PDB NEWSLETTER

NUMBER 14 ◆ SUMMER 2002 ◆ PUBLISHED QUARTERLY BY THE PROTEIN DATA BANK

Weekly PDB news is available on the Web at **http://www.rcsb.org/pdb/latest_news.html**

Links to this and previous PDB newsletters are available at **http://www.rcsb.org/pdb/newsletter.html**

Contents

Snapshot: July 1, 2002

18,528 released atomic coordinate entries

Molecule Type

16,633	proteins, peptides, and viruses
1,101	nucleic acids
776	protein/nucleic acid complexes
18	carbohydrates

Experimental Technique

15,223	diffraction and other
7,263	structure factor files
2,819	NMR
1,313	NMR restraint files

Participating RCSB Members

SDSC: www.pdb.org

Rutgers: rutgers.rcsb.org

NIST: nist.rcsb.org

E-mail: info@rcsb.org

FTP: ftp.rcsb.org

Message from the PDB

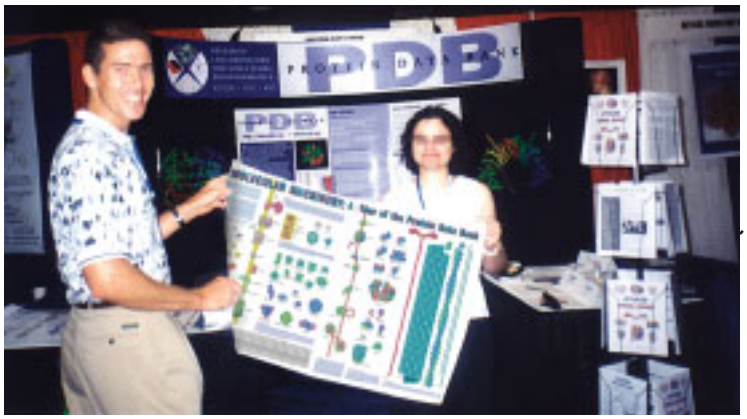
This summer, the 19th Congress and General Assembly of the International Union of Crystallography will take place in Geneva, Switzerland from August 6 -15. We are looking forward to this event, and hope you will stop by our stand (#13) in the exhibit hall or attend our PDB Users Lunch on Saturday August 10.

PDB users may be interested in the session "M65—Databases" that will be held on Tuesday August 13. The program will feature a variety of presentations on databases and database issues.

The PDB will also be exhibiting at the 10th International Conference on Intelligent Systems for Molecular Biology (August 3–7, Edmonton, Canada) and at the 16th Annual Symposium of the Protein Society (August 17–21, San Diego, CA).

We look forward to seeing you soon.

The PDB ✦



Tristan Fiedler (University of Miami Medical School) picks up a Molecular Machinery poster from PDB annotator Kyle Burkhardt at the American Crystallographic Association's Annual Meeting (San Antonio, TX, May 25–30, 2002).

The Protein Data Bank (PDB) is the single worldwide repository for the processing and distribution of 3-D biological macromolecular structure data. The PDB is operated by Rutgers, the State University of New Jersey; the San Diego Supercomputer Center (SDSC) at the University of California, San Diego; and the National Institute of Standards and Technology (NIST) — three members of the Research Collaboratory for Structural Bioinformatics, a non-profit consortium dedicated to improving our understanding of biological systems.

MIRROR SITES

Cambridge Crystallographic Data Centre (UK): **http://pdb.ccdc.cam.ac.uk/**

National University of Singapore: **http://pdb.bic.nus.edu.sg/**

Osaka University (Japan): **http://pdb.protein.osaka-u.ac.jp/**

Universidade Federal de Minas Gerais (Brazil): **http://www.pdb.ufmg.br/**

Data Deposition and Processing

PDB Deposition Statistics

During April - July 2002, more than 950 structures were deposited to the PDB. Approximately 68% of all of the structures received during this period were deposited with a "hold until publication" release status; 9% were deposited with a specific hold date; and 23% were deposited with a "release immediately" status. 74% were the result of X-ray crystallographic experiments; 13% from NMR.

