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## The definitive source for protein structures

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## Abstract

Protein Data Bank (PDB) is the recognized public repository for protein structure information.

## Mirror sites

[Protein Data Bank mirror sites](#) are available.

## Content

Protein Data Bank (PDB) is the recognized public repository for protein structure information. Most scientific journals will not allow structural biologists to publish a new experimentally determined structure unless the authors also deposit the three-dimensional coordinates with the PDB. The data bank now contains more than 13,000 structures, the majority of which have been determined by X-ray crystallographic or nuclear magnetic resonance (NMR) methods. The data bank also contains some structures that are theoretical models. The coordinates for the structures can be downloaded in the PDB's text-based format, and then viewed using rendering software such as RasMol. The site also provides an excellent 'Structure Explorer' feature, with which users can investigate an individual structure after locating it using the search interface. The Structure Explorer includes the ability to view the structure, either as a still image or interactively, using a variety of methods. It also provides a wealth of information to structural biologists and other scientists who work extensively with protein structures, such as a table of the dihedral angles in the structure, and the sequence of the protein with the associated secondary structure indicated.

## Navigation

The site makes use of good standard navigational design features, such as a link to the home page from each page. Access to the information in the data bank is, however, primarily via the search interface. Three main types of search are provided. If the user knows the PDB unique identifier of a particular structure, he or she can enter this and quickly retrieve the file for that structure. The

SearchLite feature provides quick, easy searches by keyword, such as the name of the protein or its enzymatic function. There is also an advanced search feature that allows users to perform detailed searches on fields such as the type of molecule (for example, protein or DNA), ligands or prosthetic groups (such as heme) included in the structure, and experimental crystallographic details (such as resolution and unit cell dimensions). It is also possible to search by sequence.

## Reporter's comments

### Timeliness

New structures are constantly being added to the data bank. The last update at the time of reporting was 24 October 2000.

### Best feature

When the RCSB took over administration of the PDB, they introduced the summary information page, which allows the user to view important information about the structure, such as the primary literature citation and basic experimental details, before downloading the entire coordinates file. This is useful, because the download of the complete file can take time.

### Wish list

The RCSB has introduced many new search features specific for structures determined by X-ray crystallography. It would be nice to see similarly specialized search features for structures determined by NMR. For instance, it would be useful to be able to search on the number of NMR restraints per residue used in the structure calculations. A new task force has been formed to address issues specific to NMR structures, so perhaps these search features will appear soon.

### Related websites

The PDB website includes an excellent page of links to [Protein Data Bank mirror sites](#), particularly resources about protein structure, sequence and function.

# Table of links

[Protein Data Bank \(PDB\)](#)

[San Diego Supercomputer Center](#)

[Rutgers University](#)

[National Institute of Standards and Technology](#)

[Protein Data Bank mirror sites](#)

[Macromolecular structure related resources](#)

## References

1. [Protein Data Bank \(PDB\)](#).