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RCSB PDB PROTEIN DATA BANK

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NEWSLETTER

Weekly RCSB PDB news is available online at www.pdb.org

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SNAPSHOT: OCTOBER 1, 2008

53,384 released atomic coordinate entries

49,279	proteins, peptides, and viruses
1918	nucleic acids
2154	protein/nucleic acid complexes
33	other

EXPERIMENTAL TECHNIQUE

45,587	X-ray
7502	NMR
195	electron microscopy
100	other

34,726 structure factor files
4196 NMR restraint files

Participating RCSB Members:
Rutgers • SDSC/SKAGGS/UCSD
E-mail: info@rcsb.org
Web: www.pdb.org • FTP: ftp.wwpdb.org

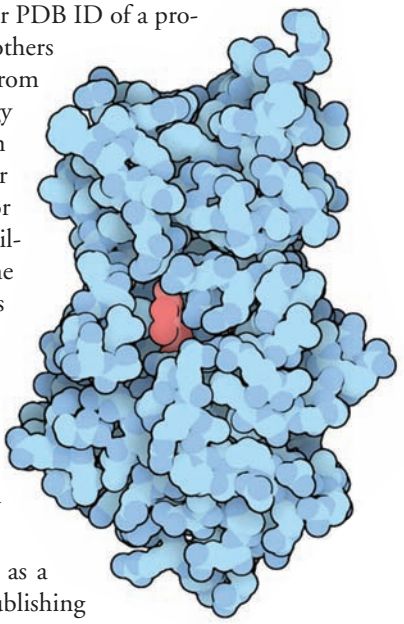
The RCSB PDB is a member of the wwPDB (www.wwpdb.org)

Message from the RCSB PDB

PSI SGKB: A Resource for Structural Genomics and Structural Biology

An increasing number of novel structures in the PDB archive are being deposited by structural genomics centers located worldwide. The RCSB PDB now links to a resource that makes all the structural genomics products generated by the Protein Structure Initative (PSI) available to the greater scientific community.

First established in the spring of 2008, the PSI Structural Genomics Knowledgebase (PSI SGKB; **kb.psi-structuralgenomics.org**) is an entry point to all of the protein structure and production resources created by the PSI. From the home page, researchers can enter the sequence or PDB ID of a protein to find the corresponding structure and others like it, structural and functional annotations from key external databases, comparative homology model structures available through the Protein Models Portal, experimental progress of similar protein targets through TargetDB, protocols for protein production through PepcDB, and availability of those DNA clone materials through the PSI Materials Repository. Keyword searches return other useful information including descriptions of new technologies and methods, a list of publications detailing key findings, and links to related resources provided by the PSI centers. The PSI SGKB makes it possible for researchers to access a wealth of information from one site.



In September, the PSI SGKB was re-launched as a Gateway in collaboration with the Nature Publishing Group (NPG). The expansion of the PSI SGKB has added a research library, RSS feeds, editorials about new research advances, news, and an events calendar to present a broader view of research activities in structural biology and structural genomics.

The PSI SGKB is funded by the NIGMS.

2p69. S.C. Almo, J.B. Bonanno, J.M. Sauder, S. Emtage, T.P. Dilorenzo, V. Malashkevich, S.R. Wasserman, S. Swaminathan, S. Eswaramoorthy, R. Agarwal, D. Kumaran, M. Madegowda, S. Ragumani, Y. Patskovsky, J. Alvarado, U.A. Ramagopal, J. Faber-Barata, M.R. Chance, A. Sali, A. Fiser, Z.Y. Zhang, D.S. Lawrence, S.K. Burley (2007) Structural genomics of protein phosphatases. J.Struct.Funct.Genom. *8: 121-140.*
Image by David Goodsell from the PSI SGKB [doi:10.3942/psi_sgkb/fm_2008_5]

Data Deposition and Processing

Announcement: Comprehensive Format Guide Version 3.2

During the past year, wwPDB annotators have collaborated on a project to clarify the details and procedures related to data processing and annotation. The result is a PDB Contents Guide Version 3.2 that more fully describes the PDB file format. This document is available either as a PDF or *via* HTML from the wwPDB website, and is accompanied by a document highlighting these clarifications.

