

The 54th Ann. Meeting of BSJ Tsukuba, 25 November 2016

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 (ww-PDB), 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

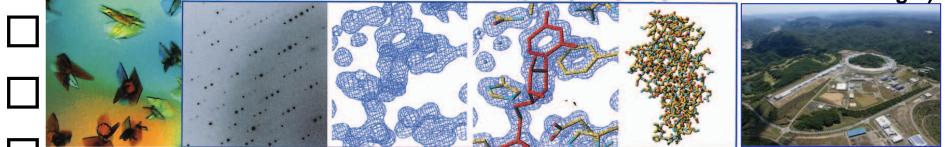


PDB: Protein Data Bank since 1971

Collects 3D structural information of biomolecules

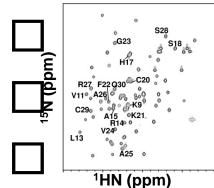
• X-ray Crystallography

XFEL & Synchrotron (SACLA & SPring-8)



Crystal ⊞ III -ray diffraction ⊟ Electron density map ⊟ I tomic model □

Nuclear Magnetic Resonance (NMR)





NMR spectrometer with superconducting 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)□

CRYSTALLOGRAPHY

Protein Data Bank

A repository system for protein crystallographic data will be operated jointly by the Crystallographic Data Centre, Cambridge, and the Brookhaven National Laboratory, The system will be responsible for storing atomic coordinates, structure factors and electron density maps and will make these data available on request. Distribution will be on magnetic tape in machine-readable form whenever possible. There will be no charge for the service other than handling costs. Files will be updated as new material is received. The total holding will be



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"



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.

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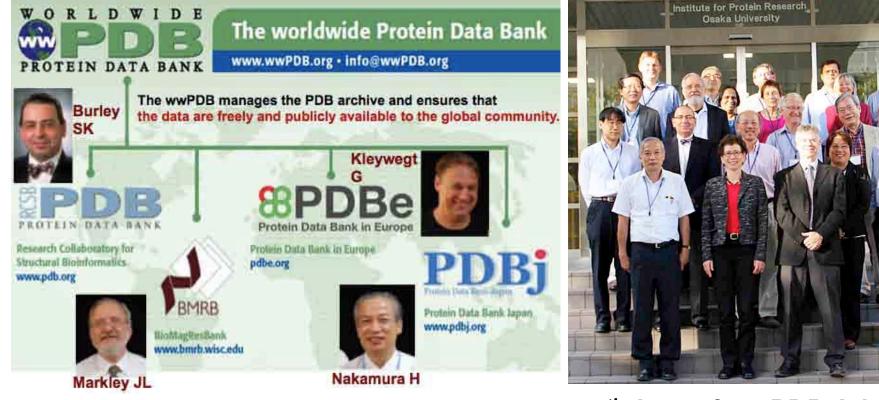
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The wwPDB (world-wide PDB)

wwPDB since 2003



wwpdb.org

12th 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

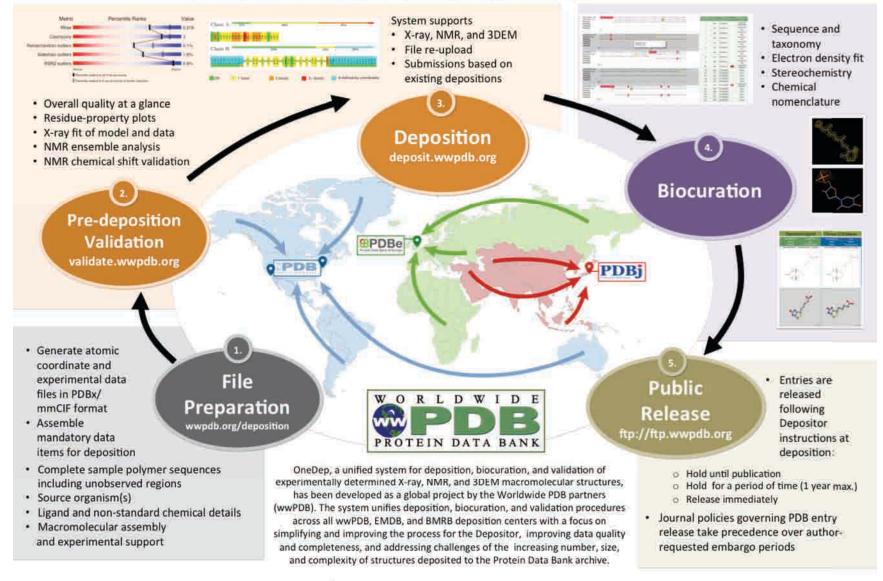


Acknowledgements

OneDep: Unified Deposition Portal for the Protein Data Bank



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



PDBe _____

OneDep: Unified Deposition Portal for the wwPDB

VALIDATION + DEPOSITION + DATA DICTIONARIES + DOCUMENTATION + TASK FORCES + STATISTICS - ABOUT +

wwpdb.org

WORLDWIDE

P.P.E

and complex assemblies.

community.

