Protein Data Bank

Quarterly Newsletter

Release #77 *July 1996*

July 1996 CD-ROM Release

4652 full-release atomic coordinate entries

Molecule Type

4207	proteins, peptides, and viruses
108	protein/nucleic acid complexes
325	nucleic acids
12	carbohydrates

Experimental Technique

136	theoretical modeling
651	NMR
3865	diffraction and other

The total size of the atomic coordinate entry database is 1802 Mbytes uncompressed.

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Internet Sites

WWW .... http://www.pdb.bnl.gov
FTP .... ftp.pdb.bnl.gov

What's New at the PDB

The PDB is an archive of experimentally determined three-dimensional structures of biological macromolecules, serving the world community of researchers, educators, and students. The database contains atomic coordinates, bibliographic citations, primary and secondary structure information, as well as crystallographic structure factors and NMR experimental data.

During the past two years, the PDB has significantly improved world-wide access to its information, *via* the widely used WWW PDB browser [D.R. Stampf, C.E. Felder, and J.L. Sussman, PDBBrowse — a Graphics Interface to the Brookhaven Protein Data Bank, *Nature* **374**, 572-574 (1995)]. In parallel, a new easier-to-fill-in electronic deposition form was introduced during the summer of 1994.

To streamline the deposition procedure, both to reduce the depositors' time spent in filling out the deposition form and to increase the accuracy and information content of a PDB entry, a WWW-based graphical user interface, AutoDep, was designed by Dave Stampf and coworkers at the PDB. AutoDep is now in the final stages of "beta" testing and will be demonstrated and released this August at the IUCr XVII International Congress in Seattle, Washington, USA.

The depositor may fill in the AutoDep form with data from any released PDB entry or a previously submitted, but not yet released entry; also, it may be filled out from scratch. Additionally, PDB-formatted output from refinement programs, *e.g.*, the new release of X-PLOR (version 4.0) which contains most of the fields now required in a full PDB entry, can be submitted and will automatically be merged into the form.

Preliminary verification of each field in the form is done during an interactive session *via* the WWW. The depositor can view the resultant header portion of the PDB entry at any time to check his or her progress. A simple script is provided that can be copied to a window on the home computer which will FTP the coordinates and related files to the PDB.

The AutoDep procedure is based on CIF and uses CIF-based data dictionaries. Any changes to the deposition procedures or information content of PDB entries are easily accommodated by editing the dictionary files. For more details on AutoDep see the article in this Quarterly Newsletter entitled "Get Ready for AutoDep — PDB's New WWW Deposition Tool".

— Joel L. Sussman

BNL Wins Award to Continue Operating the PDB

Press release issued by Brookhaven National Laboratory on June 3, 1996.

Four government agencies, spearheaded by the National Science Foundation (NSF), have jointly given the U.S. Department of Energy's Brookhaven National Laboratory an award to continue to operate the Protein Dank Bank (PDB).

The PDB is a unique international clearinghouse for three-dimensional structural information about proteins, nucleic acids, and other biological macromolecules. Scientists around the world contribute structures to the PDB and use it on a daily basis. The scientific community depends on convenient access to this information as an invaluable aid to research because the exact three-dimensional arrangement of molecules determines their biological function. The PDB has become a major resource for research in a wide variety of areas besides structural biology, including a better understanding of the molecular basis of certain diseases and the design of new therapeutics. The structural data on proteins and nucleic acids also helps scientists to use the information generated by the Human Genome Project.

The PDB originated at Brookhaven and was supported for twenty-five years by renewable NSF grants. Recently, there has been a tremendous growth in the number of structures deposited as well as in the number of scientists accessing the information — currently over one per minute on the World Wide Web. The crucial role played by the PDB in biological research and this dramatic growth has spurred the National Science Foundation (NSF) to provide operating funds using a cooperative agreement, a significant change from the standard renewable NSF grant used to fund the PDB since 1971. The current award, granted after an open competition, took effect May 1, 1996 and is funded by the NSF, the U.S. Department of Energy, the National Institute of General Medical Sciences, and the National Library of Medicine; the latter two are part of the National Institutes of Health. The NSF administers the award and oversees the operations of the PDB to assure its effectiveness. The combined funding for fiscal year 1996 is $2.5 million.

The head of PDB, Dr. Joel L. Sussman, a protein crystallographer at Brookhaven and a professor at the Weizmann Institute of Science, said, “On behalf of Brookhaven National Laboratory, I am eager to accept the challenge of keeping the Protein Data Bank a vital international resource for research institutions and industry. We expect this new cooperative agreement will facilitate the efficient operations of the fast-growing facility.”

In April, the PDB and its eighteen-member staff moved from Brookhaven's Chemistry Department to a new, specially-designed annex of the Biology Department. With research programs in structural biology, molecular genetics, and DNA sequencing for the Human Genome Project, the Biology Department is an ideal location for the PDB.

With its new award, the PDB will also get a new name. While not yet finalized, the new name is expected to be 3DB, for Three-Dimensional Database of Biomacromolecules, which emphasizes both the three-dimensional nature of the data and the archiving of other biomolecules besides proteins.

The information contained in the PDB is available to anyone who has access to the WWW at **http://www.pdb.bnl.gov.** Transfer of information across the WWW is sometimes slow, so to improve the service to the international community, 'mirror' copies of the PDB information are available at a number of sites around the world. Mirror sites are already running at the Weizmann Institute of Science, Israel, at Peking University, China, and at the EMBL Outstation — the European Bioinformatics Institute — in the United Kingdom.

Brookhaven National Laboratory is a natural host for the PDB as it carries out basic and applied research in the physical, biomedical, and environmental sciences, and in selected energy technologies. It is the only site in the United States with both a synchrotron light source and a research reactor. Many molecular biologists and crystallographers come to Brookhaven each year to use facilities at the National Synchrotron Light Source and the High Flux Beam Reactor. Brookhaven is operated by Associated Universities, Inc., a nonprofit research management organization, under contract with the U.S. Department of Energy.

