NAME: ASIF ERFAN KHAN
ROLL NUMBER: 546
COURSE: MSc CS
SUBJECT: BIOINFORMATICS
TOPIC: RETRIEVING 3D STRUCTURE FROM PDB

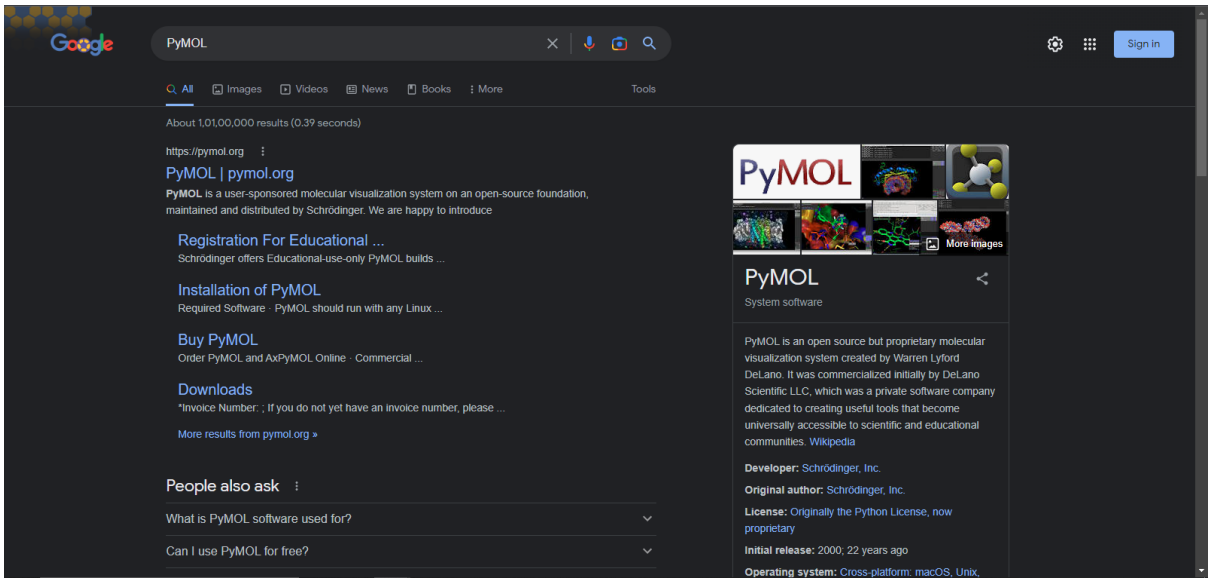
Aim: Retrieving 3D structure from PDB

To perform the current practical, you'll be needing two things

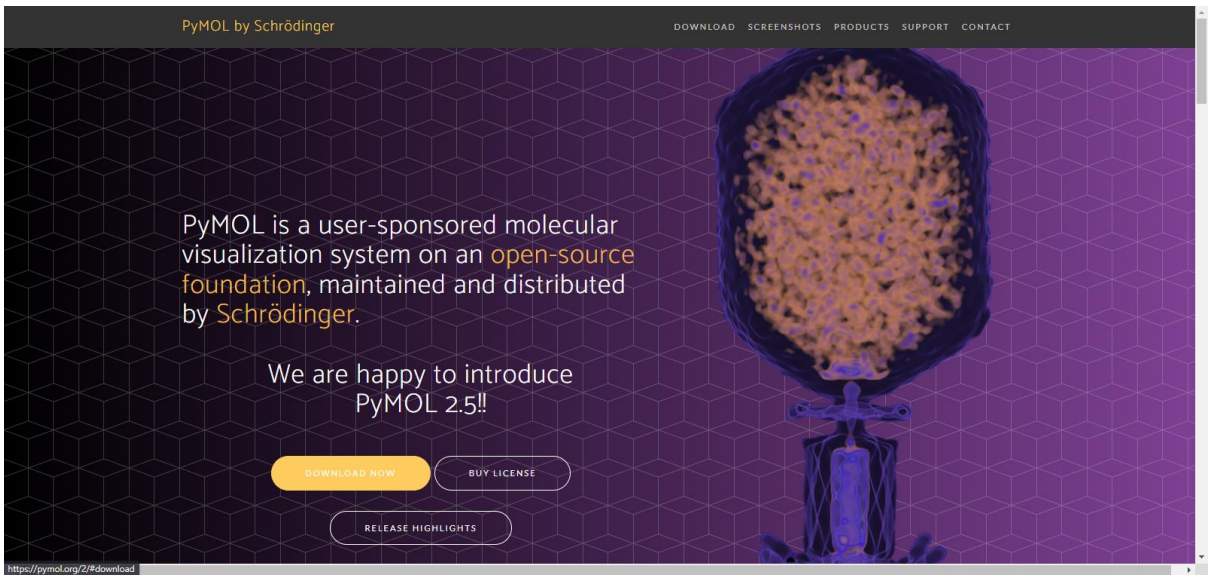
I. PyMOL (software)
II. Protein in .pdb format

