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

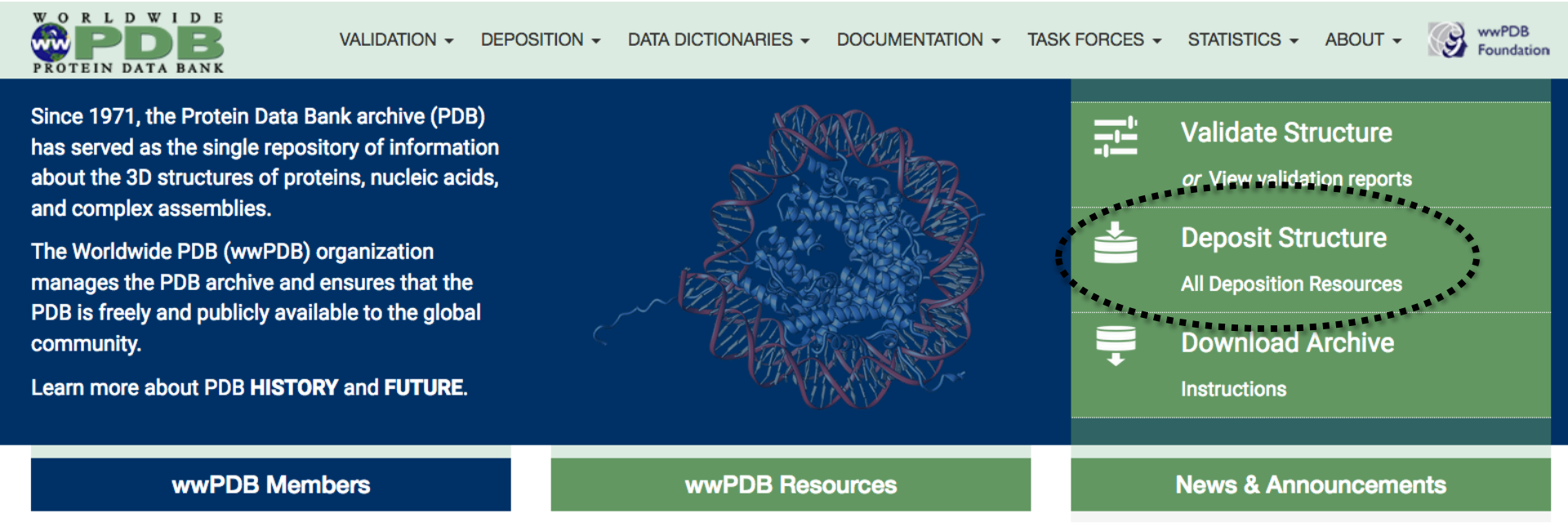
WORLDWIDE PDB
PROTEIN DATA BANK

wwpdb.org

After Solving Structure, what we should do?

