



X-tal Raw Data Archive (XRDa):

A crystallographic raw diffraction image archive in Asia

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Institute for Protein Research, Osaka University

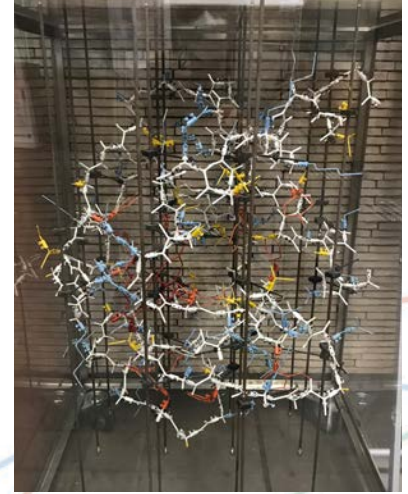
In 1971:

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

Nature New Biology **233**, page 223 (1971)



Cytochrome c @4.5 Å in 1971 and @2.3 Å in 1975, which was the 1st Asian and 21st PDB entry in the entire archive.

J. Biochem. (Tokyo) **70**, 913-924 (1971)

J. Biochem. (Tokyo) **77**, 147-162 (1975)

Early Data-out services of PDB in Japan

J. Mol. Biol. (1977) **112**, 535–542

The Protein Data Bank: A Computer-based Archival File for Macromolecular Structures

The Protein Data Bank is a computer-based archival file for macromolecular structures. The Bank stores in a uniform format atomic co-ordinates and partial bond connectivities, as derived from crystallographic studies. Data included in each data entry gives pertinent information for the structure at hand (e.g. species from which the molecule has been obtained, resolution of diffraction data, literature citations and specifications of secondary structure). In addition to atomic co-ordinates and connectivities, the Protein Data Bank stores structure factors and phases, although these latter data are not placed in any uniform format. Input of data to the Bank and general maintenance functions are carried out at Brookhaven National Laboratory. All data stored in the Bank are available on magnetic tape for public distribution, from Brookhaven (to laboratories in the Americas), Tokyo (Japan), and Cambridge (Europe and worldwide). A master file is maintained at Brookhaven and duplicate copies are stored in Cambridge and Tokyo. In the future, it is hoped to expand the scope of the Protein Data Bank to make available co-ordinates for standard structural types (e.g. α -helix, RNA double-stranded helix) and representative computer programs of utility in the study and interpretation of macromolecular structures.

J. Mol. Biol., **112**, 535–342, 1977

THE PROTEIN DATA BANK

NEWSLETTER

Number 10

October 1979

This brief newsletter provides up-to-date holdings information (Tables 1-5) and a Request Form. A full Newsletter will be distributed in January, and any of the persons listed below will be happy to answer inquiries.

We would like Japanese users to note that the center of Data Bank activity in Japan has been transferred to the Institute for Protein Research at Osaka University. Professor Masao Kakudo of Osaka has assumed the data distribution functions formerly carried out by Professor Mitsuo Tasumi of the University of Tokyo. We wish to thank Professor Tasumi for all his efforts on behalf of the Bank.

It is expected that the Protein Data Bank be acknowledged in publications which result from work making use of the Bank's services. In citing the Protein Data Bank in print, we suggest that a reference be included to F. C. Bernstein, T. F. Koetzle, G. J. B. Williams, E. F. Meyer, Jr., M. D. Brice, J. R. Rodgers, O. Kennard, T. Shimanouchi, and M. Tasumi, *J. Mol. Biol.* **112**, 535–42 (1977). When papers are published describing structures for which coordinates have been deposited, we suggest that this same citation be used and our address also supplied.

PDB Newsletter, No.10, Oct. 1979

Table 24.1.3.2. *PDB mirror sites as of May 1999*

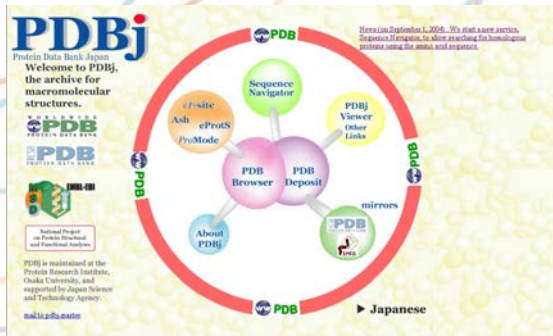
Official PDB mirror sites

Argentina: University of San Luis
 Australia: Australian National Genomic Information Service, Sydney;
 The Walter and Eliza Hall Institute of Medical Research, Melbourne
 Brazil: ICB UFMG, Inst. de Ciencias Biologicas, Univ. Federal de Minas Gerais
 China: Institute of Physical Chemistry, Peking University, Beijing
 France: Institut de Génétique Humaine, Montpellier
 Germany: GMD, German National Research Center for Information Technology, Sankt Augustin
 India: Bioinformatics Centre, University of Pune
 Israel: Weizmann Institute of Science, Rehovot
 Japan: Institute of Protein Research, Osaka University
 Poland: ICM Interdisciplinary Centre for Modelling, Warsaw University
 Taiwan: National Tsing Hua University, HsinChu
 United Kingdom: Cambridge Crystallographic Data Centre, Cambridge;
 EMBL Outstation, EBI, Hinxton
 United States: Bio Molecular Engineering Research Center, Boston University; North Carolina Supercomputing Center, Research Triangle Park; University of Georgia, Athens, Georgia; PDB at Brookhaven National Laboratory

