

# **New Issues in the wwPDB and the PDBj**

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***http://pdbj.org/, http://wwpdb.org/***

# PDBj Publication

*Kinjo et al. (2017) Nucl. Acids Res. doi: 10.1093/nar/gkw962.*

## Protein Data Bank Japan (PDBj): updated user interfaces, resource description framework, analysis tools for large structures

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### ABSTRACT

The Protein Data Bank Japan (PDBj, <http://pdbj.org>), a member of the worldwide Protein Data Bank (wwPDB), accepts and processes the deposited data of experimentally determined macromolecular structures. While maintaining the archive in collaboration with other wwPDB partners, PDBj also provides a wide range of services and tools for analyzing structures and functions of proteins. We herein outline the updated web user interfaces together with RESTful web services and the backend relational database that support the former. To enhance the interoperability of the PDB data, we have previously developed PDB/RDF, PDB data in the Resource Description Framework (RDF) format, which is now a wwPDB standard called wwPDB/RDF. We have enhanced the connectivity of the wwPDB/RDF data by incorporating various external data resources. Services for searching, comparing and analyzing the ever-increasing large structures determined by hybrid methods are also described.

major changes regarding user interfaces and analysis tools as well as additional data provided. The previously described Resource Description Framework (RDF) format, PDB/RDF, is now one of the wwPDB standard formats called wwPDB/RDF and is enhanced with supplementary information in order to connect PDB data with other biological data resources.

### USER INTERFACES

User interfaces include interactive (and graphical) web interfaces for humans and RESTful web services for computer programs. We also expose our backend database in the forms of web services or dump files for enabling very complex queries. These are described in turn.

#### Web interface

The web interface of PDBj was updated to provide a uniform integrated interface for the available services as well as to provide a scalable interface for devices ranging from smartphones to workstations. This update incorporates several innovative/renovative features as described below. We have implemented various functionalities to ease

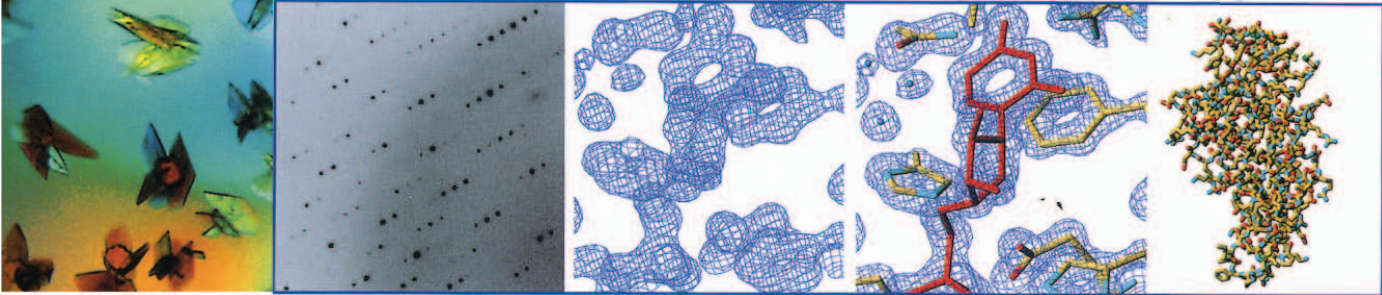

# PDB: Protein Data Bank since 1971

Collects 3D structural information of biomolecules ☐

## • X-ray Crystallography

XFEL & Synchrotron  
(SACLA & SPring-8) ☐

☐  
☐  
☐

☐ Crystal ☐ X-ray diffraction ☐ Electron density map ☐ Atomic model ☐

## • Nuclear Magnetic Resonance (NMR)

☐  
☐  
☐




NMR  
spectrometer  
with super-  
conducting  
magnet  
(@IPR) ☐

CryoEM (@IPR) ☐



## • Cryo-Electron Microscopy ☐

# Protein Data Bank: PDB

## PDB History

**1960s:** Protein crystallography started

□ Myoglobin, Hemoglobin,

Lysozyme, etc

**1970s** □ PDB started with **7 data**

(October, 1971) at Brookhaven

□ National Laboratory, USA

□ PR-Osaka Univ. determined

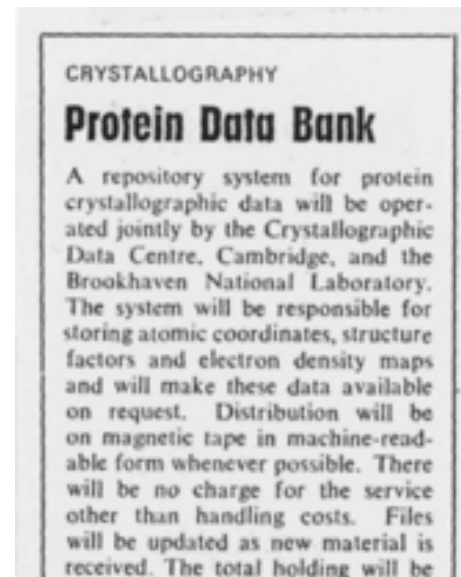
cytochrome c and deposited it to PDB

□ Magnetic tapes were distributed



Max Perutz & □□

□□ John Kendrew (Nobel Prize in Chemistry, 1962) □



# Protein Data Bank: PDB

**1980s**: Rapid data increase (IUCr recommendation  
“**Data deposition to PDB is mandatory** for  
paper submission to journals”)

**1990s**: **RCSB-PDB** started in USA

**2000s**: Foundation of **wwPDB** in 2003

Further many data by **structural genomics**

**2010s**: New methodologies are applied

More than **124,000 data**

Towards “Big Data”



# Protein Data Bank Japan

<http://pd bj.org/>

Since 2001, PDBj has been managed at **Institute for Protein Research, Osaka University** as a member of the **wwPDB**, to curate and process the deposited data for an open and single archive.



