PDB NEWSLETTER

NUMBER 17 ◆ SPRING 2003 ◆ PUBLISHED QUARTERLY BY THE PROTEIN DATA BANK

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

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

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Snapshot: April 1, 2003

20,533 released atomic coordinate entries

Molecule Type

18,492	proteins, peptides, and viruses
1,168	nucleic acids
855	protein/nucleic acid complexes
18	carbohydrates

Experimental Technique

17,386	diffraction and other
9,147	structure factor files
3,147	NMR
1,511	NMR restraint files

Participating RCSB Members

SDSC: www.pdb.org

Rutgers: rutgers.rcsb.org

NIST: nist.rcsb.org

E-mail: info@rcsb.org

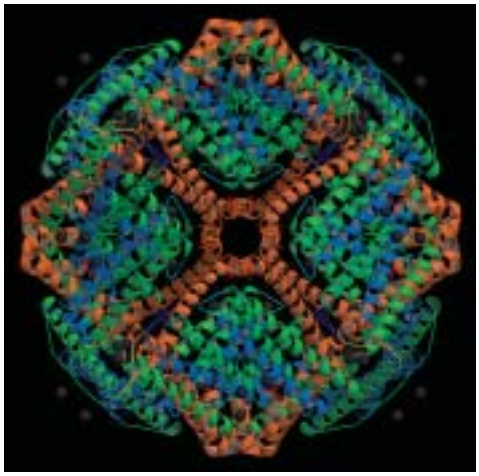
FTP: ftp.rcsb.org

Message from the PDB

During the past quarter, the PDB has added a variety of features for data query and reporting to our beta and production sites. The beta site (**beta.rcsb.org/pdb**) is a place where new developments can be tested by the PDB community before they are added to the main production PDB sites worldwide (**beta.rcsb.org/pdb/mirrors.html**). Comments about features being tested at the PDB Beta Test Site should be sent to **notify@rcsb.org**. We thank all of you who have used this site and have provided feedback!

This newsletter includes the inaugural "PDB Education Corner" article. This section is intended to highlight the different ways the PDB is used in all types of classrooms. This quarter's feature is written by Prof. Gale Rhodes (University of Southern Maine), who writes about the use of graphics in introductory biochemistry courses, as well as workshops and other resources as part of his "Molecular Level" outreach program.

The PDB ✦



The biological unit of L-chain horse apoferritin

PDB ID: ***1aew***

Hempstead, P. D., Yewdall, S. J., Fernie, A. R., Lawson, D. M., Artymiuk, P. J., Rice, D. W., Ford, G. C., Harrison, P. M. (1997): Comparison of the three-dimensional structures of recombinant human H and horse L ferritins at high resolution. J. Mol. Biol. ***268****, p. 424.*

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): **pdb.ccdc.cam.ac.uk**

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

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

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

Max Delbrück Center for Molecular Medicine (Germany): **www.pdb.mdc-berlin.de**

Data Deposition and Processing

PDB Deposition Statistics

In the first quarter of 2003, approximately 1,200 structures were deposited to the PDB. 76% 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 15% were deposited with a "release immediately" status. 85% were the result of X-ray crystallographic experiments; 11% from NMR.

PDB Annotation Manual Online in PDF and Postscript Formats

The manual used as a guide by the PDB ADIT annotators for PDB Data Processing and Annotation is now available in PDF as well as PostScript format.

This document, a reference for the annotation staff, describes how the PDB data processing software system is used to produce the files that are released into the PDB archive. It is available from **www.rcsb.org/pdb/info.html#File_Formats_and_Standards**.

PDB Focus: ADIT Annotators

PDB data are processed by an international effort. Structures deposited using ADIT are processed by staff from the RCSB (at Rutgers University in New Jersey and remotely at the Center for Complex Molecular Systems and Biomolecules in the Czech Republic) and from the Institute for Protein Research at Osaka University.

Structures are also deposited using AutoDep at the European Bioinformatics Institute (EBI) in the United Kingdom. Data deposited using AutoDep are processed by the Macromolecular Structure Database (MSD) group at the EBI.

