

日本蛋白質構造データバンク (PDBj: Protein Data Bank Japan) と wwPDB (worldwide PDB)

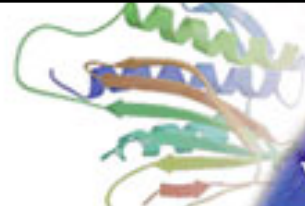
大阪大学蛋白質研究所
PDBj 日本蛋白質構造データバンク

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<http://www.pdbj.org/>





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wwPDBAC

The Worldwide Protein Data Bank (wwPDB) consists of organizations that act as deposition, data processing and distribution centers for PDB data. The founding members are **RCSB PDB** (USA), **PDBe** (Europe) and **PDBj** (Japan)¹. The **BMRB** (USA) group joined the wwPDB in 2006. The mission of the wwPDB is to maintain a single Protein Data Bank Archive of macromolecular structural data that is freely and publicly available to the global community.

This site provides information about services provided by the individual member organizations and about projects undertaken by the wwPDB.

wwPDB Statement on Retraction of PDB Entries

18-February-2010

Changes to the wwPDB Policy for Depositing Polypeptide Structures

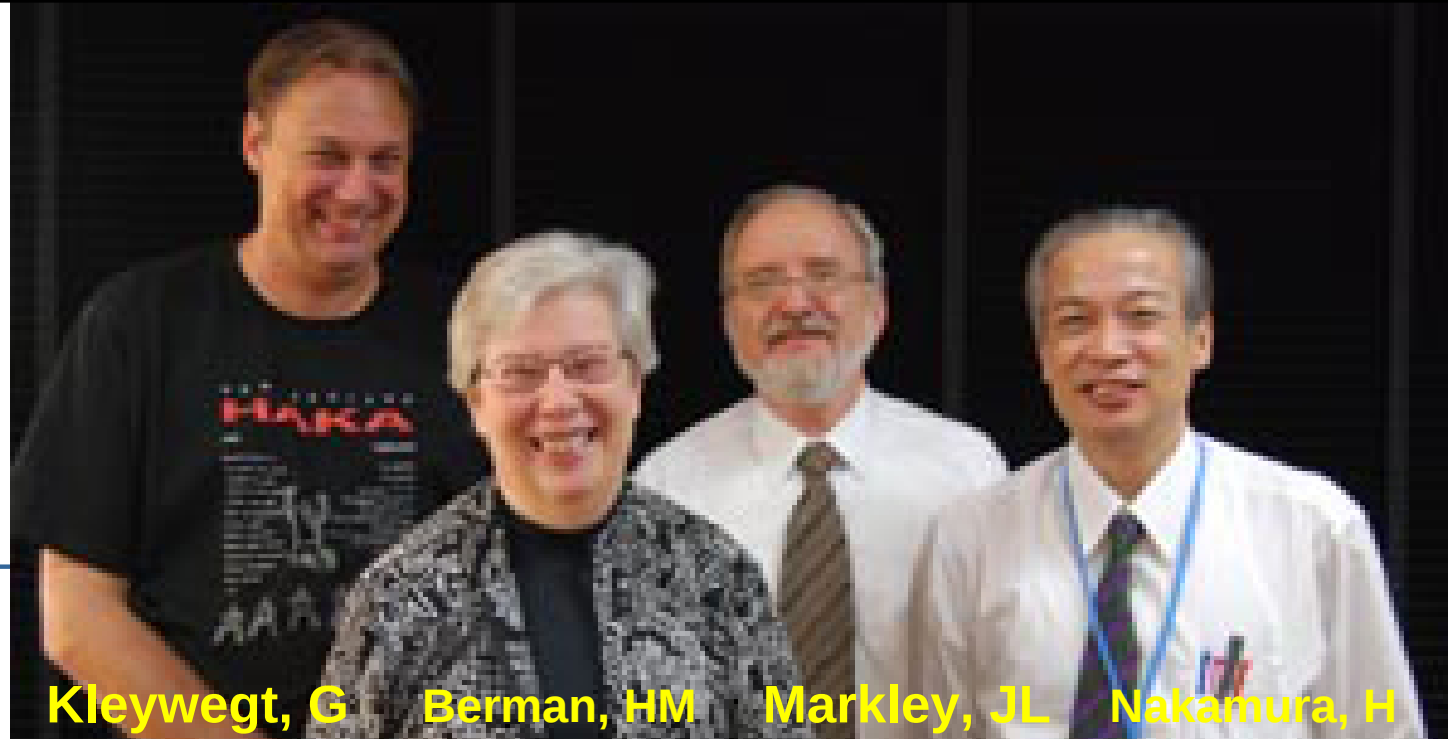
The wwPDB now accepts polypeptide structure depositions of all gene products; all naturally-occurring, non-ribosomally synthesized peptides, such as antibiotics; and all peptidic repeat units of larger polymers, such as fibrous and amyloid polymers. In addition, non-naturally occurring synthetic peptides with at least 24 residues will be accepted for deposition.

Consistent with earlier policy, depositions of polynucleotide and polysaccharide structures of 4 or more residues are also accepted. For more information, see the wwPDB Policy Guide at <http://www.wwpdb.org/policy.html>.

2-February-2010

wwPDB FTP Advisory Notice

The PDB archive can be accessed at FTP sites at the RCSB PDB, PDBe, and PDBj. The update schedules for these sites have been coordinated to be simultaneous. All updates now occur at the target time of Wednesday 00:00 UTC (**Coordinated Universal Time**).



PDBj Protein Data Bank Japan

Protein Data Bank Japan

日本蛋白質構造データバンク

<http://www.pdbj.org/>

大阪大学蛋白質研究所にて実施。
(独立行政法人)科学技術振興機構
バイオインフォマティクス推進センタ
ー(<http://www-bird.jst.go.jp/>)が
2001年から支援

原子種とその座標、アミノ酸残基、実験手法、
実験時の情報、実験観測データ(構造因子)
を整理して登録。Webから無料公開。

The screenshot displays the PDBj website. At the top, there are language links: English, Japanese, simplified Chinese, traditional Chinese, and Korean. A statistics bar shows 66961 entries available as of August 4, 2010. The left sidebar contains a 'トップページ' (Top Page) link and a 'データ登録' (Data Registration) section with links for ADIT (PDB Deposition), ADIT-NMR, and a search section. The main content area features a 'データ登録のご案内' (Data Registration Guide) with links for PDB and NMR data registration. Below this is a search section with a 'PDB検索 Mine' (PDB Search Mine) link and a search box. The right sidebar includes logos for PDB, eProTS, Protein Globe, DBCLS, and Tanpaku.org. The bottom section, '最新情報' (Latest Information), contains news items dated 2010/7/13, 2010/7/1, 2010/6/30, and 2010/5/19, detailing updates to the database and new features.



代表: 中村春木

PDBj データベース管理運営グループ:

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陳 旻瑜

ツール・サービス開発グループ:

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池川恭代, 清水有希子, 鎌田知左

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研究開発協力者:

Daron M. Standley (阪大免疫フロンティア), 木下賢吾 (東北大情報),
藤博幸 (産総研CBRC), 加藤和貴 (産総研CBRC), 輪湖博 (早大),
伊藤暢聡 (東京医歯大)

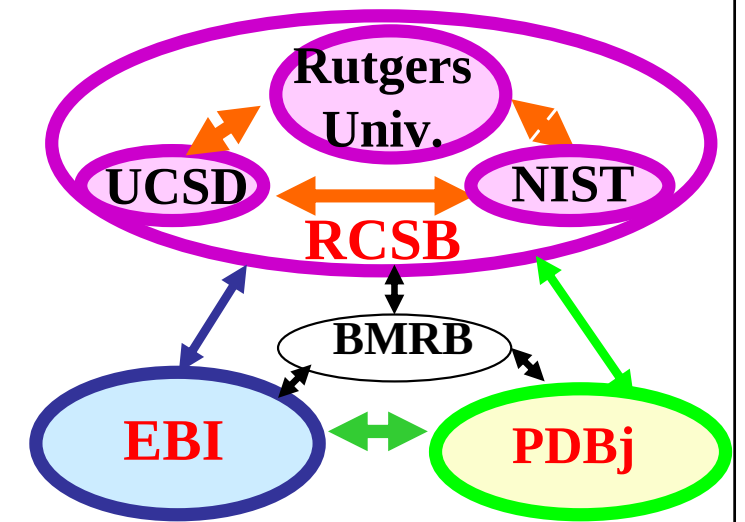
wwPDBにおける国際協力

1) データ編集・登録作業を、wwPDBのメンバーで協力しながら実施する。

2) 唯一のデータアーカイブを持ち、米国のRCSB-PDBがアーカイブ・キーパーとして書き込み権限をもつ。

3) データ・フォーマットや新たな記述法については、各メンバー間内の討議により決定する。(V3.1→V3.2)

