

PDB NEWSLETTER

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PUBLISHED QUARTERLY BY THE RESEARCH COLLABORATORY FOR STRUCTURAL BIOINFORMATICS

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SNAPSHOT: JUNE 30, 2001

15,488 released atomic coordinate entries

MOLECULE TYPE

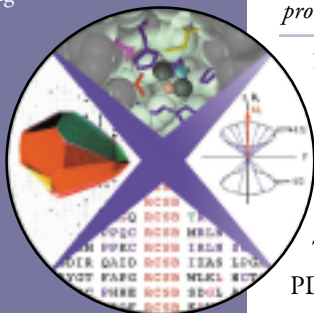
- 13,836 proteins, peptides, and viruses
- 986 nucleic acids
- 648 protein/nucleic acid complexes
- 18 carbohydrates

EXPERIMENTAL TECHNIQUE

- 12,780 diffraction and other
- 5,517 structure factor files
- 2,378 NMR
- 1,081 NMR restraint files
- 330 theoretical modeling

RCSB

SDSC: www.rcsb.org
RUTGERS: rutgers.rcsb.org
NIST: nist.rcsb.org
E-MAIL: info@rcsb.org
FTP: <ftp.rcsb.org>



MESSAGE FROM THE PDB

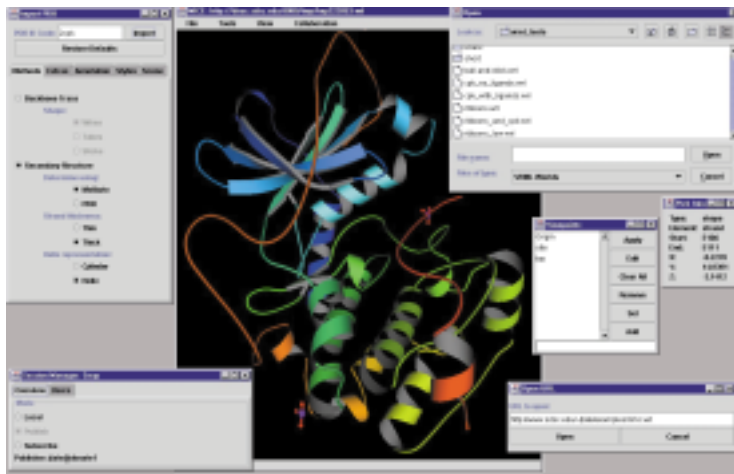
During the summer, the PDB has the opportunity to meet with our users at several different conferences:

JULY 21–26, LOS ANGELES, CA. American Crystallographic Association’s Annual Meeting. The PDB will be exhibiting in booth number 111 and will be having a users lunch on Tuesday, July 24 at noon in room Beaudry B. Anne Kuller will also be available at the PDB booth to answer questions about the BioSync Web Resource.

JULY 21–25, COPENHAGEN, DENMARK. Intelligent Systems for Molecular Biology 9th International Conference. PDB members will be exhibiting at the ISMB meeting in the Foyer of the Tivoli Concert Hall.

JULY 28–AUGUST 1, PHILADELPHIA, PA. 15th Symposium of the Protein Society. The PDB will be presenting a poster (d50) on all three poster session days at this meeting.

We look forward to seeing you and discussing recent PDB developments, including the integration of MICE with the PDB and the beta release of our validation software. *The PDB* ♦



MICE's 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.

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

This newsletter will soon be available on the Web in HTML and PDF formats at <http://www.rcsb.org/pdb/newsletter/>

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

DATA DEPOSITION AND PROCESSING

Beta Version of PDB Validation Software Released

The PDB Validation Suite is a set of programs that create validation reports about 3-D structure data. It is designed to work with files in *mmCIF* or PDB format.

The beta version of this software can be downloaded in binary form for SGI, SUN, and Linux platforms from <http://pdb.rutgers.edu/software/>.

This software is used in the Validation step of ADIT (AutoDep Input Tool) at <http://pdb.rutgers.edu/adit/> and at the Validation Server at <http://pdb.rutgers.edu/validate/>.

