

PDBjとwwPDBの活動方針について

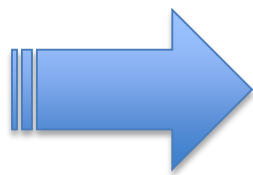
栗栖源嗣

大阪大学蛋白質研究所



wwpdb.org

After Solving Structure, what we should do?



<https://wwpdb.org>

wwPDB provides the Deposition Site



VALIDATION ▾

DEPOSITION ▾

DATA DICTIONARIES ▾

DOCUMENTATION ▾

TASK FORCES ▾

STATISTICS ▾

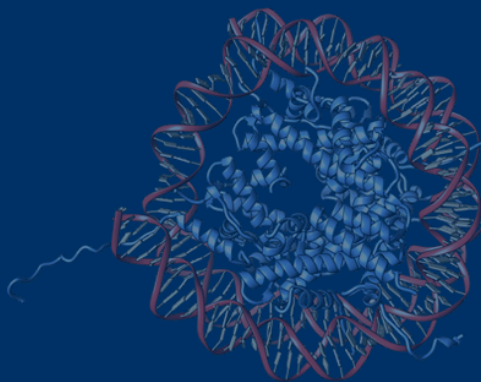
ABOUT ▾



Since 1971, the Protein Data Bank archive (PDB) has served as the single repository of information about the 3D structures of proteins, nucleic acids, and complex assemblies.

The Worldwide PDB (wwPDB) organization manages the PDB archive and ensures that the PDB is freely and publicly available to the global community.

Learn more about PDB **HISTORY** and **FUTURE**.



Validate Structure

or View validation reports



Deposit Structure

All Deposition Resources



Download Archive

Instructions

wwPDB Members

wwPDB Resources

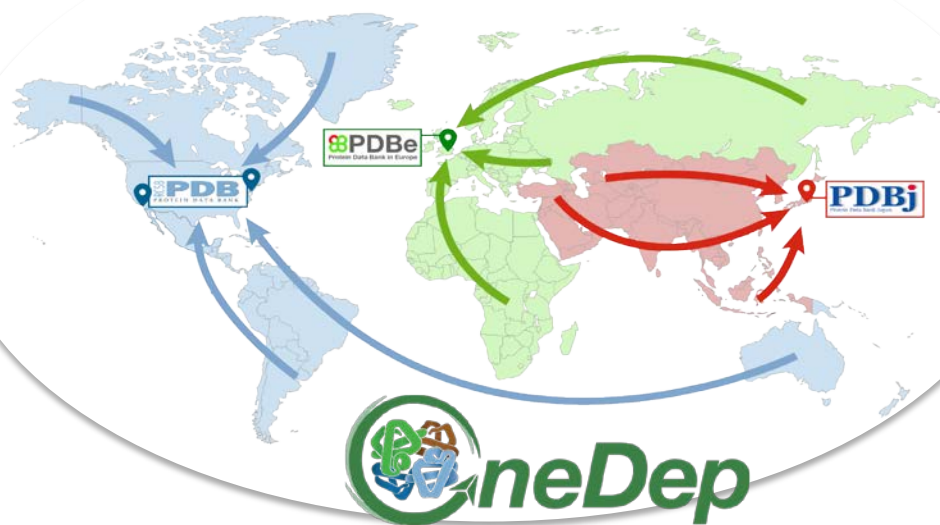
News & Announcements

<https://wwpdb.org>

wwPDB Common Deposition & Annotation

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

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	10958	4845	2100	4013
2016	11614	5326	2238	4050
2017	2577	1579	394	604
TOTAL	131815	77266	28745	25804



OneDep

- OneDep system
 - Accepting PX, 3DEM and NMR data deposition
 - Collaboration with SASBDB
 - Ver. 2.19 was implemented
- OneDep logo



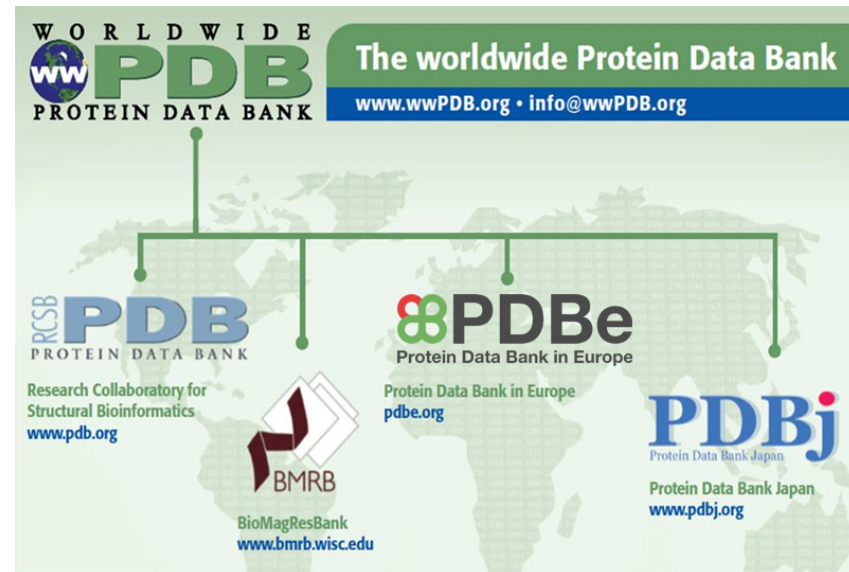
→ 詳細はこの後の中川敦史先生のご講演
で



Protein Data Bank Japan

<https://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.



