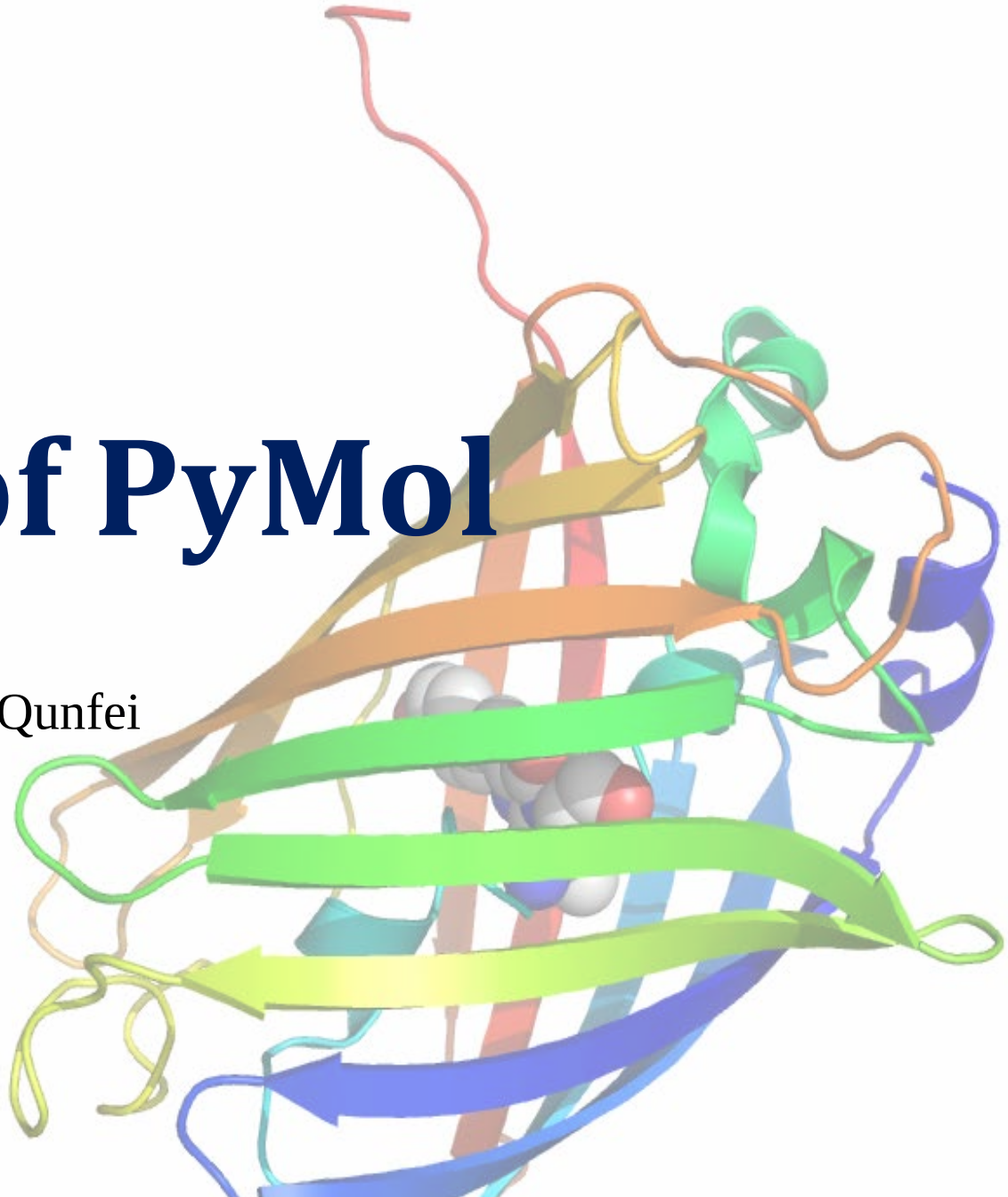
Learning notes of PyMol

Zhou Qunfei



Content

- **What is PyMol?**
- **What PyMol looks like?**
- **Why PyMol can draw amazing pictures?**
- **What can we do by using PyMol?**

  -Measurement

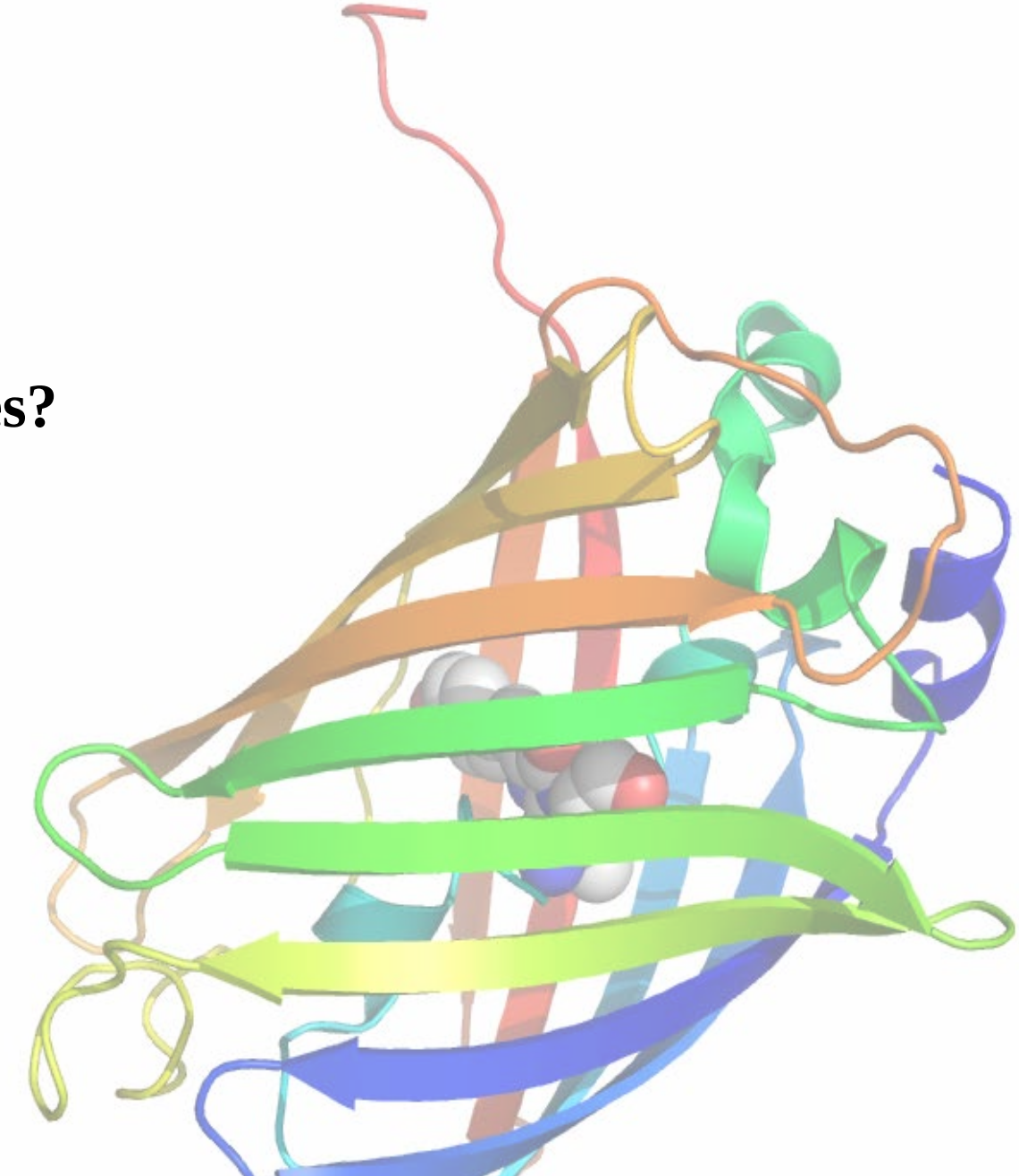
  -Structure alignment

  -Electrostatics surface

  -Highlight the ligand and the interactions

  -Electron density map

  -Making movies



What is PyMol?

