PDBj
Protein Data Bank Japan

http://www.pdbj.org/

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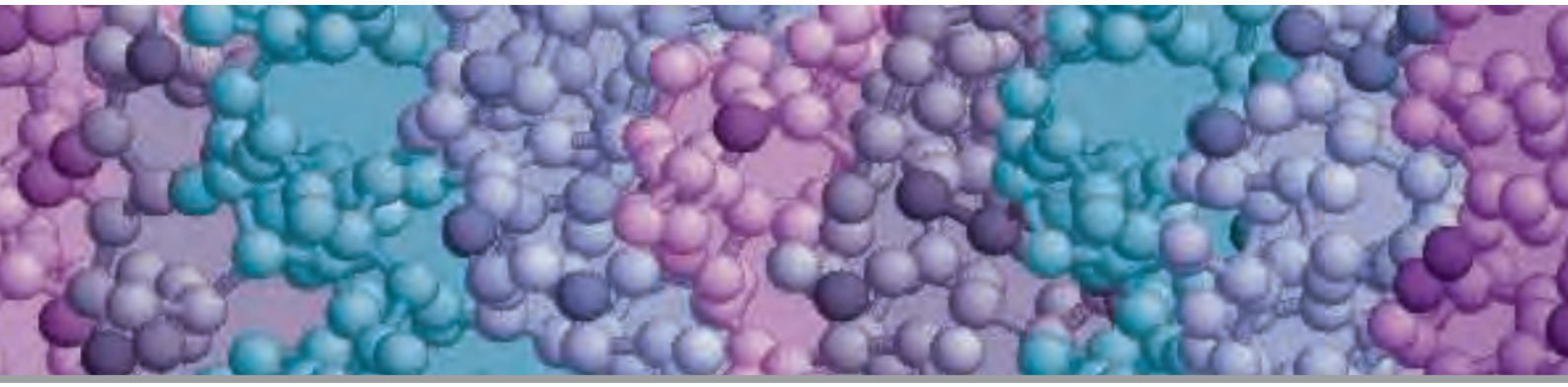


PDBj is maintained at the Protein Research Institute, Osaka University, and supported by Japan Science and Technology Agency.

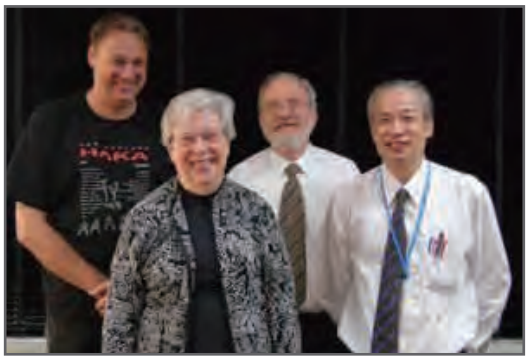
News

The 6th wwPDBAC meeting

PDBj manages the PDB database and develops several services and software tools as a member of the wwPDB (worldwide PDB), which was founded in 2003, collaborating with RCSB-PDB and BMRB in the USA, and PDBe-EBI in the EU.

On November 6, 2009, the 6th wwPDBAC (wwPDB Advisory Committee) meeting was held at the Institute for Protein Research, Osaka University, Japan, by PDBj. The current situation and the future issues were presented and discussed by the participants: The members of the wwPDB, Prof. Helen M. Berman (RCSB-PDB), Dr. Martha Quesada (RCSB-PDB), Dr. Gerard J. Kleywegt (PDBe-EBI), Prof. Haruki Nakamura (PDBj), Prof. John L. Markley (BMRB), the AC members who are specialists in several fields of structural biology: X-ray crystallography, NMR, and Bioinformatics, Dr. Stephen K. Burley (Chair), Prof. Michael G. Rossmann, Prof. Andreas Engel, Prof. Randy J. Read, Prof. Masatsune Kainosho, Prof. Ichio Shimada, Prof. Masahiro Shirakawa, Prof. Kei Yura, and Prof. Soichi Wakatsuki. In addition, as representatives of the International Societies of Crystallography and NMR, Prof. Edward N. Baker (IUCr) and Dr. Andrew Byrd (ICMRBS) attended the meeting. This time, Prof. Manju Bansal (Indian Institute of Science) and Prof. Zihe Rao (Tsinghua University) were also invited as Associate members of the wwPDBAC, and to represent India and China, following recommendations made at the previous 5th wwPDBAC meeting held in 2008. Dr. Matthew Day (NPG, Nature Publishing Group) also attended the meeting as an Observer to discuss publishing issues with the wwPDB.

