Protein Data Bank

Quarterly Newsletter

Release #80 April 1997

April 1997 CD-ROM Release

5811 Released Atomic Coordinate Entries

Molecule Type

5152	proteins, peptides, and viruses
235	protein/nucleic acid complexes
412	nucleic acids
12	carbohydrates

Experimental Technique

151	theoretical modeling
865	NMR
4795	diffraction and other

The total size of the atomic coordinate entry database is 2402 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

— Joel L. Sussman

The release in October 1996 of AutoDep, PDB's Web-based data submission system, as well as the release in February 1996 of the PDB Contents Guide, represent our major attempts at addressing data deposition and data representation problems that arose starting in the late 1980's as a result of the rapid increase in the number of data entries being deposited at the PDB. Although these products are now contributing significantly to our efforts to improve our operations, the amount of work and resources that were needed to complete these products have had a negative impact on our data production schedule. It took two years of PDB staff involvement, along with a great deal of interaction with the scientific community, to complete these projects. The average time from data deposition to release climbed from about ninety days to almost two hundred days by the fall of 1996. We are pleased to announce that we now have been able to reduce this time to approximately one hundred days, and we are now in the process of testing new procedures that are expected to further reduce the turn-around time.

AutoDep, the Web-based data submission tool developed by the PDB, was made available on the WWW on October 15, 1996 and by March 30, 1997 we had received 441depositions using this program. The number of users that login to AutoDep is increasing significantly. Our experience in processing entries submitted with AutoDep shows them to be more complete, to be of very high quality, and, concurrently, to require less staff time to process. Following are highlights of the system:

- The ability to automatically populate the required tokens from an existing PDB entry or from a previous deposition. AutoDep enters data from the designated file to the appropriate fields in the new deposition. The author merely has to update fields to reflect the new structure. Internally, all data are stored in CIF using PDB's AutoDep dictionary.
- X-ray structural refinement software is available to write PDB records that may be automatically merged into AutoDep. We worked closely with the authors of X-PLOR and SHELX-96, so that the latest versions of these programs now write refinement details as PDB records which are read directly by AutoDep and entered in the relevant sections. We are working with authors of other programs that are used during various stages of the entire structure determination process, and we anticipate that increasing numbers of programs will be integrated with the PDB deposition process.
- An extensive help facility is available, with links to related documentation and useful URLs to support the author during the AutoDep session.
- The resultant header portion of the PDB file may be previewed during the AutoDep session to check progress.

- The AutoDep session may be interrupted and resumed hours, days, or even weeks later. The session ID number and password are required to continue with the same deposition.
- When all required fields are completed, the author pushes the submit button that initiates a syntax check of the coordinates. If it fails, the depositor is asked by AutoDep to correct the problem and resubmit the coordinates. If it passes, the depositor is immediately sent an acknowledgment letter containing the PDB ID code, and the entry enters the PDB processing flow.

We are currently completing a major revision of AutoDep, which should be ready for release shortly. It includes a greatly simplified user interface as well as a much easier way to upload files to the PDB. It also permits a user to PreCheck a structure (with or without actually submitting it) using the PDB validation tools. These tools include those developed at the PDB as well as the verification program WHAT_CHECK, developed by Hooft and Vriend and explained in detail in a following article.

For additional information pertaining to AutoDep, please refer to articles in previous PDB Quarterly Newsletters — July 1996, October 1996, and January 1997 — which may be found at http://www.pdb.bnl.gov/newsletter.html.

Archive Management

— Nancy Manning

— Full Tables to be Eliminated

The current PDB contains approximately six thousand structural entries. Due to the large size and inherent complexity of the archives, the PDB provides several searching and browsing tools for finding specific entries of interest (see the following section). In light of changing practices and increasingly sophisticated searching and indexing tools, the PDB plans to eliminate the printed Full Tables.

Electronic indexing now allows quick and easy searching, whereas ordering the entries for a printed list is becoming more and more problematic. For instance, should all viruses continue to be listed with the V's? Should p-hydroxy benzoate hydroxylase be with the P's or the H's, and should alpha-thrombin be listed with the A's or the T's? How should hundreds of DNA structures be sorted? What served us well when the database contained a few hundred entries doesn't function as well now that there are several thousand.

There are many powerful tools available for searching the contents of the PDB. The next section gives details on those provided by the PDB. Elimination of the Full Tables will allow us to better utilize our resources while continuing to serve our users' needs.

— Searching the Archives

The PDB may be easily searched using tools we provide on the World Wide Web and the PDB CD-ROM, as well as on our FTP server. To quickly and easily search the PDB on the Web, go from the Home Page at http://www.pdb.bnl.gov to the "Searching and Browsing the PDB" page. Several options are available there, including:

- **3DB Browser** — The PDB Browser allows the user to rapidly search through the contents of the entire PDB archives for entries obeying certain constraints. A full-text search may be made for any string appearing in the text of a PDB entry, excluding the coordinate records. Many specific fields may be searched for regular expressions or numerical limits. You may further choose to constrain your search to entries with a particular type of annotation or associated file — stating concurrently whether all should be present or at least one of them be present. The result of this selection will be ANDed with all other fields (like "PDB ID" or "Full text query") that you choose.

