PDB NEWSLETTER

NUMBER 15 ◆ FALL 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: October 1, 2002

18,838 released atomic coordinate entries

Molecule Type

16,956	proteins, peptides, and viruses
1,092	nucleic acids
772	protein/nucleic acid complexes
18	carbohydrates

Experimental Technique

15,913	diffraction and other
7,742	structure factor files
2,925	NMR
1,373	NMR restraint files

Participating RCSB Members

SDSC: www.pdb.org

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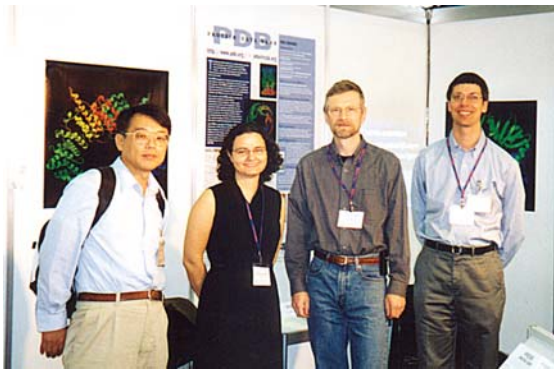
Message from the PDB

The PDB has been very busy working on two major projects: structural genomics and a redesign of the PDB Web site and query engine.

As described in this newsletter, the PDB maintains the centralized registration database for target sequences (TargetDB; **http://targetdb.pdb.org/**). The PDB has also been actively involved in coordinating the development of data deposition specifications for structural genomics and the data dictionary supporting these specifications (**http://deposit.pdb.org/mmcif/**). We recently sponsored a workshop on Structural Genomics Informatics and Software Integration. We will be participating in the International Structural Genomics Organisation (ISGO) International Conference on Structural Genomics (October 10–13, 2002; Berlin, Germany) and the High Throughput Synchrotron Crystallography Meeting (November 20–22, 2002 in Argonne, IL).

A major reengineering effort to expand the extensibility, maintainability, and scalability of the PDB query and analysis capabilities has begun. This effort will provide novel ways to query, report and visualize structure data, as well as improved navigation of the PDB Web site. In the coming months, we will be asking our PDB users for opinions and feedback on this new project.

The PDB ✦



Masami Kusunoki (Osaka University) with Kyle Burkhardt, Bohdan Schneider, and Wolfgang Bluhm at the PDB booth at the IUCr 2002 Meeting.

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

Over the summer, more than 860 structures were deposited to the PDB. Approximately 70% of all of the structures received during this period were deposited with a "hold until publication" release status; 10% were deposited with a specific hold date; and 20% were deposited with a "release immediately" status. 83% were the result of X-ray crystallographic experiments; 13% from NMR.

New mmCIF and Data Processing Software Available

RCSB-developed programs for mmCIF and data processing—including MAXIT, PDB_EXTRACT, and an mmCIF database loader—are now available from the PDB's software page for download. These programs are available in source and binary versions.

RCSB-developed applications available for use with mmCIF and for data processing include:

- **CIFTr**—An application program for translating files in mmCIF format into files in PDB format
- **PDB Validation Suite**—A tool for processing and checking structure data
- **MAXIT**—An application for processing and curation of macromolecular structure data
- **ADIT**—A package for editing and checking structure data entries
- **PDB_EXTRACT**—Tools and examples for extracting mmCIF data from structure determination applications
- **mmCIF Loader**—An application to load mmCIF data into relational databases and XML

The PDB's Software page is a portal to software developed by the RCSB and others in the macromolecular structure community. 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**.✦

Structural Genomics

Structural Genomics Informatics and Software Integration Workshop Web Site Available