The participants of the wwPDBAC meeting held on Nov. 6, 2009 at PDBj, Institute for Protein Research, Osaka University, Japan



The members of the wwPDB: From left to right, G. J. Kleywegt, H. M. Berman, J. L. Markley, and H. Nakamura.

At the beginning of this wwPDBAC meeting, Prof. Haruki Nakamura made a summary overview: 1) How the wwPDB members have responded to the 2007/2008 wwPDBAC meeting recommendations, 2) Recent progress of the wwPDB, and 3) Outreach of the wwPDB. Next, Dr. Martha Quesada gave an update on a joint project, the Common Deposition and Annotation tool, that was developed by the wwPDB members.

Prof. John L. Markley and Dr. Gerard J. Kleywegt described the continuous effort to increase data quality in NMR and X-ray data, respectively. Prof. John L. Markley has constructed the NMR Validation Task Force, which is developing the necessary tools for chemical shift deposition. The Small Molecular Structure Deposition (SMSDep) system has been developed jointly by BMRB, PDBj and RCSB-PDB, for small peptides and nucleic acids analyzed by NMR. Dr. Gerard J. Kleywegt described the recent activities of the X-ray Validation Task Force, which had made a great effort to ensure structure quality. In particular, following the Task Force proposal, development and implementation of the new and powerful validation software pipeline in the above Common Deposition and Annotation

system has been supported by the wwPDBAC members. Increasing numbers of structures determined by SAXS/SANS (Small Angle X-ray Scattering / Small Angle Neutron Scattering) and EM (Electron Microscopy) were also discussed, and new Task Forces for the both will be established.

Prof. Helen M. Berman introduced several policy issues. 1) The definition of molecules accepted by wwPDB is clarified for structures of polypeptides, polynucleotides and polysaccharides (In particular, for polypeptide structures, gene products, naturally-occurring peptides that are non-ribosomal in origin, peptidic repeat units of larger polymers, and synthetic peptides of at least 24 residues are acceptable), 2) the necessary improvement of the PDB format, which is limited to 80 column records, 62 polymeric chains and 100,000 atoms, 3) the wwPDB Foundation, which is a new Non Profit Organization to financially promote the activities of the wwPDB, was proposed.

Finally, discussion was made about the possibility of a new wwPDB journal, which was proposed by Dr. Matthew Day from NPG. The initial aim is to publish papers that cover all of the PDB entries. The wwPDBAC looks forward to further discussion including results from market research, which will be made by NPG.

The next 7th wwPDBAC meeting will be held on October 1, 2010, at Rutgers University, USA, by RCSB-PDB.

The 9th Annual Meeting of the Protein Science Society of Japan

The 9th Annual Meeting of the Protein Science Society of Japan was held from May 20th to 22nd, 2009 at the ANA Hotel Kumamoto New SKY. We introduced our activities and services, and the methods to post the eProtS Wiki page.

The workshop in the University of Tokyo, Komaba Campus

We had the workshop in the University of Tokyo, Komaba Campus on August 7th, 2009. We introduced our services and had training using PCs, and received requests from the participants.

The 47th Annual Meeting of the Biophysical Society of Japan

The 47th Annual Meeting of the Biophysical Society of Japan was held from October 30th to November 1st, 2009 at the ASTY Tokushima in Tokushima prefecture. We introduced our activities, the latest PDB search page and ProMode service.