  Report options include the asymmetric unit as found in the PDB entry as header only, header with coordinates, and in mmCIF format [1], as well as the generated full biological unit when available.

  Extensions to the 3DB Browser are being written to allow heterogen group searching with links to the HET Dictionary and CHIME display of the HET group.

  Visualization of each hit may be done using RasMol [2], and, if other graphical annotations have been provided, they may also be accessed. Hot links are provided to other resources on the Web that contain information on the selected structure.

  The 3DB Browser gives you the option of saving object sets resulting from queries. The saved set may be used as a starting point for further database operations or as a reference for your work. Every saved set includes the date of the search and the query from which it was generated.

- **PDB's WWW Browser** — This WWW Browser [3] also allows the user to quickly search the contents of the PDB archives for entries obeying certain constraints. Some of these constraints are regular expressions, while others are numerical limits. Once the constraints are set, the user may choose to view the results in a number of different ways. When the search has been concluded, one may display any entry in the archive — either as a document or as a manipulatable image using the public domain program RasMol.

  This browser has some unique features making it useful for certain queries.

  PDB's WWW Browser may be installed locally. The program and associated files may be accessed from our anonymous FTP server (ftp.pdb.bnl.gov), in the directory pub/pdb_software/WWWBrowse.

- **PDB UNIX Browse** — This browser, which looks and acts similarly to the WWW Browser, may also be installed locally to run over an FTP server. The perl scripts have a GUI (graphical user interface) front end that will work on any workstation with X, Tcl, and Tk. The program and associated files may be accessed from our anonymous FTP server, in the directory pub/pdb_software/Browse.
- **PDB-Shell** — This is a FOXPRO-based browser for use on an IBM PC or compatible machine. The program and associated files may be accessed from our anonymous FTP server, in the directory pub/pdb_software/pdbshell, and are also distributed on the PDB CD-ROM.

- **Search of the Pending/Waiting/Holding List** —This is a keyword search of all entries being processed at the PDB. The entry description, author list, current status, deposition date, and hold-release date are provided. This list is updated daily.

- **SWISS-3DIMAGE** — This is a database of annotated 3D images. SWISS-3DIMAGE [3] strives to provide high quality pictures of biological macromolecules with known three-dimensional structures. The database contains primarily images of experimentally-elucidated structures, but also provides views of well-accepted theoretical protein models. The images are provided in several formats, and both mono and stereo pictures are generally available.

- **Archive of Obsolete PDB Entries** — This is a joint initiative of the San Diego Supercomputer Center and the PDB. This Web Site (http://www.sdsc.edu/PDBobsolete) may be used to locate obsolete entries from the PDB. Full text keyword searches and searches for PDB ID codes are supported. The summarizer used for the indexing system has been designed to be expandable to allow more powerful query capabilities to be added in the future. For further information, see the article pertaining to this in our January 1997 Quarterly Newsletter.

Other useful files for searching the PDB are provided on the "Searching and Browsing the PDB" page at the PDB Web Site. They are:

- List of the pending and waiting entries.
- List of the entries on hold.
- Indexed lists of released entries.
- HET Group Dictionary.
- Indexed list with links to the prepared biological molecules.
- List of molecule types for all released entries.
- List of all molecular sequences contained in the current PDB archives in FASTA format.

There are also many other Web sites and outside programs available for searching the PDB. For instance, see a following article on WPDB by I. Shindyalov and P. Bourne. WPDB is a combined 3-D macromolecular structure database and query tool, available for Windows 3.1, Windows95, and Windows NT platforms. Our January 1997 Quarterly Newsletter contains articles on PDBsum, which gives summaries and structural analyses of PDB data files (R.A. Laskowski, E.G. Hutchinson, A. Michie, A.C. Wallace, and J.M. Thornton), and on PDBCONS, a searcher and browser for the PDB, designed to run with PCs on a DOS platform, developed at the Bioinformatics Centre, School of Biotechnology, Madurai Kamaraj University, India.

Several other starting points for searching the PDB are available from the PDB Home Page by accessing the "Molecular Biology Servers/Databases/Web Sites of Interest" page.

E-mail comments on searching the archives as well as other questions and comments are welcome and should be sent to the PDB Help Desk at pdbhelp@bnl.gov.

1. H.J. Bernstein, F.C. Bernstein, and P.E. Bourne, CIF Applications. pdb2cif: Translating PDB Entries into mmCIF Format, *J. Appl. Crystallogr.*, submitted.

2. Sayle and E.J. Milner-White, RasMol: Biomolecular Graphics for All, *Trends in Biochemical Sciences* **20**, 374-376 (1995).

3. M.C. Peitsch, D.R. Stampf, T.N.C. Wells, and J.L. Sussman, The Swiss-3DImage Collection and PDB-Browser on the World-Wide Web, *Trends in Biochemical Sciences* **20**, 82-84 (1995).

4. 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).

Staff Changes

— Pam Esposito

In January 1997, Dr. Otto Ritter joined the PDB as Head of Informatics. Otto, whose background is in mathematics and molecular biology, has spent most of the last seven years involved in biocomputing — developing theoretical models and practical information management systems (primarily for human genome data) at the German Cancer Research Center (DKFZ) in Heidelberg. Please see the following article in which Otto summarizes his plans for PDB Informatics.