Inter. Table of Cryst. Vol F, 1999

Magnetic Tape ➡ CD-ROM ➡ Internet (BNL PDB mirror site @Osaka 1998)

PDBj was founded in 2000



Data-in and Data-out services in Japan.



<https://pdj.org>. in English, Japanese,
Chinese and Korean

wwPDB was founded in 2003

CORRESPONDENCE

Announcing the worldwide Protein Data Bank

In recognition of the growing international and interdisciplinary nature of structural biology, three organizations have formed a collaboration to oversee the newly formed worldwide Protein Data Bank (wwPDB; <http://www.wwpdb.org/>). The Research Collaboratory for Structural Bioinformatics (RCSB), the Macromolecular Structure Database (MSD) at the European Bioinformatics Institute (EBI) and the Protein Data Bank Japan (PDBj) at the Institute for Protein Research in Osaka University will serve as custodians of the wwPDB, with the goal of maintaining a single archive of macromolecular structural data that is freely and publicly available to the global community.

The wwPDB represents a milestone in the evolution of the Protein Data Bank (PDB; <http://www.pdb.org/>)^{1,2}, which was established in 1971 at Brookhaven National Laboratory as the sole international repository for three-dimensional structure data of biological macromolecules. Since July 1, 1999, the PDB has been managed by three member institutions of the RCSB: Rutgers, The State University of New Jersey; the San Diego Supercomputer Center at the University of California, San Diego; and the Center for Advanced Research in Biotechnology of the National Institute of Standards and Technology.

The wwPDB recognizes the importance of providing equal access to the database—both in terms of depositing and retrieving data—from different regions of the world. Therefore, the wwPDB members will continue to serve as deposition, data processing,

mentation will be kept publicly available and the distribution sites will mirror the PDB archive using identical contents and subdirectory structure. However, each member of the wwPDB will be able to develop its own web site, with a unique view of the primary data, providing a variety of tools and resources for the global community.

An Advisory Board consisting of appointees from the wwPDB, the International Union of Crystallography and the International Council on Magnetic Resonance in Biological Systems will provide guidance through annual meetings with the wwPDB consortium. This board is responsible for reviewing and determining policy as well as providing a forum for resolving issues related to the wwPDB. Specific details about the Advisory Board can be found in the wwPDB charter, available on the wwPDB web site.

The RCSB is the 'archive keeper' of wwPDB. It has sole write access to the PDB archive and control over directory structure and contents, as well as responsibility for distributing new PDB identifiers to all deposition sites. The PDB archive is a collection of flat files in the legacy PDB file format³ and in the mmCIF⁴ format that follows the PDB exchange dictionary (<http://deposit.pdb.org/mmCIF/>). This dictionary describes the syntax and semantics of PDB data that are processed and exchanged during the process of data annotation. It was designed to provide consistency in data produced in structure laboratories, processed by the wwPDB members and used in bioinformatics applications. The PDB archive does not include the websites,

description conventions of the PDB exchange dictionary. In addition, the legacy PDB format would not be modified unless there is a compelling reason for a change. Should such a situation occur, all three wwPDB members would have to agree on the changes and give the structural biology community 90 days advance notice.

The creation of the wwPDB formalizes the international character of the PDB and ensures that the archive remains single and uniform. It provides a mechanism to ensure consistent data for software developers and users worldwide. We hope that this will encourage individual creativity in developing tools for presenting structural data, which could benefit the scientific research community in general.

ACKNOWLEDGMENTS
The RCSB PDB is supported by funds from the National Science Foundation, the Department of Energy, and the National Institutes of Health. The MSD-EBI is supported by funds from the Wellcome Trust, the European Union (TEMBLOR, NMRQUAL, SPINE, AUTOSTRUCT, and IIMS awards), CCP4, the Biotechnology and Biological Sciences Research Council (UK), the Medical Research Council (UK), and the European Molecular Biology Laboratory. PDBj is supported by grant-in-aid from the Institute for Bioinformatics Research and Development, Japan Science and Technology Corporation (JST), and the Ministry of Education, Culture, Sports, Science and Technology (MEXT).

Helen Berman¹, Kim Henrick² & Haruki Nakamura³

¹RCSB, Piscataway, New Jersey; Rockville,

Maryland and La Jolla, California, USA.

