PDB NEWSLETTER

NUMBER 9 ◆ SPRING 2001 ◆ RCSB

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CONTENTS

SNAPSHOT: MARCH 31, 2001

14,731 released atomic coordinate entries

MOLECULE TYPE

13,158	proteins, peptides, and viruses
939	nucleic acids
616	protein/nucleic acid complexes
18	carbohydrates

EXPERIMENTAL TECHNIQUE

12,137	diffraction and other
5,032	structure factor files
2,273	NMR
968	NMR restraint files
321	theoretical modeling

RCSB

SDSC: www.rcsb.org

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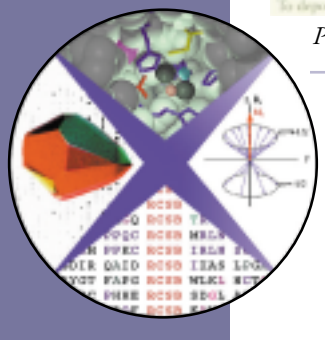


MESSAGE FROM THE PDB

The beginning of the twenty-first century has been a time of high activity for the PDB. In addition to maintaining the data flow from structure deposition to release, we continue to be actively involved in developing the resource and working with the user community.

We are very pleased that the Board of Directors of the Object Management Group (OMG) voted to adopt our proposal for the Common Object Request Broker Architecture (CORBA) Macromolecular Structure Specification. Details about this exciting development are available in this newsletter.

A poster was presented and the NMR Task Force met as part of the Frontiers of NMR in Molecular Biology VII Keystone Meeting in Big Sky, Montana (January 20-26). The PDB also exhibited at the Biophysical Society's Annual Meeting in Boston, MA (February 17-21) and at the Pittsburgh Conference (PITTCON) in New Orleans, LA (March 5-8). These were great opportunities to meet our user community, and we look forward to the meetings coming up this summer. We thank everyone who stopped by the booths.

We would like to especially thank the members of the PDB Advisory Board Committee and the representatives from our funding agencies who met with the PDB at our San Diego Supercomputer Center site on March 16-18.

The PDB

PDB paraphernalia from the Biophysical Society's Annual Meeting.

The Research Collaboratory for Structural Bioinformatics (RCSB) is a non-profit consortium dedicated to improving our understanding of biological macromolecular structure.

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.**

Data Deposition and Processing

PDB Deposition Statistics

Over 800 structures were deposited to the PDB in the first quarter of the year 2001. Among all of these many interesting structures, we received seven structures of ribosomal subunits, as well as the complete Thermus thermophilus 70S ribosome structure.

Approximately 64% of all of the structures received during this period were deposited with a "hold until publication" release status; 21% were deposited with a specific hold date; and 14% were deposited with a "release immediately" status. 83% were the result of X-ray crystallographic experiments; 14% from NMR.

Structures may be deposited using ADIT at **http://pdb.rutgers.edu/adit/** (at the RCSB-Rutgers site) or at **http://pdbdep.protein.osaka-u.ac.jp/adit/** (at the Institute for Protein Research at Osaka University, Japan). AutoDep is also available for PDB depositions at the EBI at **http://autodep.ebi.ac.uk/**. The RCSB also maintains a copy of AutoDep at **http://pdb.rutgers.edu/~adbnl/**.

Data Uniformity and *mmCIF*

New mmCIF *Resources Page*

The PDB has compiled a list of *mmCIF* (macromolecular Crystallographic Information File) resources at **http://pdb.rutgers.edu/mmcif/**. The *mmCIF* dictionary and a set of dictionary extensions are used by the PDB team for all aspects of data processing. The *mmCIF* resources page provides links to articles, data dictionaries, format correspondences, the RCSB's response to the OMG RFP for a CORBA API for Macromolecular Structure, and tutorials. This page also provides links to various software programs, including Star CIF Parser, a new program developed by the PDB.