A Powerful Desktop Molecular Graphical Tool which is also making progress to become a research tool!!

Why we choose PyMol?

Visualization is essential to understanding structural biology.

(1) Visualize multiple conformations of a single structure;

(2) Interface with external programs;

(3) Provide professional strength graphics under both Windows and Unix;

(4) Prepare publication quality images;

(5) Fit into a tight budget.

What’s the differences between PyMol and Swiss-pdbViewer?

I think…

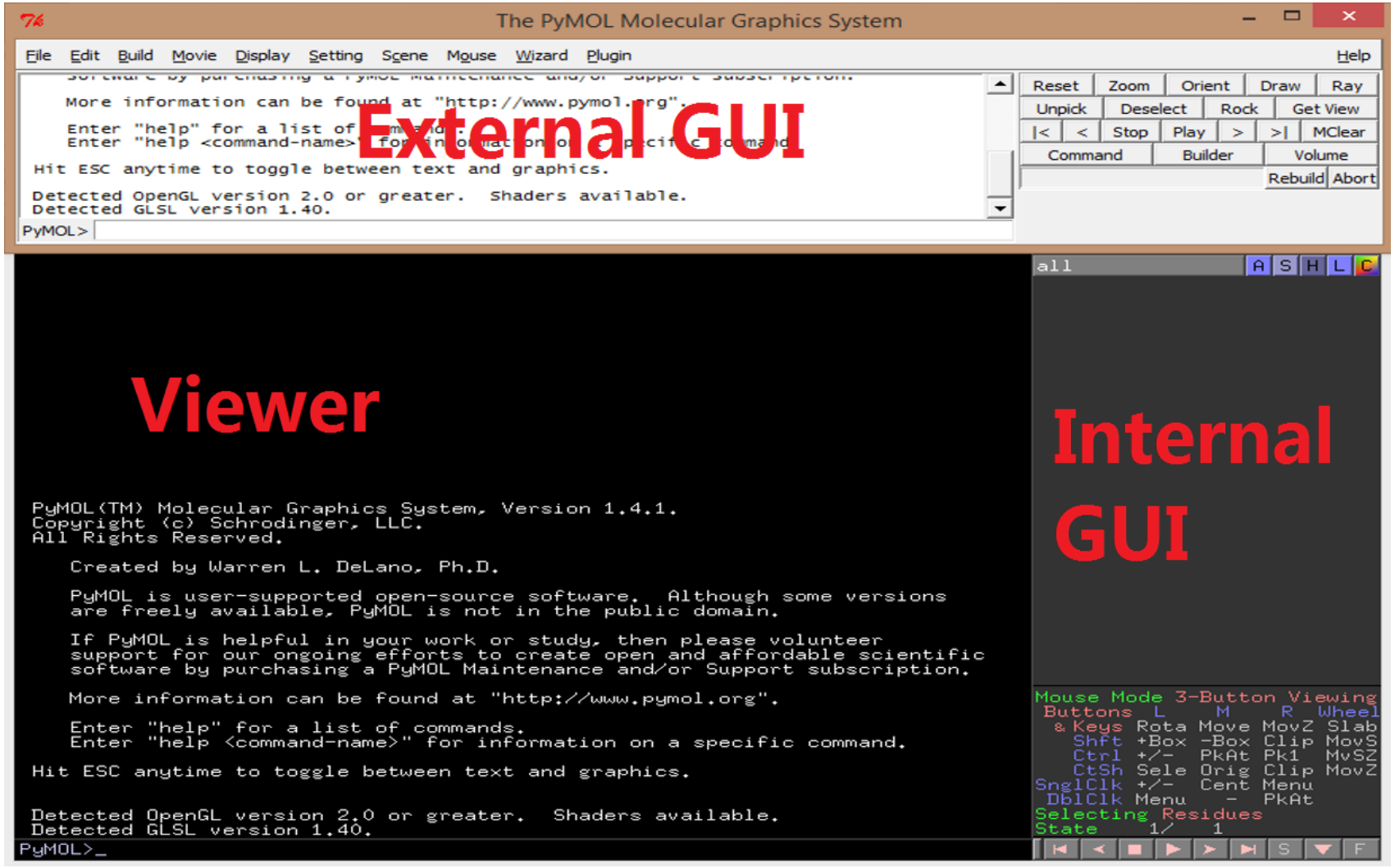
Swiss-pdbViewer is more likely to be a tool for scientific research,

Pymol is more likely to be a tool for scientific results presentation.

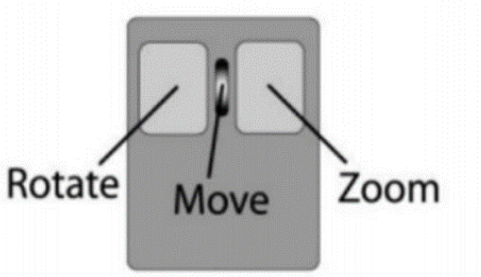
What PyMol looks like?