Minette Cummings has left the PDB to move to upstate New York where her husband, John, will be a postdoctoral researcher at Rensselaer Polytechnic Institute — they are also awaiting the exciting arrival of their first child. In her four years with the PDB, Minette has filled many valuable roles. Most recently, some of her responsibilities included receiving and tracking all incoming data and dealing with authors throughout the submission and processing procedure; corresponding with the general public in response to their varied questions; and coordinating PDB's batch quality-control checks, where all entries about to be released undergo final review procedures. We sincerely wish Minette, John, and their child much happiness and success in the future.

Christine Metz, who had been handling the Help Desk as well as preparing newly submitted entries for validation since joining the PDB in January 1996, has taken over Minette's responsibilities — we are very confident that work in this area will continue to run smoothly. Christine also attends Stony Brook University and is completing her Bachelor of Science degree in environmental chemistry.

Also joining the PDB this January was Michael J. Miley, a Stony Brook University student, currently working on his senior research project at Brookhaven which involves structure-activity relationships between HIV protease inhibitors and the HIV-I protease. Upon graduation with a Bachelor of Science degree in pharmacology, Michael hopes to attend graduate school to earn a Ph.D. in pharmacology with an emphasis on computer-based rational drug design and begin a career in the pharmaceutical industry.

Plans for PDB Informatics

— Otto Ritter

Since joining the PDB in January, I have been working with the Group to develop a conceptual model of the whole PDB enterprise to include all aspects of the resource. My objectives in regard to this are twofold:

- First, there is a plan to reengineer the current computing infrastructure and optimize informatics support for data processing and associated activities. This will be comprised of upgrades to hardware and generic software platforms; deployment of modern database and work-flow management systems; and, most significantly, the remodeling, documentation, and optimization of the PDB-specific processes and individual software components. This reengineering is intended to make current PDB editing and archiving processes more efficient and meticulous with respect to a comprehensive definition of exactly what it should or shouldn't be doing.
- The second plan relates to work on PDB's future as a comprehensive, knowledgeable resource of macromolecular structures, in pace with the growing volume and complexity of deposited data. This resource would address the new and demanding content and functionality requirements of the scientific community, would offer a rich selection of services to a variety of specific user communities, and would be aware of — and, where possible, interoperable with — other related biomedical information resources on the Internet. Work on the "next generation" PDB will be carried out in synergetic collaboration with the European Bioinformatics Institute (EBI); the European IGD - Genome Information System project; and, hopefully, with the help of users' suggestions, feedback, criticism, and/or direct participation.

As informatics plans develop and are implemented, details will be forthcoming in future Newsletter articles.

WHAT_CHECK: Verify a Protein Structure Before Submission

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Proteins are the marvels of nature that, in our bodies, are responsible for all the work, construction, energy, metabolism, and even our creative forces. On the other hand, the construction plan for these molecules is so complicated that we are not even approaching the first understanding of it. Protein structures are art.

Due to protein structures being too complex for the human mind to grasp, it is all too easy to oversee a small mistake upon model building. Modern refinement programs like X-PLOR are much more sophisticated than the software available ten years ago, and, combined with faster computers, this means a much larger radius of convergence. However, refinement programs have not gotten much smarter over the last ten years; no high-level knowledge about protein structures has been added to the standard refinement protocols. Programs still do not know what to do with a small mistake made by a human being under great time pressure, e.g., by wrongly positioning a side-chain in what looks like residual density. Current programs will just refine the molecule to the "nearest reasonable conformation" using only the low-level knowledge they have — atoms described as balls that have bonded and non-bonded contacts. The "nearest reasonable conformation" may have a very reasonable energy based on these low-level evaluations, but still represents a lousy protein conformation.

This is where verification of a protein structure using WHAT_CHECK comes in. WHAT_CHECK combines high-level information from published protein structures as well as from small-molecule crystal structures to present an evaluation of a protein structure that is independent of the refinement procedure. This allows many small "not so important at the moment" mistakes to be found and corrected quickly. After all, a small mistake at one position in a structure reduces the accuracy of all atomic coordinates.

WHAT_CHECK will:

- Verify completeness and consistency of information on symmetry cards.
- Verify simple geometry — bond lengths, bond angles, and chirality.
- Compare "identical" molecules in the asymmetric unit.
- Study side-chain planarity, and puckering of proline rings.
- Verify plausibility of B-factor distributions.
- Study ϕ, ψ torsions, ω torsions, and χ torsions.
- Make an inside/outside preference profile, and see if it looks normal.
- Look for forbidden van der Waals collisions between atoms.
- Calculate a threading potential to judge the chain fold.
- Perform extensive mid-range backbone conformation checks.
- Look for peptide flips.
- Verify positions of water molecules.
- Check histidine-type assignments as well as histidine, asparagine, and glutamine side-chain conformations using a sophisticated hydrogen-bond analysis.