Reports produced include an Atlas entry, a summary report, and a collection of structural diagnostics including bond distance and angle comparisons, torsion angle comparisons, base morphology comparisons (for nucleic acids), and a molecular graphic image. In addition, reports from PROCHECK¹, NUCHECK², and SFCHECK³ are also made available.

Questions, comments, and suggestions should be sent to help@rcsb.rutgers.edu.

PDB Deposition Statistics

In the first half of the year 2001, approximately 1,500 structures have been deposited to the PDB.

About 80% of these depositions were from X-ray experiments, and 17% were from NMR experiments. 67% were deposited with a release status of HPUB; 13% HOLD; and 20% were released as soon as the annotation process was complete.

PDB Focus: PDB File Format Documentation

In response to questions about the PDB file format, we have compiled relevant documents at http://www.rcsb.org/pdb/info.html#File_Formats_and_Standards.

The PDB file format is mainly described in the PDB Contents Guide that was released by Brookhaven National Laboratory on December 20, 1996.

Any changes made to the PDB file format by the RCSB have been distributed to the PDB mailing list for discussion and review before they have been incorporated. These notices are archived at

¹R.A. Laskowski, M.W. McArthur, D.S. Moss, J.M. Thornton (1993): PROCHECK: a program to check the stereochemical quality of protein structures. *J. APPL. CRYST.* **265**, pp. 283-291.

²Z. Feng, J. Westbrook, H.M. Berman (1998): NUCHECK. NDB-407 Rutgers University, New Brunswick, NJ.

³A.A. Vaguine, J. Richelle, S.J. Wodak (1999): SFCHECK: a unified set of procedures for evaluating the quality of macromolecular structure-factor data and their agreement with the atomic model. *ACTA CRYSTALLOGR.* **D55**, pp. 191-205.

this site.

The RCSB has written several documents to accompany the PDB Contents Guide, including a Format FAQ to answer frequently asked questions about the PDB format, and a list of common format errors that have been submitted to the PDB.

Please bookmark this link where we will continue to post information about the PDB file format.

DATA QUERY, REPORTING, ACCESS, AND DISTRIBUTION

New Look for the PDB Home Page

The PDB home page now has a new look, thanks to feedback from PDB users and Prof. Cherrri Pancake of Oregon State University, a usability engineer on sabbatical at SDSC. The redesign improves the PDB's home page as a portal to information for experts and newcomers alike. Links to mirror sites, help topics, and a query tutorial are prominently displayed. Searches by keyword or PDB

ID are immediately available. The PDB will continue to improve the design and layout of the PDB Web site.

Prereleased Sequences Now Available from the PDB Web Site

After a favorable period of testing on the beta site, the PDB production site now offers sequence data before the release of the corresponding coordinate data through the PDB status search at <http://www.rcsb.org/pdb/status.html>. Users may query all available sequences, or query based on criteria such as title or deposition date.

PDB depositors are given the opportunity to prerelease a sequence in advance of the coordinates. This decision is solely at the discretion of the depositor, who may also choose to hold the sequence until the structure is released.

The prerelease of sequence data will allow users to conduct blind tests of structure prediction and modeling techniques. It could also help prevent unintended duplication of effort in structure determination.

This feature was developed in response to requests made to the PDB.

The expedited availability of sequence information is part of PDB's efforts to enable all areas of science. Questions regarding this new feature can be sent to info@rcsb.org.

PDB Web Site Statistics

A glance at the access statistics for the primary PDB Web site at <http://www.rcsb.org/pdb/> reveals that the Web site hits received and files downloaded continue to be on the rise.



The www.rcsb.org address continues to receive the most traffic, though use of the mirror sites and beta test site is increasing. PDB users are encouraged to access their most proximate RCSB mirror site at:

- Rutgers (<http://rutgers.rcsb.org/>)
- NIST (<http://nist.rcsb.org/>)
- Cambridge Crystallographic Data Centre in the United Kingdom (<http://pdb.ccdc.cam.ac.uk/>)
- National University of Singapore (<http://pdb.bic.nus.edu.sg/>)
- Osaka University in Japan (<http://pdb.protein.osaka-u.ac.jp/>)
- Universidade Federal de Minas Gerais in Brazil (<http://www.pdb.ufmg.br/>).