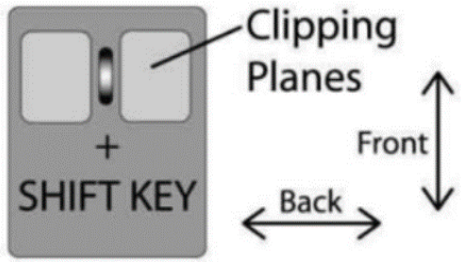
PyMol's Interface

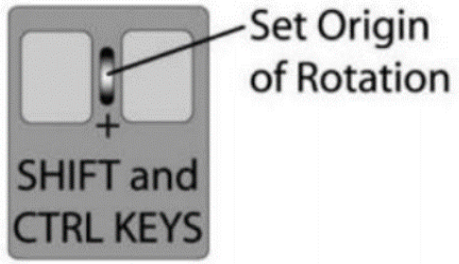
GUI:
Graphical User Interface

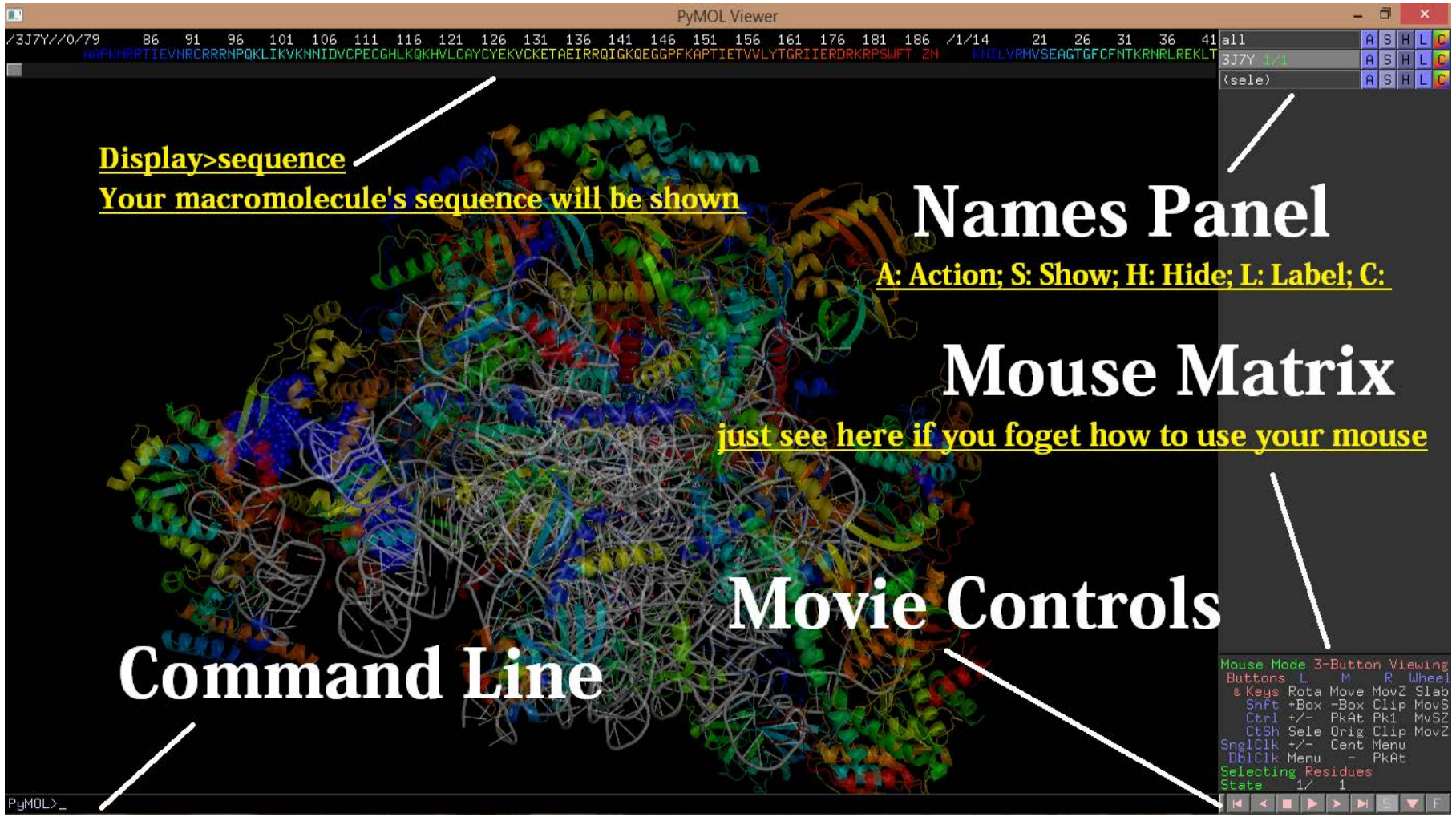


Viewer Window & Mouse Using







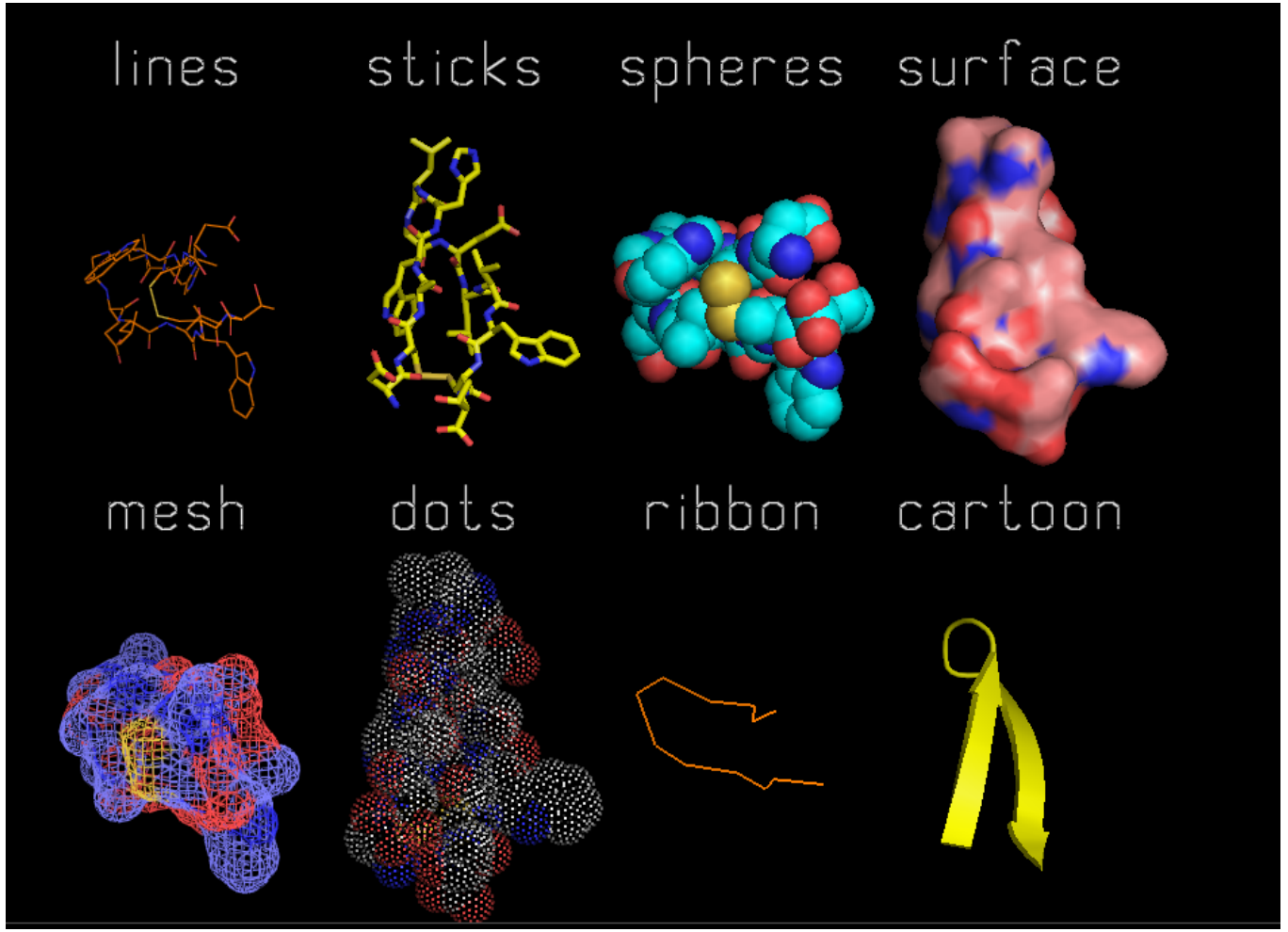


Why PyMol can draw amazing pictures?

