

NAME: ASIF ERFAN KHAN

ROLL NUMBER: 546

COURSE: MSc CS

SUBJECT: BIOINFORMATICS

TOPIC: RETRIEVING 3D

STRUCTURE FROM PDB

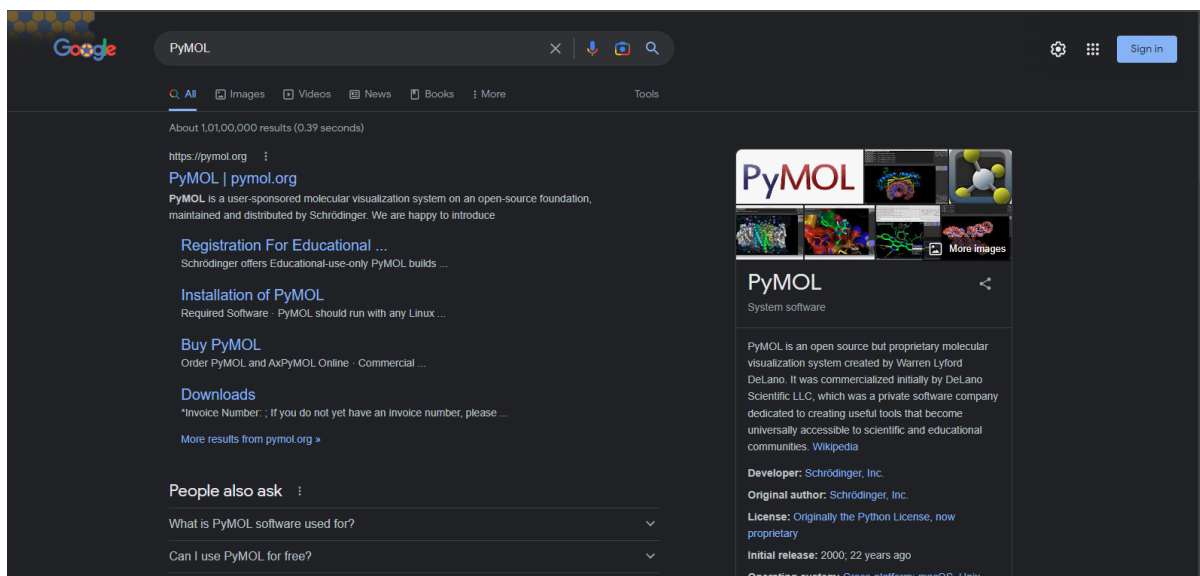
Aim: Retrieving 3D structure from PDB

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

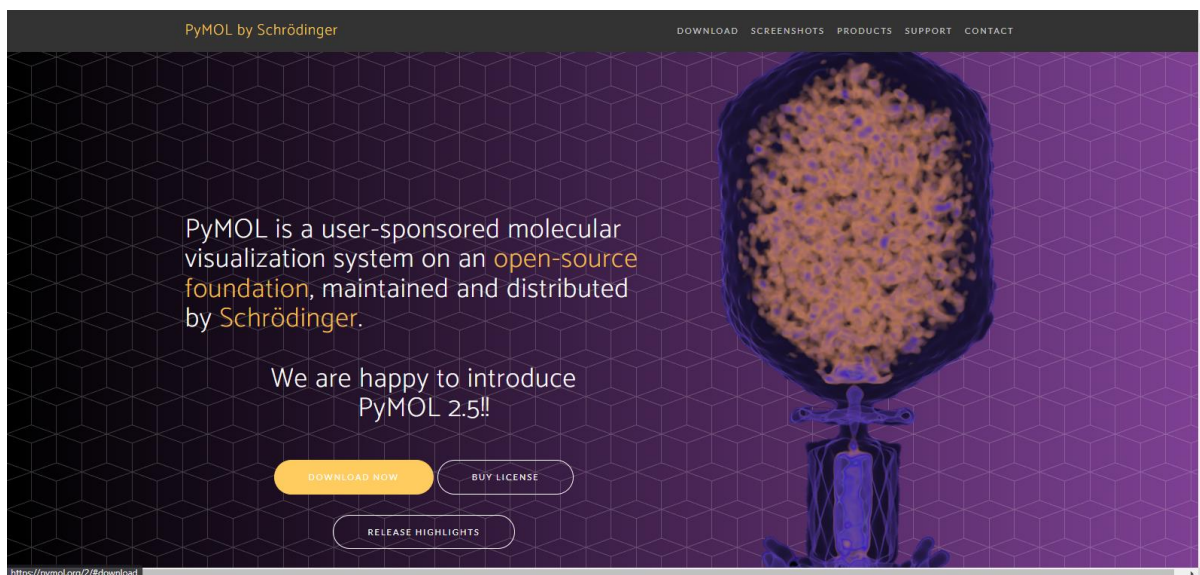
- I. PyMOL (software)
- II. Protein in .pdb format