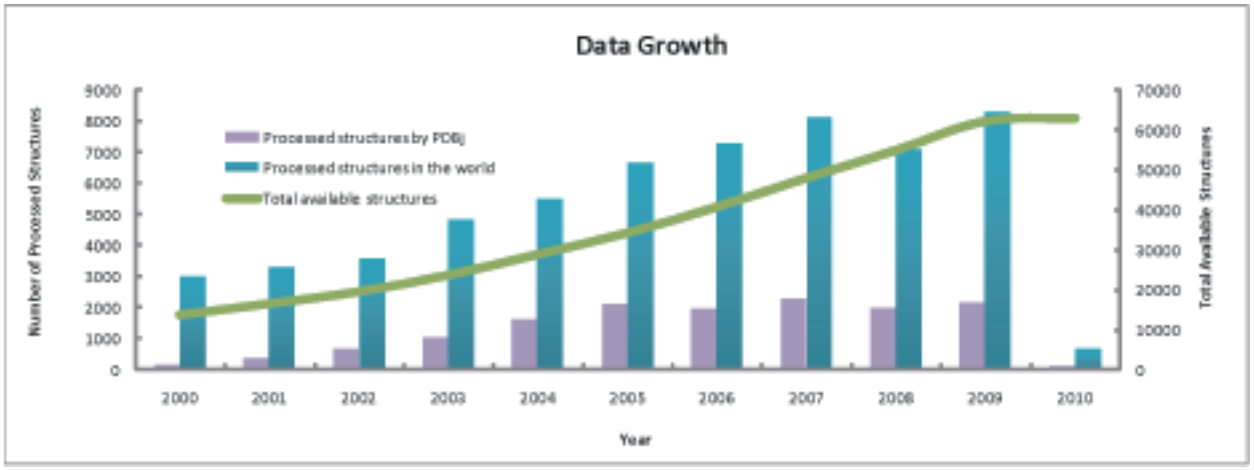
AsCA' 09 (Joint Conference of the Asian Crystallographic Association and Chinese Crystallographic Society) in Beijing

AsCA' 09 was held from October 22nd to 25th at the Jingyi Hotel in Beijing. We exhibited the booth.

Snapshots of the workshops. From left to right: the 9th PSSJ in Kumamoto, the workshop in Komaba Campus, the University of Tokyo, the 47th BSJ in Tokushima and AsCA' 09 in Beijng.

Statistics

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



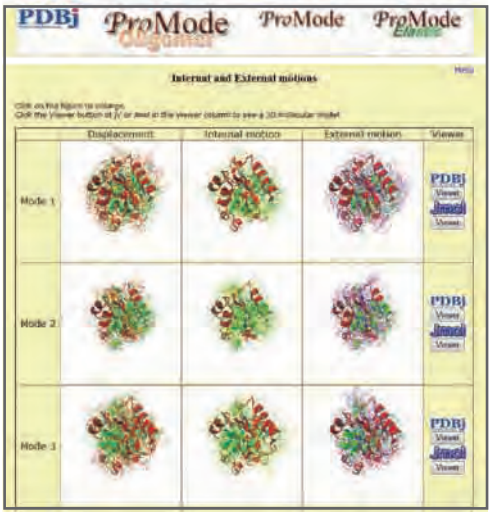
* Last updated : February 4, 2010

Services

ProMode, ProMode-Oligomer, ProMode-Elastic

In order to derive dynamic properties from static conformational information in PDB data, normal mode analysis (NMA) has been performed for PDB entries and the results have been released in the database ProMode [1]. However, the NMA calculation in ProMode was limited to systems composed of either monomer proteins or one subunit out of a multimeric complex. Now, the NMA program has been improved to cover multimeric proteins. The results have been released in a database named ProMode-Oligomer [2]. Not only the same type of data as ProMode, but also a new type of data characteristic to dynamics of the multimeric proteins, i.e., internal and external motions of atoms in individual subunits, is provided in ProMode-Oligomer. The results can be observed in the molecular viewers, jV and Jmol.

Another problem in ProMode (and also in ProMode-Oligimer) is that it cannot perform NMA for a system including a non-polypeptide molecules, such as DNA or other ligands. In addition, ProMode requires much computational time, particularly for large proteins. To overcome this problem we have developed a computational program for NMA with an elastic network model using dihedral angles as independent variables. Although it is not as accurate as ProMode and ProMode-Oligmer, the computational time is much faster and it is possible, at least in principle, to perform NMA for any system, provided in the PDB. Some results are tentatively released in a database named ProMode-Elastic [3]. Fpr full-scale service, not only much more entries but also an application, with which users can perform the NMA calculation by themselves, will be released.



Logos on the page top and a display example of internal and external motions of individual subunits in ProMode-Oligomer.

[1] http://promode.socs.waseda.ac.jp/
[2] http://promode.socs.waseda.ac.jp/promode_oligomer/
[3] http://promode.socs.waseda.ac.jp/promode_elastic/

Hybrid template modeling with Spanner

A screenshot of the Spanner web server.