Before starting learning PyMol, you can click:

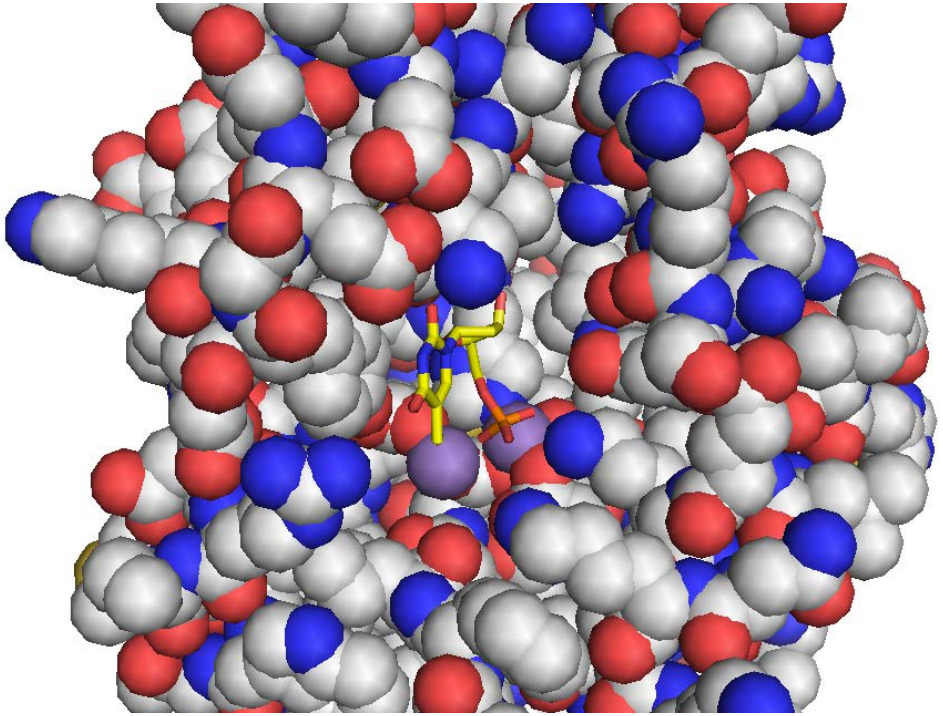
>Wizard>Demo>…

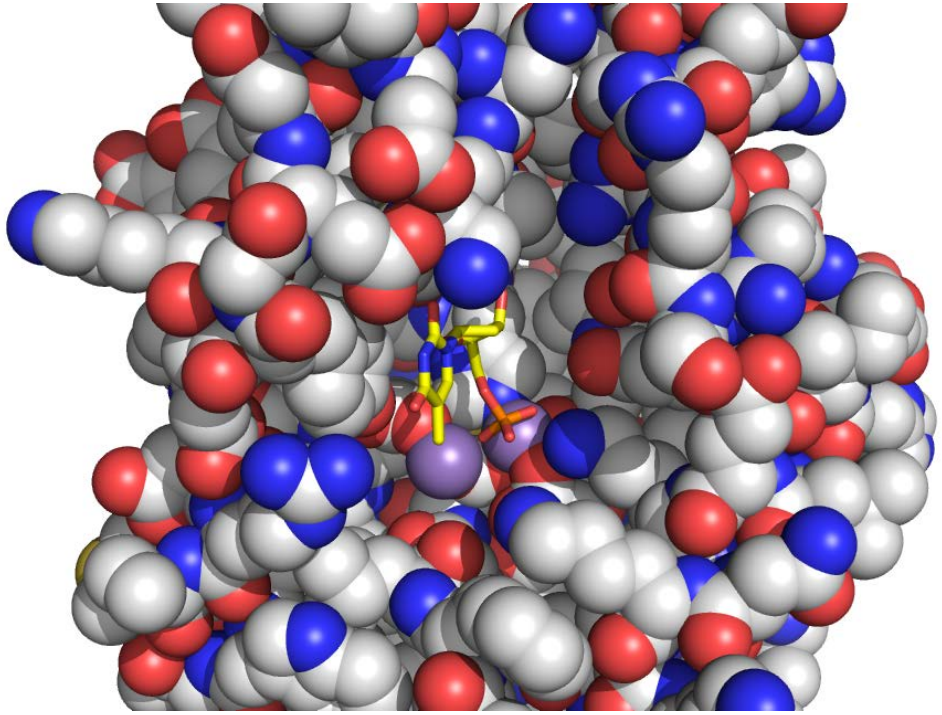
To see what PyMol can do for you.



