

# PDBj (PDB Japan)の活動と NBDCおよびwwPDBとの連携

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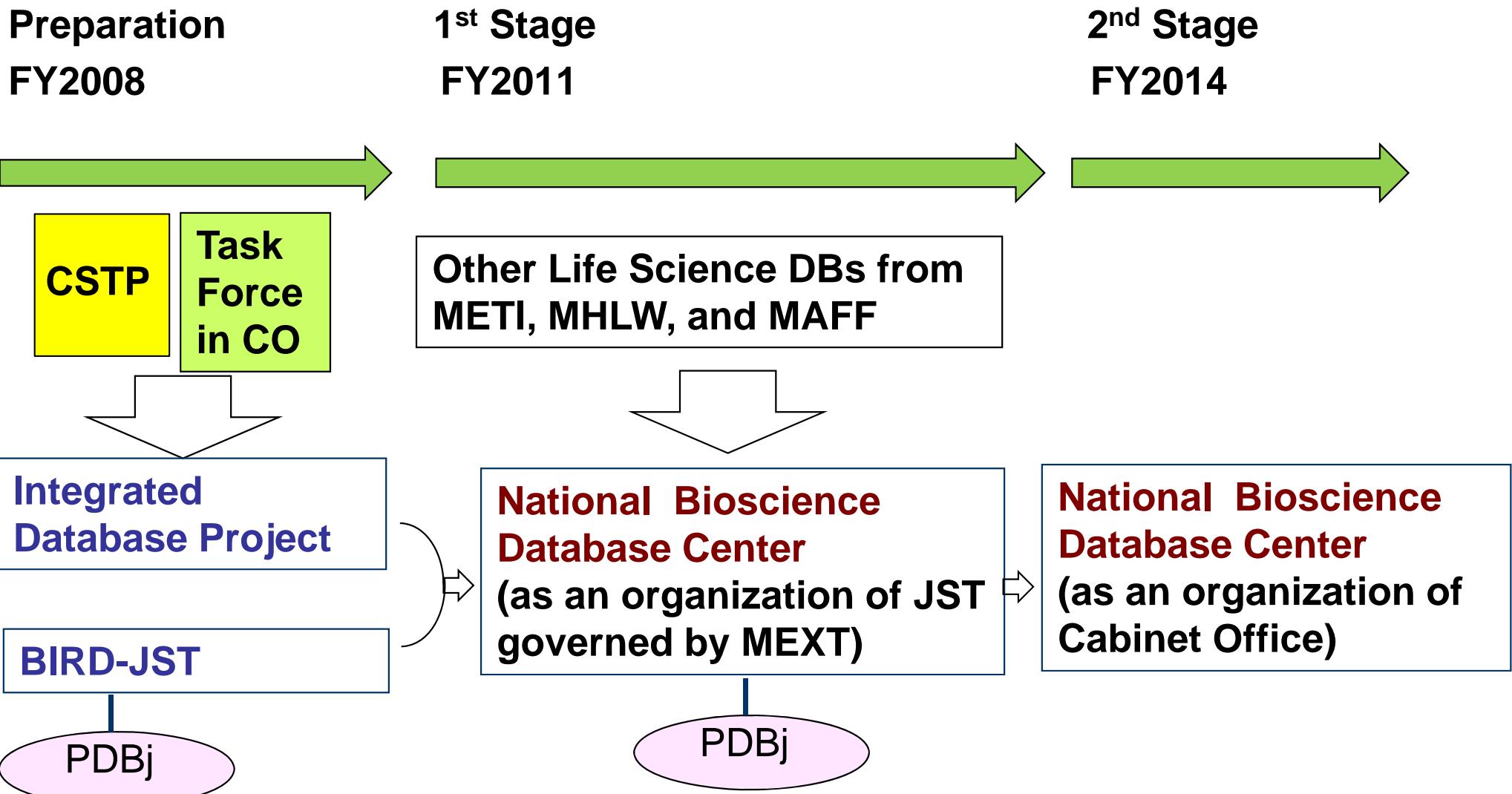
*<http://pdbj.org/>*