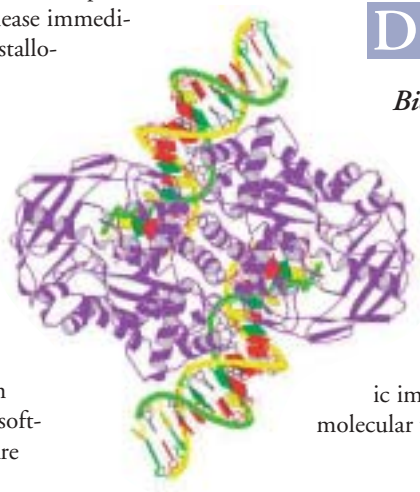
ADIT

RCSB: **pdb.rutgers.edu/adit**

Osaka University: **pdbdep.protein.osaka-u.ac.jp/adit**

AutoDep

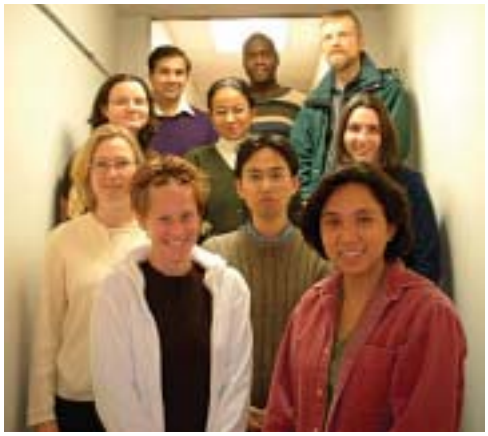
MSD-EBI: **autodep.ebi.ac.uk** ✦



The biological unit of Tn5 transposase complexed with Me DNA

PDB ID: ***1mm8***

Steiniger-White, M., Bhasin, A., Lovell, S., Rayment, I., Reznikoff, W. S. (2002): Evidence for "Unseen" Transposase—DNA Contacts. J. Mol. Biol. ***322****, p. 971.*



Annotators Takashi Kosada (Osaka University) and Bohdan Schneider (Center for Complex Molecular Systems and Biomolecules in the Czech Republic) on a visit to the RCSB-Rutgers site.

PDB Annotators (top row, left to right): Shri Jain, Anthony Adelakun, Bohdan Schneider; (middle row): Kyle Burkhardt, Shuchismita Dutta, Suzanne Richman; (bottom): Rose Oughtred, Jessica Marvin, Takashi Kosada, Tania Rose Posa.

Data Query, Reporting, and Access

New Features Available for Beta Testing: Biological Unit, Curated (Beta) mmCIF Files, Redundancy Reduction Cluster Data

During the past quarter, several new features have been released for beta testing:

Biological Unit

The biological unit images for applicable structures are now accessible from the Structure Explorer pages on the PDB Beta Web Site at **beta.rcsb.org/pdb**.

The View Structure section of the Structure Explorer now offers still ribbon images of the assumed biological unit(s) for structures, where relevant, in addition to static images of the asymmetric unit. The interactive molecular viewers available from this page continue to provide a variety of ways to visualize the asymmetric unit. Links to the coordinate files that are used to generate the biological unit images are also accessible here, as well as from the Download/Display File section of the Structure Explorer.

Curated (Beta) mmCIF Files

The Download/Display File section of the Structure Explorer pages on the Beta Web Site now provides links to view or download the curated mmCIF files. These files include remediated data from the Data Uniformity Project (**www.rcsb.org/pdb/uniformity**). The files follow the latest version of the mmCIF dictionary supplemented by an exchange dictionary developed by the RCSB and the MSD-EBI. This exchange dictionary can be obtained from **deposit.pdb.org/mmcif**.

The curated mmCIF files for a set of query results can be downloaded by selecting the Download Structures or Sequences option from the pull down menu at the top of the Query Result Browser page.

Curated mmCIF files for all PDB structures are available in gzip (.gz) format at **ftp://beta.rcsb.org/pub/pdb/uniformity/data/mmCIF.gz/**. UNIX-compressed versions of these files (**.Z**) remain available at **ftp://beta.rcsb.org/pub/pdb/uniformity/data/mmCIF/**.

Redundancy Reduction Cluster Data

The results of the weekly clustering of protein chains in the PDB are now available for beta testing at **ftp://ftp.rcsb.org/pub/pdb/derived_data/NR/**.