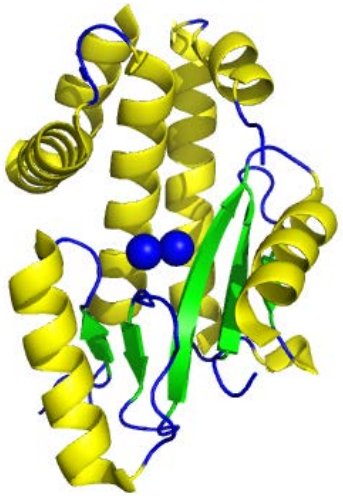
- **Fancy ray**

>ray

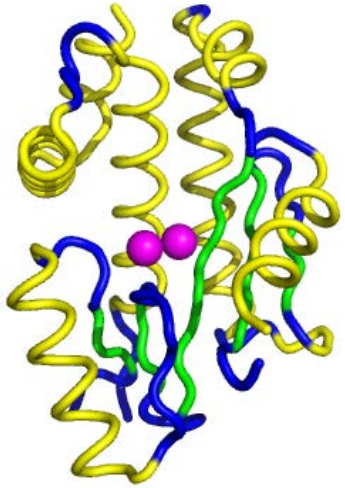




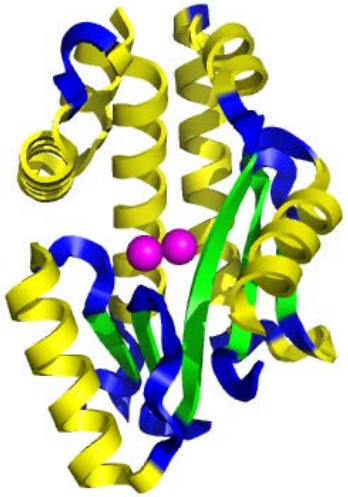
- **Fancy cartoon**



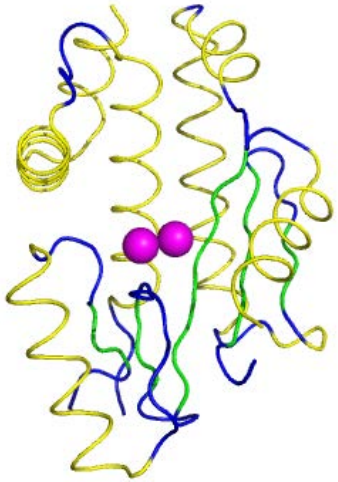
Automatic



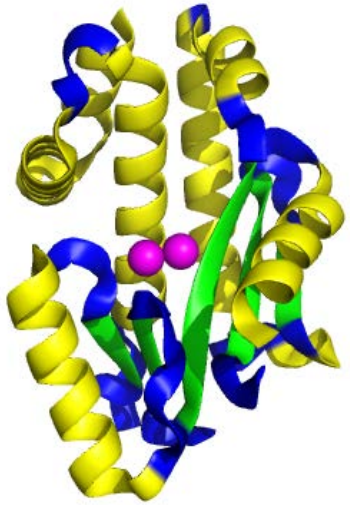
Tube



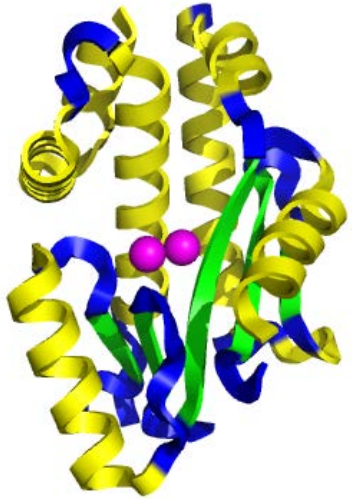
Arrow



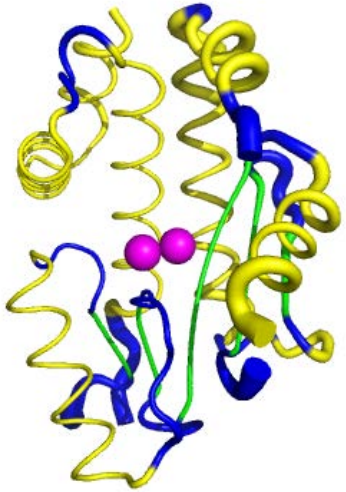
Loop



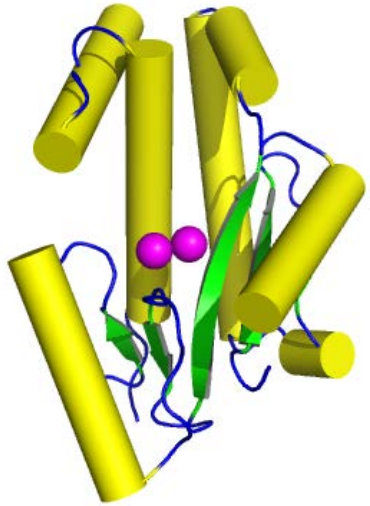
Oval



Rectangle



putty



Setting > Cartoon >….

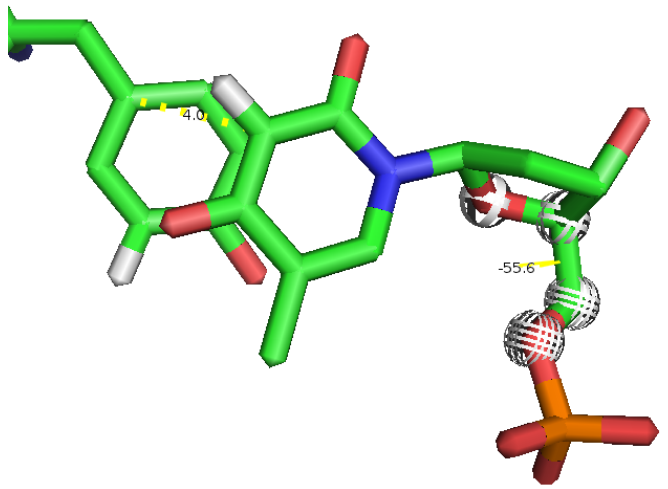
You can define the cartoon as what you like.

How to use PyMol ?

Measurement-Advanced Mouse operation

- Measure the distance between two atoms:
  Mouse:
  Ctrl+R; %select the first atom;
  Ctrl+M; %select the second atom;
  Command:
  >distance/dist
- Measure the angle between three atoms:
  Mouse:
  Ctrl+R; %select the first atom;
  Ctrl+M; %select the second atom;
  Ctrl+M; %select the third atom;
  Command:
  >angle/ang

- Measure the dihedral formed by four atoms:
  Mouse:
  Ctrl+R; %select the first atom;
  Ctrl+M; %select the second atom;
  Ctrl+M; %select the third atom;
  Ctrl+M; %select the forth atom;
  Command:
  >dihedral/dih



Structure alignment

Fit by protein sequence

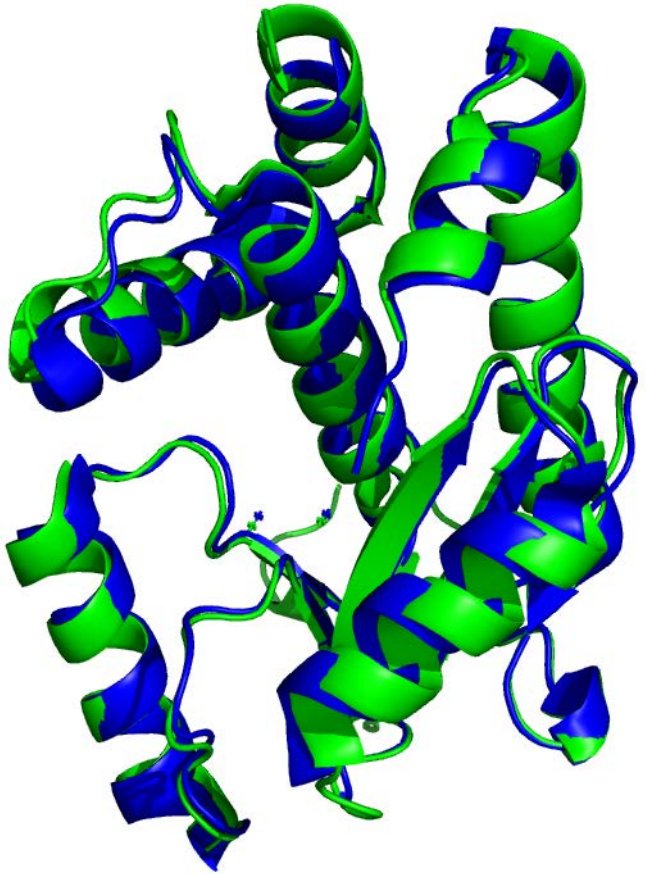
- Mouse:
- First molecule>A>align>to molecule Second molecule;
- Command:
- >Align (A and name ca), (B and name ca)

Fit by overall structure

- Command:
- >cealign A, B

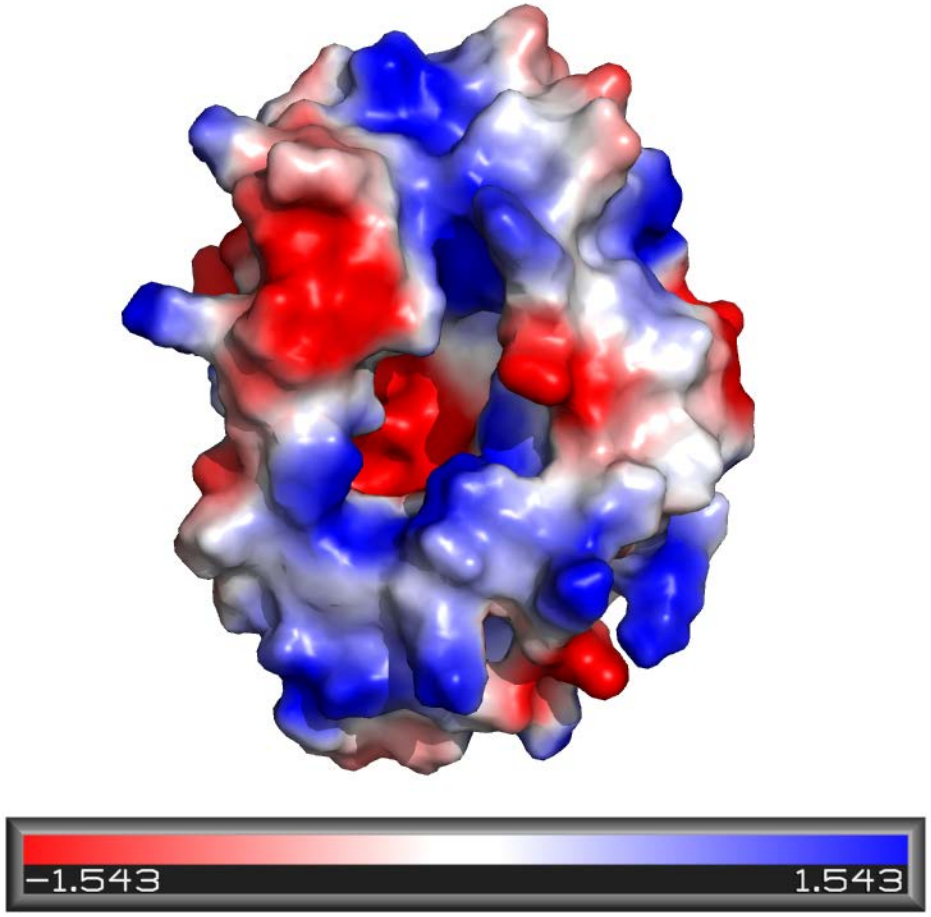
Fit by atom pair

- Mouse:
- Wizard>Pair Fitting



Show the simple electrostatics surface

- Your protein>A>generate>vacuum electrostatics>protein contact potential (local)
- Note: Due to short cutoffs, truncations, and lack of solvent “screening”, these computed potentials are only qualitatively useful.
- You can install the package “APBS” for accurate calculation.