BMRB

PDBe

PDB

RCS8 PD8

Data Bank

Data Bank

Since 1971, the Protein Data Bank archive (PDB)

about the 3D structures of proteins, nucleic acids,

PDB is freely and publicly available to the global

Learn more about PDB HISTORY and FUTURE.

wwPDB Members

wwPOB data centers serve as deposition, annotation,

Collects NMR data from any experiment and captures

assigned chemical shifts, coupling constants, and peak

lists for a variety of macromolecules; contains derived annotations such as hydrogen exchange rates, pKa

Rich information about all PDB entries, multiple search

visualisation and validation of NMR and EM structures.

and browse facilities, advanced services including

PDBePISA, PDBeFold and PDBeMotif, advanced

Supports browsing in multiple languages such as

Japanese, Chinese, and Korean; SeSAW identifies

functionally or evolutionarily conserved motifs by locating

and annotating sequence and structural similarities, tools

Simple and advanced searching for macromolecules and

ligands, tabular reports, specialized visualization tools,

sequence-structure comparisons, RCSB PDB Mobile, Molecule of the Month and other educational resources

Biological Magnetic Resonance

values, and relaxation parameters.

Protein Data Bank in Europe

tools for bioinformaticians.

Protein Data Bank Japan

for bioinformaticians, and more.

» Research Collaboratory for

Structural Bioinformatics Protein

and distribution sites of the PDB archive. Each site offers tools for searching, visualizing, and analyzing PDB data.

The Worldwide PDB (wwPDB) organization manages the PDB archive and ensures that the

has served as the single repository of information

wwPDB Resources

Data Dictionaries

- Macromolecular Dictionary (PDBx/mmCIF) Small Molecule Dictionary (CCD)
- Peptide-like antibiotic and inhibitor molecules (BIRD)

Annotation

BMRB

8PDBe

PDB

Procedures and policies > improvements for consistency and accuracy

Community Input: Task Forces and Working Groups

- Validation Task Forces (X-ray, NMR, 3DEM)
- Small Angle Scattering Task Force
- PDB/mmCIF Working Group
- Hybrid/Integrative Methods Task Force Ligand Validation Workshop

PDB Data Growth & Usage Statistics

- Depositions: by data center, by year, and by depositor location
- > Downloads: by year for all entries

Workshops & Symposia

» Summaries and presentations from past meetings and events

Information for Journals

 Policies, procedures, coordination with publishers, and preferred Instructions to Authors

Cite www.RDB:

Nature Structural Biology 10, 980 (2003) doi: 10.1038/nsb1203-980 More publications

News & Announcements

wwPD8

Validate Structure

Deposit Structure

All Deposition Resources

Download Archive

Instructions

https://validate.wwpdb.org now generates preliminary validation reports for structures solved by NMR and 3D Electron Microscopy, in addition to X-ray crystallography.

Read more

EMDB Will Be Mandatory for PDB Depositions of 3DEM models Starting September 6th, 2016

Read more

06/23/2016

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.

Read more

All News

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News & Announcements

at PDB-101, and more

Download Archive

RCSB PDB ftp PDBe ftp PDBj ftp Instructions

CITE WWFOR

Nature Structural Biology 10, 980 (2003) doi: 10.1038/nsb1203-980

08/05/2016 wwPDB Validation Server Upgrade The new wwPDB Validation Server at

07/06/2016

Announcement: Map Volume Deposition to

Effective September 6th, 2016, deposition to the PDB of atomic models determined by 3D Electron cryo-Microscopy (3DEM) will require prior or simultaneous deposition of the associated 3DEM volume maps to EMDB.