*<http://wwpdb.org/>*

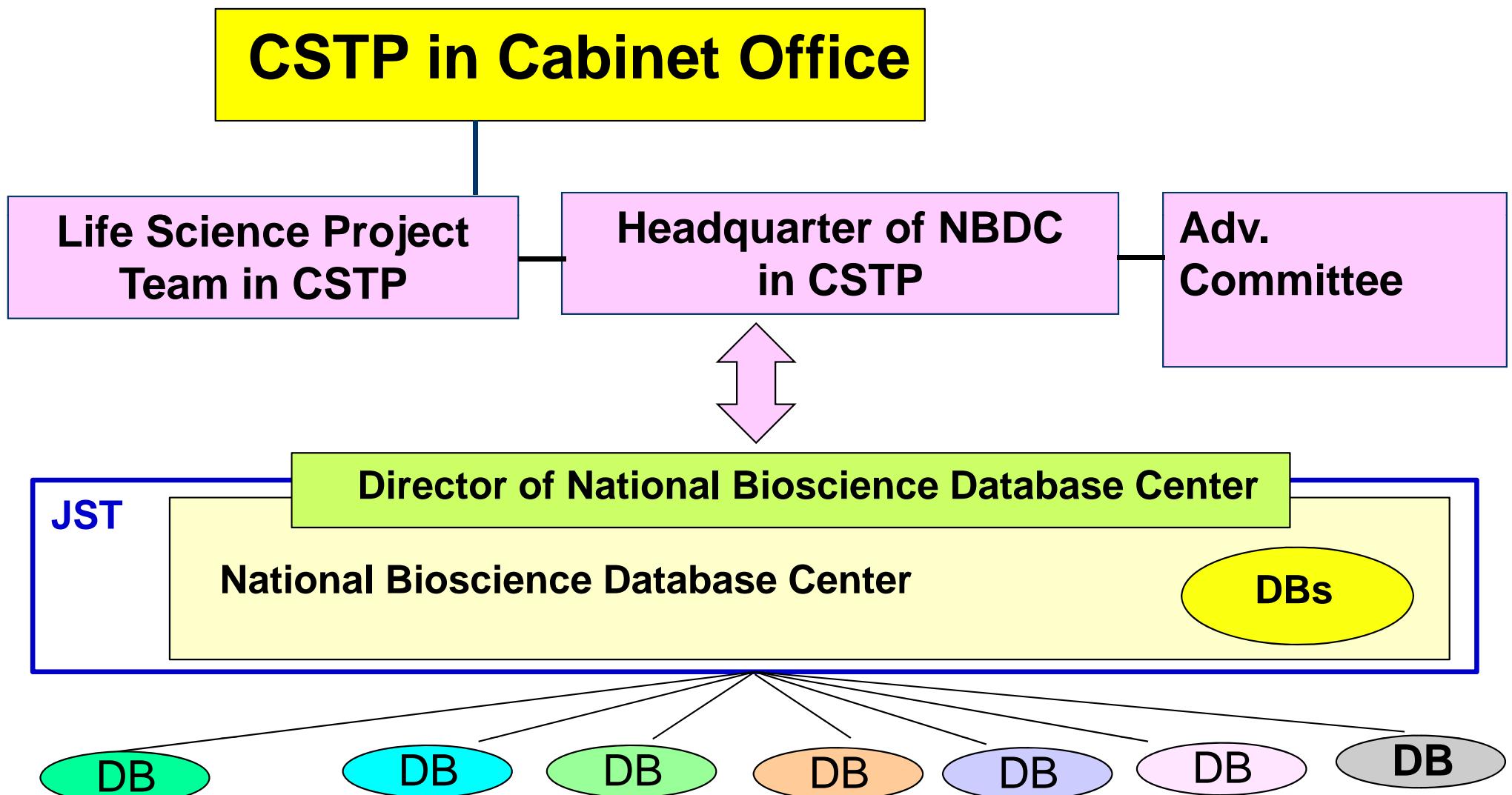
## Staff

- **Head**
  - Nakamura, Haruki, Ph. D. (Prof., IPR, Osaka Univ.)
- **Group for PDB Database Curation**
  - Nakagawa, Atsushi, Ph. D. (Group Leader, Prof., IPR, Osaka Univ.)
  - Igarashi, Reiko (IPR, Osaka Univ.)
  - Kengaku, Yumiko (IPR, Osaka Univ.)
  - Cho, Hasumi (IPR, Osaka Univ.)
  - Ikegawa, Yasuyo (IPR, Osaka Univ.)
  - Takano, Tomoko (IPR, Osaka Univ.)
- **Group for Development of new tools and services**
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  - Iwasaki, Kenji, Ph. D. (IPR, Osaka Univ.)
  - Suzuki, Hirofumi, Ph. D. (IPR, Osaka Univ.)
  - Yamashita, Reiko (IPR, Osaka Univ.)
  - Kudou, Takahiro (IPR, Osaka Univ.)
  - Nishikawa, Ken, Ph. D. (Guest Prof., IPR, Osaka Univ.)
- **Group for BMRB**
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  - Akutsu, Hideo, Ph. D. (Prof., IPR, Osaka Univ.)
  - Kojima, Chojiro (IPR, Osaka Univ.)
  - Kobayashi, Naohiro (IPR, Osaka Univ.)
  - Harano, Yoko (IPR, Osaka Univ.)
  - Iwata, Takeshi (IPR, Osaka Univ.)
- **Collaboratory Researchers**
  - Wako, Hiroshi, Ph. D. (Prof., Waseda Univ.) (**for ProMode**)
  - Ito, Nobutoshi, Ph. D. (Prof., Tokyo Medical and Dental Univ.)
  - Kinoshita, Kengo, Ph.D. (Prof., Tohoku Univ.) (**for eF-site**)
  - Standley, Daron, Ph. D. (iFReC, Osaka Univ.) (**for SeqNavi, StructNavi, SeSAW, and ASH**)
  - Katoh, Kazutaka, Ph. D. (CBRC, AIST) (**for ASH**)
- **Secretary**
  - Haruki, Nahoko (IPR, Osaka Univ.)

# Roadmap for Foundation of National Bioscience Database Center (NBDC)



# Organization of National Bioscience Database Center (NBDC)



# PDBj is a member of NBDC, Japan

*<http://biosciencedbc.jp/>*

**NBDC** National Bioscience Database Center

独立行政法人  
科学技術振興機構  
JST  
Japan Science and Technology Agency

Font size L M S search

Home About Us Contact Us Link

Organization

Welcome from the Director-General  
Projects and Activities  
Organization  
List of Members

**Council for Science and Technology Policy (CSTP)**  
Life Science Project Team DB Integration Promotion Task Force

**National Bioscience Database Center (NBDC)**

Director-General Michio Oishi, Ph.D.  
Deputy Director-General Toshihisa Takagi, Ph.D.

Steering Committee

Program Concerning Technology Development for Database Integration  
Research Supervisor Takeshi Nagase, Ph.D.  
Research Advisor  
Research Advisor  
Research Advisor

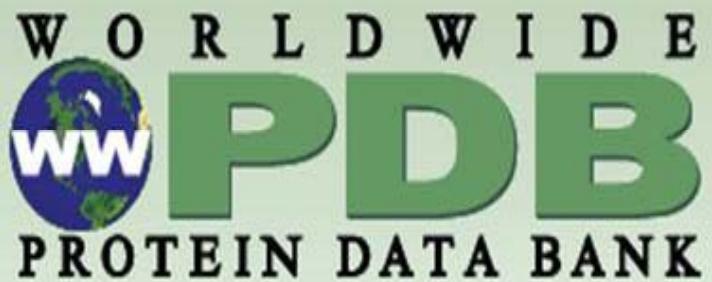
Program for Coordination Toward Integration of Related Databases  
Research Supervisor Toshihisa Takagi, Ph.D.  
Research Advisor  
Research Advisor  
Research Advisor

Department of Planning and Management  
Researchers

About the Director-General (Michio Oishi, Ph.D.)

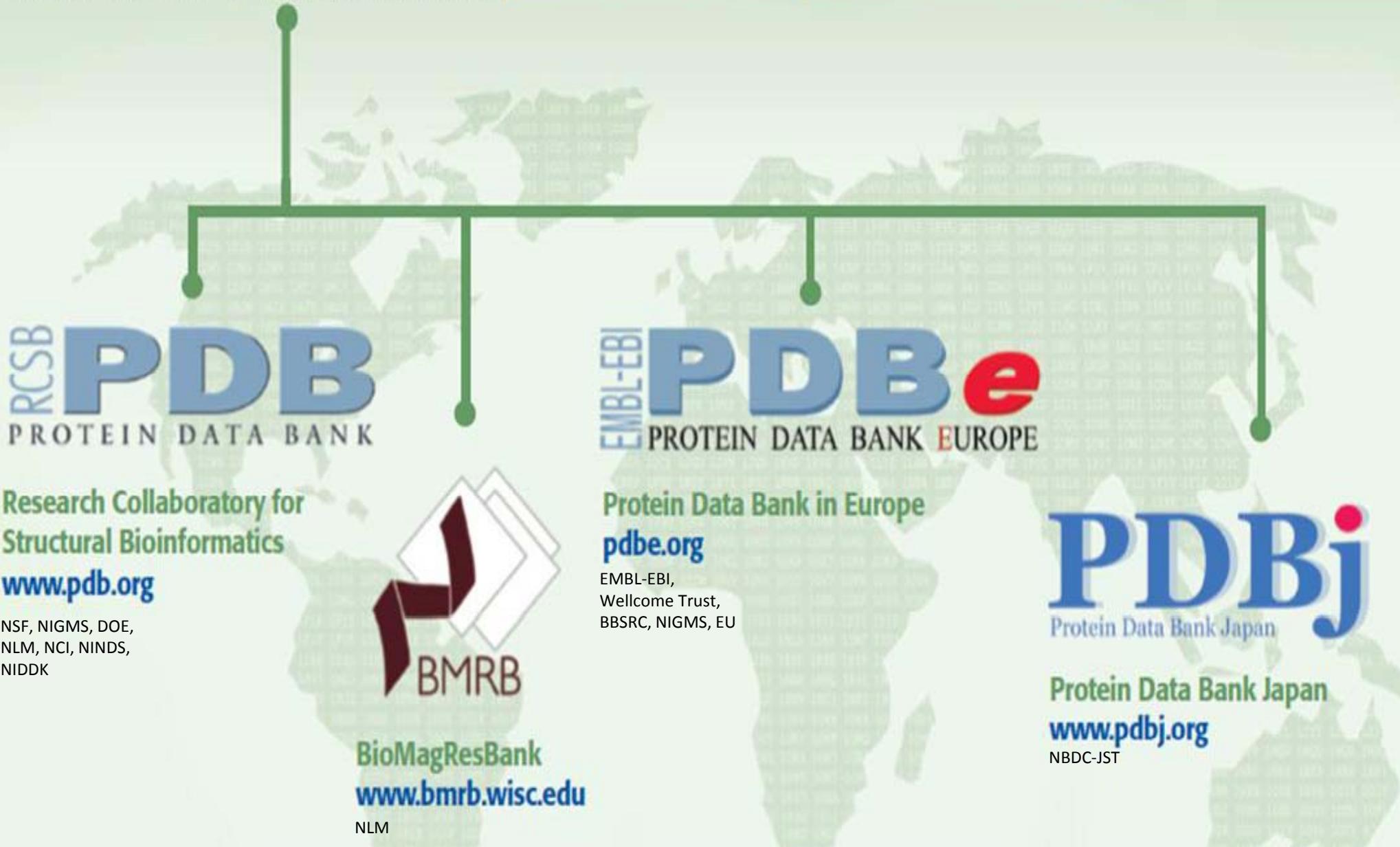


Education :  
1958 B. S. Dept. of Biology, Faculty of Sciences, The University of Tokyo  
1963 Ph.D. Dept. of Biochemistry and Biophysics, Faculty of Sciences, The University of Tokyo



# The worldwide Protein Data Bank

[www.wwPDB.org](http://www.wwPDB.org) • [info@wwPDB.org](mailto:info@wwPDB.org)



Research Collaboratory for  
Structural Bioinformatics  
[www.pdb.org](http://www.pdb.org)

