

# Protein Databank



**PDBj**  
<https://pdbj.org/>

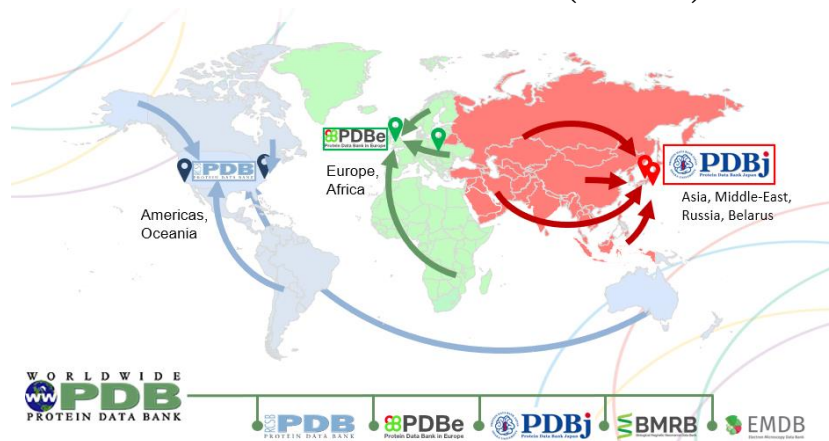


The Protein Data Bank Japan (PDBj) (<https://pdbj.org/>) is a key member of the Worldwide Protein Data Bank (wwPDB), which is comprised of data from Japan, the United States, and Europe. As a result, it has established the PDB (Protein Data Bank) and the BMRB (NMR Experimental Data Bank). The total number of publicly available data in wwPDB is 240,291 (196,681 X-ray crystal structures, 14,571 NMR structures, 28,335 cryo-electron microscopy structures, and 704 others) (as of August 2025). Within this, PDBj is mainly responsible for registering data from the Asian region, and approximately 30% of the data registered in wwPDB comes from PDBj.

As part of PDBj's unique activities, it has integrated data quality validation reports for all experimental methods and provided them to wwPDB. In addition, it has developed and provides its own services and tools for searching, visualizing, and analyzing protein three-dimensional structure data, contributing to the advancement of structural biology data utilization.

It is widely used as a reference for experimental data and is utilized not only in basic biology but also in applied fields such as drug discovery.

## Worldwide Protein Data Bank (wwPDB)



## Usage Status

### • Average monthly access count over the past four years

(Number of visits to the PDBj and BMRBj sites)

FY2021: Approximately 120,000 cases, FY2022: Approximately 170,000 cases, FY2023: Approximately 260,000 cases, FY2024: Approximately 1,020,000 cases

After Dr. John M. Jumper and others received the Nobel Prize in Chemistry in September 2024, access to PDBj, which contains the PDB data used as training data for AlphaFold, surged.

### • Number of papers and number of citations (As of August 2025, surveyed by Scopus)

From 2002 to 2025, the number of papers published in this database, under the names wwPDB and BMRB, totaled 48, and these papers were cited a total of 7,545 times.

### • Case Studies

#### 1) Design of Novel Non-Natural Proteins

By elucidating structural rules from the three-dimensional structures of many known proteins, it is possible to design proteins with entirely new three-dimensional structures that have not been observed in nature before. Professor Koga and his colleagues at Osaka University artificially designed a novel protein with a completely new  $\alpha\beta$ -fold combination that had not been previously seen, using PDB data, and then synthesized the protein and determined its NMR structure (Nature Struct. Mol. Biol. 2023).

#### 2) Development of AlphaFold2

Dr. John M. Jumper and his colleagues, who received the Nobel Prize in Chemistry for their research on protein structure prediction, further developed AlphaFold3, which enhances protein complex prediction technology, by using PDB data to train AlphaFold2, which was trained on PDB data (Nature 2024).

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# Integrated website summarizing 3D structures, mutation information, and interaction information for each protein



## PDBj UniProt Portal

<https://pdbj.org/uniprot>



3D structural data of various bio-macromolecules analyzed by research groups around the world are registered with the Protein Data Bank (PDB), an international collaborative organization, and made available worldwide. These structural data are actively utilized not only in basic biology but also in applied fields such as drug discovery.

PDBj (<https://pdbj.org/>) collaborates with centers in the United States and Europe to publish all PDB data and register protein 3D structure data analyzed in the Asian region. It also develops and provides unique services and tools for searching, visualizing, and analyzing protein 3D structure data.

In Nov 2024, PDBj launched a new integration portal for UniProt. This portal site compiles PDB structural data for each amino acid sequence (UniProt ID) in UniProt, along with gene mutation information and interaction information derived from jMorp (Japanese Multi Omics Reference Panel) and MGenD (Medical Genomics Japan Variant Database), enabling users to comprehensively view various types of information related to the 3D structure of any protein.

This portal page shows unique quality evaluation scores for each 3D structure data set. If multiple structure data sets are registered for a single protein, this information can be used as a reference when deciding which structure data set to select for a given purpose.

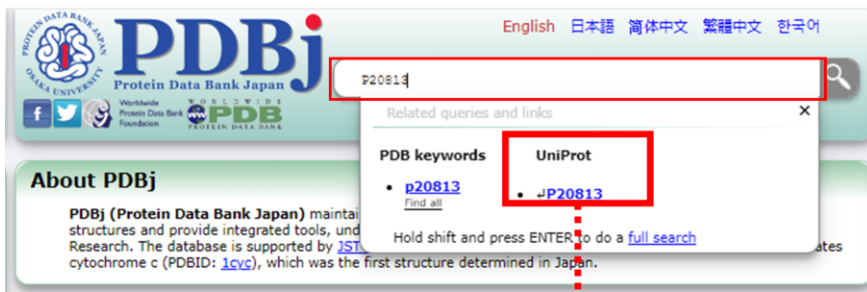
In addition, gene mutation information is displayed in the amino acid sequence viewer, and the position of any amino acid residue can be confirmed in the 3D structure viewer. This can be useful, for example, in speculating on the effects of gene mutations related to diseases on protein function.

### How to access the UniProt Integrated Portal

Enter the UniProt ID of the protein you want to search for in the search box on the PDBj top page, and click the link under “UniProt” to display the UniProt integrated portal page.

### Reference

Gert-Jan Bekker *et al.*, Protein Data Bank Japan: Improved tools for sequence-oriented analysis of protein structures. *Protein Science* 2025 (<https://doi.org/10.1002/pro.70052>)



An example of PDBj UniProt Portal page (P20813)

The screenshot shows the PDBj UniProt Portal page for P20813. Key features include:

- 3D Structure Viewer Panel:** A 3D ribbon diagram of the protein structure.
- AA sequence data panel:** A sequence viewer showing the amino acid sequence with various annotations.
- Information on Proteins:** A table with protein details such as Name (Cytochrome P450 2B6), Modification date (2025-06-18), and Organism (Homo sapiens (Human)).
- List of 3D Structure Data:** A table listing available PDB IDs and their coverage percentages.
- Interaction Information Panel:** A circular diagram showing interaction partners.
- List of sequence changes:** A table listing mutations such as Met 20, Asp 22, and Thr 24.
- List of genetic mutations:** A table listing mutations like A120, A121, and A122.
- Verification report panel for 3D structural data:** A chart showing quality metrics like Clashscore, Ramachandran outliers, and RSMD outliers.
- Information on the 3D structure:** A section providing details about the structure, including the PDB ID (PDB: 20813) and the X-ray diffraction resolution (1.76 Å).



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