TOOLS FOR PROTEIN SCIENCE

New tools and functions in data-out activities at Protein Data Bank Japan (PDBj)

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Yuko Tsuchiya,¹ Hiromu Sato,⁴ Hafumi Nishi,⁴ Kengo Kinoshita,⁴
Hirofumi Suzuki,¹ Takeshi Kawabata,¹ Masashi Yokochi,¹ Takeshi Iwata,¹
Naohiro Kobayashi,¹ Toshimichi Fujiwara,¹ Genji Kurisu,¹ and Haruki Nakamura^{1*}**

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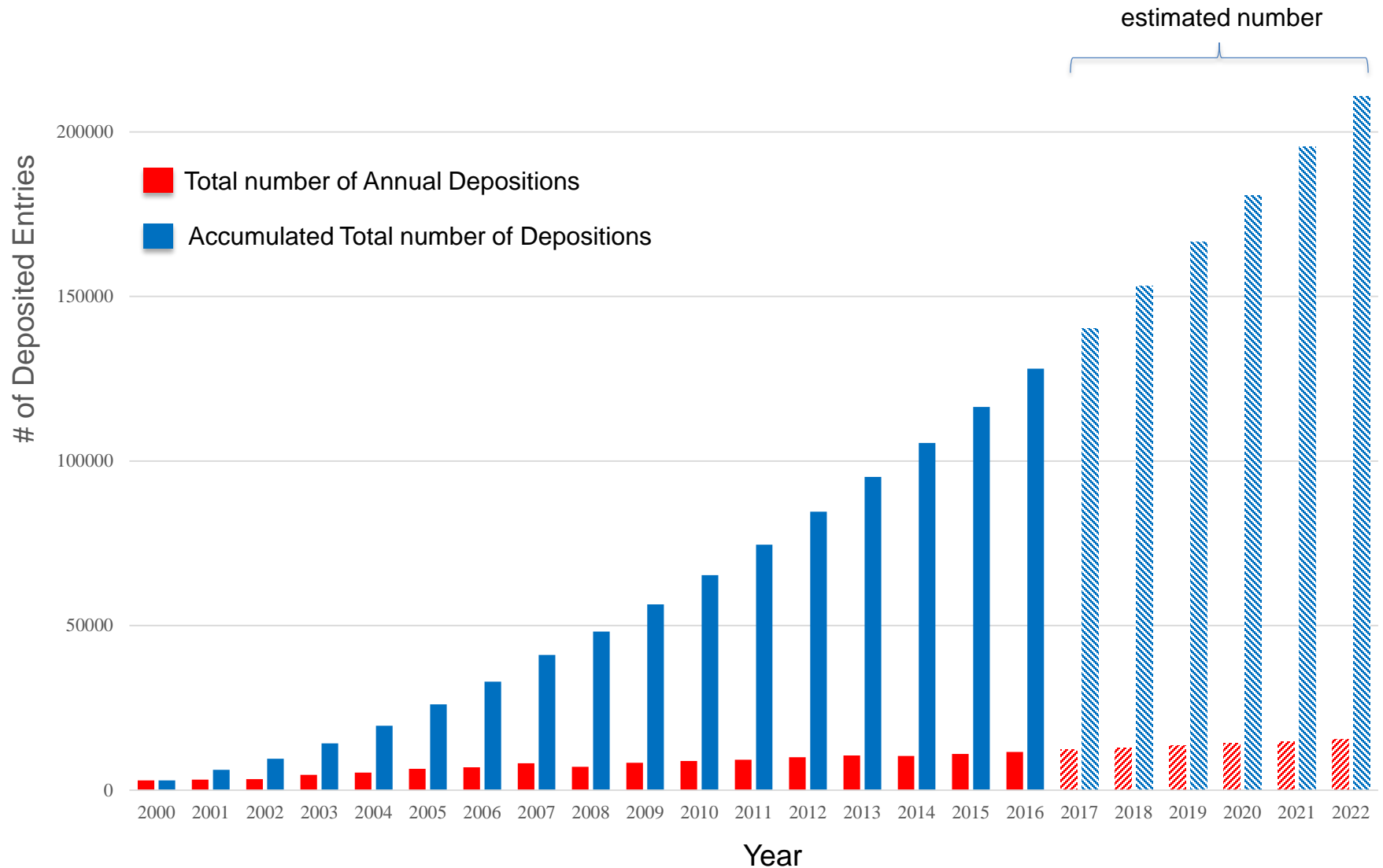
⁴Graduate School of Information Sciences, Tohoku University, 6-3-09 Aoba, Aramaki-aza Aoba-ku, Sendai 980-8579, Japan