CIF Parsing Modules Available

The CIF (Crystallographic Information File) format, a subset of STAR (Self-defining Text Archival and Retrieval format), is suitable for archiving all types of text and numerical data, in any order. CIF's usefulness derives from its generality, upward compatibility, and flexibility. Recently, the RCSB released a set of simple object-oriented Perl modules and scripts for parsing STAR-compliant data files and dictionaries like *mmCIF*. Users with a working knowledge of Perl and a basic familiarity with CIF or other STAR-compliant data file formats will benefit from these tools. Modules included in this distribution are:

STAR::Parser Perl extension for parsing STAR-compliant files (with no nested loops)

STAR::DataBlock class and object methods for dealing with DataBlock objects created by *STAR::Parser*, for such tasks as reading objects from disk or querying their data structures

STAR::Dictionary a subclass of *STAR::DataBlock*, which supports all methods from S*TAR::DataBlock*, as well as the additional method *get_save_blocks*

STAR::Writer provides several methods for writing *STAR::DataBlocks* as files in different formats

STAR::Checker contains the checker object, with methods for checking DataBlock object against STAR rules and against a specified dictionary

STAR::Filter contains the filter object for filtering DataBlock objects

The included scripts are a mixture of basic utility scripts (e.g., *parse.pl* or *check.pl*) and very simplistic examples that are meant to test certain methods in the modules (e.g., *create.pl*). Users can also write their own custom scripts.

To download these modules or for more information, please refer to the documentation at **http://pdb.sdsc.edu/STAR/**.

CORBA Specification for Macromolecular Structure Adopted by OMG

On Tuesday, February 27, 2001, the Board of Directors of the Object Management Group (OMG) voted to adopt the Common Object Request Broker Architecture (CORBA) Macromolecular Structure Specification. This specification opens the door to seamless and more specific access to PDB data. It will provide a standard application programming interface (API) that allows direct access by remote programs to the binary data structures of the PDB. Designed in collaboration with the International Union of Crystallography (IUCr), the new standard is based on the Macromolecular Crystallographic Information File (*mmCIF*) data representation**. Unlike current access in which users are required to retrieve and parse complete PDB files, an implementation of this CORBA API will allow applications to retrieve a single data item from a remote PDB server and import it for use in a local application.

CORBA provides a platform- and programming language-neutral mechanism for specifying distributed, object-oriented interfaces. The OMG, which oversees the development of CORBA and several other open standards for object-oriented computing, also charters groups such as the Life Sciences Research (LSR) Task Force for work in specific application domains. In addition to macromolecular structure, the LSR has also defined or is currently working on interface specifications in areas such as sequence analysis, gene expression, and laboratory equipment control. Collectively, these specifications should provide a robust framework for the development and integration of key data resources required by the structural biology community.

This initiative was led by Dr. Douglas Greer of the San Diego Supercomputer Center (SDSC). Dr. Greer is also the chair of the Macromolecular Structure Finalization Task Force (FTF), a newly created entity within the OMG with the charter of making any necessary changes to the specification necessary for implementation. A reference implementation with source code is expected to be publicly available from the PDB in the next year.

*** P.E. Bourne, H.M. Berman, B. McMahon, K. Watenpaugh, J. Westbrook, and P.M.D. Fitzgerald (1997): The Macromolecular CIF Dictionary.* Methods in Enzymology **277**, *pp. 571-590.*

Additional information is available at the following sites:

OMG and LSR: **http://www.omg.org/**

IUCr: **http://www.iucr.org/**

Data Uniformity Project Web Page

Data Uniformity is the name given to the PDB's efforts to provide a consistent and standard data archive. Links and update notices about this project are archived at the Data Uniformity Project Web page at **http://www.rcsb.org/pdb/uniformity/index.html.**

The latest additions include links to the *mmCIF*-formatted files on the PDB beta FTP site and to the *CIFTr* translation software. The *mmCIF* data files are for approximately 1,000 protein-nucleic complexes determined by X-ray crystallographic experiments. These files include consistent nomenclature for polymer chains, ligands, ligand atoms, consistent representation of disorder, and self-consistent descriptions of sequence and coordinate data. These files have been placed on the beta site to obtain comments on their content and to give programmers a head start in developing code that uses the richer *mmCIF* data representation. The PDB will release *mmCIF* files for all released entries this coming summer.