NSF, NIGMS, DOE,  
NLM, NCI, NINDS,  
NIDDK



BioMagResBank  
[www.bmrb.wisc.edu](http://www.bmrb.wisc.edu)

NLM

Protein Data Bank in Europe  
[pdbe.org](http://pdbe.org)

EMBL-EBI,  
Wellcome Trust,  
BBSRC, NIGMS, EU

PDBj  
Protein Data Bank Japan

Protein Data Bank Japan  
[www.pdbj.org](http://www.pdbj.org)  
NBDC-JST



WORLDWIDE  
WW PDB  
PROTEIN DATA BANK



PDB<sup>e</sup>  
PROTEIN DATA BANK EUROPE

PDBj  
Protein Data Bank Japan

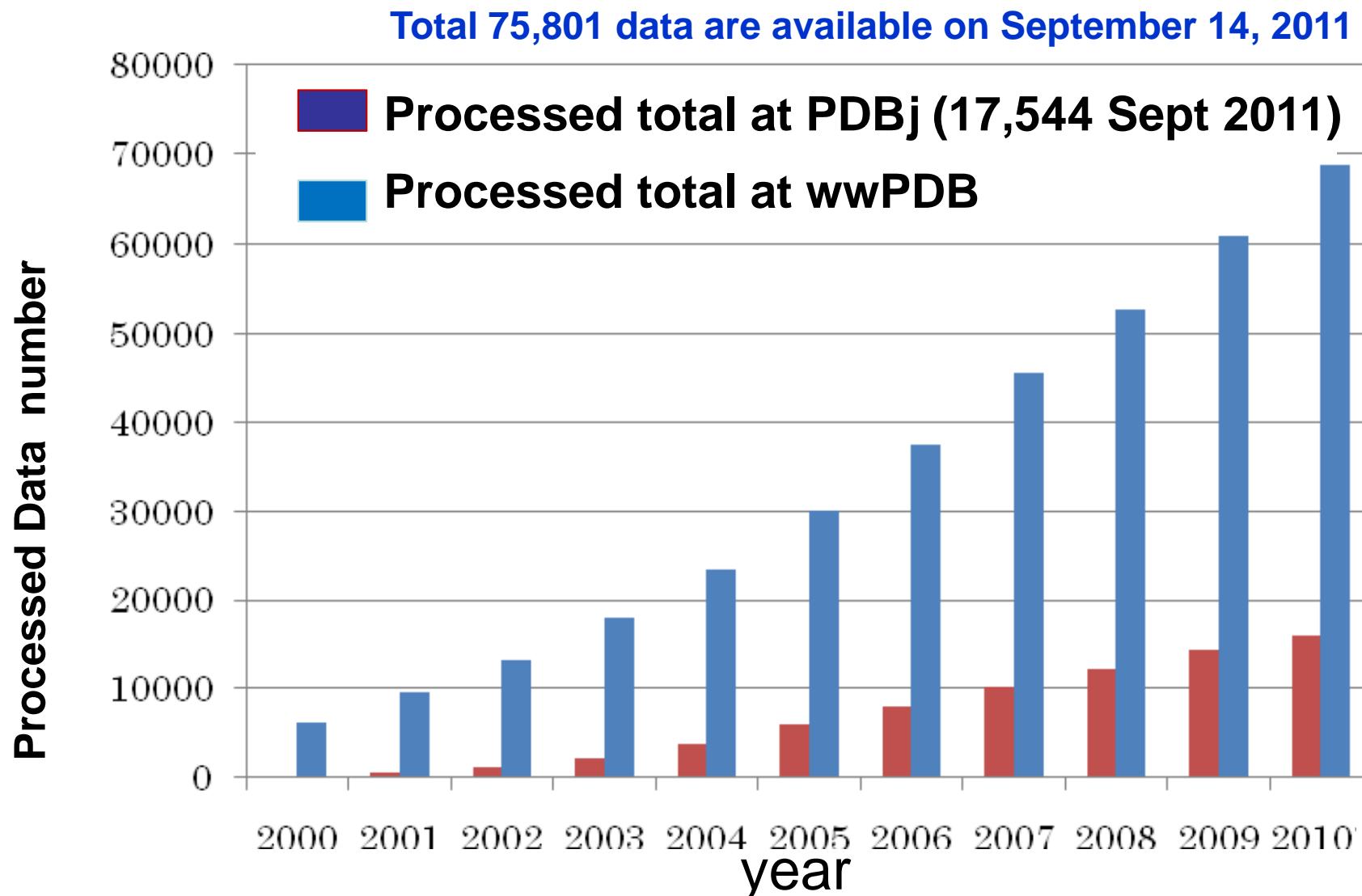


RCSB PDB  
PROTEIN DATA BANK

# New Launching Activities of PDBj

- PDB and BMRB **Data-in**, Collaborating with Other wwPDB Members
- **PDB on the Semantic Web** for Database Integration in NBDC
- Development of a **Validation Tool** for PDB Data Description
- Development of a **New Pipeline Service** from Sequence to Biological Function Through Structure
- Development of **New Service Tools** for BMRB Data-in and NMR Data Analysis

# Data Processed at PDBj and wwPDB



PDBj curates and processes about a Quarter of the deposited data, mainly from Asian and Oceania regions.

# PDB/RDF for Semantic Web

(Recently developed by PDBj: Akira R. Kinjo et al.)

*<http://pdbj.org/rdf>*

**PDB/RDF** *About PDB/RDF  
chem\_comp/RDF Search*

**PDB ID:**  (e.g., '7RSA')  
**property:**  (e.g., 'PDBo:entity.pdbx\_description')  
**keywords:**  (e.g., 'alcohol')

Download XSLT stylesheet for converting PDBML to RDF: [PDBML2rdf.xsl.gz](#)  
(gzipped 22KB)

\*) Some web browsers such as Internet Explorer will display the plain XML file. Please use other browsers that can handle XSLT, e.g. Firefox, Google Chrome, or Safari etc..

**PDB/RDF is a collection of PDB data in the Resource Description Framework (RDF) format. The RDF format is the standard format for the Semantic Web. An ontology defined in the Web Ontology Language (OWL) is also provided for the PDB/RDF, which is a straightforward translation of the PDB mmCIF Exchange Dictionary.**

**Home**[Data Deposition >>](#)

ADIT: PDB Deposition

ADIT-NMR

[Search >>](#)[Search PDB \(Mine/xPSSS\)](#)[PDB/RDF, chem\\_comp/RDF](#)[Latest Release Search](#)[Sequence-Navigator](#)[Structure-Navigator](#)[SeSAW](#)[Ligand Binding Sites \(GIRAF\)](#)[EM Navigator](#)[Search NMR Data \(BMRB\)](#)[Status Search](#)[Service and Software >>](#)[JV: Graphic Viewer](#)[Yorodumi](#)[Protein Globe](#)[ASH](#)[MAFFTash](#)[SEALA](#)[Structure Prediction >>](#)[CRNPRED](#)[Spanner](#)[SFAS](#)[Derived database >>](#)[eF-site/eF-seek/eF-surf](#)[eProtS](#)[ProMode / ProMode Elastic /  
ProMode Oligomer](#)[Download >>](#)[PDB Archive/Snapshot Archive](#)[Links](#)

PDBj (Protein Data Bank Japan) maintains a centralized PDB archive of macromolecular structures and provides integrated tools, in collaboration with the RCSB, the BMRB in USA and the PDBe in EU. PDBj is supported by JST-NBDC and Osaka University.

**Deposition**[Data Deposition Information >>](#)**PDB Deposition****NMR Data Deposition****Search****Search PDB**

PDB ID or Keyword

[Advanced Search >>](#)**Search NMR Data**

- Accession number  
 Deposition code


**What's new**

18-Aug-2011

PDB/RDF service has started. For more details, please refer to the [help page](#).

13-July-2011

New PDBMLplus schema (PDBMLplus\_v40.xsd) has been released. For more details, please refer to the [help page](#).

13-July-2011

The latest version of JV (JV4.0) has been released, supporting the new version of PDBML format (ver 4.0). Please note that the older version of JV may not be able to parse the new PDBML data (v4.0). Please download the newest version from [here](#).

