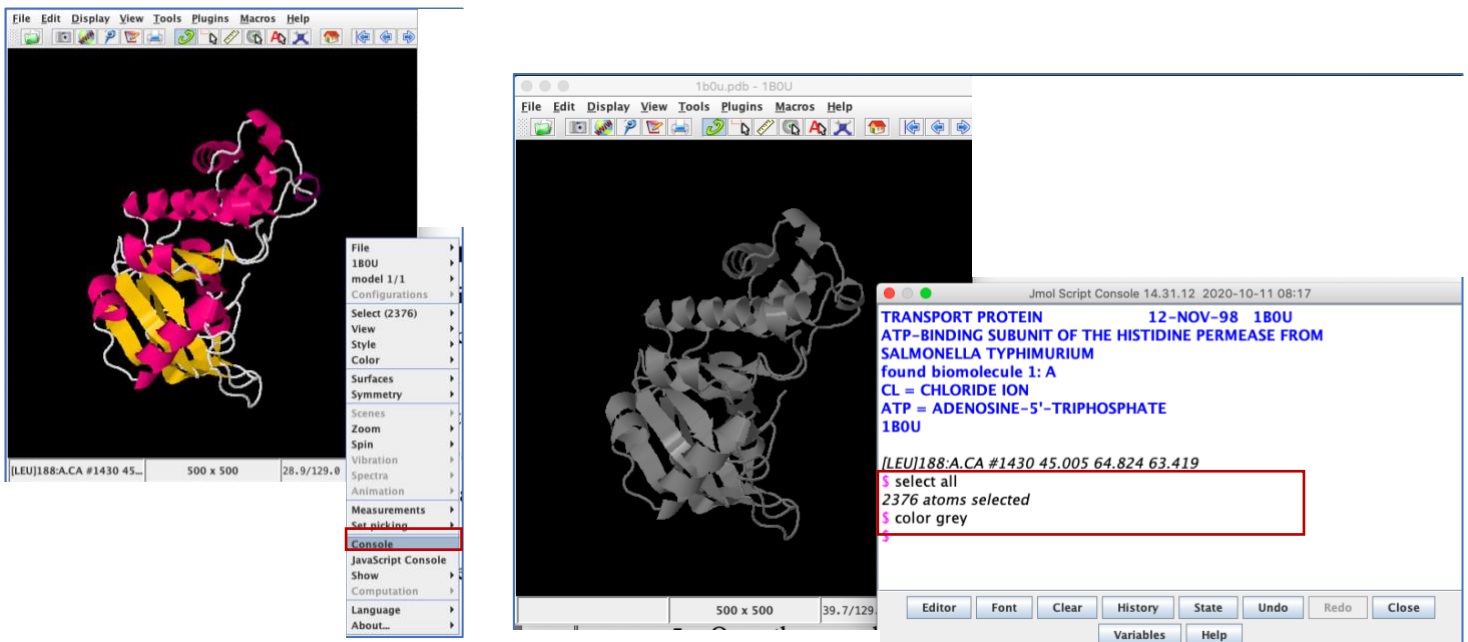
3. Change Style display from Atom style to **Cartoon** scheme style

(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).



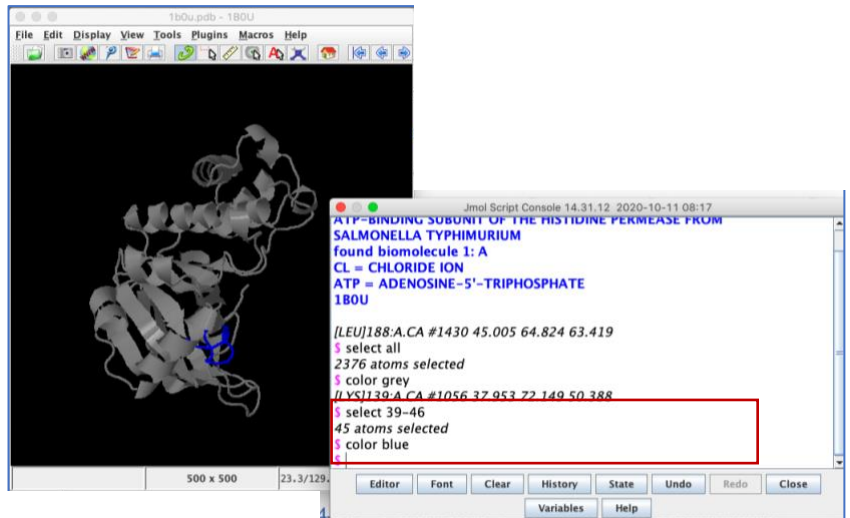
- Open the protein page in **protein database (NCBI)** to know the different motifs of the protein and their location.