https://wwpdb.org

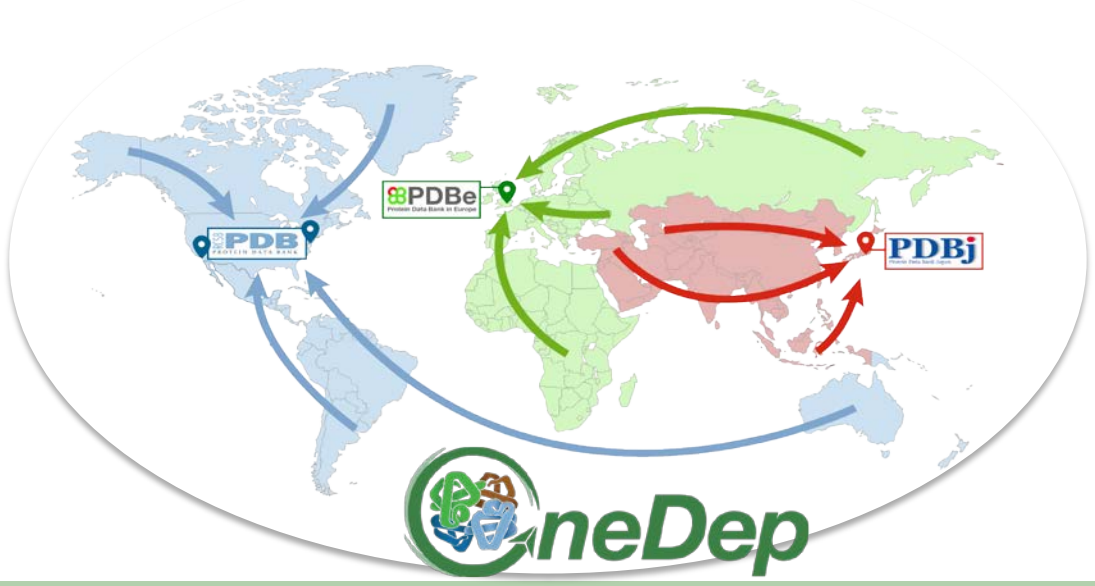
wwPDB provides the Deposition Site



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

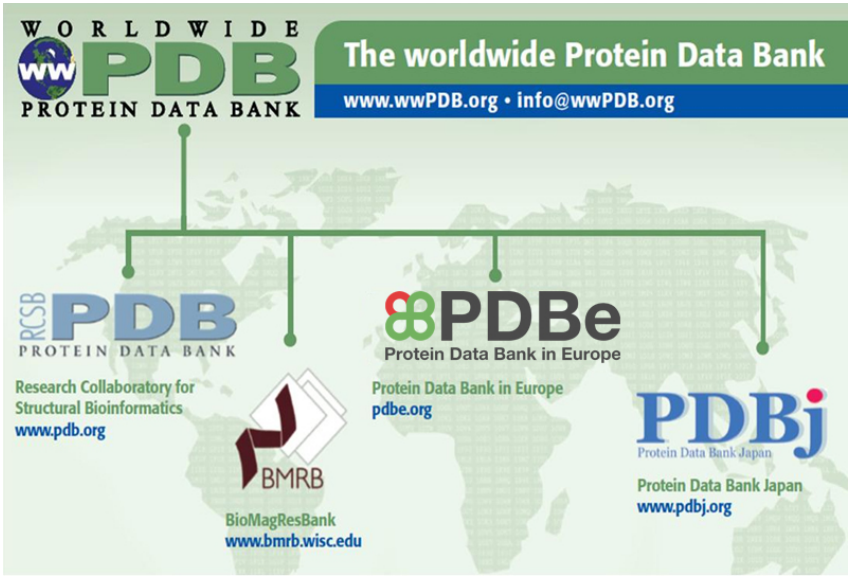
→ 詳細はこの後の中川敦史先生のご講演で

PDBj
Protein Data Bank Japan

Protein Data Bank Japan

https://pdbj.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 Publication

TOOLS FOR PROTEIN SCIENCE

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

Akira R. Kinjo,[1] Gert-Jan Bekker,[1] Hiroshi Wako,[2] Shigeru Endo,[3] 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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[2]School of Social Sciences, Waseda University, 1-6-1 Nishi-Waseda, Shinjuku-ku, Tokyo 169-8050, Japan
[3]School of Science, Kitasato University, 1-15-1, Kitasato, Minami-ku, Sagamihara, Kanagawa 252-0373, Japan
[4]Graduate School of Information Sciences, Tohoku University, 6-3-09 Aoba, Aramaki-aza Aoba-ku, Sendai 980-8579, Japan