These clusters are used in the "remove sequence homologs" feature on the PDB web sites. Files that list the clusters and their rankings at 50%, 70% and 90% sequence identity are available. Smaller rank numbers indicate higher (better) ranking. Chains with rank number 1 are ranked as the best representative of their cluster.

The contents of these files and the details of the clustering and ranking are further described at **ftp://ftp.rcsb.org/pub/pdb/derived_data/NR/README** and **www.rcsb.org/pdb/redundancy.html**.

Comments on these new features are appreciated and may be sent to **notify@rcsb.org**.

New Features on the Structure Explorer Pages of the PDB Web Site: Author and Ligand Searches, BioMagResBank Links

The following new features have been implemented on the Structure Explorer pages of the PDB Web Site:

Author and Ligand Searches

For any PDB entry, the Summary Information section of the Structure Explorer page now supports queries for all other entries by a specific primary citation author, or that include a particular ligand listed on that page. By clicking on any individual primary citation author's name, all PDB entries by that author will be returned. A query for all entries that contain an individual ligand is performed by clicking on any ligand in the "Retrieve all PDB IDs Containing" column in the "HET groups" table.

BioMagResBank Links

Links to the BioMagResBank (BMRB) are now included on the Structure Explorer pages for NMR-solved PDB structures that are also available in the BMRB resource. These links return a BMRB NMR restraints grid for the particular PDB structure being explored. The BMRB database contains NMR chemical shifts derived from proteins and peptides, reference data, amino acid sequence information, and data describing the source of the protein and the conditions used to study the protein. Images of the structures are also available. The BMRB links on the Structure Explorer pages are directed to the BMRB site maintained at the University of Wisconsin-Madison, an RCSB partner site.

Feedback on these new features is appreciated and may be sent to **info@rcsb.org**.

PDB Focus: Redundancy Reduction Capability

A subset of structures from which homologous sequences have been largely removed can be obtained from the result list of a query. This option—which is activated by selecting the "remove sequence homologs" option on SearchLite, SearchFields, and the PDB home page—filters subsets of structures that match a particular query. The default threshold for sequence similarity removal for queries from the home page or SearchLite is 90%; SearchFields provides the option of selecting 50, 70, or 90% similarity as cut-off values. Users can toggle between the complete set of results and the reduced subset by using the options menu at the top of the Query Result Browser.

Further information about this feature is available at **www.rcsb.org/pdb/redundancy.html**.

PDB Focus: Maintaining a Local PDB FTP Mirror Site

There are several freely available methods for establishing and maintaining a local copy of the PDB FTP Site. The methods described below have the added benefit of preserving the timestamps on files:

rsyncPDB.sh

The RCSB-created *rsyncPDB.sh* script is a template for using rsync to mirror the FTP archive from an anonymous rsync server. The script can be found at **ftp://ftp.rcsb.org/pub/pdb/software/**, and the comments in the script explain its usage. Before successfully running it, users will need to set three variables in *rsyncPDB.sh* to suit their local setup. This script is now used by the PDB to maintain its FTP mirrors.

mirror.pl

The non-RCSB *mirror.pl* script, which had been used to mirror the PDB FTP archive in the past, is available under the GNU public license from **ftp://sunsite.org.uk/packages/mirror/**. It is recommended to install the *ftp.pl_wupatch* security patch with the script, also available from this site.

The RCSB-created *getPdbUpdate.pl* script can also be useful for providers of new FTP mirror sites in obtaining the files from any one particular update.

The script can be found at **ftp://ftp.rcsb.org/pub/pdb/software/**, and its usage is explained at **ftp://ftp.rcsb.org/pub/pdb/software/getPdbUpdate.html**.

Be aware that only *LWP::UserAgent*, but not *wget*, preserves the original time stamps of the files.

PDB FTP mirroring procedures are further explained at **www.rcsb.org/pdb/ftpproc.final.html**, and the layout of the PDB FTP archive is accessible at **www.rcsb.org/pdb/ftp_plan.html**. For more information about mirroring the PDB FTP Site, please send e-mail to **info@rcsb.org**.