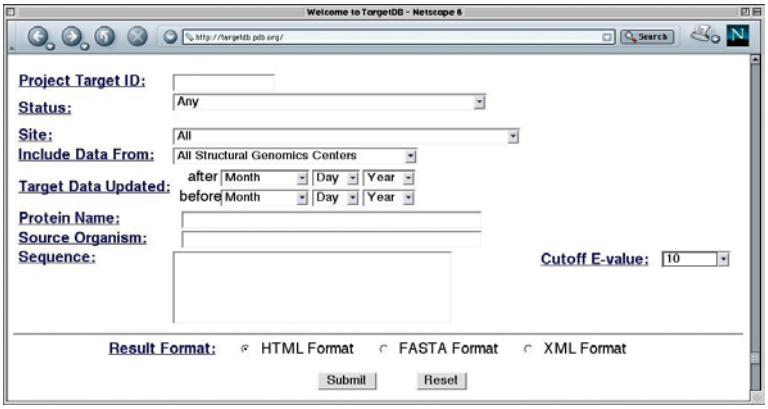
The Structural Genomics Informatics and Software Integration (SG ISI) workshop was held at the Hyatt Regency Hotel in San Antonio, Texas, on May 24-25, 2002. This workshop organized by Helen Berman, Tom Terwilliger and John Westbrook was attended by more than forty people including software developers, people involved in data management for structural genomics projects, and representatives of the Protein Data Bank.

The workshop focused on data specification, software integration, and data management issues associated with automated deposition of data into the PDB from high-throughput structure determinations.

The materials from this meeting have been made available at **http://deposit.pdb.org/sgisi02/**.

Target Registration Database Available for Structure Genomics Projects Worldwide

TargetDB (**http://targetdb.pdb.org/**) is a target registration database that was originally developed to provide registration and tracking information for NIH P50 structural genomics centers. TargetDB has now been expanded to include target data from worldwide structural genomics and proteomics projects. The scope of TargetDB is to provide timely status and tracking information on the progress of the production and solution of structures.



The TargetDB query form. Search options include ID, target status, and structural genomics center. HTML reports include the current status of the target and the one-letter code sequence, and additional information when provided by the center (source organism, structure database references, links to project data, and other related remarks. Reports may also be created in FASTA and XML formats.)

The target database can be searched by sequence using FASTA (Pearson, W.R. and Lipman, D.J. (1988) "Improved tools for biological sequence comparison" *PNAS* **85**:2444-2448). Sequence searches may include only the target sequences or the PDB sequences. Target sequences may also be searched by contributing site, protein name, project tracking identifier, date of last modification, and the current status of the target (e.g. cloned, expressed, crystallized, ...). Search results may be viewed as HTML reports, FASTA data files, or in XML.

Information on target classification is also available from **http://presage.berkeley.edu** and **http://proteome.umbi.umd.edu**. ✦

Data Query, Reporting, and Access

New Features on the PDB Web Site

Three new features are now available from the primary PDB Web site and its mirror sites:

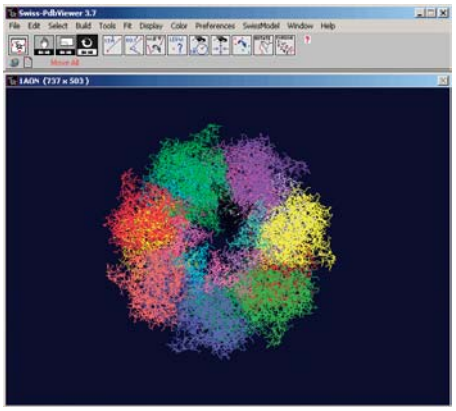
- After a period of testing on the PDB beta Web site, the Swiss-Pdb Viewer is now linked from the View Structure section of the Structure Explorer page for each PDB entry.
- The Citation Tabular Reports, which can provide bibliographic information for each structure in a search results set, now include links to search Medline either by PDB ID or Medline ID.
- A Perl script to download PDB files from any given update date is now available from **ftp://ftp.rcsb.org/pub/pdb/software/**. This script has three usages:

  getPdbUpdate.pl dates—retrieves and prints a list of valid update dates;

  getPdbUpdate.pl latest—retrieves all files from the latest update; and

  getPdbUpdate.pl 20020603—retrieves all files from that particular update.

Questions or comments on these new features may be sent to **info@rcsb.org**.



An image of PDB entry ***1aon*** *viewed with the Swiss-Pdb Viewer. This program offers functions such as comparison of alignments of multiple structures and determining distances between atoms.*

Xu, Z., Horwich, A.L., Sigler, P.B. (1997): The crystal structure of the asymmetric GroEL-GroES-(ADP)7 chaperonin complex. Nature ***388****, pp. 741.*

Experimental Data Reporting and Model Access Enhancements

Enhancements have been made to the PDB site for reporting the availability of experimental data and for accessing model data.