Installing PyMOL Software

First, we need to install PyMOL. To do so open google and simply search PyMOL

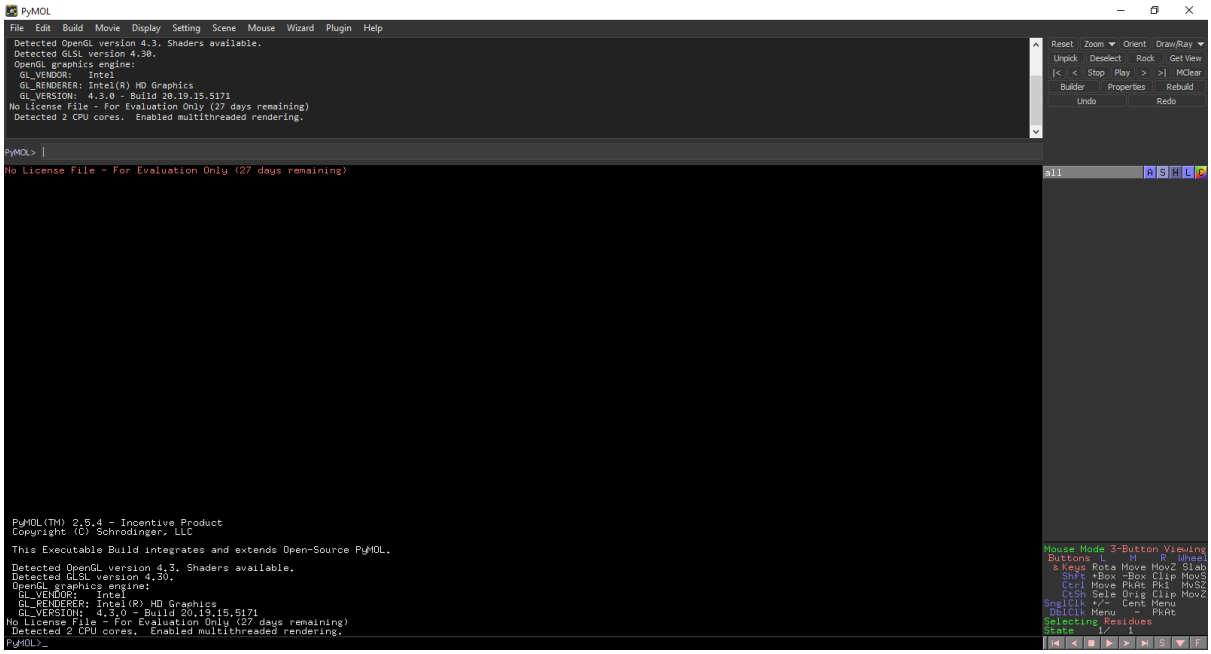


Open the first link and click Download Now



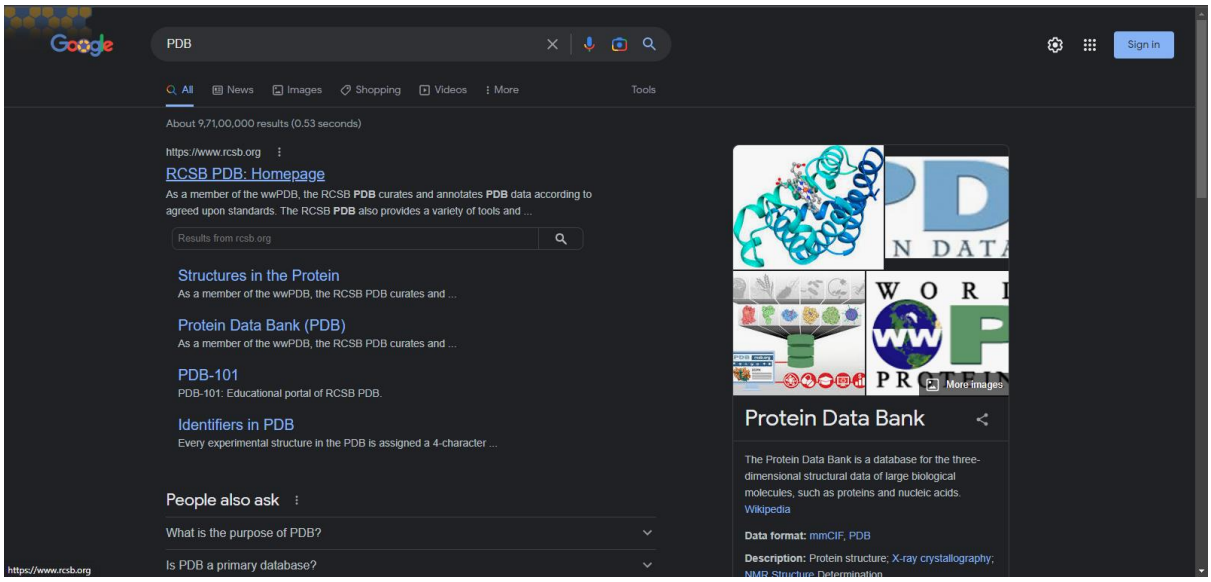