These sites are now directly accessible from the PDB home page.

Access Statistics for www.rcsb.org

MONTH	DAILY AVERAGE			MONTHLY TOTALS		
	HITS	FILES	SITES	BYTES	FILES	HITS
June 01	104,227	82,073	46,736	67,434,031	2,462,202	3,126,834
May 01	123,466	96,143	51,429	75,910,537	2,980,441	3,827,457
Apr. 01	127,135	99,293	55,472	75,817,080	2,978,802	3,814,062

Users are also invited to preview new features at the PDB beta test site, accessible at <http://beta.rcsb.org/pdb/>. We appreciate your feedback! ♦

PDB OUTREACH

PDB Paper Cited in Science Watch®

The publication *Science Watch®* has named “The Protein Data Bank” (H.M.Berman, J.Westbrook, Z.Feng, G.Gilliland, T.N.Bhat, H.Weissig, I.N.Shindyalov, P.E.Bourne (2000): *Nucleic Acids Research* 28, pp. 235-242) as the second-most cited research paper of 2000. (“The Hottest Research of 1999-2000” (2001): *Science Watch®* 12, p. 1). ♦

Second International Structural Genomics Meeting

The Second International Structural Genomics Meeting was held at the Airlie Conference Center in Warrenton, Virginia, on April 4-6, 2001. The meeting focused on fostering and formalizing international interactions in structural genomics. Task forces reported on the goals of the efforts and policies on data release and deposition, publication, intellectual property, and cooperation with industry.

There was general agreement at the meeting for projects with public funding to deposit the coordinates immediately after their determination to the PDB, and to release these data soon thereafter in most cases. Release can be delayed (by six months) after deposition in some cases.

For these structural genomics entries, the PDB will capture the details generally presented in the Materials and Methods section

of a published paper. The data items and their definitions are being developed by the International Task Force on Deposition, Archiving, and Curation of the Primary Information.

Further information, including the Agreed Principles and Procedures, is available at

<http://www.nigms.nih.gov/news/meetings/airlie.html>. ♦

“The Structures of Life” Booklet Published

Images from the PDB were used in the booklet “The Structures of Life.”

This free booklet is geared toward an advanced high school or early college-level audience. It explains how structural biology provides insight into health and disease. The booklet contains a general introduction to proteins, a chapter each on X-ray crystallography and NMR, and a chapter on structure-based drug design. It also features “Student Snapshots” designed to inspire young people to consider careers in biomedical research.

This resource is available online at

http://www.nigms.nih.gov/news/science_ed/structlife.pdf.

“The Structures of Life,” and other science education booklets, are published by the National Institute of General Medical Sciences, a component of the National Institutes of Health. To order any or all of these free booklets, call 301-496-7301, send e-mail to pub_info@nigms.nih.gov, or order online at

<http://www.nigms.nih.gov/news/publist.html>. ♦

PDB CD-ROM Set 96 Released

The latest PDB CD-ROM (release #96) is currently being distributed. This release contains the macromolecular structure entries and the experimental data (where available) for the 14,731 structures available as of the March 28, 2001 update of the PDB Web site.

Further information is available at

<http://www.rcsb.org/pdb/cdrom.html>. ♦

Molecules of the Quarter: Aminoacyl-tRNA Synthetases, Cyclooxygenase, and Myosin

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:

Aminoacyl-tRNA Synthetases: Twenty Flavors

April, 2001—When a ribosome pairs a “CGC” tRNA with “GCG” codon, it expects to find an alanine carried by the tRNA. It has no way of checking; each tRNA is matched with its amino acid long before it reaches the ribosome. The match is made by a collection of remarkable enzymes, the aminoacyl-tRNA synthetases. These enzymes charge each tRNA with the proper amino acid, thus allowing each tRNA to make the proper translation from the genetic code of DNA into the amino acid code of proteins.