PDBi



OneDep: Unified Deposition Portal for the wwPDB

| 1 | Welcome to the Worldwide Proton Data B |
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| Existing deposition | Start a new deposition |
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OneDep: Unified Deposition Portal for the wwPDB



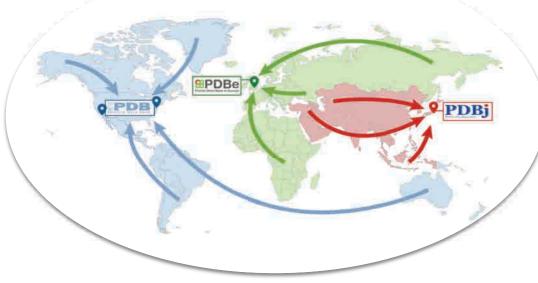


| Existing deposition | | | Start a new deposition | |
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| To enable better annotation and tracking, the wwPDB partners encourage depositors to provide ORCID identifiers and information on relevant grants funding their research when depositing PDB data. 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 | Country Experimental method X-Ray Diffraction Electron Microscopy Solution NMR Neutron Diffraction Electron Crystallography Solid-state NMR Fiber Diffraction Requested accession codes PD8 EMD8 6MRB | Japon | Reset country 0 | |
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PDB Depositions & Annotations

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

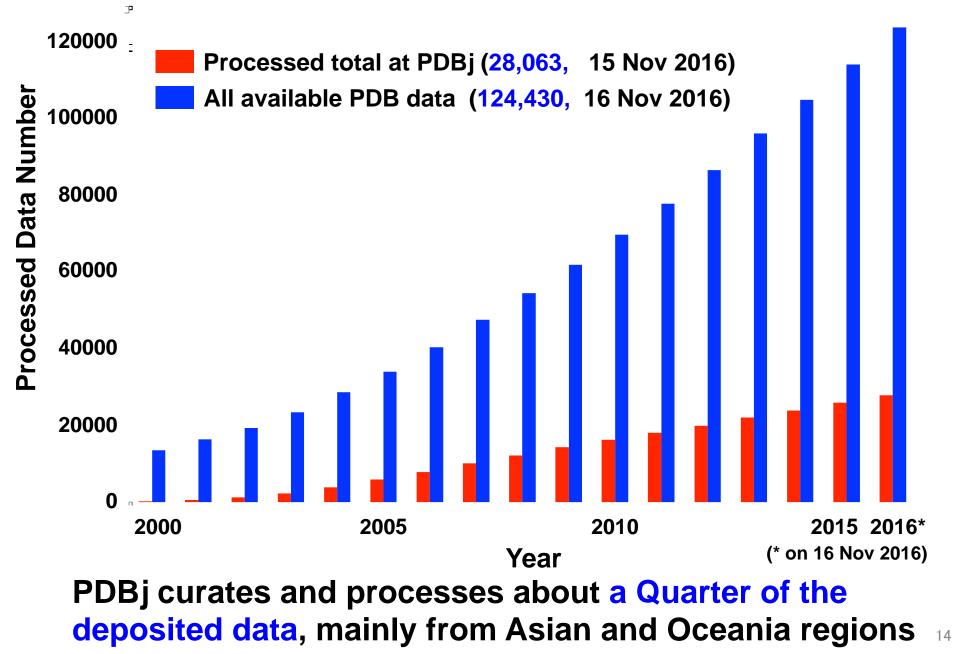


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Last Updated: 15 September 2015

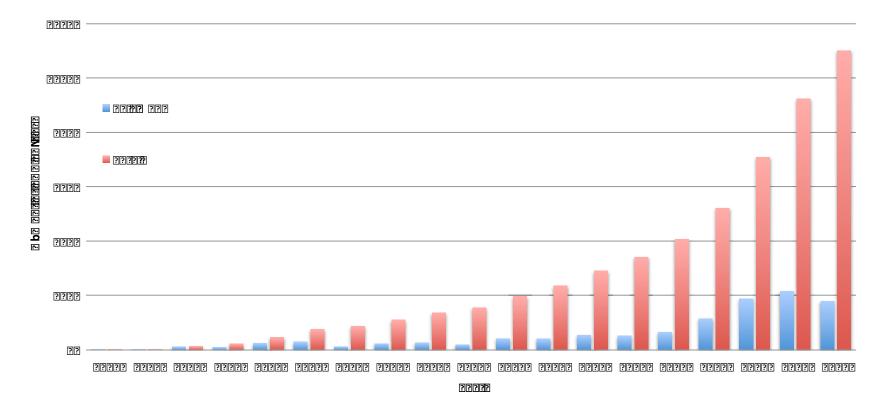


Data-in at PDBj and wwPDB





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

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| ORCID | FOR RESEARCHERS | FOR ORGANIZATIONS | ABOUT | HELP | SIGN IN | |
| Connecting Research and Researchers | | | 11 | 11 | | |

DISTINGUISH YOURSELF IN THREE EASY STEPS

ORCID provides a persistent digital identifier that distinguishes you from every other researcher and, through integration in key research workflows such as manuscript and grant submission, supports automated linkages between you and your professional activities ensuring that your work is recognized. Find out more.