PDB Focus: Weekly Updates to the PDB

The PDB is updated with new structures each week by Wednesday, 1:00 A.M. Pacific time. This schedule is maintained each week; any changes that may occur are announced in the PDB news. Users can access structures from any previous update using the *getPdbUpdate.pl* script, which can be found at **ftp://ftp.rcsb.org/pub/pdb/software/**. Usage of this script is explained at **ftp://ftp.rcsb.org/pub/pdb/software/getPdbUpdate.html**.

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 **eta.rcsb.org/pdb**.

The access statistics are given on page 4 for the main PDB Web site at **www.pdb.org**.

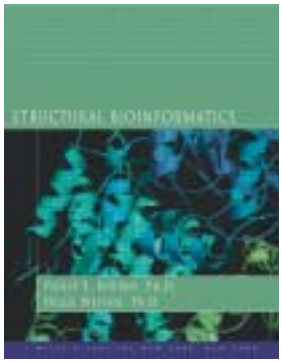
Access Statistics for **www.pdb.org**

	DAILY AVERAGE			MONTHLY TOTALS		
MONTH	HITS	FILES	SITES	KBYTES	FILES	HITS
Mar 02	174,789	132,651	109,763	149,005,949	4,112,207	5,418,463
Feb 02	177,358	135,209	101,844	133,377,215	3,785,855	4,966,025
Jan 02	177,832	132,344	91,520	160,156,911	4,102,694	5,512,795

PDB Web Mirrors

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

PDB Outreach



Structural Bioinformatics *Book Includes Chapters on the PDB*

The recently published book, *Structural Bioinformatics*, includes several chapters about the PDB, which describe its history, function, development, and future goals, as well as the different data formats and protocols used to represent PDB structures:

The PDB Team (2003). The Protein Data Bank. *Structural Bioinformatics.* P. E. Bourne and H. Weissig. Hoboken, NJ, John Wiley & Sons, Inc. pp. 181-198.

Westbrook, J and Fitzgerald, PM (2003). The PDB format, mmCIF formats and other data formats. *Structural Bioinformatics*. P. E. Bourne and H. Weissig. Hoboken, NJ, John Wiley & Sons, Inc. pp. 161-179.

Structural Bioinformatics facilitates an understanding of the theories, algorithms, resources, and tools that are used to study biomacromolecular structures such as those included in the PDB. The topics covered—including protein, DNA, RNA, carbohydrate, and complex structures—offer the reader a better understanding of biological function.

Structural Bioinformatics. P. E. Bourne and H. Weissig. Hoboken, NJ, John Wiley & Sons, Inc. (2003). ISBN: 0-471-20199-5

PDB Paper Published in Nucleic Acids Research

The PDB recently published a paper, "The Protein Data Bank and structural genomics", in the latest Database Issue of *Nucleic Acids Research*. This paper describes some of the resources available from **www.rcsb.org/pdb/strucgen.html**, including the target registration database, TargetDB.

J. Westbrook, Z. Feng, L. Chen, H. Yang, and H.M. Berman (2003): The Protein Data Bank and structural genomics. *Nucl. Acids Res.* **31**, pp. 489-491.

New Distribution Procedure for Protein Data Bank CD-ROM Sets

The January 2003 release of the PDB CD-ROM sets, issue 103, is a full release of 19,623 experimentally determined structures that were available as of January 1, 2003. The structures, on five CD-ROM disks, have been shipped.

Starting with the April 2003 release, an incremental set of structures released

since the January 2003 Issue will be sent to subscribers. Structures re-released for any reason between January and April will be included in this update. A list of files that have become obsolete since the last update will be included so users can update their set of structures.

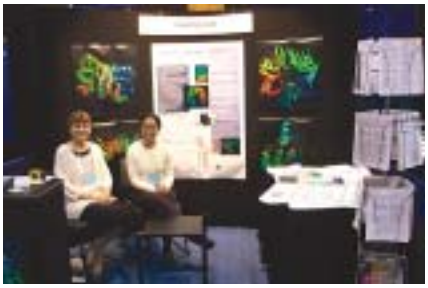
July and October Issues will only contain the structures released during those quarters. New subscribers will receive the January release and all subsequent updates.

The index files in the *pub/resource* sub-directory will continue to include all structures in the current PDB FTP site as of that release.

