PDB NEWSLETTER

Number 3 ◆ FALL 1999 ◆ RCSB

Published quarterly by the Research Collaboratory for Structural Bioinformatics

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RCSB

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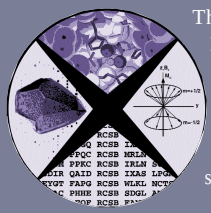

The Research Collaboratory for Structural Bioinformatics (RCSB) is a non-profit consortium dedicated to improving our understanding of the function of biological systems through a study of 3-D biological macromolecular structure.

Message from the RCSB

June 30, 1999, was the day that the address **http://www.rcsb.org/** became the single home of the Protein Data Bank. All queries to the old BNL-PDB are being redirected to the new site. This final step marked the end of the transition period that began in October 1998, for the RCSB to assume responsibility for the PDB. During this time, features of the RCSB-PDB were introduced as the BNL-PDB was phased out. The ultimate goal of the transition period was to make these changes as seamless as possible.

What did this entail? It meant introducing a new deposition tool while not abruptly discontinuing the older one. The AutoDep Input Tool (ADIT: **http://pdb.rutgers.edu/adit/**) was introduced by the RCSB in April and has been extensively utilized. AutoDep was kept online at BNL and EBI, with the data deposited after January 26, 1999, successfully processed to completion by the RCSB staff. To ensure that depositors were not adversely affected by the BNL closing, the RCSB ported a version of AutoDep and the current BNL AutoDep sessions to its site.

The transition also meant coordinating with the BNL team, who continued to process structures in the queue as of January 26, 1999. Every Monday, the two sets of structures and updated status information were combined and sent to SDSC for distribution.

At SDSC, the distribution team uploaded the data into the database and into two FTP servers. Again, the RCSB team has attempted to minimize the disruption to the community. The original BNL-style FTP archive is maintained at **ftp://bnlarchive.rcsb.org/** and a new and simpler RCSB-style ftp archive is available at **ftp://ftp.rcsb.org/**.

The past few months have also found the RCSB staff cataloging the PDB paper files and magnetic media that have been stored at BNL since 1971. These data have been moved to NIST where the master archive is maintained.

Most importantly, the transition period was a time for the RCSB to tell the community what we were doing via e-mail lists, newsletters, meetings, and workshops. Our goal was to eliminate any possible surprises and to keep open the lines of communication. To this end, we have changed the PDB network address so that all PDB traffic is sent to the RCSB.

None of this could have been accomplished without the dedication of the project teams and the institutional support at the RCSB sites — Rutgers, SDSC, and NIST. We are indebted to the countless conversations and e-mails from the members of the community offering suggestions, advice, and questions. We are especially appreciative of the efforts of our beta testers, the PDB Advisory Board, Herb and Frances Bernstein, and the dedicated efforts of the agencies that fund the PDB: the NSF, NIH, and DOE. Finally, the transition would not have been complete without the BNL group under the direction of Joel Sussman, who worked until the last day to make sure the PDB would endure as

the single archive of macromolecular structures. Special thanks also go to Regina Shea and John McCarthy for their contributions.

We look forward to working with you in the years to come, and will welcome your input to help maintain the integrity of the resource and to make it a vital and enabling technology for biology.

The RCSB Project Leaders
Helen M. Berman
Phil Bourne
Gary Gilliland
John Westbrook
Peter Arzberger
Phoebe Fagan ✦

PDB at IUCr Meeting

XVIII International Union of Crystallography Congress and General Assembly

It was a wonderful experience for those of us in the RCSB to meet the PDB users who attended IUCr Congress and General Assembly in Glasgow, Scotland, this year.

Our PDB booth in the Exhibition Hall allowed us to meet those of you whom we have known by e-mail and structure only! In addition, this was a great opportunity to get all kinds of feedback from the community — we greatly appreciate your comments. It was also a pleasure to have an opportunity to distribute our CD-ROMs, as well as our PDB mugs and pencils.

Thanks to everyone who attended the PDB Users Meeting on August 7, 1999.