Example: 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 (i)

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 : 2013-06-20
 - 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 A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

Top page of Validation report

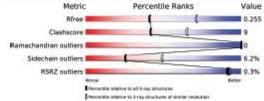
Mandatory Experimental data

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

¹ Overall quality at a glance (i)

The reported resolution of this entry is 260 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 (i)

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 colorcoded 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 above 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

Chain A:



Nature Structural & Molecular Biology 23, 871 (2016) doi:10.1038/nsmb.3307, Published online 05 October 2016



nature structural & molecular biology

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/validationreports). 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

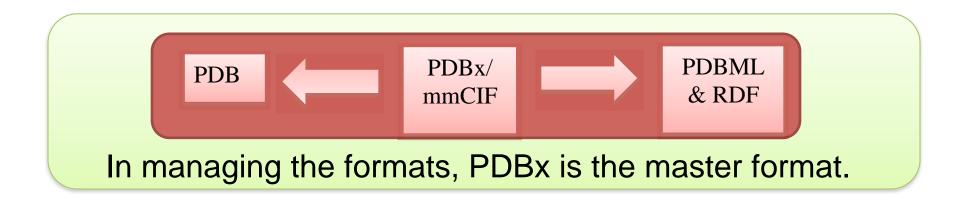
- As of December 2014, large structures are no longer split into multiple PDB entries but are released as single PDBx/mmCIF and PDBML files
 - Existing split entries were consolidated into single entries
 - A bundle of best-effort PDB files (PDB bundle) is available for every large structure through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

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Current Supported Archival Formats protein structure format universe

PDB (*ca.* 1974) PDBx/mmCIF (*ca.* 1997) PDBML (*ca.* 2005) RDF (*ca.* 2011)



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| ATOM | 3 | C | GLN A | 39 | 23.990 | -25.379 | 23.905 | 1.00 59. | 98 C | |
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| ATOM | 5 | CB | GLN A | 39 | 23.136 | -26.685 | 25.878 | 1.00 60. | 69 C | |
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| 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 | 0 | 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 | |
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loop_

PDB

PDBx/mmCIF

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| _atom_s: | ite.Ca | rtn_ | У | | | | | | | | | | |
| _atom_s: | ite.Ca | rtn_ | z | | | | | | | | | | |
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| _atom_s: | ite.oc | cupa | ncy | | | | | | | | | | |
| | - | | | | d | | | | | | | | |
| _atom_s: | ite.B_ | iso_ | or_e | quiv | | | | | | | | | |
| ATOM | | | N | GLN | A | 39 | 24.690 | -27.754 | | 1 | 1.000 | • | 60.760 |
| ATOM | 2 | CA | C | GLN | A | 39 | 23.581 | -26.768 | 24.416 | 1 | 1.000 | • | 60.980 |
| ATOM | | | C | GLN | A | | 23.990 | -25.379 | | 1 | | • | 59.980 |
| ATOM | | 0 | 0 | GLN | A | 39 | 25.070 | -25.209 | 23.330 | 1 | 1.000 | • | 60.250 |
| ATOM | | CB | C | GLN | A | | 23.136 | -26.685 | 25.878 | 1 | | • | 60.690 |
| ATOM | | N | N | VAL | A | 40 | 23.115 | -24.395 | 24.122 | 1 | | • | 59.580 |
| ATOM | | CA | C | VAL | Α | 40 | 23.342 | -23.010 | 23.690 | 1 | | • | 57.260 |
| ATOM | | | - | | Α | | | | | 1 | | • | 56.000 |
| ATOM | | - | - | VAL | Α | | | | | 1 | | • | 55.530 |
| ATOM | | - | - | | Α | | | | | _ | | • | 57.320 |
| ATOM | 11 | N | N | ALA | Α | 41 | 24.560 | -22.804 | 25.797 | 1 | 1.000 | • | 54.570 |
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GLN A 39 23.581 ATOM 3 C C GLN A 39 23.581 ATOM 3 C C GLN A 39 23.990 ATOM 4 0 0 GLN A 39 23.090 ATOM 5 CB C GLN A 39 23.136 ATOM 6 N N VAL A 40 23.115 ATOM 7 CA C VAL A 40 23.342 ATOM 8 C C VAL A 40 23.992 ATOM 9 0 0 VAL A 40 23.992 ATOM 10 CB C VAL A 40 22.015</pre></th> <th><pre>_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.Cartn_z _atom_site.cartn_z _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 ATOM 2 CA C GLN A 39 23.581 -26.768 ATOM 3 C C GLN A 39 23.581 -26.768 ATOM 3 C C GLN A 39 23.990 -25.379 ATOM 4 0 0 GLN A 39 23.136 -26.685 ATOM 5 CB C GLN A 39 23.136 -26.685 ATOM 6 N N VAL A 40 23.115 -24.395 ATOM 6 N N VAL A 40 23.342 -23.010 ATOM 8 C C VAL A 40 23.342 -23.010 ATOM 8 C C VAL A 40 23.992 -20.920 ATOM 9 0 0 VAL A 40 23.992 -20.920 ATOM 10 CB C VAL A 40 22.015 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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/