Received 28 June 2017; Accepted 14 August 2017

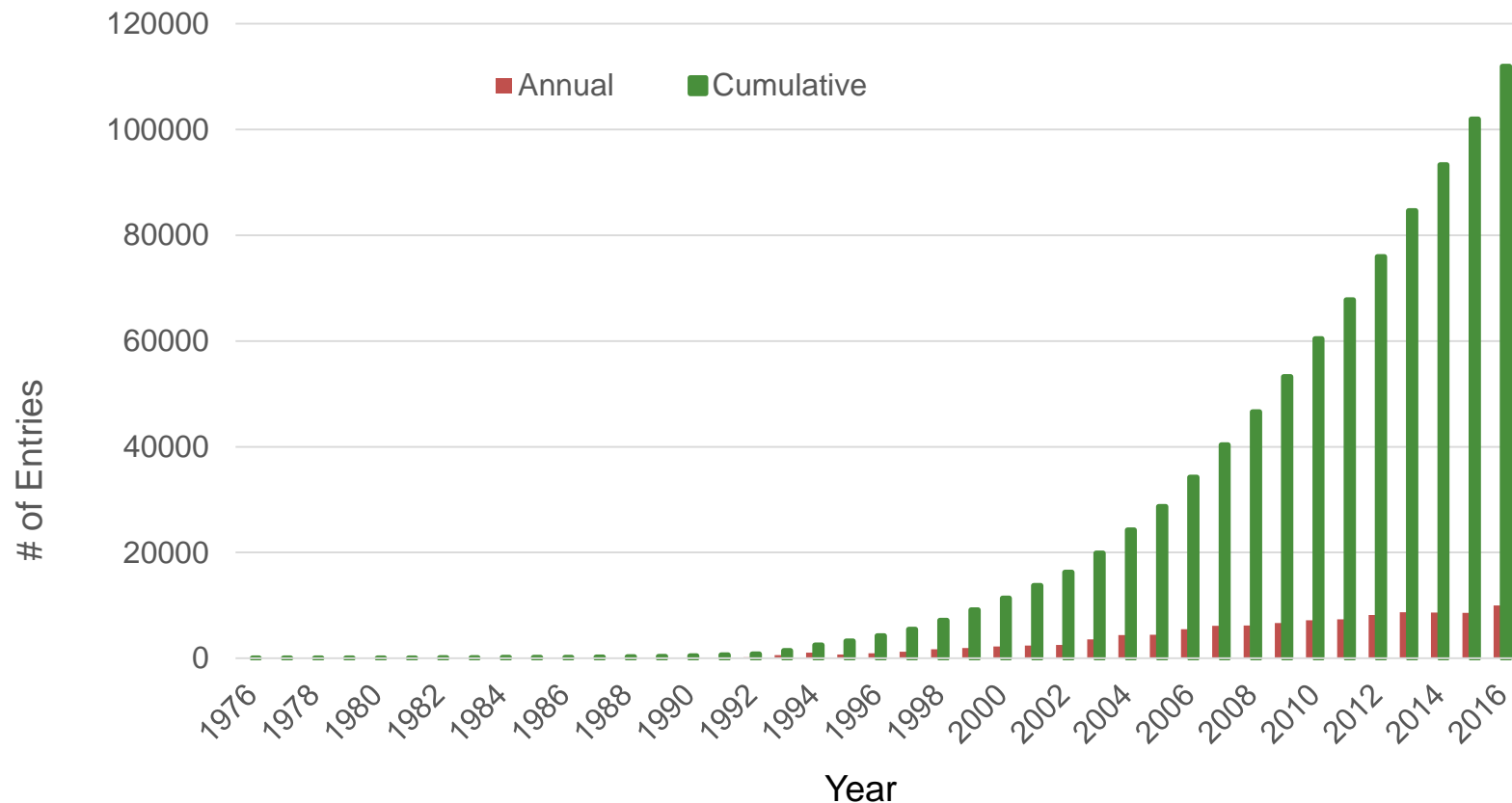
DOI: 10.1002/pro.3273

Published online 00 Month 2017 proteinscience.org

Growing Number of Depositions



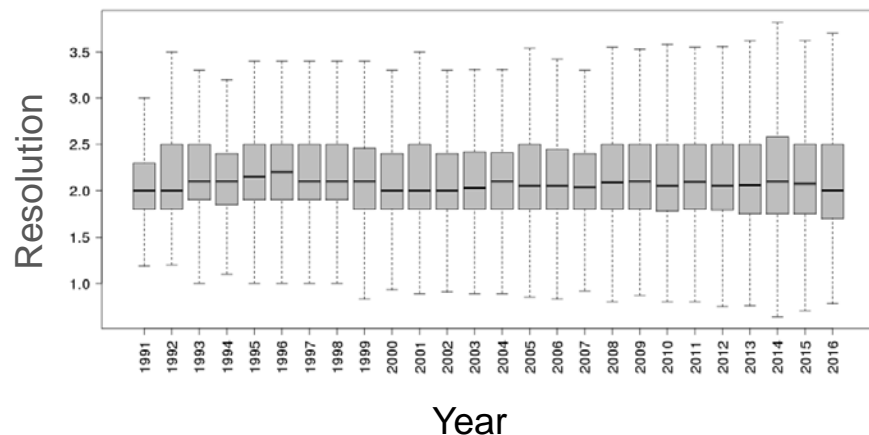
Growth of Released PX Entries



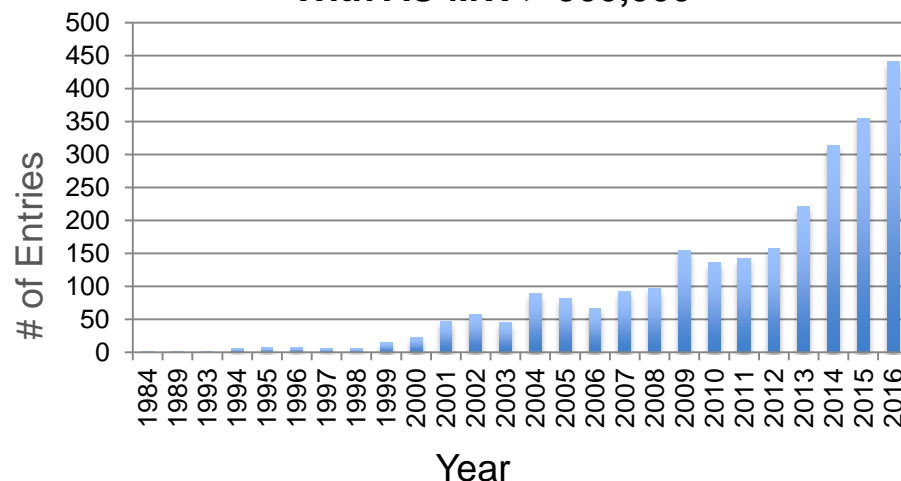