This meeting was a major highlight of our continuing conversations with the PDB user community. We look forward to discussing these issues further in the next few months at meetings and on the listserv, and towards the PDB developments that will result. Watch the PDB News section on the Web site for updates.

We hope to meet you all again at future conferences. ◇

Data Deposition and Processing Update

Data deposited at the RCSB PDB is fully processed within a few days of deposition. The data is deposited via the following channels:

ADIT, the AutoDep Input Tool (http://pdb.rutgers.edu/adit/)

ADIT was developed by the RCSB to make structure deposition simple and easy. ADIT allows the user to check the format of coordinate and structure factor files and to perform a variety of validation tests on a structure prior to deposition in the database. These checks can be done without intervention by the database staff.

RCSB Leadership Team left to right: Gary Gilliand (National Institute of Standards and Technology), John Westbrook (Rutgers University), Helen Berman (Rutgers University), Phil Bourne (San Diego Supercomputer Center), Phoebe Fagan (National Institute of Standards and Technology), Peter Arzberger (San Diego Supercomputer Center)

To deposit a structure, the user uploads the relevant coordinate and structure factor files, and then usiing ADIT, adds any additional information to the submission.

RCSB AutoDep

Deposition sessions that were started using the BNL AutoDep have been moved over to the RCSB site. These sessions (those with restart IDs similar to "BNL-XXXXXX") can be completed using the RCSB's copy of AutoDep at **http://pdb.rutgers.edu/~adbnl/**.

EBI AutoDep

The EBI AutoDep will continue to be available at **http://autodep.ebi.ac.uk/**. Structures deposited using the EBI AutoDep from June 15, 1999, onwards are processed by the EBI and, after consolidation with other recent depositions, are released in the PDB archive. ✦

PDB Change Advisory Notices

Introduction to Structure Checking by the RCSB

Modifications to established PDB services will be implemented after community review. PDB Advisory Notices are sent out as a means of communicating and refining any changes to the PDB.

These Advisory Notices will be posted on the PDB listserv at least 60 days before any modification is implemented. During a period of public review, we will collect the recommendations and revisions received about the initial notice. A final announcement will be made on the listserv before the change is made.

On July 9, 1999, the RCSB posted its first PDB Change Advisory, which is summarized below. For the full announcement, please see **http://www.rcsb.org/pdb/lists/pdb-l/199907/msg00013.html.**

Synopsisof PDB Change Advisory Notice (#19990709)

The PDB is fully committed to providing and maintaining the current PDB format in as standard a manner possible; however, as with any standard, there is the occasional need for clarification and amendment. We hope that the changes proposed in this Advisory Notice will be reviewed in the spirit for which they are intended — small changes to an existing mature standard format.

Summary of Proposed Changes:

In short, the changes proposed are:

1. Raise the criteria used in REMARK 500 to flag bond distance and bond angle outliers.
2. Provide improved descriptions for biological assemblies.
3. Standardize the protein hydrogen atom nomenclature following IUPAC recommendations.
4. Permit single PDB ID assignment for NMR ensembles.
5. Provide support for new experimental techniques.
6. Simplify/clarify the specification of macromolecule content within COMPND records.
7. Add new identifying codes for common entry revisions.
8. Obsolete the coden publication identifier.
9. Remove the SEGID field from ATOM, HETATM, SIGUIJ, SIGATM and ANISOU records in the archival format.

The changes proposed here are primarily content changes. Only item 2 above involves a change in the column layout of the PDB file. The remainder of this document provides complete descriptions of each of the proposed changes.

(For a complete description of PDB Change Advisory Notice [#19990709], see **http://www.rcsb.org/pdb/lists/pdb-l/199907/msg00013.html.**) ✦

Status of PDB WWW Mirrors

RCSB PDB Mirrors

In addition to the existing RCSB mirrors at Rutgers and NIST, over the past few months the RCSB PDB has been working to establish a world-wide set of mirrors. Our immediate focus is to establish a relatively small number of mirror sites at strategic locations around the globe.

