

Repositories of coordinates and structural information

Protein Data Bank (PDB)

<http://www.wwpdb.org/>

The Protein Data Bank archive serves as the single repository of information about the 3D structures of proteins, nucleic acids, and complex assemblies. The Worldwide PDB (wwPDB) organization manages the PDB archive and ensures that the PDB is freely and publicly available to the global community.

PDB mirrors:

(US) <http://www.rcsb.org/pdb/home/home.do>

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

(Europe) <http://www.ebi.ac.uk/pdbe/>

PDBe is the European resource for the collection, organisation and dissemination of data on biological macromolecular structures.

Teaching materials: <http://www.ebi.ac.uk/pdbe/training/tutorials>

Structure validation: <http://www.ebi.ac.uk/pdbe/modval1>

(Japan) <https://pdbj.org/>

Nucleic Acid Database (NDB):

<http://ndbserver.rutgers.edu/>

The NDB contains information about experimentally-determined nucleic acids and complex assemblies. Use the NDB to perform searches based on annotations relating to sequence, structure and function, and to download, analyze, and learn about nucleic acids.

Guide to understanding PDB data:

<http://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/introduction>

Biological Magnetic Resonance Data Bank (BMRB)

<http://www.bmrwisc.edu/>

A Repository for Data from NMR Spectroscopy on Proteins, Peptides, Nucleic Acids, and other Biomolecules

**NMR data related analysis tools <http://www.ebi.ac.uk/pdbe/nmr-resources>*

EMDataBank

<http://www.emdatabank.org/>

EMDataBank is a unified global portal for deposition and retrieval of 3DEM density maps, atomic models, and associated metadata, as well as a resource for news, events, software tools, data standards, validation methods for the 3DEM community.

**How to search in EMdata <https://www.youtube.com/watch?v=aXDK6owQovw&feature=youtu.be>*

EMPIAR

<http://www.ebi.ac.uk/pdbe/emdb/empiar/>

EMPIAR, the Electron Microscopy Public Image Archive, is a public resource for raw, 2D electron microscopy images. Here, you can browse, upload, and download and reprocess the thousands of raw, 2D images used to build a 3D structure.

Small angle scattering biological databank (SASBDB)

<https://www.sasbdb.org/>

Curated repository for small angle scattering data and models. SASBDB is a fully searchable curated repository of freely accessible and downloadable experimental data, which are deposited together with the relevant experimental conditions, sample details, derived models and their fits to the data. About the SAXS data <https://www.sasbdb.org/help/>

Software for structure visualisation

LiteMol

<http://webchemdev.ncbr.muni.cz/Litemol/>

Fast, handles 3D data in the browser

PyMOL

<https://www.pymol.org/>

The leading software package for customization of 3-D biomolecular images. Using PyMOL, data can be represented in nearly 20 different ways. Spheres provides a CPK-like view, surface and mesh provide more volumetric views, lines and sticks put the emphasis on bond connectivity, and ribbon and cartoon are popular representations for identifying secondary structure and topology.

- * PyMOL wiki https://pymolwiki.org/index.php/Main_Page
- * PyMOL plugin for PDB annotations https://pymolwiki.org/index.php/PDB_plugin
- * PyMOL plugin for SAXS data <https://www.embl-hamburg.de/biosaxs/manuals/saspy.html>
- * PyMOL movie school <https://pymolwiki.org/index.php/MovieSchool>

UCSF Chimera

<https://www.cgl.ucsf.edu/chimera/>

UCSF Chimera is a highly extensible program for interactive visualization and analysis of molecular structures and related data, including density maps, supramolecular assemblies, sequence alignments, docking results, trajectories, and conformational ensembles. High-quality images and animations can be generated. Chimera includes complete documentation and several tutorials, and can be downloaded free of charge for academic, government, nonprofit, and personal use.

- * Chimera 'wiki' <https://www.cgl.ucsf.edu/chimera/docindex.html>

UCSF ChimeraX

<https://www.cgl.ucsf.edu/chimerax/>

UCSF ChimeraX (or simply ChimeraX) is the next-generation molecular visualization program from the Resource for Biocomputing, Visualization, and Informatics (RBVI), following UCSF Chimera. ChimeraX can be downloaded free of charge for academic, government, nonprofit, and personal use. Advantages over Chimera: <https://www.cgl.ucsf.edu/chimerax/docs/user/advantages.html>

Jmol

<http://jmol.sourceforge.net/>

Jmol is a free, open source molecule viewer for students, educators, and researchers in chemistry, biochemistry, physics, and materials science.

Educational resources

PDB Molecule of the month:

<http://pdb101.rcsb.org/motm/motm-by-title>

Paper models of molecules:

http://pdb101.rcsb.org/learn/resources/paper_models