13-July-2011

**PDB Archive Version 4.0 has been released on July 13, 2011.**

wwPDB has released the new version of the PDB data, which reflects the review and resulting changes and

remediation have been updated as version 3.3. ([wwPDB News...](#))

12-Jan-2011

From January 15, 2011(JST), the wwPDB will resume the practice of providing advance notification of PDB entries that

**75801**[entries available](#)[on 14 Sep.,](#)[2011](#)

00:00(UTC) / 09:00(JST)



# Get Entry Data from our browser

Access to <http://pdbj.org/>

PDBj

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- Search NMR Data (BMRB)
- Status Search

サービス&ソフトウェア >>

- JV: Graphic Viewer
- Protein Globe
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  - Spanner
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二次データベース >>

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- eProtS
- ProMode
- Molecule of the Month

ダウンロード >>

- PDB Archive/Snapshot Archive

リンク集

日本蛋白質構造データバンク (PDBj: Protein Data Bank Japan)は、JST-BIRDの支援を受け、米国RCSB、BMRB、および欧州PDBeと協力して、生体高分子の立体構造データベースを国際的に統一化されたアーカイブとして運営するとともに、様々な解析ツールを提供しております。

データ登録

PDB登録 AP Auto PDB Input Tool

NMRデータ登録 AP NMR

検索

PDB検索 Mine Mine日本語ページについて

12as PDB ID or Keyword Go

詳細条件検索 >>

最新情報

2010/7/13 PDBj が開発しておりますフリーの分子グラフィックス・ビューア: JVの最新版 (JV3.8)がリリースされました。displayatom on/off のコマンド機能が追加され、多様な表示が容易にできるようになっております。どうぞ、こちらからダウンロードしてお使いください。

2010/7/1 2010年8月9日(月)、10日(火)に、「ライフサイエンス・データベース講習会 in 名大」を名古屋大学情報文化学部棟にて開催いたします。(詳細 / お申し込み)

2010/6/30 NMR距離制限情報ファイルバージョン2が公開されました。(詳細...)

2010/5/19 JVの最新版(JV3.7.1)が公開されました。

PDBj

Japanese 統計情報 ヘルプ FAQ お問い合わせ

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検索 >>

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Ligand Binding Sites (GIRAF)

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PDB Archive/Snapshot Archive

トピック集

66961 entries available on 4 Aug., 2010 00:00(UTC) / 09:00(JST)

WORLDWIDE PDB PROTEIN DATA BANK

eProts Encyclopedia of Protein Structures

Protein Globe

DBCLS Database Center for Life Science

Tanaku.org

National Project on Protein Structural and Functional Analyses

Bio R&D

Mine

概要 [12as]

日本蛋白質構造データバンク(PDBj: Protein Data Bank Japan)は、JST-BIRDの支援を受け、米国RCSB、BMRB、および欧州PDBeと協力して、生体高分子の立体構造データベースを国際的に統一化されたPDBアーカイブとして運営するとともに、様々な解析ツールを提供しております。

日本語ページについて PDBj Mineについて 更新情報

概要 構造情報 実験情報 機能情報 相同蛋白質 ダウンロード/画面表示 外部データベース PDB ID or Keyword 検索

<非対称単位>

(回転なし) 他の画像...

3次元構造ビューア JV3 / Jmol (JV3 と Jmol には Java(TM)Plug-in 1.5以上が必要です。)

エントリーID (PDB ID) 12as 配列情報 (FASTA形式) PDBファイルのダウンロード

分子名称 ASPARAGINE SYNTHETASE, L-ASPANAGINE, ADENOSINE MONOPHOSPHATE

タイトル ASPARAGINE SYNTHETASE MUTANT C51A, C315A COMPLEXED WITH L-ASPANAGINE AND AMP

機能のキーワード LIGASE, ASPARAGINE SYNTHETASE, NITROGEN FIXATION

由来する生物種 Escherichia coli K12

細胞内の位置 [UNP-P00963] Cytoplasm

ポリマー鎖の合計数 2

分子量の合計 74226 (詳細は 構造情報のページ)

著者 Nakatsu, T., Kato, H., Oda, J. (登録日: 1998-12-30)

引用文献 Crystal structure of asparagine synthetase reveals a close evolutionary relationship to class II aminoacyl-tRNA synthetase. Nature Struct. Biol., 5:15 - 19, 1998. (PubMed: 9437423) (DOI: 10.1038/nsb0198-15)

実験手法 X-RAY DIFFRACTION (2.2Å)

他のデータベース情報 CATH, CE, FSSP, SCOP, VAST, UniProt (P00963), eF-site, KEGG (EC 6.3.1.1), GDB, EzCatDB, PISA, PQS

PDBID (e.g. 12as) or Key-word is input in a box and GO



Summary for each PDBID is displayed.

# Get Entry Data from our browser, PDBj Mine

## Keyword search in Japanese



# Summary for each PDBID

<http://pdbj.org/>

PDBj (Protein Data Bank Japan) maintains a centralized PDB archive of macromolecular structures and provides integrated tools, in collaboration with the RCSB, the BMRB in USA and the PDBe in EU. PDBj is supported by JST-BIRD.

**Mine**

**Summary [1gof]**

[About PDBj Mine](#) [Update Information](#)

[Summary](#) [Structural Details](#) [Experimental Details](#) [Functional Details](#) [Sequence Neighbor](#) [Download/Display](#) [External DB](#)

PDB ID: 1gof sequence information (FASTA format) [download PDB format file](#)

**Descriptor:** GALACTOSE OXIDASE (E.C.1.1.3.9) (PH 4.5)

**Title:** NOVEL THIOETHER BOND REVEALED BY A 1.7 ANGSTROMS CRYSTAL STRUCTURE OF GALACTOSE OXIDASE

**Functional Keywords:** OXIDOREDUCTASE(OXYGEN(A))

**Biological source:** Hypomyces rosellus

**Cellular location:** [UNP - Q01745] Secreted

**Total number of polymer chains:** 1

**Total molecular weight:** 68785.9 (the details in [Structural Details Page](#))

**Authors:** Ito, N. , Phillips, S.E.V. , Knowles, P.F. (deposition date : 1993-09-30, release date : 1994-01-31)

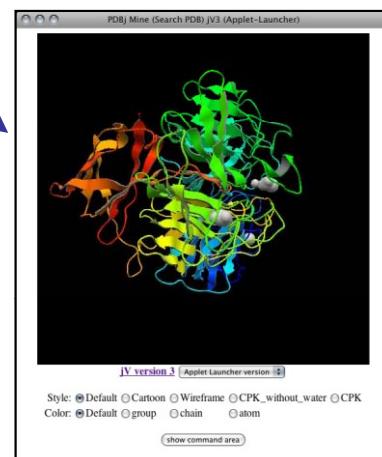
**Primary citation:** Ito, N. , Phillips, S.E. , Stevens, C. , Ogel, Z.B. , McPherson, M.J. , Keen, J.N. , Yadav, K.D. , Knowles, P.F. Novel thioether bond revealed by a 1.7 Å crystal structure of galactose oxidase. *Nature*, 350:87 - 90, 1991. (PubMed : 2002850) (DOI: [10.1038/350087a0](https://doi.org/10.1038/350087a0))

**Experimental method:** X-RAY DIFFRACTION ( 1.7[Å] )

**Other Database Information:** CATH , CE , FSSP , SCOP , VAST , UniProt ( Q01745 ), eF-site , KEGG ( EC 1.1.3.9 ) , EzCatDB , PISA , PQS