Most cells make twenty different aminoacyl-tRNA synthetases, one for each type of amino acid. These twenty enzymes are widely different, each optimized for function with its own particular amino acid and the set of tRNA molecules appropriate to that amino acid. PDB entry **1asz**, which charges aspartic acid onto the proper tRNA, is a dimer of two identical subunits. Others are small monomers or large monomers, or dimers, or even tetramers of one or more different types of subunits. Some have wildly exotic shapes, such as the serine enzyme (PDB entry **1set**). The structures of nearly all of these different enzymes are available in the PDB.

As you might expect, many of these enzymes recognize their tRNA molecules using the anticodon. But this may not be possible in some cases. Take serine, for instance. Six different codons specify serine, so seryl-tRNA synthetase must recognize six tRNA molecules with six different anticodons, including AGA and GCU, which are entirely different from one another. So, tRNA molecules are also recognized using segments on the acceptor end and bases elsewhere in the molecule.

One base in particular, number 73 in the sequence, seems to play a pivotal role in many cases, and has been termed the discriminator base. In other cases, however, it is completely ignored.

Note also that each enzyme must recognize its own tRNA molecules, but at the same time, it must not bind to any of the other ones. So, each tRNA has a set of positive interactions that match up the proper tRNA with the proper enzyme, and a set of negative interactions that block binding of improper pairs. For instance, the aspartyl-tRNA synthetase found in PDB entry **1asz** recognizes the discriminator base and 4 bases around the anticodon. But, one other base, guanine 37, is not used in binding, but must be methylated to ensure that the tRNA does not bind improperly to the arginyl-tRNA synthetase.

Recent analyses of entire genomes revealed a big surprise: some organisms don't have genes for all twenty aminoacyl-tRNA synthetases. They do, however, use all twenty amino acids to construct their proteins. The solution to this paradox revealed, as is often the case in living cells, that more complex mechanisms are used. For instance, some bacteria do not have an enzyme for charging glutamine onto its tRNA. Instead, a single enzyme adds glutamic acid to all of the glutamic acid tRNA molecules and to all of the glutamine tRNA molecules. A second enzyme then converts the glutamic acid into glutamine on the latter tRNA molecules, forming the proper pair.

Aminoacyl-tRNA synthetase enzymes approach the tRNA from different angles. Isoleucine (entry **1ffy**), valine (entry **1gax**) and glutamine (entry **1euq**) enzymes cradle the tRNA, gripping the anticodon loop (at the bottom in each tRNA), and placing the amino-acid acceptor end of the tRNA in the active site (at the top right in each tRNA). These all share a similar protein framework, known as "Type I," approaching the tRNA similarly and adding the amino acid to the last 2' hydroxyl group in the tRNA. The phenylalanine (entry **1eiy**) and threonine (entry **1qf6**) enzymes are part of a second class of enzymes, known as "Type II." They approach the tRNA from the other side, and add the amino acid to the other free hydroxyl on the last tRNA base.

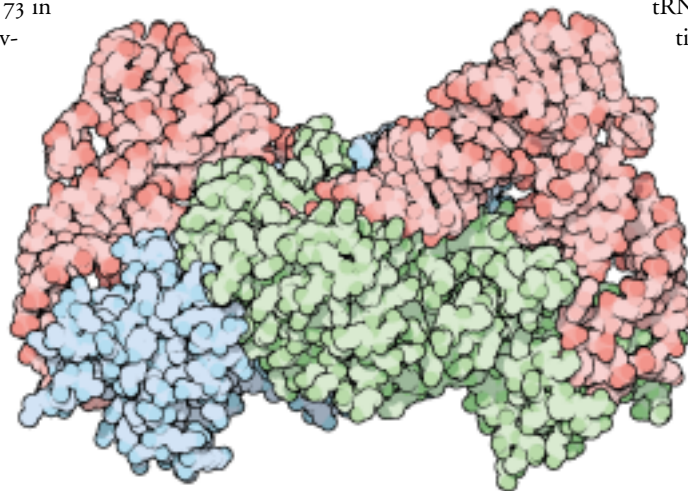
Aminoacyl-tRNA synthetases must perform their tasks with high accuracy. Every mistake they make will result in a misplaced amino acid when new proteins are constructed. These enzymes make about one mistake in 10,000. For most amino acids, this level of accuracy is not too difficult to achieve. Most of the amino acids are quite different from one another, and, as mentioned

before, many parts of the different tRNA are used for accurate recognition. But in a few cases, it is difficult to choose just the right amino acids and these enzymes must resort to special techniques.