Experimental data—NMR constraints and X-ray structure factors—will be handled in the same manner as the structures: a complete set in January, and incremental updates for the three subsequent quarters.

Questions should be directed to **info@rcsb.org**. Ordering information is available at **www.rcsb.org/pdb/cdrom.html**.

PDB at the Biophysical Society Meeting



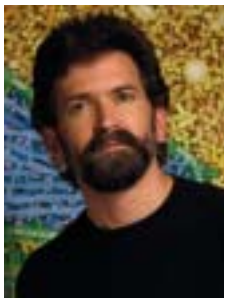
PDB staff members Judith Flippen-Anderson and Shuchismita Dutta at the PDB booth at the Biophysical Society Annual Meeting

The PDB would like to thank everyone who visited the PDB booth at the 47th Annual Meeting of the Biophysical Society, that was held March 1-5, in San Antonio, TX. We appreciate the feedback that we received from the community, and hope to see you at future meetings!

PDB Focus: David Goodsell and the Molecule of the Month

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 **www.rcsb.org/pdb/molecules/molecule_list.html**.

Recently, the PDB interviewed Dr. Goodsell to find out how he creates these beautiful and informative works of art.



Dr. David S. Goodsell

***PDB:** How did this idea emerge initially?*

Goodsell: When I started, I wanted to create a friendly doorway to the PDB. The PDB contains many interesting structures, but it can be daunting to people who aren't experienced with atomic coordinates and molecular viewers.

One great challenge is the sheer magnitude of the PDB. For instance, if you are interested in hemoglobin, you are faced with dozens of structures, and it may be difficult to choose one for further exploration. My goal these days is to present a general introduction to each molecule, and then give a few suggestions for PDB entries that show the major features of the molecule. A place for visitors to start in their own exploration of these fascinating molecular machines.

***PDB:** How do you create the illustrations?*

Goodsell: Most of the pictures are created with a computer program that I developed back when I was doing postdoctoral work with Dr. Art Olson here at The Scripps Research Institute. I've been using this style of illustration—with flat colors and black outlines—for about 10 years now. I like the way that this style simplifies the molecule, giving a feeling for the overall shape and form of the molecule, but at the same time you can still see all the individual atoms. On the last page of each Molecule of the Month—"Exploring the Structure"—I always use RasMol, to give visitors an idea of the kinds of pictures that they can create themselves with off-the-shelf software.

Proteins are challenging subjects to illustrate. I try to find views that show off the unusual features of the molecules. I like to work with molecules where there is a clear relationship between the structure and the function, such as the way that the ribosome clamps around the messenger RNA or the power stroke motion of myosin. I am also fascinated by the beautiful symmetry of proteins, and always create pictures that highlight this symmetry. Every Molecule of the Month is a new adventure.

***PDB:** How do you select the featured structures?*

Goodsell: I try to pick molecules that play a familiar role in human life and health. My favorites are molecules where we can see how the molecular structure and function are directly related to something that we experience in our lives. Myosin is a good example--we can easily imagine those countless little engines crawling up actin as we bend our arm. For each new Molecule of the Month, I try to pick 4-5 PDB entries that, in my opinion, best show the functional features that I am describing.

***PDB:** Has it been popular?*

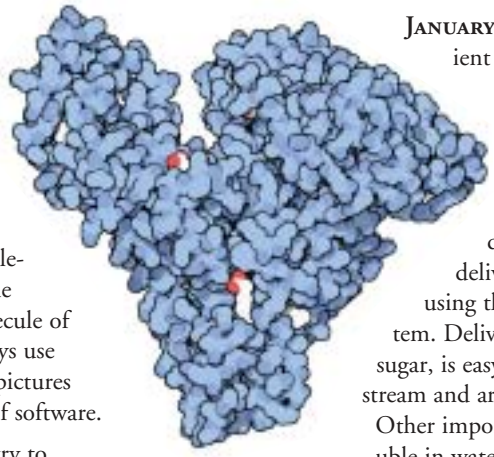
Goodsell: Well, I hope so! I have gotten a bunch of great letters from visitors—students, teachers, researchers, and all sorts of other people. I always like it when people use my pictures in their own assignments or presentations, to aid in their own exploration of the subject.