- 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).

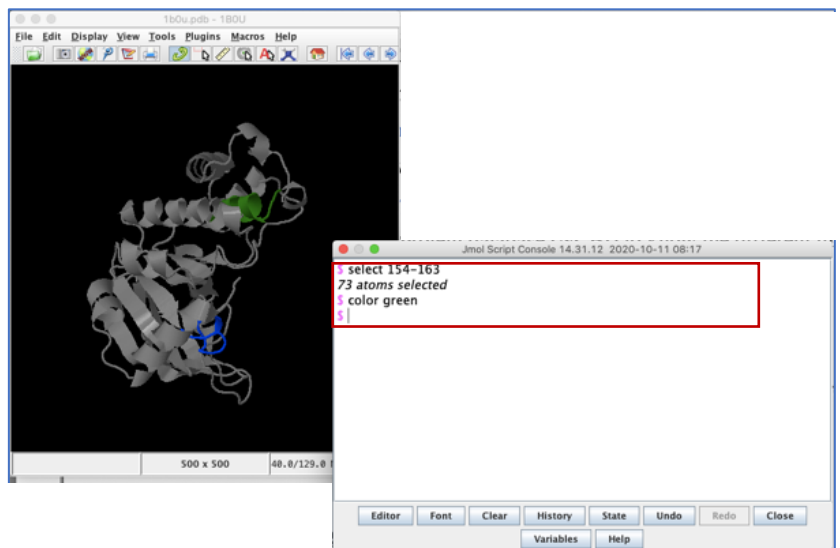
```
Site 39..46
/site_type="other"
/note="Walker A/P-loop"
/db_xref="CDD:213229"
```



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

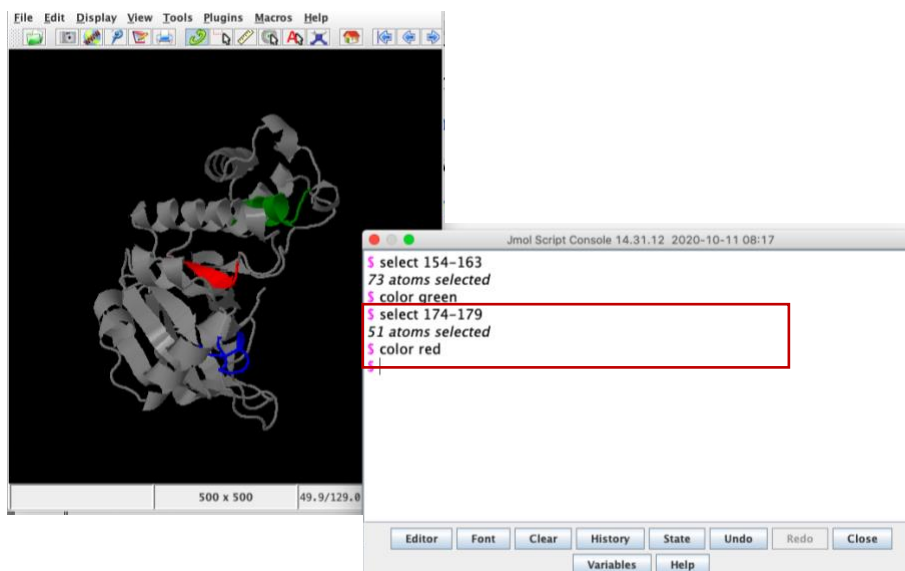
(Type: select 154-163 → Press enter → Type: color green → Press enter).