PDBj staffs  
(April 2016)

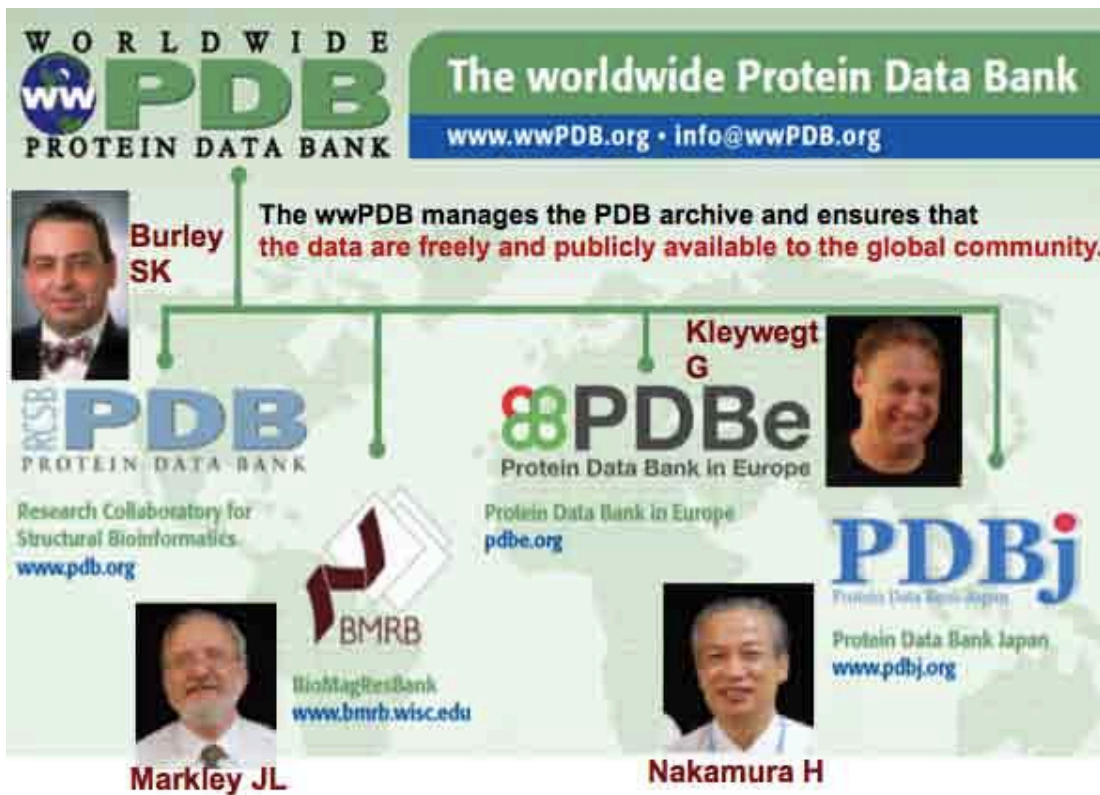


PDBj-BMRB staffs



# The wwPDB (world-wide PDB)

*wwPDB since 2003*



***wwpdb.org***

**12<sup>th</sup> Annual wwPDB Advisory Committee meeting held on 2 Oct 2015 at IPR, Osaka University**

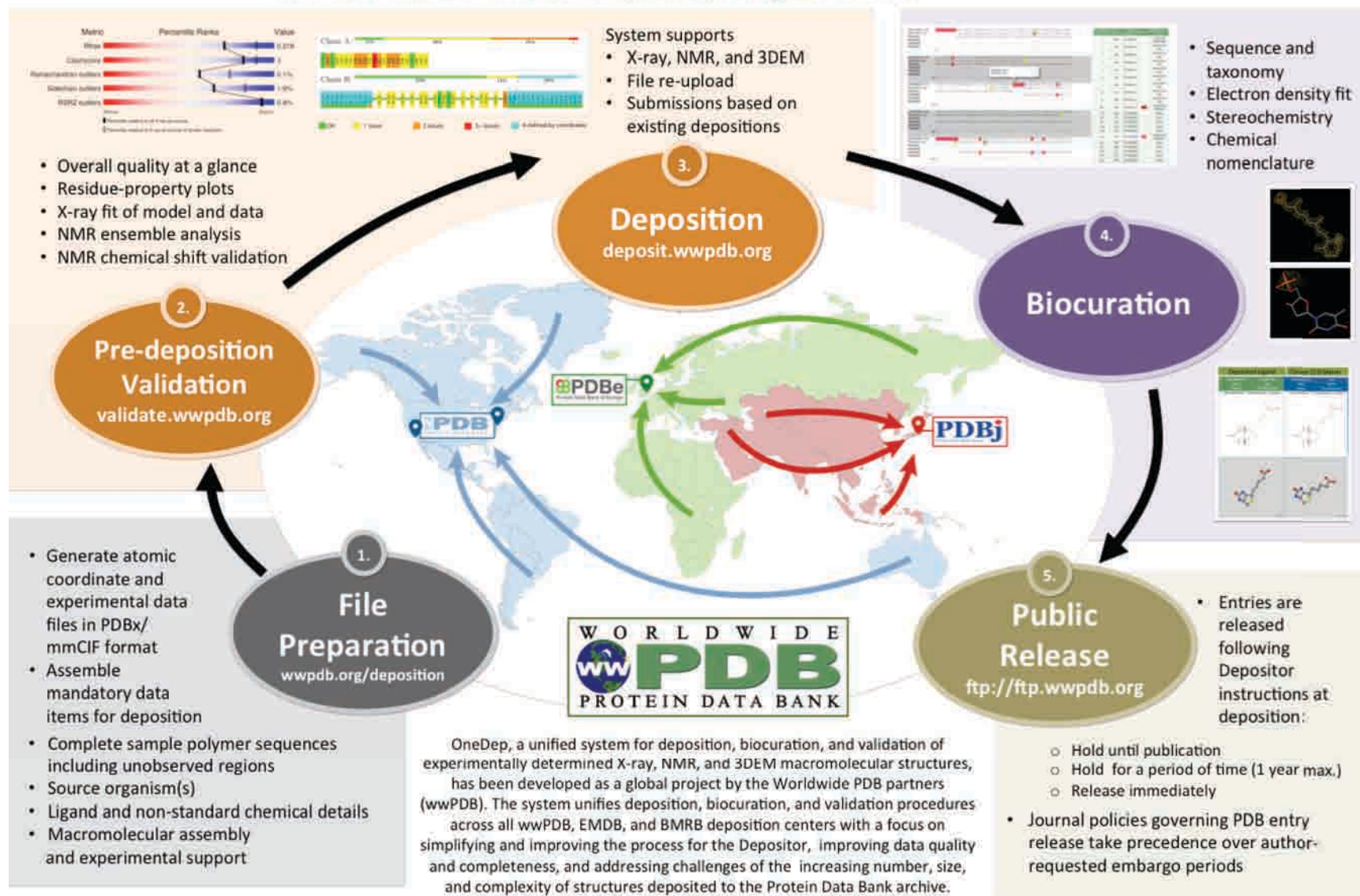
# Activities/Services of each member of the wwPDB