Isoleucine is a particularly difficult example. It is recognized by an isoleucine-shaped hole in the enzyme, which is too small to fit larger amino acids like methionine and phenylalanine, and too hydrophobic to bind anything with polar sidechains. But, the slightly smaller amino acid valine, different by only a single methyl group, also fits nicely into this pocket, binding instead of isoleucine in about 1 in 150 times. This is far too many errors, so corrective steps must be taken. Isoleucyl-tRNA synthetase (PDB entry **1ffy**) solves this problem with a second active site, which performs an

editing reaction. Isoleucine does not fit into this site, but errant valine does. The mistake is then cleaved away, leaving the tRNA ready for a properly-placed leucine amino acid. This proofreading step improves the overall error rate to about 1 in 3,000.

These enzymes are not gentle with tRNA molecules. The structure of glutaminyl-tRNA synthetase with its tRNA (entry **1gtr**) is a good example. The enzyme firmly grips the anticodon, spreading the three bases widely apart for better recognition. At the other end, the enzyme unpairs one base at the beginning of the chain, and kinks the long acceptor end of the chain into a tight hairpin. This places the 2' hydroxyl on the last nucleotide in the active site, where ATP and the amino acid are bound.



PDB ID: **1asz**

J. Cavarelli, G. Eriani, B. Rees, M. Ruff, M. Boeglin, A. Mitschler, F. Martin, J. Gangloff, J.C. Thierry, D. Moras (1994): *The active site of yeast aspartyl-tRNA synthetase: structural and functional aspects of the aminoacylation reaction*. EMBO. J. **13**, p. 327.

A list of Aminoacyl-tRNA Synthetases in the PDB as of April, 2001, is available at

http://www.rcsb.org/pdb/molecules/pdb16_report.html. For suggestions for further information on aminoacyl-tRNA synthetases, please see http://www.rcsb.org/pdb/molecules/pdb16_5.html.

Cyclooxygenase: A Complex Enzyme

May, 2001—What is the most commonly-taken drug today? It is an effective pain-killer. It reduces fever and inflammation when the body gets overzealous in its defenses against infection and damage. It slows blood clotting, reducing the chance of stroke and heart attack in susceptible individuals. And, there is growing evidence that it is an effective addition to the fight against cancer. This wonder drug, with manifold uses in medicine, is aspirin. Aspirin has been used professionally for a century, and traditionally since ancient times.

A similar compound found in willow bark, salicylic acid, has a long history of use in herbal treatment. But only in the last few decades have we understood how aspirin works, and how it might be improved.

As you might expect from a drug with such diverse actions, aspirin blocks a central process in the body. Aspirin blocks the production of prostaglandins, key hormones that are used to carry local messages. Unlike most hormones, which are produced in specialized glands and then delivered throughout the body by the blood, prostaglandins are created by cells and then act only in the surrounding area before they are broken down. Prostaglandins control many of these neighborhood processes, including the constriction of muscle cells around blood vessels, aggregation of platelets during blood clotting, and constriction of the uterus during labor.

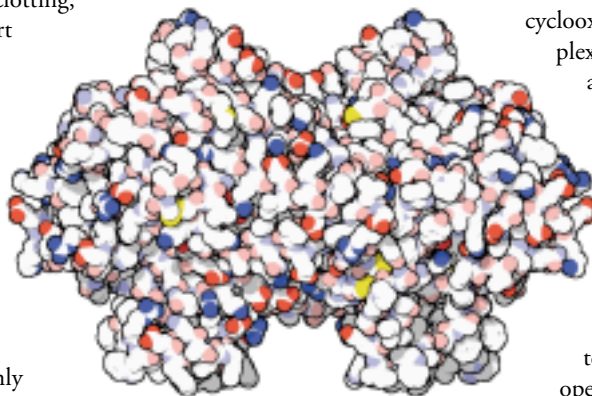
Prostaglandins also deliver and strengthen pain signals and induce inflammation. These many different processes are all controlled by different prostaglandins, but all created from a common precursor molecule.