Examples of the kind of problems that may be located using WHAT_CHECK (taken from actual PDB structures) are given in two illustrations which are available from EMBL at http://www.sander.embl-heidelberg.de/rob/pdb-newsletter/ and from PDB at http://www.pdb.bnl.gov/newsletter.html. The first illustration shows two threonine residues from the same protein, one of them having the wrong side-chain chirality. The second illustration shows a superposition of parts of two C-alpha traces of two identical molecules, where one of the two has most probably been modeled incorrectly — the average threading Z-scores for the stretches indicated by thick lines are -1.45 (green) and -2.44 (red), respectively. Although these are only two examples out of a long list of possible anomalies that may be detected, they clearly indicate that WHAT_CHECK may be helpful to the crystallographer at many stages during the structure solution process.

WHAT_CHECK is available from both the EMBL home page at ftp://swift.embl-heidelberg.de/whatcheck/ and the PDB home page at http://www.pdb.bnl.gov/software.html. We are currently producing a complete explanation to the WHAT_CHECK output, found at http://www.sander.embl-heidelberg.de/rob/checkhelp/, which should be very useful to first-time users.

Journals Coordinate Deposition Policy: Enforcement and How Users Can Help

Kurt Giles, Departments of Structural Biology and Neurobiology, Weizmann Institute of Science, Rehovot, Israel (kurt@sgjs4.weizmann.ac.il).

The usefulness of ensuring macromolecular coordinate deposition [1, 2] is hopefully something I don't need to preach to readers of the PDB Quarterly Newsletter. This sentiment is fortunately shared by nearly all journals, and coordinate deposition is a requirement for publication. Regrettably, the vague wording and enforcement of policies vary significantly between journals.

After discovering a 1996 article in *Nature* without any reference to the availability of the coordinate data, I contacted the journal to remind them of their recent change in policy — requiring data to be made freely available [3]. I was doubtful of my ability to have any influence, but, to my pleasant surprise, ten days later the coordinates were received by the PDB. However, similar letters to *Nature* and other journals are not always so productive (A. Wlodawer, personal communication).

One of the reasons the omission of a PDB ID code is overlooked may be its usual relegation to a footnote buried somewhere near the end of the references. The recent suggestion in *Nature Structural Biology* to publish PDB ID codes "in a prominent position in the front of the journal" (editorial note to [2]) is warmly welcomed. Other journals, especially those dealing mainly with macromolecular structures, should be encouraged to follow suit.

Just as producing an article without figures to help explain the findings would seem absurd, explaining a three-dimensional concept without the ability to view it as such greatly diminishes comprehension. Thanks to the invention of AutoDep, PDB ID codes are issued almost immediately for automated depositions. Authors should be encouraged to put PDB ID codes in a prominent position in the paper, encouraging readers to simultaneously view the structure. In addition, papers describing analyses of structures, or any other mention of a structure, should be accompanied by the relevant PDB ID codes. Encouraging literature abstracting services to include these codes will greatly enhance the ability to automatically search related references.

The easiest way to check if data has been submitted to the PDB is to use the 3DB Browser at Brookhaven [4]; this will check both released data and the pending/waiting list data (PDB mirror sites are, by their nature, slightly behind the original, and may not contain the most recently submitted data). On identifying a published but not deposited structure, I believe it is better to contact the journal rather than the authors — making journals enforce their policy will remind them of their obligations. The omission should also be pointed out to other users, for example, through the pdb-l mailing list [5]. If an editor receives multiple complaints then he or she is more likely to act. Reviewers of manuscripts have an additional responsibility to ensure data has been submitted, and those on editorial boards should pay particular attention to their journal's policy and its enforcement.

1. E.N. Baker, T.L. Blundell, M. Vijayan, E. Dodson, G. Dodson, G.I. Gilliland, and J.L. Sussman, *Nature* **379**, 202 (1996).
2. A. Wlodawer, *Nat. Struc. Biol.* **4**, 173-174 (1997).
3. Editorial opinion, *Nature* **379**, 191 (1996).
4. 3DB Browser URL: http://www.pdb.bnl.gov/cgi-bin/pdbmain.
5. PDB Listserver URL: http://www.pdb.bnl.gov/pdb-l.html.

WPDB v2.2

Ilya Shindyalov, San Diego Supercomputer Center, San Diego CA, USA and Philip Bourne, San Diego Supercomputer Center and Department of Pharmacology, University of California, San Diego CA, USA (http://www.sdsc.edu; bourne@sdsc.edu).

WPDB is a combined 3-D macromolecular structure database and query tool for the analysis of a single structure or for comparative analysis of multiple structures. It is available for Windows 3.1, Windows95, and Windows NT platforms. It runs on any Intel 386 processor or higher. An earlier version was described in I. Shindyalov and P. Bourne, *J. App. Cryst.* **28(6)**, 847-852 (1995). The current version has an improved 3-D rendering tool. All display windows interoperate so that selecting a feature, e.g., a region of polypeptide chain, in one display window will display that feature in all open windows. This capability facilitates an intuitive mode of operation.