- “**Data-in**” activity, common in all the wwPDB members with high quality control. For the purpose, data deposition, validation system, versioning system, and new format are developed
- “**Data-out**” services, common archive as the ftp site and the characteristic services by each wwPDB member



# OneDep: Unified Deposition Portal for the Protein Data Bank

wwPDB Partners - RCSB PDB, PDBe, PDBj, and BMRB



# OneDep: Unified Deposition Portal for the wwPDB

[wwpdb.org](http://wwpdb.org)



The screenshot shows the wwPDB website interface. At the top, there is a navigation bar with links: VALIDATION, DEPOSITION, DATA DICTIONARIES, DOCUMENTATION, TASK FORCES, STATISTICS, and ABOUT. The main header features the wwPDB logo and a central image of a protein structure. Below the header, there are three main columns:

- wwPDB Members:** Lists various data centers including BMRB (Biological Magnetic Resonance Data Bank), PDBe (Protein Data Bank in Europe), PDBj (Protein Data Bank Japan), and RCSB PDB (Research Collaboratory for Structural Bioinformatics Protein Data Bank).
- wwPDB Resources:** Includes Data Dictionaries (Macromolecular Dictionary, Small Molecule Dictionary, Peptide-like antibiotic and inhibitor molecules), Annotation (Procedures and policies, Improvements for consistency and accuracy), Community Input (Task Forces and Working Groups), PDB Data Growth & Usage Statistics, Workshops & Symposia, and Information for Journals.
- News & Announcements:** Features several news items, including a validation server upgrade, an announcement about mandatory 3DEM model deposition, and deposit ORCID and grant information.

On the right side of the main header, there is a sidebar with three buttons: 'Validate Structure or View validation reports', 'Deposit Structure' (highlighted with a red circle), and 'Download Archive'. Below these buttons is a 'OneDep' logo.





# OneDep: Unified Deposition Portal for the wwPDB

**wwPDB OneDep System**

[FAQ](#)
[Tutorials](#)

Existing deposition

Deposition ID

Password

[Log in](#)

[Forgot Password](#)

wwPDB regions

wwPDB news

**Deposit ORCID and Grant Information with PDB Data**

To enable better annotation and tracking, the wwPDB partners encourage depositors to provide ORCID identifiers and information on relevant grants funding their research when depositing PDB data. ORCID identifiers are unique to each researcher; usage will help avoid ambiguity in

Start a new deposition

Welcome to the wwPDB OneDep system.

To continue with an existing deposition, please login on the left.  
Please note that un-submitted sessions will expire 3 months after last login. Un-submitted sessions and uploaded files will be removed once they expire.

If you have any feedback, please write to us at [deposit-help@mail.wwpdb.org](mailto:deposit-help@mail.wwpdb.org)  
At this time this deposition system does not work with Internet Explorer versions 8 or less.

**Warning: Please note the current system does not support multiple simultaneous depositions.**

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Please select the location of the institute of your PI.  
This will automatically direct to the closest wwPDB data center (RCSB PDB/US, PDBe/UK, or PDBj/Japan) for faster response times for communication and computation.

Country:

- ✓ Select...
- United Kingdom
- United States
- Japan**
- Afghanistan
- Aland Islands
- Albania
- Algeria
- American Samoa
- Andorra
- Angola
- Anguilla
- Antarctica
- Antigua And Barbuda
- Argentina
- Armenia
- Aruba
- Australia
- Austria
- Azerbaijan
- Bahamas
- Bahrain

Version: V2.6

<http://deposit.wwpdb.org/deposition/>

# OneDep: Unified Deposition Portal for the wwPDB



## wwPDB OneDep System



Existing deposition:

Deposition ID

Password

Log in

Forgot Password

wwPDB regions

wwPDB news

**Deposit ORCID and Grant Information with PDB Data**  

To enable better annotation and tracking, the wwPDB partners encourage depositors to provide ORCID identifiers and information on relevant grants funding their research when depositing PDB data. ORCID identifiers are unique to each researcher, usage will help avoid ambiguity in attributing the correct authorship of PDB, BMRB, and EMDB entries. In order to register an ORCID, please visit <http://orcid.org>. Provision of funding agency and grant information will enable better impact tracking and statistics.

Start a new deposition

Welcome to the wwPDB OneDep system.

To continue with an existing deposition, please login on the left. Please note that un-submitted sessions will expire 3 months after last login. Un-submitted sessions and uploaded files will be removed once they expire.

To start a new deposition, please complete the form below. Upon completion, you will be emailed login information specific to your new deposition.

**Question about an in-progress deposition? For fastest response, login into your session and select the "Communication" page from the left hand navigation panel.**

If you have any feedback, please write to us at [deposit-help@mail.wwpdb.org](mailto:deposit-help@mail.wwpdb.org). At this time this deposition system does not work with Internet Explorer versions 8 or less.

**Warning: Please note the current system does not support multiple simultaneous depositions.**

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Access to the Deposition sessions: On initiation of a deposition session the wwPDB OneDep system will provide the Corresponding Author, the Project PI and additional contact authors, as designated by the Principal Investigator with a deposition session password. Responsibility for managing the access information to each deposition session, and hence the privacy of this information, rests with the Principal Investigator.

Your e-mail address

Password (optional, or we will provide one)

This is a shared "group password" (8 to 16 alphanumeric characters)

Country  


Reset country

Experimental method  
☐ X-Ray Diffraction  
☐ Electron Microscopy  
☐ Solution NMR  
☐ Neutron Diffraction  
☐ Electron Crystallography  
☐ Solid-state NMR  
☐ Fiber Diffraction