Deposition Checklists Available

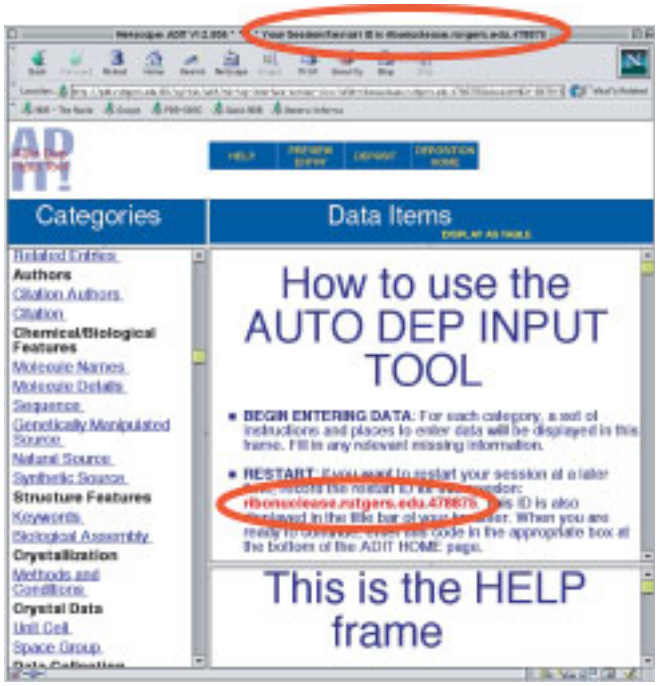
Checklists of the data items to have on hand when depositing structures via ADIT are available for both X-ray and NMR depositions. These checklists highlight the information that will be requested when depositing.

ADIT is accessible from **http://deposit.pdb.org/adit/** (RCSB-US) and **http://pdbdep.protein.osaka-u.ac.jp/adit/** (Osaka University, Japan). Further information about PDB depositions is available at **http://deposit.pdb.org/**.

NMR: **http://deposit.pdb.org/nmr-cklist.html**
X-ray: **http://deposit.pdb.org/xray-cklist.html**

PDB Focus: Restarting ADIT Depositions

Depositing a structure using ADIT can be done in more than one session by using the "Session Restart ID". This identifier appears in red in the center of the browser window when the ADIT "deposit" step is first started. It also appears in the title of the browser throughout the deposition session.



The restart ID appears in the center of the browser window when the session is first started. It also appears in the title of the browser throughout the deposition session.

ADIT stores the data entered in a category every time the user presses the SAVE button. These data will be available with the restart ID until the user deposits the entry by selecting the "DEPOSIT NOW" button.

The restart ID is entered in the space provided on the ADIT home page to return to the undeposited ADIT entry. Restart IDs are case-sensitive.

ADIT is available at **http://deposit.pdb.org/adit/** (RCSB-US) and **http://pdbdep.protein.osaka-u.ac.jp/adit/** (Osaka University, Japan).

A tutorial guide to using ADIT is available in English at **http://deposit.pdb.org/adit/docs/tutorial.html** and in Japanese at **http://www.protein.osaka-u.ac.jp/pdb/**. Example "in progress" ADIT depositions are available at **http://deposit.pdb.org:81/**.

Data Query, Reporting, and Access

New PDB Features

The Swiss-PdbViewer and new external links are now available from the Structure Explorer page for each PDB entry.

The Swiss-PdbViewer is now included as an option in the View Structure section of Structure Explorer pages on the PDB beta Web site. This molecular graphics viewing program allows users to load and display several molecules simultaneously, create layered image files, and more. Instructions for downloading and configuring the Swiss-PdbViewer can be found at **http://www.rcsb.org/pdb/help-graphics.html#spdbv_download**.

New external links to PDBsum, CATH, and SCOP are now accessible from the Summary Information section of the Structure Explorer pages on the PDB Web site and its mirrors. Additionally, external links to analysis resources, such as Contacts of Structural Units, are now available from the Geometry section of the Structure Explorer pages on these sites.

Questions about these new features may be sent to **info@rcsb.org**.

Theoretical Model Files Moved to Separate Directory on PDB FTP Site

As previously announced, the PDB theoretical model coordinate files were separated from the main archive beginning July 1, 2002. After this date, the main archive consists of structures determined using experimental methods only. Theoretical models will only be available for download from the PDB FTP site as follows:

- All theoretical models are in a separate location in the FTP archive, and a subdirectory for obsoleted models is also available:
  pub/pdb/data/structures/models/current
  pub/pdb/data/structures/models/obsolete
- Any newly deposited or released theoretical model will go directly into the /models/current directory. If it supersedes an earlier model, that earlier model will be obsoleted, and moved from /models/current to /models/obsolete.
- An index file is available in the models directory to facilitate browsing.