Some typical applications of WPDB are:

- Analysis of protein-protein and protein-ligand interactions.
- Analysis of internal interactions in proteins to reveal different folds (e.g., helix-helix hydrophobic stacking).
- Analysis of sequence-structure correlations using a sequence search and static property profiles.
- As above with sequence homology [S.B. Needleman and C.D. Wunsch, *Mol. Biol.* **48(3)**, 443-453 (1970)] and structure superposition (least-squares minimization of differences in C-alpha positions).
- Analysis of thermal motion profiles.
- Secondary structure calculation according to the method of W. Kabsch and C. Sander [*Biopolymers* **22**, 2577-2637 (1983)].
- Analysis of exposure based on the method of B. Lee and F.M. Richards [*J. Mol. Biol.* **55**, 379-400 (1971)].
- Locate structures based on string searches of combinations of PDB record types and/or sequence patterns and resolution ranges.
- Basic molecular rendering.

Specific examples are given on the Web pages.

Databases of one hundred random structures (2 MB) for testing purposes, unique structures according to U. Hobohm and C. Sander [*Protein Sci.* **3(3)**, 522-524 (1994)] (currently 420 structures, 9.7 MB), and the complete PDB built from the PDB's CD-ROM distribution (currently 83.5 MB for the October 1996 version) are available via the Internet. As you can see, a key feature of WPDB is the compression algorithm that is applied when building a WPDB database. A ten- to twenty-fold compression of PDB files is achieved, depending on the amount of derived information included in the database. An accompanying WPDBL program can be used to build your own database from files in PDB format.

WPDB is fully documented with a manual as well as on-line help. Manuals may be downloaded via the Internet; bound versions may be requested from *consult@sdsc.edu*. A Listserver exists to discuss issues relating to WPDB. To join the mailing list, send mail to *majordomo@sdsc.edu* with the body of the message containing the words "subscribe wpdb." Over one thousand copies of WPDB have been distributed, and feedback indicates that it is particularly useful for teaching the principles of protein structure at both undergraduate and graduate levels as well as for conducting basic research. WPDB remains an active area of development — improved search capabilities and support for 3-D glasses, similar to the Stereographics glasses found on SGI workstations, may be expected in the future. WPDB is maintained by the San Diego Supercomputer Center and may be found at http://www.sdsc.edu/pb/wpdb/wpdb.htm or ftp://ftp.sdsc.edu/pub/sdsc/biology/WPDB/.

Internet-Based Database of HIV Protease Structures

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We have created a database dedicated to providing structural information about a single enzyme — HIV protease (HIV PR)[1]. This enzyme plays a crucial role in HIV infection and has been, without doubt, the subject of structural studies involving the largest number of laboratories and resulting in the largest number of independently determined crystal structures. These studies have helped in the discovery and development of a new class of efficient AIDS drugs, four of which were recently approved by the U.S. Food and Drug Administration, with others in advanced clinical studies [2-4].

The database contains structural data for three PR variants: namely, HIV-1, HIV-2, and simian immunodeficiency virus PRs. One of the main reasons why this database is being constructed is the concern that the very success of the field may lead to the loss of relevant data. Most of the structures have been determined by pharmaceutical companies and were never published, nor were the coordinates released, despite their importance and variety. Only a fraction of the structures are publicly available, mainly through the PDB. We believe that statistical evaluation of common structural features of the inhibitor complexes of HIV PR could help efforts to create new types of ligands in improving inhibitor design strategies and also be useful in approaching new areas in the future.

The database is designed as a WWW service accessible from http://www-fbsc.ncifcrf.gov/HIVdb. The structure of the home page supports the aim of providing information in two distinct ways. The database will be the source of all available structures in a unified and fully annotated format. This part of the database, called "Informal," contains information about both the protein and the inhibitor present in the complexes of HIV PR, as well as the original sets of coordinates. The information about complexes, PRs, and inhibitors is available separately. Descriptions of the complexes, database-unique labels, PDB names, descriptions of the inhibitors, and references are in the main table which is the gateway between the more detailed information about the PRs, such as the names of viral isolates, and the data on inhibitors. The latter includes chemical formulas, two- and three-dimensional models, a more detailed description of the compounds, and conditions of the Ki measurements, if available. All of the original coordinate files have unified annotation and are stored in PDB format, which is widely used as input for molecular modeling programs. To allow visualization of the structural information contained in these files, we have included a PDB-fluent Java applet. Using a Java-enabled Web browser, such as the current version of Microsoft Internet Explorer or Netscape Navigator, one can view simplified, three-dimensional models of the enzymes. The Java applet uses an integer mathematics package and is adapted from software originally developed by Dr. Scott M. Le Grand [5]. Graphics calculations in an integer coordinate system, combined with the rendering of the large PR molecule as a backbone model, maximize efficiency and minimize the computing hardware and network bandwidth necessary for effective on-line three-dimensional modeling. Alternatively, more complex renderings are available with simple molecular graphics packages such as RasMol [6]. All of these programs are publicly available and work on many different computing platforms. For users who have no access to commercial molecular modeling software, this will be the only way to manipulate the structures in real time.