When done downloading install the software.

This is how the interface of the software looks like.



Downloading Protein in .pdb format

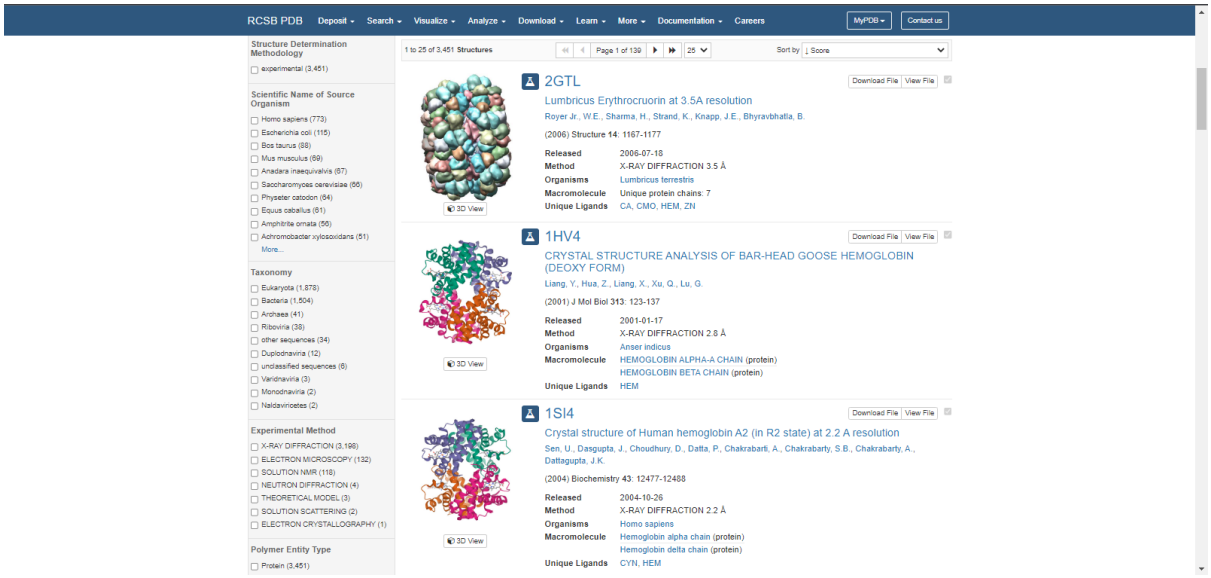
To download Protein open, google and search pdb or simply visit https://www.rcsb.org/