- From the Web interfaces, a theoretical model file will only be accessible by entering its PDB ID. All other queries (SearchLite, SearchFields, Status) will not return model entries.
- Searches by the PDB ID of a model through the Web will return a hyperlink to that model's coordinate file in the FTP archive.
- Theoretical models will be removed from the PDB Contents Growth and PDB Holdings statistics at **http://www.rcsb.org/pdb/holdings.html**.
- Theoretical models will also be moved to a separate location on the PDB CD-ROMs after July 1.

Models may still be deposited after this date, using ADIT: **http://deposit.pdb.org/adit/**, **http://pdbdep.protein.osaka-u.ac.jp/adit/**; or AutoDep: **http://autodep.ebi.ac.uk/**. These depositions will be forwarded to the models directory of the PDB FTP server without further annotation or validation.

PDB Focus: Query Result Browser Options

Any set of structures returned from a PDB search can be included in a tabular report, downloaded in one file, queried further in a refined search, and more when using the Query Result Browser.

The pulldown menu at the top of the Query Result Browser page can be used to:

- **Perform a New Search**—returns either SearchFields or SearchLite, depending on which was used for the previous search.
- **Download Structures or Sequences**—search results can be downloaded in a single file in a variety of file and compression formats
- **Refine Your Query**—the resulting set can be searched further with the option to remove files that contain certain parameters or keywords
- **Create a Tabular Report**—choose from a variety of prepared reports (Structure Summary, Sequence, Crystallization Description, Unit Cell, Data Collection, Refinement, Citation) or customize your own
- **Select/Deselect All Structures**—all the entries can be selected/deselected with one click. This is useful when performing further operations on a result set in which the majority, but not all, structures are desired
- **Remove Sequence Homologues**—creates a subset of the structures from which sequence homologues have been largely removed
- **Show Only Selected Structures**—removes unselected structures from the browser view
- **Show Structures on Hold**—returns a list of unreleased structures which match the query
- **Review Your Query**—shows the search parameters used and the number of structures found, selected, and on hold

These options are activated by selecting one and clicking on the "Go" button.

More information on using the options available from the Query Result Browser is available at **http://www.rcsb.org/pdb/help-results.html**.

PDB Focus: Software Page

The PDB's Software page is a portal to software developed by the RCSB and others in the macromolecular structure community. RCSB-developed software, such as the CIFTr application for translating files between mmCIF and PDB formats, the STAR (CIF) modules for parsing mmCIF files, and the ADIT workstation version are available for download. Links to external software resources relating to mmCIF, crystallography, NMR, structure analysis and verification, modeling and simulation, and molecular graphics are also available here.

This page is accessible from the "SOFTWARE" link on the PDB home page and at **http://www.rcsb.org/pdb/software-list.html**. Requests to add macromolecular-related software links to this page may be sent to **info@rcsb.org**.

PDB Web Site Statistics

The PDB is available from several Web and FTP sites located around the world. Users are also invited to preview new features at the PDB beta test site, accessible at **http://beta.rcsb.org/pdb/**.

The access statistics are given below for the main PDB Web site at **http://www.pdb.org/**.

Access Statistics for **www.pdb.org**

	DAILY AVERAGE			MONTHLY TOTALS		
MONTH	HITS	FILES	SITES	KBYTES	FILES	HITS
Jun 02	130,469	100,509	66,347	96,614,937	3,015,287	3,914,098
May 02	149,367	114,677	75,831	142,094,035	3,440,328	4,481,031
Apr 02	169,904	129,524	84,374	195,524,851	3,885,741	5,097,149

PDB Mirrors

SDSC/UCSD (US) **http://www.pdb.org/**
Rutgers (US) **http://rutgers.rcsb.org/**
NIST (US) **http://nist.rcsb.org/**
CCDC (UK) **http://pdb.ccdc.cam.ac.uk/**
National University of Singapore **http://pdb.bic.nus.edu.sg/**
Osaka University (Japan) **http://pdb.protein.osaka-u.ac.jp/**
Universidade Federal de Minas Gerais (Brazil) **http://www.pdb.ufmg.br/**

PDB Outreach

Three PDB Papers Published

As highlighted on its cover, the July-August 2002 issue of the *American Scientist* contains an article that explores the history of protein structure determination and the PDB. "Protein Structures: From Famine to Feast" also reports how structural genomics initiatives will populate the PDB with many unique structures in the future. The illustrations were created by David S. Goodsell, author and illustrator of the PDB's Molecule of the

Month feature and Molecular Machinery poster.