The *CIFTr* software that is now available translates this richer *mmCIF* into a PDB formatted file, with several nomenclature options.

mmCIF Files: **ftp://beta.rcsb.org/pub/pdb/uniformity/data/mmCIF/**

CIFTr: **http://pdb.rutgers.edu/software/**

Data Query, Reporting, Access, and Distribution

Molecular Interactive Collaborative Environment (MICE) Now Available from the PDB Web Site

The PDB is pleased to announce the availability of MICE on its Web site and mirrors. The MICE collaborative molecular viewer is now available from the View Structure page for each entry. MICE permits remote users to share a VRML-based view of a molecule via the Internet. This view is referred to as the "molecular scene." One user publishes the scene and any number of users subscribe to the scene. By mutual consent, usually via telephone, any participant can become the publisher.

At this time, MICE is supported as a signed applet on Windows machines. Further details can be obtained by visiting the MICE Web site at **http://mice.sdsc.edu/** or by clicking on the help link accessible from the View Structure page.

Questions about this feature may be sent to **info@rcsb.org**.

Custom Reports Now Available from the PDB Web Site

An additional feature has been added to the PDB Web site which allows users to create their own customized tabular reports. By selecting "Create A Tabular Report" from the option scroll bar at the top of the Query Result Browser page, users can choose from a variety of parameters that will be used to generate a report from a result list. For example, choices are available for either entire citations or authors only, or for both citations and structure summaries. Previously available report options remain accessible as well: Cell Dimensions, Primary Citation, Structure Identifier, Sequence, Experimental Technique, Refinement Information, and Data Collection information.

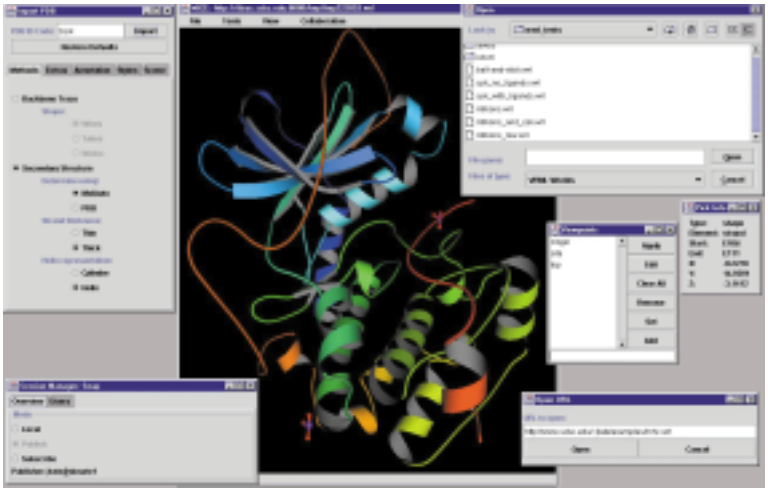
Please send your comments on this new feature to **info@rcsb.org**.

Access Statistics for **www.rcsb.org**

	DAILY AVERAGE			MONTHLY TOTALS		
MONTH	HITS	FILES	SITES	BYTES	FILES	HITS
Mar. 01	131,473	99,482	57,284	90,821,384	3,083,944	4,075,674
Feb. 01	133,337	102,748	52,936	78,840,299	2,876,954	3,733,444
Jan 01	113,143	87,024	45,084	76,445,093	2,523,706	3,281,151

PDB Web Site Statistics

The access statistics for the primary PDB Web site at **http://www.rcsb.org/pdb/** show that the numbers of hits received and files downloaded continue to increase.



As an example of a simple three-dimensional scene, the image at left shows a screenshot of a cAMP dependent protein kinase molecule (PDB ID: ***2cpk****), represented in VRML within a Web browser. This structure can be manipulated and examined from any angle. The interactive view of a molecule provides an intuitive and natural way to examine the structure.*

PDB ID: ***2cpk***

D. R. Knighton, J. Zheng, L. F. Ten Eyck, V. A. Ashford, N.-H. Xuong, S. S. Taylor, J. M. Sowadski (1991): Crystal structure of the catalytic subunit of cyclic adenosine monophosphate-dependent protein kinase. Science ***253****, p. 407.*

While the **www.rcsb.org** address continues to receive the most traffic, use of the mirror sites and beta test site is on the rise. PDB users are encouraged to access their proximate RCSB mirror sites at Rutgers (**http://rutgers.rcsb.org/**), NIST (**http://nist.rcsb.org/**), the Cambridge Crystallographic Data Centre in the United Kingdom (**http://pdb.ccdc.cam.ac.uk/**), the National University of Singapore (**http://pdb.bic.nus.edu.sg/**), Osaka University in Japan (**http://pdb.protein.osaka-u.ac.jp/**), and the Universidade Federal de Minas Gerais in Brazil (**http://www.pdb.ufmg.br/**). The beta test site is accessible at **http://beta.rcsb.org/pdb/**.