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 Resources

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

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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 »

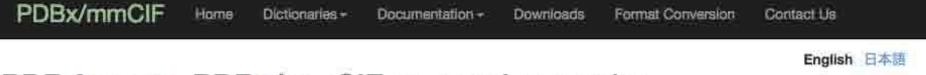
FAQs

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



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. 選択...ファイルが選択されていません。 Submit Reset

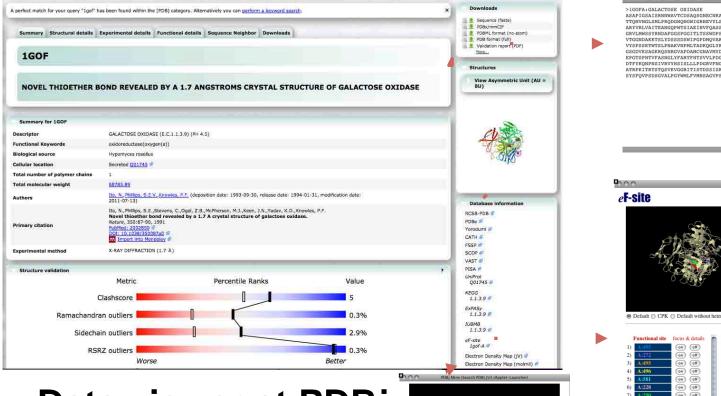
2. Confirm the contents of operations

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 rewrited 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.

http://pdbj.org/



Data viewer at PDBj

Graphic viewer: *N* and *Molmil http://pdbj.org/jV/*





Color:

Default

group

chain

ator

(show command area)

Amino acid sequence (FASTA)

 Image: State of the state

| TTQNVNGLSMLPRQDGNQNGWIGRH ARYVRLVAITEANGQPWTSIAEINV | EVYLSSDGTNWGSFVASGSWFADSTTKYSNFET FQASSYTAPQPGLGRWGPTIDLPIVPAAAAIEF | RP TS |
|---|--|--|
| VTGGNDAKKTSLYDSSDSNIFGPD VYSPSKTWTSLPNAKVNPHLTADK GSGDVKSAGKRQSNRGVAPDAMCGN EPGTSPNTVFASNGLYFARTFHTSV DTFYKQPPNSIVRVYHSISLLLPDG ATRFKITRTSTQSVKVGGRITISTD | MQVARGYQSSATMSDGRVFTIGGSWSGGVEEK QQLYRSDHHAMLFGWKKGSVFQAGPSTAANWY IAVMYDAVKGKILTFGGSPDYQDSDATTNAHIIT VLPDGSTFITGQQRRGIPFDSSTVFTPEIYV RVFNGGGGLCGCTTNHFDAQIFTPNYLYNSM SSISKASLIRYGTATHTVNTDQRFIPLTLTNNG | GE TS LG EQ NL |
| | | |
| B 00 | eF-site/Structure 1q | A 0f-A |
| | 1gof-A | |
| O Efault ① CPK ② Default witho | nu hetero atoris | lik |
| Functional site focus & details 1 \$195 (m) (m) 2 \$1272 (m) (m) 3 \$195 (m) (m) 4 \$1531 (m) (m) 5 \$1532 (m) (m) 6 \$1253 (m) (m) 7 \$1290 (m) (m) 8 \$1292 (m) (m) 9 \$1365 (m) (m) 11 \$1294 (m) (m) 12 \$12722 (m) (m) | Ac405 ACT_SITE sequence Y description Proton acceptor, source Swise-Prot : 1 | |
| | - ar surfaco | DB· <i>oF-si</i> |
| | Transacture Transacture ARTVALAUMSSYNNDAPGOSPORTTER Transacture GRUAUMSSYNNDAPGOSPORTTER Transacture GRUAUMSSYNNDAPGOSPORTTER Transacture VTGBDAKATSLIDDSSDBTIPGT Transacture VTGBDAKATSLIDDSSDBTIPGT Transacture VTGBDAKATSLIDDSSDBTIPGT Transacture PETGSFNTAL Transacture PETGSFNTAL Transacture PETGSFNTAL Transacture VTGBDAKATSJUDSSDAU Transacture VTGBDAKATS | ef-site lgof-A Image: Signed State Sta |