The second part of the database, "Analytical," is organized either by services giving access to various tools or by results of specific analyses, which may be viewed immediately. Some of the computationally complex calculations are run in batch mode at the National Cancer Institute's Frederick Biomedical Supercomputing Center, and the results are returned via e-mail. The Analytical part contains coordinates of the complexes transformed into a common frame of reference, as well as separate files of coordinates for the PRs, inhibitors, and water molecules. Although the database exclusively utilizes the PDB format to specify atomic coordinates, we provide conversion to approximately forty other common formats through the program Babel [7,8]. Assuming that many users will be interested in different modes of superpositioning of structures, we provide the program ProFit [9] to compute different sets of transformations, performed with the McLachlan algorithm [10]. The users may apply their own criteria of alignment of the complexes, PRs, and inhibitors. It may be observed that the known inhibitors share a strong pattern of two "rings," containing the P3, P1, and P3′, P1′ side chains, with part of the main chain of each inhibitor. An additional, less evident "ring" is also found between the P2′ and P1 side chains. On the basis of such data, one can speculate about the ideal shape of a template for the construction of potentially improved inhibitors. On the other hand, the plasticity of the binding site of HIV PR clearly makes it possible for different areas of the inhibitors to assume a variety of conformations.

As part of the analytical services, we also provide Internet access to a program that measures distances, angles, and torsion angles. The user interested in particular geometrical parameters needs only to fill out a simple form of input data, and the results will be immediately released by e-mail or written directly to the screen.

Among the different quantitative measures that characterize PR-inhibitor interactions, we paid particular attention to volume and surface calculations. We used the program Surfnet [11] to compute the surface areas and volumes of the PRs, inhibitors, and gaps between them. Such analysis can help the process of understanding the properties of binding subsites. Grid files of volumes for two of the most widely used molecular modeling programs, InsightII and SYBYL, are stored on the WWW server, and these grids may be visualized as contour surfaces. A single PostScript® image of each volume-based analysis is available for investigators who do not have either of the above-mentioned programs. Such information may be combined to derive minimal and maximal binding cavity volumes and, when combined with reasonable template structures, could be used to direct a search for novel inhibitors [12,13].

Although the database, in its current form, is composed largely of previously released structures found in the PDB, new structures may be deposited using the WWW service — depositors may supply all of the necessary information using the on-line form. The coordinates (in PDB format) may then be copied to the on-line form, or they may be sent via anonymous FTP to mars.ncifcrf.gov in the /hivpr/incoming directory. We also encourage deposition of these structures in the PDB.

We are currently planning to add the following capabilities to the database:

- To include in the Informal part certain data from computations, such as molecular dynamics and Monte Carlo simulations, as well as the results from ab initio and semi-empirical calculations.
- To include results of the simulation of solvated and unsolvated states of the inhibitors and empirical calculations of the complexes with respect to their interaction energy or to their free energy.
- To prepare more sophisticated templates for inhibitor design.
- To more fully develop the Web-accessible services and compare the database with similarly organized network services and information systems.

The database is linked to a number of other sites. One of them is the Protease Inhibitors server (IAPAC) (http://www.iapac.org/consumer/proinbk.html), which contains, almost exclusively, data about clinical trials of HIV PR inhibitors. Another link is the PROLYSIS server, dedicated to all proteases and protease inhibitors (http://delphi.phys.univ-tours.fr/Prolysis/). A particularly close two-way link was established with the PDB. It is possible to move between these two databases with ease, and the data formats are completely compatible. We anticipate that upon completion of the projects in approximately one year, the database will be transferred to PDB and will be maintained there in the future.

All software modules are in place, and full access to the database for outside users has been provided since February 1997. We hope that the availability of the database will convince the laboratories that have unpublished structures of these enzymes to make them available to the scientific community as a whole by depositing them in the manner discussed above. We also hope that the user community will suggest to us additional topics for inclusion.

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IUCr Macromolecular Crystallography School

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The International Union of Crystallography (IUCr) Macromolecular Crystallography Computing School was held at Western Washington University in Bellingham, Washington, USA on August 17 - 22, 1996. The School was the seventh in a series of IUCr Crystallographic Symposia. There were 106 attendees from 16 countries; of these, 38 were either speakers or tutors. Of the remaining 68 attendees, 29 were graduate students, 12 were postdoctoral fellows, 9 were faculty, and 18 were from industry or elsewhere.

The School covered the latest developments in macromolecular crystallographic computing — beginning with data collection and processing; continuing with phasing, model building, and refinement; and ending with visualization. There were also sessions dealing with the quantity and quality of structures being generated as well as updates of many of the common software packages being used. Finally, there were sessions on ancillary topics important to macromolecular crystallographers, for example, object-oriented programming, macromolecular CIF, and the use of the Internet. Refer to the on-line editorial, at http://www.sdsc.edu/Xtal/IUCr/CC/School96/Ed.html, for details on the speakers and specific topics.

A draft of the Proceedings were distributed to attendees, and final papers will appear in the published Proceedings. For the first time at a Computing School, the Proceedings are available electronically at http://www.sdsc.edu/Xtal/IUCr/CC/School96/ or by anonymous FTP at ftp.sdsc.edu in the /pub/sdsc/societies/IUCr/School96 directory. Individual papers may be downloaded as PostScript® files.

This is an exciting time for macromolecular crystallography because it is contributing enormously to our understanding of biological processes. This excitement was evident at the School and is now evident in the electronically available Proceedings.

Notes of a Protein Crystallographer

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— On Gold Rings and Synchrotron Rings

...Dedicated to all people working in synchrotrons...