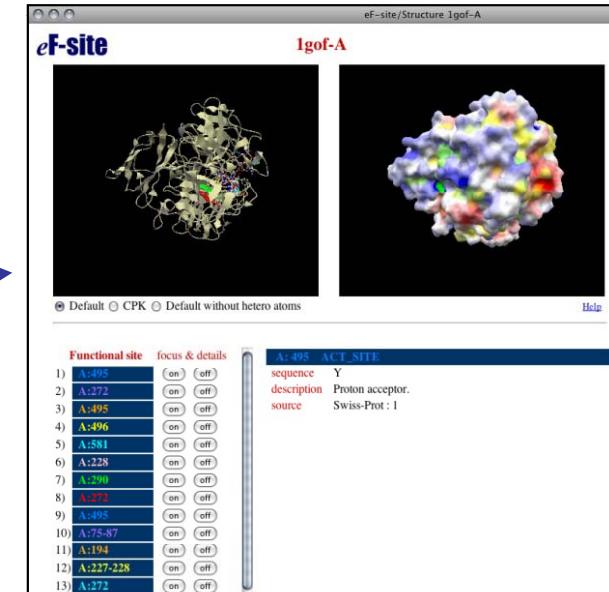
## Data viewer at PDBj

Graphic viewer: JV  
<http://www.pdbj.org/jV/>



## Amino acid sequence (FASTA)

```
>1GOFA:GALACTOSE OXIDASE
ASAPIGSAISRNNWAVTCDSAQSNECNAIDGNKDTFWHFTYGGANGDPKPPTHTIDMK
TTQVNGLSLMLPRQDGQNQNGWIGIREVEYLSSDGTNWGSFVAGSGWFADSTTKYSNFETRP
ARYVRVLVAITEANGQPMITSIAEINVFGAASSYTAPOPGFLGRWGPFTIDLPIVPAAAIEPTS
GRVLWMSYRNDAFGSPGCGITLTSMDPSTGIVSDRTVTVTHDMFCPGISMDNGQIV
VTGNDAAKETSLYDSSDWIPGPDPMOVARGYSSATMSDGRVFTIGGSWSGGVERKNGE
VYSPSKTWTSILPNAKVNPLMTADKQCLYRSNDHAMLFGWKXGSVQAGPSPTANWNYWTS
GSGDVKSAGRKQSQSLSGVADAMCGNAAVMDAVKGILTFGGSPDYQDSDATTNAHIIITLG
EGFTSNTVPAFSNLVYARTHTSVLFDGSTFTTGGQRGIPFEDSTPFTVTPTEIYVPEQ
DTFYKQNPNISVYHHSISLLLPDGRVFNNGGICGDCTTNHFDQIIFTPNYLNNSNGL
ATRPKITRTSQTQSVKVGGRITISTDSSISKASLIRYGTATHTVNTDQRRIPLTNNNGN
SYSFQVPSDGSVALPGYWMLFVMNSAQPVSASTIRVTO
```



Molecular surface DB: eF-site  
<http://ef-site.hgc.jp/eF-site/>

# Annotation of Protein Function from Molecular Surface Similarity: eF-site / eF-seek

**PDBj** **eF-site**  
electrostatic surface of Functional-site

[About eF-site](#) | [References](#) | [Links](#) | [Acknowledgements](#) | [Feedback](#)

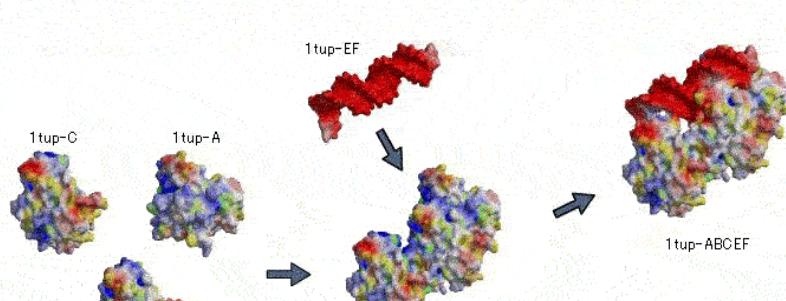
175033 Entries, Last Update: 20-Aug-2005

Keyword Search  
  PDB code only  and  or

Category Search

- [Antibody](#)
- [Prosite](#)
- [Active Site](#)
- [Membrane](#)
- [Binding Site](#)

Examples of molecular surface

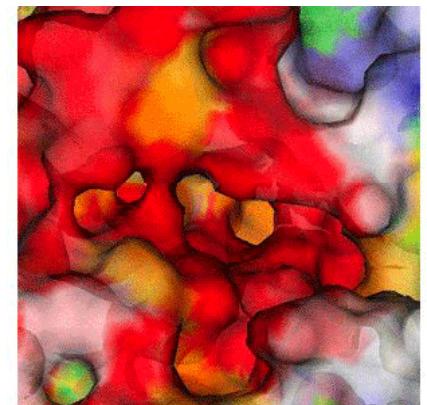


Protein Molecular Surface DB

[TOP](#) [Help](#) [FAQ](#) [References](#) [Links](#)

**PDBj** **eF-seek**

**ABOUT eF-seek:**  
Molecular function of proteins are determined by their three dimensional structures, thus the similarity of protein structure can give some clues to infer their functions. In many cases, the molecular function are begun with the molecular interaction with small molecules (ligands). **eF seek** is a web server to search for the similar ligand binding sites for the uploaded coordinate file with PDB format. The representative binding sites in **eF-site\_database** are search by our own algorithm based on the clique search algorithm.



Submission STEP-1:  
Specify a PDB format file:    
E-mail address:   
Keyword: \*1   
Title: (optional)

Search for Similar Surface

# Viewing Folds and Dynamics @ PDBj

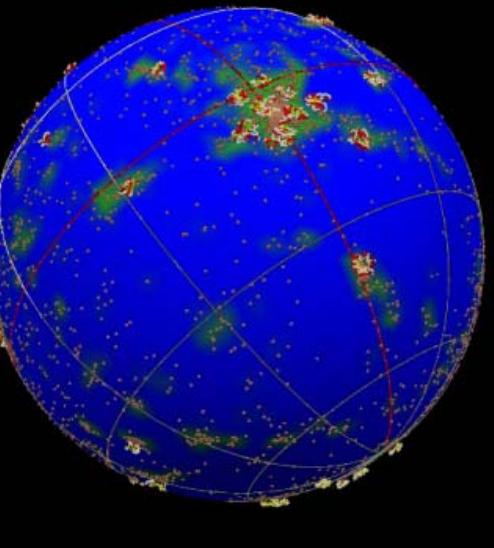
**PDBj Protein Globe (pre-beta)**  
A graphical user interface (GUI) to the PDBj database. [[Description](#) | [Tutorial](#)]

↔ ZOOM↔ +  
xPSSS SeqNavi StructNavi rF-site JV SCOP CATH reset

Select Display  
 1. globe.xml.g  
 2. latlong.xml.l  
 3. cartoons.xml.c  
 4. sphere0.xml.s

PDB ID: 1d13  
Chain: B  
Domain: 0  
xPSSS

This domain:



In PDB:



JV> welcome to PDBj Globe!  
JV>  
1 Atom Selected.  
JV>  
Atom: 1d13 1647 Group: sco 1647 Chain: B Model: 0 File: 1  
JV>

**PDBj** Protein Data Bank Japan **ProMode Elastic** **ProMode** **ProMode Oligomer**

Database of normal mode analysis of PDB data using elastic network model in torsional angle space

Home | What is ProMode-Elastic | Help Japanese

No. of entries 13

PDB code (4 chars)  Find Example 1abc

Select from a list of entries

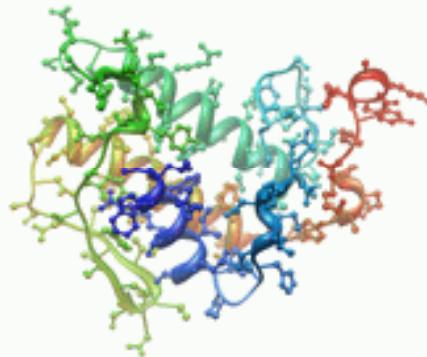
Submission of your data to be analyzed. (In preparation)

Download of

ProMode-E using the pr Torsional A atoms in PD ligand molec molecules a

Reference:

TOPICS 2009.12.12



PDB id: 7rsa Name: Hydrolase (phosphoric diester) Title: Structure of phosphate-free ribonuclease a refined at 1.26 angstroms Structure: Ribonuclease a Chain: E

\*Click on image for an enlarged image and more information.