PDB Outreach

Structural Genomics Web Page at PDB

The PDB has compiled a variety of structural genomics links as part of the Web site at **http://www.rcsb.org/pdb/strucgen.html**. This page is a portal to additional information on structural genomics relevant to PDB users. Links and other structural genomics-related developments may be provided to the PDB by sending e-mail to **info@rcsb.org**.

PDB CD-ROM Set 95 Now Available

The latest PDB CD-ROM (release #95) is currently being distributed. This release contains the macromolecular structure entries (and experimental data when available) for the 14,040 structures deposited as of the December 26, 2000 update of the PDB Web site. With this release, the CD-ROM set has grown to six disks.

To assist Microsoft Windows platform users, additional resources for uncompressing the *.gz* files are included in the set.

The PDB CD-ROM set documentation is available for browsing at **http://www.rcsb.org/pdb/cdrom.html**. On-line ordering information is also available from that site.

PDB Annual Report Available On-line

The PDB Annual Report is now available from the PDB Web site in PDF format at **http://www.rcsb.org/pdb/annual_report00.pdf**. This document features a detailed look at the first full year of the RCSB's operation of the PDB from July 1, 1999, through June 30, 2000. It highlights PDB functions, accomplishments during this period, and plans for the coming year. Printed copies can also be obtained by sending your postal address to **AnnualReport@rcsb.org**.

PDB Highlighted in Genome Biology

The Protein Data Bank was reviewed in a Web Report in Genome Biology which is available at **http://genomebiology.com/2000/1/6/reports/2056/**.

Upgrade to the pdb-l@rcsb.org List

The *pdb-l* list is a forum for PDB users to collaborate and distribute information. While the RCSB maintains this resource for the community and does not moderate the list, the recent dissemination of a computer virus has made it necessary to for us to modify our policy.

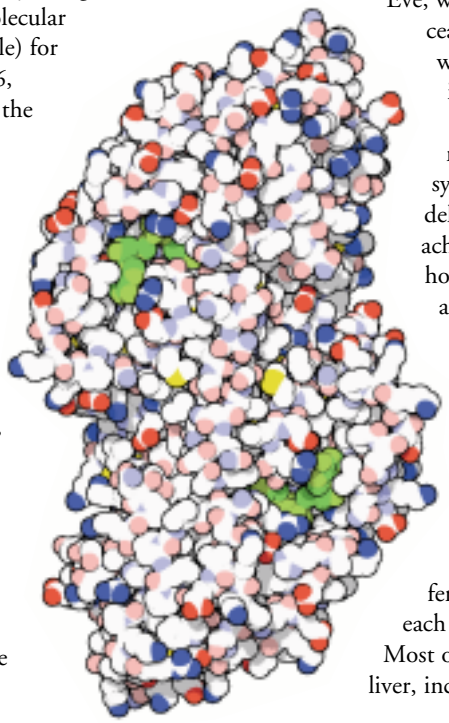
Effective February 1, 2001, messages with attachments that are sent to **pdb-l@rcsb.org** will not be accepted. Subscription information and an archive of *pdb-l* messages is available at **http://www.rcsb.org/pdb/forum.html**.

Molecules of the Quarter: Alcohol Dehydrogenase, Insulin, and Transfer RNA

The PDB has continued to feature its popular "Molecule of the Month" piece. Written and drawn by David S. Goodsell, an assistant professor of molecular biology at The Scripps Research Institute in La Jolla, California, these articles provide an overview of significant milestones in the growth of the PDB's macromolecular structure data for a diverse audience. Here is a sample of the information that is presented in this feature:

Alcohol Dehydrogenase: Our Precarious Line of Defense

January, 2001—Here's a toast to alcohol dehydrogenase. While recovering from the excesses of New Year's Eve, we might ponder the enzyme that ceaselessly battles the champagne that we consume. Alcohol dehydrogenase is our primary defense against alcohol, a toxic molecule that compromises the function of our nervous system. The high levels of alcohol dehydrogenase in our liver and stomach detoxify about one stiff drink each hour. The alcohol is converted to acetaldehyde, an even more toxic molecule, which is then quickly converted into acetate and other molecules that are easily utilized by our cells. Thus, a potentially dangerous molecule is converted, through alcohol dehydrogenase, into a mere foodstuff.



