PDBj

Protein Data Bank Japan

http://www.pdbj.org/

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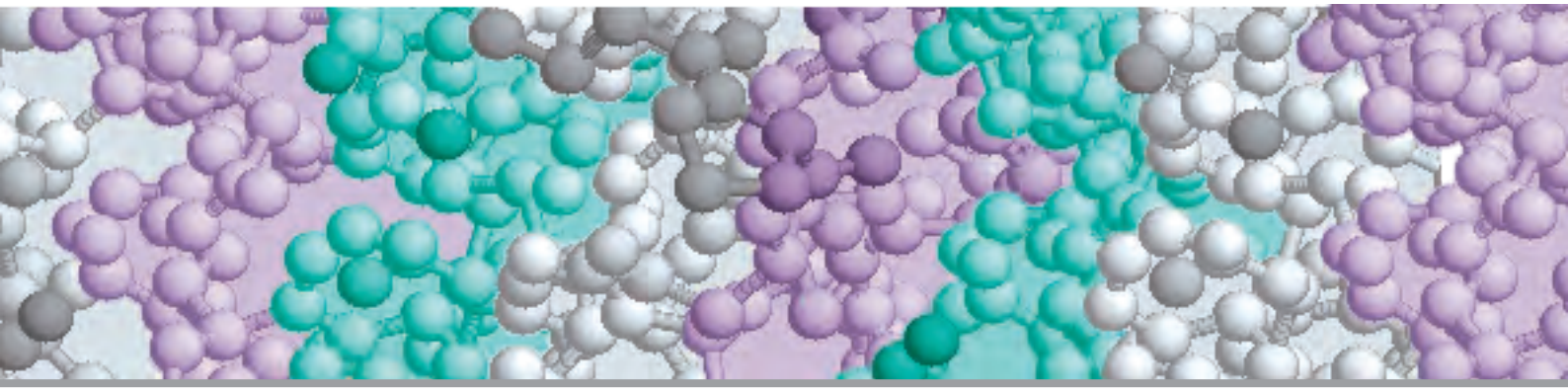


PDBj is maintained at the Protein Research Institute, Osaka University, and supported by Japan Science and Technology Agency.

News

New treatment for theoretical models

The wwPDB has recently decided to restrict PDB depositions to atomic coordinates that are substantially determined by experimental measurements on specimens containing biological macromolecules. Namely, molecular structures determined by X-ray crystallography, NMR, and cryo electron microscopy are included, but models purely constructed in silico with homology modeling or ab-initio methods will not be included.

This decision is the result of a workshop held November 19-20, 2005 at the RCSB PDB to discuss the archiving of theoretical models. Dr. Daron M. Standley of PDBj participated as one of the members. A paper describing this Workshop on Biological Macromolecular Structure Models has been published (Berman et al. Structure, 14, 1211-1217, 2006).

On October 15, 2006, such theoretical model deposition will be stopped. The announcement was made on August 15, 2006, and a letter was sent to journal editors to inform them of our new policy on theoretical models. In the meantime from August 15 to October 15, 2006, theoretical models can be deposited to the wwPDB, but we will not validate or process the data.

The details of the transition plan for our new policy are as follows:

2.3.1.1 At the RCSB, PDBj, and MSD: The PDB format files for theoretical models will not include REMARK 500 (no validation) and would also have a statement in the HEADER to indicate this fact. The following statement would be added in REMARK 220 in the HEADER section of the PDB format file:

"This theoretical model entry was not annotated and not validated by the wwPDB staff and therefore may not conform to the PDB format."