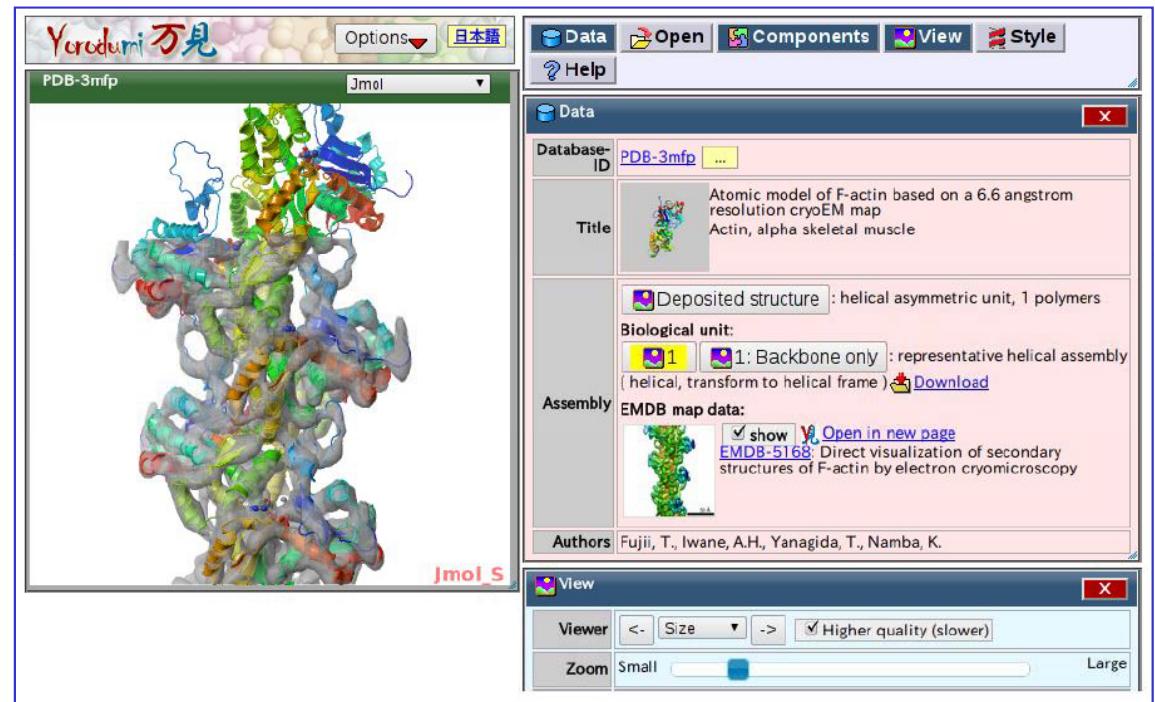
PageTop | Back (Latest update 2009.12.21)

Copyright © WASEDA Univ.Japan. All rights reserved. Email: [promode@list.waseda.jp](mailto:promode@list.waseda.jp)

**Protein Globe: Protein Folds Browser**

**ProMode: Protein Dynamics Database by NMA**

# Viewing both EM Image and Atomic Structure



**EM Navigator:** Viewer of Images of EM-DB

**Yorodumi:** Viewer of both Image and Atomic Structure

# New PDB format

- 1) PDB format is still the most widely used format
- 2) However, there are several limitations, which become problematic more and more
  - For Large and Complex molecules
  - For Meta-data description
  - .....
- 3) PDBx (mmCIF) or PDBML are for machines, and not very human readable.

# Size Matters

- PDB column format limitations
  - 1-character for polymer chain labels
  - 5-characters for atom serial numbers
  - 3-characters for monomers and ligand identifiers
  - 5-characters for atom names
  - F8.3 for model coordinates
- Implications –
  - Maximum of **62 chains** (upper and lower case!)
  - Maximum of **99,999 atoms**
    - Requires splitting structures across multiple entries (5 ribosomes in ASU stored in 10 PDB entries!)
    - Map and experimental validation are difficult for split entries
  - Cannot use **standard monomer & ligand nomenclatures** (e.g. carbohydrates & protonation variants)
  - Cannot use **conventional atom names in large ligands**
  - Limits molecular dimension (< 9999.999 Angstroms)

# Example: Vault by Kato et al. (2zuo, 2zv4, 2zv5)

CRYST1	702.246	383.796	598.480	90.00	124.69	90.00	C	1	2	1	52
ORIGX1	1.000000	0.000000	0.000000			0.000000					
ORIGX2	0.000000	1.000000	0.000000			0.000000					
ORIGX3	0.000000	0.000000	1.000000			0.000000					
SCALE1	0.001424	0.000000	0.000986			0.000000					
SCALE2	0.000000	0.002606	0.000000			0.000000					
SCALE3	0.000000	0.000000	0.002032			0.000000					
ATOM	1	N	MET	A	1	-82.230	143.797	30.257	1.00224.78		N
ATOM	2	CA	MET	A	1	-81.386	143.353	31.410	1.00224.78		C
ATOM	3	C	MET	A	1	-82.092	142.602	32.579	1.00224.78		C
ATOM	4	O	MET	A	1	-81.529	142.546	33.672	1.00224.78		O
ATOM	5	CB	MET	A	1	-80.532	144.526	31.950	1.00238.55		C
ATOM	6	CG	MET	A	1	-80.944	145.901	31.411	1.00238.55		C
ATOM	7	SD	MET	A	1	-81.051	147.196	32.668	1.00238.55		S
ATOM	8	CE	MET	A	1	-82.566	148.018	32.159	1.00238.55		C
ATOM	9	N	ALA	A	2	-83.281	142.021	32.391	1.00183.83		N
ATOM	10	CA	ALA	A	2	-83.718	140.956	33.340	1.00183.83		C
ATOM	11	C	ALA	A	2	-85.047	140.283	32.983	1.00183.83		C
ATOM	12	O	ALA	A	2	-85.544	140.452	31.862	1.00183.83		O
ATOM	13	CB	ALA	A	2	-83.676	141.427	34.858	1.00153.13		C
ATOM	14	N	THR	A	3	-85.601	139.498	33.914	1.00241.98		N
ATOM	15	CA	THR	A	3	-86.810	138.720	33.602	1.00241.98		C
ATOM	16	C	THR	A	3	-88.021	139.162	34.413	1.00241.98		C
ATOM	17	O	THR	A	3	-87.885	139.702	35.529	1.00241.98		O
ATOM	18	CB	THR	A	3	-86.748	137.233	33.902	1.00168.86		C
ATOM	19	OG1	THR	A	3	-87.140	136.275	32.867	1.00168.86		O
ATOM	20	CG2	THR	A	3	-86.525	136.850	35.263	1.00168.86		C

# Example: Vault by Kato et al. (2zuo, 2zv4, 2zv5)

HEADER STRUCTURAL PROTEIN 24-OCT-08 2ZUO  
TITLE THE STRUCTURE OF RAT LIVER VAULT AT 3.5 ANGSTROM RESOLUTION  
SPLIT 2ZUO 2ZV4 2ZV5  
COMPND MOL\_ID: 1;  
COMPND 2 MOLECULE: MAJOR VAULT PROTEIN;  
COMPND 3 CHAIN: A, B, C, D, E, F, G, H, I, J, K, L, M;  
COMPND 4 SYNONYM: MVP  
SOURCE MOL\_ID: 1;  
SOURCE 2 ORGANISM\_SCIENTIFIC: RATTUS NORVEGICUS;  
SOURCE 3 ORGANISM\_COMMON: RAT;  
SOURCE 4 ORGANISM\_TAXID: 10116;  
SOURCE 5 TISSUE: LIVER  
KEYWDS 9 REPEAT DOMAINS, PROTEIN-PROTEIN COMPLEX, CYTOPLASM,  
KEYWDS 2 RIBONUCLEOPROTEIN, STRUCTURAL PROTEIN  
EXPDTA X-RAY DIFFRACTION  
AUTHOR K.KATO, Y.ZHOU, H.TANAKA, M.YAO, E.YAMASHITA, M.YOSHIMURA,  
AUTHOR 2 T.TSUKIHARA  
REVDAT 2 03-FEB-09 2ZUO 1 JRNL  
REVDAT 1 18-JAN-09 2ZUO 0  
JRNL AUTH H.TANAKA, K.KATO, E.YAMASHITA, T.SUMIZAWA, Y.ZHOU,  
JRNL AUTH 2 M.YAO, K.IWASAKI, M.YOSHIMURA, T.TSUKIHARA  
JRNL TITL THE STRUCTURE OF RAT LIVER VAULT AT 3.5 ANGSTROM  
JRNL TITL 2 RESOLUTION  
JRNL REF SCIENCE V. 323 384 2009  
JRN