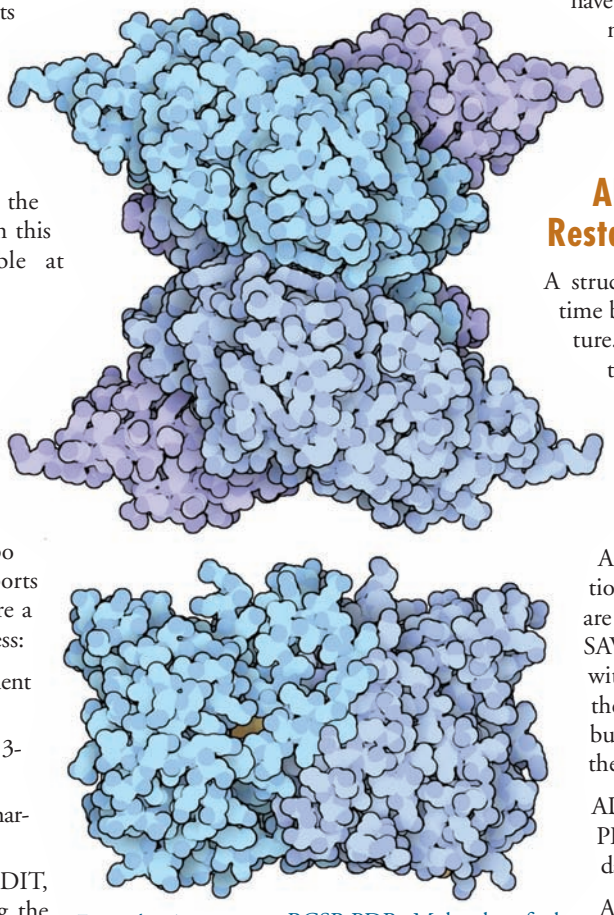
In the coming months, all files released by the wwPDB will follow the format as described in this document. Details will be made available at **www.pdb.org** and at **www.wwpdb.org**.

Ligand Expo: A Resource for Depositing Structures

The Chemical Component Dictionary archives chemical and structural information about all residue and small molecule components found in PDB entries. Ligand Expo is a tool that can access, visualize, and build reports about these data. It can also be used to prepare a file for deposition through the following process:

- Search Ligand Expo for a chemical component that matches your ligand
- If a match is found, use that corresponding 3-character code for the ligand in your coordinates
- If the ligand is not found, choose a new 3-character code for the ligand
- When depositing your structure with ADIT, upload the chemical name and a file showing the chemical image for the new ligand into the Ligand Information section

Ligand Expo (**ligand-expo.rcsb.org**) is an update of the Ligand Depot[1] resource.



From the August 2008 RCSB PDB Molecule of the Month *on Selenocysteine Synthase. Top: 3bc8. O.M. Ganichkin, X.M. Xu, B.A.Carlson, H. Mix, D.L. Hatfield, V.N. Gladyshev, M.C. Wahl (2008) Structure and catalytic mechanism of eukaryotic selenocysteine synthase. J.Biol.Chem. 283: 5849-5865. Bottom: 2yye. Y. Itoh, S. Sekine, E. Matsumoto, S. Yokoyama, Crystal structure of selenophosphate synthetase [doi: 10.2210/pdb2yye/pdb]*

PDB Focus: What is the Smallest Polymer Structure That Can Be Deposited to the PDB?

The PDB contains biomolecular polymers including polypeptides, polynucleotides, polysaccharides, and their complexes.

Polypeptide structures containing 24 or more residues can be deposited to the PDB. Smaller peptides that are complexed with a larger polymer (greater than the minimum length defined above) may be deposited to the PDB. Crystal structures of peptides with fewer than 24 residues, such as antibiotics, should be sent to the Cambridge Crystallographic Data Centre (CCDC; **www.ccdc.cam.ac.uk**).

Polynucleotide structures with 4 or more residues are accepted at the PDB. Smaller oligonucleotides (dinucleotides and trinucleotides) can be deposited at the Nucleic Acid Database (NDB; **ndbserver.rutgers.edu**).

Coordinates for the repeating unit of fibrous polymers and polysaccharide structures with 4 or more sugar residues may be deposited at the PDB archive. Molecules that do not conform to these guidelines but have been previously deposited in the archive will not be removed.

Structures may be deposited to the archive *via* the wwPDB.

ADIT Focus: Restarting Deposit Sessions

A structure can be deposited over a period of time by using ADIT's "Session Restart ID" feature. This identifier appears in red in the center of the browser window when ADIT's "deposit" step is first started. It is also seen in the title of the browser throughout the deposition session.

The case-sensitive restart ID should be entered in the space provided on the ADIT home page to return to the deposition session. Any data entered in a category are stored every time the user selects the SAVE button. All entered data associated with a particular entry can be accessed using the restart ID until the "DEPOSIT NOW" button is selected, for up to six months after the session has been last updated.