nttp://ef-site.hgc.jp/eF-site/

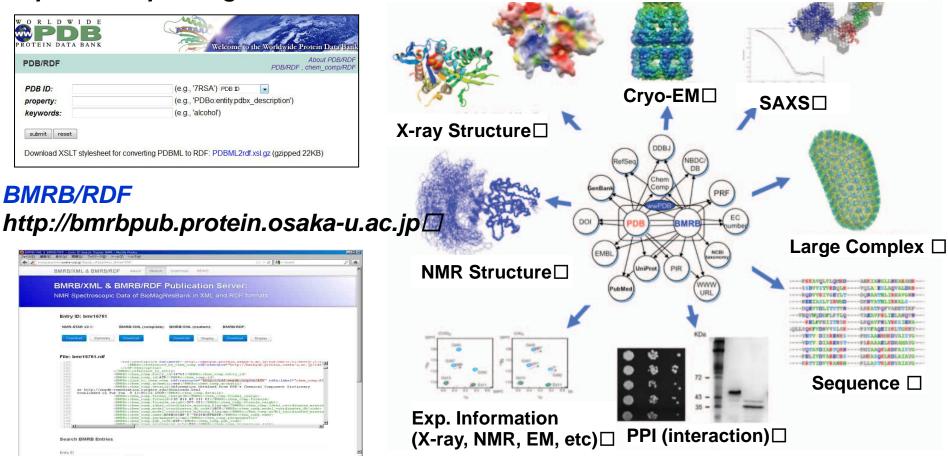
Kinjo et al. NAR 40, D453 (2012)

PDBJ WORLDWED WWPDB/RDF format for Semantic Web

Service from wwPDB

wwPDB/RDF http://rdf.wwpdb.org/

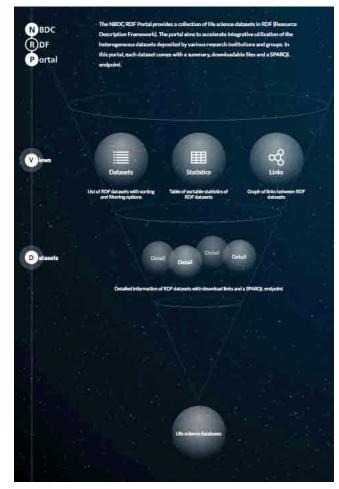
Kinjo et al. (2017) Nucl. Acids Res. doi: 10.1093/nar/gkw962. Yokochi et al. (2016) J. Biomed. Semantics, 7:16.



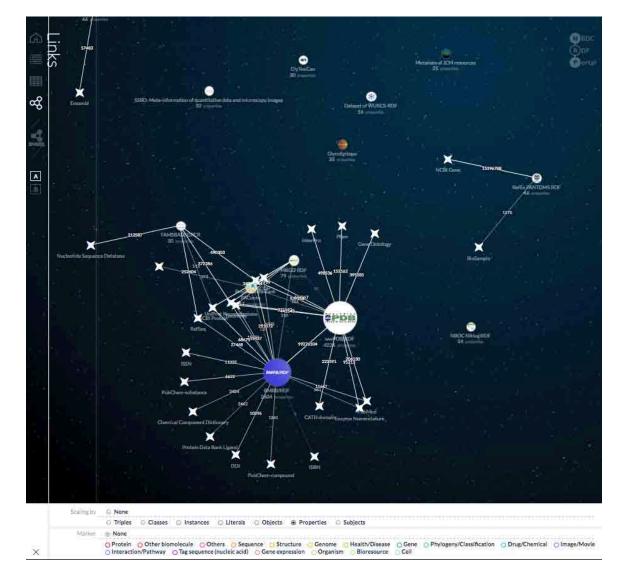
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Integration to NBDC RDF-portal



NBDC RDF-Portal https://integbio.jp/rdf/





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