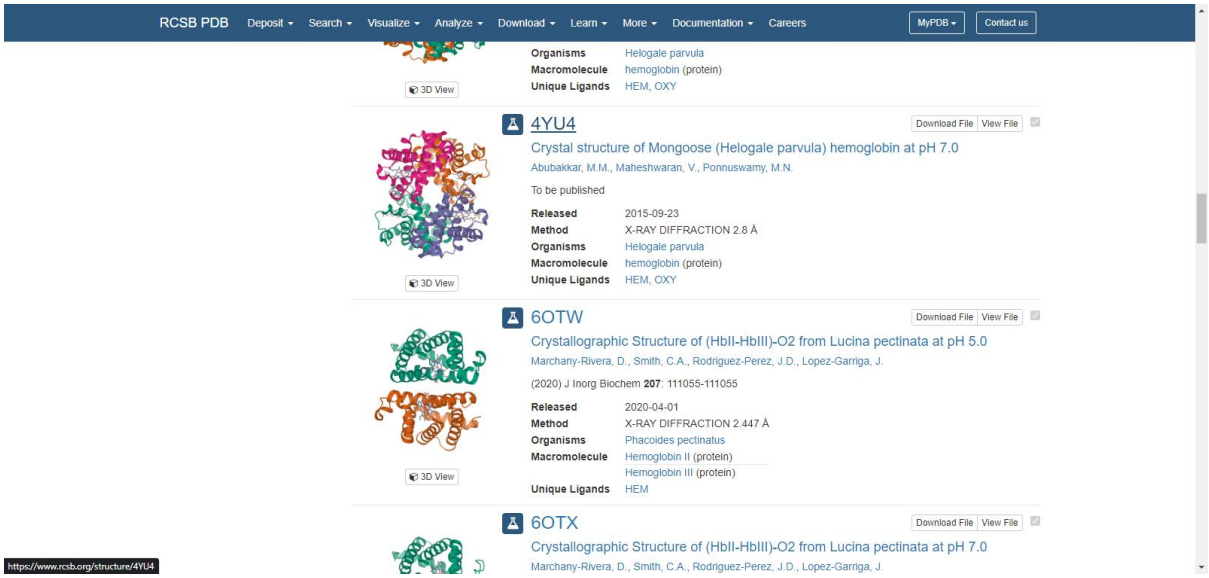
Open the first link named “RCSB PDB: Homepage”

On the search bar search for “hemoglobin”

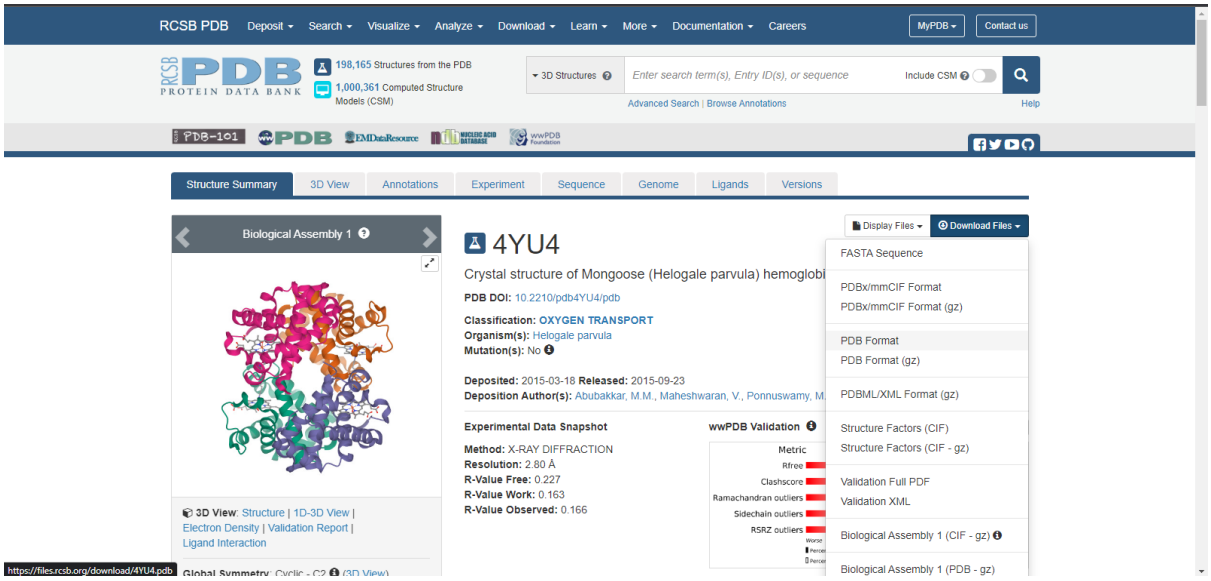
You'll see all the proteins listed below like this