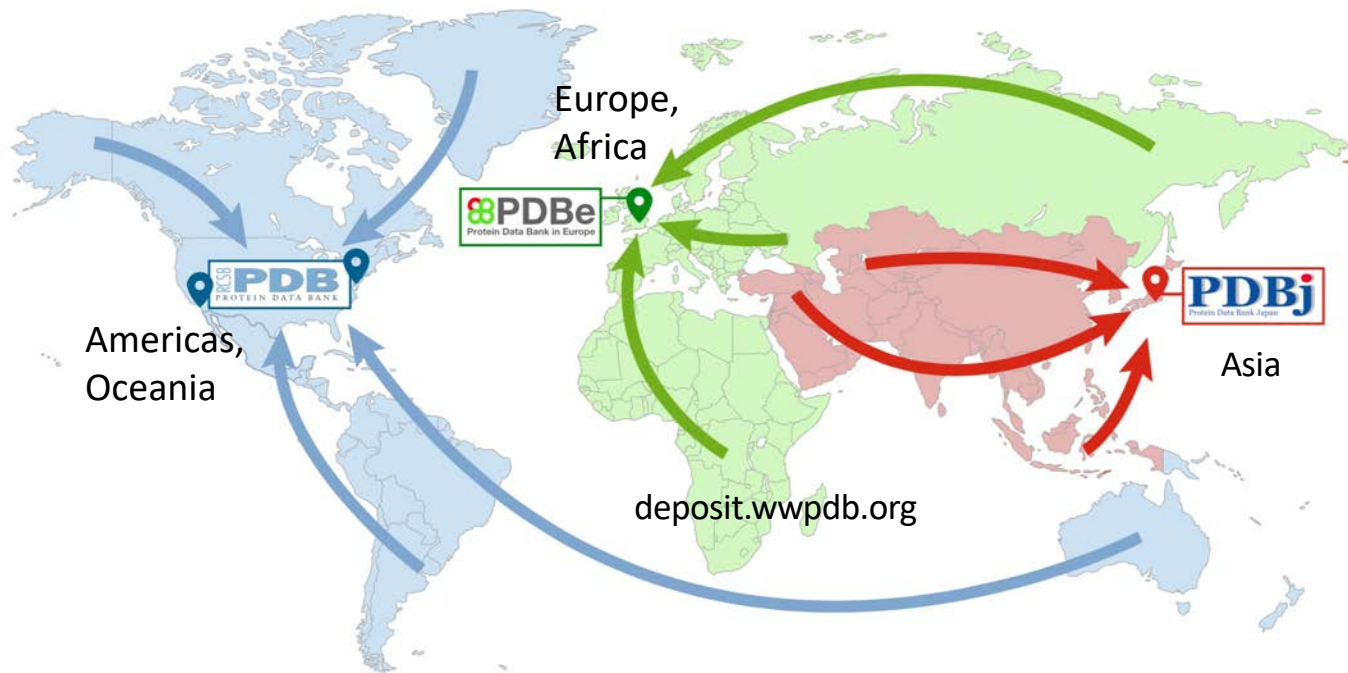
²MSD-EBI, Hinxton, UK. ³PDBj, Institute for Protein Research, Osaka University, Osaka,

Nature Structural Biology **10**, 980 (2003)
[doi: 10.1038/nsb1203-980](https://doi.org/10.1038/nsb1203-980)



Helen Berman
Kim Henrick
Haruki Nakamura

PDBj is in charge of processing and annotating the depositions from Asia



*PDB China started contributing to Data Processing of Asian depositions from 2022.
Acta Cryst. D. available *online ahead of print* DOI:[10.1107/S2059798323006381](https://doi.org/10.1107/S2059798323006381)

The history of PDBj from 2000

PDBj founded



SF become mandatory

CS become mandatory



PDBx/mmCIF become mandatory



2000 01 02 03 04 05 06 07 08 09 2010 11 12 13 14 15 16 17 18 19 2020 21 23

Launch of *Promote* service at PDBj

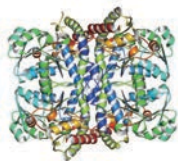
Launch of *eF-site* service at PDBj

20,000 depositions at PDBj

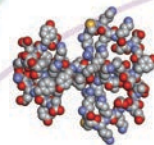
20th Anniversary of PDBj,

50,000 depositions at PDBj

The 1st MX structure processed by PDBj was 1GC0 (L-Met γ -lyase), deposited from Japan



The 1st NMR structure processed by PDBj was 1EJQ (Syndecan-4), deposited from Korea



Structural Biology Data Archiving in Asia

1. NMR Spectroscopy



Spectral Data

Chemical shifts
Coupling constants
Time-domain data
Spectral peak lists



Relaxation Data

R1/T1, R2/T2, R1rho/T1rho, NOEs



→ Coordinates (XYZ)