ADIT is available at the RCSB PDB and PDBj. ADIT-NMR can be used to deposit data to both the PDB and BMRB.

A tutorial guide to using ADIT is available in English and Japanese. Simulation sessions for "in progress" deposition are available to practice learning how to use ADIT at **rcsb-deposit-demo-1.rutgers.edu**.

Deposition Statistics

In the third quarter of 2008, 1924 experimentally-determined structures were deposited to the PDB archive. The entries were processed by wwPDB teams at the RCSB PDB, PDBe, and PDBj.

Of the structures deposited, 76.9% were deposited with a release status of "hold until publication"; 18.1% were released as soon as annotation of the entry was complete; and 5.0% were held until a particular date. 92.2% of these entries were determined by X-ray crystallographic methods; 6.8% were determined by NMR methods.

During the same time period, 1928 structures were released in the PDB.

[1]Z. Feng, L. Chen, H. Maddula, O. Akcan, R. Oughtred, H.M. Berman, J. Westbrook (2004) Ligand Depot: a data warehouse for ligands bound to macromolecules. *Bioinformatics* **20**:2153-2155.

Data Query, Reporting, and Access

Exploring Structures Through PubMed Abstracts

PubMed[2] abstracts for the primary citations of PDB entries are integrated into the RCSB PDB website.

When reviewing query results of multiple structures at the RCSB PDB site, the Citations Tab provides a PubMed-like list of the corresponding primary citations. This list can be downloaded in Medline format for use with bibliographic programs such as Endnote and RefWorks by selecting the "Medline Format" option from the lefthand menu. The Citations Tab also links to all structures that share a primary citation, and to related articles in PubMed.

For each PDB structure, the "Abstract" link on a Structure Summary page provides information downloaded from PubMed about the citation. The keywords, title, and abstract on this page can be used to query the PDB for other entries that have the same words in their abstracts. The citation information can be downloaded in Medline format by selecting the "Medline Format" option from the lefthand menu. Selecting the PubMed icon takes users to the abstract in PubMed.

Using the Advanced Search, PubMed keyword searches can be combined with any other query option.

Website Statistics

Access statistics for **www.pdb.org** and **ftp://ftp.wwpdb.org** for the third quarter of 2008 are given below.

MONTH	UNIQUE VISITORS	NUMBER OF VISITS	BANDWIDTH	HTTP DOWNLOADS	FTP DOWNLOADS
JUL 08	161567	355065	636.25 GB	3735223	12876019
AUG 08	133412	296024	514.27 GB	3157620	11587553
SEP 08	168114	366983	631.13 GB	4614066	10354741

Enhanced RSS Feed from the RCSB PDB

The RCSB PDB offers an RSS (Really Simple Syndication) feed that provides users with a list of newly updated structures as soon as they are released. Based upon user feedback, this weekly feed now includes each PDB ID and structure title. Subscribers to this feed can quickly scan the list for structures of interest.

To start, select an RSS reader. Many RSS feed readers are already packaged with web browsers and email programs, while others are available as dedicated programs or websites.

To incorporate the RCSB PDB feed, either drag or select the orange RSS icon from the top of the RCSB PDB home page (located just next to the latest release date) and add the URL for new structures to your reader.

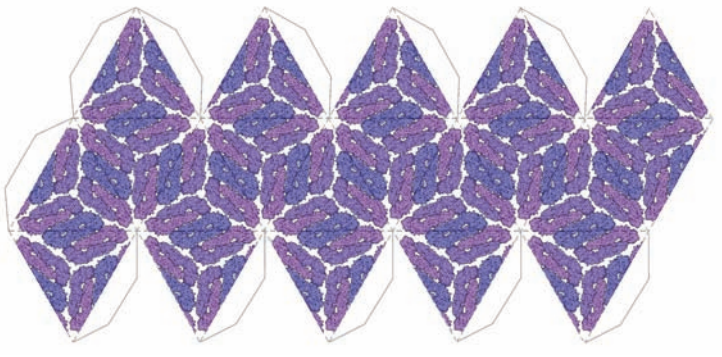
Outreach and Education

Handheld 3D Virus Model

A template is available to create a 3D model of the dengue virus as illustrated by David S. Goodsell. From the RCSB PDB's *Educational Resources* page, download and print the PDF, cut out the protein structure, and fold on the dotted lines. The flaps can then be taped or glued into place to form an icosahedron.

The RNA genome, which contains 10,649 nucleotides, can be modeled using a piece of string approximately 5.4 meters long and placed inside of the paper structure.

For more information on the dengue virus, please see the July 2008 *Molecule of the Month* (10.2210/rcsb_pdb/mom_2008_7).