Requested accession codes:  
☐ PDB ☐ EMDB ☐ BMRB

Structural genomics

Please copy this code 53959

Start deposition

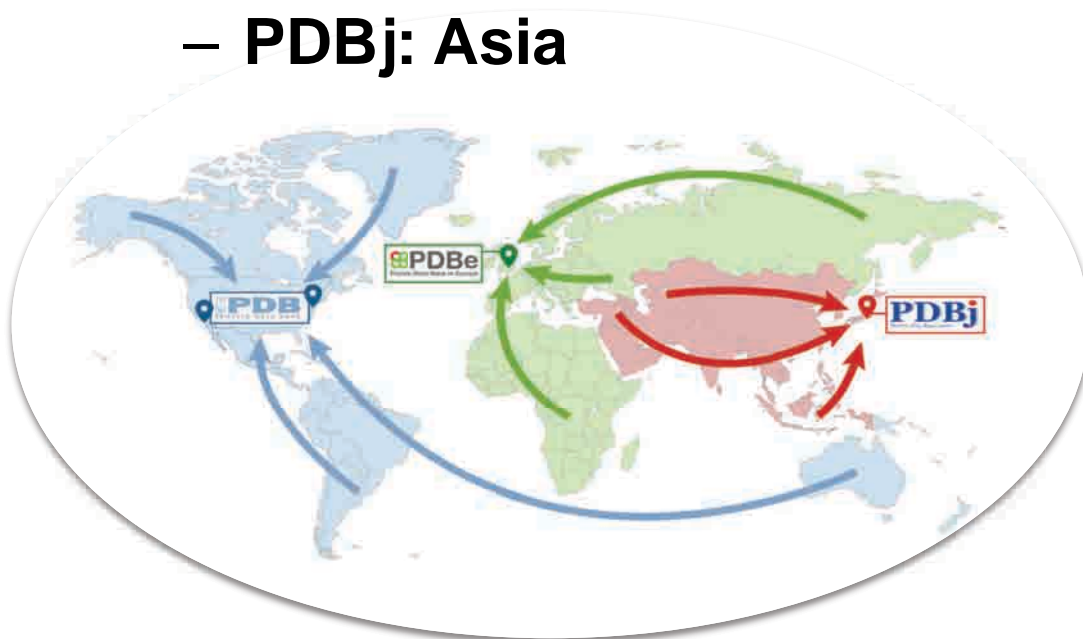
Re-directed to PDBj site

<http://deposit-pdbj.wwpdb.org/deposition>



# PDB Depositions & Annotations

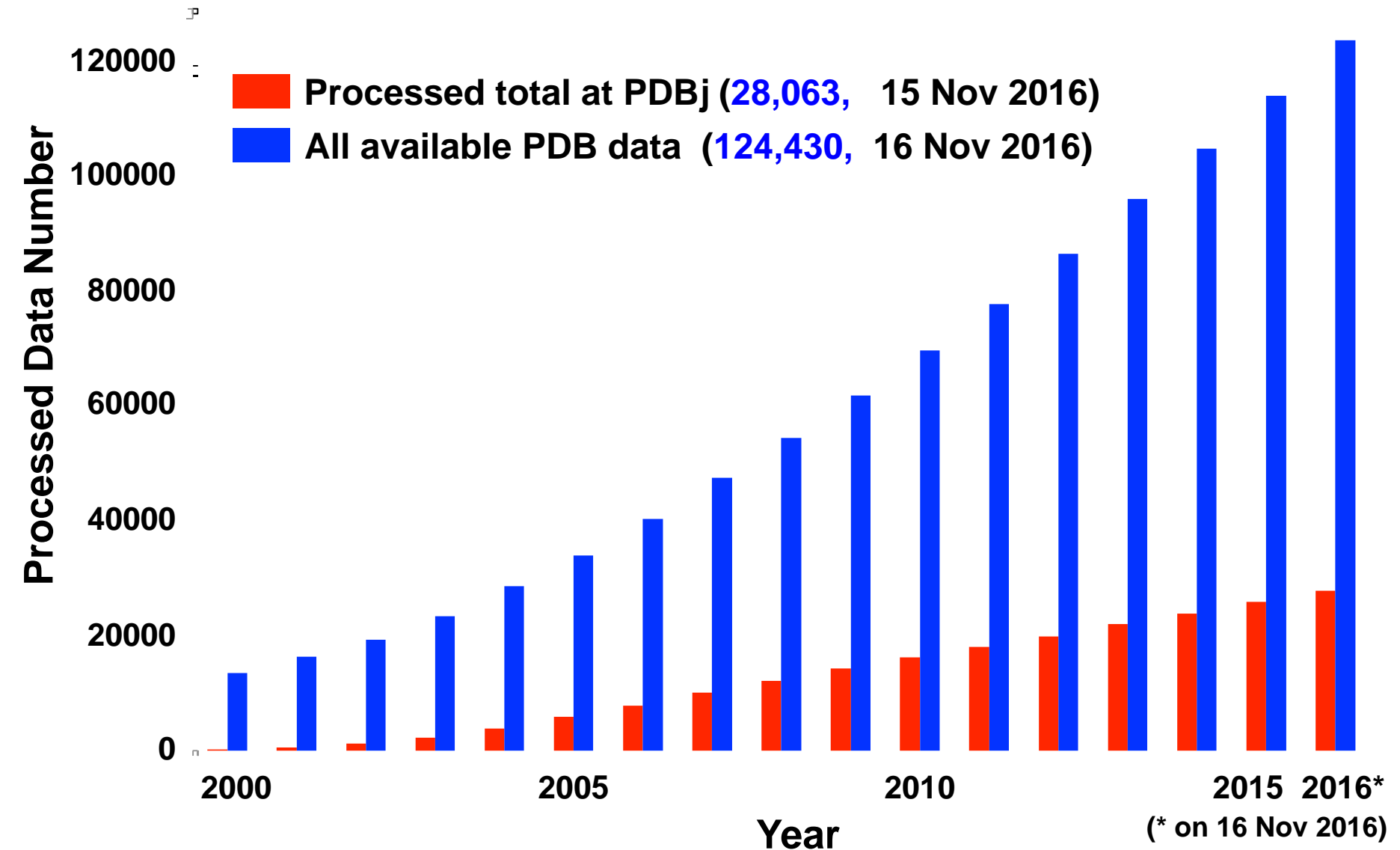
- As of 2016 region-based processing of D&A-deposited entries:
  - RCSB PDB: Americas & Oceania
  - PDBe: Europe & Africa
  - PDBj: Asia



Year	Total Depositions	Processed By		
		RCSB PDB	PDBj	PDBe
2000	2983	2297	158	528
2001	3287	2408	383	496
2002	3565	2401	657	507
2003	4830	3135	1026	669
2004	5508	3082	1614	812
2005	6678	3563	2110	1005
2006	7282	4252	1945	1085
2007	8130	4703	2299	1128
2008	7073	4106	1994	973
2009	8300	5069	2173	1058
2010	8878	5464	2041	1373
2011	9250	5938	1816	1496
2012	9972	6408	1888	1676
2013	10566	6652	2128	1786
2014	10364	6038	1781	2545
2015	10954	4843	2100	4011
2016	8641	4034	1666	2941
TOTAL	126261	74393	27779	24089