The availability of experimental data for a particular structure can now be included in reports generated for a set of structures resulting from a PDB search. This new column indicates whether there is a structure factor or NMR restraint file available for each structure. This feature is included in the Structure Summary report and is offered as an option for the customizable reports. Tabular reports of results can be saved in HTML format or plain text format; the latter can also be imported into a spreadsheet program such as Excel.

Links to the models directory on the PDB FTP site (**ftp://ftp.rcsb.org/pub/pdb/data/structures/models/**) have been added to the SearchLite and SearchFields pages to facilitate access to these entries from the PDB Web site. This directory includes links to released theoretical model files, a set of index files containing the keyword, author, source organism, compound, resolution, crystal dimensions for these files, and the obsoleted theoretical model files.

Limited search capability for theoretical models will be made available in the near future.

PDB Focus: Author Searches

Users can query for a particular author of a structure or a primary citation using the SearchFields interface at **http://www.rcsb.org/pdb/cgi/queryForm.cgi.** In the Citation Author field, enter the two initials and last name of the target author. An example of an author query would be:

```
S.S.Taylor
```

The initials should be separated by "."s without spaces between them or the last name. If the query is not formed this way, no results will be returned. For authors with a title included in their name, the format should be:

```
W.E.Royer Jr.
H.Brumer III
```

A search can also be performed using the author's last name only, for example:

```
Matthews
```

This will return all authors with the last name "Matthews" that are referenced in the PDB archive, as listed in the JRNL records or PDB REMARK 1 records in the structure entries. To remove a particular author from this result list, select the Refine Your Query option from the pull down menu at the top of the Query Results Browser page, which will return the SearchFields page. At the top, select the BUTNOT logic button and enter the author to be removed from the results list in the Citation Author field. For example:

```
B.W.Matthews
```

will remove all entries that reference "B.W.Matthews" from the "Matthews" result list.

Multiple authors can be queried for by performing a search for a single author as noted above, then selecting Refine Your Query from the pull down menu at the top of the results page, and entering the second author in the Citation Author field (note: the AND logic button on the SearchFields page must be selected; it is the default).

The Text Search field can also be used to query for part or all of one or more author names in a single query, such as:

```
Taylor and Zheng
```

However, users should be aware that this type of search scans the entire text of each PDB file and will return entries that include text that literally matches the query, so some undesired results may occur.

Requests for assistance with queries may be sent to **info@rcsb.org**

PDB Focus: PDBOBS

The PDBOBS database at **http://pdbobs.sdsc.edu/** archives versions of PDB entries that have been obsoleted or superseded by more recent versions. These entries are made available for historical purposes, and to allow new versions of software to be tested against the same data sets as earlier versions of the software.

The PDBOBS search interface can be used to locate obsolete entries by PDB ID or keyword. A list of obsolete PDB ID's is also available for browsing.

The result of all queries and the links in the browsing pages will graphically display the history of all versions of the PDB entry as well as a textual comparison of the key features of the structure.

A simple view of the sequence and backbone of any obsolete entry can be seen through the QuickPDB applet linked from the PDBOBS home page.

This feature also includes a simple search by PDB ID capability. Content statistics and a list of enhancements are also accessible from the PDBOBS home page.

Obsolete PDB entries are also available from the FTP Web site at **ftp://ftp.rcsb.org/pub/pdb/data/structures/obsolete/**.

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
Sept 02	153,319	117,024	84,916	126,612,164	3,510,725	4,599,589
Aug 02	114,067	88,895	61,287	112,125,145	2,666,874	3,422,023
July 02	121,727	94,732	62,595	108,313,045	2,841,977	3,651,821

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

PDB at ISMB, IUCr, and the Protein Society Symposium

The PDB thanks everyone who visited our exhibit booths at several meetings earlier this month: the Intelligent Systems for Molecular Biology (ISMB) conference in Edmonton, Canada, the Protein Society's Annual Symposium in San Diego, CA, and the XIX Congress and General Assembly of the International Union of Crystallography (IUCr) in Geneva, Switzerland.