— BNL Public Affairs Office

Get Ready for AutoDep — PDB's New WWW Deposition Tool

In August 1996, a new interactive tool will be introduced that will greatly simplify the process of preparing depositions to the PDB. Known as AutoDep, it is a WWW-based graphical interface to the deposition form which leads the author through the entire process of deposition [1]. In addition, AutoDep verifies some data and checks validation [2]. Thus, many problems or errors are flagged and corrected before the deposition is sent to the PDB.

Users of PDB are requesting an increasing amount of information with every released structure. They demand more detailed information, as well as access to the experimental data such as X-ray crystallographic structure factors to better judge the structure’s quality. In response, PDB has increased the number of reported experimental and refinement statistics, and expects to continue to enhance the information content of entries in accordance with these demands. AutoDep simplifies the reporting and submission of these data, and because the program uses CIF-based data dictionaries, it has a straightforward means of responding to the changing needs of the community.

AutoDep's most important features include the following:

- The ability to fill in the form automatically from an existing PDB entry or a previous deposition. As easy as pushing a button, AutoDep will enter data from the designated file to the appropriate fields in the new form. The author merely has to update fields to reflect the new structure.
- Software is available to write PDB records that can be automatically merged into the deposition form. For example, the

new releases of X-PLOR [3] and SHELX-96 write refinement details as PDB records which will be read by the program and entered into the relevant sections. We are continuing to work with authors of various programs and anticipate that increasing numbers of programs will be integrated with PDB.

- Each session has help files, examples, and links to related documentation and useful URLs in each section to support the author during the AutoDep session.
- At any time during the AutoDep session, the Deposition Form or the resultant header portion of the PDB file can be viewed to check progress.
- The AutoDep session can be interrupted at any time and returned to hours, days, or even weeks later. The session id number and password must be recorded to continue with the same deposition.
- When an author is satisfied with the completed deposition form, a script is provided which allows cutting and pasting to your local computer to automatically download the completed form and all associated files to the PDB.

It is useful to gather certain information before beginning AutoDep. Here are some items which should be on hand while making a deposition.

- Name of the file that has the coordinates in PDB format.
- Complete description of the molecular contents of the entry, including any heterogens present.
- Name of the sequence database entry or entries for the molecules present.
- Description of the biological source(s) of the molecules.
- Details of data collection, such as temperature, pH, number of crystals used; description of the radiation and equipment used for collection; the resolution range, completeness (%), data redundancy, merging R value, and average I/sigma(I) — both overall and in the highest resolution shell.
- Unit cell data.
- Structure refinement statistics.
- References for papers being cited.

We wish to extend our deepest appreciation to all those who have given their time and effort to developing AutoDep. Many people have brainstormed with us, given valuable help and suggestions, or served as alpha and beta testers. Axel Brünger and George Sheldrick, in collaboration with the PDB, have modified the output of X-PLOR and SHELXPRO (part of the SHELX-96 package) for direct inclusion into a PDB file *via* AutoDep.

The PDB will be demonstrating AutoDep at the XVII Congress and General Assembly of the IUCr, August 8 - 17 in Seattle, Washington. Please come to our exhibit booth for an introduction and some hands-on practice.

Watch for announcement of the release of AutoDep on PDB's WWW Home Page (**http://www.pdb.bnl.gov** and mirror sites) and on several popular mailing lists. If you have any questions on how to use AutoDep, support will be available from our Help Desk at **pdbhelp@bnl.gov**, telephone 516-344-6356. We gladly welcome your comments and suggestions.

1. D.R. Stampf, E.E. Abola, N.O. Manning, D. Xue, and J.L. Sussman, AutoDep — Facilitating Deposition to the Protein Data Bank Through the New Web-Based Submission Form, IUCr Abstract No. PS22.03.10, IUCr XVII Congress and General Assembly, Seattle, WA (1996).

2. J.P. Rose, S. Swaminathan, E.E. Abola, N.O. Manning, and J.L. Sussman, PDB Validation Procedures — Past, Present and Future, IUCr Abstract No. PS22.03.11, IUCr XVII Congress and General Assembly, Seattle, WA (1996).

3. J.-S. Jiang, N.O. Manning, E.E. Abola, A.T. Brünger, and J.L. Sussman, PDB Submission with X-PLOR, IUCr Abstract No. PS22.03.12, IUCr XVII Congress and General Assembly, Seattle, WA (1996).

— Nancy O. Manning

Update on International Conference on Bioinformatics <---> Structure

*This article was written by Michal Harel, Department of Structural Biology, Weizmann Institute of Science, Rehovot, Israel **(csharel2@weizmann.weizmann.ac.il)**.*

The 24th Aharon Katzir-Katchalsky Conference on BIOINFORMATICS <--> STRUCTURE celebrating the Twenty-fifth Anniversary of the Brookhaven Protein Data Bank and the Tenth Anniversary of SwissProt will be held in Jerusalem, Israel on November 17 - 21, 1996.

The registration date has been extended to September 1, 1996.