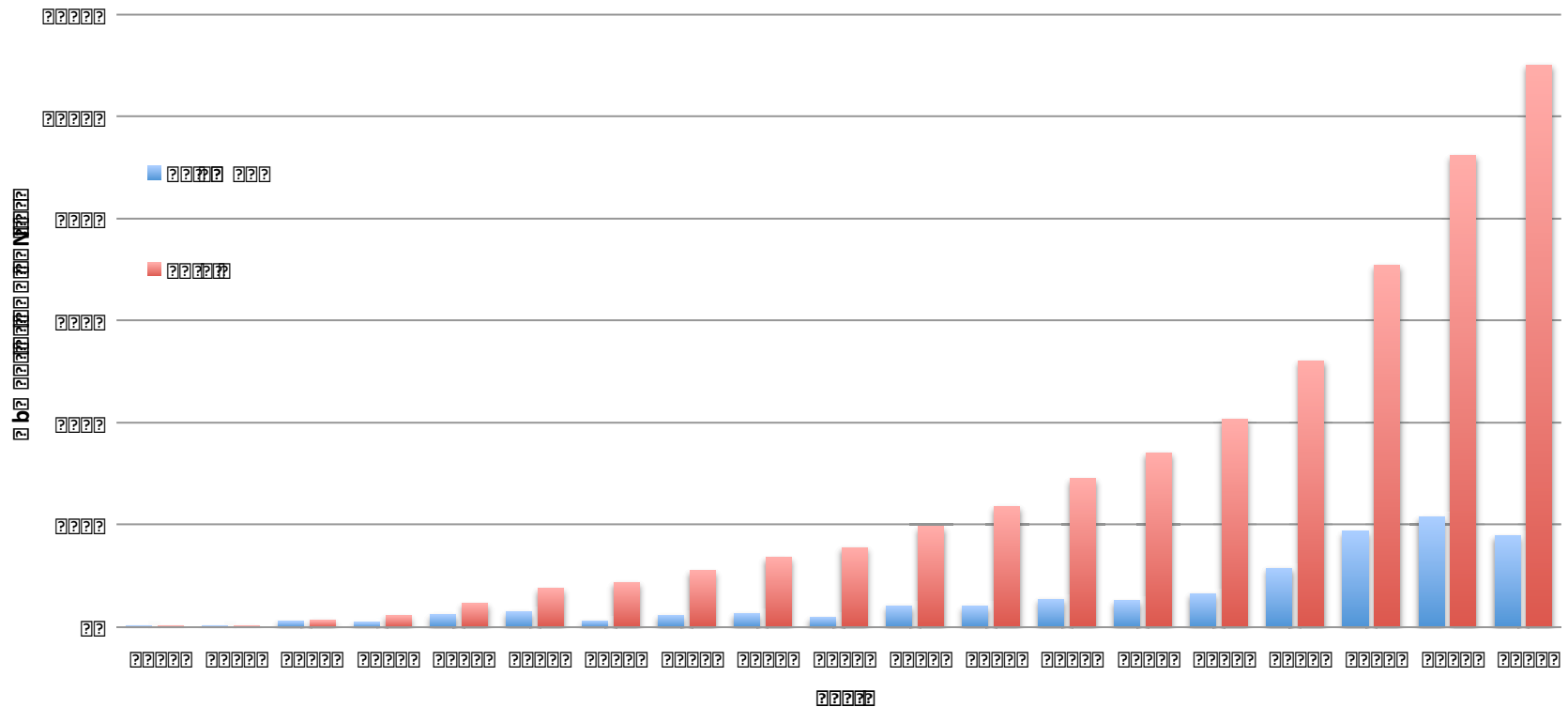
**125K      74K   28K   24K**

# Data-in at PDBj and wwPDB



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

# Growth of PDB EM Entries



As of August 1, 2016, >1100 EM entries in the PDB archive  
 178 new entries released Jan 1 - Aug 1, 2016

# Collection of ORCID IDs

## Open Researcher and Contributor ID

<http://orcid.org>



***Example: [orcid.org/0000-0001-6690-5863](http://orcid.org/0000-0001-6690-5863)***

- **wwPDB Begins to use in April 2016**
- **Mandatory going forward in 2018**



# Validation Report with experimental data

wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:13 AM GMT

PDB ID : 3WDZ  
 Title : Crystal Structure of Keap1 in Complex with phosphorylated p62  
 Authors : Fukutomi, T.; Takagi, K.; Mizushima, T.; Tanaka, K.; Komatsu, M.; Yamamoto, M.  
 Deposited on : 2013-06-26  
 Resolution : 2.60 Å (reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
 We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
 A user guide is available at <http://www.pdb.org/ValidationPDFNotes.html>

Top page of  
Validation report

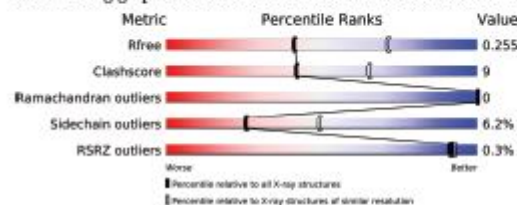
## Mandatory Experimental data

- X-ray: Structure Factor
- NMR: Chemical Shifts and Distance restraints
- EM: 3DEM volume map

### 1 Overall quality at a glance

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 2: Peptide from Sequestosome-1



Validation report

## EDITORIAL

# nature structural & molecular biology

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## Where are the data?

Here, we announce two policy changes across Nature journals: data-availability statements in all published papers and official Worldwide Protein Data Bank (wwPDB) validation reports for peer review.

... We are now taking a further step and are **requesting official wwPDB validation reports for peer review**. These reports are made available by the wwPDB after data deposition (<http://www.wwpdb.org/validation/validation-reports>). **Other Nature journals will soon follow suit.**

# Versioning of PDB entries

## Current Issue

- Loss of connection between **PDB ID and Publication**

## Introduction of a new PDB ID code format

- Allow more informative and transparent delivery of revised data files
- With PDB prefix and extension of 4 characters (e.g. from “**1ABC**” to “**PDB\_00001ABC**”)
- Example: **PDB\_00001ABC\_XYZ\_V2-2.cif.gz**

## Implementation plan

- **Create new versioned ftp tree** containing the latest minor revision to each major version
- **Continue current ftp tree with current file naming** convention.