***PDB:** What do you plan for the future?*

Goodsell: Lots more molecules! I'm planning a new column on hemoglobin with Dr. Shuchismita Dutta (PDB-Rutgers), who helped out on the one on potassium channels a few months ago--look for it later this Spring. I don't have any plans to enlarge the Molecule of the Month--the PDB is growing too fast to think of doing anything more comprehensive. I'm planning to keep it small and informal—a new tidbit each month.

PDB Molecules of the Quarter: Serum Albumin, Potassium Channels, and lac Repressor

A sample of the molecules featured during this past quarter are included below:



PDB ID: **1e7i**

Bhattacharya, A. A., Grune, T., Curry, S. (2000): Crystallographic Analysis Reveals Common Modes of Binding of Medium and Long-Chain Fatty Acids to Human Serum Albumin. J. Mol. Biol. ***303****, p. 721.*

Serum Albumin: Carrying Fatty Acids

January, 2003—Think about how convenient it is to be able to eat. Each one of your ten trillion cells requires a constant supply of nourishment. But we don't have to worry about this--we merely eat our dinner and our body does the rest. The food is digested and the useful pieces are delivered to cells throughout the body, using the bloodstream as the delivery system. Delivery of water-soluble molecules, like sugar, is easy. They float in the watery bloodstream and are picked up by cells along the way. Other important nutrients, however, are not soluble in water, so special carriers must be made to chaperone them to hungry cells.

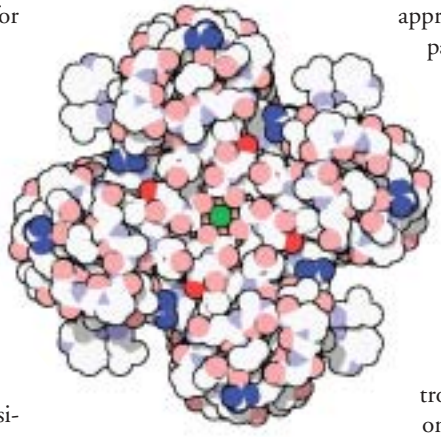
Serum albumin, shown in PDB entry **1e7i**, is the carrier of fatty acids in the blood. Fatty acids are essential for two major things in your body. They are the building blocks for lipids, which form all of the membranes around and inside cells. They are also rich sources of energy, and may be broken down inside cells to form ATP. Thus, your body maintains a storehouse of fatty acids, stored as fat. When your body needs energy or needs building materials, fat cells release fatty acids into the blood. There, they are picked up by serum albumin and delivered to distant parts of the body.

Further information about serum albumin can be found at **www.rcsb.org/pdb/molecules/pdb37_1.html**.

Potassium Channels: Open and Shut

February, 2003—All living cells are surrounded by a membrane that separates the watery world inside from the environment outside. Membranes are effective barriers for small ions (as well as for large molecules like proteins and DNA), providing a novel oppor-

tunity: differences in ion levels may be used for rapid signaling. For instance, a cell can raise the level of potassium ions inside it. Then, at a moment's notice, potassium can be released through channels in the membrane, creating a large change in the potassium level that will be felt throughout the cell. This process is used in all types of cells - bacteria, plants and animals. Two common examples of ion channels at work are seen in muscle contraction (which is started by the release of calcium ions), and nerve signaling (which involves a complex flow of sodium and potassium ions).



PDB ID: **1bl8**

Doyle, D. A., Morais Cabral, J., Pfuetzner, R. A., Kuo, A., Gulbis, J. M., Cohen, S. L., Chait, B. T., MacKinnon, R. (1998): The structure of the potassium channel: molecular basis of K+ conduction and selectivity. Science ***280****, p. 69.*

When you smell a flower and know that it is a rose, or touch a hot object and immediately pull your hand away, nerves from your nose and hands use the release of ions to send signals to your brain and relay back the appropriate response. Nerve cells ready themselves for sending a signal by concentrating potassium ions inside and selectively pumping sodium ions out. This creates a difference in electrical potential across the cell membrane. To send a signal, sodium channels along the nerve open, allowing sodium to enter and reducing the voltage across the membrane. Potassium channels then open, letting the potassium ions out and re-establishing the original voltage.