Philip E. Bourne, David Padilla, and Gregory Vasquez respond to questions from PDB user Michael Braxenthaller at PDB's exhibit at the ISMB 2002 Conference.

The PDB Users Lunch held at the IUCr meeting set the stage for feedback from our users and a very productive discussion. We would like to thank our sponsors for their support at this lunch: Area Detector Systems Corporation, Blake Industries, Inc., deCODE genetics Emerald BioStructures Products, GlaxoSmithKline, Hampton Research, IBM, Merck Co., Inc.—USA, Proctor & Gamble Pharmaceuticals, and the Schering-Plough Research Institute.

PDB CD-ROM Set #101 Released

The current Protein Data Bank CD-ROM set (release #101) is now being distributed. This release contains the macromolecular structure entries for the 18,528 structures available on the PDB Web site as of July 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.

CD-ROM News: Experimental Data to be Offered as Separate CD-ROM Set

The number of entries in the PDB archive is ever-increasing, and this is reflected in the number of CD-ROMs required to contain each quarterly release. In order to reduce the number of disks in each set, beginning with the October 2002 CD-ROM release, subscribers will receive only the coordinate files for structure entries. This will include structures solved by X-ray and NMR experimental techniques as well as those determined theoretically.

The experimental data files will no longer be included automatically. This will reduce the number of CD-ROM disks to be loaded by 50%. Requests to receive either the X-ray structure factors or NMR constraint files can be submitted at **http://www.nist.gov/srd/o_nist801.htm**.

All recipients of the current release, July 2002, received a flyer with the CD set that can be returned to request the experimental data as well as update their address. That same flyer is included as a README file on the first CD-ROM disk in directory pub and can thus be attached to an email to use in requesting the experimental data.

All CD-ROM services will continue to be available free of charge.

PDB ID: **1olg**

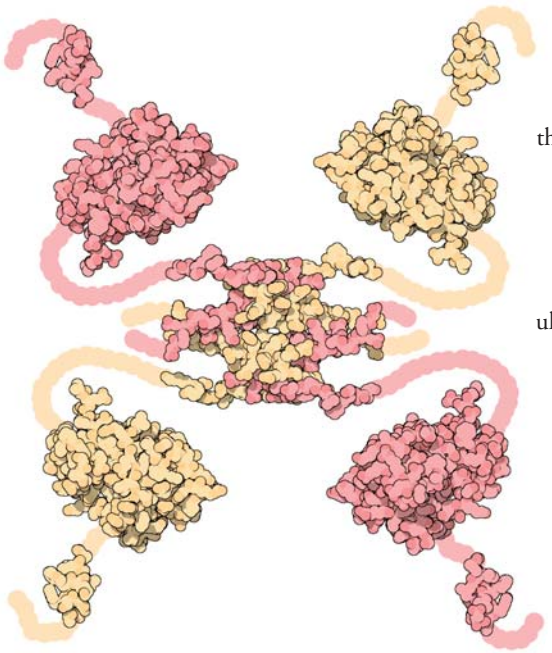
Takano, K., Yamagata, Y., Fujii, S., Yutani, K. (1997): Contribution of the hydrophobic effect to the stability of human lysozyme: calorimetric studies and X-ray structural analyses of the nine valine to alanine mutants. Biochemistry ***36****, pp. 688.*

PDB ID: **1tup**

Cho, Y., Gorina, S., Jeffrey, P.D., Pavletich, N.P. (1994): Crystal structure of a p53 tumor suppressor-DNA complex: understanding tumorigenic mutations. Science ***265****, pp. 346.*

PDB ID: **1ycq**

Kussie, P.H., Gorina, S., Marechal, V., Elenbaas, B., Moreau, J., Levine, A.J., Pavletich, N.P. (1996): Structure of the MDM2 oncoprotein bound to the p53 tumor suppressor transactivation domain. Science ***274****, pp. 948.*



ization domain (PDB entry **1olg**) that ties the four chains together. A long flexible region in each chain then connects to the second stable domain: a large DNA-binding domain (PDB entry **1tup**) that is rich in arginine residues that interact with DNA. This domain recognizes specific regulatory sites on the DNA. The third stable domain studied thus far is the transactivation domain (PDB entry **1ycq**), found near the end of each arm, that activates the DNA-reading machinery.