The current list of speakers includes the following people:

Enrique Abola (USA)	Olga Kennard (UK)
Ron Appel (Switzerland)	Doron Lancet (Israel)
Rolf Apweiler (UK)	Michael Levitt (USA)
Amos Bairoch (Switzerland)	Victor Markowitz (USA)
Helen Berman (USA)	Edgar Meyer (USA)
Tom Blundell (UK)	John Moult (USA)
Peer Bork (Germany)	Manuel Peitsch (Switzerland)
Stephen Bryant (USA)	Jaime Prilusky (Israel)
Graham Cameron (UK)	Jane Richardson (USA)
Cyrus Chothia (UK)	Chris Sander (Germany/UK)
David Eisenberg (USA)	Manfred Sippl (Austria)
Ken Fasman (USA)	William Studier (USA)
Osnat Herzberg (USA)	Joel L. Sussman (Israel/USA)
Barry Honig (USA)	Yoshio Tateno (Japan)
Leroy Hood (USA)	Tomitake Tsukihara (Japan)
Rod Hubbard (UK)	Keith D. Watenpaugh (USA)
Ephraim Katchalski-Katzir (Israel)	Keith Wilson (UK/Germany)
John Kendrew (UK)	Ada Yonath (Israel)

For registration and program details contact:

e-mail: pdb25sw10@bioinformatics.weizmann.ac.il
URL: http://bioinformatics.weizmann.ac.il/conf/pdb25sw10
http://www.pdb.bnl.gov/pdb25sw10 or its mirror sites

Meeting secretary: Ruth Goldstein, Katzir Center
e-mail: jkgold@weizmann.weizmann.ac.il
fax: 972-8-9474425
phone: 972-8-9342148

Growth of Data at the PDB

For twenty-five years the PDB has been accepting, verifying, annotating, and releasing three-dimensional coordinate entries of biological macromolecules. For many years the number of entries submitted was well below 100 per year. Then, in 1988, twice as many coordinates were submitted as in any previous year. The number increased steadily from that point on, as Figure 1 shows. In 1995 we received 1,269 entries for deposition, close to ten times as many as in 1988.

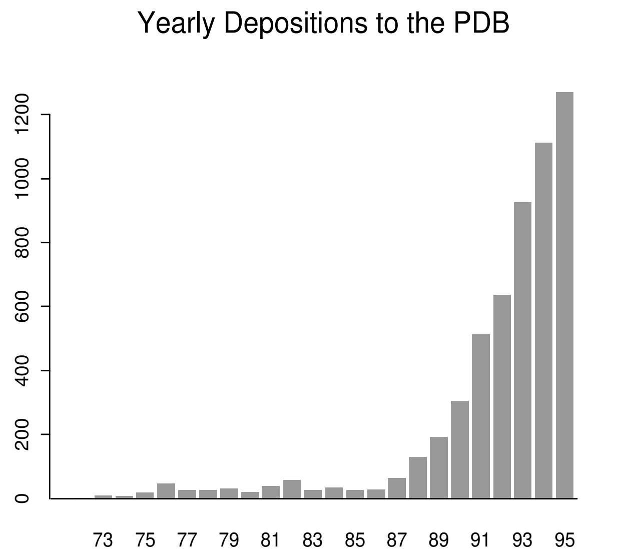

Figure 1

This increase in submissions greatly affected the number of entries accessible to researchers. Figure 2 shows the dramatic increase in the availability of coordinates that became evident in 1988.

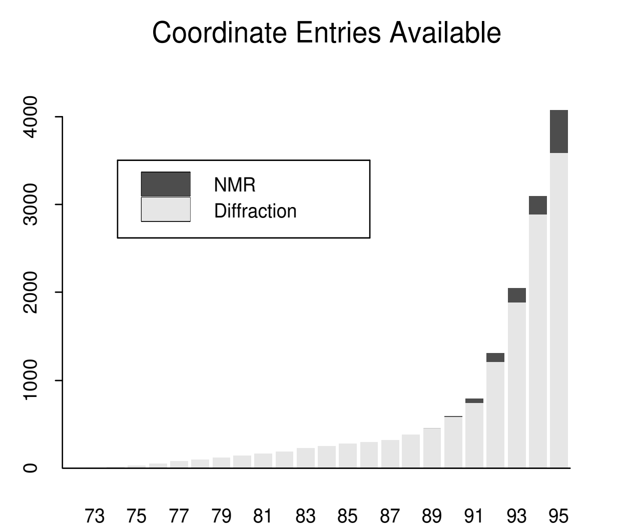

Figure 2

Today, more than 4,500 entries are accessible. If the number of depositions continues to increase at the present rate, it is anticipated that between 12,000 and 25,000 entries will be available by the year 2000, depending on the type of projection used. Joel Sussman's lead article in the April 1996 Protein Data Bank Quarterly Newsletter discussed the factors that affected the deposition rates over the past several years.

Please see URL **http://www.pdb.bnl.gov/statistics.html** for the current statistics.

— Regina K. Shea

New Bioinformatics Server in China

This article was written by Luhua Lai and Dawei Lin, Institute of Physical Chemistry, Peking University, Beijing, China ***(lai@ipc.pku.edu.cn)****.*

We are pleased to announce that the first bioinformatics server in China has been established and is being maintained by the Molecular Design Lab, Institute of Physical Chemistry, Peking University, Beijing, China. At this infant stage, it is only mirroring protein-related databases; however, other molecular biology databases will soon be mirrored, as requested.

Under the direction of Professor Luhua Lai, all the mirror work and database interconnections were implemented by Dawei Lin. The Home Pages were designed by Renxiao Wang and Dawei Lin. The work is supported by the Chinese National Commission of Science and Technology.

At present, we are one of three official mirror sites of the Protein Data Bank (see the listing of Affiliated Centers and Mirror Sites at the end of this Newsletter) and provide WWW browsing capability and access to all of PDB's FTP directories. We are one of SCOP's five official mirror sites. The PDB and SCOP mirror sites have been cross-linked for the convenience of local users. We also mirror the FTP services of SWISSPROT, PIR, PROSITE, and BLOCKS. The molecular graphics software, RasMol, is attached to the databases to enable graphical viewing. Users in China and nearby countries may find this server helpful.

We would like to thank all the people who have given us help and valuable suggestions, especially Joel Sussman, Enrique Abola, Jaime Prilusky, Dave Stampf, and Nancy Manning for their help in setting up our PDB mirror site; Steven Brenner and Tim Hubbard for their help in setting up our SCOP mirror site; and Amos Bairoch for his help in setting up our SwissProt mirror site.