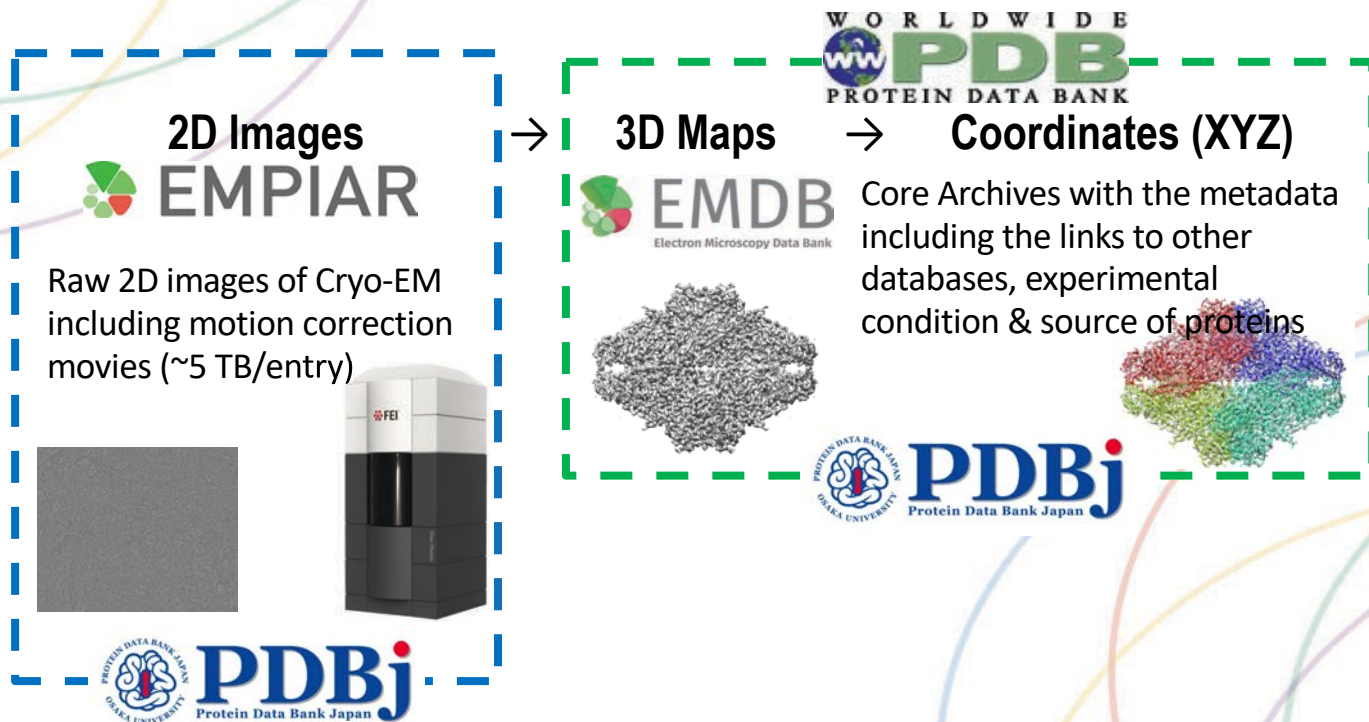


PDB Core Archive with the
metadata including the
links to other databases &
source of proteins



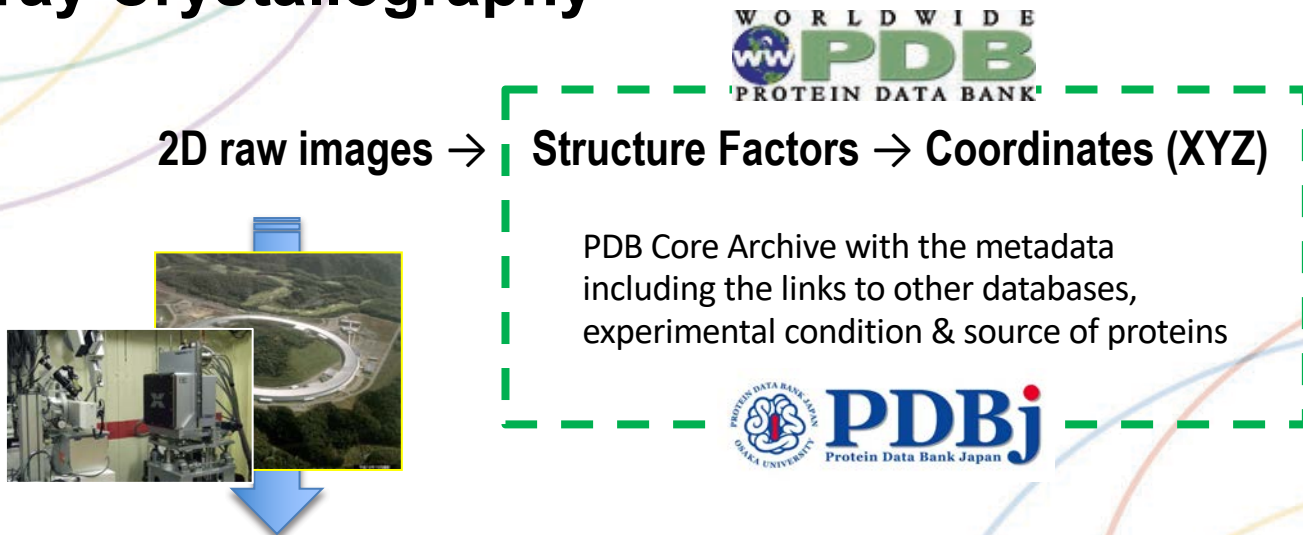
Structural Biology Data Archiving in Asia