4) 各メンバーは、各々独自のデータ・ブラウザ、ビューア、検索ツール、Web サービスを開発することが期待される。



日本蛋白質構造データバンク:PDBj

1. 国際蛋白質構造データバンク([wwPDB](http://www.pdb.org))の運営
2. 蛋白質立体構造データベース登録作業
3. 蛋白質構造情報の記述フォーマット(v3.2, [mmCIF](#), [PDBML](#))の開発(validation)とその応用
4. 蛋白質構造解析実験および蛋白質機能に関する文献情報の付加
5. 蛋白質立体構造に関する新規二次データベースの構築と解析ツールの開発

Japanese

PDBj
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日本蛋白質構造データバンク (PDBj: Protein Data Bank Japan)は、JST-BIRDの支援を受け、米国RCSB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おります。

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最新情報
2009/10/22
2009年10月22日 (木) から、PDBjでは、主要なページおよびデータ登録に関するページについて、**繁体中国語**のページを公開しました。

2009/10/9
2009年10月14日 (水) から、wwPDBでは、毎週のデータアップデートを、原則として、日本時間の毎水曜日午前9時 (UTC0時) に行います。
このデータ更新は、米国のRCSB-PDB、欧州のPDBe、PDBjにおいて、同時刻に行われます。

2009/10/9
2009年10月14日 (水) から、PDBjにおけるデータ検索システムとして新たに開発した「**PDBj Mine**」の稼働を始めます。
PDBj Mineは、relational DBを用いているため、XPath/XQueryの利用はできなくなります。また、これまでの検索システム「xPSSS」も、しばらくの間はご利用できます。

61248
entries available
on 4 Nov., 2009
00:00(UTC) / 09:00(JST)

Korean

PDBj
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PDB (Protein Data Bank Japan)는 미국의 구조 생물 정보학 연구 공동체(RCSB)와 유럽 생물 정보학 연구소(EBI)와 협력하여 고분자 입체구조와 구조 해석 일을 제공하고 있습니다. PDB는 독립적인 과학기술 진흥기구 생물 정보학 추진센터(JST-BIRD)의 후원을 받고 있습니다.

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새로운 뉴스
22-Oct-2009
On October 22, 2009, PDBj main pages and deposition pages in "traditional Chinese" have been released.

9-Oct-2009
On October 14, 2009, the weekly data update will be made, in principle, at 9:00 AM (JST) of every Wednesday, which corresponds to 0:00 (UTC). This update is simultaneously made at every member of the wwPDB: RCSB-PDB, PDBe, and PDBj.

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On October 14, 2009, we will start to use a new data viewer, **PDBj Mine**, which has been recently developed by PDBj. Because PDBj Mine uses a relational database, XPath/XQuery is not available. Our XML-based database, xPSSS, is still available for another couple of months.

25-Sep-2009
The changes to the wwPDB FTP site has been announced as "The advisory notice" at <http://www.wwpdb.org/>. (September 25, 2009)

61248
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Simplified Chinese

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日本蛋白质结构数据库 (PDBj: Protein Data Bank Japan), 由JST-BIRD提供支持, 与美国的RCSB和欧洲PDBe共同合作。在对国际性的生物大分子立体结构数据库的档案文件进行维护的同时, 还提供各种结构解析的应用工具。

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Traditional Chinese

PDBj
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wwPDB FTP Traffic



32,276,101 ファイルが2010年3月の1ヶ月間に世界中のwwPDBメンバーサイトからダウンロードされている (RCSB-PDB, EBI-PDBe, and PDBj)

データの品質管理・保守について

- 登録時に、各立体構造の品質が厳しく検査・鑑定される。登録者本人と、wwPDBのアノテータが、それぞれ検証する。この検証に合格しないと、PDBIDが発行されない。
- 実験情報(X線結晶解析の場合には構造因子、NMRの場合には原子間距離情報) が、2008年2月1日から、登録時に座標と同時に必須の項目となった。NMR化学シフトデータも近い将来に必須となる予定。

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PDB登録



NMRデータ登録



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Mine

Mine日本語ページについて

NMRデータ検索



PDB ID or Keyword

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☒ Accession number

☐ Deposition code

Go

最新情報

2010/7/13

PDBj が開発しておりますフリーの分子グラフィックス・ビューア: **jvの最新版(jv3.8)**がリリースされました。displayatom on/off のコマンド機能が追加され、多様な表示が容易にできるようになっております。どうぞ、[こちら](#)からダウンロードしてお使いください。

2010/7/1

2010年8月9日(月)、10日(火) に、「ライフサイエンス・データベース講習会 in 名大」を名古屋大学情報文化学部棟にて開催いたします。(詳細 / お申し込み)

2010/6/30

NMR距離制限情報ファイルバージョン2 が公開されました。(詳細...)

66961

[entries available
on 4 Aug., 2010](#)

00:00(UTC) / 09:00(JST)