Installing PyMOL Software

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

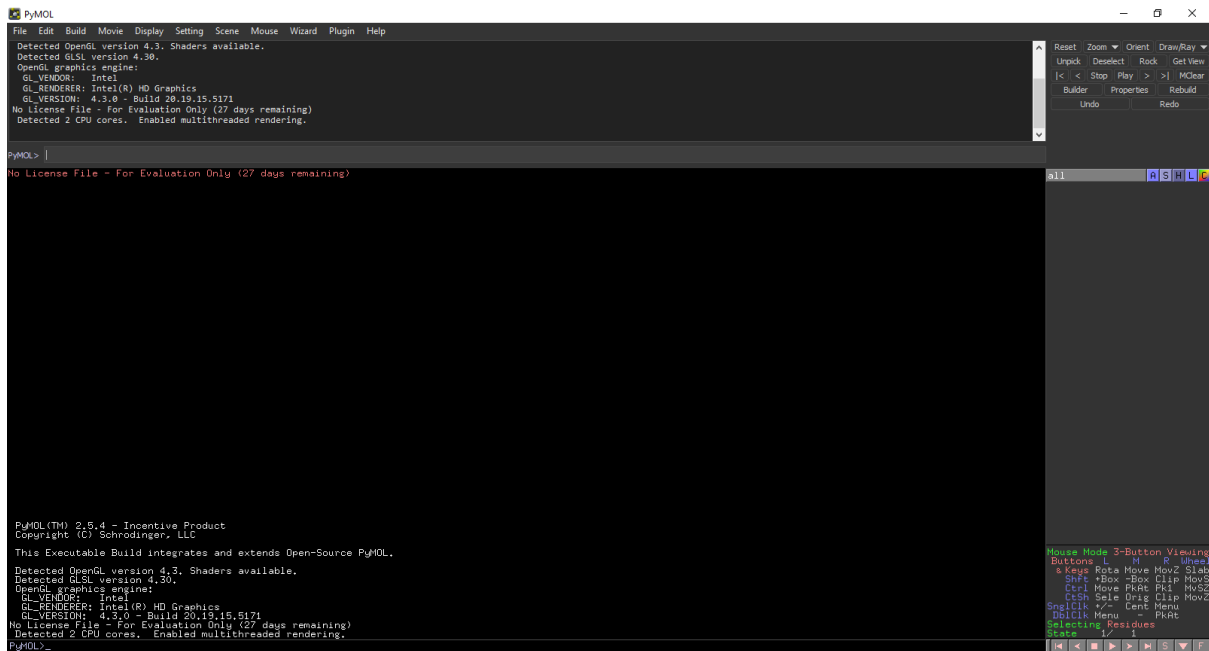


Open the first link and click Download Now



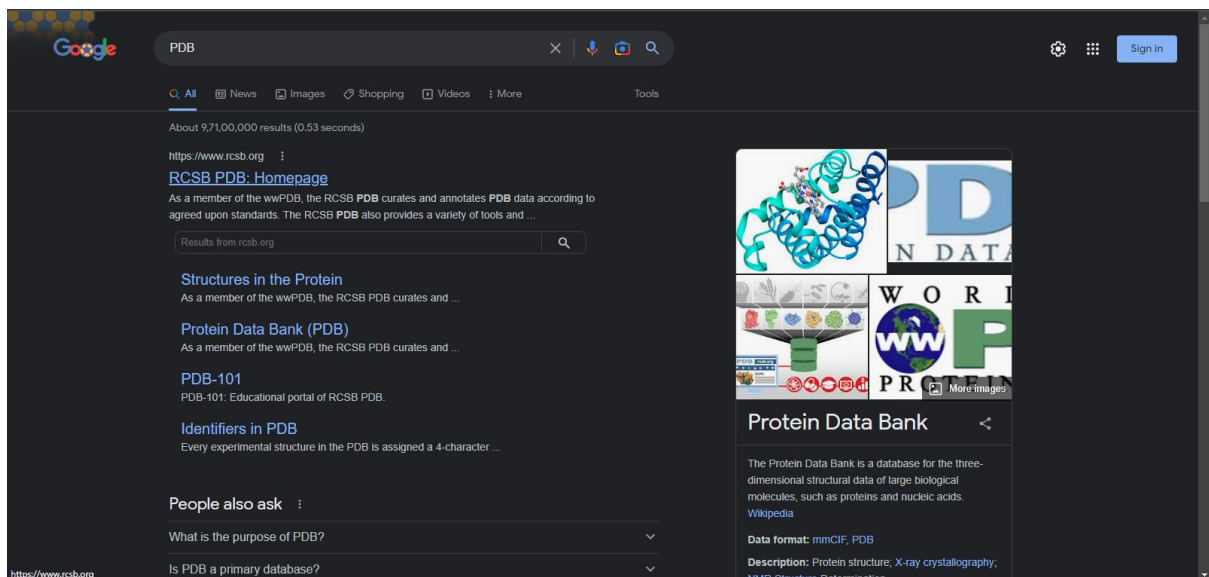
When done downloading install the software.