The first set of WWW mirrors will include sites in Brazil (Universidade Federal de Minas Gerais), Singapore (BioInformatics Centre, NUS), United Kingdom (Cambridge Crystallographic Data Center) and Japan (Institute for Protein Research, Osaka University). Most of these sites are now partially or fully established and are in the final stages of testing before their web site addresses are made accessible to the PDB user community. Notification to the community as to when these sites are publicly available will be made on the PDB web site and PDB discussion list.

Our current expectation is that it will not be necessary to provide as many RCSB PDB WWW mirrors as BNL PDB WWW mirrors in order to achieve good PDB access in all parts of the world. The situation will be evaluated once this first tier of mirrors is fully established and operating in a routine manner.

BNL PDB Mirrors

Prior to the shutdown of Brookhaven National Laboratory on June 30, 1999, all the official BNL PDB mirror sites were notified that the RCSB would provide the means for them to continue their key activities as (a) repositories of the PDB entries and (b) providers of query capability.

To facilitate the continuation of these services, these sites were provided with information on accessing the RCSB maintained copy of the FTP archive (**ftp://bnlarchive.rcsb.org/**) with the same structure as BNL's PDB FTP archive. Access to this archive allows these sites to continue to update their structure entries with only minimal changes to their mirroring scripts. In addition, these sites were provided with a static Web page to launch the 3DB/PDBLite and to link to RCSB resources.

The RCSB's intention in this process was to provide the BNL PDB's mirrors with a simple path, requiring minimal ongoing effort to continued operation.

Of the 17 official BNL PDB web site mirrors, 11 sites changed their PDB home pages to the page supplied by the RCSB, and most of these sites have been updating their structure holdings on a weekly basis. All but two of these sites (the two US mirrors) have continued to offer the 3DB/PDBLite query capability from this Web page.

The PDB mirrors that have changed their Web sites from the BNL to the RCSB-created page are:

Argentina
- University of San Luis
  http://pdb.unsl.edu.ar/

Australia
- ANGIS
  http://molmod.angis.org.au/pdb/
- The Walter and Eliza Hall Institute of Medical Research, Melbourne
  http://pdb.wehi.edu.au:8181/pdb/

France
- Institut de Genetique Humaine, Montpellier
  http://pdb.igh.cnrs.fr/

India
- Bioinformatics Centre, University of Pune
  http://202.41.70.33/

Israel
- Weizmann Institute of Science, Rehovot
  http://pdb.weizmann.ac.il/

Taiwan
- National Tsing Hua University, HsinCh
  http://pdb.life.nthu.edu.tw/

United Kingdom
- Cambridge Crystallographic Data Centre, Cambridge
  http://pdb.ccdc.cam.ac.uk/
- EMBL Outstation
  European Bioinformatics Institute, Hinxton
  http://www2.ebi.ac.uk/pdb/

United States
- Bio Molecular Engineering Research Center,
  Boston University, Massachusetts
  http://www.pdb.bu.edu/
- North Carolina Supercomputing Center
  Research Triangle Park, North Carolina
  http://pdb.ncsc.org/

It should be emphasized that although these sites are offering a valuable service, they are not RCSB PDB mirrors. The RCSB's only role in their operation is to provide access to the data that they need to continue. The level of performance of these sites may vary and is outside the RCSB's control. For example, Eric Martz lists a smaller subset of sites at **http://www.umass.edu/microbio/rasmol/pdblite.htm** that appear to be maintaining a fully functional PDBLite. ◇

PDB CD-ROM

The PDB CD-ROM set for structures released through July 1, 1999, is now available. Distribution began at the IUCr meeting in Glasgow, Scotland, August 4-13, 1999.

The CD-ROMs contain the full release of PDB structure files, structure factor files, and some contributed software and resources. The structure of the directories will be that of earlier CD-ROMs. The CD-ROM set includes the 10,213 structures. Four CD-ROMs are required to contain these structures in compressed (gzip) format. To order a CD-ROM set, go to the RCSB CD-ROM information page at **http://www.rcsb.org/pdb/cdrom.html**. There is no charge for this CD-ROM set.