Protein Structures: From Famine to Feast. Helen M. Berman, David S. Goodsell and Philip E. Bourne. *American Scientist* (2002) **90:4**, pp. 350-359.

The recent special issue of *Acta Crystallographica B/D* on crystallographic databases features two PDB articles. "The Protein Data Bank" introduces and describes the goals of the PDB, the systems in place for data deposition and access, and plans for the future development of the resource. "Protein structure resources" describes and classifies the web-accessible resources derived from data in the PDB. These include resources for protein structure and functional classification, as well as links to primary genomic information, protein-protein interactions, protein dynamics, and protein-modeling resources.

The Protein Data Bank. H.M. Berman, T. Battistuz, T.N. Bhat, W.F. Bluhm, P.E. Bourne, K. Burkhardt, Z. Feng, G.L. Gilliland, L. Iype, S. Jain, P. Fagan, J. Marvin, D. Padilla, V. Ravichandran, B. Schneider, N. Thanki, H. Weissig, J.D. Westbrook and C. Zardecki. *Acta Cryst.* (2002). **D58**, pp. 899-907.

Protein structure resources. H. Weissig and P.E. Bourne. *Acta Cryst.* (2002). **D58,** pp. 908-915.

The July-August 2002 issue of the American Scientist.

PDB at the ACA and the International School of Crystallography

The PDB participated in two meetings in May. Thanks to everyone who stopped by the PDB exhibit at the American Crystallographic Association's Annual Meeting in San Antonio, Texas (May 25-30).

On May 24, a PDB talk was given as part of the International School of Crystallography Meeting in Erice, Italy. We appreciate the support shown by those who were able to join us at these events!

PDB CD-ROM Set #100 Now Available

The current Protein Data Bank CD-ROM set (release #100) is now being distributed. This release contains the macromolecular structure entries for the 17,679 structures available on the PDB Web site as of April 1, 2002.

The CD-ROMs are produced quarterly as of the last update of the PDB Web site for March, June, September and December. Further information is available at **http://www.rcsb.org/pdb/cdrom.html** where the CD-ROM documentation can also be accessed.

BioSync: A Structural Biologist's Guide to Synchrotron Facilities

The Structural Biology Synchrotron Users Organization (BioSync) offers a portal to resources for crystallographers through the BioSync Web site at **http://biosync.sdsc.edu/**. This site contains information for prospective synchrotron users in the field of macromolecular crystallography, including technical descriptions of U.S. beamlines. Hyperlinks to beam time request forms, synchrotron usage training, site contact information and directions are also available. Further details can be obtained by visiting the BioSync Web site or by sending email to **biosync@sdsc.edu**. Further information on BioSync can also be found in the article:

A biologist's guide to synchrotron facilities: the BioSync Web resource

Anne Kuller, Ward Fleri, Wolfgang F. Bluhm, Janet L. Smith, John Westbrook and Philip E. Bourne

Trends in Biochemical Sciences **27:4**, pp. 213-215. (1 April 2002)

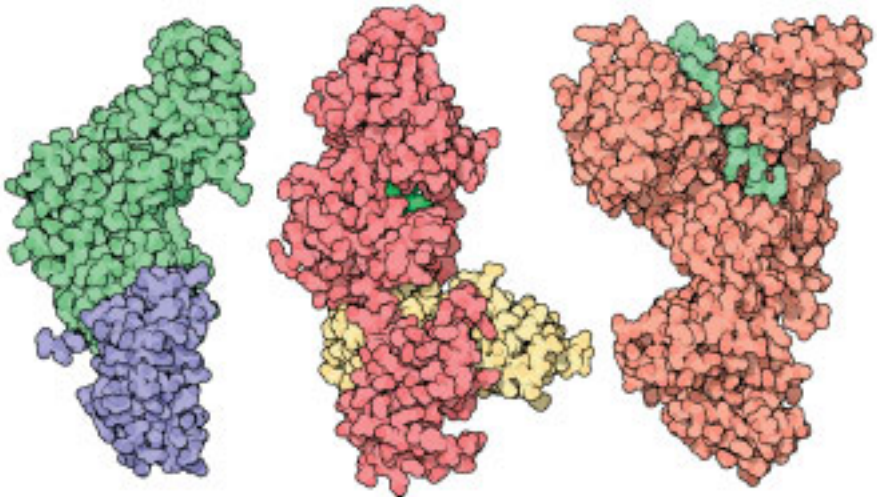
PDB Molecules of the Quarter: Anthrax Toxin, Penicillin-binding Proteins, and Glutamine Synthetase