>120,000 Total Released MX Entries Projected for End 2017

MX Deposition Complexity

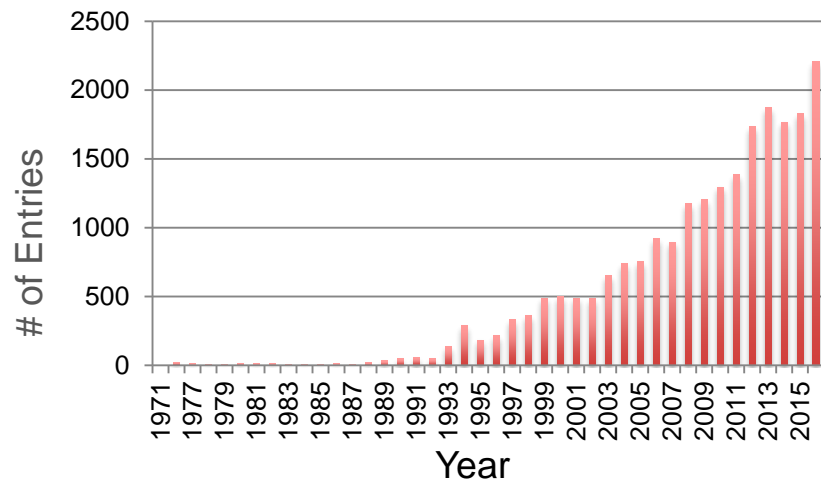
**Annual Distribution for
High Resolution Limit**



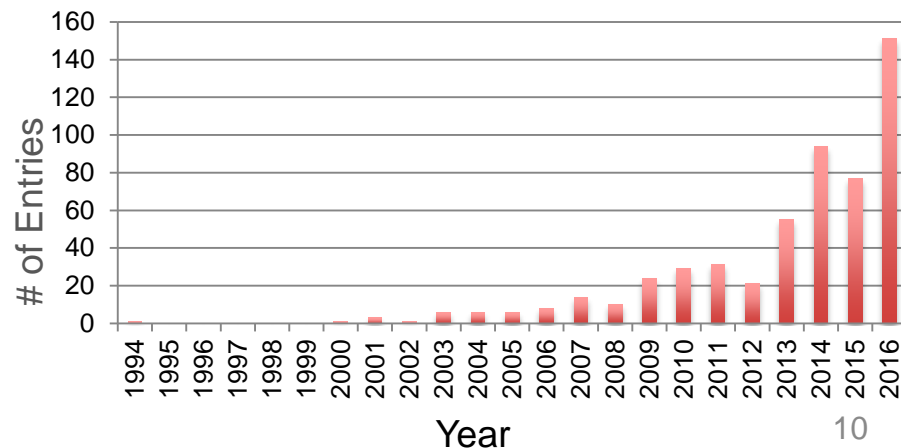
**Annual Released Structures
With AU MW > 500,000**