Files in this branch will serve up the latest version of each data file

# New format of PDB: PDBx/mmCIF

- PDB format is almost **40 years old** and does not support today's science.
- PDB Record format limitations
  - **Max. 62 chains**
  - **Max. 99,999 atoms**
  - No bond orders or chirality specified for ligands
  - No support for NMR, EM, hybrid methods, ...
  - Meta-data specification cumbersome and inflexible

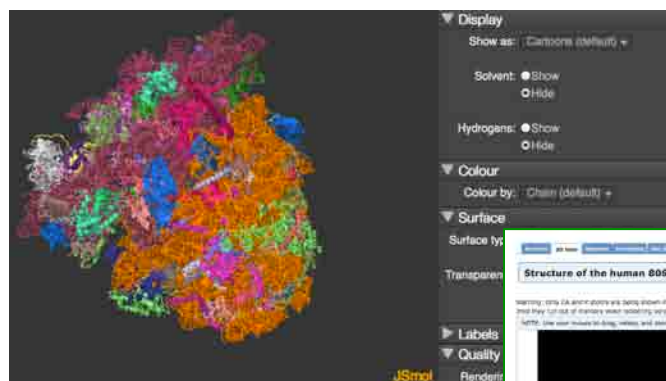


- **Preserve backward compatibility where possible**
- **web service to create PDB format data files**
- **Start in 2014**

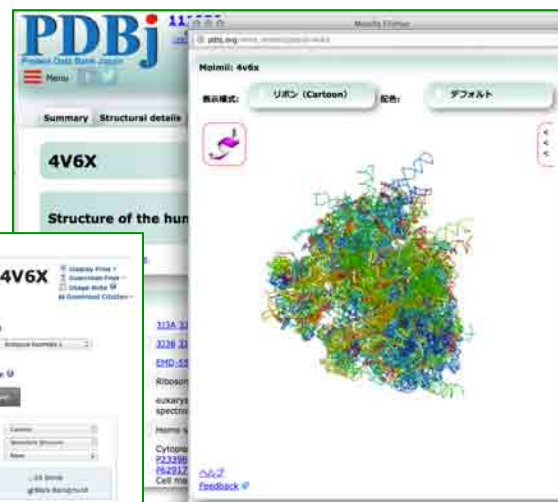


# Large Structures (476) in PDB

- As of December 2014, large structures are no longer split into multiple PDB entries but are **released as single PDBx/mmCIF and PDBML files**
  - Existing split entries were consolidated into single entries
  - A bundle of best-effort PDB files (PDB bundle) is available for every large structure through the wwPDB FTP sites
- Each wwPDB member provides **tools to view large structures**

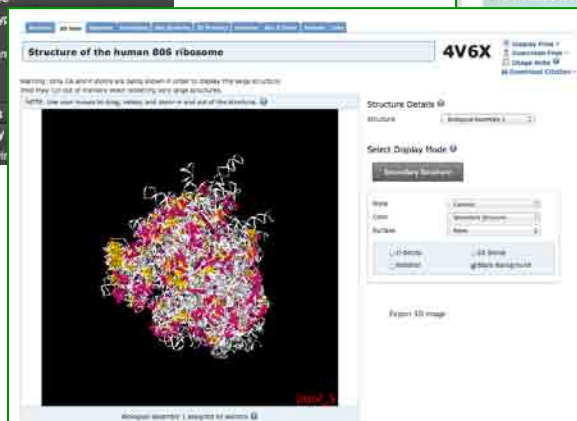


**PDBe**

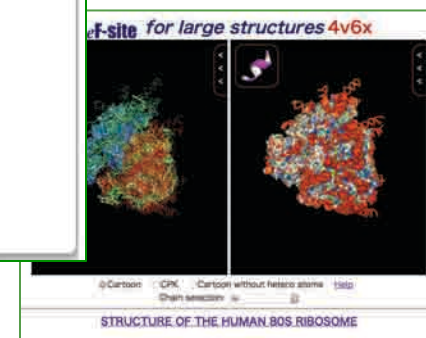


**PDBj**

**4v6x: structure of human 80S ribosome, 89 chains, 4 MDa**



**RCSB-PDB**



# Current Supported Archival Formats

## *protein structure format universe*

**PDB (*ca.* 1974)**

**PDBx/mmCIF (*ca.* 1997)**

**PDBML (*ca.* 2005)**

**RDF (*ca.* 2011)**



In managing the formats, PDBx is the master format.

ATOM	1	N	GLN	A	39	24.690	-27.754	24.275	1.00	60.76	N
ATOM	2	CA	GLN	A	39	23.581	-26.768	24.416	1.00	60.98	C
ATOM	3	C	GLN	A	39	23.990	-25.379	23.905	1.00	59.98	C
ATOM	4	O	GLN	A	39	25.070	-25.209	23.330	1.00	60.25	O
ATOM	5	CB	GLN	A	39	23.136	-26.685	25.878	1.00	60.69	C
ATOM	6	N	VAL	A	40	23.115	-24.395	24.122	1.00	59.58	N
ATOM	7	CA	VAL	A	40	23.342	-23.010	23.690	1.00	57.26	C
ATOM	8	C	VAL	A	40	24.000	-22.152	24.778	1.00	56.00	C
ATOM	9	O	VAL	A	40	23.992	-20.920	24.692	1.00	55.53	O
ATOM	10	CB	VAL	A	40	22.015	-22.337	23.275	1.00	57.32	C

PDB

```

loop_
_atom_site.group_PDB
_atom_site.id
_atom_site.auth_atom_id
_atom_site.type_symbol
_atom_site.auth_comp_id
_atom_site.auth_asym_id
_atom_site.auth_seq_id
_atom_site.Cartn_x
_atom_site.Cartn_y
_atom_site.Cartn_z
_atom_site.pdbx_PDB_model_num
_atom_site.occupancy
_atom_site.pdbx_auth_alt_id
_atom_site.B_iso_or_equiv