This is how the interface of the software looks like.



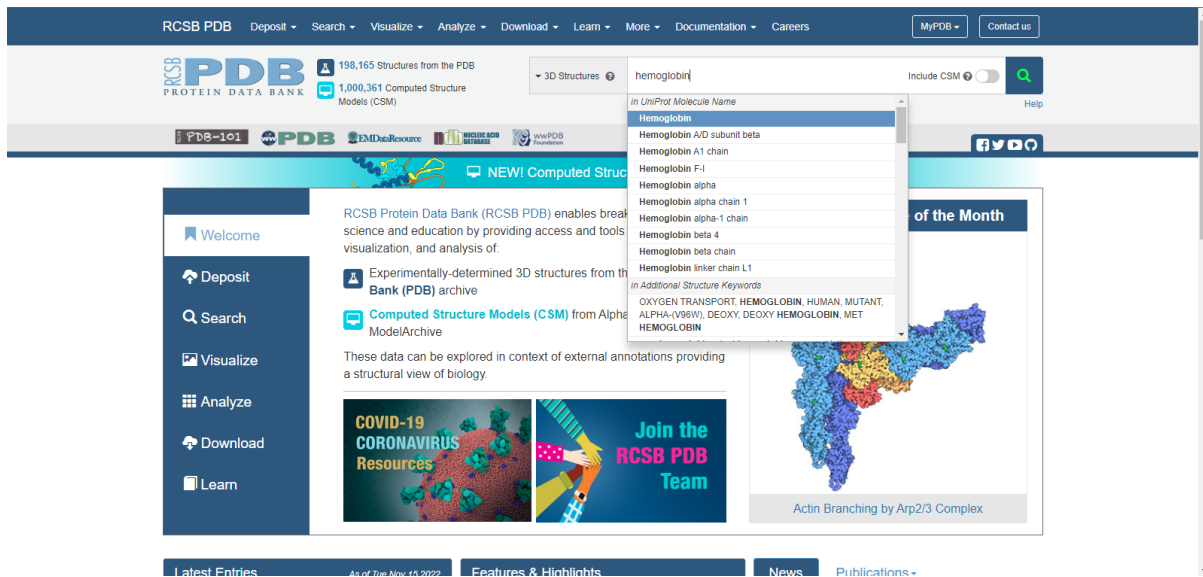
Downloading Protein in .pdb format

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

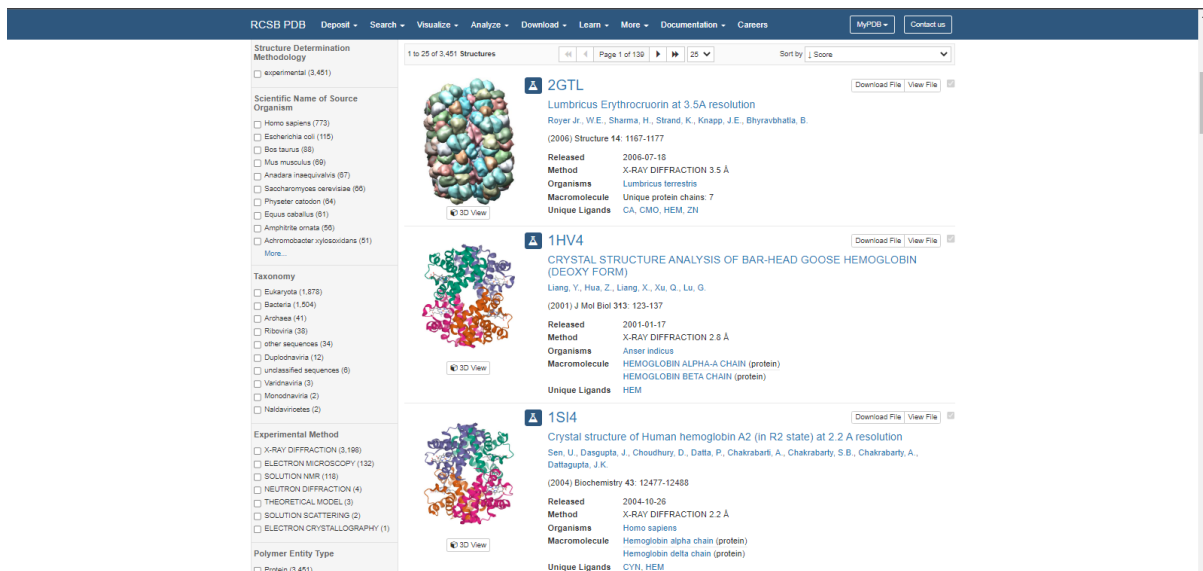


Open the first link named “RCSB PDB: Homepage”

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”

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4YU4
Crystal structure of Mongoose (Halogale parvula) hemoglobin at pH 7.0
Abubakkar, M.M., Maheshwaran, V., Ponnuswamy, M.N.
To be published
Released: 2015-09-23
Method: X-RAY DIFFRACTION 2.8 Å
Organisms: Halogale parvula
Macromolecule: Hemoglobin (protein)
Unique Ligands: HEM, OXY

6OTW
Crystallographic Structure of (HbII-HbIII)-O₂ from *Lucina pectinata* at pH 5.0
Marchany-Rivera, D., Smith, C.A., Rodriguez-Perez, J.D., Lopez-Garriga, J.
(2020) J Inorg Biochem **207**: 111055-111055
Released: 2020-04-01
Method: X-RAY DIFFRACTION 2.447 Å
Organisms: Phacoides pectinatus
Macromolecule: Hemoglobin II (protein)
Unique Ligands: Hemoglobin III (protein)
HEM

6OTX
Crystallographic Structure of (HbII-HbIII)-O₂ from *Lucina pectinata* at pH 7.0
Marchany-Rivera, D., Smith, C.A., Rodriguez-Perez, J.D., Lopez-Garriga, J.

<https://www.rcsb.org/structure/4YU4>

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

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RCSB PDB PROTEIN DATA BANK 198,165 Structures from the PDB 1,000,361 Computed Structure Models (CSM)

3D Structures Enter search term(s), Entry ID(s), or sequence Include CSM Help

Advanced Search Browse Annotations

PDB-101 PDB EMDB Resource

Structure Summary 3D View Annotations Experiment Sequence Genome Ligands Versions

4YU4
Crystal structure of Mongoose (Halogale parvula) hemoglobin
PDB DOI: 10.2210/pdb4YU4/pdb
Classification: OXYGEN TRANSPORT
Organism(s): Halogale parvula
Mutation(s): No
Deposited: 2015-03-18 Released: 2015-09-23
Deposition Author(s): Abubakkar, M.M., Maheshwaran, V., Ponnuswamy, M.
Experimental Data Snapshot
Method: X-RAY DIFFRACTION
Resolution: 2.80 Å
R-Value Free: 0.227
R-Value Work: 0.163
R-Value Observed: 0.166