1k4r: R.J. Kuhn, W. Zhang, M.G. Rossmann, S.V. Pletnev, J. Corver, E. Lenches, C.T. Jones, S. Mukhopadhyay, P.R. Chipman, E.G. Strauss, T.S. Baker, J.H.Strauss (2002) Structure of dengue virus: implications for flavivirus organization, maturation, and fusion. Cell *108: 717-725.*

Meetings and Presentations

The RCSB PDB and the wwPDB have been participating in several meetings:

• At the **22nd Annual Symposium of The Protein Society** (July 19-23; San Diego, CA), Peter Rose presented the poster "Effective Mining of the Protein Data Bank" which explored the many different search functions available from **www.pdb.org**.

• Many PDB users stopped by the RCSB PDB's exhibit booth at the **16th Annual International Conference for Intelligent Systems for Molecular Biology (ISMB;** July 19-23; Toronto, Canada), the official conference of the International Society for Computational Biology (ISCB). Associate Director Phil Bourne was involved in many presentations and discussions, and delivered a 3DSig Keynote Lecture at the Structural Bioinformatics and Computational Biophysics satellite meeting.

• At the **XXI Congress & General Assembly of the International Union of Crystallography (IUCr;** August 23 – 31; Osaka, Japan) wwPDB members from around the globe hosted a joint exhibition stand for demonstrations, met with users, and participated in a variety of sessions and commission meetings.

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[2]D.L. Wheeler, T. Barrett, D.A. Benson, S.H. Bryant, K. Canese, V. Chetvernin, D.M. Church, M. Dicuccio, R. Edgar, S. Federhen, M. Feolo, L.Y. Geer, W. Helmberg, Y. Kapustin, O. Khovayko, D. Landsman, D.J. Lipman, T.L. Madden, D.R. Maglott, V. Miller, J. Ostell, K.D. Pruitt, G.D. Schuler, M. Shumway, E. Sequeira, S.T. Sherry, K. Sirotkin, A. Souvorov, G. Starchenko, R.L. Tatusov, T.A. Tatusova, L. Wagner, E. Yaschenko (2008) Database resources of the National Center for Biotechnology Information. *Nucleic Acids Res.* **36**: D13-21.

1

2


3

4

The wwPDB exhibit stand at the IUCr meeting: 1. John Westbrook at the wwPDB booth, which highlighted resources at all member sites; 2. James Watson (EMBL); 3. IUCr attendees; 4. Helen Berman and Haruki Nakamura (PDBj)

Also at the IUCr meeting, RCSB PDB Director Helen M. Berman presented a keynote lecture entitled *What the Protein Data Bank tells us about the past, present, and future of structural biology*, and John Westbrook presented *Data Quality in the PDB Archive*. Professor Berman also participated in a Question and Answer session at the Commission on Biological Macromolecules.

• As part of the International Structural Genomics Organization's Conference on Structural Genomics (Sept. 20-24; Oxford, UK), RCSB PDB Director Helen Berman described the PSI Structural Genomics Knowledgebase.

• At the **EMBO 08** Practical Course on Computational Aspects of the Protein Target Selection, Protein Production Management and Structure Analysis Pipeline (Sept. 22-26; Hinxton, UK), Helen Berman and John Westbrook (RCSB PDB), Haruki Nakamura (PDBj), and Kim Henrick, Dimitris Dimitropoulos, Eugene Krissinel, and Tom Oldfield (PDBe) led tutorial sessions about various resources and tools from wwPDB sites.

• **At the European Conference in Computational Biology (ECCB 08;** Sept. 22-26; Sardinia, Italy), Martha Quesada and Andreas Prlic (RCSB PDB) gave an overview of the multifaceted wwPDB collaboration and demonstrated features found at the RCSB PDB, PDBe, PDBj, and BMRB websites.

Andreas Prlic at ECCB08

• Upcoming RCSB PDB events include the **New Jersey Science Convention** for science teachers (October 14-15; Somerset, NJ), **eCheminfo Community of Practice Meeting on Advances in Drug Discovery and Development** (October 13-17; Philadelphia, PA), the meeting of the **Association of Science and Technology Centers** (October 18-21; Philadelphia, PA) and the **Pittsburgh Diffraction Conference** (October 30-November 1; Pittsburgh, PA).