2. Cryo Electron Microscopy



Structural Biology Data Archiving in Asia

3. X-ray Crystallography



- o ProteinDiffraction.org - <https://proteindiffraction.org>
- o SBGrid - <https://sbgrid.org>
- o CXIDB - <http://www.cxidb.org>

No public database for X-ray images available in Asia

Archive for X-ray Diffraction Images

ORIGINAL

English 日本語

XRDa
Xtal Raw Data Archive

OneDep IUCr

Login using ORCID Help Browse Statistics

Help menu

- Help top page
- How to submit a new entry
- File upload system
- How to set a graphical abstract
- How to request publication of an entry
- How to download data

Welcome to XRDa

The Xtal Raw Data Archive (XRDa for short) top page.

We welcome depositions of raw X-ray diffraction images corresponding to PDB entries.
[To submit new entries, please login using your ORCID ID.](#)

If you have any questions, please [contact us](#).
Please note that this archive is still under development and thus we appreciate any feedback you might have.

2020-04-09 (last edited: 1 month ago)

Latest entries All entries Covid-19 entries Electron Diffraction entries

XRDa-00001 (6L4P: Crystal structure of the complex between the axonemal outer-arm dynein light chain-1 and microtubule binding domain of gamma heavy chain)

Structure resolution: 1.70 Å

Toda, A., Nishikawa, Y., Tanaka, H., Yagi, T., Kurisu, G.

Primary citation: [10.1074/jbc.RA119.011541](#)

XRDa entry DOI: [10.51093/xrd-00001](#)

Deposition date: 2020-05-02

Release date: 2020-05-02

XRDa-00002 (6KUM: Ferredoxin I from C. reinhardtii, low X-ray dose)

Structure resolution: 1.40 Å

Onishi, Y., Kurisu, G., Tanaka, H.

1 2 3 4 >

English 日本語

XRDa
Xtal Raw Data Archive

OneDep IUCr

Login using ORCID Help Browse Statistics

XRDa-00024 (7dmu: Structure of SARS-CoV-2 spike receptor-binding domain complexed with high affinity ACE2 mutant 3N39)

Entry type: X-ray Diffraction

PDB entry authors: Arimori, T., Takagi, J.

R-work: 0.17880

R-free: 0.19790

Unit cell edges (Å): 227.8 x 227.8 x 147.03

Unit cell angles (°): 90, 90, 90

Resolution: 48.13 Å - 3.2 Å

Space group: P 43

Primary citation

PDBj website for 7dmu

Entry: [Download](#) (107.52 GB)

XRDa entry DOI: [10.51093/xrd-00024](#)

Dataset SARS-CoV-2 spike receptor-binding domain complexed with ACE2 mutant 3N39

Number of frames 3600

Distance (mm) 300

Oscillation width (°) 0.1

Omega (°) 0

Wavelength (Å) 0.9

Equipment DECTRIS EIGER X 16M

Beamline SPRING-8 BEAMLINE BL44XU

<https://xrda.pdbj.org>

Now 81 entries are released

Archive for X-ray Diffraction Images

<https://xrda.pdbj.org>

ORIGINAL

XRDa
Xtal Raw Data Archive

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• My entries Help Browse Statistics

My entries

The following entries for your ORCID ID were found in OneDep:

Entries only in XRDa (not yet registered in the PDB):

- [XRD-00081](#)
- [XRD-00119](#)
- [XRD-00120](#)
- [XRD-00082](#)
- [XRD-00064](#)
- [XRD-00067](#)

Entries only in the PDB (not yet registered in XRDa):

[5h57](#)
[6aa2](#)
[7bw2](#)
[8cab](#)
[8jc1](#)
[8hn2](#)
[7v5y](#)
[8i3j](#)
[7akt](#)
[5h59](#)
[7xn8](#)
[8h2u](#)
[6j13](#)
[8hn3](#)
[6m1b](#)
[8cjk](#)
[2h2c](#)

XRDa
Xtal Raw Data Archive

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• My entries Help Browse Statistics

Options

Release mechanism has moved to the preview page.