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



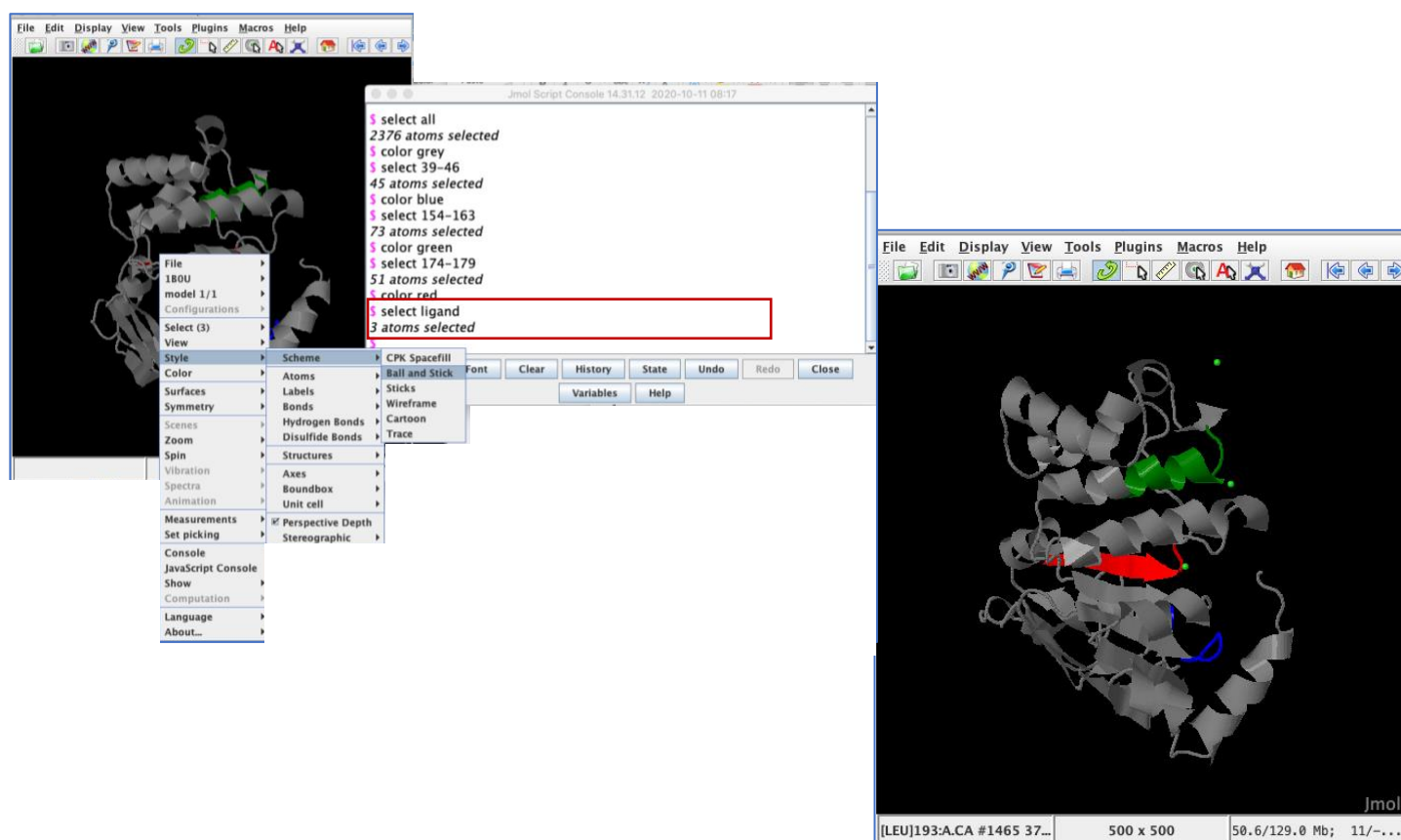
8. Select **Walker B motif** (174-179), and color it red.

