




That's a great question, Srushti 🌸 — and it's **very important** to understand before working with protein visualization and BioPython scripts like the one you just ran.

Let's go step-by-step 👉

What is PDB?

PDB stands for **Protein Data Bank** — it's both a **file format** and a **global database** of 3D structures of biological molecules (like proteins, DNA, and RNA).

♦ 1. PDB as a Database

- The **Protein Data Bank (PDB)** is an **online repository** that stores experimentally determined **3D structures** of biomolecules.
- Scientists deposit structures obtained from techniques like:
 - o  **X-ray crystallography**
 - o  **NMR spectroscopy**
 - o  **Cryo-electron microscopy (Cryo-EM)**

 Website: <https://www.rcsb.org>

You can search by protein name or PDB ID (like 1A3N, 3RGK, 6LU7, etc.)
Each structure has a unique **4-character PDB ID**.

♦ 2. PDB as a File Format

A **PDB file** (extension .pdb or .ent) contains:

- **3D coordinates** of all atoms in the molecule
- **Residue and chain information** (e.g., amino acid number, chain A/B)
- **Experimental data** (optional)
- **Metadata** like title, method, and authors

Example of a PDB file snippet



```
HEADER  OXYGEN TRANSPORT          07-JUL-97  1A3N
TITLE   HEMOGLOBIN (DEOXY FORM)
ATOM    1  N  VAL A  1    11.104 13.207  2.120 1.00 16.44    N
ATOM    2  CA VAL A  1    12.560 13.367  2.309 1.00 15.69    C
ATOM    3  C  VAL A  1    13.183 12.067  2.838 1.00 15.41    C
ATOM    4  O  VAL A  1    12.526 11.025  2.708 1.00 15.84    O
ATOM    5  CB VAL A  1    12.963 14.587  3.171 1.00 16.14    C
TER
END
```

Explanation:

- ATOM → Each atom entry
- Columns give:
 - Atom number
 - Atom name (N, CA, C, O, etc.)
 - Residue name (like VAL = Valine)
 - Chain ID (A, B, etc.)
 - 3D coordinates (X, Y, Z)
 - Occupancy, temperature factor, element type

So basically, a PDB file tells your program **where every atom is located in 3D space**.

♦ 3. Purpose of PDB Files

Purpose	Description
 Structural Biology	Understand 3D shapes of proteins/DNA
 Drug Design	Study how drugs fit into protein binding sites