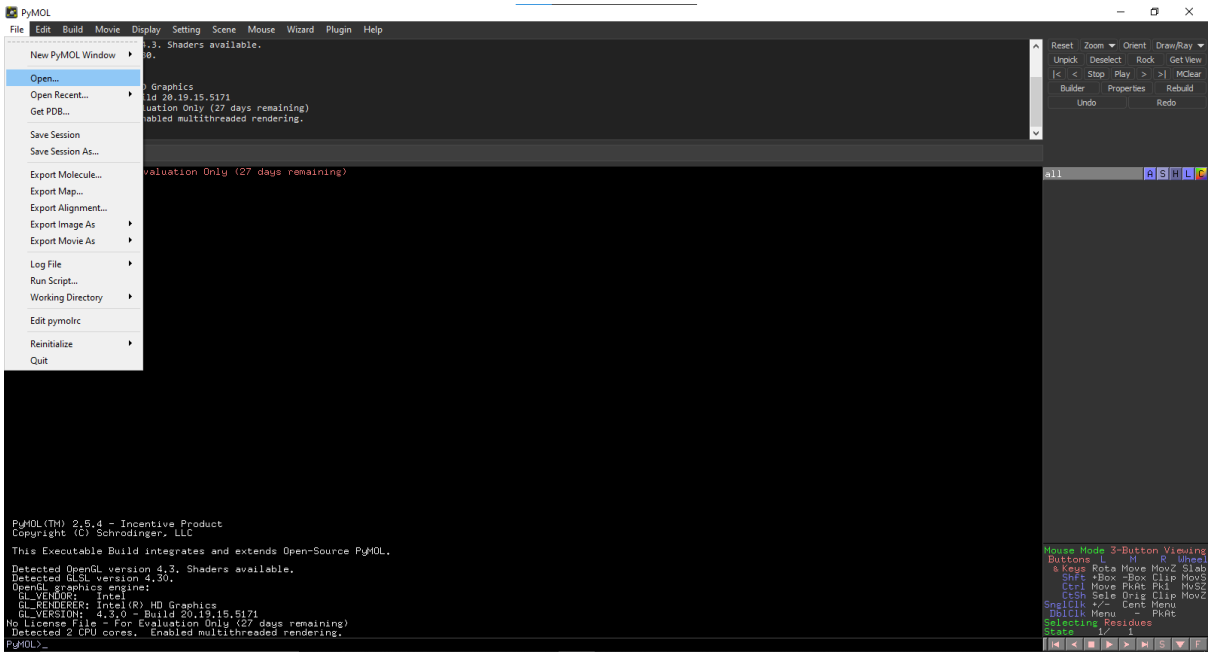
Scroll down until you find "4YU3" and open it or you can directly search for "4yu4"