The following are useful URLs related to the bioinformatics server:

- Home page: The first China Bioinformatics Server:
  http://www.ipc.pku.edu.cn/mirror/mirror.html
- Home page: Institute of Physical Chemistry, Peking University:
  http://www.ipc.pku.edu.cn/
- PDB mirror site:
  http://www.ipc.pku.edu.cn/npdb/index.html
- SCOP mirror site:
  http://www.ipc.pku.edu.cn/scop/
- Anonymous FTP server: Institute of Physical Chemistry:
  ftp.ipc.pku.edu.cn

Suggestions and encouragement are welcome — please send them to **lai@ipc.pku.edu.cn**.

Appeal for Structures to be Predicted for the Second Meeting on the Critical Assessment of Techniques for Protein Structure Prediction

*This article was written by John Moult on behalf of the CASP2 organizers, CARB, University of Maryland Biotechnology Institute, Rockville, MD, USA **(jmoult@indigo5.carb.nist.gov)**.*

The second Asilomar protein structure prediction experiment, called CASP2, is well underway, with the prediction season running through October 1 (see relevant article in the April 1996 PDB Quarterly Newsletter). The meeting to evaluate the results of the prediction experiment will be held December 12-16, 1996 in Asilomar, California. The goal of the experiment is to obtain as objective a view as possible of the capabilities of current methods of predicting protein structure methods. The approach is to obtain information about soon-to-be-solved structures from experimentalists, to pass that on to the predictors, and to collect their models before the structure is made public. The first experiment, held during 1994, produced a large amount of interesting and provocative data. A special issue of *Proteins: Structure, Function and Genetics*, **23**(3) (Nov. 1995) contains papers describing the outcome of the first experiment. We hope the second experiment will be as informative. In particular, a big question now is the extent to which the key problems identified two years ago have been solved.

As of July 1, we have seventy groups registered as intending to make predictions. Thirty-five teams predicted last time, so we are on the way to doubling participation. In contrast to this, we have only twenty-three targets and would like to get close to fifty. Therefore, we need your help in providing targets. We need targets in all four categories: comparative modeling, fold recognition (‘threading’), *ab initio* structure prediction, and docking (new). Even if you do not have any targets available yourself, please pass this request on to other experimentalists you think may be interested. We cannot make this experiment work without again getting the help of the experimental community. The rules are spelled out on the general target request found on the CASP2 WWW pages.

Additional information, including the target situation, may be obtained from two Web sites, **http://iris4.carb.nist.gov/casp2** and **http://www.mrc-cpe.cam.ac.uk/casp2**. If you would like to receive the mailings associated with the experiment, please register your interest.

A Library of Protein Family Cores

*This article was written by Russ B. Altman, Robert Schmidt, and Mark Gerstein, Stanford University, Stanford, CA, USA **(e-mail: altman@camis.stanford.edu; http://www-camis.stanford.edu/projects/helix/LPFC)**.*

The growing number of protein structures that fall within well-defined families (and share structural features) allows statistical analysis of the commonalities and differences between members of these families. The PDB is now linked to the Library of Protein Family Cores (LPFC). Starting with structural alignments specified in a standard format, we use a recently published algorithm [1] to compute the spatial variation of the residues in each column of the multiple alignment. The spatial variation then can be used to separate residues which have high spatial variability across the family from those with low variability. The low variability atoms can be considered the core of the family, since they represent residues that are in essentially the same position in all members. They can serve as a starting point for accurate model building, threading applications, and functional analysis of the families.

The basic core-finding methodology was applied to the globin and immunoglobulin family with some success. We showed that the average core structures defined by this procedure have biological significance, corresponding to functional significance, exon organization, data on the order of protein folding, and identifying submotifs that are re-used in other families [1,2].

The LPFC is divided into sections based on the multiple structural alignment algorithm used. Currently, the library contains alignments from the HOMALDB database by Sali and Overington [3], and the FSSP database by Holm and Sander [4]. It also contains some hand alignments. The library is generated automatically from a set of scripts and requires only the set of structural multiple alignments in a standard file format as input. Thus, it is relatively easy to update as new releases of various alignment databases are made available. The code for computing protein family cores is given at the LPFC Web site as well. Those wishing to incorporate other multiple structural alignment methods into the library are encouraged to contact the authors at **lpfc@camis.stanford.edu**.

For each multiple structural alignment of a protein family, LPFC has a Web page. These pages contain the names of the proteins included in the alignment, the number of aligned residues, and the number of core residues (a subset of the aligned residues). They also give access to data files providing detailed information about the actual volume of spatial variation for each residue, the coordinates of an unbiased average structure based on the low variance atoms alone, and numerous display files, including files for generating ellipsoids using the proteanD program for SGI machines [5] which may be found at **ftp://camis.stanford.edu/pub/altman/proteand.tar.Z**, as well as VRML files for interactively viewing ellipsoidal representations of residue variability. The main pages are also linked to a grid that shows all the RMS deviations between members of the family, as well as a new parameter, the SD-RMS [1] that measures the deviation between two structures in the context of the known variation within the family. Finally, each page has links to other popular Internet resources, such as the PDB, SCOP, Swiss-Prot and the Protein Motions Database (see relevant article in the July 1995 PDB Quarterly Newsletter).

Access into the LPFC can be gained at the WWW home page: **http://www-camis.stanford.edu/projects/helix/LPFC**.

From the home page, a user may access the source code, explanations of file formats, and references to publications describing the alignment techniques. The LPFC also has a search capability. A rudimentary textual search is possible, although the full-text search of the PDB is a more sensitive search tool. Given a PDB ID code, a user may search by the ID code alone or a set of PDB ID codes. The LPFC will create a page listing all occurrences of the provided ID codes in the families (some structures are part of more than one family within a set of multiple alignments or across multiple alignment methodologies). The user may select a family from this list. Additionally, the LPFC allows the user to specify a PDB ID code and an amino-acid number. The user is once again presented with a list of choices, if there are more than one. The result of this search is a page listing the amino-acid sought, as well as all aligned residues from other proteins (the entire relevant column of the multiple alignment) and information about the spatial variability of these residues in the protein family selected. The user may traverse the multiple alignment to the left or right by following pointers on these pages.