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

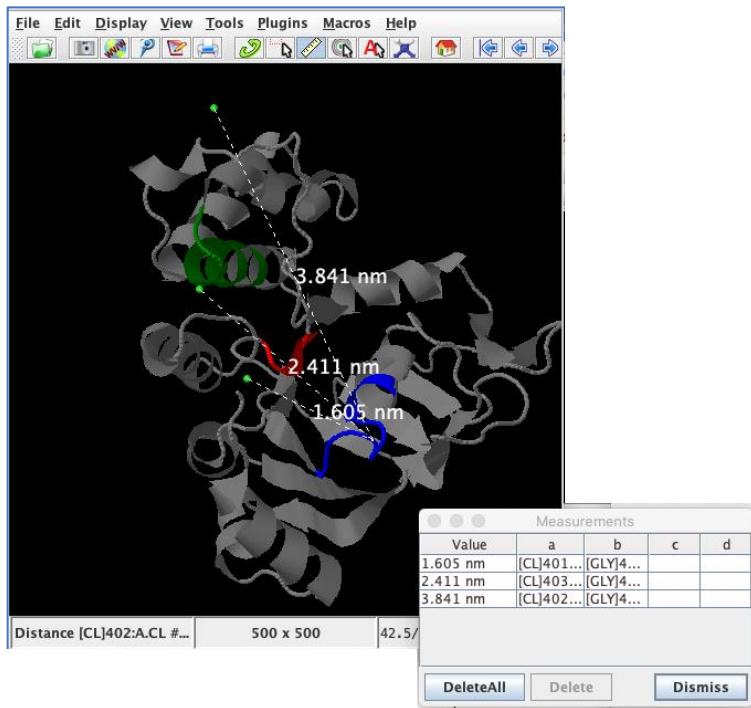


9. Show the ATP ligand as **Ball and stick** scheme style.

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

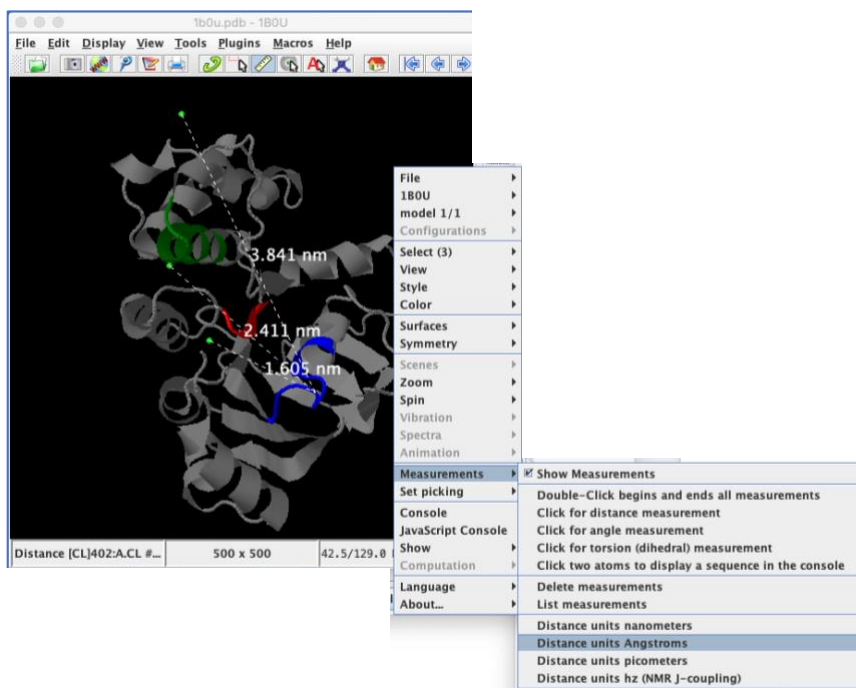


10. Show which one is closest to **Walker A/P-loop motif** and measure the **distance** between them. (Toolbar → Click the ruler icon)