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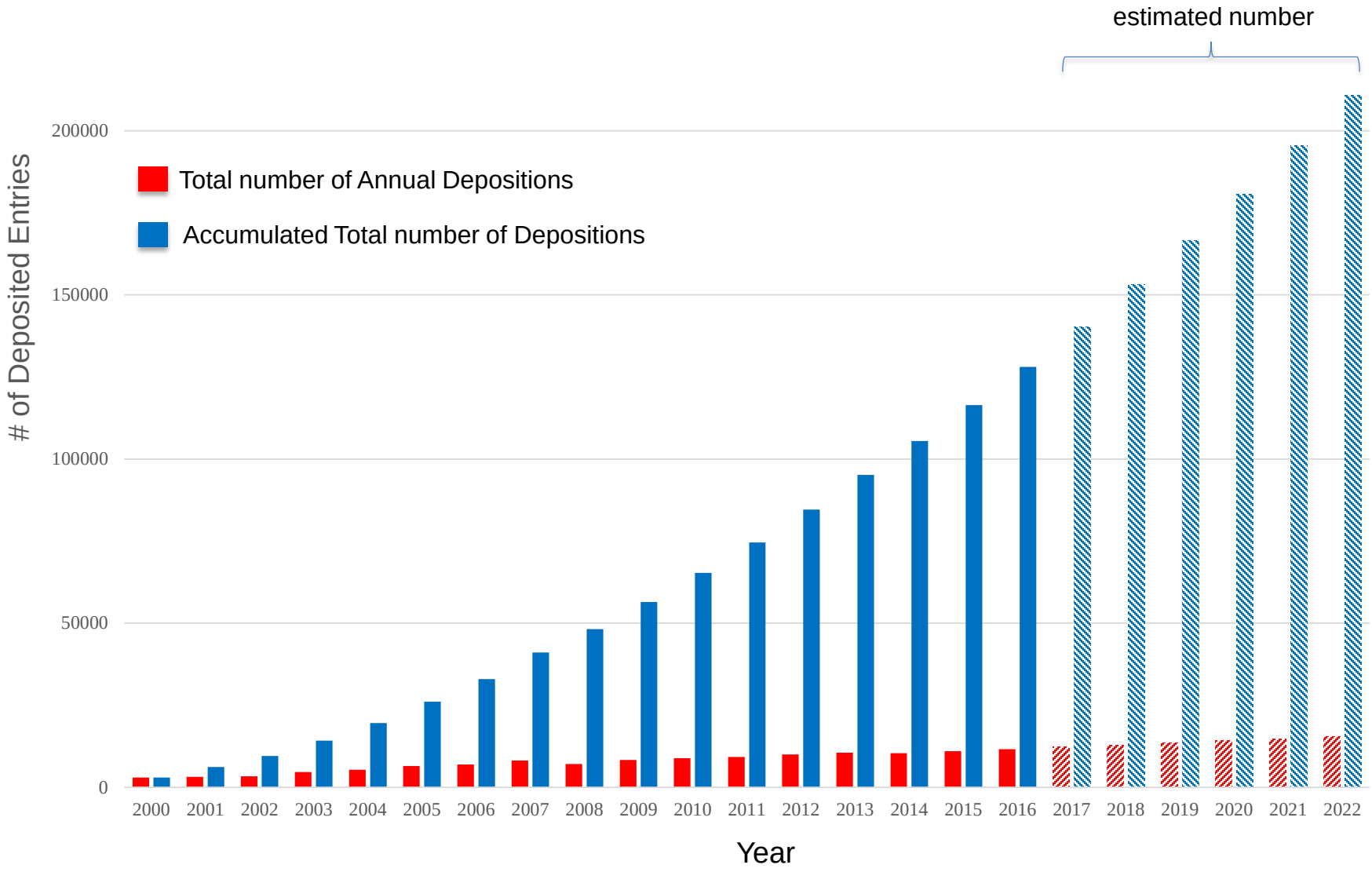
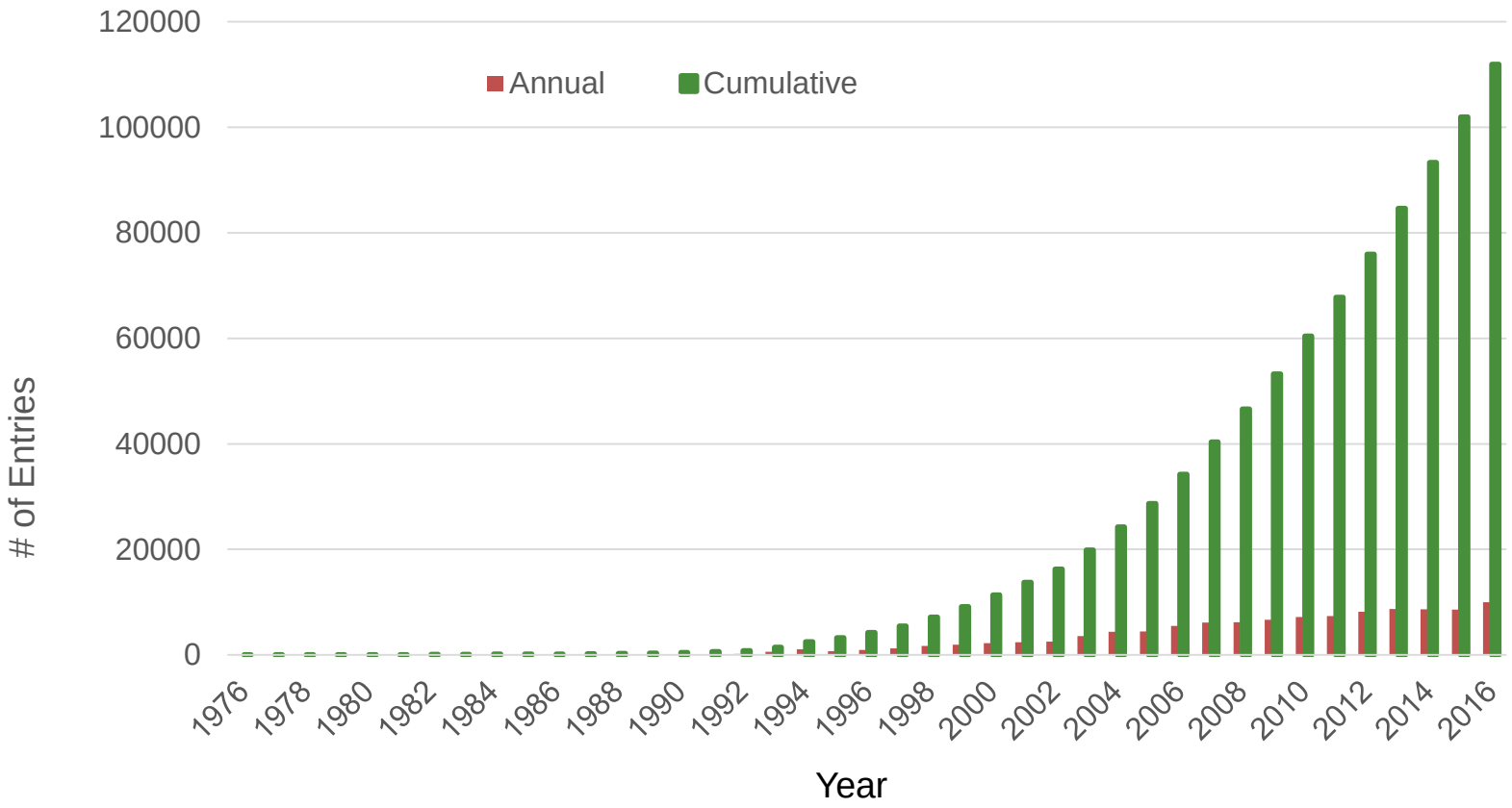
DOI: 10.1002/pro.3273
Published online 00 Month 2017 proteinscience.org