PDB ID: ***1htb***

G. J. Davis, W. F. Bosron, C. L. Stone, K. Owusu-Dekyi, T. D. Hurley (1996): X-ray structure of human beta3beta3 alcohol dehydrogenase. The contribution of ionic interactions to coenzyme binding. J. BIOL. CHEM. *271,* p. 17057.

Our bodies create at least nine different forms of alcohol dehydrogenase, each with slightly different properties. Most of these are found primarily in the liver, including the beta3 form (PDB entry **1htb**) and the similar enzyme from horse liver (PDB entry **6adh**). The sigma form, available in PDB entry **1agn**, is found in the lining of the stomach. Each enzyme is composed of two subunits, and quite remarkably, you can mix and match subunits between these different forms, creating mixed dimers that are still

active. Ethanol is not the only target of these enzymes; they also make important modifications to retinol, steroids, and fatty acids. The range of different types of alcohol dehydrogenase ensures that there will always be one that is perfect for the current task.

Alcohol dehydrogenase provides a line of defense against a common toxin in our environment. But this protection carries with it some dangers. Alcohol dehydrogenase also modifies other alcohols, often producing dangerous products. For instance, methanol, which is commonly used to "denature" ethanol, rendering it undrinkable, is converted into formaldehyde by alcohol dehydrogenase. The formaldehyde then does the damage, attacking proteins and embalming them. Small amounts of methanol cause blindness, as the sensitive proteins in the retina are attacked, and larger amounts, perhaps a glassful, lead to widespread damage and death.

Alcohol dehydrogenase also plays a central role in the most ancient business of biotechnology: alcoholic fermentation. Yeast and many bacteria build a larger alcohol dehydrogenase, like the one shown on the right (PDB entry **1ykf**). It performs the last step in the conversion of food into metabolic energy, creating ethanol instead of detoxifying it. Sugars are broken down and used for energy, forming ethanol as the waste product, which is excreted into liquid surrounding the cell. We have harnessed this process to produce alcoholic beverages: yeast is allowed to ferment grain sugars to form beer, and yeast is allowed to ferment grape juice to form wine.

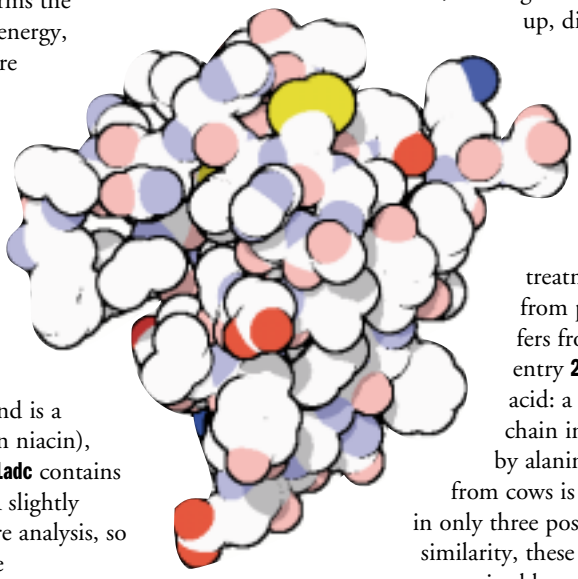
Alcohol dehydrogenase uses two molecular "tools" to perform its reaction on ethanol. The first is a zinc atom, which is used to hold and position the alcoholic group on ethanol. The second is a large NAD cofactor (constructed using the vitamin niacin), which actually performs the reaction. PDB entry **1adc** contains ethanol molecules bound to the two active sites. A slightly modified version of NAD was used in the structure analysis, so that the enzyme would not immediately attack the ethanol. The zinc atom is cradled by three amino acids from the protein: cysteine 46, cysteine 174, and histidine 67. The ethanol binds to the zinc and is positioned next to the NAD cofactor.