DOIs for PDB Structures and the *Molecule of the Month*

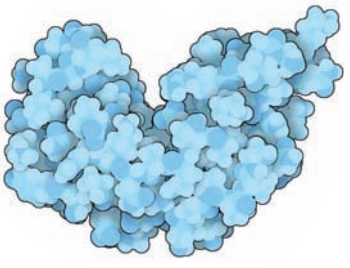


Image of ribonuclease A from the September 2008 RCSB PDB Molecule of the Month *feature (10.2210/rcsb_pdb/mom_2008_9) by David Goodsell*

PDB structures can be cited using their PDB ID and related published citation. Structures may also be referenced using their Digital Object Identifier (DOI). PDB DOIs are formatted as 10.2210/pdbXXXX/pdb, where XXXX is the PDB ID. For example, the DOI for entry 4hhb is "10.2210/pdb4hhb/pdb".

DOIs can be used in a URL (**dx.doi.org/10.2210/pdb4hhb/pdb**) or entered in a DOI resolver (such as **www.crossref.org**) to automatically link to file pdb4hhb.ent.gz on the main PDB FTP archive.

DOIs are also available for *RCSB PDB Molecule of the Month* features in the format: 10.2210/rcsb_pdb/mom_YYYY_MM (where YYYY is the year and MM the number of the month, using one or two digits). For example, the DOI for the May 2003 feature on hemoglobin by Shuchismita Dutta and David S. Goodsell is "10.2210/rcsb_pdb/mom_2003_5". These features are referenced with the DOI and the author/s of the article.

A page describing policies & references for using and citing PDB data and RCSB PDB resources is available at **www.pdb.org**.

RCSB PDB Poster Prizes

The RCSB PDB Poster Prize for best student poster related to structure and function prediction at the ISCB's ISMB meeting went to Dariya Glazer for *Clustering Across Space and Time* (Dariya Glazer, Randy Radmer, Russ Altman; Stanford University).

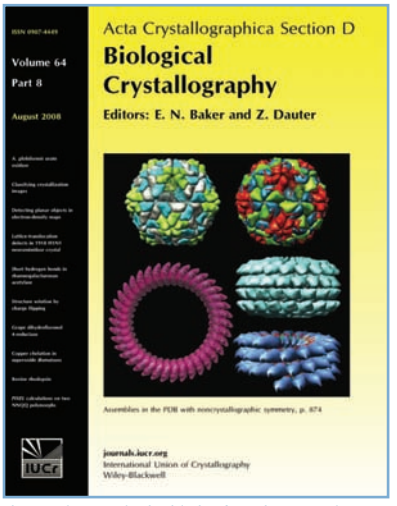
At the IUCr meeting, the judges found that the best student poster related to macromolecular crystallography was "Structural insights into the mitochondrial import complex, TIM9.10" by Chaille T. Webb,[1,2] Michael Baker,[1] Michael T. Ryan,[1] Peter M. Colman,[1] and Jacqueline M. Gulbis[1]([1]The Walter and Eliza Hall Institute of Medical Research and [2]The University of Melbourne, Australia).

Chaille T. Webb

The winners will receive a subscription to *Science* and a related reference book.

Special thanks to our judges and the conference organizers.

wwPDB Paper: Representation of Viruses in the Remediated PDB



The article was also highlighted on the journal cover.

The 2007 release of remediated data improved the representation of deposited and experimental coordinate frames, symmetry, and frame transformations in the archive. A paper describing the scheme used by the wwPDB to represent viruses and other biological assemblies with regular noncrystallographic symmetry has been published:

C.L. Lawson, S. Dutta, J.D. Westbrook, K. Henrick and H. M. Berman (2008) Representation of viruses in the remediated PDB archive *Acta Cryst.* **D64**: 874-882

Education Corner by Brad Larson, Ph.D., Sunset Lake Software

Molecular Visualization in your Pocket

BRAD LARSON *is the sole proprietor of Sunset Lake Software, a software company devoted to the development of applications aimed at engineering and the sciences.* Molecules *for the iPhone and iPod Touch is the first public product of this company, with others planned. His day job is Chief Technology Officer of SonoPlot, Inc., a company he co-founded as a spin-off of research at the University of Wisconsin-Madison. SonoPlot (www.sonoplot.com) manufactures high-precision fluid dispensers, called Microplotters, that can print microelectronic circuits and high-density protein microarrays.*

He holds a B.S. in Chemical Engineering, with a minor in Computer Science, from the Rose-Hulman Institute of Technology in Terre Haute, IN, and a M.S. and Ph.D. in Materials Science from the University of Wisconsin-Madison. Additional background information and publication PDFs are at ***www.sunsetlakesoftware.com/about****.*