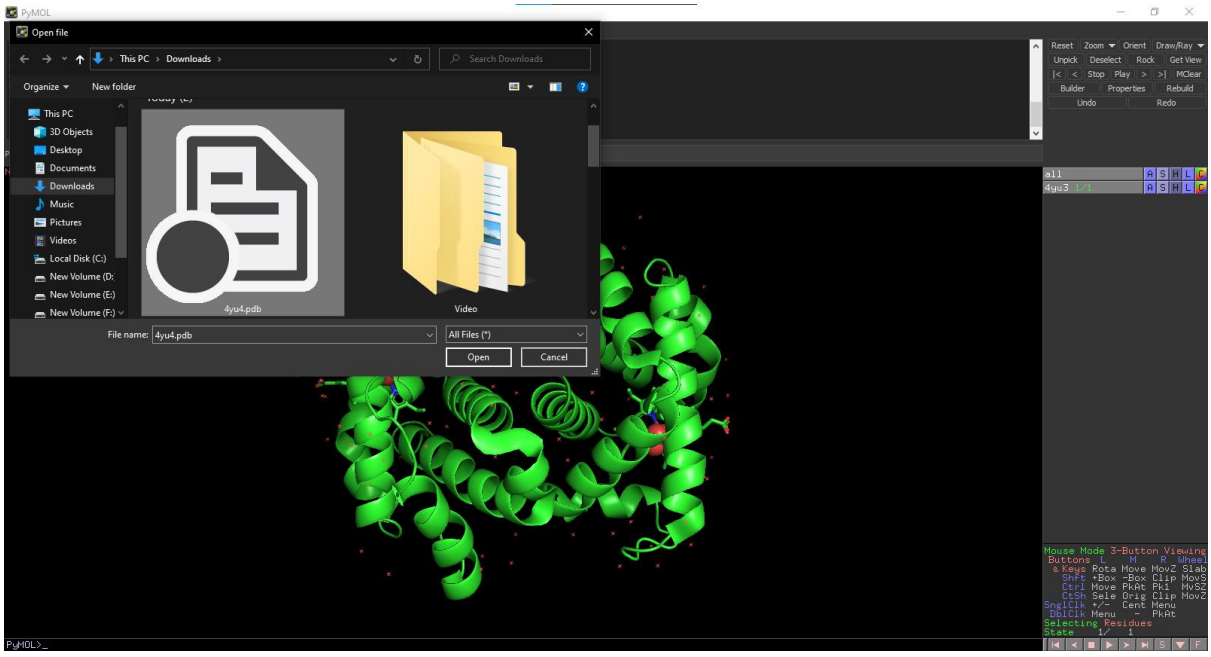
On the right-hand side, you'll the download option. Click on it and download as PDB format



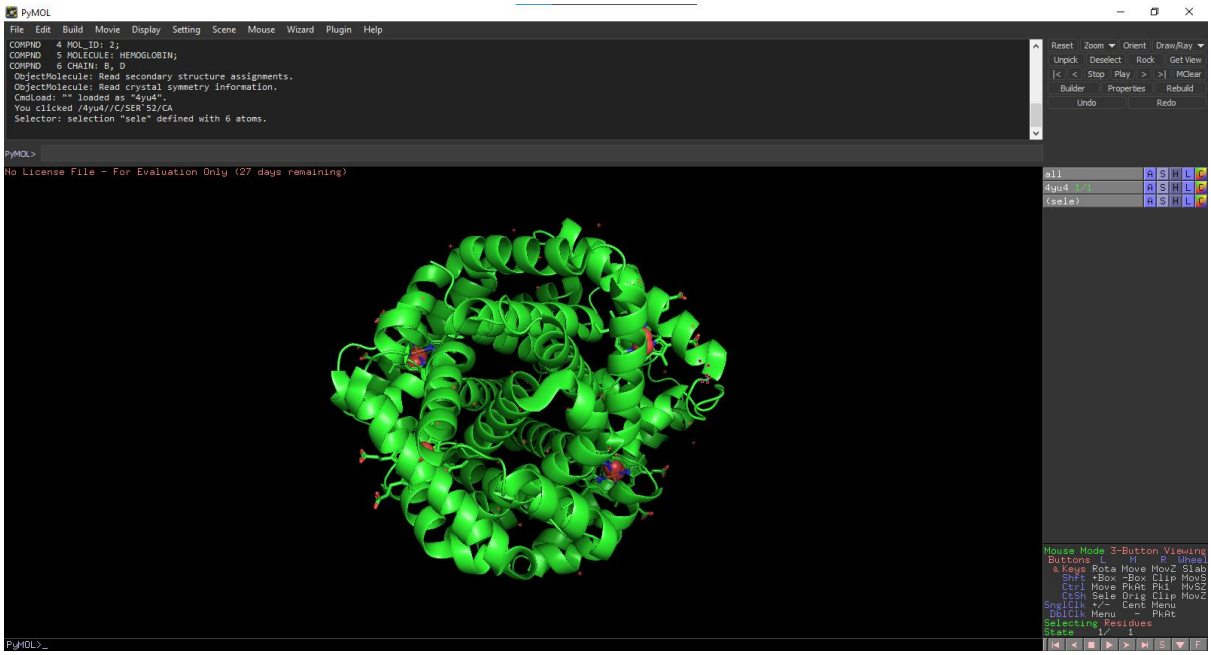
Now that protein is downloaded open PyMOL and on top left corner click File > open