I have written before on these lines about the technical specifications of synchrotron rings and about the immense possibilities that the power and brilliance of these third-generation sources will offer for the investigation of the atomic universes that surround us (see article in the April 1996 Newsletter). This time, I would like to take a different, more philosophical, viewpoint.

Rings are very special artifacts and icons in Western culture and most likely in many other societies also. Gold rings or rings of other precious metals, engraved and decorated with precious stones, have always been the attributes of kings, queens, and other high dignitaries. Quite often throughout history, their owners may claim special privileges of power, property, or influence in both religious and secular organizations. Additionally, they are commonly associated with material wealth and used as tokens of special liaisons, alliances, or compromises.

Among human beings, the most special, and at the same time the most common, are the agreements of engagement or marriage. Rings are exchanged between the bride (or the bride-to-be) and the groom (or the groom-to-be) as a symbol of eternal fidelity and unending love. I will only mention the “claddagh” ring in the Irish culture, a heritage from their Gaelic ancestors as a symbol of love and friendship also used as a betrothal ring. The claddagh presents a prominent heart in the middle of the ring which, by the way it is pointing, indicates whether the carrier of the ring is free or engaged to another person.

In the realm of dramatic musical arts, there is a monumental composition which unfolds around a gold ring — collectively referred to as *“The Ring”* or *“The Ring Cycle.”* I am referring to *Der Ring des Nibelungen* by Richard Wagner (1813-1883), arguably the most massive, complex, and expressive dramatic music of the Western culture. In its final form, *The Ring Cycle* consists of the introduction (a major opera) *Das Rheingold* (The Gold of the Rhine), followed by three complete operas entitled: Die Walküre, Siegfried, and Götterdämmerung (The Valkyrie, Siegfried, and The Twilight of the Gods). *The Ring* represents the culmination of the complete work of art (“Gesamtkunstwerk”) conceived by Richard Wagner as the perfect enmeshing of music, words, and action. This composition is arguably the most ambitious, most complex, and most expressive of the musical drama.

The text (I would not dare to call it libretto) of *The Cycle* originates from the research that Wagner did on the mythology and Sagas of the Teutonic and Norse cultures that he sketched circa 1849. The most important characters are a god (Wotan) and a goddess (Fricka) who would like to live in a magnificent and impregnable palace in heaven (Valhalla); a hero (Siegfried); a disobedient heroine (Brünnhilde) who turns into a sleeping princess atop a fire-girth rock; villainous, shrew dwarfs (Alberich and Mime) who anneal the magic *Ring* and forge a magic helm (Tarnhelm); and strong, brutish giants (Fafner and Fasolt) who agree to build Wotan’s fortress in exchange for Freia (the goddess of beauty), and one of which later transforms into a dragon to guard the gold of the Rhine.

From the first literary sketches to the time that the last note was written, it took twenty-six years to complete *The Ring Cycle*. This includes a long pause of twelve years during which Wagner broke off the composition of *The Ring* (in the middle of Act II of Siegfried) and concentrated on *Tristan und Isolde* and *Die Meistersinger*. When *The Ring* was resumed in 1869 and completed in 1874, Wagner had evolved considerably, both musically and philosophically, and the work did not have the concise logic that guided its original gestation. In addition, Wagner had written to his imprisoned revolutionary friend, August Röckel, of the 1849 Dresden [1] uprising:

> *“I believe that it was a true instinct that led me to guard against excessive eagerness to make things plain, for I have learned to feel that to make one’s intentions too obvious risks impairing the proper understanding of the work in question; in drama — as in any work of art — it is a question of making an impression, not by parading one’s opinions, but by setting forth what is instinctive.”*

All these factors compound to make the full, complete, logical understanding of *The Ring* almost impossible, and certainly beyond the scope of these lines. The first complete public performance of *The Ring* took place in Bayreuth, directed by Hans Richter in August 1876, a quarter of a century after it was first conceived. Overall, we can take *The Ring* tetralogy as an allegory and a conspectus of human relations and society — possibly also, as a testament of a disillusioned would-be reformer [2].

Yet, what is *The Ring* about? In spite of the disagreements concerning the meaning of *The Ring*, most people will agree that it is about the conflict between love and power. In the opening scene of *Das Rheingold*, Wellgunde, one of the Rhinemaids, says:

> *“The inheritance of the world would be won by him who made The Ring from the Rhinegold, it would vouchsafe him limitless power.”*

This was followed immediately by the chilling strings and the announcement by Woglinde, the other Rhinemaid:

> *"Only he who forswears love...."*

Immediately after, the chief villain, Alberich, tears the gold from the rock, renounces love as a prerequisite to the power and possession of *The Ring*, and henceforth gets the action of the entire drama underway. The tension increases when Alberich, dispossessed of the gold of the Rhine, *The Ring* that he was able to craft from it, and the magic helmet by Wotan, curses *The Ring* to be the cause of death to whoever owns it. What Wagner means or implies by love during the duration of *The Ring Cycle* changes; yet, from a simple viewpoint, it seems as if Wotan and Alberich provide the essential dynamic force of the drama by renouncing love for power. In fact, Wotan, this very human god, says to Brünnhilde at the beginning of his monologue in Act II of *Die Walküre:*

> *"When the joy of young love departed from me, my spirit longed for power."*

Back then to synchrotron rings. We have amassed the "gold of the Rhine" and from it we have built not one, but many synchrotron rings around the earth. These rings have given us a tremendous amount of power to pierce and penetrate matter and to uncover many of its well-hidden secrets. We can probe the material universe at the atomic level for the animate and inanimate domain. We have gathered, and we will continue to gather, enormous amounts of data which will translate into new forms of knowledge. We know ... knowledge is power. Do we have to renounce love and beauty? The answer should be a resounding "No!"