Cyclooxygenase performs the first step in the creation of prostaglandins from a common fatty acid. It adds two oxygen molecules to arachidonic acid, beginning a set of reactions that will ultimately create a host of unusual molecules. Aspirin blocks the binding of arachidonic acid in the cyclooxygenase active site. The normal messages are not delivered, so we don't feel the pain and don't launch an inflammation response.

We actually build two different cyclooxygenases (termed COX-1 and COX-2) for different purposes. COX-1 is built in many different cells to create prostaglandins used for basic housekeeping messages throughout the body. The second enzyme is built only in special cells and is used for signaling pain and inflammation. Unfortunately, aspirin attacks both. Since COX-1 is targeted, aspirin can lead to

unpleasant complications, such as stomach bleeding. Fortunately, specific compounds that block just COX-2, leaving COX-1 to perform its essential jobs, are now becoming available. These new drugs are selective pain-killers and fever reducers, without the unpleasant side-effects.

This enzyme actually has two different active sites, collectively termed prostaglandin synthase. On one side, it has the cyclooxygenase active site discussed previously. On the opposite side, it has an entirely separate peroxidase site, which is needed to activate the heme groups that participate in the



PDB ID: **1prh**

D. Picot, P.J. Loll, R.M. Garavito (1994): The X-ray crystal structure of the membrane protein prostaglandin H2 synthase-1. NATURE 367, p. 369.

cyclooxygenase reaction. The enzyme complex is a dimer of identical subunits, so altogether, there are two cyclooxygenase active sites and two peroxidase active sites in close proximity. Each subunit has a small carbon-rich knob. These knobs anchor the complex to the membrane of the endoplasmic reticulum. The cyclooxygenase active site is buried deep within the protein, and is reachable by a tunnel that opens out in the middle of the knob.

This acts like a funnel, guiding arachidonic acid out of the membrane and into the enzyme for processing. In the structure found at PDB entry **4cox**, a drug is blocking the active site in both subunits. The heme groups are also shown above the drug in each subunit.

PDB entry **1pth** shows how aspirin blocks the cyclooxygenase active site. Aspirin is composed of two parts: an acetyl group attached to salicylic acid. When it attacks cyclooxygenase, it connects its acetyl group to a serine amino acid, permanently inactivating the enzyme. After aspirin has performed its job, the acetyl group becomes attached to the serine amino acid, and the salicylic acid is bound close by.

A list of all cyclooxygenases as of May, 2001, is available at http://www.rcsb.org/pdb/molecules/pdb17_report.html. For suggestions for further reading on cyclooxygenase, please see http://www.rcsb.org/pdb/molecules/pdb17_4.html.

Myosin: Molecular Motion

June, 2001—All of the different movements that you are making right now—your fingers on the computer keys, the scanning of your eyes across the screen, the isometric contraction of muscles in your back and abdomen that allow you to sit comfortably—are powered by myosin. Myosin is a molecule-sized muscle that uses chemical energy to perform a deliberate motion. Myosin captures a molecule of ATP, the molecule used to transfer energy in cells, and breaks it, using the energy to perform a “power stroke.” For all of your voluntary motions, when you flex your biceps or blink your eyes, and for all of your involuntary motions, each time your heart beats, myosin is providing the power.

Myosin requires huge amounts of ATP when muscles are exerted. When you start running, the supply of ATP in your muscles lasts

only about a second. Then, the muscle cells shift to phosphocreatine, a backup source of energy, which can be converted quickly into about 10 seconds worth of ATP. Then, if you are still running full tilt, your muscles start using glycogen, a molecule that stores glucose. This lasts for a minute or two, building up toxic acids as the sugar is used up. Then, the sprint is over and you have pushed your muscles to the limit. If, however, you slow down and pace yourself, your muscles can perform much longer. The blood vessels will dilate and your heart rate will increase, bringing twenty times as much blood through the muscles.