The Molecule of the Month series explores the functions and significance of selected biological macromolecules for a general audience. These features, written and illustrated by Dr. David S. Goodsell of the Scripps Research Institute, are available at **http://www.rcsb.org/pdb/molecules/molecule_list.html**. A sample of the molecules featured during this past quarter are included below:

Anthrax Toxin: A Lethal Combination

April, 2002—Anthrax is a household word, in spite of the fact that anthrax is not a common disease. For humans, anthrax is difficult to contract. It is not transmitted from person to person—it is usually contracted when people come into contact with infected animals or their products. But recently, anthrax has gained the potential to be a major threat through bioterrorism. It is an effective weapon because it forms sturdy spores that may be stored for years, that rapidly lead to lethal infections when inhaled.

Anthrax is caused by an unusually large bacterium, *Bacillus anthracis*. Once its spores lodge in the skin or in the lungs, it rapidly begins growth and produces a deadly three-part toxin. These toxins are designed for maximum lethality, and are frighteningly effective. Part of the toxin is a delivery mechanism that seeks out cells; another part is a toxic enzyme that rapidly kills the cell. In anthrax toxin, there is one delivery molecule, termed "protective



PDB ID: ***1acc*** *(left)*

Petosa, C., Collier, R. J., Klimpel, K. R., Leppla, S. H., Liddington, R. C.: Crystal structure of the anthrax toxin protective antigen. Nature ***385*** *pp. 833 (1997)*

PDB ID: ***1k90*** *(center)*

Drum, C. L., Yan, S.-Z., Bard, J., Shen, Y.-Q., Lu, D., Soelaiman, S., Grabarek, Z., Bohm, A., Tang, W.-J.: Structural Basis for the Activation of Anthrax Adenylyl Cyclase Exotoxin by Calmodulin Nature ***415*** *pp. 396 (2002)*

PDB ID: ***1jky*** *(right)*

Pannifer, A. D., Wong, T. Y., Schwarzenbacher, R., Renatus, M., Petosa, C., Bienkowska, J., Lacy, D. B., Collier, R. J., Park, S., Leppla, S. H., Hanna, P., Liddington, R. C.: Crystal Structure of the Anthrax Lethal Factor Nature ***414*** *pp. 229 (2001)*

antigen" because of its use in anthrax vaccines (shown on the left from PDB entry **1acc**). It delivers the other two parts, edema factor and lethal factor (center and right, from PDB entries **1k90** and **1jky**), which are the toxic components that attack cells.

These types of multiple-part toxins are quite common in the bacterial world because they are exquisitely effective. Many other examples, such as toxins from the bacteria that cause cholera and whooping cough, may be found in the PDB. The delivery component specifically seeks out cell surfaces and inserts the toxic component where it can do the most damage. The toxic component is far more effective than poisons like cyanide and arsenic. Those poisons attack one-on-one, with a single cyanide molecule poisoning a single protein molecule. But toxic enzymes are compact cell-killing machines. Once inside the cell, they hop from molecule to molecule, destroying each in turn. These molecules are so effective that in some cases a single molecule can kill an entire cell.

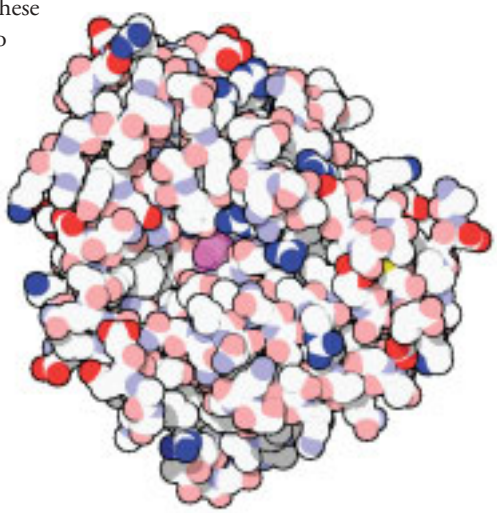
Penicillin-binding Proteins: Magic Bullets

May, 2002—Bacteria pose a continual threat of infection, both to humans and to other higher organisms. Thus, when looking for new ways to fight infection, it is often productive to look at how other plants, animals and fungi protect themselves. This is how penicillin was discovered. Through a chance observation in 1928, Alexander Fleming discovered that colonies of Penicillium mold growing in his bacterial cultures were able to stave off infection. With more study, he found that the mold was flooding the culture with a molecule that killed the bacteria, penicillin.