Insulin: A Molecular Messenger

February, 2001—Our cells communicate using a molecular postal system: the blood is the postal service and hormones are the letters. Insulin is one of the most important hormones, carrying messages that describe the amount of sugar that is available from moment to moment in the blood. Insulin is made in the pancreas and added to the blood after meals when sugar levels are high. This signal then spreads throughout the body, to the liver, muscles and fat cells. Insulin tells these organs to take glucose out of the blood and store it, in the form of glycogen or fat.

Insulin is a tiny protein. It moves quickly through the blood and is easily captured by receptors on cell surfaces, delivering its message. Small proteins pose a challenge to cells: it is difficult to make a small protein that will fold into a stable structure. Our cells solve this problem by synthesizing a longer protein chain, which folds into the proper structure. Then, the extra piece is clipped away, leaving two small chains in the mature form. The structure is further stabilized by three disulfide bridges.

When insulin function is impaired, either by damage to the pancreas or by the rigors of aging, glucose levels in the blood rise dangerously, leading to diabetes mellitus. For people totally deficient in insulin, such as children who develop diabetes early in life, this can be acutely dangerous. High glucose levels lead to dehydration as the body attempts to flush out the excess sugar in urine, and life-threatening changes in blood pH as the body turns to other acidic molecules for delivery of energy. Diabetes mellitus has severe long-term effects as well. It is one of the major chronic diseases in the industrialized world. Lowered levels of insulin that may occur as we age allow elevated levels of sugar in the blood over extended periods of time. Sugar molecules attach to proteins throughout the body, compromising their function, and sugars derived from glucose build up, distorting and clogging cells.



PDB ID: **4ins**

E. N. Baker, T. L. Blundell, J. F. Cutfield, S. M. Cutfield, E. J. Dodson, G. G. Dodson, D. M. Hodgkin, R. E. Hubbard, N. W. Isaacs, C. D. Reynolds, et al. (1988): The structure of 2Zn pig insulin crystals at 1.5 A resolution. PHILOS. TRANS. R. SOC. LOND. B. BIOL. SCI. *319,* **p. 369.**

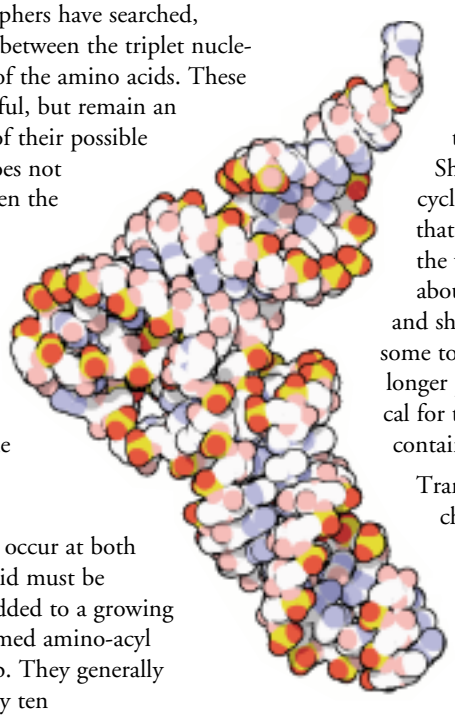
Diabetes mellitus may be treated by manually replacing the insulin that is missing in the blood. Of course, we need a plentiful source of insulin for use in these treatments. Fortunately, insulin from pigs (PDB entry **4ins**) differs from human insulin (PDB entry **2hiu**) by only one amino acid: a threonine at the end of the chain in human insulin is replaced by alanine in pig insulin. Insulin from cows is also very similar, differing in only three positions. Because of their similarity, these forms of insulin are also recognized by our own cells and may be used in therapy. Today, human insulin is also created by biotechnology, using engineered bacteria to produce a protein exactly identical to our own protein.