We should continue to illuminate our samples with evermost brilliant sources of radiation and use all possible ranges of the electromagnetic spectrum as well as all possible experimental configurations. However, we should also retain the admiration and awe for the cosmos around us. We must convey a sense of beauty for what we discover and respect for the "mysteries" that are still the undiscovered facets of this multisided microcosm. We should consider our new structures, not as climbing rungs in our career ladders, but as prodigious pebbles — precious jewels — that we have been fortunate enough to unveil and privileged enough to present to humankind. We have to retain the joy and enthusiasm of young love toward the puzzles that still have to be discovered within the current paradigms of science. In addition, we should cultivate an insatiable thirst for the "unknown unknowns" [3] that exist both inside ourselves and outside in our surrounding universes. Only in this way will the immense power of our Synchrotron Rings not destroy us.

An illustration which appeared on the invitation card to the dedication of the Advanced Photon Source on May 1, 1996 is available from PDB's Home Page. It was this representation of the APS ring that inspired this article. The illustration is a courtesy of Argonne National Laboratory, Susan H. Barr, 9700 South Cass Avenue, Argonne, IL 60439-4800. ■

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OPM (Object-Protocol Model) Data Management Tools .... gizmo.lbl.gov/DM_TOOLS/OPM/OPM.html
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Squid: Analysis and Display of Data from Crystallography and Molecular Dynamics www.yorvic.york.ac.uk/%7Eoldfield/squid/
VMD - Visual Molecular Dynamics .... www.ks.uiuc.edu/Research/vmd/
X-PLOR Home Page .... xplor.csb.yale.edu/

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--> Check payable to Brookhaven National Laboratory in US dollars and drawn on a US bank. Foreign checks cannot be accepted and will be returned.

--> Original purchase order payable to Brookhaven National Laboratory. After your order is processed, you will be invoiced by Brookhaven National Laboratory. Please indicate exact address to which invoice should be sent:

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A wire transfer is acceptable only ***AFTER*** we have received an original purchase order from your organization and you have been invoiced by Brookhaven. After receiving Brookhaven's invoice, your bank may send a wire transfer to:

Bank name : Morgan Guaranty Trust Company of New York
Account name : Brookhaven National Laboratory
Account number : 076-51-912

Please send all required items together *via* postal mail to:

Protein Data Bank Orders
Biology Department, Building 463
Brookhaven National Laboratory
P.O. Box 5000
Upton, NY 11973-5000

1 Protein Data Bank CD-ROM Set — ISO 9660 Format *$357.25*

(tax and shipping charges not applicable)

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STATEMENT OF SUPPORT

The PDB is supported by a combination of Federal Government Agency funds (work supported by the U.S. National Science Foundation; the U.S. Public Health Service, National Institutes of Health, National Center for Research Resources, National Institute of General Medical Sciences, and National Library of Medicine; and the U.S. Department of Energy under contract DE-AC02-76CH00016) and user fees.

ACCESS TO THE PDB

Main Telephone	1 516-344-3629
Help Desk Telephone	1 516-344-6356
Fax	1 516-344-5751
Help Desk	pdbhelp@bnl.gov
General Correspondence	pdb@bnl.gov
WWW Home Page	http://www.pdb.bnl.gov
FTP Server	ftp.pdb.bnl.gov
Network Services	sysadmin@pdb.pdb.bnl.gov
Entry Error Reports	errata@pdb.pdb.bnl.gov
Order Information	orders@pdb.pdb.bnl.gov
User Group	PDBusrgrp@suna.biochem.duke.edu
Listserver Postings	pdb-l@pdb.pdb.bnl.gov
Listserver Subscriptions	listserv@pdb.pdb.bnl.gov
to subscribe, the text of your message should be	subscribe PDB-L Your Name

FTP DIRECTORY STRUCTURE FOR ENTRIES

The PDB has updated the FTP server (ftp.pdb.bnl.gov) in order to have a more standardized directory structure. This will facilitate use of mirror software to keep local copies of the database current. Links have been put in so the server still “looks” the same to users.

Entry files are now found under the directory pub/pdb/.

all_entries/	coordinate entry files in compressed and uncompressed format
biological_units/	generated coordinates for the biomolecules
current_release/	current database, with entries removed or added since the last CD-ROM
fullrelease/	static copy of the database as found on the last CD-ROM
latest_update/	entries added or removed in the most recent FTP update
newly_released/	entries released since the last CD-ROM
nmr_restraints/	compressed NMR restraint files
obsolete_entries/	withdrawn and/or replaced entries
structure_factors/	compressed structure factor files

fullrelease, newly_released, and current_release are divided into multiple subdirectories.

Protein Data Bank
Biology Department, Bldg. 463
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(516) 344-3629

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