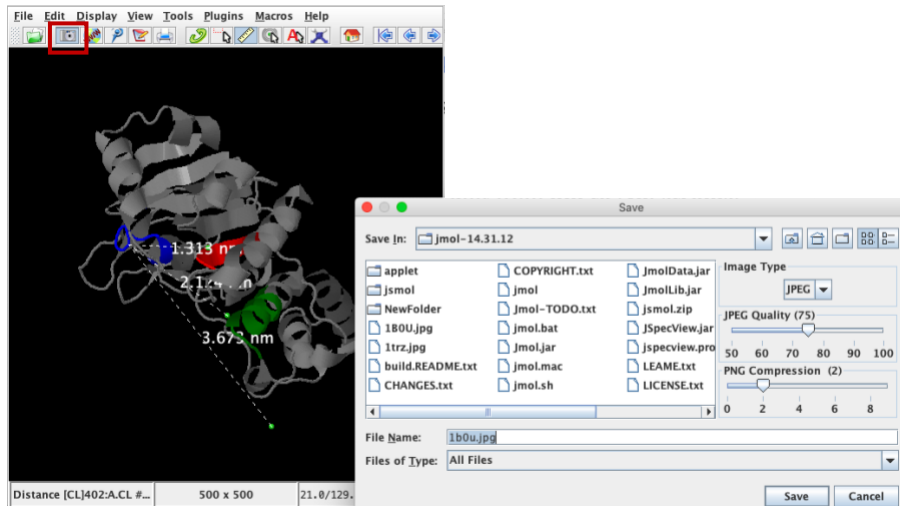


11. Change the measurement unit from **nm to Angstroms**.

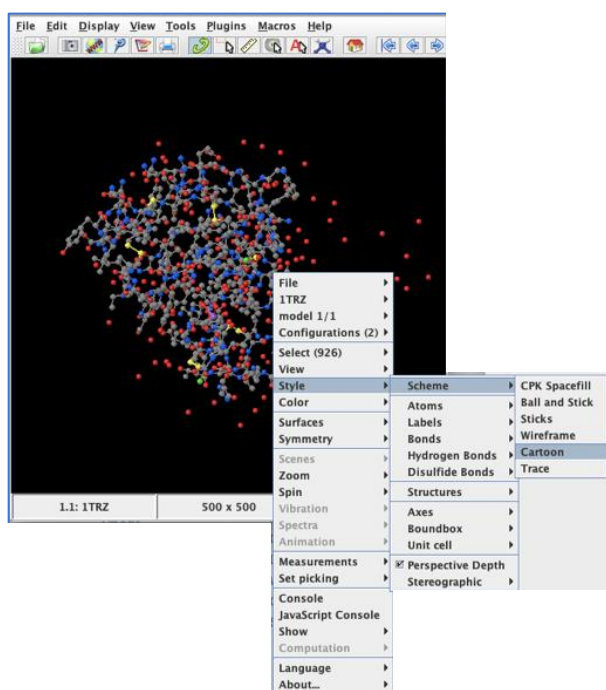
(Click right → Measurements → Distance units angstroms)



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

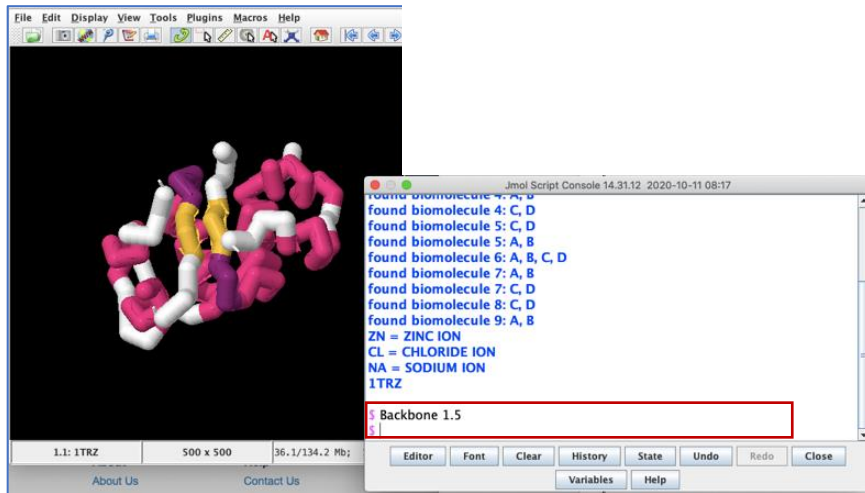


1. Open Protein Data Bank (**PDB**) website, Search for **1TRZ** protein; which is the PDB ID of Human Insulin hexamer.
2. Change Style display from Atom style to **Cartoon** scheme style.
(Click right → Style → Scheme → Cartoon).