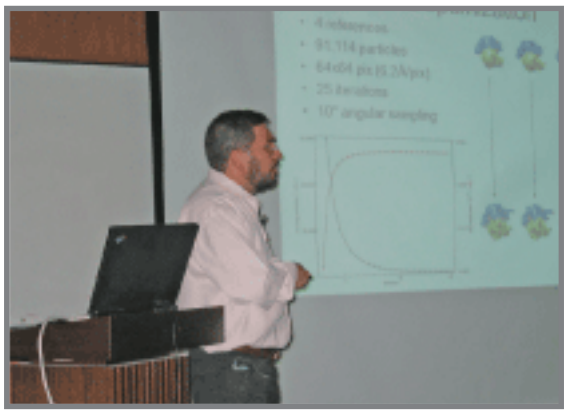
2.3.1.2 The authors of theoretical models that have already been deposited will receive email to state that the PDB format files will be released as-is on the web site according to the status set at the time of deposition. Author corrections will not be incorporated. Authors will have the option of withdrawing the entry. The status authors may choose for newly deposited theoretical models is either REL or HOLD until a certain date. HPUB will no longer be an allowed option.

2.3.1.3 Entries that have previously been processed and returned to the authors for review (on AUTH) status will be updated and released.

2.3.1.4 Theoretical models already on HPUB or HOLD status will continue to be released after the October 15, 2006 date into the theoretical model archives, which is separate from the experimental structures.

Finally, several archives have already been constructed, including those for only theoretical models. Moreover, Berman et al. (Structure, 14, 1211-1217, 2006) have proposed a new portal system, where such theoretical model databases serve model structures just as the wwPDB serves experimental structures.

The seminar by Prof. José-María Carazo



Prof. Carazo at the seminar.

Two topics, “Large macromolecules and their (expected) conformational changes: An image processing approach” and “Flexible Fitting in 3D-EM Guided by the Structural Variability of Protein Superfamilies” , were discussed by Prof. Jose-Maria Carazo on September 1st at IPR Main Hall, Osaka University. In the first lecture, a maximum likelihood method was used to account for conformational heterogeneity in three-dimensional electron microscopy (3D-EM) data. Maximum likelihood is especially suitable for this problem because it allows uncertainty in the conformational state of the macromolecule to be incorporated into the fitting procedure.

The second talk described a method for flexible fitting of molecular models into 3D-EM reconstructions. The approach utilized structural variability among protein domains of a given superfamily rather than normal mode analysis. The method was applied to both simulated and experimental data and flexible fitting was able to produce better results than rigid body fitting. Both topics focus on structural analysis of flexible biomolecules, an important aspect for future studies using 3D-EM.

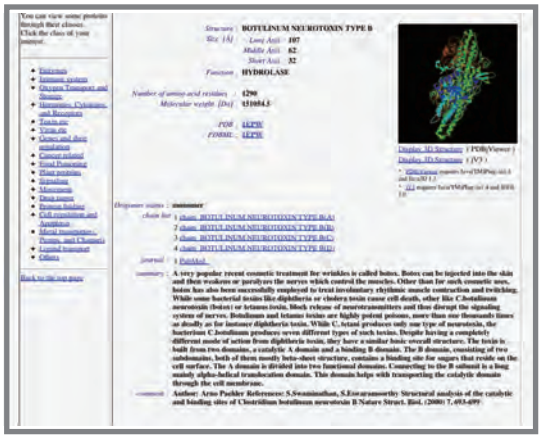
Statistics

The statistics data is available at the wwPDB page (http://www.wwpdb.org/stats.html.).

* Last updated : September, 2006

Services

eProtS: Encyclopedia of Protein Structures



eProtS of example (1EPW).

Have you taken a look at eProtS (encyclopedia of Protein Structures)? eProtS is one of PDBj's services in which various PDB entries (their biological context and structure descriptions) are explained to the layperson and non-specialist. Both English and Japanese versions are available. There are at present about 300 entries registered in eProtS, and more entries are being added constantly. Targeted audiences are assumed to be advanced high school students or those with higher education. However, the contents of eProtS may be enjoyable for the professional structural biologists such as the reader of this News Letter, because, in eProtS, protein structures are described from a somewhat different perspective than that of scientific journals. eProtS can be accessed from PDBj's Homepage.