```

ATOM	1	N	N	GLN	A	39	24.690	-27.754	24.275	1	1.000	.	60.760
ATOM	2	CA	C	GLN	A	39	23.581	-26.768	24.416	1	1.000	.	60.980
ATOM	3	C	C	GLN	A	39	23.990	-25.379	23.905	1	1.000	.	59.980
ATOM	4	O	O	GLN	A	39	25.070	-25.209	23.330	1	1.000	.	60.250
ATOM	5	CB	C	GLN	A	39	23.136	-26.685	25.878	1	1.000	.	60.690
ATOM	6	N	N	VAL	A	40	23.115	-24.395	24.122	1	1.000	.	59.580
ATOM	7	CA	C	VAL	A	40	23.342	-23.010	23.690	1	1.000	.	57.260
ATOM	8	C	C	VAL	A	40	24.000	-22.152	24.778	1	1.000	.	56.000
ATOM	9	O	O	VAL	A	40	23.992	-20.920	24.692	1	1.000	.	55.530
ATOM	10	CB	C	VAL	A	40	22.015	-22.337	23.275	1	1.000	.	57.320
ATOM	11	N	N	ALA	A	41	24.560	-22.804	25.797	1	1.000	.	54.570

PDBx/mmCIF

# PDBx/mmCIF Software Support

- **Phenix and Refmac** – produce native PDBx files for deposition
- **MMDB** - macromolecular object library in CCP4
- **iotbx.cif/ucif** - CCTBx C++/Python IO library with dictionary validation
- **CCIF** – CCP4 C++ library with FORTRAN support and dictionary validation
- **CBFLib** - ANSI-C library for CIF & imgCIF files
- **mmLIB** - Python toolkit supporting CIF & mmCIF
- **BioPython** - Python toolkit for computational biology
- **PyCifRW** - Python CIF/mmCIF parsing tools
- **BioJava** - Java mmCIF IO package
- **STAR::Parser** – Perl mmCIF parser and molecular object library
- **RCSBTools** - C++/Python parsing and dictionary validation tools plus many other supporting format conversion and data management applications
- **Visualization** - **UCSF Chimera, Jmol, OpenRasMol, Coot, CCP4mg, jV, Molmil**



# wwPDB Service site for a new format

***<http://mmcif.wwpdb.org/> or <http://mmcif.pdbj.org/>***

PDBx/mmCIF Home Dictionaries Documentation Downloads Contact Us

Search current dictionary

## PDBx/mmCIF Dictionary Resources

This site provides information about the format, dictionaries and related software tools used by the Worldwide Protein Data Bank ([wwPDB](http://wwpdb.org/)) to define data content for deposition, annotation and archiving of PDB entries.

[Browse the current dictionary »](#)

### Dictionaries

- [Browse the current dictionary»](#)
- [Download/view all dictionaries »](#)
- [Search dictionaries»](#)

### Documentation

- [PDB -> PDBx/mmCIF correspondences »](#)
- [PDBx/mmCIF for large structures »](#)
- [Software resources »](#)
- [C++ »](#) and [Python »](#) programming examples
- [File syntax »](#) and [dictionary organization »](#)
- [Atomic »](#) and [molecular »](#) descriptions
- [References »](#)
- [Glossary »](#)

### FAQs

Questions about PDBx/mmCIF format, and data content, or software tools? Check out the [FAQ»](#)

# wwPDB Service site for a new format

***<http://mmcif.pdbj.org/converter/index.php?l=en>***

**PDBx/mmCIF**

[Home](#)

[Dictionaries](#)

[Documentation](#)

[Downloads](#)

[Format Conversion](#)

[Contact Us](#)

[English](#) [日本語](#)

## PDB format - PDBx/mmCIF conversion service

You can convert a molecular structural data into another format. The type of uploaded file is determined automatically. When the type is mmCIF and PDB format, it is converted into PDB format and mmCIF, respectively. The gzip compressed files that end ".gz" of the name, are also available. When they are gzipped, the converted files are also gzipped.

### 1. Specify a source file to convert

Specify a source file to convert. The maximum size of the file is 1GB.

ファイルが選択されていません。

### 2. Confirm the contents of operations

### 3. Execute conversion & Download the converted file

When you convert a large structure mmCIF file into the PDB format, it will be treated as following:

- When it includes more than 99999 atoms, all the atomids larger than 99999 are rewritten to 99999.
- When the chain id (auth\_asym\_id) has two letters, it will be described as it is by using unused 21th column and defined 22th column.

# Data-out from PDBj

<http://pd bj.org/>

## Amino acid sequence (FASTA)

```
ftp://ftp.pdbj.org/XML/pdbmlplus/fasta_seq_data/Igof_seq.txt
>1GOF: GALACTOSE OXIDASE
ASAPIGSAISNNNAVTCDSAGSGNECNKAIDGNKDTFWHTFYGANDPKFPHTYITDMK
TTQNVNGLSHLFRQDNQNGWIGRIHEVYLSDDGTHWGSFVAGSWFADSTKYSNFTETP
ARYVRLVAITEANGQWTSIAEINIVQASSTAPQFGLRWGPTIDLPVFAAAIEPTS
GRVLARSTYNDAPGGPGIPLTSSDPSTVISRVTYVTKHDFCPGISMDQNGQIV
VTGNDARKSLYDSSDSWPGDMQVARGVQSSATMSDGRVTFIGSSSGVFENGE
VYSPSKTWTSLPNAKVNPHLTADKQGLYRSNHAHLFGWKGVSFQAGPSTAMNWTYS
GSDVKSAGKQSGNRGVPADMCNNAVYDVGKILTFGSPDYQSDATTNAHIITLG
EPGTSNPTVFADNGLIARTFTHSVULPDGSTFIQGGRCIPFEDSTVFTPEIVPEQ
DTFYKQNPBIVVYVTEISILLPGGRVFNQGGGLCCCTTFNDAQITFFNYLNSNGL
ATRPKITRTSTQSVVGGRITISTDSSISKASLIRYGTATHTVHTQRRIPILTNNHGG
SYSFQVDSGVALPGYVNLVFNNSAGVPSVASTIRVTQ
```

A perfect match for your query "Igof" has been found within the [PDB] category. Alternatively you can [perform a keyword search](#).