Your muscle cells can then use this extra oxygen to produce far more ATP from the sugar in glycogen. Instead of collapsing after a short sprint, you now have the resources for a mountain hike or a marathon.

Myosin is composed of several protein chains: two large “heavy” chains and four small “light” chains.

The structures available in the PDB, such as PDB entry **1b7t**, contain only part of the myosin molecule.

The whole molecule is much larger, with a long tail that has been clipped off to allow the molecule to be studied. Fortunately, the crystal structures include most of the “motor” domain, the part of the molecule that performs the power stroke, so we can look at this process in detail.

Each myosin performs only a tiny molecular motion. It takes about 2 trillion myosin molecules to provide the force to hold up a baseball. Our biceps have a million times this many, so only a fraction of the myosin molecules need to be exerting themselves at any given time. By working together, the tiny individual power stroke of each myosin is summed to provide macroscopic power in our familiar world. Inside muscle cells, about 300 myosin molecules bind together, with all of the long tails bound tightly together into a large “thick filament.” The many myosin heads extending from the thick filament then reach over to actin fila-

ments, and together climb their way up.

ATP contains a key phosphate-phosphate bond that is difficult to create and is used to power many processes inside cells. You might be surprised to find, however, that breakage of this phosphate-phosphate bond is not directly responsible for the power stroke in myosin. Instead, it is release of the phosphate left over after ATP is cleaved that powers the stroke. Think of myosin like

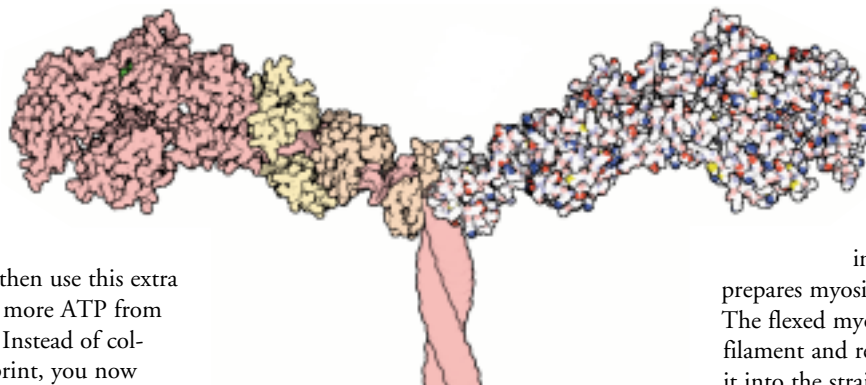
an arm that can flex towards you or push away. The cleavage of ATP is used in a priming step. When ATP is cleaved, myosin adopts a bent, flexed form, like in PDB entry **1br1**. This

prepares myosin for the power stroke. The flexed myosin then grabs the actin filament and release of phosphate snaps it into the straight “rigor” form. This power stroke pushes the myosin molecule along the actin filament. When finished, the remaining ADP is replaced by a new ATP, the myosin lets go of the actin filament. Then, it is ready for the next stroke.

The myosin motor domain, from entry **1b7t**, is nearly straight, close to the rigor

form. You can explore several interesting features. At the tip of the molecule is a cleft that binds to the actin filament. Notice that the ADP molecule is bound at the base of this deep cleft. It is thought that changes in the nucleotide, as it cycles from ATP, to ADP and phosphate, to ADP alone, are transmitted along this cleft to change the way that myosin interacts with actin. In the middle of the molecule is the “converter” domain that changes shape when phosphate is released. On one side of the molecule is a long alpha helix with the two light chains bound around it. This is the “lever arm” that amplifies the converter shape change into a large power stroke.

A list of all myosin structures as of June, 2001, is available at http://www.rcsb.org/pdb/molecules/pdb18_report.html. For suggestions for further reading about myosin, please see http://www.rcsb.org/pdb/molecules/pdb18_5.html. ♦



PDB ID: **1b7t**

A. Houdusse, V.N. Kalabokis, D. Himmel, A.G. Szent-Gyorgyi, C. Cohen (1999): *Atomic structure of scallop myosin subfragment S1 complexed with MgADP: a novel conformation of the myosin head.* CELL 97, p. 459.

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 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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