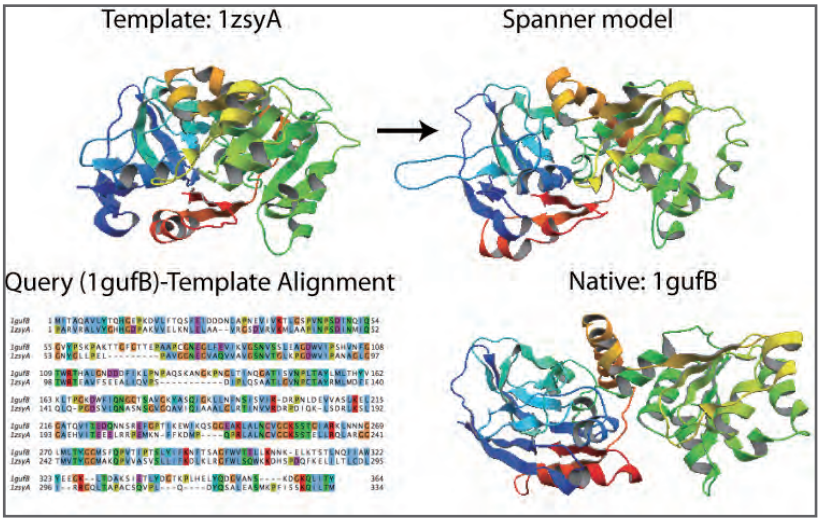
Protein structural modeling plays an important role in biomedical research. Knowledge of even an approximate three-dimensional structure can provide valuable information about the biochemical and biological function of the protein. Currently, the most accurate methods for protein structure modeling are extensions of the fragment assembly method originally implemented by Baker and co-workers in the program Rosetta, and now found in several newer, more accurate methods. In this class of methods, short fragments of known structures are mapped on to the query sequence and then assembled by combinatorial optimization to create a hybrid template model. The drawback of this approach, at least in its current state, is that the optimization procedure takes a very long time. Waiting times on the most popular servers can be weeks to months, and users are usually limited to one query at a time. For this reason, single-template threading and profile-based approaches are far more widely used. Results can be computed in minutes to hours, which fits well with a typical researcher' s timeframe. Unfortunately, the single-template methods typically result in a significant number of insertions and deletions for queries with low homology. Large insertions present problems for constraint-based modeling software, such as Modeller, since the inserted sequence is effectively unconstrained and appears as a random coil, when no further structural information is added to the structural modeling step.

Here we introduce a novel modeling method, Spanner, which uses fragment assembly to extend an initial single-template such that there are no insertions or deletions. Because Spanner starts with an initial 'anchor' template, the search for fragments is very efficient. Furthermore, since the fragments are selected based on sequence and secondary structure similarity to the query, the insertions have the potential to be structured.

The current Spanner is a β-version and it is still under development, but the server can be accessed from the PDBj homepage or through Immunology Frontier Research Center (IFReC) at http://sysimm.ifrec.osaka-u.ac.jp/cgi-bin/spanner.

As shown above, Spanner requires a template structure in PDB format, a query-template alignment, and an email address to which the resulting structure will be sent. In addition, there are options for energy minimization (Presto or Gromacs) as well as internal parameters that might affect the final model.

On the right, we show the structure-based sequence alignment of PDB entry 1guf, chain B (query) and 1zsyA (template). The overall shape and some of the detailed structural features of the final model resemble the native query structure more than the original template.



An example of a structural model built with the Spanner web server using a structure-based sequence alignment between 1gufB and 1zsyA.

PDBj Mine and RESTful Web Services

PDBj Mine is the new relational database and web interface for search and retrieval of entries from Protein Data Bank Japan (http://www.pdbj.org). The underlying data used in PDBj Mine are derived from PDBMLplus files which are PDBML (noatom) XML files with enhanced annotations added at PDBj. PDBj Mine has been on operation since October, 2009. Recently, we have added two RESTful web service interfaces based on PDBj Mine (http://doc.pdbj.org/help.cgi?PDBj%20Mine%3aREST%20API).

Since the relational database of PDBj Mine is based on PDBMLplus XML files, we can retrieve arbitrary XML elements of each PDB entry by using XPath expressions. For example, by accessing the URL http://service.pdbj.org/mine/xpath/1gof/datablock/citationCategory/citation[@id='primary'], you can retrieve the primary citation elements of the PDB entry 1GOF. That is, by simply appending a PDB ID and an XPath expression to the URL http://service.pdbj.org/mine/xpath, the corresponding XML elements can be retrieved.

Furthermore, since PDBj Mine is essentially a relational database, more general searches using SQL queries are also possible based on HTTP POST protocol. For a brief description of the usage, simply access the URL http://service.pdbj.org/mine/sql.

The PDBj frontpage.

The PDBj Mine frontpage.

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