**Summary** | Structural details | Experimental details | Functional details | Sequence Neighbor | Downloads

### 1GOF

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

**Summary for 1GOF**

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

**Functional Keywords** oxidoreductase(oxygen(a))

**Biological source** Hypomyces rosellus

**Cellular location** Secreted [Q01745](#)

**Total number of polymer chains** 1

**Total molecular weight** [58785.89](#)

**Authors** Ito, N., Phillips, S.E.V., Knowles, P.F. (deposition date: 1993-09-30, release date: 1994-01-31, modification date: 2011-07-13)

**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: 10.1038/35087a0](#) [Import into Mendeley](#)

**Experimental method** X-RAY DIFFRACTION (1.7 Å)

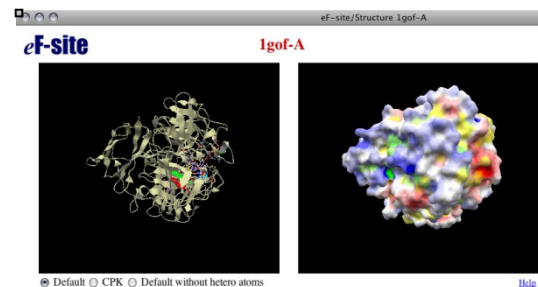
**Structure validation**

Metric	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.3%
Sidechain outliers		2.9%
RSRZ outliers		0.3%

Worse Better

**Database information**

- RCSB-PDB
- PDBe
- Yorodumi
- CATH
- FSSP
- SCOP
- VAST
- PISA
- UniProt [Q01745](#)
- KEGG [1.1.3.9](#)
- ExPASy [1.1.3.9](#)
- JUBMB [1.1.3.9](#)
- eF-site [Igof-A](#)
- Electron Density Map (JV)
- Electron Density Map (molmil)



Functional site	focus & details	A:495	ACT_SITE
1) A:495	on	off	Y
2) A:272	on	off	Proton acceptor.
3) A:495	on	off	Swiss-Prot: 1
4) A:496	on	off	
5) A:581	on	off	
6) A:228	on	off	
7) A:290	on	off	
8) A:272	on	off	
9) A:495	on	off	
10) A:75-87	on	off	
11) A:194	on	off	
12) A:227-228	on	off	
13) A:372	on	off	

## Data viewer at PDBj

Graphic viewer: *jv* and *Molmil*

<http://pd bj.org/jv/>



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

Kinjo et al. NAR 40, D453 (2012)



**Yokochi et al. (2016) J. Biomed. Semantics, 7:16.□**

**X-ray Structure** ☐

**Cryo-EM** ☐

**SAXS** ☐

**Large Complex** ☐

**Sequence** ☐

**Exp. Information (X-ray, NMR, EM, etc)** ☐

**PPI (interaction)** ☐

**c.jp** ☐

**NMR Structure** ☐

**PDB** **BMRB**

RefSeq, GenBank, DOI, EMBL, PubMed, UniProt, PIR, WWW URL, NCBI taxonomy, EC number, PRF, NBDC/DB, Chem Comp, DDBJ

File: bmr16761.rdf

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Summary

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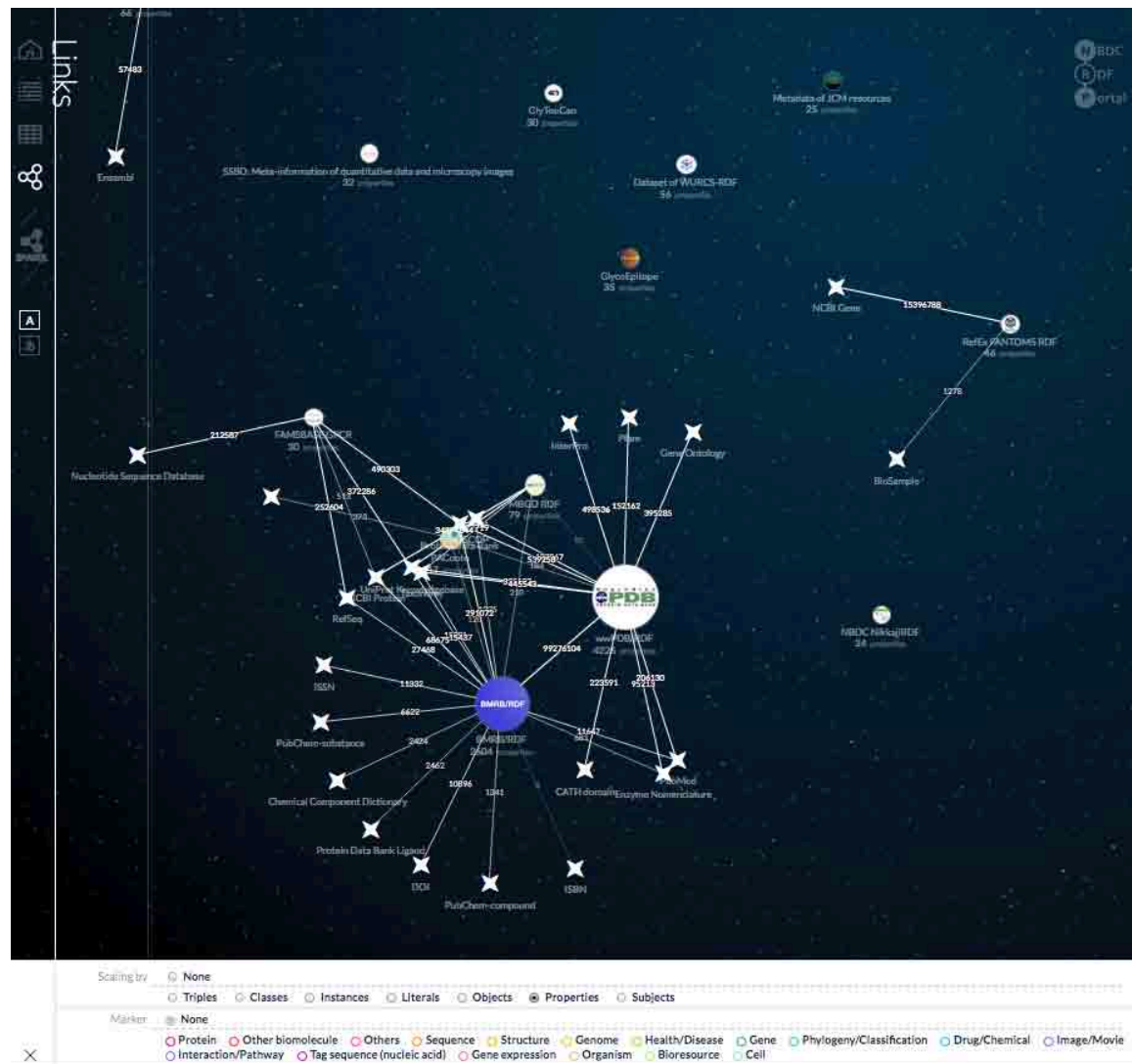
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