Growing Number of Depositions



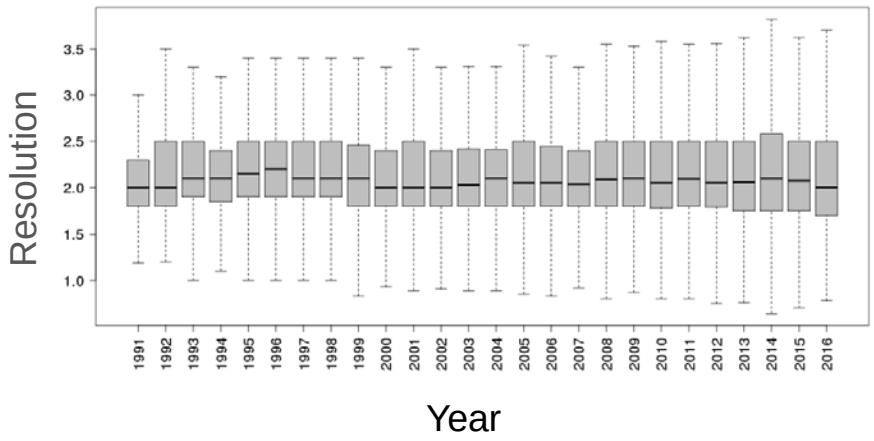
Growth of Released PX Entries



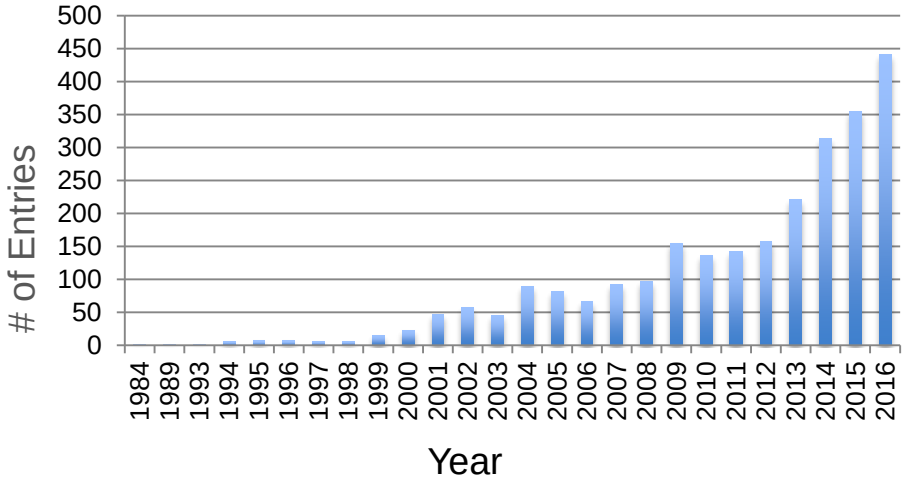
>120,000 Total Released MX Entries Projected for End 2017

MX Deposition Complexity

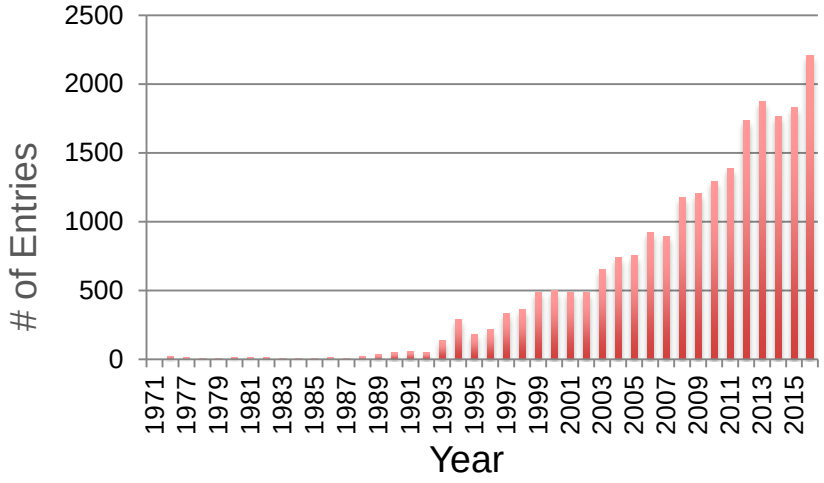
Annual Distribution for High Resolution Limit