Total Number of New CCD Entries



**Annual Released Large Structures
(chains > 62 & atoms > 99999)**



PDB Data Download Statistics

Year	Total	Total FTP Archive	Total Website	RCSB PDB FTP Archive	RCSB PDB Website	PDBe FTP Archive	PDBe Website	PDBj FTP Archive	PDBj Website
2009	328,362,536	271,116,934	57,245,602	222,984,760	53,507,785	30,141,339	1,475,116	17,990,835	2,262,701
2010	294,326,976	213,180,966	81,146,010	159,248,214	64,569,658	34,383,219	14,017,349	19,549,533	2,559,003
2011	383,131,048	276,952,286	106,178,762	204,939,406	81,560,098	40,960,368	18,515,245	31,052,512	6,103,419
2012	376,944,070	255,837,735	121,106,335	213,510,347	90,438,501	21,601,103	23,982,801	20,726,285	6,685,033
2013	441,262,210	296,176,290	145,085,920	215,331,908	97,549,580	43,684,850	37,762,496	37,159,532	9,773,844
2014	512,227,251	339,193,721	173,033,530	237,168,615	110,115,316	52,362,370	48,031,414	49,662,736	14,886,800
2015	534,339,871	368,244,766	166,095,105	255,346,630	111,802,897	48,544,330	41,127,219	64,353,806	13,164,989
2016	591,876,087	366,677,897	225,198,190	293,648,366	161,208,456	30,274,284	44,432,830	42,755,247	19,556,904

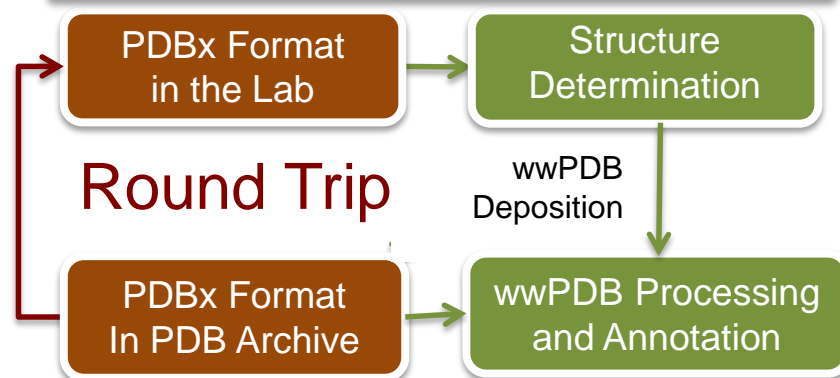
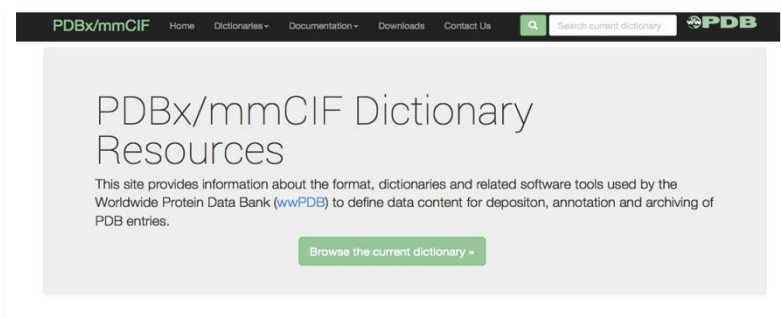
More than 1.5 million/day

Geographic origins of FTP downloads, 2012-2015



2017 PDBx/mmCIF Working Group

- PDBx/mmCIF is the archival data standard for the repository
- wwPDB together with the PDBx/mmCIF Working Group of community experts and methods developers oversee the evolution of the standard
- Working Group ensures that the standard is well supported by key community software tools.
- PDB hosts community workshops and maintains mmcif.wwpdb.org serving PDBx/mmCIF data dictionaries, schema and software tools
- **2017 PDBx/mmCIF Working Group meeting finalized new content recommendations for diffraction data and ligand refinement restraint data**



PDBx/mmCIF Workshop Participants, July 2017

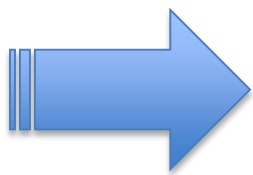
File Versioning: Planning Process

- User feedback solicited
- Enable revisions to entries updated by the Depositor of Record (e.g., Version 1-0 → 1-1; 1-0 → 2-0)
 - wwPDB will NOT assign a new PDB ID going forward (for Depositor of Record revision only)
- Introduce 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

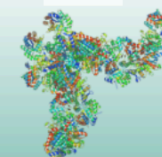
Collection of ORCID IDs

- Successfully Implemented Apr 11, 2016
- Metrics (Apr 11 – Aug 31, 2016):
 - ~8% of Depositions have ORCID ID (374/4713)
 - 170 unique ORCID IDs (92 identified as PIs)
- Plans to Increase ORCID Adoption
 - Expand to all entry authors to provide ORCID (2017)
 - Distribute collected ORCID IDs at ftp archive (2017)
 - Mandatory going forward (2018)

When you want to know the 3D structure?