Preview entry

Assign PDB entry

[How to submit a new entry](#)

Notices

Entry editor

entry

xrldid*	type*	pdbid	entry_doi*	set_dirfile*	repr_image*	description	title
67	X-ray Diffraction						

set

ordinal*	name	number_of_frames	distance	oscillation_width	omega	wavelength	equipment	beamline	flux	description	dirfile
1											

Add new dataset

author

ordinal*	name	orcid	manager
134		0000-0003-2035-954x	true
135		0000-0001-7804-102x	true
136		0000-0003-3434-6678	true
137	GENJI KURISU	0000-0002-5354-0807	true

Add new author

external_databases

ordinal*	dbname	accession
----------	--------	-----------

Further development

- 1) Semi-automatic data upload
- 2) Automatic data quality check

Please deposit your experimental data to PDBj

ORIGINAL

<https://xrda.pdbj.org>

XRD-00001 (6L4P: Crystal structure of the complex between the axonemal outer-arm dynein light chain-1 and microtubule binding domain of gamma heavy chain)

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XRDa entry DOI: [10.51093/xrd-00001](https://doi.org/10.51093/xrd-00001)
Deposition date: 2020-05-02
Release date: 2020-05-02

XRD-00002 (6KUM: Ferredoxin I from C. reinhardtii, low X-ray dose)

Structure resolution: 1.40 Å
Onishi, Y., Kurisu, G., Tanaka, H.

ORIGINAL

<https://empiar.pdbj.org>

EMPIAR-13309 Cryo electron microscopy micrographs of yeast Enx1 complex [6472 multi-frame micrographs composed of 32 frames each in MRC format]

Wang, W., Guo, W., Li, Y., Mei, K.
[PubMed: 39320462]
[DOI: 10.5580/EMPIAR-13309-22]

EMPIAR-13305 Combining high-resolution cryo-electron microscopy and mutagenesis to develop a new model virus for biosecurity [16419 multi-frame micrographs composed of 16 frames each in MRC format]

Hoshikawa, Y., Durrant, A., Hoshikawa, Y., Kuroki, M., Lomonosov, G.P.
[PubMed: 39320462]
[DOI: 10.5580/EMPIAR-13305-22]

<https://deposit-bmrdb.pdbj.org>

Welcome to BMRBdep!

Start a new deposition

Click to select a deposition type *

Please enter your e-mail. *

Please enter a brief nickname for this deposition. *

Please enter your ORCID if you have one.

[Click here to start a new deposition.](#)

Resume deposition

To resume your deposition, simply click the link in the e-mail you were sent when you created the deposition with the subject 'Please validate your e-mail address for BMRBdep deposition...'

If you have lost that e-mail, please [contact us](#).

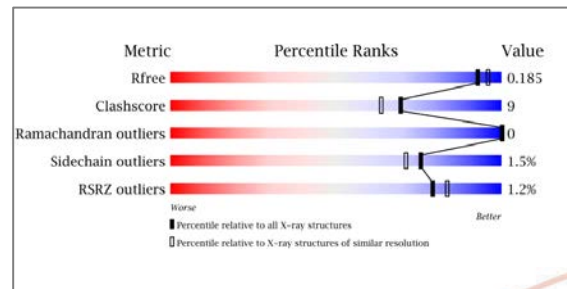


All three experimental data types are now archived in Asia!

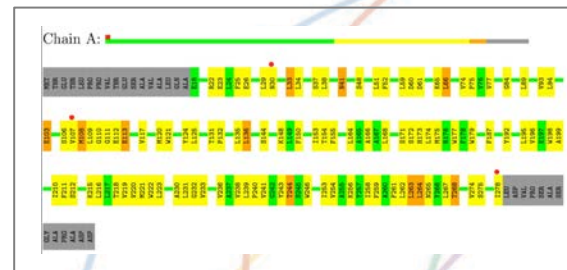
wwPDB validation report

- Model Quality
 - Bond lengths and angles (outlier info, RMS-Z)
 - Chirality, planarity
 - Close contacts (including worst clashes, MolProbity clash score)
 - Torsion angles (Ramachandran statistics, protein rotamers)
 - Ligand geometry (Mogul analysis)
- Residue Plots
 - Residues with model-quality outliers (0, 1, 2, >2)
 - Residues with RSR-Z > 5 are highlighted
 - Residues not observed

Overall Quality Summary



Residue Plots



wwPDB/RDF-validation graph

PDBj-BMRB Data Server:

common open representations of BMRB NMR-STAR data in XML, RDF and JSON formats

<https://bmrpub.pdbj.org>

[Home](#) [Search](#) [Examples](#) [Download](#) [Resources](#) [NEWS](#)

Virtuoso SPARQL Query Editor

[About](#) | [Namespace Prefixes](#) | [Inference rules](#)

Default Data Set Name (Graph IRI)

<https://rdf.wwpdb.org/pdb-validation>

Query Text

```
select distinct ?Concept where {[ ] a ?Concept} LIMIT 100
```

(Security restrictions of this server do not allow you to retrieve remote RDF data, see [details](#).)