 WORLDWIDE

 PROTEIN DATA BANK

 蛋白質構造百科事典

 eProtS
 Encyclopedia of
 Protein Structures

 Protein
 Globe

 DBCLS
 Database Center for Life Science

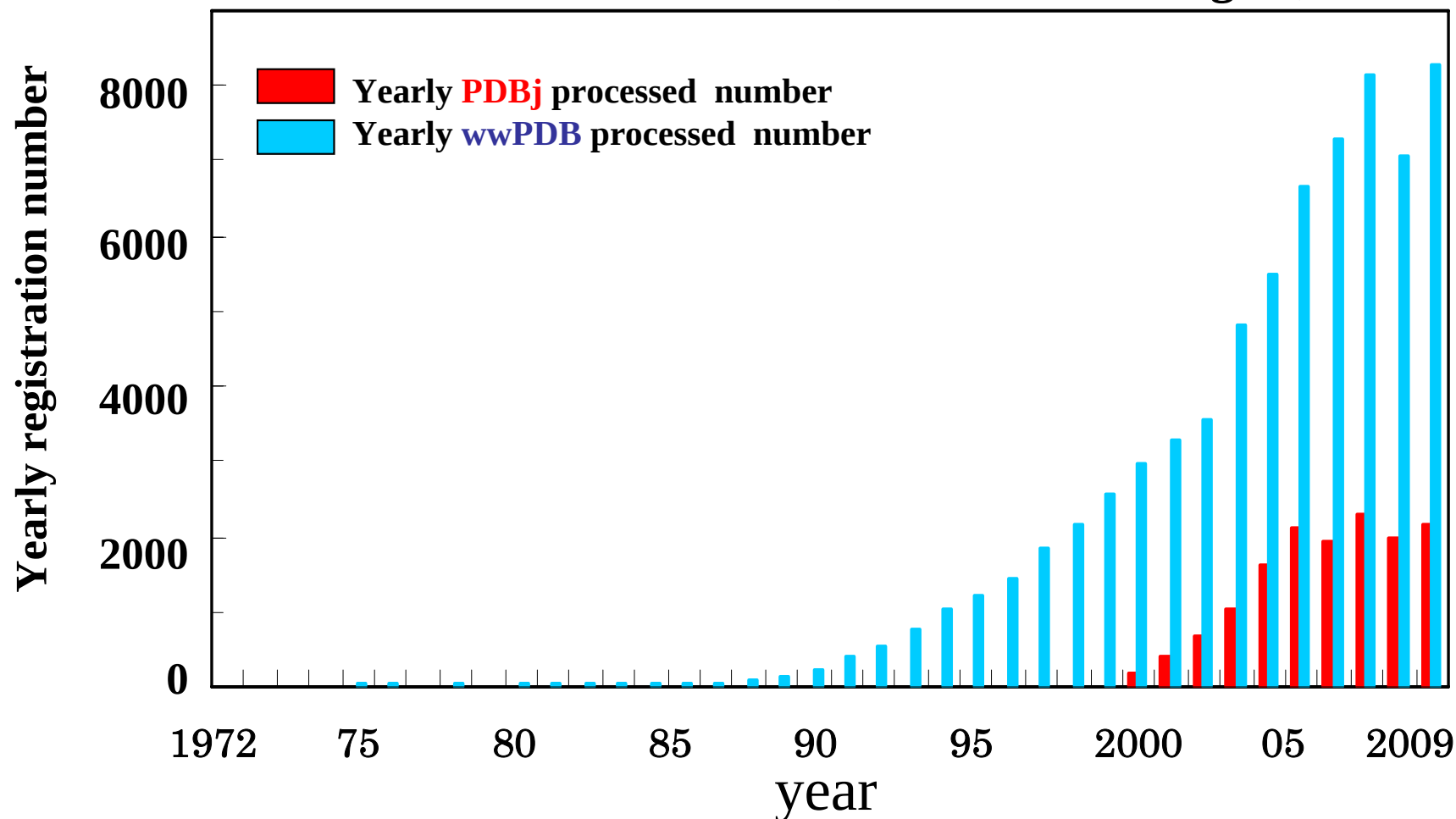
Tanpaku.org

 National Project
 on Protein Structural
 and Functional Analyses

BioIT

PDBj と wwPDBにおけるデータ登録数

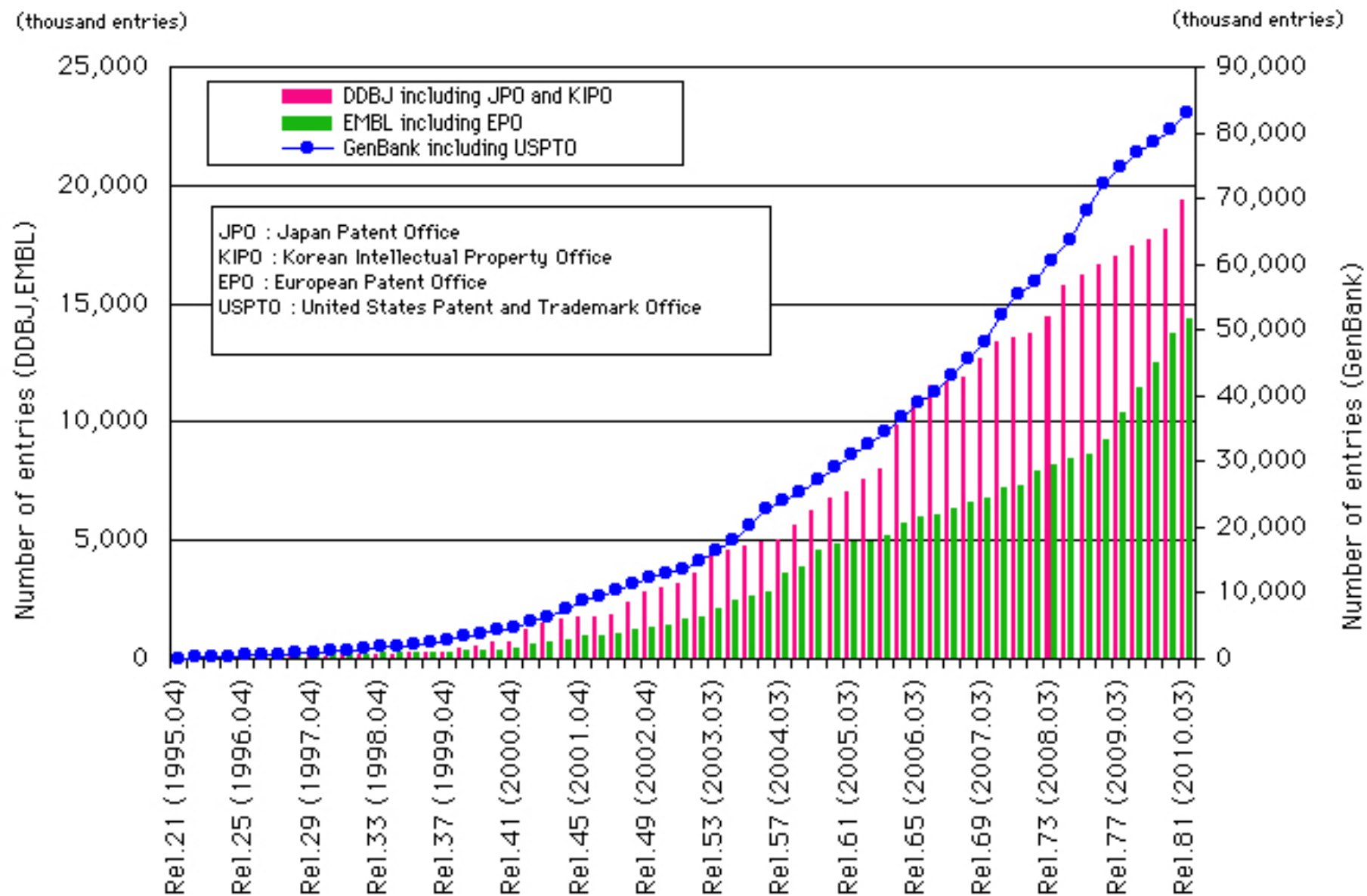
Total 66,961 data on 4 August, 2010



PDBjでは、世界中で登録されるエントリーのうち **25-30 %** を登録している。日本からの登録はすべてPDBjが行い、またアジア、オセアニア地区からの登録もPDBjが担当している。

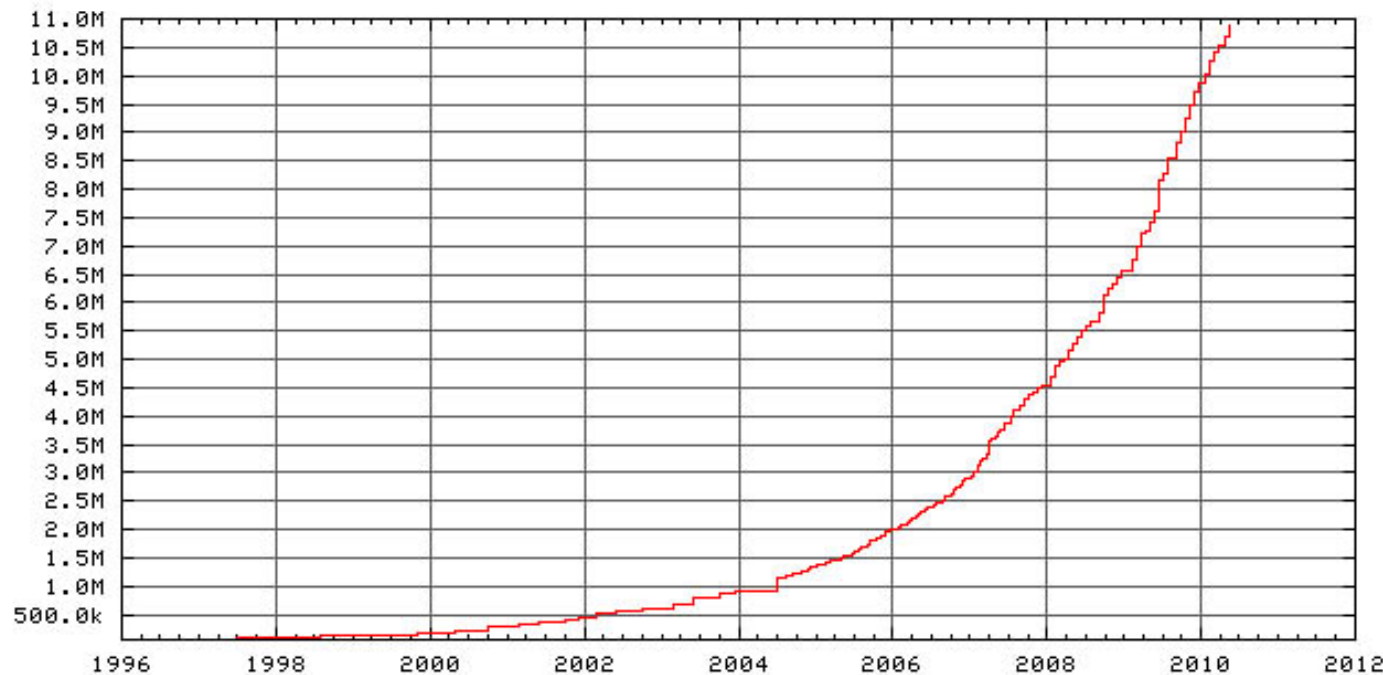
The Number of Entries by Contributors to DDBJ Release
(1995/01-2010/03)

Rapid increase of gene information (from DDBJ).