How about doing something that Swiss-pdbViewer can not do?

Before that…

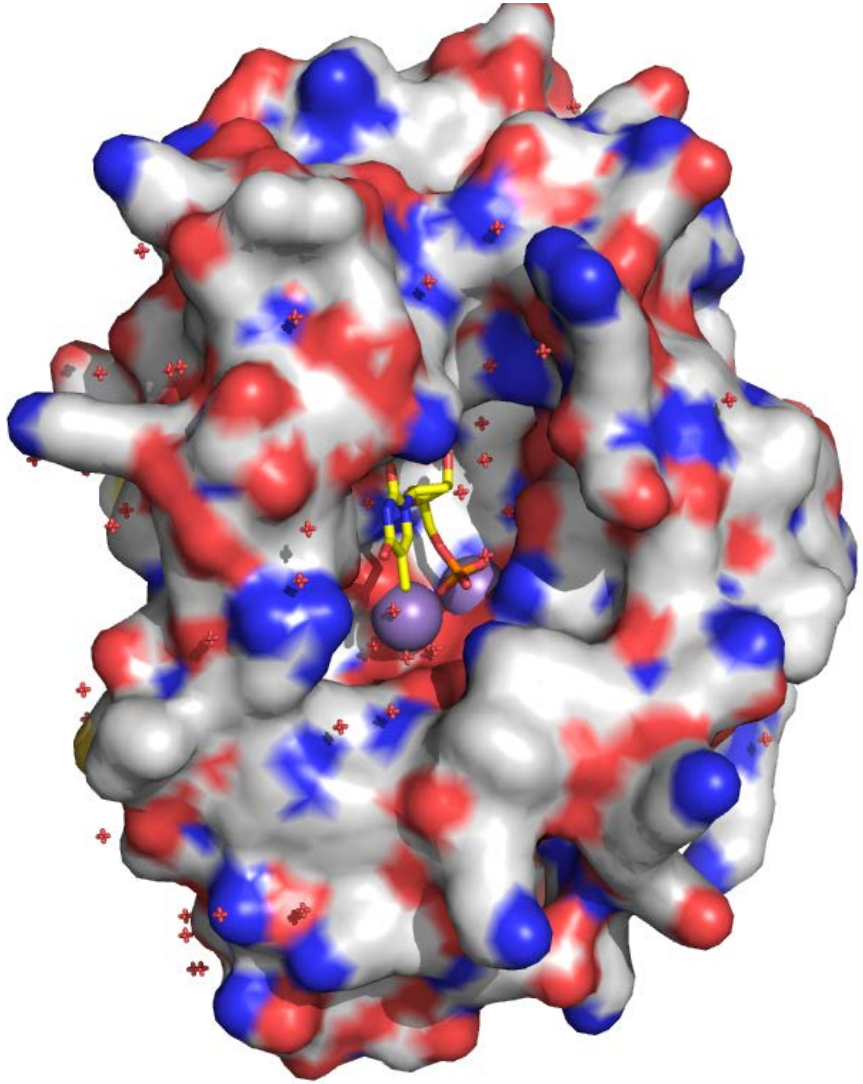
The example protein will be used: PA polymerase of Influenza virus.

PDB code: 4AVL

Function: “Cap snatching” of host pre-mRNA

Active site: 3000 Å^2; Metal coordination; highly conserved

Ligand: TMP



Highlight the ligand and the interactions

1. Draw the scaffold;

4AVL>H>everything;

4AVL>S>cartoon;

4AVL>C>by ss;

2. Draw the ligand;

Display>Sequence;

Select TMP with mouse;

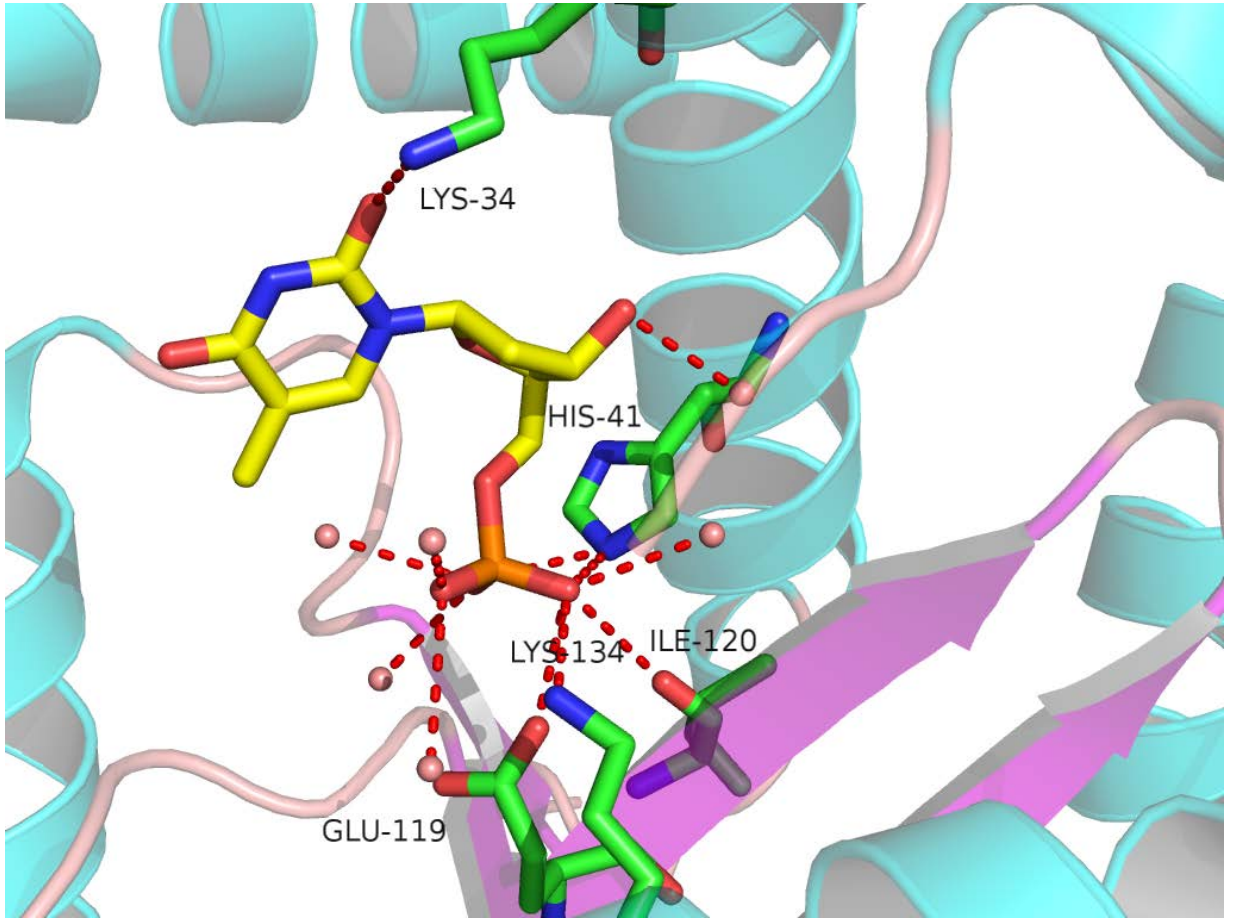
(sele)>A>find>polar contacts>to other atoms in the object;