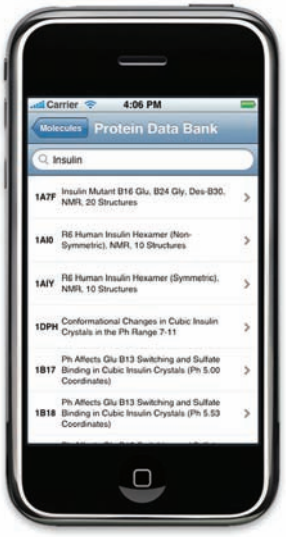
In recent years, we've seen an explosion in processing power within portable devices such as cell phones and media players. Current devices more closely resemble general-purpose computers, especially Apple Inc.'s new iPhone and iPod Touch. Both use a form of the OS X operating system found on Macintosh computers, and can run custom applications designed using a desktop-caliber software development kit (SDK). Additionally, these applications are available worldwide through Apple's iTunes Store and can be downloaded with a single click. Many high school and college students will carry these devices into classes this fall, providing a opportunity for educational software to be used in unique ways. *Molecules* is one such application that will hopefully introduce students to the fascinating world of biomolecules and their 3D structures.

One of the inspirations for *Molecules* was a conversation I had with my brother, Matt Larson, who is using X-ray crystallography to determine the structure of a protein as part of his Ph.D. work at the University of Alabama at Birmingham. He was preparing to present a poster with an early structure for this protein, and I couldn't help but think that a static image wasn't the best means of displaying that structure. After witnessing the capabilities of the iPhone and iPod Touch, I imagined what it would be like if he could take an iPod to a conference and pull it out of his pocket every time he wanted to show off the full 3D structure of his protein or even download and research on the spot any PDB molecule mentioned in a presentation.

Molecules for the iPhone/iPod Touch: *Molecules* is a free, open-source molecular visualizer that uses the built-in 3D hardware acceleration, touch interface, and always-on data networking capability of the iPhone to deliver an intuitive means of viewing molecular models away from a desktop

B-DNA rendered in the ball-and-stick visualization mode in Molecules. *1bna: H.R. Drew, R.M. Wing, T. Takano, C. Broka, S. Tanaka, K. Itakura, R.E. Dickerson (1981) Structure of a B-DNA dodecamer: conformation and dynamics.* Proc.Natl.Acad.Sci.USA **78***: 2179-2183.*

computer. (I will refer to the iPhone for the remainder of the article, but the iPod Touch shares all of the same hardware, minus the cell phone connection, and thus can also run *Molecules*). *Molecules* allows users to look up and download files from the PDB to the iPhone, even over the cell phone data network.



A direct keyword search of the RCSB PDB results in a list of structures that can be downloaded.

Once the files are on the device, molecules currently can be displayed in ball-and-stick, spacefilling, and cylinder (colored by amino acid or nucleotide residue) visualization modes. To rotate the models, users simply move their finger across the display. A molecule can be zoomed out by pinching two fingers together or zoomed in on by reversing the gesture. Panning across the molecule is accomplished by dragging it using two fingers.

Initial response: Because of reasonably fast rendering performance, these easy-to-learn controls provide the impression that you are manipulating the molecule itself with your fingers. The response I've heard over and over from non-scientific users who have tried this out is "That's so cool!" This is exactly what you'd like to hear from students, especially impressionable younger ones. What they have viewed as just their cell phone or music player suddenly becomes a scientific tool with the addition of one program. This capability, coupled with a savvy educator, could make a significant impact.

This is not just wishful thinking on my part. I've received correspondence from professors and high school teachers who will be using this as an aid in their upcoming classes. I've also heard from many researchers across the world who are very excited about the prospects of using this as an extension of their desktop software, and as a tool that allows them to look up structures while out in the lab or at a conference.

Most surprising to me has been the number of people who have used *Molecules*. In the first three months of availability, it has been downloaded by more than 230,000 unique users. Some of its popularity comes from being a free iPhone application, among the first 500 released, and from being listed as a Staff Favorite on the front page of iTunes. Still, that is a rather large number of users for a niche application.

Future plans: Along with all the positive reviews and messages have come some complaints. The first was about how difficult it was to find and load new structures onto the iPhone. Initially, I required users to type in the four-character ID code to download new structures. Even with an integrated web browser to search within the RCSB PDB website, many users found this frustrating.

With the help of the RCSB PDB, I was able to use Web Services to integrate keyword searching into *Molecules* itself. Web Services allow you to communicate directly with the RCSB PDB's data store and retrieve values without having to go through the website; this is ideal for a portable device on a bandwidth-limited connection.