1. M. Gerstein and R.B. Altman, Average Core Structures and Variability Measures for Protein Families: Application to the Immunoglobulins, *J. Mol. Biol.* **251**(1), 161-175 (1995).

2. M. Gerstein and R.B. Altman, Using a Measure of Structural Variation to Define a Core for the Globins, *CABIOS* **11**(6), 633-644 (1995).

3. A. Sali and J. Overington, Derivation of Rules for Comparative Protein Modeling from a Database of Protein Structure Alignments, *Prot. Sci.* **3**(9), 1582-1596 (1994).

4. L. Holm and C. Sander, The FSSP Database of Structurally Aligned Protein Fold Families, *Nucl. Acids Res.* **24**, 204-210 (1994).

5. R.B. Altman, C. Hughes, and M.B. Gerstein, Methods for Displaying Macromolecular Structural Uncertainty: Application to the Globins, *J. Mol. Graphics* **13**, 142-152 (1995).

PKDB: The Protein Kinase Database Project

This article was written by Phil Bourne, Michael Gribskov, Lynn Ten Eyck, and Susan Taylor, San Diego Supercomputer Center and University of California at San Diego, San Diego, CA, USA ***(e-mail: bourne@sdsc.edu; http://www.sdsc.edu/kinases)****.*

Members of the serine/threonine/tyrosine protein kinase family of enzymes play key roles in regulating cellular differentiation and the proliferation of diverse cell types. Cellular functions, such as cell proliferation and signal transduction, are frequently regulated, in part, by the balance between protein kinases and phosphatases. Perturbation of this balance can lead to disease or oncogenesis. The protein kinase database (PKDB) project **(http://www.sdsc.edu/kinases)** is an ongoing effort to bring together a variety of on-line information about this diverse family of enzymes. PKDB is a prototype for a new type of biological data resource. Unlike the majority of existing resources*, e.g.,* PDB and GenBank which cover a large diverse body of biological information in limited detail, PKDB covers a relatively small area — in this case a single protein family, in considerable detail. Other groups are developing similar resources, for example, the following:

- cytokines:
  http://www.ocms.ox.ac.uk/~smb/cyt_web/
  http://www.lmb.uni-muenchen.de/groups/ibelgaufts/cytokines.html
- esterases:
  http://ensam.inra.fr/cholinesterase
- transmembrane proteins:
  ftp://ulrec3.unil.ch/pub/tmbase/
- g protein-coupled receptors:
  http://receptor.mgh.harvard.edu/GCRDBHOME.html
- glucoamylase:
  http://www.public.iastate.edu/~pedro/glase/glase.html

PKDB currently organizes data by family classification, sequence, 3-D structure, and known relationships to diseases. It is possible to search for any text string (including subsequences) across all this information using the Harvest search system developed at the University of Colorado. The available sequences, of which there are 390, as compared to about 600 in the PIR or SWISS-PROT databases, have been manually aligned by kinase experts [1]. Alignments are organized by protein family classification.

We are adding analytical tools having the ability to show the alignments of novel kinase-related sequences to the known kinase families and expanding the alignment information to include all known kinase sequences.

Disease information was extracted from the On-line Mendelian Inheritance in Man (OMIM) database, found at **http://www3.ncbi.nlm.nih.gov/omim**, which, in turn, has links to bibliographic data in Medline.

Structural information is available on nineteen separate structures. Several of them have either not been submitted to the PDB, or are on hold. Notable are MAP kinase ERK2 complexed with MgATP and cyclin-dependent protein kinase (complexed with cyclin). While still under development, details on each structure include a brief synopsis, references, crystallographic information (provided by Ketan Patel and Helen Berman at **http://rutchem.rutgers.edu/faculty/berman/berman.html**), and a structure walk-through, which uses the frames capability of recent Netscape browsers. The goal of the walk-through is to provide a level of annotation and explanation of structural features not possible within the page constraints of traditional journals (for an example see **http://www.sdsc.edu/CompSci/Biomed/Kinases/mlundy/html/frame.htm**). Moreover, helper applications can be used to render structural views as necessary. Beyond a discussion of each individual structure is the opportunity to compare structures, though in a limited way. While this, too, is in an early stage of development, there is a collage available showing temperature factors and C-alpha superposition of apo and bound forms of several structures.

As accessibility and acceptance of the Web as a delivery system for quality scientific information improves, our goal is to operate the resource as an electronic journal, complete with peer review. There are some technical barriers to be overcome before this goal can be realized.

Presently, PKDB is not a true database, but rather, a collection of related information with appropriate hyperlinks added manually. To be successful, such resources must be current with respect to the primary sources of information, must contain additional detail, and must have powerful capabilities to answer questions. Staying current and automatically adding hyperlinks requires automatic updating, which, in turn, requires a higher level of data organization than presently available. Thus, in addition to our immediate tasks of better organizing the available data and providing analytical tools, our long-term task is to maintain the information in a database permitting better validation and more flexible support for questions. Comments, suggestions, and contributions to PKDB are welcome at **kinase_maint@sdsc.edu**.

1. D.G. Hardie and S.K. Hanks, eds., *The Protein Kinases Factsbook*, Academic Press, San Diego, 1996.

Swiss-PdbViewer: A Fast and Easy-to-use PDB Viewer for Macintosh and PC

This article was written by Nicolas Guex and Manuel C. Peitsch, Geneva Biomedical Research Institute, CH-1228, Geneva, Switzerland ***(ng45767@ggr.co.uk)****.*

As the number of experimentally determined, three-dimensional structures dramatically increased over the past years, comparative modeling has become a convenient way to look at proteins not yet crystallized but similar to ones with a known three-dimensional structure. Moreover, since mutagenesis experiments are time-consuming, many molecular biologists need to predict the effect that a specific mutation would have on their protein before performing the experiment.