To assure easy use, the format and content of the CD-ROM set are the same as on previous issues. Minor exceptions are that separate structure deposition files are provided for X-ray and NMR, and all the software is consolidated in the public, external (**/pub/xtrnl**) directory. The structures and structure factors are in the same directories as in the past, organized by the two letter subdirectories as before. A documentation booklet will be shipped with the CD set to assist new users.

The RCSB plans to make changes to the CD-ROM for future releases and is asking the user community to comment on possible changes. Both print and electronic copies of a form laying out possible areas for change and requesting comments and suggestions are included with the CD-ROM. ◇

WPDB — Access to the PDB for Windows Users

WPDB is a software package for maintaining a database of macromolecular structures derived from the PDB and exploring those structures with a variety of supplied tools. WPDB is available for all Intel processors running a version of the Microsoft Windows operating system (Windows 3.1, Win95, and Win98 Wintel platforms). A comprehensive description of WPDB can be found on the Web at **http://www.sdsc.edu/pb/wpdb/**. This article intends simply to introduce those not familiar with WPDB to the available features, indicate how to obtain a copy of WPDB, and to provide existing users with an update on WPDB developments.

Features of WPDB

WPDB is not new — it was first described in Shindyalov and Bourne (1995) J. Appl. Cryst. 28(6) 847-852. Over 2,000 copies have been distributed and feedback indicates it is used most in education at the undergraduate level. Central to WPDB is a database of structures in compressed form. Three databases are available: the complete PDB of currently 10,000 structures (300MB); a unique set of structures defined by Holbohm and Sander based on sequence identity (20MB); and 100 randomly selected structures (2MB). Users can increment these databases or create their own with the supplied loader program (WPDBL) which loads PDB files into a database. Complete documentation is available both online and in a printed manual.

Simple queries permit locating a subset of structures of interest

that can then be manually augmented as needed. Structures can then be displayed in a variety of ways — 3D visualization, Calpha contact maps, sequence-based property profiles, and plots showing stereochemical quality. Limited comparative structure analysis is possible, specifically, sequence alignment (Needleman and Wunsch) followed by least-squares based superposition of aligned structures and difference contact maps.

How to Obtain WPDB

WPDB is free and available via anonymous ftp from **ftp://ftp.sdsc.edu/pub/sdsc/biology/WPDB/** and on CD-ROM. Our goal is to update the FTP site quarterly and the CD-ROM once per year to include new structures. A new CD-ROM with 10,000 structures will be available soon. CD-ROMs can be obtained by sending e-mail to **pdbadmin@sdsc.edu** including a full mailing address. Please note that this is a separate distribution from the PDB CD-ROM (see the article in this issue of Newsletter), which contains the PDB data files in a standard compressed text (ASCII) format.

Future Developments

WPDB is now part of the RCSB-PDB and will slowly be integrated. A long-term goal as specified in the RCSB's grant application (**http://www.rcsb.org/pdb/docs/grant/toc.html**) is to convert WPDB to a Java-based application which will make it available on all major computing platforms. At that time, the interface will be redesigned based on the feedback we have received in the past.

Acknowledgements

WPDB was developed by Ilya Shindyalov and Phil Bourne with funding from the National Science Foundation and the San Diego Supercomputer Center.

First NMR Task Force Workshop

The RCSB has reached out to the NMR community by bringing together experts in the field to form a task force to provide us with advice and guidance in those aspects of the PDB that are unique to the NMR structure files. Among these issues are protein nomenclature, multiple ID codes, ensemble data, constraint files, and validation concerns. Additionally, we desire task force counsel in our development of a new deposition tool and its underlying data dictionary. Task Force members are:

- R. Andrew Byrd – NCI-FCRDC
- Iain Campbell – Univ. of Oxford
- Marius Clore – NIH-NIDDK
- PeterDomaille – Dupont Pharmaceuticals
- Juli Feigon – UCLA
- Robert Kaptein – Univ. of Utrecht
- John Markley -Univ. of Wisconsin
- Michael Nilges – EMBL, Heidelberg
- Michael Summers – Univ. of Maryland, Baltimore
- Peter Wright – Scripps Institute
- Kurt Wuthrich – Swiss Federal Institute of Technology

The Task Force held a short organizational meeting at the Keystone Frontiers of NMR in Molecular Biology VI Symposium in Breckenridge, CO, in January, followed by a one-day workshop in Rockville, MD, on April 23, 1999. The workshop format included morning sessions of short presentations and discussions and an afternoon session devoted to working on the deposition tool and validation needs.