Results Format:

HTML

Execution timeout:

0

milliseconds (values less than 1000 are ignored)

Options:



Strict checking of void variables

(The result can only be sent back to browser, not saved on the server, see [details](#))

[Run Query](#)

[Reset](#)

Query examples

Category holders

1. Select all [category holders](#) of datablock class of BMRB entry 15400: [Show](#)
2. Select all [category holders](#) of datablock class of Metabolomics entry bmse000400: [Show](#)

Entry statistics

3. Count entries per [submission year](#) and [experimental method \(subtype\)](#): [Show](#)

Assembly descriptions

4. Select all [assembly names](#), [asym IDs](#), [entity IDs](#), [polymer types](#), [formula weights](#) and [functions](#) in a [assembly](#): [Show](#)

Entity descriptions

5. Select all [entity names](#) and [sequences](#) of polymer [entities](#) expressed using one-letter code: [Show](#)
6. Select all [original source information](#) of molecular [entities](#) and external links to NCBI Taxonomy: [Show](#)
7. Select all [biological systems](#) to produce molecular [entities](#) and external links to NCBI Taxonomy: [Show](#)

Citation information

8. Select [citation information](#) of all entries together with external links to PubMed and DOI, if available: [Show](#)

Example: Entry search based on wwPDB/RDF-validation

"4CK1",

"INTEGRASE",

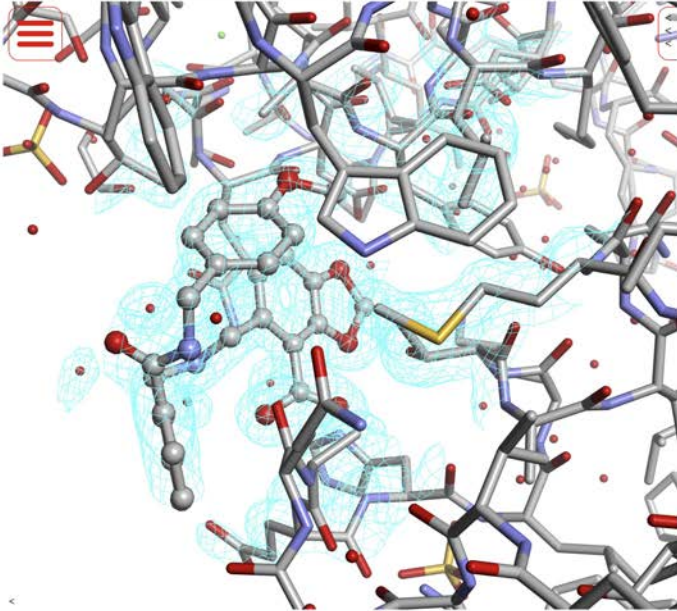
"(4-CARBOXY-1,3-BENZODIOXOL-5-YL)METHYL-[[2-[(4-METHOXYPHENYL)METHYLCARBAMOYL]PHENYL]METHYL]AZANIUM",

"OM1",

"0.081"

EDmap (Molmil): 4ck1

Style: ☒ Wireframe ☐ Color: ☐ Atom



Parameters for Electron Density Map

[About the PDB Electron Density Map Viewer](#)

Type of the map: ☒ contour mesh ☐ iso surface

Map position:

☐ atom nearest to the center of the map

* Atom ID: , ,

You can select "Atom ID" by clicking in the viewer!

☐ coordinates (x: y: z:

mapped area: Å
(this is the length of edge of a cube)

contour level: σ

color: R: G: B:

isosurface transparency level:

Electron Density Map Download/Delete

file format	filename	
structure factor	r4ck1sf.ent.gz	<input type="button" value="Download"/>
refinement file	4ck1_ref.tar.gz	<input type="button" value="Download"/>
ccp4 file	4ck1.ccp4.gz	<input type="button" value="Download"/>
edmap file	2018103203127_4ck1.c.xml.gz	<input type="button" value="Delete"/> <input type="button" value="Download"/>

Depositor-Initiated Atomic Coordinate Versioning

- Improve the quality of PDB structures
- Preserve original PDB IDs and maintain connections to the scientific literature
- Reasoning captured
- The latest versioned file can be accessed at FTP
- The latest minor version of each major version is available at versioned FTP
ftp-versioned.wwpdb.org

wwPDB Deposition: D_1300000002 -- ID: 5AUI(REL)

Deposition locked

All items
Mandatory items

Navigation

- Instructions
- Communication
- Review
- Assembly Review
- Validation reports
- File-upload files
- Admin
- Contact information
- Grant information
- Release status
- Entry site & author
- Citation information
- Macromolecules
- 1j Ferredoxin-1
- Data collection
- Crystal information
- Collection Source
- Software Used
- Collection Statistics
- Refinement
- Refinement
- Ligands
- Related entries
- Summary & conditions

Log out

Communication with the wwPDB

This page shows you the current messages associated with this deposition and allows you to send a new message to the wwPDB.