As you might guess from its name, p53 tumor suppressor plays a central role in the protection of your body from cancer. Cancer cells typically contain two types of mutations: mutations that cause uncontrolled growth and multiplication of cells, and other mutations that block the normal defenses that protect against unnatural growth. p53 is in this second category and mutations in the p53 gene contribute to about half of the cases of human cancer. Most of these are missense mutations, changing the information in the DNA at one position and causing the cell to build p53 with an error, swapping an incorrect amino acid at one point in the protein chain. In these mutants, the normal function of p53 is blocked and the protein is unable to stop multiplication in the damaged cell. If the cell has other mutations that cause uncontrolled growth, the cell will develop into a tumor.

Further information about p53 tumor suppressor can be found at **http://www.rcsb.org/pdb/molecules/pdb31_2.html.**

PDB Molecules of the Quarter: p53 Tumor Suppressor, Chaperones, and Reverse Transcriptase

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:

p53 Tumor Suppressor: Guardian of the Cell

July, 2002—Our cells face many dangers, including chemicals, viruses, and ionizing radiation. If cells are damaged in sensitive places by these attackers, the effects can be disastrous. For instance, if key regulatory elements are damaged, the normal controls on cell growth may be blocked and the cell will rapidly multiply and grow into a tumor. p53 tumor suppressor is one of our defenses against this type of damage. p53 tumor suppressor is normally found at low levels, but when DNA damage is sensed, p53 levels rise and initiate protective measures. p53 binds to many regulatory sites in the genome and begins production of proteins that halt cell division until the damage is repaired. Or, if the damage is too severe, p53 initiates the process of programmed cell death, or apoptosis, which directs the cell to commit suicide, permanently removing the damage.

p53 tumor suppressor is a flexible molecule composed of four identical protein chains. Flexible molecules are difficult to study by X-ray crystallography because they do not form orderly crystals, and if they do crystallize, the experimental images are often blurry. So, p53 has been studied in parts, by removing the flexible regions and solving structures of the pieces that form stable structures. Three of these compact, globular portions, termed "domains", have been studied. At the center of p53 is a tetramer-

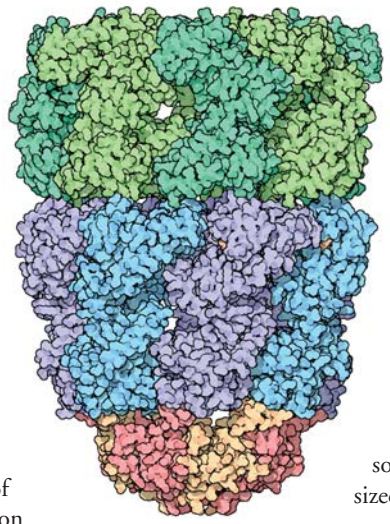
Chaperones: Guides Along the Folding Pathway

August, 2002—As you can see when looking through the many structures in the PDB, most active proteins have a stable, globular structure. However, proteins are built as formless chains, pieced together one amino acid at a time by ribosomes. Most protein chains then fold spontaneously into their final structure, driven by the need to shelter their carbon-rich portions from the surrounding water. But some--large proteins or proteins with several domains--need some assistance. As they fold into a compact shape, they might get stuck somewhere along the way.

This is not a trivial problem. Cells cannot merely wait for proteins to fold properly. Misfolded proteins often have carbon-rich amino acids on their surfaces, instead of tucked safely inside. These carbon-rich patches associate strongly with similar patches on other proteins, forming large aggregates. Random aggregates are death to cells: diseases such as sickle cell anemia, mad cow disease, and Alzheimer's disease are caused by unnatural aggregations of proteins into cell-clogging fibrils.

Chaperones are proteins that guide proteins along the proper

pathways for folding. They protect proteins when they are in the process of folding, shielding them from other proteins that might bind and hinder the process. Many chaperone proteins are termed "heat shock" proteins (with names like HSP-60) because they are made in large amounts when cells are exposed to heat. Heat, in general, destabilizes proteins and makes misfolding more common. So when it gets really hot, cells need some extra help with their proteins.