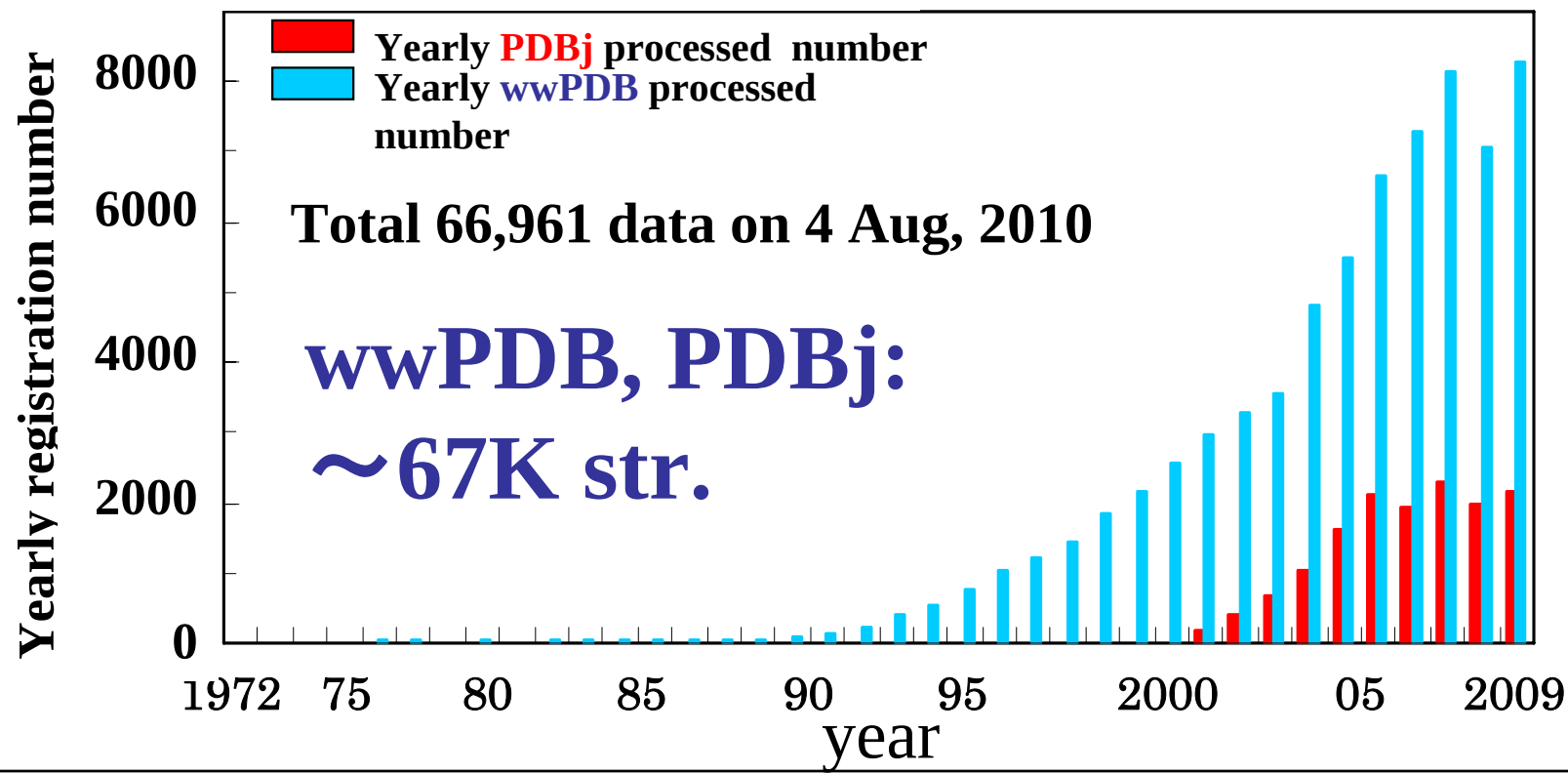


* Note: CON and TPA divisions are not counted in the Release statistic

Rapid increase of protein information.



UniProt:
~11M seq.



Different Growth of SDAs (Single-Domain Architecture) and MDAs (Multi-Domain Architecture)

Michael Levitt, Nature of the protein universe.
Proc. Natl. Acad. Sci. USA (2009) 27, 11079-11084

The number of MDA families is growing rapidly with time, the number of SDA families appears to be saturating. Structural information is known for $\frac{1}{4}$ of sequence profiles.

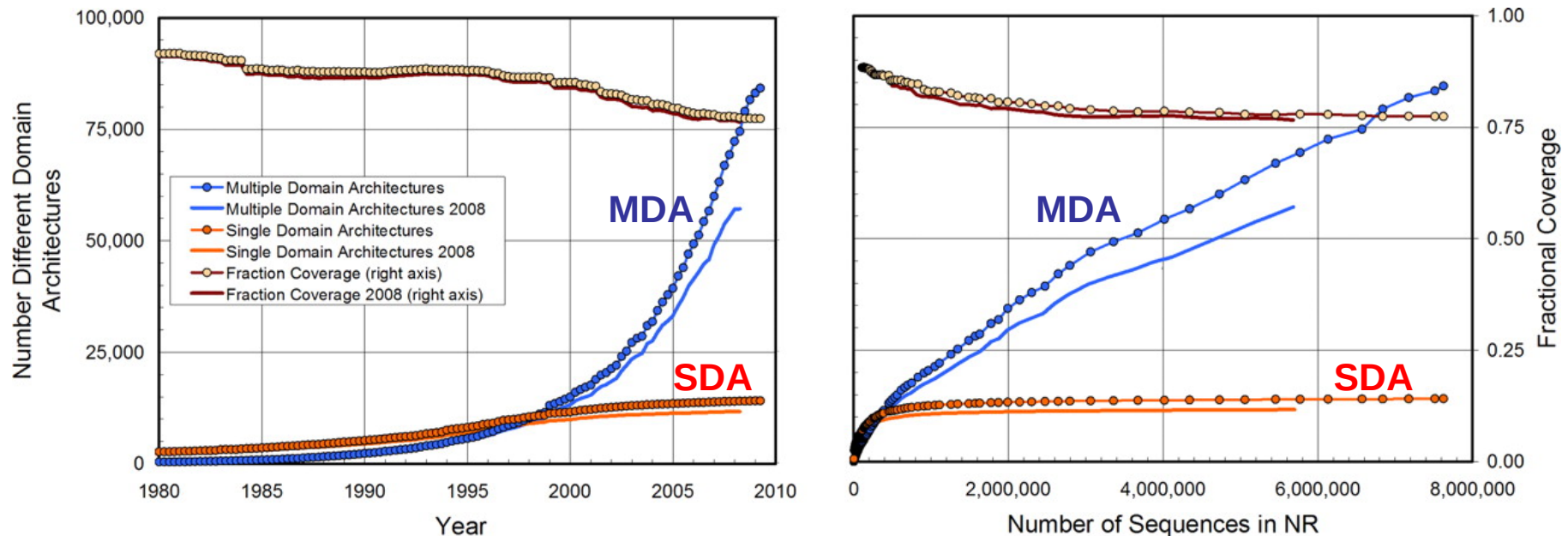


Fig. 1: As the NR database grows, the number of different multidomain architecture (MDA) families found by CDART is increasing rapidly with year (Left) or added sequence (Right)

ホモロジー・モデリング

(homology modeling / comparative modeling)

アミノ酸配列の類似性を基に構造既知の蛋白質の立体構造を鋳型(テンプレート)として構造未知の蛋白質の立体構造モデルを作成すること

● ホモロジーモデリングの必要性

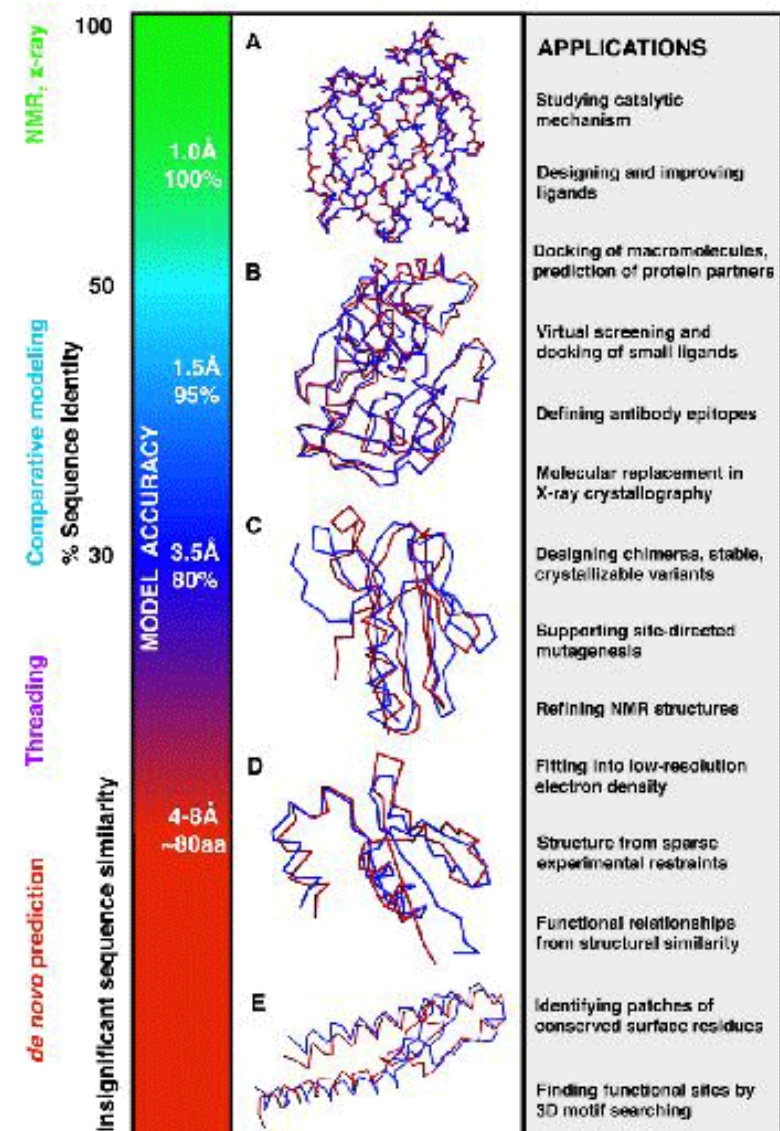
- 配列情報: 約 **1,163 万** 配列 (UniProt)
 - 立体構造: 約 **6万7千** 分子 (wwPDB)
- ファミリー代表の構造がデータベースにあれば、構造モデルを作成できる。
- ファミリー数: 約 **30,000** (30% identity)
 - フォールド数: 約 **2,000** (loose definition)