Penicillin and other beta-lactam antibiotics (named for an unusual, highly reactive lactam ring) are very efficient and have few side effects (apart from allergic reactions in some people). This is because the penicillin attacks a process that is unique to bacteria and not found in higher organisms. As an additional advantage, the enzymes attacked by penicillin are found on the outside of the cytoplasmic membrane that surrounds the bacterial cell, so the drugs can attack directly without having to cross this strong barrier.

When treated with low levels of penicillin, bacterial cells change shape and grow into long filaments. As the dosage is increased, the cell surface loses its integrity, as it puffs, swells, and ultimately ruptures. Penicillin attacks enzymes that build a strong network of carbohydrate and protein chains, called peptidoglycan, that braces the outside of bacterial cells. Bacterial cells are under high osmotic pressure; because they are concentrated with proteins, small molecules and ions are on the inside and the environment is dilute on the outside. Without this bracing corset of peptidoglycan, bacterial cells would rapidly burst under the osmotic pressure.

Penicillin is chemically similar to the modular pieces that form the peptidoglycan, and when used as a drug, it blocks the enzymes that connect all the pieces together. As a group, these enzymes are called penicillin-binding proteins. Some assemble long chains of sugars with little peptides sticking out in all directions. Others, like the D-alanyl-D-alanine carboxypeptidase/transpeptidase shown here (PDB entry **3pte**), then crosslink these little peptides to form a two-dimensional network that surrounds the cell like a fishing net.



PDB ID: ***3pte***

Kelly, J. A., Knox, J. R., Zhao, H., Frere, J. M., Ghaysen, J. M.: Crystallographic mapping of beta-lactams bound to a D-alanyl-D-alanine peptidase target enzyme. J Mol Biol ***209*** *pp. 281 (1989)*

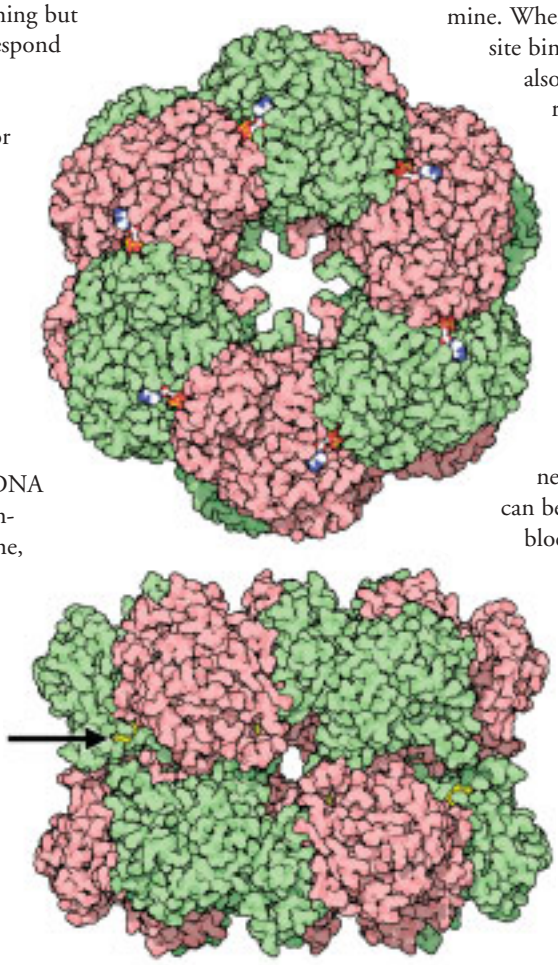
Glutamine Synthetase

June, 2002—Our cells are continually faced with a changing environment. Think about what you eat. Some days you might eat a lot of protein, other days you might eat a lot of carbohydrate. Sometimes you may eat nothing but chocolate. Your body must be able to respond to these different foods, producing the proper enzymes for capturing the nutrients in each. The same is doubly true for small organisms like bacteria, which do not have as many options in choosing their diet. They must eat whatever food happens to be close by, and then mobilize the enzymes needed to use it.