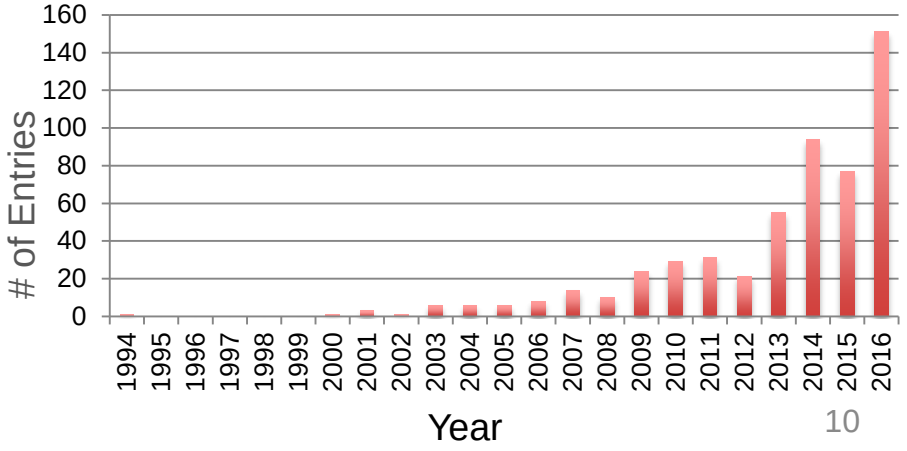
Annual Released Structures With AU MW > 500,000



Total Number of New CCD Entries



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



PDB Data Download Statistics

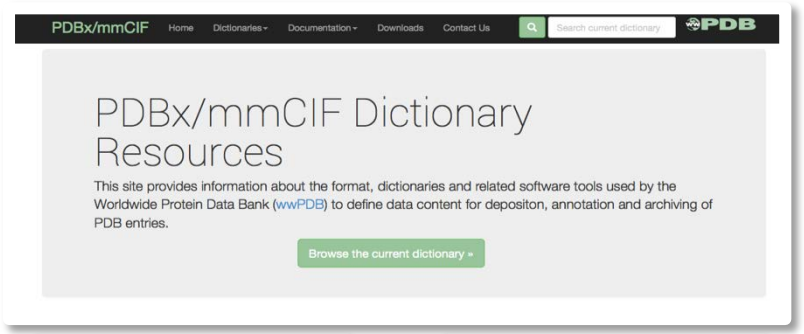
Year	Total	Total FTP Archive	Total Website	RCSB PDB FTP Archive	RCSB PDB Website	PDBe FTP Archive	PDBe Website	PDBj FTP Archive	PDBj Website
2009	328,362,536	271,116,934	57,245,602	222,984,760	53,507,785	30,141,339	1,475,116	17,990,835	2,262,701
2010	294,326,976	213,180,966	81,146,010	159,248,214	64,569,658	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

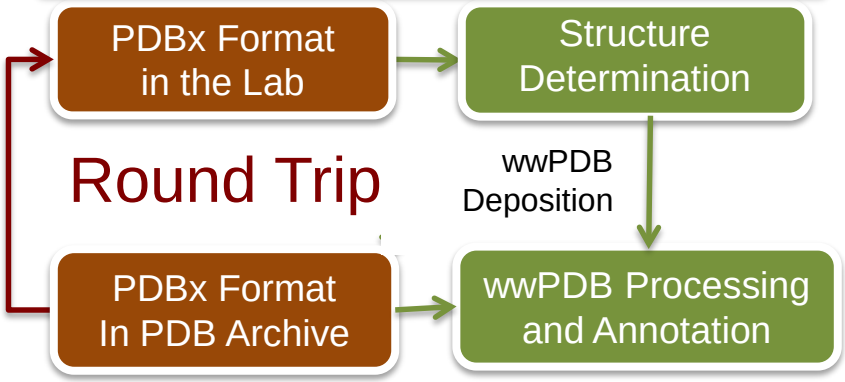
More than 1.5 million/day

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

Protein Data Bank Japan - PDBj

PDBj
Protein Data Bank Japan
Worldwide Protein Data Bank Foundation

Menu

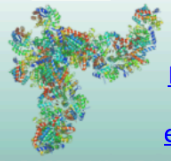
131905 entries (2017-07-11)

English ▼

Search pdbj.org

wwPDB RCSB PDB PDBe BMRB Legacy
Adv. Search Search help

5OCW



Latest new entries

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

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

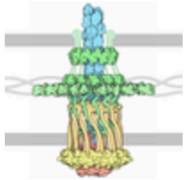
Choose a keyword listed below or input keywords into the textbox at the right of the keyword list. The brief explanation of the matched services will be displayed.