● 原則

- 配列が似ていれば構造は似ている
- 構造未知でも、配列の似た蛋白質で構造既知のものがあれば、その構造を参考に構造を予想できる

● モデリングの具体的作業

- 似た配列を探す
- 配列のalignmentを作る
- 配列の違う部分のつじつまを合わせる(主鎖と側鎖)



New! *Spanner*

Hybrid-Template Modeling

<http://www.pdbj.org/spanner/>

Developed by

Mieszko Lis (MIT),

Daron M. Standley (iFREC, Osaka U),

Haruki Nakamura (IPR, Osaka U)

Spanner v1.0.1
Hybrid-template Structural Modeling

REQUIRED INPUTS

Template Structure in PDB format:
(ファイルを選択) ファイルが選...ていません

Sequence alignment in FASTA format (1st sequence = template and 2nd sequence = query):
(ファイルを選択) ファイルが選...ていません

Email address for results:

ADVANCED OPTIONS

Job Name (optional):

Model (optional): ☐

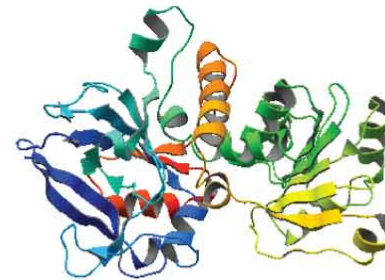
Chain (optional): ☐

Energy Minimization: ☒ Presto ☐ Gromacs

Margin:

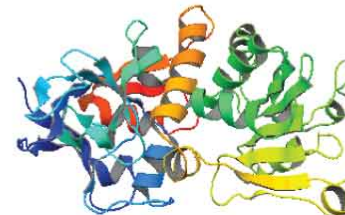
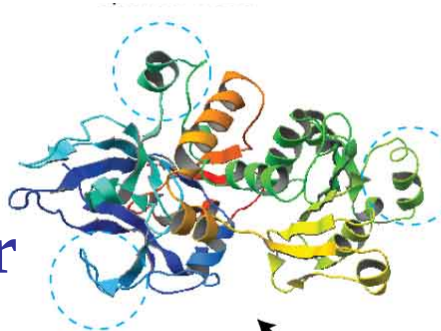
Anchor Tolerance:

START!

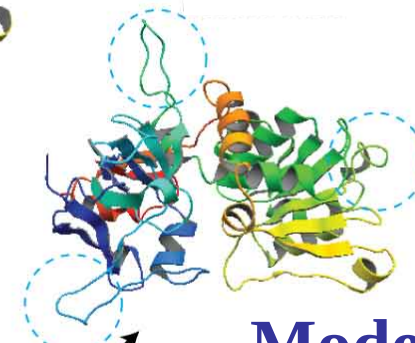


Native: 1guf B

**Spanner
model**



Template: 1zsy A



**Modeller model
without no loop
information**

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PDB Archive/Snapshot

日本蛋白質構造データバンク (PDBj: Protein Data Bank Japan)は、JST-BIRD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おります。

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NMRデータ登録



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PDBj
Mine

Mine日本語ページについて

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Go

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NMRデータ検索

☒ Accession number☐ Deposition code

Go

最新情報

2010/7/13

PDBj が開発しておりますフリーの分子グラフィックス・ビューア: **jvの最新版(jv3.8)**がリリースされました。displayatom on/off のコマンド機能が追加され、多様な表示が容易にできるようになっております。どうぞ、[こちら](#)からダウンロードしてお使いください。

2010/7/1

2010年8月9日(月)、10日(火) に、「ライフサイエンス・データベース講習会 in 名大」を名古屋大学情報文化学部棟にて開催いたします。(詳細 / お申し込み)

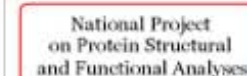
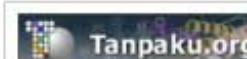
2010/6/30

NMR距離制限情報ファイルバージョン2 が公開されました。(詳細...)

66961

[entries available
on 4 Aug., 2010](#)

00:00(UTC) / 09:00(JST)



フォーマットのupdate: v3.2

1) SPLIT レコードの新設:

巨大な蛋白質複合体の原子座標の記載

2) 情報の追加:

複合体情報: PISA/PQS

SITEレコード: 実験/リガンド近傍原子

3) 低分子リガンドのdictionary: CCD

(Chemical Compound Dictionary

<http://www.wwpdb.org/ccd.html>) の整備

Example: Vault by Kato et al. (2zu0, 2zv4, 2zv5)

```
CRYST1  702.246  383.796  598.480  90.00 124.69  90.00 C 1 2 1      52
ORIGX1      1.000000  0.000000  0.000000      0.000000
ORIGX2      0.000000  1.000000  0.000000      0.000000
ORIGX3      0.000000  0.000000  1.000000      0.000000
SCALE1      0.001424  0.000000  0.000986      0.000000
SCALE2      0.000000  0.002606  0.000000      0.000000
SCALE3      0.000000  0.000000  0.002032      0.000000
ATOM      1  N  MET A  1  -82.230 143.797  30.257  1.00224.78      N
ATOM      2  CA MET A  1  -81.386 143.353  31.410  1.00224.78      C
ATOM      3  C  MET A  1  -82.092 142.602  32.579  1.00224.78      C
ATOM      4  O  MET A  1  -81.529 142.546  33.672  1.00224.78      O
ATOM      5  CB MET A  1  -80.532 144.526  31.950  1.00238.55      C
ATOM      6  CG MET A  1  -80.944 145.901  31.411  1.00238.55      C
ATOM      7  SD MET A  1  -81.051 147.196  32.668  1.00238.55      S
ATOM      8  CE MET A  1  -82.566 148.018  32.159  1.00238.55      C
ATOM      9  N  ALA A  2  -83.281 142.021  32.391  1.00183.83      N
ATOM     10  CA ALA A  2  -83.718 140.956  33.340  1.00183.83      C
ATOM     11  C  ALA A  2  -85.047 140.283  32.983  1.00183.83      C
ATOM     12  O  ALA A  2  -85.544 140.452  31.862  1.00183.83      O
ATOM     13  CB ALA A  2  -83.676 141.427  34.858  1.00153.13      C
ATOM     14  N  THR A  3  -85.601 139.498  33.914  1.00241.98      N
ATOM     15  CA THR A  3  -86.810 138.720  33.602  1.00241.98      C
ATOM     16  C  THR A  3  -88.021 139.162  34.413  1.00241.98      C
ATOM     17  O  THR A  3  -87.885 139.702  35.529  1.00241.98      O
ATOM     18  CB THR A  3  -86.748 137.233  33.902  1.00168.86      C
ATOM     19  OG1 THR A  3  -87.140 136.275  32.867  1.00168.86      O
ATOM     20  CG2 THR A  3  -86.525 136.850  35.263  1.00168.86      C
```

Example: Vault by Kato et al. (2zuo, 2zv4, 2zv5)

```
HEADER      STRUCTURAL PROTEIN                               24-OCT-08   2ZUO
TITLE       THE STRUCTURE OF RAT LIVER VAULT AT 3.5 ANGSTROM RESOLUTION
SPLIT       2ZUO 2ZV4 2ZV5
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: MAJOR VAULT PROTEIN;
COMPND      3 CHAIN: A, B, C, D, E, F, G, H, I, J, K, L, M;
COMPND      4 SYNONYM: MVP
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: RATTUS NORVEGICUS;
SOURCE      3 ORGANISM_COMMON: RAT;
SOURCE      4 ORGANISM_TAXID: 10116;
SOURCE      5 TISSUE: LIVER
KEYWDS      9 REPEAT DOMAINS, PROTEIN-PROTEIN COMPLEX, CYTOPLASM,
KEYWDS      2 RIBONUCLEOPROTEIN, STRUCTURAL PROTEIN
EXPDTA      X-RAY DIFFRACTION
AUTHOR      K.KATO,Y.ZHOU,H.TANAKA,M.YAO,E.YAMASHITA,M.YOSHIMURA,
AUTHOR      2 T.TSUKIHARA
REVDAT      2   08-FEB-09 2ZUO   1       JRNL
REVDAT      1   13-JAN-09 2ZUO   0
JRNL        AUTH   H.TANAKA,K.KATO,E.YAMASHITA,T.SUMIZAWA,Y.ZHOU,
JRNL        AUTH 2 M.YAO,K.IWASAKI,M.YOSHIMURA,T.TSUKIHARA
JRNL        TITL   THE STRUCTURE OF RAT LIVER VAULT AT 3.5 ANGSTROM
JRNL        TITL 2 RESOLUTION
JRNL        REF    SCIENCE                               V. 323   384 2009
JRNL        REF    1004 0000 0075
```