Gary Gilliland, RCSB Project Team Member, NIST, welcomed the Task Force in his opening remarks. Helen Berman, director of the RCSB, presented an overview of the RCSB and stressed our desire to work with the community to develop a database that would best serve both the NMRand the user communities. John Westbrook presented an overview of the deposition/annotation system used by the RCSB and discussed the dictionary on which the system is built. He briefly reviewed the current validation procedures and discussed format issues that need to be addressed.

Eldon Ulrich, representing the BioMagResBank (BMRB: **http://www.bmrb.wisc.edu/**), provided an update on the BMRB. The BMRB has been receiving a substantial portion of their chemical shift data through PDB/EBI, and the RCSB will continue to accept chemical shift data and send it on to BMRB. The BMRB and the RCSB are committed to working together to develop and implement a single interface for NMRdeposition of coordinates and experimental data.

Diane Hancock, RCSB Member, NIST, discussed the current deposition process, addressed format issues in detail, and described ADIT, the AutoDep Input Tool (**http://pdb.rutgers.edu/adit/**). ADIT's goal is to facilitate access to the maximum amount of deposited data while not placing an undue burden on the depositor. Discussion followed as to what are the essential data that must be collected from the depositor to populate the database, and what items, while not essential, would be useful to have in the database. It was clearly recognized that there are a substantial number of data items that, while useful, might preclude a timely deposition due to their number — i.e., if we ask for more, we might get less. The deposition form that is being developed relies heavily on pull down menus, so that many data entries require only the click of a mouse.

Highlights of Task Force discussions on a number of issues follow.

Proton Nomenclature

Task Force members were in consensus as to the advisability of adopting IUPAC nomenclature[1,2] in the coordinate files. It was recognized that this would involve substantial changes in the files as IUPAC nomenclature will require:

- Changing the numbering of methylene hydrogens.
- Establishing aromatic ring numbering on a model by model basis since CD1 and CE1 designations are dependent on chi2 torsion angles — further discussion maybe be warranted with respect to model by model numbering.
- Correction of side chain-NH2 hydrogen nomenclature in Asn and Gln residues (currently done in the RCSB validation procedure)
- Correction of Arg side chain nitrogen nomenclature as needed (currently done in the RCSB validation procedure).

[1] *J. L. Markley, et al., "Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids,"* Pure and Appl. Chem., *70 (1998): 117-142.*

[2] *C. Liebecq,* Compendium of Biochemical Nomenclature and Related Documents, *2d ed., Portland Press: London and Chapel Hill, 1992.*

Although these changes will establish consistency with the BMRB nomenclature, they will create inconsistencies with existing literature and constraint files. Efforts will have to be made to document these differences.

Multiple ID Codes

There was consensus among the Task Force members present for assignment of one accession code for a single study, i.e., put all members of the ensemble and the minimized average structure under one code rather than the multiple codes that now exist. In the old PDB files, the atoms have been numbered sequentially from model to model, with the result that the field limit for the atom number often necessitated the creation of multiple files with multiple accession codes, e.g., 1SAF, 1SAJ, 1SAH. In the newly deposited PDB files, the atom serial numbers are sequential within each model of the ensemble so that all models of the ensemble have the same atom serial numbers. The CONECT records, provided for the first model, are now applicable to all the models.

The minimized average structure will need to be identified so that those structures are not inadvertently downloaded and treated as just another member of the ensemble. A suffix tag, e.g. .ave and .rep could be used to identify the minimized average structure and the representative structures, respectively. Hence a single accession code might include the ensemble (.model1, .model2, .model3 ...) and the average (.ave), or representative (.rep) structures.