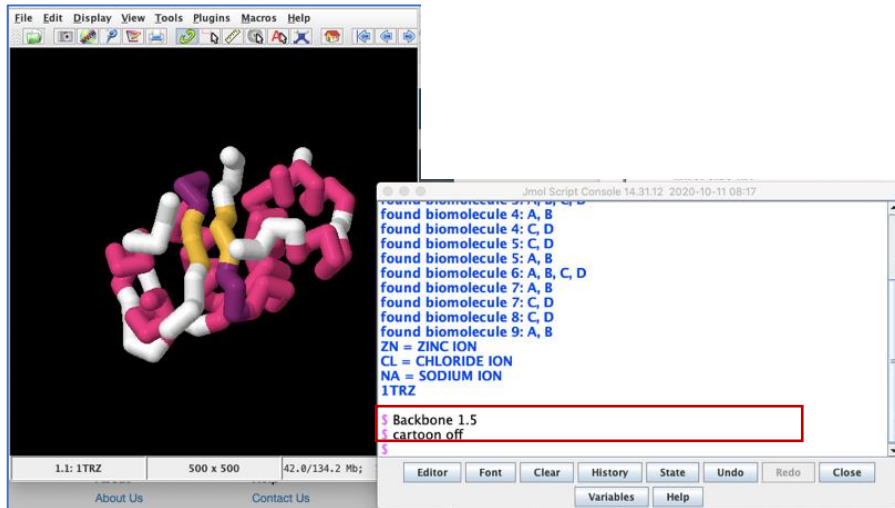


3. Change Style display to **Backbone 1.5** scheme style.

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

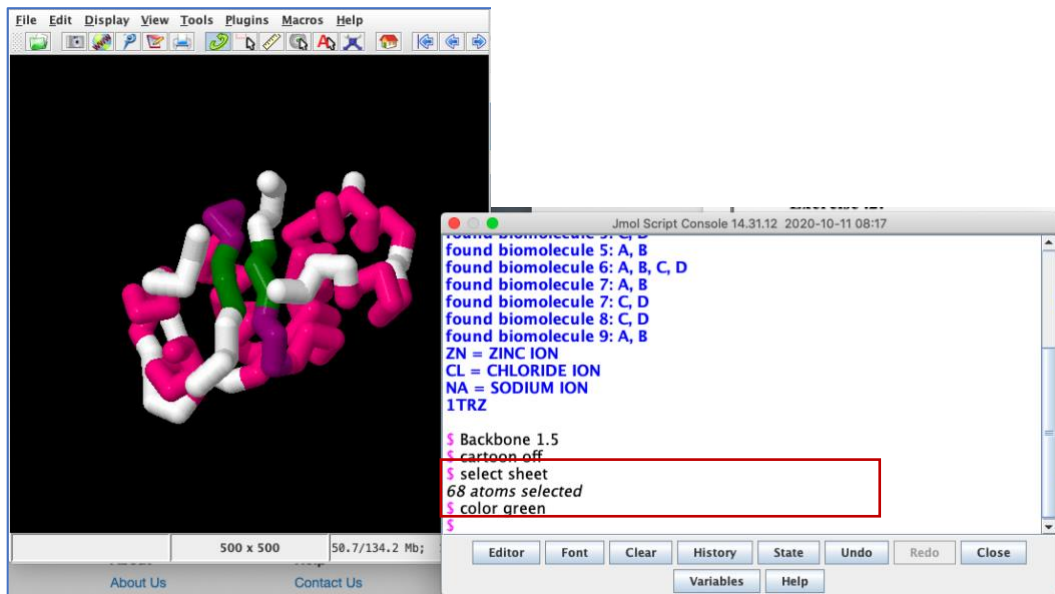


4. Turn cartoon style off. (Type: cartoon off → Press enter)