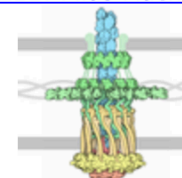


<https://pdbj.org>



Molecule of the Month

211: Pilus Machine



[Molecule of the Month listing](#)

WORLDWIDE
PDB
PROTEIN DATA BANK

[wwPDB](#)

[Enriched Model Files Conforming to OneDep Data Standards Now Available in the PDB FTP Archive](#)

[5 Easy Steps to PDB Deposition](#)

[Revise Your Structure Without Submitting the PDB](#)

Guide for first time visitors

For an introduction to the new web interface, please read [Using PDBj's web interface](#). An introduction to the customization features offered by the new PDBj web interface can be found [here](#). To get a more in-depth explanation on the various features of the PDBj website, please take a look at the [Interactive tutorial series](#).

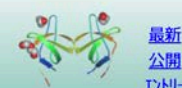
The [legacy PDBj website](#) will no longer be updated after July 12, 2017 and will be closed at the end of August, 2017.

Find the service you need

Choose a keyword listed below or input keywords into the textbox at the right of the keyword list. The brief explanation of the matched services will be displayed.

- Click the 'Show all services' button to display the explanation for all services.
- Input some keywords into the 'Word Search Box' to narrow down the search results.

- ☐ PDB ☐ BMRB
- ☐ search ☐ deposition
- ☐ education/dictionary
- ☐ NMR ☐ electron microscopy



今月の分子

211: 線毛機械 (Pilus Machine)

日本蛋白質構造データバンク (PDBj: Protein Data Bank Japan) は、[JST-NBDC](#) と [大阪大学蛋白質研究所](#) 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

Example1: Gleevec using PDBj-Mine

PDBj **132905**
Protein Data Bank Japan
entries
(2017-08-16)

English 日本語 简体中文 繁體中文 한국어

Search pdbj.org

Menu    Worldwide Protein Data Bank Foundation

[wwPDB](#) [RCSB PDB](#) [PDBe](#) [BMRB](#) [Legacy](#) [Adv. Search](#) [Search help](#)

Chemie search ?

Search of [Chemical Component Dictionary](#)

Quick search: 


Code (comp_id):

Molecular name:

Formula:

SMILES:

InChi:

   **PDB**  Worldwide Protein Data Bank Foundation  EMDDataBank
Unified Data Resource for 2020

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Explore 1T46: Gleevec using PDBj-Mine (cont.)

132905

entries available on 2017-08-16
00:00 UTC / 09:00 JST

PDBj
Protein Data Bank Japan



English 日本語 简体中文 繁體中文 한국어

Search pdbj.org

wwPDB RCSB PDB PDBj BMRB Legado Adv. Search Search help

PDB: 8 results Info pages: 0 results Status search: 0 results Chemie search: 0 results

Gleevec

1XBB



CRYSTAL STRUCTURE OF THE SYK TYROSINE KINASE DOMAIN WITH GLEEVEC

Descriptor: 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE, Tyrosine-protein kinase SYK

Authors: Nienaber, V.L., Atwell, S., Adams, J.M., Badger, J., Buchanan, M.D., Feil, I.K., Froning, K.J., Gao, X., Hendle, J., Keegan, K., Leon, B.C., Muller-Deickmann, H.J., Noland, B.W., Post, K., Rajashankar, K.R., Ramos, A., Russell, M., Burley, S.K., Buchanan, S.G.

Deposit date: 2004-08-30

Release date: 2004-11-02

Last modified: 2011-07-13

Method: X-RAY DIFFRACTION (1.57 Å)

Cite: A Novel Mode of Gleevec Binding Is Revealed by the Structure of Spleen Tyrosine Kinase J.Biol.Chem., 279, 2004

3GVU



THE CRYSTAL STRUCTURE OF HUMAN ABL2 IN COMPLEX WITH GLEEVEC

Descriptor: 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE, Tyrosine-protein kinase ABL2

Authors: Ugochukwu, E., Salah, E., Barr, A., Mahajan, P., Shrestha, B., Savitsky, P., Chaikwad, A., Filippakopoulos, P., Roos, A., Pike, A.C.W., von Delft, F., Bountra, C., Arrowsmith, C.H., Welgelt, J., Edwards, A., Knapp, S., Structural Genomics Consortium (SGC)

Deposit date: 2009-03-31

Release date: 2009-04-21

Last modified: 2011-07-13

Method: X-RAY DIFFRACTION (2.05 Å)

Cite: The crystal structure of human ABL2 in complex with GLEEVEC To be Published

1XBA



CRYSTAL STRUCTURE OF APO SYK TYROSINE KINASE DOMAIN

Descriptor: Tyrosine-protein kinase SYK

Authors: Atwell, S., Adams, J.M., Badger, J., Buchanan, M.D., Feil, I.K., Froning, K.J., Gao, X., Hendle, J., Keegan, K., Leon, B.C., Muller-Deickmann, H.J., Nienaber, V.L., Noland, B.W., Post, K., Rajashankar, K.R., Ramos, A., Russell, M., Burley, S.K., Buchanan, S.G.