(sele)>A>copy to object;

obj01>A>rename object: lig;

lig>S>sticks;

lig>C>by element>yellow…



3. Draw the interactions

Lig>A>orient;

4AVL>show lines;

Find the residues that contact with the lig, select them with mouse;

(sele)>A>copy to object;

obj02>A>rename object: resi_cont;

resi_cont>S>sticks;

resi_cont>C>by element>blue…

4AVL>H>lines;

4AVL>S>nb_sphere;

Find the HOHs that contact with the lig, select them with mouse;

(sele)>A>copy to object;

obj03>A>rename object: HOH_cont;

4AVL>H>nb_sphere;

HOH_cont>S>nb_sphere;

HOH_cont>C>red;

4. Draw the metal ions;

Find the MN in the sequence list, select them with mouse;

(sele)>A>copy to object;

obj04>A>rename object: metal

5. Optimize the picture

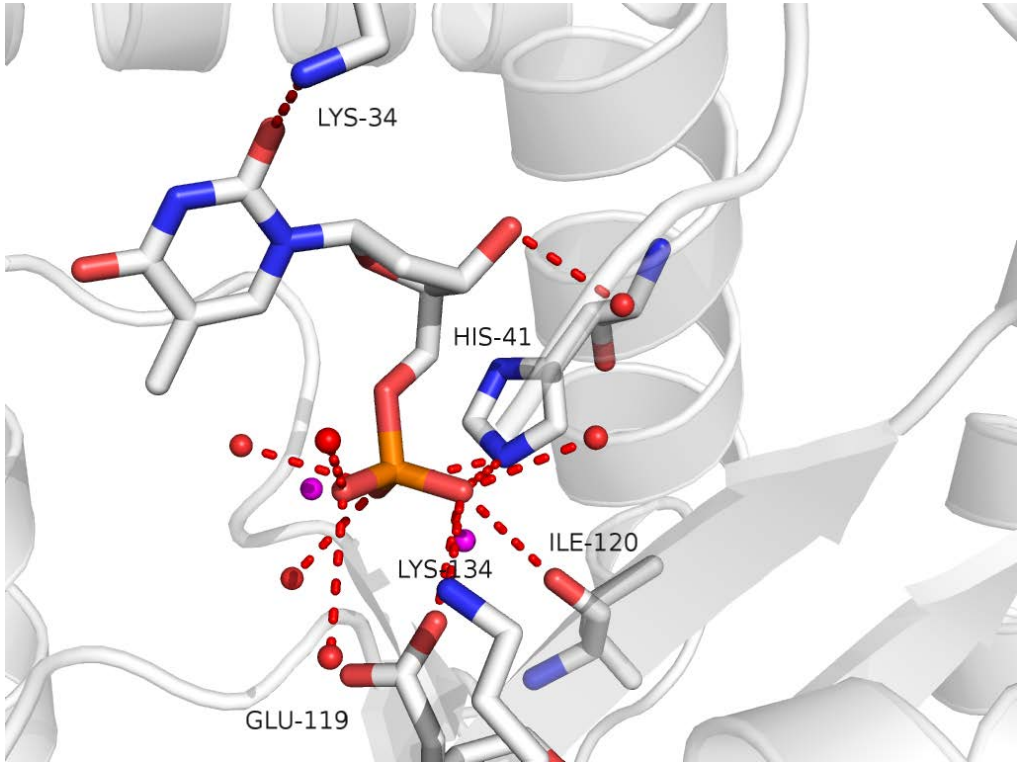
Display>background>white;

Setting>cartoon>fancy helices;

Setting>cartoon>highlight colors;

Setting>transparency>caroon>50%;

Command: ray 1024, 768



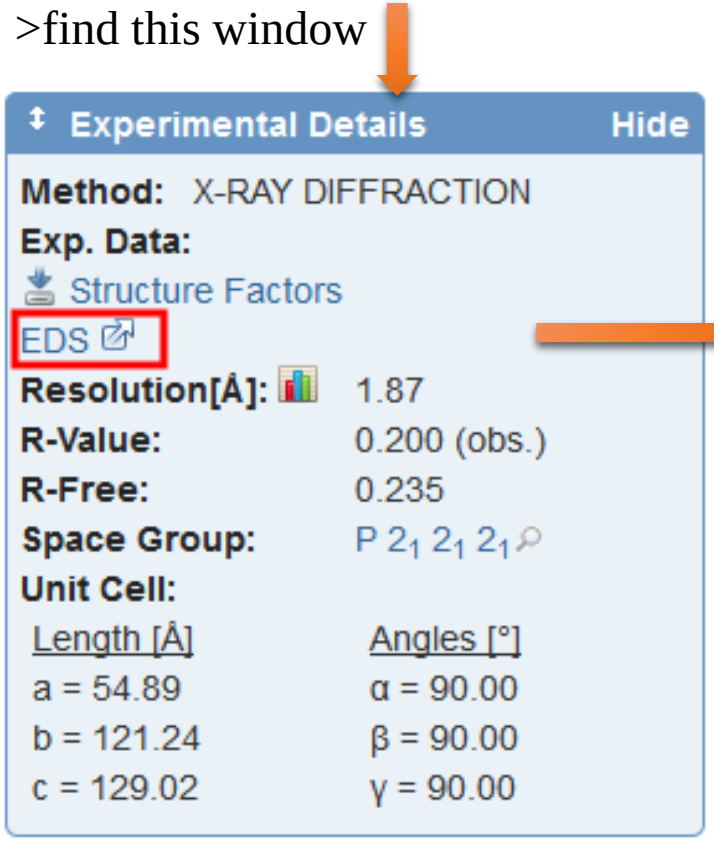
Electron Density Map

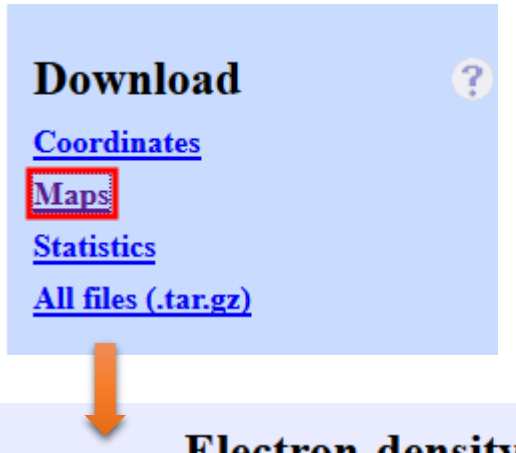
First Step: Download an electron density map