Example: Vault by Kato et al. (2zuo, 2zv4, 2zv5)

PDBj
Protein Data Bank Japan

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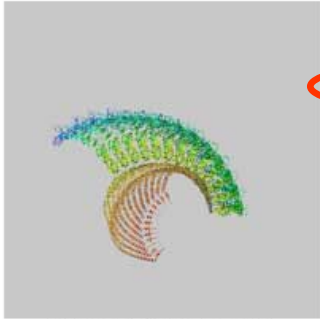
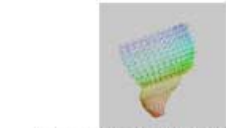
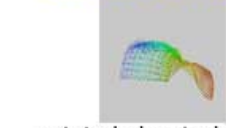
Links

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	PDB ID	2zuo sequence information (FASTA format) download PDB format file
	SPLIT PDB ID	2zv4, 2zv5
	RELATED PDB ID	2zv4, 2zv5
	Descriptor	Major vault protein
	Title	The structure of rat liver vault at 3.5 angstrom resolution
	Functional Keywords	9 REPEAT DOMAINS, PROTEIN-PROTEIN COMPLEX, Cytoplasm, Ribonucleoprotein, STRUCTURAL PROTEIN
	Biological source	Rattus norvegicus (rat)
	Cellular location	[UNP - MVP_RAT] Cytoplasm
	Organ source	[UNP - MVP_RAT] Lung
	Total number of polymer chains	13
	Total molecular weight	1246973 (the details in Structural Details Page)
	Authors	Kato, K. , Zhou, Y. , Tanaka, H. , Yao, M. , Yamashita, E. , Yoshimura, M. , Tsukihara, T. (<i>deposition date</i> : 2008-10-24, <i>release date</i> : 2009-01-13)
	Primary citation	Tanaka, H. , Kato, K. , Yamashita, E. , Sumizawa, T. , Zhou, Y. , Yao, M. , Iwasaki, K. , Yoshimura, M. , Tsukihara, T. The structure of rat liver vault at 3.5 angstrom resolution <i>Science</i> , 323:384 - 388, 2009.(PubMed : 19150846) (DOI: 10.1126/science.1164975)
	Experimental method	X-RAY DIFFRACTION (3.5[Å])
	Other Database Information	CATH , CE , FSSP , SCOP , VAST , UniProt (UNP - Q62667) , eF-site

Structure Viewers
[jV3](#) / [Jmol](#)
jV and Jmol require [Java\(TM\)Plug-in 1.5 or later.](#)

rotated about x by 90°
[250X250](#) [500X500](#)

rotated about y by 90°
[250X250](#) [500X500](#)

Get Entry Data from our browser

Access to <http://www.pdbj.org/>

The screenshot shows the PDBj homepage with a search bar containing the text "12as" and a "Go" button. The search bar is highlighted with a red circle. The page includes navigation links for English, Japanese, simplified Chinese, traditional Chinese, and Korean. It also features a sidebar with links to various PDBj services and a main content area with a search bar and a "Go" button.

The screenshot shows the PDBj summary page for entry 12as. The page includes a 3D ribbon diagram of the protein structure, a table of entry details, and a list of references. The table contains the following information:

フィールド名	値
エントリID (PDB ID)	12as 配列情報 (FASTA形式) PDBファイルのダウンロード
分子名義	ASPARAGINE SYNTHETASE, L-ASPARAGINE, ADENOSINE MONOPHOSPHATE
タイトル	ASPARAGINE SYNTHETASE MUTANT C51A, C315A COMPLEXED WITH L-ASPARAGINE AND AMP
構造のキーワード	LIGASE, ASPARAGINE SYNTHETASE, NITROGEN FIXATION
由来する生物種	Escherichia coli K12
細胞内の位置	[UNP - ASNA_ECOLI] Cytoplasm
ポリマー鎖の合計数	2
分子量の合計	74228 (詳細は 構造情報のページ)
著者	Nakatsu, T., Kato, H., Oda, J. (登録日: 1997-12-02, 公開日: 1998-12-30)
引用文献	Nakatsu, T., Kato, H., Oda, J. Crystal structure of asparagine synthetase reveals a close evolutionary relationship to class II aminoacyl-tRNA synthetase. <i>Nature Struct. Biol.</i> , 5:15 - 19, 1998 (PubMed: 9437423) (DOI: 10.1038/1580198-15)
実験手法	X-RAY DIFFRACTION (2.2Å)
他のデータベース情報	CATH, CE, FSSP, SCOP, VAST, UniProt (UNP - P00903), eF-site, KEGG (EC 6.3.1.1), GDB, EoCatDB

PDBID (e.g. 12as) is input
in a box and GO



Summary for each PDBID is
displayed.

Get Entry Data from our browser

Access to <http://www.pdbj.org/>



The screenshot shows the PDBj homepage in Japanese. The search bar is highlighted with a red circle. The search bar contains the text "PDB検索 Mine" and a search button. Below the search bar is a "Go" button and a link to "詳細条件検索 >>".



The screenshot shows the PDBj search results page in Japanese. The page displays search results for the query "トリプトファン合成酵素" (tryptophan synthase). The results are shown in a table with columns for "分子名称" (Molecule Name), "タイトル" (Title), "著者" (Author), "実験手法" (Experiment Method), "登録日" (Registration Date), and "公開日" (Release Date). The first result is "TRYPTOPHAN SYNTHASE ALPHA CHAIN (E.C.4.2.1.20), TRYPTOPHAN SYNTHASE BETA CHAIN (E.C.4.2.1.20)" with a title of "TRYPTOPHAN SYNTHASE IN COMPLEX WITH (NAPHTHALENE-2'-SULFONYL)-2-AMINO-1-ETHYLPHOSPHATE (F19)".

日本語のキーワード
を入力

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Structure Viewers

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rotated about x by 90°
[250X250](#) [500X500](#)



rotated about y by 90°
[250X250](#) [500X500](#)

PDB ID

Descriptor

Title

Functional

Biological

Cellular loc

Total num

polymer ch

Total mole

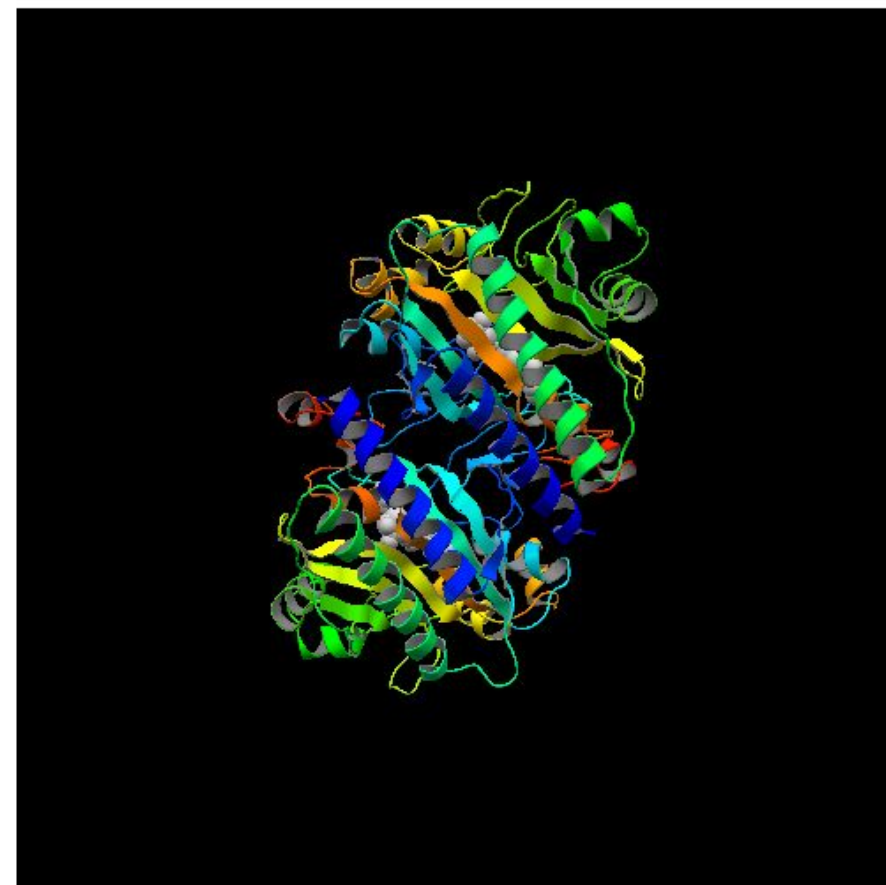
Authors

Primary cit

Experimen

**Other Data
 Information**

http://pdbjs3.protein.osaka-u.ac.jp - xPSSS (xml-based Protein Structure Search Serv...