One impressive type of chaperone forms an enclosed environment for folding proteins which totally protects them as they fold. The GroEL-GroES complex of the bacterium *E. coli* can be seen in PDB entry **1aon**. It is composed of two stacked rings of GroEL proteins, and a cap on one side composed of GroES. Seven GroEL proteins form a ring with a protein-sized cavity inside. Unfolded proteins enter this cavity and fold up inside.

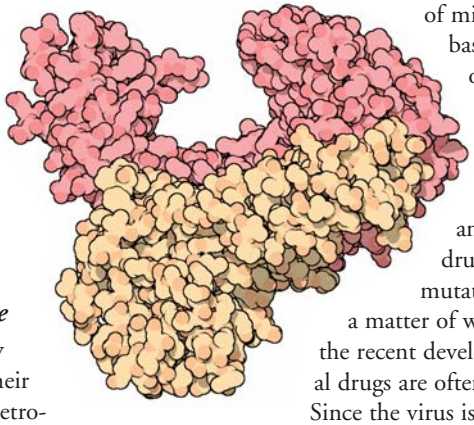
Further information about chaperones can be found at **http://www.rcsb.org/pdb/molecules/pdb32_2.html.**

PDB ID: ***1aon***

Xu, Z., Horwich, A.L., Sigler, P.B. (1997): The crystal structure of the asymmetric GroEL-GroES-(ADP)7 chaperonin complex. Nature ***388****, pp. 741.*

PDB ID: ***3hvt***

Wang, J., Smerdon, S.J., Jager, J., Kohlstaedt, L.A., Rice, P.A., Friedman, J.M., Steitz, T.A. (1994): Structural basis of asymmetry in the human immunodeficiency virus type 1 reverse transcriptase heterodimer. Proc. Natl. Acad. Sci. U.S.A. ***91****, pp. 7242.*



Reverse Transcriptase: A Sloppy Enzyme

September, 2002—Viruses are tricky. They use all sorts of unusual mechanisms during their attacks on cells. HIV is no exception. It is a retrovirus, which means that it has the ability to insert its genetic material into the genome of the cells that it infects. But, infectious HIV particles carry their genome in RNA strands. Somehow, during infection, the virus needs to make a DNA copy of its RNA genome. This is very unusual, because all of the normal cellular machinery is designed to make RNA copies from DNA, but not the reverse. DNA is normally only created using other DNA strands as a template.

This tricky reversal of synthesis is performed by the enzyme reverse transcriptase, as found in PDB entry **3hvt**. Inside its large, claw-shaped active site, it copies the HIV RNA and creates a double-stranded DNA version of the viral genome. This then integrates into the cell's DNA, and later instructs the cell to make additional copies of the virus.

Viruses are tiny. They only carry enough genetic material to encode a few proteins. Many viruses, such as poliovirus and rhinovirus, carry the bare minimum—just enough to specify their own structure and get synthesis started once they get inside cells. The genome of HIV, on the other hand, carries instructions for building a few enzymes that are used in the reproduction of the virus. Reverse transcriptase is one of these enzymes. But, space in the HIV genome is still at a premium, so reverse transcriptase is encoded in a tricky way. It is composed of two different subunits, but both are encoded by the same gene. After the protein is made, one of the subunits is clipped to a smaller size so that it can form the proper mate with one full-sized subunit.

Reverse transcriptase performs a remarkable feat, reversing the normal flow of genetic information, but it is rather sloppy in its job. The polymerases used to make DNA and RNA in cells are very accurate and make very few mistakes. This is essential because they are the caretakers of our genetic information, and mistakes may be passed on to our offspring.

Reverse transcriptase, on the other hand, makes lots of mistakes, up to about one in every 2,000 bases that it copies (if this same error rate occurred in the "Molecule of the Month," there would be two typos in this month's installment). You might think that this would cause severe problems. But, in fact, this high error rate turns out to be an advantage for the virus in this era of drug treatment. The errors allow HIV to mutate rapidly, finding drug resistant strains in a matter of weeks after treatment begins. Fortunately, the recent development of treatments that combine several drugs are often effective in combating this problem. Since the virus is simultaneously attacked by several different drugs, it cannot mutate to evade all of them at the same time.

Further information about reverse transcriptase can be found at **http://www.rcsb.org/pdb/molecules/pdb33_2.html**. ✦

RCSB PDB Project Team Leaders

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