Another area where *Molecules* falls short is the amount of time it takes to load large structure files, render them to the screen, and refresh the display after changes are made in orientation or scale. This makes working with structures containing over 10,000 atoms a chore. While you might think that this is a natural limitation of the portable hardware, the truth is that the iPhone has a surprisingly fast processor and graphics chip, and I believe it is capable of much more. I am currently testing a series of enhancements that should make file loading and initial rendering much faster, and am learning from other open source projects such as QuteMol (**qutemol.sourceforge.net**) that appear to have far more efficient 3D engines than *Molecules*.

Finally, other reviewers have identified two additional requirements to make this more useful as a scientific tool: additional visualization modes, primarily ribbon representations, and the ability to load custom structures not contained within the PDB. Both of these enhancements will take a little work, but I would expect to accomplish them within the next few months.

One pleasant result of the initial exposure of this program has been the offers of help from other developers, some experienced in writing other visualization applications. Their assistance should speed along the implementation of ribbon and other display modes.

Loading custom molecules onto the device presents a tricky problem, given some of the limitations of the mobile platform, but other iPhone programmers have suggested a solution. I will be crafting a desktop version of this application that can load whatever custom structures you would like and store them locally in a manner similar to iTunes. A desktop client would then be able to synchronize to a users' iPhone through a network connection to provide iPhone access to whatever structures are on the computer.

Conclusion: When it came to choosing data sources to use for *Molecules*, the RCSB PDB was first on my list. I have been a fan of the work they have done for years. I'd like to thank them again for providing this resource and being so helpful in the development of this program. This whole experience has been a lot of fun and hopefully will result in an application that students and researchers alike will find useful.

I am excited to see what other scientific applications will emerge for portable devices, once people realize that these are no longer just pieces of consumer electronics but powerful mobile computers.

For more information: Blog posts and tips on programming the iPhone's 3D hardware are at **www.sunsetlakesoftware.com/molecules**. A direct link to the free *Molecules* download from iTunes is provided for users with a compatible device (iPhone or iPod Touch with the 2.0 firmware update installed). To participate in a discussion or read what others have had to say, stop by the forums at **www.sunsetlakesoftware.com/forum**.

Finally, the source code to *Molecules* has been released under the BSD license at the first page mentioned above. In addition to the educational opportunities of the application itself, I hope that the availability of the code will help others develop similar portable scientific tools.

USING *MOLECULES* IN THE CLASSROOM

Imagine a university biochemistry class in which the professor is about to begin a lesson on antibodies. He starts by asking how many in attendance have either an iPod Touch or iPhone. About a third of those in the audience raise their hands, so he instructs those people to download Molecules directly to their devices *via* the campus WiFi network and find the structure 1igt: an intact IgG2a monoclonal antibody. As the professor explains the structure of an antibody, these students can rotate and zoom in on the molecule themselves (of course, sharing with their neighbors who lack a compatible device). This kind of an interactive demonstration could convey more information than a presentation using a projected screen at the front of the class. At the end of the day, the students can take this capability home to play with later.

PDB Community Focus

Paul D. Adams, Ph.D., Lawrence Berkeley Laboratory

Q: *You have had a long history in the development of crystallographic software. Your latest project is PHENIX–what can you tell us about it?*

A: At the beginning of this century, the field of structural genomics really took off and it was clear that there would be an increased emphasis on automated crystallographic structure solution. The development of PHENIX was a response to this. A number of us got together, including Randy Read, Tom Terwilliger, Tom Ioerger, and more recently Jane and David Richardson, and decided that it was the right time to do something new. PHENIX has been designed with automation in mind and is based on the Python scripting language. There are tools for automated structure solution using experimental phasing and molecular replacement, structure refinement, ligand coordinate and restraint generation, and structure validation. Although PHENIX has been created with automated structure solution in mind, it is pleasing to see that it is also being used for a number of very challenging structures. PHENIX can be downloaded on the web by academic researchers at **www.phenix-online.org**.

Q: *A recent article in* Science *highlighted the Technology Portal of the PSI SGKB site. What is your vision for this resource?*

A: Although there is currently much debate about the best future direction for structural genomics research in the US, I think most would agree that this branch of research has generated a large number of tools that are of benefit to all structural biologists. However, one of the problems, not unusual in science, is the communication of these innovations to the scientific community. NIH very wisely decided to put some funding into developing a web-based resource for dissemination of information generated in the US by PSI-funded structural genomics projects. I see this PSI Knowledgebase, lead by Helen Berman, as an essential vehicle for making the broader scientific community aware of these advances. The Technology Portal of the Knowledgebase lets anyone read about new technologies that might be helpful to their own research. Our goal is to provide information so that these researchers can easily get in touch with the technology developers and thus expand the adoption of new technologies. We are also going to set up forums to promote more discussions about technology development in the general scientific community.