- All messaging on this page will be archived permanently with this deposition.
- This page can ONLY be used to communicate information about this deposition.
- This page shows:
 - All messages as a list.
 - A box for you to create and send a new message.
 - If you are communicating changes to be made in the annotation of your file, please do so preferably using CIF format.

Old messages

TimeStamp	Sender	Subject	Content (click to show more)
2015-09-14 06:41:01	auto	DEPOSITION ID "D_1300000002" -- Release of PDB ID "SAUI"	Dear Depositors, This message...
2015-05-07 23:41:26	RI	Acknowledgement of Structure Approval	Dear Dr. Kurisu, Thank you fo...
2015-05-01 11:24:58	depositor	Re: PDB ID SAUI	Dear Igarashi-san, Thank you...

Last message from annotator

Time stamp: 2015-09-14 06:41:01
Sender: auto
Subject: DEPOSITION ID "D_1300000002" -- Release of PDB ID "SAUI"

Full Text

Dear Depositors,

This message is to inform you that your structure PDB ID SAUI (Deposition ID D_1300000002) and the associated experimental data which were deposited with release instructions, 'HPUB', will be released on 2015-09-23. The entry is entitled:

D_1300000002_val-data-annotate_P1.xml.V2
D_1300000002_val-report-annotate_P1.pdf.V2
D_1300000002_model-annotate_P1.pdf.V2
D_1300000002_model-review_P1.pdf.V2
D_1300000002_sf-annotate_P1.cif.V2
D_1300000002_val-report-full-annotate_P1.pdf.V2

Attachments

New message

Subject: Other

Dear Biocurator,

I'd like to replace the coordinate file as a versioned entry. Could you kindly unlock the session for this SAUI entry? Thank you very much.

Message

Best regards,
Genji Kurisu

Sender: Kurisu, Genji (principal investigator/group leader)

Send this message to the wwPDB

Depositor-Initiated Atomic Coordinate Versioning

- Improve the quality of PDB structures
- Preserve original PDB IDs and maintain connections to the scientific literature
- Reasoning captured
- The latest versioned file can be accessed at FTP
- The latest minor version of each major version is available at versioned FTP

<ftp-versioned.wwpdb.org>

▼ New message

Subject

Message

Sender

[Send this message to the wwPDB](#)

Diffraction Data Case Study for GOSC

Deliverables

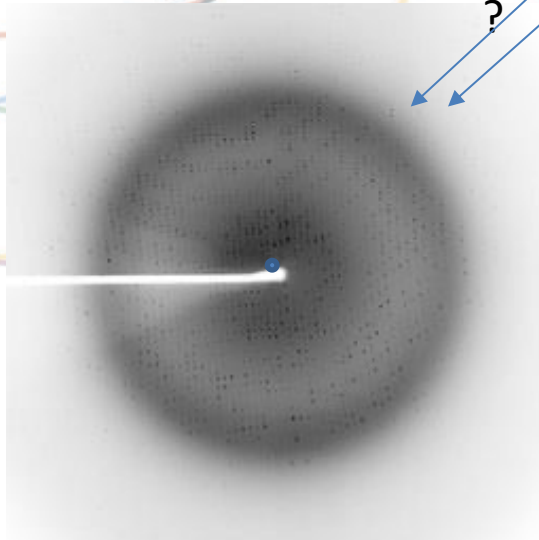
Reproducibility of data sets is paramount.

The team aim for a single point of contact for definitive molecular models, namely at the PDBj and its XRDa, the X-ray Diffraction Data Archive based at the Institute for Protein Research in Japan.

We aim to avoid dispersed multiple versions of a protein model derived from a single raw diffraction data set. Controlled versioning procedure of PDB entries should be tightly linked.

A critical deliverable is to realise metrics of 'definitive reusability' which would then be applicable to the individual diffraction data sets held in the XRDa. These metrics and the definitive diffraction data files are a bedrock of interoperability.

A glimpse of the variation of X-ray diffraction resolution limit choice involving the commonly used metrics in macromolecular crystallography:-



Resolution cut off estimates:-

resolution of all data	:	1.913
based on $CC(1/2) \geq 0.33$:	1.946
based on $\text{mean}(I/\sigma) \geq 2.0$:	3.037
based on $R\text{-merge} < 0.5$:	2.411
based on $R\text{-meas} < 0.5$:	2.497
based on <u>completeness</u> $\geq 90\%$:	2.335
based on completeness $\geq 50\%$:	2.155

Via the Diederichs and Karplus method, using the XRDa entry the resolution limit should be 2.40 Å.
The depositor, Sato et al (Biochem. J. 478, 1023–1042) used 2.40 Å.

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CCD ID becomes 5-letters

- 3-letter ID codes of the Chemical Component Dictionary (CCD) will run out in 2022.
- Only the PDBx/mmCIF format will be provided for CCD IDs with 5-letters.