The aim of Swiss-PdbViewer is to help biologists compare protein structures, as well as decide which amino-acids could be worth mutating.

As molecular biologists tend to work more with Macintoshes and PCs than with UNIX systems, Swiss-PdbViewer was initially developed on microcomputers, although an X-Window version is also planned.

— Current Features

Swiss-PdbViewer allows one to load up to ten PDB files simultaneously. Proteins can then be “piled-up” in 3D space, either by picking three corresponding reference atoms of the structures to align or by performing a least-squares fit of selected parts of the molecules. RMS deviations then can be calculated on selected amino-acids of the superimposed proteins using alpha-carbon atoms, backbone atoms, side-chain atoms, or all atoms. Comparing active sites and other relevant regions is, therefore, very easy.

The workspace is divided into two windows. The main window essentially displays the molecules, but also contains a few tools to measure distances, angles, and torsion angles between atoms. The content of the main window can be exported as a PDB file, an image, or a POV scene description (POV is a popular multi-platform free ray-tracer capable of rendering very high quality images).

The second window is a control panel that lists all amino-acids and other groups of each molecule, together with their current display status. It is possible to individually display/undisplay amino-acid side chains, names, and van der Waals dotted surfaces, as well as change their color with simple mouse clicks. In addition, various shortcuts allow one to directly center specific amino acids on the screen, as well as to automatically rescale and recenter visible parts, eliminating the need to manually “search the space” to obtain the desired view.

Other key features of Swiss-PdbViewer are the ability to evaluate hydrogen bonds for the whole molecule, even if the PDB file does not provide explicit hydrogen atoms, and the ability to mutate amino-acid side chains by browsing a rotamer library. The best rotamer is automatically suggested. In addition, during the mutation process, H-bonds and steric hindrances are automatically estimated and displayed in real time, facilitating the best rotamer choice.

— Future Developments

Swiss-PdbViewer is under constant improvement. By the end of 1996, it should allow biologists to do multiple alignments threading, as well as to directly submit comparative modeling requests to “Swiss-Model”, the automated knowledge-based protein modeling server running at the Geneva Biomedical Research Institute at **http://expasy.hcuge.ch/swissmod/SWISS-MODEL.html**.

For further information, consult the Swiss-PdbViewer user guide (**http://expasy.hcuge.ch/swissmod/Swiss-PdbViewer/mainpage.html**). Executables may be downloaded from there or directly by anonymous FTP **(ftp://expasy.hcuge.ch/pub/PDBViewers/Prot3Dviewer)**.

VMD — A Molecular Graphics and Analysis Program

This article was written by Andrew Dalke, Theoretical Biophysics Group, Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL, USA ***(dalke@ks.uiuc.edu)****.*

VMD (Visual Molecular Dynamics) is a relatively new program for interactive visualization and analysis of molecular simulations. While most people use it for research in structural biology, others use VMD for fields ranging from quantum chemistry and solid-state physics to making videos for chemistry education. VMD is part of the MDScope project, which is a computational environment for structural biology. VMD and MDScope were developed and freely distributed by the NIH Resource for Concurrent Biological Computing/Theoretical Biophysics Group at the Beckman Institute, University of Illinois at Urbana-Champaign.

VMD directly reads PDB files and X-PLOR style PSF and DCD (trajectory) files and can be configured to use the program Babel for transparent translation from a wide number of structure formats to the PDB format before loading (including animations from XYZ and Gaussian formats). The structure may originate from the local file system, a Web browser, or may be automatically down-loaded from any URL, including the PDB FTP site. Multiple files may be loaded simultaneously and there is no limit to the number of atoms in each file. The largest system loaded to date is a 500,000 atom structure of the complete polio-virus capsid.

Once loaded the structure or a selected substructure may be drawn in many styles including wire-frame, cylinder bonds, licorice, CPK, van der Waals spheres, ribbons, cartoon (using Frishman and Argos' STRIDE to determine the secondary structure), and molecular surface (using Varshney's SURF to find the surface triangulation). The representations may be colored by various schemes, including coloring by atom name, residue type, structure, position, or beta value.

VMD does not directly export any bitmap image formats like GIF or SGI RGB. Instead, the final scene description can be saved as an input script for one of several popular image rendering programs, including Raster3D, POV-Ray, and Radiance. VMD can also read and display Raster3D input files.

All of the basic operations may be done with the mouse and graphical user interface (implemented with the XForms library). The display may be rotated or scaled about a given center, or translated. Molecular structure features may be selected with the mouse to find information about an atom, bond, angle, or dihedral value. Atom coordinates may be modified, allowing for some types of placement and docking of atoms as well as Kabsch least-squares alignment. The new coordinates may be saved to a PDB or DCD file.

One of the more flexible aspects of VMD is its Tcl-based scripting language. Tcl, developed by John Ousterhout, is a widely used scripting language designed to be embedded in other applications. It contains basic programming concepts, like variables, loops, and procedures, as well as more advanced features, such as file I/O, process spawning, and remote procedure calls. In VMD, the Tcl language was extended to include commands relevant to molecular modelling including commands to load molecules, move and scale the display, and change the graphics selections. Indeed, nearly all mouse actions may be logged to a script file, then edited and replayed, making it easy to produce tutorials or high-quality movies.