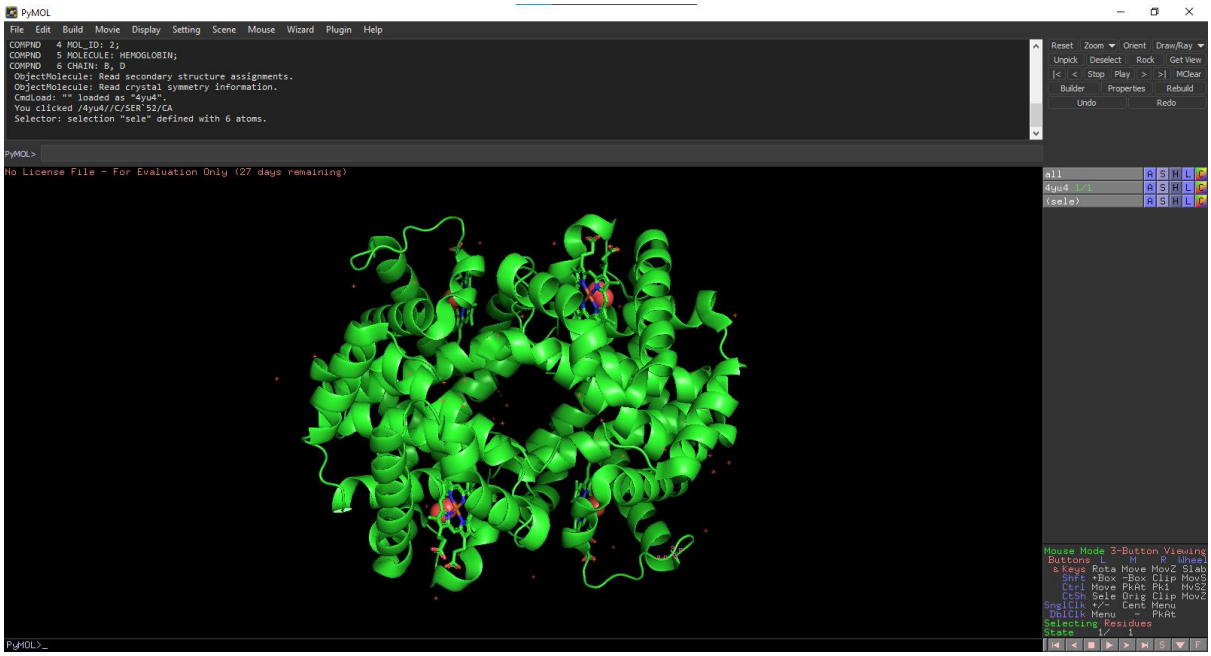


Now browse for the file you just downloaded (4yu4.PDB)



This is how the screen of imported file looks like


PyMOL
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
COMPND 4 MOL_ID: 2;
COMPND 5 MOLECULE: HEMOGLOBIN;
COMPND 6 CHAIN: B, D
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
CmdLoad: "" loaded as "4yu4".
You clicked /4yu4//C/SER`52/CA
Selector: selection "sele" defined with 6 atoms.
Reset Zoom Orient Draw/Ray
Unpick Deselect Rock Get View
Stop Play MClear
Builder Properties Rebuild
Undo Redo
PyMOL>
No License File - For Evaluation Only (27 days remaining)
all
4yu4
(sele)
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl Move PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
State 1/ 1
PyMOL>_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DblClk Menu - PkAt
Selecting Residues
State 1/ 1
PyMOL>_