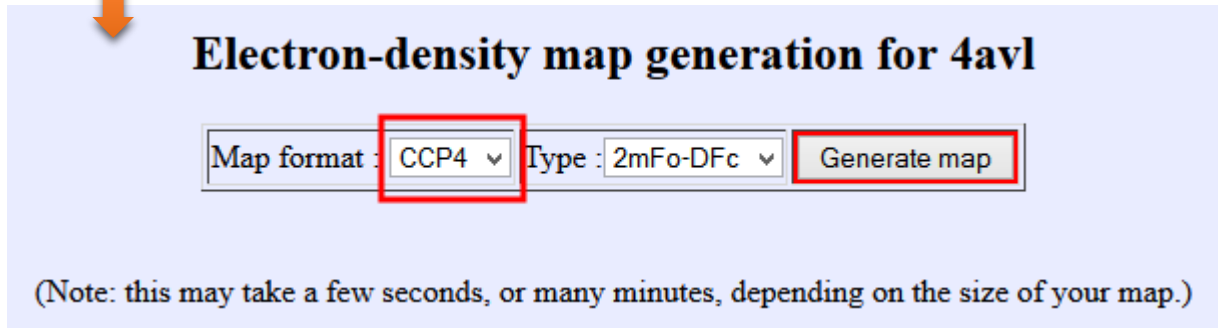
>Go to the PDB Database

>input your PDB code (eg. 4AVL)

>find this window







>Download your map file (eg. 4avl.ccp4)

>Uncompressed it;

>Rename it: 2biw.map.ccp4

(You will find it make the work convenient!!)

Second step: Display electron density map

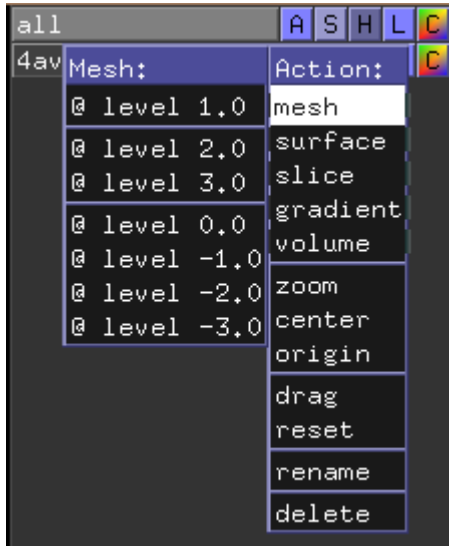
> Load your map file;

☺ Do not panic if your screen still appears black at this point! This is normal.

4avl>mesh>@ level 1.0/2.0/3.0

☺ Do not panic if you find a lot of white worms! This is normal.

(The increase of electron density map means the decreasing resolution of the map at this site)

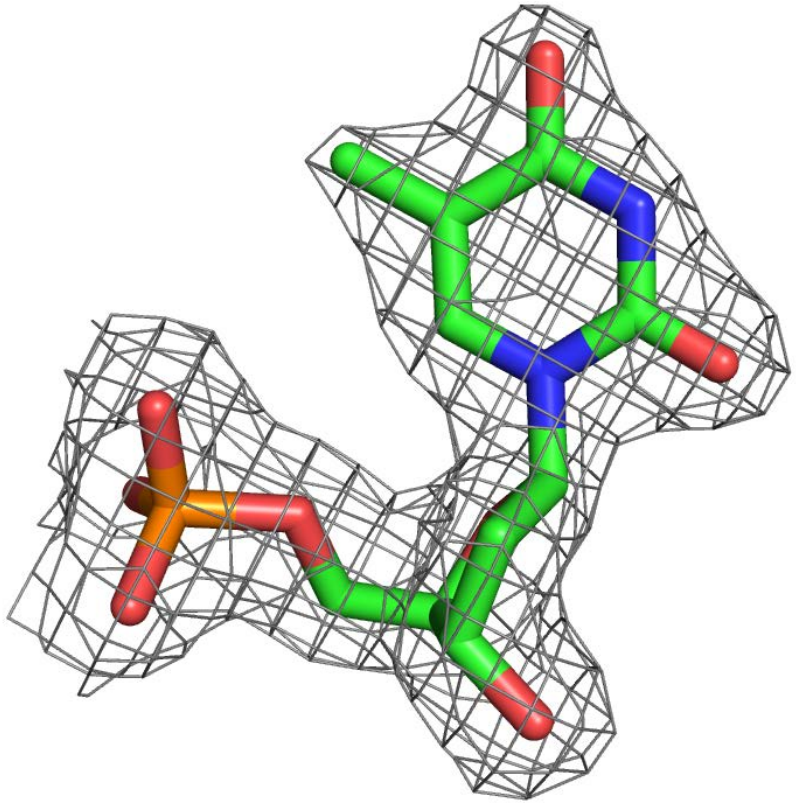


Third step: Add your PDB file

>load 4avl.pdb

Fourth step: Display electron density map for what you want

Display>Sequence;
Select TMP with mouse;
(sele)>A>rename object: lig;
lig>S>sticks;
4AVL>H>lines;
Command: isomesh lig_map, 2biw.map, 1.0, lig carve=1.6
click 4avl.map to hide the overall map.



Fifth step: Optimize the picture

center lig;
lig_map>C>gray50;
Command:
>bg_color white
>set mesh_width, 0.5
>set ray_trace_fog, 0
>set depth_cue, 0
>set ray_shadows, off

Making movies: Rotating Molecule

Command:
mset 1, 180 %make a movie that has 180 frames;
util.mroll 1, 180, 1 %make a movie that start at the 1st frame and stop at the 180th frame with each frames rotating 1 degree;
set ray_trace_frames, 1 %turn on the ray trace, it would be perfect!
set cache_frames, 0 %turn out the cache frames

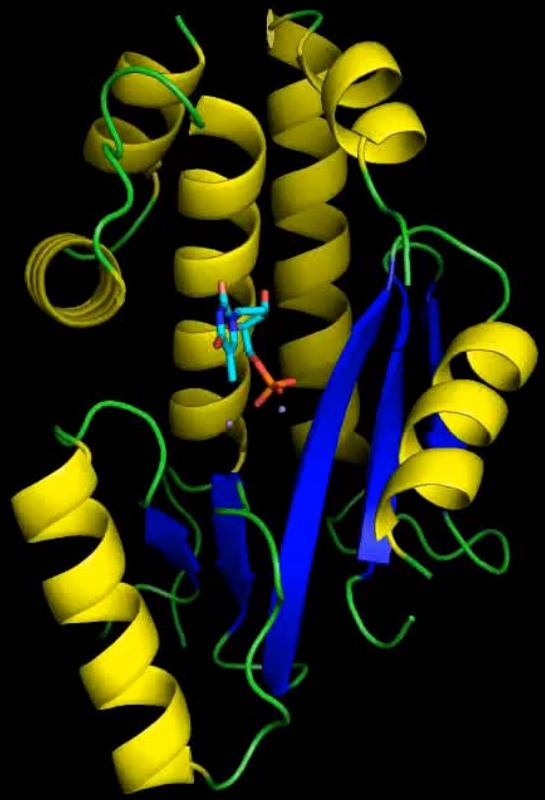
>save>movie>mpng

Making movies: Scene Translation

Making different states
State 1
>Scene>Store>F1;
State 2
>Scene>Store>F2;
State 3
>Scene>Store>F3;
……

You can check your scene by
>Scene> Recall>Fn

Making movie
>Movies>Program>Scene Loop>….
% define the time and the translation mode;
>save>movie>mpng.



My Notes for using PyMol

- You will find the importance of “(sele)>A>copy to object” !!
- You will find it very very important to save a PyMol section!!!
- Rename the default generated sele_polar_conts term.

Thank You!!!

And Good Luck to Use PyMol!