Ensemble Issues

The following ensemble issues were raised:

- Should there be a limit placed on the number of models submitted or a suggested limit?
- Should the H-bonds, salt bridges, helices, sheets, and turns be defined for the ensemble as a whole or for each model? Currently these parameters are defined for the first model. If defined for the whole ensemble, how should a consensus value be derived?
- Will IUPAC aromatic ring nomenclature present a problem if nomenclature changes from model to model?

There seemed to be no strong opinions regarding these issues and no consensus was reached.

Validation Issues

The Task Force reviewed the current RCSB validation process for the NMR data, which relies on Procheck-NMR[3] for protein ensembles, Procheck[4] for the minimized average protein structures, and Nucheck for nucleic acid structures (ADIT Validation Server: **http://pdb.rutgers.edu/validate/**). It was felt that these programs did a good job of alerting authors to geometric anomalies that might signal a structural problem. (Note: The RCSB validation procedures were discussed in detail in the April 1999 PDB Newsletter.)

[3] *R. A. Laskowski et al., "AQUA and PROCHECK-NMR: Programs for Checking the Quality of Protein Structures Solved by NMR,"* J. of Biomol. NMR, *8 (1996): 477-486.*

[4] *R.A. Laskowski et al., "PROCHECK: A Program To Check the Stereochemical Quality of Protein Structures,"* J. Appl. Cryst., *26, (1993): 283-291.*

There was a limited discussion on what should be done for validation of the experimental data. Deposition of the chemical shift data and NOE peak tables including peak areas or volumes, would allow further validation. There was some interest in constructing a template for this data. Additionally, a listing of atoms that float during structure calculations would be valuable.

The question of how constraint data should be formatted was raised and the opinion was that adoption of a standard common format would not be possible since the program contents are different, e.g., some programs use pseudo atoms and others do not, the types of constraints vary, etc. Validation of experimental data will require further consideration, both with respect to what could/should be done and what additional data the community is willing to deposit.

Data Deposition, Now and Later

The ADIT deposition/annotation system is built on the mmCIF dictionary and the NMR STAR extensions. It provides precise definitions and examples and defines data relationships, data type, range restrictions, allowed values, etc. The dictionary is organized in table-like structures called "categories." The Task Force critiqued this new deposition tool and proposed changes that are being incorporated. In the future, we hope that data harvesting can evolve to the state that the available data is increased along with a decrease in depositor effort but, in the meantime, we will have to rely on the goodwill of the depositors. ◇

PDB News Distribution Advisory

The PDB proposes to make the following changes in the way they disseminate information to the community, with the goal of being more timely and cutting production costs.

- New developments will be posted to the PDB Web site **http://www.rcsb.org/pdb/** on a weekly basis.
- These announcements will be accessible in chronological order going back to the last newsletter (a maximum of 3 months).
- On a quarterly basis, these announcements and other relevant information will be collated into a quarterly Newsletter.
- The Newsletter will be available on the Web in the form it is now (see **http://www.rcsb.org/pdb/newsletter/index.html**). Links to previous Newsletters will appear with the chronological list of recent news.
- As is the case at present, a text version will be distributed to those who have subscribed to the Newsletter mailing list.
- There will no longer be a printed version of the Newsletter distributed via standard mail.
- The PDB will produce an annual report. The annual report will be made available on the Web in PDF format and in printed form.
- Other services, for example the pdb-l list, will not change. ◇

RCSB Staff and Statement of Support

RCSB Project Team

The overall operation of the RCSB PDB is managed by the RCSB Project Team. Technical and scientific support is provided by the RCSB Members.

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Statement of Support *The RCSB's PDB is supported by funds from the National Science Foundation, the Office of Biology and Environmental Research at the Department of Energy, and two units of the National Institutes of Health: The National Institute of General Medical Sciences (NIGMS) and the National Library of Medicine (NLM), in addition to resources and staff made available by the host institutions.*

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