jV version 3

Style: ☒ Default ☐ Cartoon ☐ Wireframe ☐ CPK_without_water ☐ CPK
 Color: ☒ Default ☐ group ☐ chain ☐ atom

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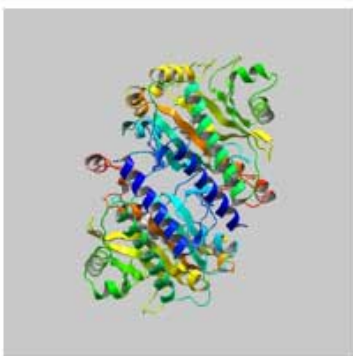
Mine**Summary [12as]**

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Summary[Structural Details](#)[Experimental Details](#)[Functional Details](#)[Sequence Neighbor](#)[Download/Display](#)[Link](#)

PDB ID or Keyword

search

**Structure Viewers****jv3 / Jmol**

jv and Jmol require
Java(TM)Plug-in 1.5 or
later.



rotated about x by 90°
250X250 500X500



rotated about y by 90°
250X250 500X500

PDB ID12as [sequence information \(FASTA format\)](#)[download PDB format file](#)**Descriptor**

ASPARAGINE SYNTHETASE, L-ASPARAGINE,
ADENOSINE MONOPHOSPHATE

KEGG**REACTION: R00483**[Help](#)

Entry	R00483	Reaction
Name	L-Aspartate:ammonia ligase (AMP-forming)	
Definition	ATP + L-Aspartate + NH3 <=> AMP + Pyrophosphate + L-Asparagine	
Equation	C00002 + C00049 + C00014 <=> C00020 + C00013 + C00152	
RPair	RP: A00116 C00049_C00152 main	
Pathway	PATH: rn00252 Alanine and aspartate metabolism PATH: rn00460 Cyanoamino acid metabolism PATH: rn00910 Nitrogen metabolism	
Enzyme	6.3.1.1	
Ortholog	KO: K01914 aspartate--ammonia ligase	
LinkDB	All DBs	

=> [Original format](#)DBGET integrated database retrieval system, [GenomeNet](#)

Summary for each PDBID

Amino acid sequence (FASTA)

PDBj (Protein Data Bank Japan) maintains a centralized archive of macromolecular structures and provides integrated tools, in collaboration with the **RCSB** in USA and the **PDBe** in EU. PDBj is supported by JST-BIRD.

Summary [1gof]

PDB ID: 1gof [sequence information \(FASTA format\)](#) [download PDB-format file](#)

Descriptor: GALACTOSE OXIDASE (E.C.1.1.3.9) (PH 4.5)

Title: NOVEL THIOETHER BOND REVEALED BY A 1.7 ÅNGSTROMS CRYSTAL STRUCTURE OF GALACTOSE OXIDASE

Functional Keywords: OXIDOREDUCTASE(OXYGEN(A))

Biological source: Hypomyces rosellus

Cellular location: [UNP - GAOA_DACDE] Secreted

Total number of polymer chains: 1

Total molecular weight: 68785.9 (the details in [Structural Details Page](#))

Authors: Ito, N., Phillips, S.E.V., Knowles, P.F. (deposition date: 1993-09-30, release date: 1994-01-31)
Ito, N., Phillips, S.E., Stevens, C., Ogel, Z.B., McPherson, M.J., Keen, J.N., Yadav, K.D., Knowles, P.F.

Primary citation: Novel thioether bond revealed by a 1.7 Å crystal structure of galactose oxidase. *Nature*, 350:87-90, 1991. [PubMed: 2002850] (DOI: 10.1038/350087a0)

Experimental method: X-RAY DIFFRACTION (1.7Å)

Other Database Information: CATH, CE, FSSP, SCOP, VAST, UniProt (UNP: P01745), eF-site, KEGG (EC 1.1.3.9), EzCaDB

Structure Viewers: jv3 / Jmol
jv and Jmol require Java(TM) Plug-in 1.5 or later.

rotated about x by 90°
250X250 500X500

rotated about y by 90°
250X250 500X500

Electron density map is available to be displayed from the Experimental Details page.

```
>1GOF:GALACTOSE OXIDASE
ASAPIGSAISRNNWAVTCDSAQSGNECNRAIDGNKDTFWHTFYGANGDKFPHTYITDMK
TTQAVNGLSMLPFGDQGNQWIGRHEVILSDQTNWGSFVAGSNFADSTFRYSNTEFP
ARYVRLVAITEAGQWPTSIABINVFQASSYTAQPLGRWGTIDLPFVFAAAIEPTPS
GRVLMSSSYRNDAFGSGPGGILTSSWDPTGIVSDRTVTVTXKDMFCPGISMDGNGQIV
VTGGNDAAKTSLYDSSDSWIFGPDQVARGYQSSATMSDGRVFTIGGWSGGVPEKNGE
VYSPSSKTWTSLPNAKVNPMLTADQKGLYRSDNHAWLFGWKKGSVFQAGPSTAMNYYTS
GSGDVKSAGKRQSNRGVAPDAMCGNAVHYDAVKGKILTFGGSPDYQSDATTAHITLG
EPFGSPWVVFASNGLYFARTHTSVLPFGSTIFGGQKGIFFEDSTVPFPEIIVVEQ
DTTYKQNEISVGVHSISLLLPQGRVYVNGGGGLCGDCTNHFAQIFPFWLYNENGL
ATRPKITRTSTQSVKVGGRITISTDSSISKASLIKYGTATHTVNTDQRRIPILTNNNGN
SYSFQVPSDSGVALPGYWMLFVMMASAGVPSVASTIRVTQ
```

eF-site **1gof-A**

ef-site/Structure 1gof-A

Default CPK Default without hetero atoms

Functional site **focus & details**

Functional site	focus & details
1) A:495	on off
2) A:272	on off
3) A:495	on off
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:272	on off

A:495 ACT SITE

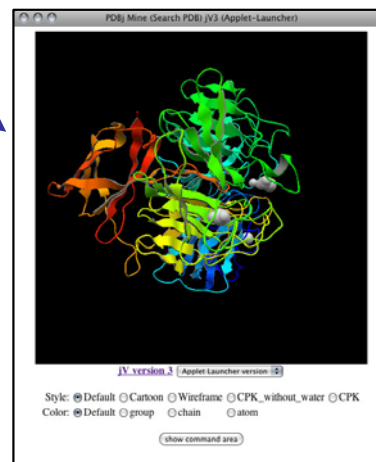
sequence Y

description Proton acceptor.

source Swiss-Prot: 1

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

Graphic viewer: jV
<http://www.pdbj.org/jV/>



Graphic viewer: *jV* version 3.8

Download from <http://www.pdbj.org/jV/>

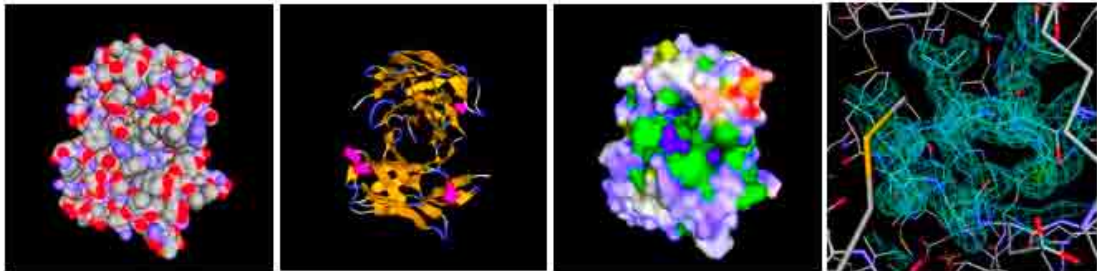
[TOP](#) [DOWNLOAD](#) [Help](#) [Links](#) [Acknowledgement](#)

 **jV version 3** 

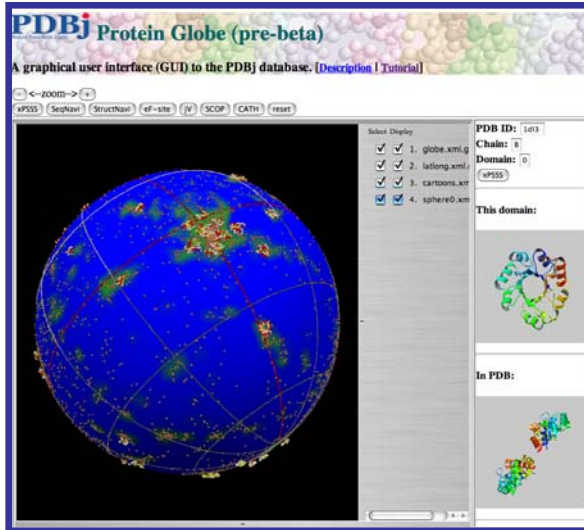
jV version 3 (formerly known as PDBjViewer) is a program to display molecular graphics of proteins and nucleic acids. jV supports the following features:

- jV can read and display PDBML files, the canonical XML format for the Protein Data Bank.
- Of course, jV can read and display the traditional PDB format files, too.
- RasMol-like usability.
- jV can process more than one molecules.
- jV can display polygons specified by XML. ([XML Schema for polygons](#) is available.)
- Multiple polygons can be processed simultaneously, and be superimposed onto molecular images.
- Animation can be realized.
- jV runs on the Java Runtime Environment ([JRE](#)) so that it can work as a stand-alone application as well as [an applet](#).
- The graphics of jV is based on OpenGL (JOGL), thereby producing fairly beautiful pictures.