Additional commands are available for molecular analysis including methods to extract information about atoms and molecules, routines for computing basic molecular properties such as the center of mass, and functions for general vector and matrix mathematics. Under development are methods for computing values more specific to biological systems, such as finding hydrogen bonds and DNA twist parameters. Graphics commands are available for adding triangles, spheres, cylinders, and other geometric objects as well as text labels anywhere in the display, giving a unique way to show analysis results in the molecular display. An example is the following script, which draws a sphere for each residue at the residue's center of mass — the sphere's radius is determined by the residue's radius of gyration.

```
## computes and returns the computes radius of gyration for a given
selection
proc find_rgyr {sel} {
  set com [measure center $sel weight mass]
  set I 0 ; set M 0
  foreach m [$sel get mass] pos [$sel get {x y z}] {
    set I [expr $I + $m * [veclength2 [vecsub $pos $com]]]
    set M [expr $M + $m]
  }
  return [expr sqrt($I/$M)]
}

### find the sphere parameters for every residue except waters
set sel [atomselect top "not water"]
set molid [$sel molindex]
foreach residue [luniq [$sel get residue]] {
  set ressel [atomselect $molid "residue $residue"]
  ## find the center of mass and radius of gyration
  set com [measure center $ressel weight mass]
  set radius [find_rgyr $ressel]
  ### draw the sphere with the correct color assigned to the residue
  lassign [$ressel get resname] resname
  draw color [colorinfo category Resname $resname]
  draw sphere $com radius $radius
}
```

Complete VMD user documentation and a pre-compiled binary file for IRIX 5.x are available. VMD can be compiled on other machines that implement the SGI GL graphics library, including some IBM RS/6000s and HPs with the NPGL emulator. An OpenGL version is nearing completion which, when used with the Mesa emulator, will allow VMD to run under most X-based systems. For those interested in modifying or porting VMD, a complete, commented C++ source is available along with documentation describing the major internal organization.

For more information about VMD, please see the VMD home page at **http://www.ks.uiuc.edu/Research/vmd/**. VMD is supported by grants from the National Institutes of Health (PHS 5 P41 RR05969-04), and the National Science Foundation (BIR-9318159).

Listed below are some relevant URLs which may be useful:

- Theoretical Biophysics Group:
  http://www.ks.uiuc.edu/
- Beckman Institute:
  http://www.beckman.uiuc.edu/
- University of Illinois at Urbana-Champaign:
  http://www.uiuc.edu/
- MDScope:
  http://www.ks.uiuc.edu/Research/mdscope/
- Babel:
  http://mercury.aichem.arizona.edu/babel.html
- STRIDE:
  http://www.embl-heidelberg.de/stride/stride_info.html
- SURF:
  ftp://ftp.cs.unc.edu/pub/projects/GRIP/SURF/surf.tar.Z

- Raster3D:
  http://www.bmsc.washington.edu/raster3d/
- POV-Ray:
  http://www.povray.org/
- Radiance:
  http://radsite.lbl.gov/radiance/HOME.html
- XForms:
  http://bragg.phys.uwm.edu/xforms/
- Tcl:
  http://www.sunlabs.com/research/tcl/
- OpenGL:
  http://www.sgi.com/Technology/openGL/opengl.html

A World Wide Web Service on Macromolecular Crystal Packing with Virtual Reality Modeling Language (VRML)

This article was written by Tai Y. Fu and Yu Wai Chen, Department of Biochemistry and Molecular Biology and the Protein Engineering Network of Centres of Excellence, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z3 ***(tony@laue.biochem.ubc.ca)****.*

One of the current hot topics on the WWW is the Virtual Reality Modeling Language (VRML), an emerging standard for describing navigable and interactive three-dimensional environments. Its goal is to bring a new dimension into visualization and perception of data on the Web and to create a new basis for multi-participant interaction. VRML originates from a subset of the Open Inventor ASCII File Format from Silicon Graphics. The term VRML was extended to represent the entire concept of 3-D environments on the Web. One of VRML's greatest strengths lies in the fact that complex 3-D environments (worlds) may be described with little textual information. This makes VRML ideal for interchanging 3-D information over the net.

To explore the use of VRML in visualizing the intermolecular interaction of macromolecules, a WWW service which transforms Brookhaven's PDB structure files into 3-D crystal packing VRML worlds was developed and may be found at URL **http://laue.biochem.ubc.ca:8080/cgi-bin/ssis/banff/xpack.html**. The user interface of this service is simple; users are required to specify only two parameters:

- The viewing radius within which the neighboring molecules are included in the virtual world.
- The source of the PDB file — this PDB source can either be a URL where the PDB files can be picked up off the Internet (FTP or HTTP protocols) or, if the Web browser being used supports the file upload feature, a full-path filename of the PDB file in the user's own file system.

The core of this Web service is a Common Gateway Interface (CGI) script written in PERL. The function of the CGI script is to accept the information (*via* the HTML form) submitted by the user, analyze the input, and finally return the VRML-world file back to the user. The script gets the unit-cell parameters and the space group information from the "CRYST1" record of the PDB file. If there is no record, only the identity molecule will be included in the output world file. The CGI script does not read the "SCALEn" lines and does not support non-standard orthogonalization of coordinates. The symmetry operation data used are extracted from a library file (symop.lib) from the CCP4 suite of crystallographic programs.

Speed is the major problem with 3-D rendering in VRML. The manipulation of complex VRML worlds requires extensive computing resources and can be painfully slow. Hence, in designing the Web service, the aim is to make the simplest VRML world (wireframe models) which allows the fastest response to the client and, at the same time, contains adequate molecular information for packing analyses. Consequently, the simpler approach of drawing all atoms and determining their connectivities by summing their covalent radii was abandoned. Instead, only the most interesting features of the macromolecule(s) are presented to achieve maximum computing performance. At present, these features include the protein alpha-carbon (C alpha) backbone, disulfide bridges, heme groups, and the phosphate backbone of nucleic acids. The resulting VRML world consists of the crystallographic unit cell and the macromolecules in various symmetry-related positions.