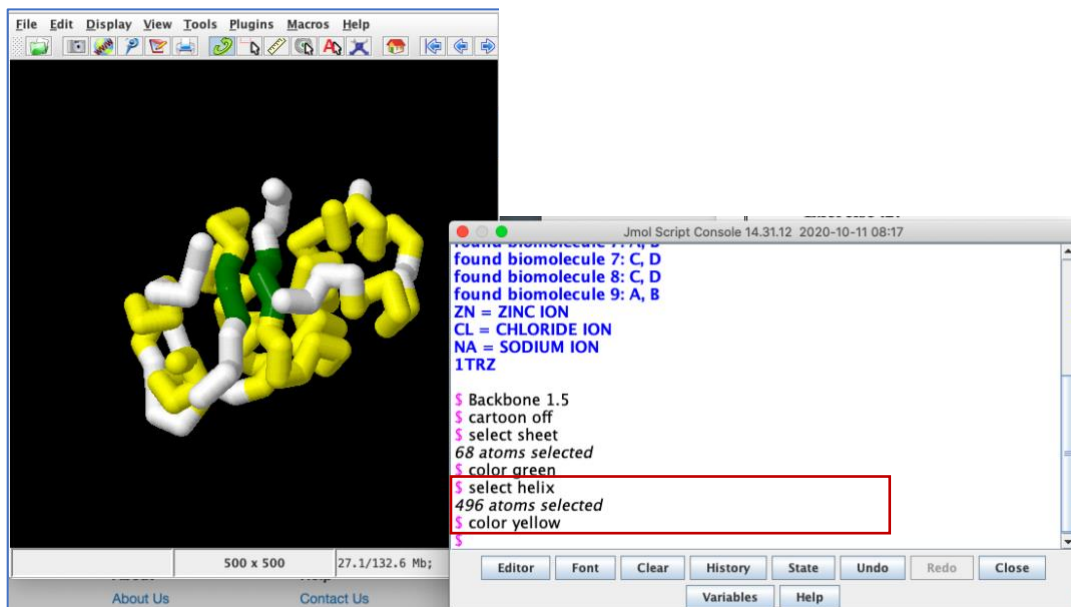
5. Select sheets and color it green.

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



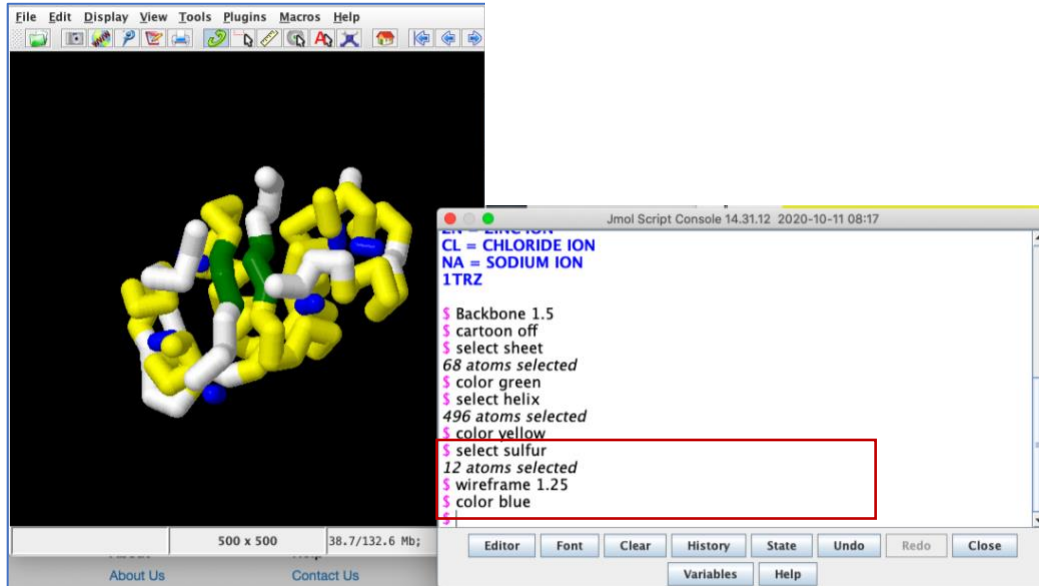
6. Select helix and color yellow.