Other channels and pumps later reset the distribution of sodium and potassium ions inside and outside the cell. By clever design, both of these channels are sensitive to the voltage across the membrane, opening when the voltage changes. So, when the channels are opened at one end of a nerve cell, the flow of ions there instantly triggers channels further down the membrane to open. The result is a wave of channel opening that rushes down the nerve cell, carrying the nerve signal to the end.

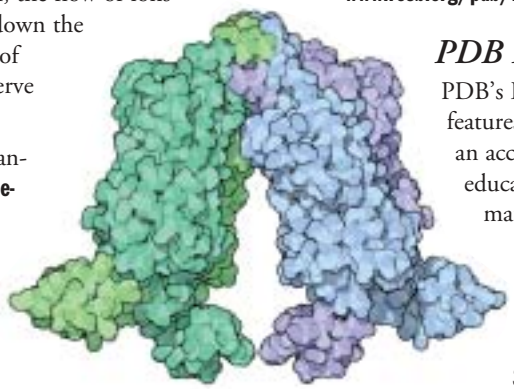
Further information about potassium channels can be found at **www.rcsb.org/pdb/molecules/pdb38_1.html**.

lac Repressor: Blocking DNA

March, 2003—DNA is filled with information. Our own DNA contains the instructions for building tens of thousands of different proteins and RNA, which perform all the different functions that keep us alive. As discovered by Watson and Crick fifty years ago, this genetic information is stored in the sequence of adenine, thymine, cytosine and guanine bases in the DNA. Their model of the DNA double helix showed how the information is read by separating the two strands of DNA and then pairing the exposed surfaces of the bases with appropriate partners, such that adenine always pairs with thymine and cytosine pairs with guanine.

The genetic information encoded in the DNA strand is far from being the whole story. A simple set of protein blueprints would hardly be useful, because each of our cells would make all of the 30,000 proteins continually. But brain cells don't need to make hemoglobin, and red blood cells don't need to make acetylcholine receptors. Each cell needs to be able to control the construction of its proteins so that it only builds the proteins needed for its own function. To solve this problem, our DNA also contains a lot of regulatory information that specifies when and where each protein should be made. Unlike the genetic information, this regulatory information is read without unwinding the DNA double helix. Instead, an army of regulatory proteins—including the lac repressor—feels along the surface of the DNA double helix, reading the parts of the bases that are exposed and looking for the appropriate instructions. Some of these proteins, when they find the appropriate instructions, bind to DNA and block the production of proteins that are encoded in the local area. Other regulators enhance the production of proteins, coaxing RNA polymerase to begin its function of transcribing messenger RNA. The nucleus is a flurry of these regulatory proteins, as they control the production of proteins that are currently needed and block synthesis of proteins that are not.

Further information about the lac repressor can be found at **www.rcsb.org/pdb/molecules/pdb39_1.html.**



PDB ID: **1tlf**

Friedman, A. M., Fischmann, T. O., Steitz, T. A. (1995): Crystal structure of lac repressor core tetramer and its implications for DNA looping. Science ***268****, p. 1721.*

PDB ID: **1efa**

Bell, C. E., Lewis, M. (2000): A Closer View of the Conformation of the Lac Repressor Bound to Operator. Nat. Struct. Biol. *7, p. 209.*

PDB Education Corner

PDB's Education Corner is a new column that features a different teacher each quarter, offering an account of how he or she uses the PDB to educate students. Educators will find this information useful to inspire their own courses and methods of teaching that incorporate the PDB.

This quarter's column is by Prof. Gale Rhodes, from the University of Southern Maine:

Students in my introductory biochemistry course learn how to visualize and study macromolecules by computer graphics at the same time they learn the basics of protein structure. They learn how to obtain macromolecular models from the Protein Data Bank and to analyze their structure with Deep View (aka Swiss-PdbViewer). After learning how to use Deep View by way of a hands-on workshop and a Web tutorial

(**www.usm.maine.edu/~rhodes/SPVTut/index.html**), they pick a protein for individual study, obtain it from the Protein Data Bank, get to know its structure, and write a structural description illustrated with a views in a Deep View project file. Throughout the rest of the course, students work problems from a graphics problems supplement. Students must obtain PDB models and study them with Deep View in order to solve the problems.