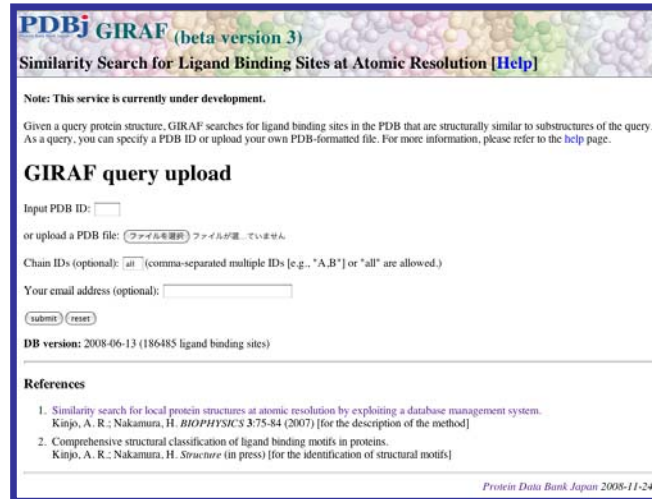
[Download](#)



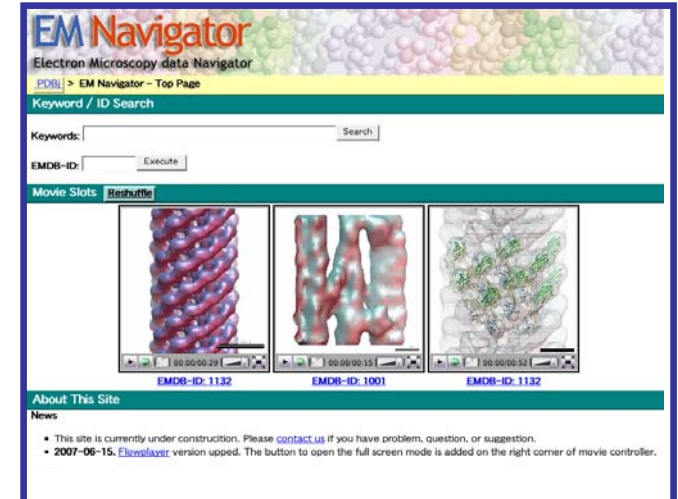
Development of other Databases and Services



Protein Folds Browser,
Protein Globe (Kinjo & Standley)



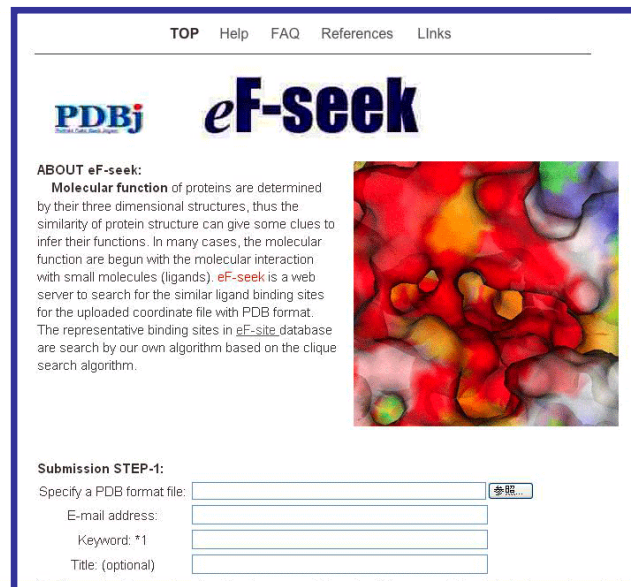
Ligand Binding Site Search,
GIRAF (Kinjo)



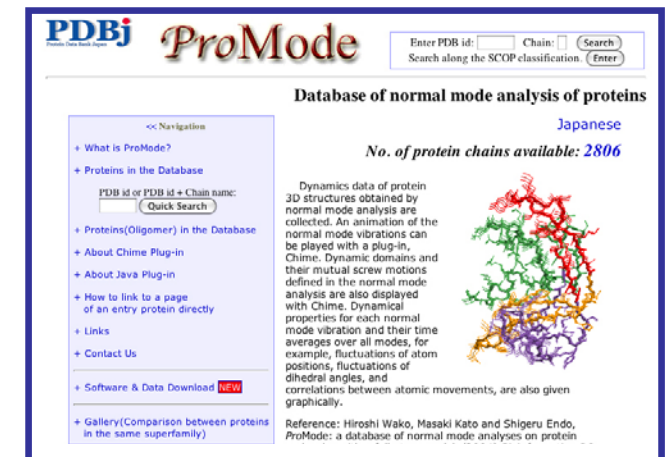
Electron Microscopy Navigator,
EM-Navi (Suzuki)



Protein Molecular Surface
Database, **eF-site**
(Kinoshita & Nakamura)



Search for Similar Surface, **eF-seek**
(Kinoshita & Nakamura)



Protein Dynamics Database,
ProMode (Wako & Endo)

Development of other Databases and Services

PDBj (Protein Data Bank Japan) maintains a centralized archive of macromolecular structures and provides integrated tools, in collaboration with the RCSB in USA and the MSD-EBI in EU. PDBj is supported by JST-BIRD.

Sequence Navigator

About Sequence Navigator

Sequence Navigator Soap Service

To Enter Navigator, input a PDB ID and Chain ID A.

OR input an AA Sequence

Clustering Options

☐ No Clustering ☐ Cluster by E-value 10^{-4}

Homolog protein search,
Sequence Navigator
(Standley)

PDBj (Protein Data Bank Japan) maintains a centralized archive of macromolecular structures and provides integrated tools, in collaboration with the RCSB in USA and the MSD-EBI in EU. PDBj is supported by JST-BIRD.

Structure Navigator

Protein Structure Search Engine

About Structure Navigator

Structure Navigator (Opal-OP)

Chain A (required)

PDB Code: OR

PDB File:

☐ return e-mail (address) ☐ return web

Similar fold search,
Structure Navigator
(Standley & Toh)

SeSAW Functional Annotation
by
Sequence-Derived Structural Alignment Weights

Enter a PDB ID or Upload a PDB-formatted file

PDB ID 2czl or ファイルが選...ていません Chain ID A (required)

☐ Send results to this email address harukin@protein.osaka-u.ac.jp

☐ Display results in browser as they are completed

If your query is a homology model, the following information is requested

Template PDB ID Template Chain ID A

PDBj About SeSAW Send feedback

Function Annotation from
Folds and Sequences,
SeSAW (Standley)

MAFFTash

alignment of multiple sequences and structures

Paste your sequences and PDB IDs (plus chain IDs) here:

Example:

```
>PDBID
>3y9c
>Q4Q899|DDX5L_MOUSE| 1-91
MTAAQQRHLQAFDYIKKILQPTLYILEYMSHLEDEVOYIAQKXNKGNHSAASLFLOY
LRLQLGQRFPQAFGLALYHAGYCCGCAIES
>Q4Q899|DDX5L_MOUSE| 101-176
EKHLLLRLEPKFATYVPRDILSELSECLINQCKKIKQIKQRTKRMGAQKMACLI
RDDEKHPYVLQALSL
>PDBID
>2plha
```

Need help picking PDB IDs? Use [Pre-MAFFTash](#).

OR upload a file ファイルが選...ていません

email address (required)

PDBj About MAFFTash Send feedback

Alignment of Sequence and
Structures. **MAFFTash**
(Kato, Toh & Standley)

PDBj eProtS

Topics

- Introduction to PDBj
- Introduction to Protein Structures
- Protein List
- Classification by Original eProtS
- Classification by Biological Functions (tentative)
- Classification by Biochemical Functions (tentative)
- Sitemap
- Questions and Comments
- RSS
- Glossary
- External Links
- Japanese version eProtS
- Japanese version Topics

eProtS: Encyclopedia of Protein Structures

The eProtS, Encyclopedia of Protein Structure, is a dictionary with pictures of the protein three-dimensional structures, for understanding the tertiary structures and the biological functions for several selected protein molecules that are particularly important for biology. This Web site can be prepared for non-specialists of protein structures. When the molecular graphics software, PDBjViewer, is available in your hardware system, you may be able to manipulate the protein molecules on the display interactively by mouse (JE 5.0 (or later) or NN 6.0 (or later) are recommended.)

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(Kinjyo, Kudo, & Ito)

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Molecule of the Month, **MoM**
(Goodsell & Kudo)