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

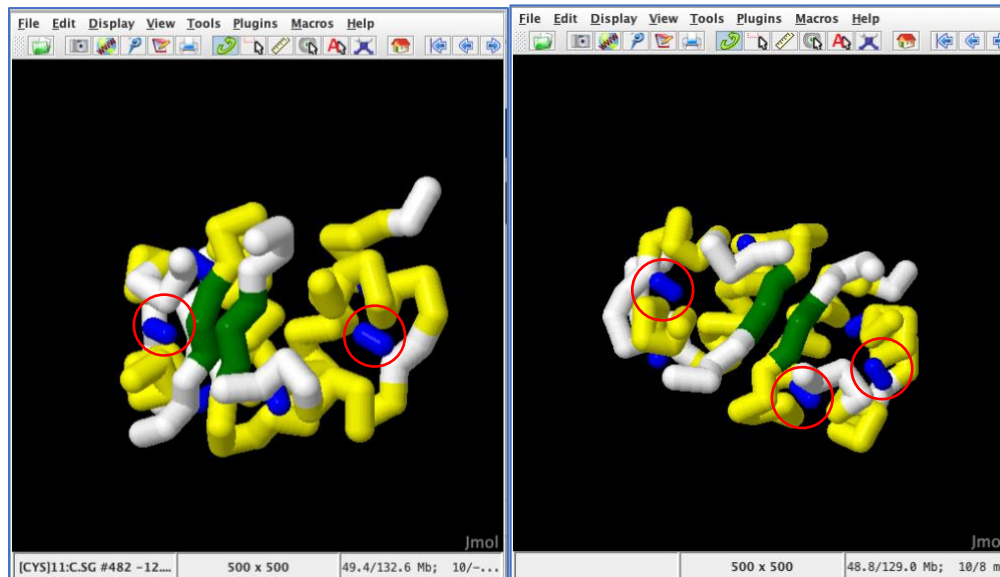


7. Show cysteines (Sulfur) that forms disulphide bridges “showing how the polypeptides hold together through S-S bonds”. Change to wireframe 1.25 and color them blue.

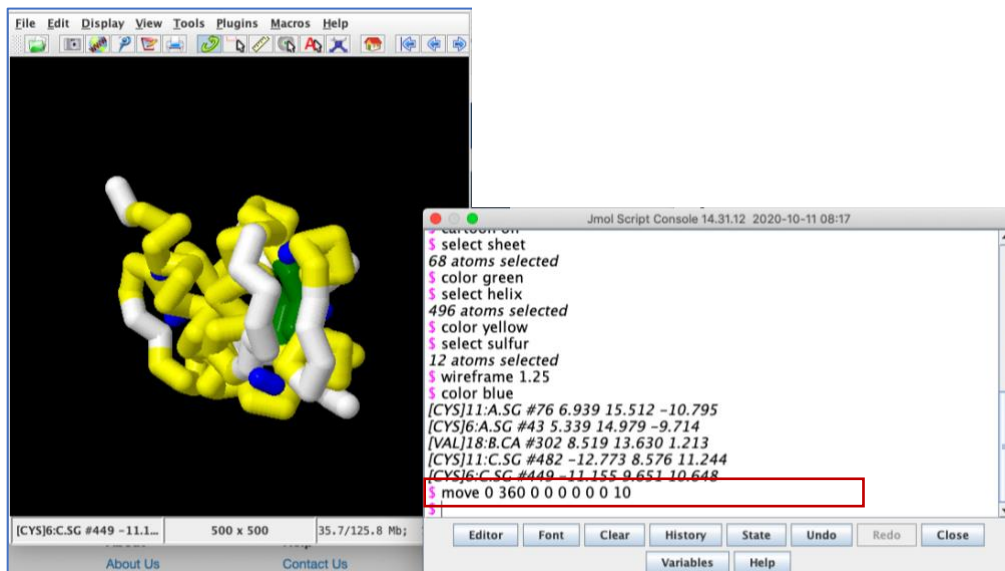
(Type: select sulfur → Press enter → Type: wireframe 1.25 → Press enter → Type: color blue).



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



9. Move the structure 360°. (Type: `move 0 360 0 0 0 0 0 10` → Press enter)



10. Save the protein structure.