Deposit date: 2004-08-30

Release date: 2004-11-02

Last modified: 2011-07-13

Method: X-RAY DIFFRACTION (2 Å)

Cite: A novel mode of Gleevec binding is revealed by the structure of spleen tyrosine kinase. J.Biol.Chem., 279, 2004

Search results info

Total results: 8
Displayed results: 8
Sorted by: Hit score (from highest)
Auto-pager: ☐

Download results

Sort by

Hit score (from highest)
PDBID ascending
PDBID descending
Deposition date (from oldest)
Deposition date (from newest)
Release date (from oldest)
Release date (from newest)
Resolution (from highest)

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Format Conversion

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Latest entries

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Search PDB (Advanced)
Chemie search
Search BMRB
Sequence-Navigator
Structure-Navigator
EM Navigator
Omokage search
wwPDB/RDRC
GSAW

132905

entries available on 2017-08-16
00:00 UTC / 09:00 JST

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EM Navigator
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Molecular Viewers

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Summary Structural details Experimental details Functional details Sequence Neighbor Downloads

1T46

STRUCTURAL BASIS FOR THE AUTOINHIBITION AND STI-571 INHIBITION OF C-KIT TYROSINE KINASE

Summary for 1T46

Related	1PKG 1T45
Descriptor	Homo sapiens v-kit Hardy-Zuckerman 4 feline sarcoma viral oncogene homolog, PHOSPHATE ION, 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE, ... (4 entities in total)
Functional Keywords	kinase, inhibitor, sti-571, gleevec, transferase activator
Biological source	Homo sapiens (human)
Total number of polymer chains	1
Total molecular weight	36072.48
Authors	Mol, C.D. , Dougan, D.R. , Schneider, T.R. , Skene, R.J. , Kraus, M.L. , Scheibe, D.N. , Snell, G.P. , Zou, H. , Sang, B.C. , Wilson, K.P. (deposition date: 2004-04-28, release date: 2004-06-15, Last modification date: 2011-07-13)
Primary citation	Mol, C.D. , Dougan, D.R. , Schneider, T.R. , Skene, R.J. , Kraus, M.L. , Scheibe, D.N. , Snell, G.P. , Zou, H. , Sang, B.C. , Wilson, K.P. Structural basis for the autoinhibition and STI-571 inhibition of c-Kit tyrosine kinase. <i>J.Biol.Chem.</i> , 279:31655-31663, 2004 PubMed: 15123710 (PDB entries with the same primary citation) DOI: 10.1074/jbc.M403319200 Import into Mendeley
Experimental method	X-RAY DIFFRACTION (1.6 Å)

Structure validation

More Asymmetric unit images



Worldwide
Protein Data Bank
Foundation



EMDataBank
Unified Data Resource for 3DEM

Copyright © 2013-2017 Protein Data Bank Japan

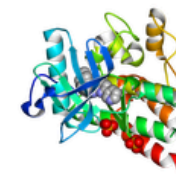
Downloads

- Sequence (fasta)
- PDBx/mmCIF
- PDBML format (no-atom)
- PDB format (full)
- Validation report (PDF)

[More...](#)

Structures

View Asymmetric Unit (AU
= BU)



Database information

- RCSB-PDB
- PDBj
- Yorodumi
- CATH
- FSSP
- SCOP
- VAST
- PISA
- UniProt
- KEGG
2.7.1.112
- ExPASy
2.7.1.112
- IUBMB
2.7.1.112
- eF-site
1T46
- Electron Density Map (molmil)
- Promote Elastic
EzCatDB (M00323)

Electron Density map (Molmil)

Explore 1T46: Gleevec using PDBj-Mine (cont.)

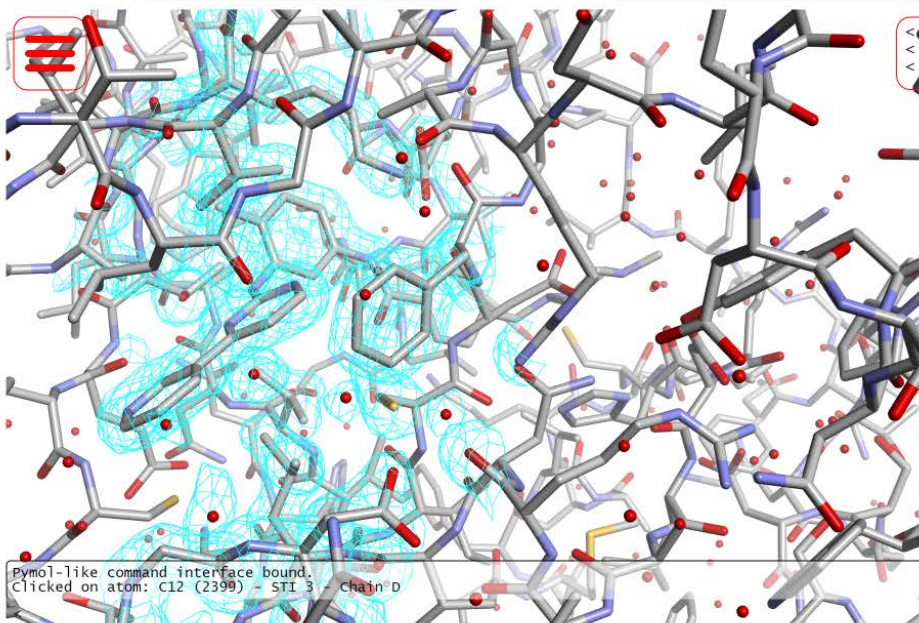
EDmap (Molmil): 1t46

Style:

Wireframe

Color:

Atom



Parameters for Electron Density Map

[About the PDBj 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:

Create map

Reset

Electron Density Map Download/Delete

file format

filename

structure factor

r1t46sf.ent.gz

Download

refinement file

1t46_ref.tar.gz

Download

ccp4 file

1t46.ccp4.gz

Download

edmap file

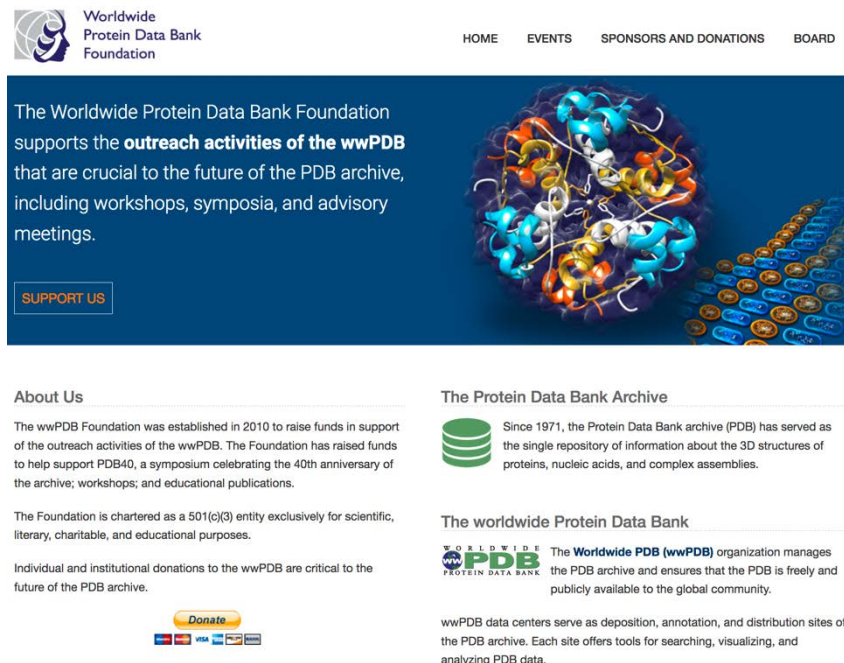
2017819153711_1t46.c.xml.gz

Delete

Download

wwPDB Foundation Progress

- 501(c)(3) entity exclusively for scientific, literary, charitable, and educational purposes
- Ongoing solicitations of Corporate donations



The screenshot shows the homepage of the Worldwide Protein Data Bank Foundation. At the top, the logo and name "Worldwide Protein Data Bank Foundation" are on the left, and navigation links "HOME", "EVENTS", "SPONSORS AND DONATIONS", and "BOARD" are on the right. The main banner features a blue background with a 3D protein structure and a path of coins leading towards it. Text on the banner states: "The Worldwide Protein Data Bank Foundation supports the **outreach activities of the wwPDB** that are crucial to the future of the PDB archive, including workshops, symposia, and advisory meetings." Below this is a "SUPPORT US" button. The page is divided into two columns. The left column, titled "About Us", contains text about the foundation's establishment in 2010, its 501(c)(3) status, and its mission. It also includes a "Donate" button with logos for Visa, Mastercard, and American Express. The right column, titled "The Protein Data Bank Archive", describes the PDB as a single repository of 3D structures since 1971. Below this, "The worldwide Protein Data Bank" section explains that the wwPDB organization manages the PDB archive and ensures it is freely available. It also mentions that wwPDB data centers serve as deposition, annotation, and distribution sites.

Worldwide Protein Data Bank Foundation

HOME EVENTS SPONSORS AND DONATIONS BOARD

The Worldwide Protein Data Bank Foundation supports the **outreach activities of the wwPDB** that are crucial to the future of the PDB archive, including workshops, symposia, and advisory meetings.

SUPPORT US

About Us

The wwPDB Foundation was established in 2010 to raise funds in support of the outreach activities of the wwPDB. The Foundation has raised funds to help support PDB40, a symposium celebrating the 40th anniversary of the archive; workshops; and educational publications.

The Foundation is chartered as a 501(c)(3) entity exclusively for scientific, literary, charitable, and educational purposes.

Individual and institutional donations to the wwPDB are critical to the future of the PDB archive.

Donate

The Protein Data Bank Archive

Since 1971, the Protein Data Bank archive (PDB) has served as the single repository of information about the 3D structures of proteins, nucleic acids, and complex assemblies.

The worldwide Protein Data Bank

The **Worldwide PDB (wwPDB)** organization manages the PDB archive and ensures that the PDB is freely and publicly available to the global community.

wwPDB data centers serve as deposition, annotation, and distribution sites of the PDB archive. Each site offers tools for searching, visualizing, and analyzing PDB data.

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