wwPDB Validation

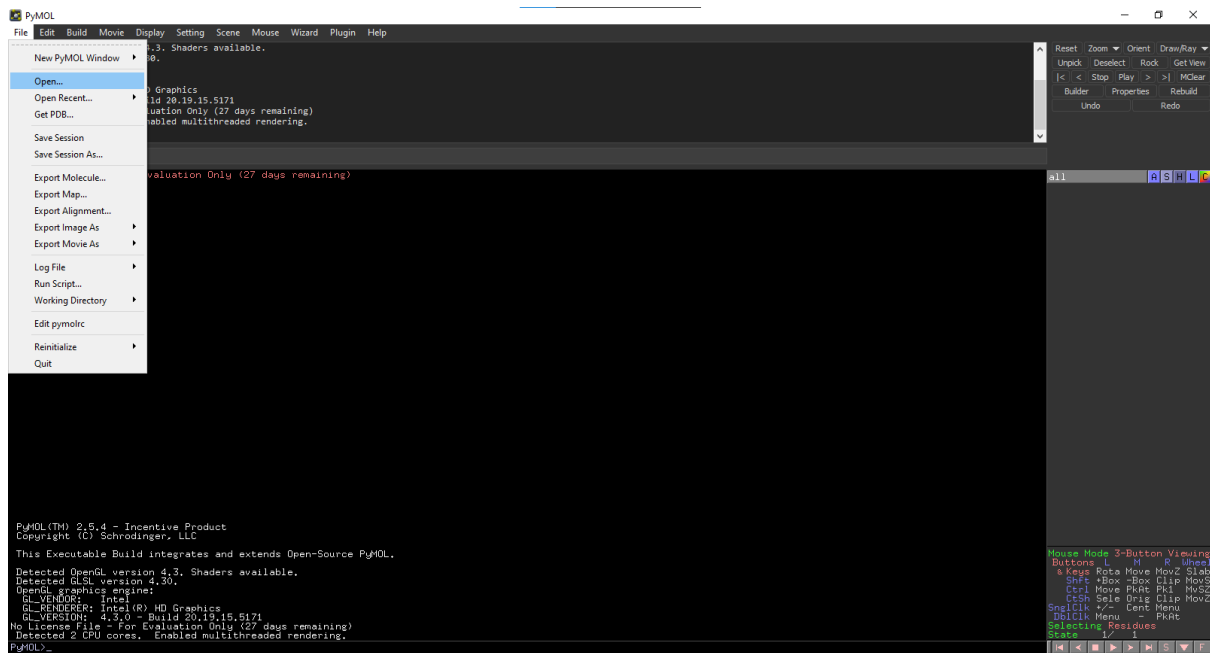
Metric
Rfree
Clashscore
Ramachandran outliers
Sidechain outliers
RSRZ outliers

Structure Factors (CIF)
Structure Factors (CIF - gz)
Validation Full PDF
Validation XML
Biological Assembly 1 (CIF - gz)
Biological Assembly 1 (PDB - gz)

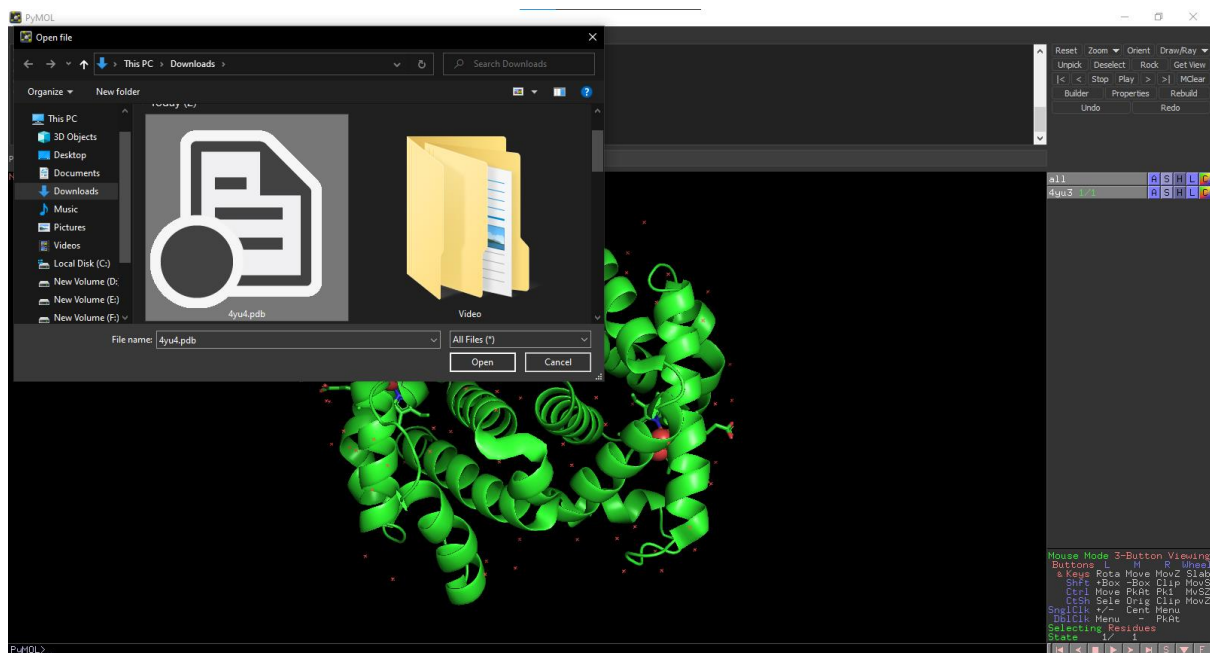
3D View: Structure | 1D-3D View | Electron Density | Validation Report | Ligand Interaction

<https://files.rcsb.org/download/4YU4.pdb>

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