The enzyme glutamine synthetase is a key enzyme controlling the use of nitrogen inside cells. Glutamine, as well as being used to build proteins, delivers nitrogen atoms to enzymes that build nitrogen-rich molecules, such as DNA bases and amino acids.So, glutamine synthetase, the enzyme that builds glutamine, must be carefully controlled. When nitrogen is needed, it must be turned on so that the cell does not starve. But when the cell has enough nitrogen, it needs to be turned off to avoid a glut.

Glutamine synthetase acts like a tiny molecular computer, monitoring the amounts of nitrogen-rich molecules. It watches levels of amino acids like glycine, alanine, histidine and tryptophan, and levels of nucleotides like AMP and CTP. If too much of one of these molecules is made, glutamine synthetase senses this and slows production slightly. But as levels of all of these nucleotides and amino acids rise, together they slow glutamine synthetase more and more. Eventually, the enzyme grinds to a halt when the supply meets the demand.

The glutamine synthetase molecule shown here (PDB entry **1fpy**) is from bacteria. It is composed of twelve identical subunits, each of which has an active site for the production of glutamine. When performing its reaction, the active site binds to glutamate and ammonia, and also to an ATP molecule that powers the reaction. But, the active sites also bind weakly to other amino acids and nucleotides, partially blocking the action of the enzyme. All of the many sites communicate with one another, and as the concentrations of competing molecules rise, more and more of the sites are blocked, eventually shutting down the whole enzyme. The cell has a more direct approach when it wants to shut down the enzyme. At a key tyrosine next to the active site, an ADP molecule can be attached to the protein, completely blocking its action.



PDB ID: ***1fpy***

Gill, H. S., Eisenberg, D.: The Crystal Structure of Phosphinothricin in the Active Site of Glutamine Synthetase Illuminates the Mechanism of Enzymatic Inhibition Biochemistry ***40*** *pp. 1903 (2001)*

We make several versions of glutamine synthetase in our own cells. Most of our cells make a version similar to the bacterial one described here, but with eight subunits instead of twelve. Like the bacterial enzyme, it is controlled by the nitrogen-rich compounds down the synthetic pipeline. We also make a second glutamine synthetase in our brain. There, glutamate is used as a neurotransmitter, and glutamine synthetase is used when the glutamate is recycled after a nerve impulse is delivered. In the brain, glutamine synthetase is in constant action, so a highly-regulated version is not appropriate. Instead, the alternate form is active all the time, continually performing its essential duty.

PDB Project Team Leaders

The overall operation of the PDB is managed by the PDB Project Team Leaders. Technical and scientific support are provided by the PDB Members.

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PDB Job Listings

PDB career opportunities are posted at **http://www.rcsb.org/pdb/jobs.html**. The current available openings are:

System and Applications Programmer

The Protein Data Bank at Rutgers University has a position open for an applications programmer to support and develop software for data processing operations at the Protein Data Bank. Programming areas include: macromolecular structure analysis and validation, molecular graphics, web application development, distributed object and relational database applications, and general scientific programming. Experience developing and maintaining object oriented software on UNIX platforms is required. Experience in the following is highly desirable: C/C++, JAVA, and Corba.

Please send resume to Dr. Helen M. Berman at **pdbjobs@rcsb.rutgers.edu**.

Biochemical Information Specialist

The Protein Data Bank at Rutgers University has a position open for a Biochemical Information Specialist to curate and standardize macromolecular structures for the Protein Data Bank. A background in biological chemistry, as well as some experience with UNIX-based computer systems, is required. Experience in crystallography and/or NMR spectroscopy is a strong advantage. The successful candidate should be well-motivated, able to pay close attention to detail, and meet deadlines. This position offers the opportunity to participate in an exciting project with significant impact on the scientific community.

Please send resume to Dr. Helen M. Berman at **pdbjobs@rcsb.rutgers.edu**.

Administrative Support

The Protein Data Bank at Rutgers University has a position open for Administrative Support. General office support including, but not limited to calendar maintenance, filing, phones, typing general correspondence. Proficiency in word processing and database applications as well as usage and creation of spreadsheets utilizing MS Office software. Requires excellent organizational and communication skills. General accounting experience a plus.

Please send resume to Dr. Helen M. Berman at **pdbjobs@rcsb.rutgers.edu**.

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