Most VRML browsers are very easy to use and are available in the most popular computer platforms. A properly installed VRML browser will automatically pop up each time a VRML file is loaded from the Web. Users may then sail into the virtual crystal packing world and interactively examine molecular packing.

See URL **http://www.construct.net/tools/vrml/browsers.html** for a list of VRML browsers.

Squid: A Program for the Analysis and Display of Data from Crystallography, NMR, and Molecular Dynamics

This article was written by T. J. Oldfield, Molecular Simulations Ltd., Department of Chemistry, University of York, Heslington, York, YO1 5DD, United Kingdom ***(e-mail: oldfield@yorvic.york.ac.uk****;* ***http://www.yorvic.york.ac.uk/~oldfield/squid).***

Squid is a graphical program designed to analyze and display molecular information and general 2D, 3D, and 4D data [1]. The basic graphics driver was developed to allow Squid to be run on powerful workstations (*i.e.*, SGI) under X-windows, or even at the level of a VT100. Hard-copy output (postscript, HPGL, *etc.*) is exactly as seen and is of publication quality.

The program is designed specifically for analyzing macromolecular structural data from crystallography, NMR, or molecular dynamics; this includes structure validation, MD trajectory data-reduction, cluster analysis, and some database facilities. All derived data are placed in one or more of the internal data tables that may be further processed by intrinsic functions, and then displayed by one of the graphing techniques.

Squid also supports a structured language which allows automated "stream" files to be run through the program, including the use of loop structures and block if structures. In particular, a stream file, which automatically validates protein structures determined by crystallography, is supplied with the current version of the program. The stream file produces a summary file indicating possible problems with the structure which then may be studied further within Squid with specific commands. The validation script concentrates on the analysis of the properties that indicate the quality of the overall structure, not just the simple analysis of bonds, angles, planes, and torsion angles. These include geometry checking, non-bond checking, hydrogen bond analysis, solvent analysis, statistical expectation of derived data, and analysis of isotropic and anisotropic temperature factors.

The techniques in Squid, providing new methods of analysis which are very useful to the crystallographic community, are now being used by the European validation collaboration as part of their protein validation suite.

The molecular dynamics simulation analysis has several primary data-reduction techniques on multiple trajectory files. These range from calculating simple atomic deviations to determining normalized covariance matrices as a function of "R" or "x, y, z" components. The derived data then can be further processed using the functions intrinsic to Squid. For example, covariance matrices may be diagonalized for principal component analysis or processed with the clustering algorithms for conformational analysis.

Squid is provided free to academic organizations and may be obtained from T. J. Oldfield **(oldfield@yorvic.york.ac.uk)**.

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1. T.J. Oldfield, SQUID: A Program for the Analysis and Display of Data from Crystallography and Molecular Dynamics, *J. Mol. Graphics* **10** 247-252 (1992).

Notes of a Protein Crystallographer

— When I Heard the Learn'd Crystallographer

*This article was written by Cele Abad-Zapatero, Abbott Laboratories, Abbott Park, IL, USA **(abad@abbott.com)**.*

Probably every high school student in the United States and in most of the Anglo-Saxon world has been exposed to a poem by the American poet Walt Whitman (Long Island, NY, 1819 -1892) entitled "When I Heard the Learn'd Astronomer." It is a poem that has been included in all too many anthologies and that has been used many times to illustrate the so-called gap between C. P. Snow's two cultures: the sciences and the humanities.

To me, however, the poem epitomizes the need for complementary approaches in our perception, depiction, and understanding of the cosmos that surrounds us. Do we have to know every single note of Händel's Messiah to appreciate it? Will all listeners mentally consult the "circle of fifths" while listening to the modulations of a piano concerto by Mozart? Probably not. Depending upon the time, the occasion, and the profession, most of us simply listen to the music and enjoy it.

Similarly, putting aside the coordinates, the bond angles, bond lengths, the tables, the diagrams, one can look at the overall protein structure for further insight, or just for sheer enjoyment. To contemplate macromolecular structures for what they can be considered to be: atomic sculptural masterpieces of intricate detail.

I do not mean to imply that the analytical, reductionistic tools are superfluous. No, and with chemical redundancy, I say 6.023×10^{23} times no. I am just arguing that there are many different approaches to "comprehend" the atomic underworld beyond our reach, and that the analytical mode is only one of them, although a very important one.

Not coming from an English-speaking culture, I discovered the poem rather late, when I was already a professional macromolecular crystallographer. Nonetheless, it immediately occurred to me that it could be adapted to many other scientific professions. Putting aside the issues of copyright for the moment, I am sure that the bard of Long Island will not object to my modifying his poem to expand its message and its audience. Besides, some of you might have seen the recent film "Il Postino" (The Postman, in the English version) where the main character argues with the famous Chilean poet, Pablo Neruda, that poetry does not belong to whomever writes it, but rather it is the property of the person who needs it.

Therefore, following this dictum, I have taken the liberty of adapting Whitman's poem to try to convey the importance of complementary insights and approaches in our perception, analysis, and understanding of the atomic microcosms that surround us.

When your crystals do not grow, or, if they grow do not diffract, or, if they diffract do not get substituted, or, if they get substituted your maps are not interpretable, or if ..... etc., etc., etc., just go to the graphics room, and, in silence, contemplate any protein structure.

WHEN I HEARD THE LEARN'D CRYSTALLOGRAPHER

When I heard the learn'd crystallographer,
When the proofs, the figures, were ranged in columns before me,
When I was shown the charts and diagrams, to add, divide, and measure them,
When I sitting heard the crystallographer where he lectured with much applause in the lecture-room,
How soon unaccountable I became tired and sick,
Till rising and gliding out I wander'd off by myself,
In the mystical dim-lighted room, and from time to time,
Look'd up in perfect silence at the protein fold.

— Adapted by C.Abad-Zapatero from "Leaves of Grass" (Walt Whitman)

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