Q: *Most recently, you have taken on a leadership role in the Joint BioEnergy Institute. What are your goals for this organization?*

A: The long-term availability of fossil fuels and concerns about global warming have made the development of carbon-neutral and renewable sources of energy a priority. The conversion of cellulosic (plant) material to transport fuels has the potential to provide a significant fraction of available fuel in the future. The Joint BioEnergy Institute (JBEI) is one of three Department of Energy (DOE) funded research centers developing the basic science and technology for biofuels production. JBEI is a collaborative effort between Lawrence Berkeley Laboratory, Sandia National Laboratory, Lawrence Livermore Laboratory, UC Berkeley and UC Davis, and the Carnegie Institution at Stanford. We're located in Emeryville, California, about three miles from UC Berkeley and Lawrence Berkeley Laboratory. There are four Divisions that are addressing different parts of the biofuels problem: Feedstocks, Deconstruction, Fuels Synthesis and Technology. As the Vice President leading the Technology Division, my goal is to create new technologies to support the development of biofuels. In the next five to ten years, JBEI researchers will have developed new feedstocks optimized for biofuels production, new methods to breakdown lignocellulose, and microbes that are optimized for the conversion of sugars to fuels.

Q: *You have been involved in many aspects of structural biology. Where do you see the future?*

A: I feel fortunate to have experience in both experimental and computational structural biology–my B.Sc. and Ph.D are in biochemistry but I got involved in crystallography, molecular modeling, molecular dynamics, and parallel computing as a graduate student and postdoc. The field has changed greatly over the last twenty years and I think the future of structural biology is already happening. In the past it was only practical for researchers to specialize in one main experimental technique, such as X-ray crystallography. Now more researchers are embracing the idea that answering a biological problem often requires multiple experimental methods, and that it is feasible to bring these methods in house. I anticipate that many of the ground breaking structural biology research projects in the future will combine multiple biophysical techniques, such as crystallography (X-ray and neutron), electron microscopy, and small angle scattering. Hopefully, the use of computational techniques, such as molecular simulation, will increase as those methods improve. Ultimately new experimental techniques will be developed, such as single particle X-ray diffractive imaging, which will undoubtedly open up new research possibilities.

PAUL D. ADAMS *is a Senior Scientist and Deputy Director of the Physical Biosciences Division at Lawrence Berkeley Laboratory, Head of the Berkeley Center for Structural Biology, Vice President for Technology at the Joint BioEnergy Institute, and an Adjunct Professor in the Department of Bioengineering at the University of California Berkeley.*

He studied biochemistry at Edinburgh University where, in 1992, he also received his Ph.D. in structural biology for work on rodent pheromone binding proteins using crystallographic and molecular modeling methods. During this time he became involved in parallel computing and spent a year working at the Edinburgh Parallel Computing Center. In 1992 he moved to Yale University for a postdoctoral position developing crystallographic and computational modeling methods. Together with Axel T. Brunger and others, he developed the Crystallography and NMR System package that has been a mainstay of structural biology for the last decade. In 1999 he moved to the Lawrence Berkeley Laboratory to start a new group developing tools for structural biology.

His current research interests span computation, structural biology and biofuels. Much of his research is focused on the development of new algorithms and computational methods for addressing problems in structural biology. He leads the NIH-funded PHENIX collaboration developing new software for the automated solution of macromolecular structures using crystallographic methods. He also collaborates with researchers at Los Alamos National Laboratory and Baylor College of Medicine to incorporate methods for neutron diffraction and analysis of high-resolution structures from single particle cryo-electron microscopy. He has collaborated with experimentalists, most recently Judith Frydman at Stanford, to understand the structure and function of chaperonins. He is the author of over 80 papers, book chapters and review articles. As Head of the Berkeley Center for Structural Biology at the Advanced Light Source, he oversees the development, maintenance and operation of five synchrotron beamlines for macromolecular crystallographic data collection. Recent upgrades to the beamlines have improved automation and X-ray flux. He is also involved in the growing field of biofuels research, leading programs at both the Joint BioEnergy Institute in Emeryville and the Energy Biosciences Institute in Berkeley. He has had a long and fruitful association with the Protein Data Bank and is a member of the wwPDB X-ray Validation Task Force. He also leads the development of the Technology Portal for the PSI Structural Genomics Knowledgebase.

RCSB PDB Partners

The RCSB PDB is managed by two partner sites of the Research Collaboratory for Structural Bioinformatics:

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