- 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

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

PDBj
Protein Data Bank Japan
Worldwide Protein Data Bank Foundation

メニュー

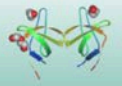
131905 エントリー (2017-07-11)

日本語 ▼

pdbj.org 全体を検索（日本語OK）

wwPDB RCSB PDB PDBe BMRB Legacy
Adv. Search Search help

5OAZ



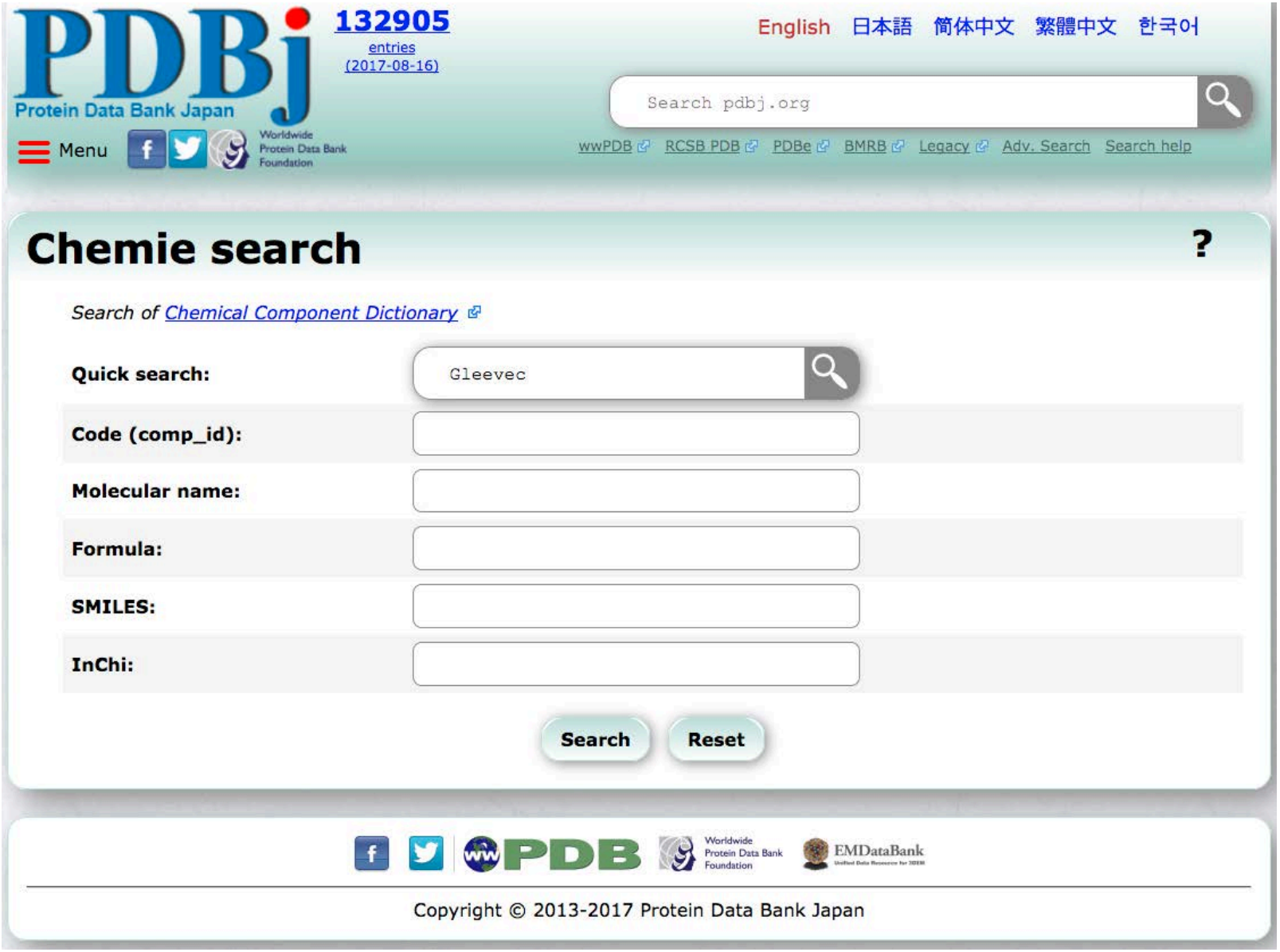
最新公開エントリー

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

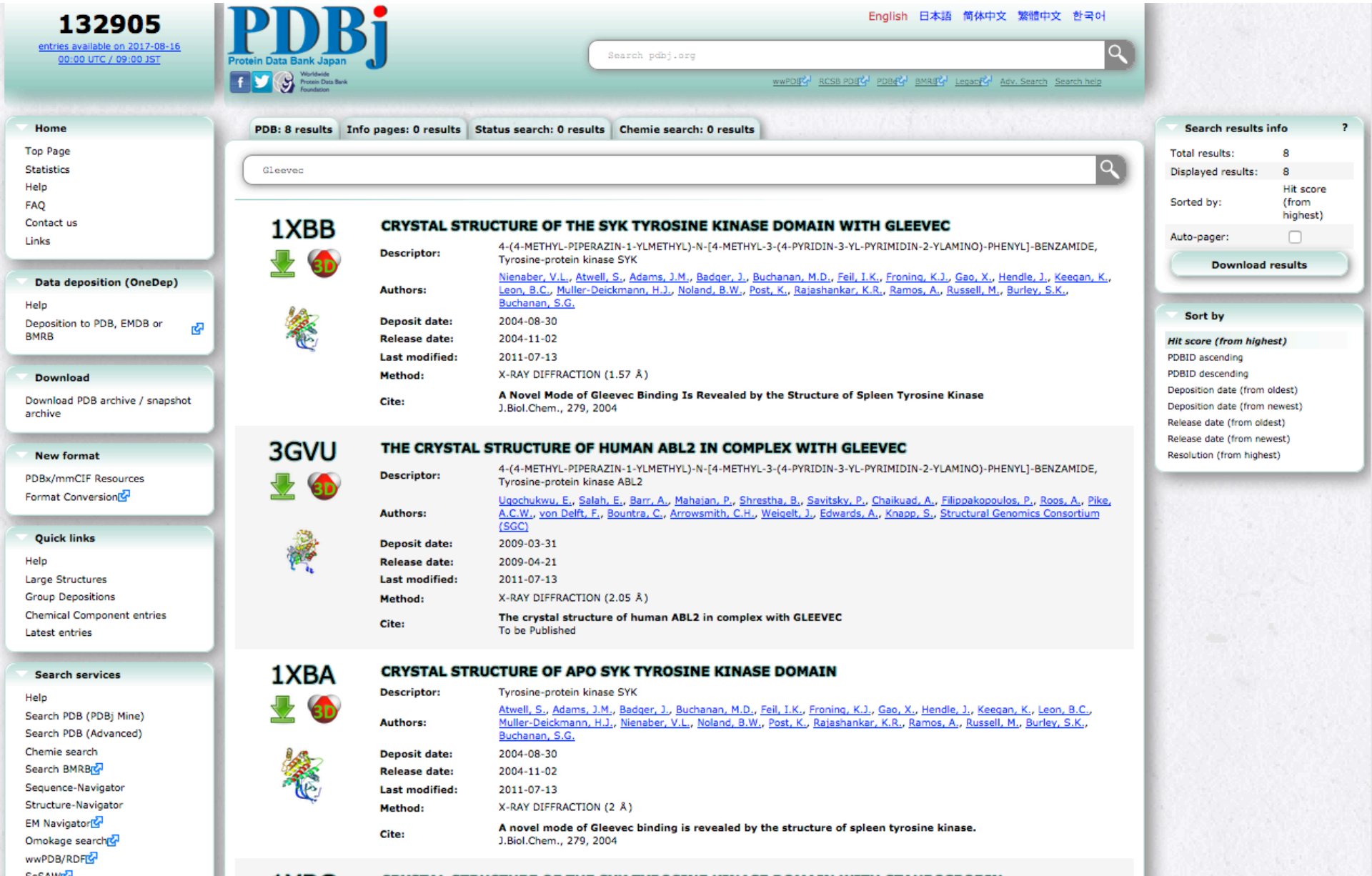
今月の分子

211: 線毛機械 (Pilus Machine)

Example1: Gleevec using PDBj-Mine



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



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Structure-Navigator
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Omokage search
wwPDB/RDF
SeSAW
Ligand Binding Sites (GIRAF)
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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.** *J.Biol.Chem.*, 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