# Example: Vault by Kato et al. (2zuo, 2zv4, 2zv5)

PDBj

Japanese 統計情報 ヘルプ FAQ お問い合わせ

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Search PDB (Mine/xPSSS) Latest Released Search Sequence-Navigator Structure-Navigator SeSAW Ligand Binding Sites (GIRAF) EM Navigator Search NMR Data (BMRB) Status Search サービス&ソフトウェア >>

JV: Graphic Viewer Protein Globe ASH MAFFTash SEALA Structure Prediction >> CRNPRED Spanner SFAS 二次データベース >> eF-site/eF-seek/eF-surf eProtS ProMode Molecule of the Month ダウンロード >> PDB Archive/Snapshot Archive

Mine 概要[2zuo]

日本語ページについて PDBj Mineについて 更新情報

概要 構造情報 実験情報 機能情報 相同蛋白質 ダウンロード/画面表示 外部データベース

PDB ID or Keyword 検索

<非対称単位> (回転なし) 他の画像... 3次元構造ビューア JV3 / Jmol (JV3 と Jmol には Java(TM)Plug-in 1.5以上が必要です。)

<生物学的単位> (x軸周りに90°回転) 他の画像... (\*) 生物学的単位の画像は、UCSF-Chimeraを使って作成しています。

エントリーID(PDB ID)	2zuo 配列情報(FASTA形式) PDBファイルのダウンロード
SPLIT PDB ID	2zv4, 2zv5
関連構造のPDB ID	2zv4, 2zv5
分子名称	Major vault protein
タイトル	The structure of rat liver vault at 3.5 angstrom resolution
機能のキーワード	9 REPEAT DOMAINS, PROTEIN-PROTEIN COMPLEX, Cytoplasm, Ribonucleoprotein, STRUCTURAL PROTEIN
由来する生物種	Rattus norvegicus (rat)
細胞内位置	[UNP - Q62667] Cytoplasm
由来する組織	[UNP - Q62667] Lung
ポリマー鎖の合計数	13
分子量の合計	1246973 (詳細は構造情報のページ)
著者	Kato, K., Zhou, Y., Tanaka, H., Yao, M., Yamashita, E., Yoshimura, M., Tsukihara, T. (登録日: 2008-10-24, 公開日: 2009-01-13)
引用文献	Tanaka, H., Kato, K., Yamashita, E., Sumizawa, T., Zhou, Y., Yao, M., Iwasaki, K., Yoshimura, M., Tsukihara, T. The structure of rat liver vault at 3.5 angstrom resolution Science, 323:364 - 368, 2009. (PubMed: 19150846) (DOI: 10.1126/science.1164975)
実験手法	X-RAY DIFFRACTION (3.5 Å)
他のデータベース情報	CATH, CE, FSSP, SCOP, VAST, UniProt (Q62667), eF-site, PISA, PQS

# Refinement Details Example

```
REMARK 3 DATA USED IN REFINEMENT.  
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 1.57  
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 23.00  
REMARK 3 DATA CUTOFF (SIGMA(F)) : 0.000  
REMARK 3 COMPLETENESS FOR RANGE (%) : NULL  
REMARK 3 NUMBER OF REFLECTIONS : 43316  
REMARK 3  
REMARK 3 FIT TO DATA USED IN REFINEMENT.  
REMARK 3 CROSS-VALIDATION METHOD : NULL  
REMARK 3 FREE R VALUE TEST SET SELECTION : NULL  
REMARK 3 R VALUE (WORKING + TEST SET) : NULL  
REMARK 3 R VALUE (WORKING SET) : 0.191  
REMARK 3 FREE R VALUE : 0.221  
REMARK 3 FREE R VALUE TEST SET SIZE (%) : NULL  
REMARK 3 FREE R VALUE TEST SET COUNT : 2189  
REMARK 3
```

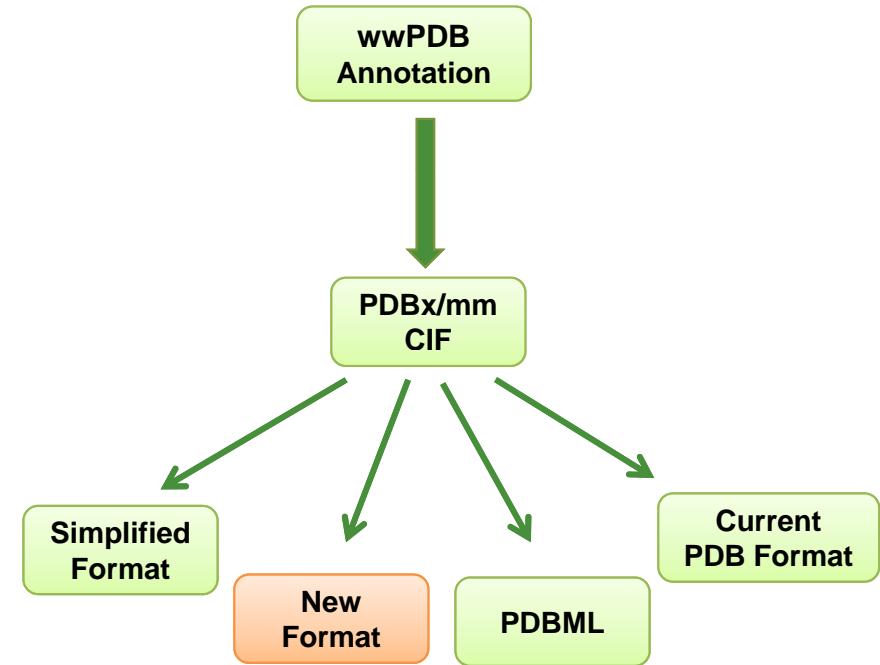
PDB

```
_refine.entry_id 1XBB  
_refine.ls_d_res_high 1.57  
_refine.ls_d_res_low 23.00  
_refine.pdbx_ls_sigma_F 0.0  
_refine.ls_percent_reflns_obs ?  
_refine.ls_number_reflns_obs 43316  
  
_refine.pdbx_ls_cross_valid_method ?  
_refine.pdbx_R_Free_selection_details ?  
_refine.ls_R_factor_obs ?  
_refine.ls_R_factor_R_work 0.191  
_refine.ls_R_factor_R_free 0.221  
_refine.ls_percent_reflns_R_free ?  
_refine.ls_number_reflns_R_free 2189
```

mmCIF

# New PDB format

- Internal data architecture of the PDB is built on mmCIF dictionary technology
- There will be continued support for mmCIF/PDBx and PDBML archival formats
- There is a critical need to adopt an alternative to the current PDB format
- A hybrid approach which takes the best of PDB & mmCIF formats is put forward as a new format