Insulin is a perfect molecule for exploring protein structure. It is small enough that you can display all of the atoms and still have a picture that is not too confusing. Human insulin, PDB entry **1trz**, contains four chains, labeled A, B, C, and D. When looking at this structure, you'll want to display only the A and B chains, which together compose one monomer of insulin. In the structure, you can see many of the key features that stabilize protein structure. Notice the cluster of carbon-rich amino acids, like leucine and isoleucine, that cluster in the middle of insulin, forming a hydrophobic core. Notice that the surface is covered with the charged amino acids lysine, arginine, and glutamate. These amino acids interact favorably with the surrounding water. Also notice

the three disulfide bridges between cysteine amino acids, which stabilize this tiny protein.

Transfer RNA: The Translator of Genetic Sequence

March, 2001—Since the process of DNA-directed protein synthesis was discovered, scientists and philosophers have searched, more or less seriously, for a relationship between the triplet nucleic acid codons and the chemical nature of the amino acids. These attempts have been uniformly unsuccessful, but remain an occasional topic of speculation because of their possible insights into the origins of life. There does not appear to be a specific interaction between the codons and the amino acids themselves. Instead, the match is made by transfer RNA, the Rosetta Stone that translates the nucleotide language of codons into the amino acid language of proteins. This translation is physical and direct: at one end of each tRNA is an anticodon that recognizes the genetic code, and at the other end is the appropriate amino acid for that code.



PDB ID: ***4tna***

B. Hingerty, R. S. Brown, A. Jack (1978): Further refinement of the structure of yeast tRNAPhe. J. MOL. BIOL. ***124,*** **p. 523.**

Errors in the production of proteins can occur at both ends of the tRNA. The proper amino acid must be added to the tip of tRNA, ready to be added to a growing protein chain. A battery of enzymes, termed amino-acyl tRNA synthases, are in charge of this job. They generally make a mistake in about one out of every ten thousand tRNA molecules that they charge with an amino acid. We'll look more carefully at these fascinating proteins next month. Errors may also occur at the other end of the tRNA, when the anticodon matches up with a codon. It may simply match improperly—this happens about one time in five hundred. Or, because each codon is three nucleotides long, it may associate in a shifted position, instead of the proper reading frame. This will throw off the rest of the protein, as each successive tRNA lines up in the wrong position after the shifted one. Fortunately, when genetic sequences are read in the wrong frame, they are filled with STOP codons, so the protein synthesis will be aborted after a few dozen more amino acids are added.

Biological evolution is remarkable in its ability to benefit from shortcomings. If there is any way that a problem can be made into an asset, the process of natural selection will find it eventually. Errors in protein synthesis are no exception. Both the mismatch of codon with anticodon and the shifting of reading frames play special functional roles in certain organisms. In many places, different codons are used as START signals. The codons may be GUG, UUG, or AUU, but all use the same methionine tRNA, which normally recognizes the codon AUG. In order for these proteins to be made, the methionine tRNA must pair with these erroneous codons. Shifting of the reading frame is essential in the lifecycle of HIV. When making the long polyprotein that contains all of the proteins that are found inside the virus, ribosomes make a mistake in one place about 5% of the time, aligning a tRNA incorrectly and shifting the reading frame. This causes the ribosome to miss the normal STOP codon, so a much longer protein is made. These occasional errors are critical for the life of the virus, because the longer proteins contain the enzymes that transcribe the viral genome.

Transfer RNA molecules are composed of one short chain of RNA, 70-90 nucleotides in length, folded into a trefoil shape. Two different examples of this structure can be found in phenylalanine tRNA (PDB entry **4tna**) and aspartate tRNA (PDB entry **2tra**). The two ends of the RNA chain are close to one another at the pointed end of the L-shaped structure. The amino acid is also added at this end. The center of the chain forms the rounded leg of the L, exposing the three nucleotides that form the anticodon. The other two loops of the trefoil are bundled into the elbow, where they provide structure to the whole molecule. The four normal RNA bases—adenine, uracil, guanine and cytosine—obviously do not provide enough latitude to form a sturdy structure, because many of the bases are modified to enhance their structures. To see two particularly exotic examples, look at the base next to the anticodon, number 37, in the initiator methionine tRNA (PDB entry **1yfg**) or the phenylalanine tRNA (PDB entries **4tna** and **6tna**).

For more information on Transfer RNA, please see the list of references at **http://www.rcsb.org/pdb/molecules/pdb15_4.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 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 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 Berman at **pdbjobs@rcsb.rutgers.edu**.

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