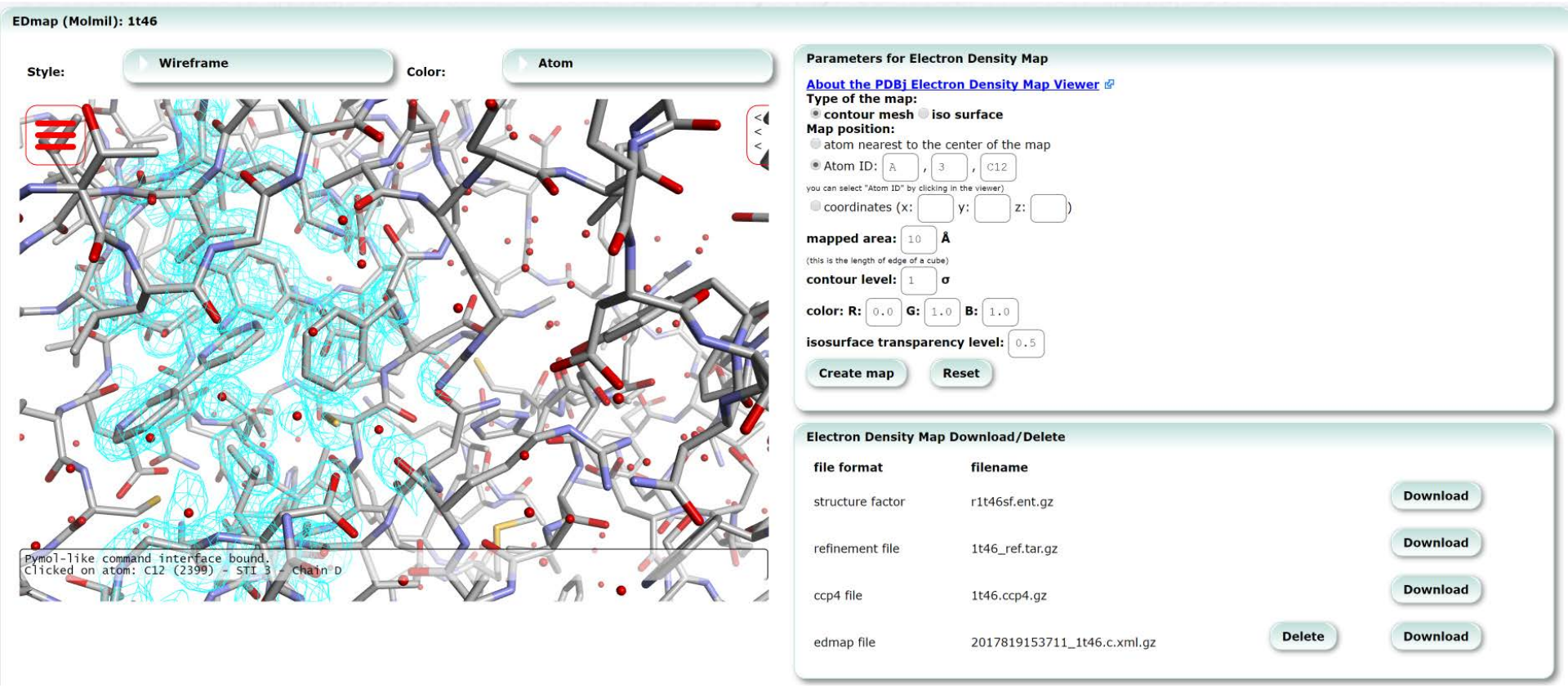
Downloads
Sequence (fasta)
PDBx/mmCIF
PDBML format (no-atom)
PDB format (full)
Validation report (PDF)
More...

Structures
View Asymmetric Unit (AU = BU)

Database information
RCSB-PDB
PDBe
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 A
Electron Density Map (molmil)
wwPDB/RDF
Promode Elastic
EzCatDB (M00323)

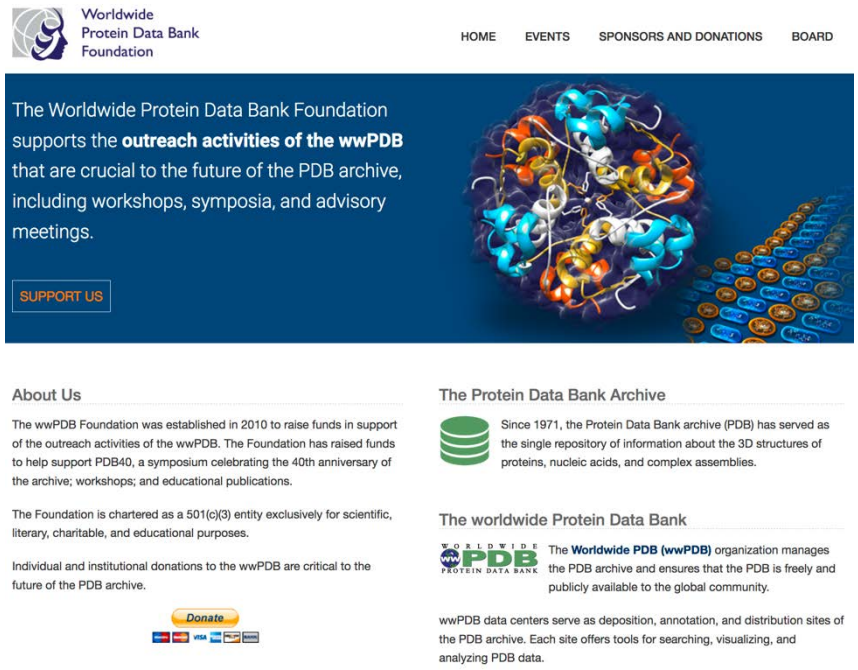
Eelectron Density map (Molmil)

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



wwPDB Foundation Progress

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



http://foundation.wwpdb.org/