# Method Specific Atom Records

## Atom Records Retain Familiar Look and Feel

```
!!BEGIN_TABLE_DATA atom_site_xray (record_name,atom_id,atom_name,element,residue_name,chain_id,residue_sequence_number,¥
insertion_code,Cartn_x,Cartn_y,Cartn_z,formal_charge,model_number,group_id,occupancy,alternate_location,B_isotropic)
ATOM      1 N           N  ARG      A          4 _    16.757    8.703   13.450  0   1   1  1 0.620 _   21.740
ATOM      2 CA          C  ARG      A          4 _    17.014    7.699   12.351  0   1   1  1 0.620 _   18.890
ATOM      3 C           C  ARG      A          4 _    16.929    8.224   10.937  0   1   1  1 0.620 _   18.590
ATOM      4 O           O  ARG      A          4 _    17.177    7.506   9.922   0   1   1  1 0.620 _   16.720
ATOM      5 CB          C  ARG      A          4 _    16.060    6.546   12.613  0   1   1  1 0.620 _   20.010
ATOM      6 CG          C  ARG      A          4 _    16.429    5.815   13.916  0   1   1  1 0.620 _   22.740
ATOM      7 CD          C  ARG      A          4 _    15.282    4.910   14.340  0   1   1  1 0.620 _   24.130
ATOM      8 NE          N  ARG      A          4 _    15.103    3.825   13.351  0   1   1  1 0.620 _   22.450
ATOM      9 CZ          C  ARG      A          4 _    14.137    2.914   13.579  0   1   1  1 0.620 _   24.510
ATOM     10 NH1         N  ARG      A          4 _    13.382    3.040   14.677  0   1   1  1 0.620 _   24.220
ATOM     11 NH2         N  ARG      A          4 _    13.920    1.913   12.748  0   1   1  1 0.620 _   24.130
ATOM     12 N           N  LYS      A          5 _    16.357    9.426   10.835  0   1   1  1 0.620 _   19.660
ATOM     13 CA          C  LYS      A          5 _    16.206   10.152   9.575   0   1   1  1 0.620 _   21.670
ATOM     14 C           C  LYS      A          5 _    15.607    9.229   8.538   0   1   1  1 0.620 _   20.880
ATOM     15 O           O  LYS      A          5 _    16.057    8.995   7.416   0   1   1  1 0.620 _   20.640
ATOM     16 CB          C  LYS      A          5 _    17.506   10.742   9.045   0   1   1  1 0.620 _   23.450
ATOM     17 CG          C  LYS      A          5 _    17.959   11.915   9.911   0   1   1  1 0.620 _   26.960
ATOM     18 CD          C  LYS      A          5 _    19.253   12.533   9.415   0   1   1  1 0.620 _   30.300
ATOM     19 CE          C  LYS      A          5 _    20.441   11.595   9.492   0   1   1  1 0.620 _   31.990
ATOM     20 NZ          N  LYS      A          5 _    21.676   12.193   8.914   0   1   1  1 0.620 _   33.340
!!END_TABLE_DATA
```

Standard



Method Specific



# Additional Records

```
!!WWPDB_PWF_VERSION 1.0
!!WWPDB_PWF_DEFINITION pwf-def-x-ray-alt.pwf
!!CREATOR wwPDB
!!TIMESTAMP 2011-08-28:10:17:22

!!BEGIN_TABLE_DATA audit_author (record_name,pdbx_ordinal,name)
AUTH      1 Kovalevsky, Y_A.Y.
AUTH      2 Hanson, Y_L.
AUTH      3 Langan, Y_P.
!!END_TABLE_DATA

!!BEGIN_TABLE_DATA cell (record_name,length_a,length_b,length_c,angle_alpha,angle_beta,angle_gamma)
CRYST    93.908     99.503    102.971   90.00   90.00   90.00
!!END_TABLE_DATA

!!BEGIN_TABLE_DATA symmetry (record_name,space_group_name_H-M)
SPGRP   IY_2Y_2Y_2
!!END_TABLE_DATA

!!BEGIN_TABLE_DATA refine (record_name,refine_id,diffrn_id,number_reflns_all,number_reflns_obs,percent_reflns_obs,Y
res_high,res_low,B_iso_min,B_iso_max,R_factor_R_work,R_factor_R_free,R_factor_R_free_error,number_reflns_R_free,Y
percent_reflns_R_free,sigma_F,R_factor_obs,solvent_model_param_bsol,solvent_model_param_ksol,R_Free_selection_details,Y
data_cutoff_high_rms_absF,method_to_determine_struct,starting_model,stereochemistry_target_values,cross_valid_method,Y
solvent_model_details)
REFINE  NEUTRONY_DIFFRACTION 1        28290     26760  81.4   2.00  20.00    9.03    72.85  0.254  0.280  0.004  ...
REFINE  X-RAYY_DIFFRACTION 2        51320     49805  93.6   1.70  20.00    9.03    72.85  0.195  0.211  0.005  ...
!!END_TABLE_DATA
```

Version details

Table section with  
inline definition

Table section for meta-  
data (hybrid)

# Chemical Description Example

```
!!BEGIN_TABLE_DATA pdbx_geom_bond (record_name,atom_id_1,atom_signature_1,atom_id_2, atom_signature_2,symmetry_oper_2,bond_order)
CONECT 2360 NZ:_:LYS:A:296:_:1      5227 C15:_:RET:A:1332:_:1    1_555 SING
CONECT 5213 C1:_:RET:A:1332:_:1      5214 C2:_:RET:A:1332:_:1    1_555 SING
CONECT 5213 C1:_:RET:A:1332:_:1      5218 C6:_:RET:A:1332:_:1    1_555 SING
CONECT 5213 C1:_:RET:A:1332:_:1      5228 C16:_:RET:A:1332:_:1   1_555 SING
CONECT 5213 C1:_:RET:A:1332:_:1      5229 C17:_:RET:A:1332:_:1   1_555 SING
CONECT 5214 C2:_:RET:A:1332:_:1      5215 C3:_:RET:A:1332:_:1    1_555 SING
CONECT 5215 C3:_:RET:A:1332:_:1      5216 C4:_:RET:A:1332:_:1    1_555 SING
CONECT 5216 C4:_:RET:A:1332:_:1      5217 C5:_:RET:A:1332:_:1    1_555 SING
CONECT 5217 C5:_:RET:A:1332:_:1      5218 C6:_:RET:A:1332:_:1    1_555 DOUB
CONECT 5217 C5:_:RET:A:1332:_:1      5230 C18:_:RET:A:1332:_:1   1_555 SING
CONECT 5218 C6:_:RET:A:1332:_:1      5219 C7:_:RET:A:1332:_:1    1_555 SING
CONECT 5219 C7:_:RET:A:1332:_:1      5220 C8:_:RET:A:1332:_:1    1_555 DOUB
CONECT 5220 C8:_:RET:A:1332:_:1      5221 C9:_:RET:A:1332:_:1    1_555 SING
CONECT 5221 C9:_:RET:A:1332:_:1      5222 C10:_:RET:A:1332:_:1   1_555 DOUB
CONECT 5221 C9:_:RET:A:1332:_:1      5231 C19:_:RET:A:1332:_:1   1_555 SING
CONECT 5222 C10:_:RET:A:1332:_:1     5223 C11:_:RET:A:1332:_:1   1_555 SING
CONECT 5223 C11:_:RET:A:1332:_:1     5224 C12:_:RET:A:1332:_:1   1_555 DOUB
CONECT 5224 C12:_:RET:A:1332:_:1     5225 C13:_:RET:A:1332:_:1   1_555 SING
CONECT 5225 C13:_:RET:A:1332:_:1     5226 C14:_:RET:A:1332:_:1   1_555 DOUB
CONECT 5225 C13:_:RET:A:1332:_:1     5232 C20:_:RET:A:1332:_:1   1_555 SING
CONECT 5226 C14:_:RET:A:1332:_:1     5227 C15:_:RET:A:1332:_:1   1_555 SING
!!END_TABLE_DATA
```

Atom Serial  
numbers

Atom  
signatures

Bond  
orders

# Definition File Example

```
!!BEGIN_TABLE_DECLARATION atom_site_xray
!!BEGIN_COLUMN_LIST 17
record_name
atom_id
atom_name
element
residue_name
chain_id
residue_sequence_number
insertion_code
Cartn_x
Cartn_y
Cartn_z
formal_charge
model_number
group_id_list
occupancy
alternate_location
B_isotropic
!!END_COLUMN_LIST
!!FORMAT_STRING_C  ROW (%-6s %8d %-10s %-2s %-10s %-10s %6d %-2s %10.3f %10.3f %10.3f %
%3d %4d %3d %5.3f %-2s %8.3f\n)
!!FORMAT STRING F77 ROW (A6,1X,I8,1X,A10,1X,A2,1X,A10,1X,A10,1X,I6,1X,A2,1X,F10.3,1X,F10.3,%
1X,F10.3,1X,I3,1X,I4,1X,I3,1X,F5.3,1X,A2,1X,F8.3)
!!END_TABLE_DECLARATION
```

Table description

Column list

Program formats

**We would appreciate any  
comments to the new PDB format**

**Please send your comments to**

***<http://pdbj.org>***