For example, Botulinum neurotoxin type B is described as follows:

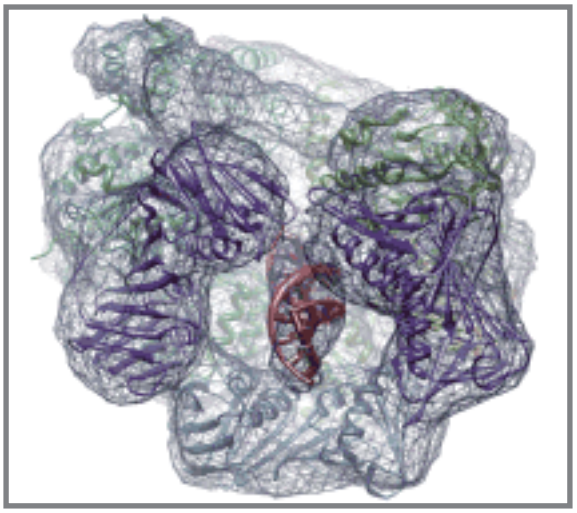
``A very popular recent cosmetic treatment for wrinkles is called botox. Botox can be injected into the skin and then weakens or paralyzes the nerves which control the muscles. Other than for such cosmetic uses, botox has also been successfully employed to treat involuntary rhythmic muscle contraction and twitching. While some bacterial toxins like diphtheria or cholera toxin cause cell death, other like C.botulinum neurotoxin (botox) or tetanus toxin, block release of neurotransmitters and thus disrupt the signaling system of nerves... "

Currently, the entries of eProtS are written by several young researchers with structural biological backgrounds. Considering the overwhelming growth rate of the number of PDB entries, it is hopeless to match eProtS entries with all the PDB entries. Also, we assume (or hope?) that there are many potential writers who are structural biologists and want to explain the structures they have determined to the general public. Hence, we are now planning to convert eProtS to the Wiki style. If many structural biologists participate in eProtS, it will serve not only as feedback of research results to the society but also as slightly different (third-party) annotations of the PDB entries (if you are interested in the Wiki version of the eProtS, visit the experimental site which is accessible from the eProtS top page).

Osaka University's Members

Database for 3D electron microscopy

The figure below shows the structure of the clamp-loading complex revealed by hybrid analysis combining electron microscopy (EM) and X-ray crystallography. The clamp loader (green) is opening the sliding clamp with toroidal shape (blue), and loading it onto the DNA (red). While we can reveal detailed atomic structures of the biological molecules by X-ray crystallography and NMR, it is very hard to obtain the overall structure of flexible and complicated macromolecules like this complex. These are, so to speak, the ways to “detailed but partial” structures. On the other hand, by 3D EM methods, such as single particle analysis and electron tomography, we can see the overall 3D structures of the macromolecules and organelles rather easily, while their resolution has not been achieved to atomic level, yet. So, these are the ways to “entire but blurred” structures. Therefore, employing EM with X-ray or NMR is one of the best approaches to “detailed and entire” structures of the flexible and complicated macromolecules. As the trend of structural research is shifting to such samples, the number of the papers about EM studies is growing.



Structure from EM and X-ray hybrid analysis.

To date, however, only limited data from EM 3D maps and atomic coordinates fitted into the maps have been shared. One of the major problems is in the data format. There are a number of formats carrying 3D maps of EM data, and it seems the same formats might have different interpretations regarding coordinate axes, origin, and scale. Thus, with current software is not possible to reliably determine the relationship between the 3D maps and coordinates. EBI has already been managing “EMDB” (http://www.ebi.ac.uk/msd-srv/emsearch/index.html) as a repository for 3D EM maps. Although the number of data entries is increasing every year, the ratio of deposited data to published works is estimated to be around one half. Furthermore, no official repository for fitted atomic coordinate data with 3D relational information to the EM 3D maps has been constructed.

In PDBj, we are starting to construct a new database for 3D EM structures and related data. Cooperating with EBI, RCSB, and the EM communities, we will contribute to overcome the problems mentioned above and construct a framework for sharing 3D EM data. The 3D models for complicated structures such as the figure above has some information, which is very hard to explain by words and figures, and is easy to understand by viewing and manipulating by oneself on the computer. Moreover, seeing and manipulating such data is a pleasure stimulating curiosity and imagination. Thus one of the goals of this database project is to share this “pleasure” with all the users.

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