I also use Deep View and PDB models throughout the course to illustrate all aspects of macromolecular structure and function. Finally I am currently developing an introduction to bioinformatics for the second semester of my biochemistry course. This teaching unit, a study of human opsins, will entail a FASTA search of the PDB for opsin structures (and finding bovine rhodopsin, no doubt), and will culminate with homology modeling of a human opsin, using a search of the ExPDB database for templates.

In addition to this use of PDB models in my teaching, I have a little outreach project called "The Molecular Level: Molecular Graphics Training for Students, Teachers, and Researchers". Through this program, I provide hands-on workshops in molecular graphics to area researchers, students in other courses at USM, and advanced-placement biology and chemistry high-school students and teachers. Workshop participants get a hands-on introduction in which they learn how to obtain models from the PDB and study them with Deep View. They can then use my tutorial to follow up the workshop.

For more information about my use of graphics in introductory biochemistry, see "Molecular Graphics Manifesto: Why and How to Integrate Molecular Graphics into Introductory Biochemistry", at **www.usm.maine.edu/~rhodes/Manifesto/index.html**.

To see my graphics exercises for a biochemistry course, see "Learning Biochemistry with Deep View: A Gallery of Graphics Exercises for Introductory Biochemistry", at **www.usm.maine.edu/~rhodes/BiochemViews/index.html**.

To see typical workshop outlines and other resources of "The Molecular Level" outreach program, go to **www.usm.maine.edu/~rhodes/MolLevel/index.html**.

My introduction to bioinformatics is under development. You can see what I've done so far (PDB and homology modeling parts not done yet) at **www.usm.maine.edu/~rhodes/Goodies/Matics.html**.

Related Links: Education

The PDB's Education Web portal links to many different resources, including:

Online Macromolecular Museum: www.clunet.edu/BioDev/omm/gallery.htm

Basics of NMR: www.cis.rit.edu/htbooks/nmr

An introduction to the nuclear magnetic resonance experimental method *Audience: Undergraduate*

Reciprocal Net: www.reciprocalnet.org

Distributed database used by research crystallographers to store information about molecular structures, including basic elements and ions, amino acids and nucleosides; also offers Flash tutorial on symmetry and point groups. *Audience: Graduate* ✦

PDB Job Listings

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

Systems/Web/Database Programmer

The Protein Data Bank has a position open for a systems programmer and database administrator who will be responsible for maintenance of software, website, and supporting databases associated with a digital library of the Protein Data Bank (PDB) archive. The duties will include maintenance of web application software and database tools to manage the historical record of the PDB. The ideal candidate will have a strong background in UNIX, website, and database administration. Proficiency in programming in a UNIX/LINUX environment with languages such as JAVA, C/C++, or PERL is required. Experience in the following is highly desireable: SQL, JDBC, and application development using ORACLE or DB2. This position is at the PDB site at the Center for Advanced Research in Biotechnology in Rockville, MD. Please send resume to Dr. Gary L. Gilliland at **gary.gilliland@nist.gov**.

Data Archive/ Digital Librarian

The Protein Data Bank has a position open for a data archivist who will organize and manage the historical record of the Protein Data Bank. The ideal candidate will have a strong background in library science and the physical sciences. Experience in the management of large document and media collections is required. The position is at the PDB site at the Center for Advanced Research in Biotechnology in Rockville, MD.

Please send resume to Dr. Gary L. Gilliland at **gary.gilliland@nist.gov**.

Lead Scientist, Structural Bioinformatics

The Protein Data Bank at the San Diego Supercomputer Center, University of California--San Diego, has a position open for a lead scientist to provide research and development leadership in the area of structural bioinformatics, genomics, and proteomics. Description: Work closely and collaboratively with the PDB software architects, programmers, and scientists, at SDSC and the PDB partner sites, to expand the PDB's functionality and reliability as a premier biological data and information resource. Identify and develop requirements for new PDB delivery, query functionality and usability. Develop innovative approaches that will satisfy users' current needs and anticipate their future needs based on progress in the science of structural biology and structural bioinformatics. Act as the PDB technology liaison to research groups at SDSC and UCSD. Conduct bioinformatics research as it relates to the needs and expanding scope of the PDB.

Qualifications and application instructions are available at **www.rcsb.org/pdb/jobs.html**.

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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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