

Protein Data Bank & Structure Deposition at PDBj

Nobutoshi Ito

Graduate School of Biomedical Science,
Tokyo Medical and Dental University
also
Protein Bank Japan

<http://www.pdbj.org>

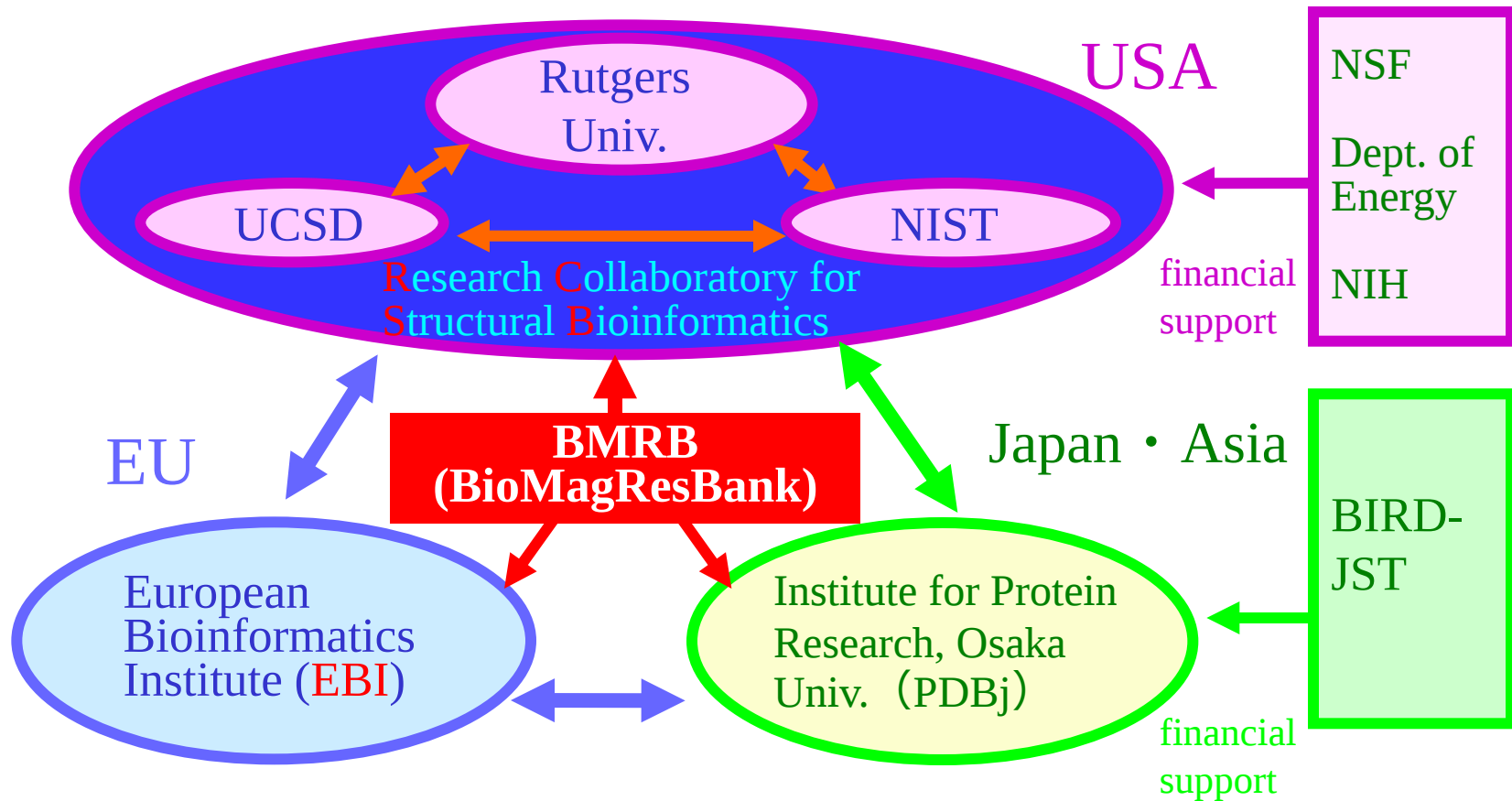
CCP4 Workshop
2 Nov 2012

PDBj
Protein Data Bank Japan

Today's menu

- wwPDB and PDBj
 - Quick tour of deposition
 - Quantity and quality of data
 - Related databases etc at PDBj
-

Protein Data Bank (PDB)



→ More international wwPDB

RCSB **PDB**
PROTEIN DATA BANK

Research Collaboratory for
Structural Bioinformatics
www.pdb.org

NSF, NIGMS, DOE,
NLM, NCI, NINDS,
NIDDK



BioMagResBank
www.bmrwisc.edu

NLM

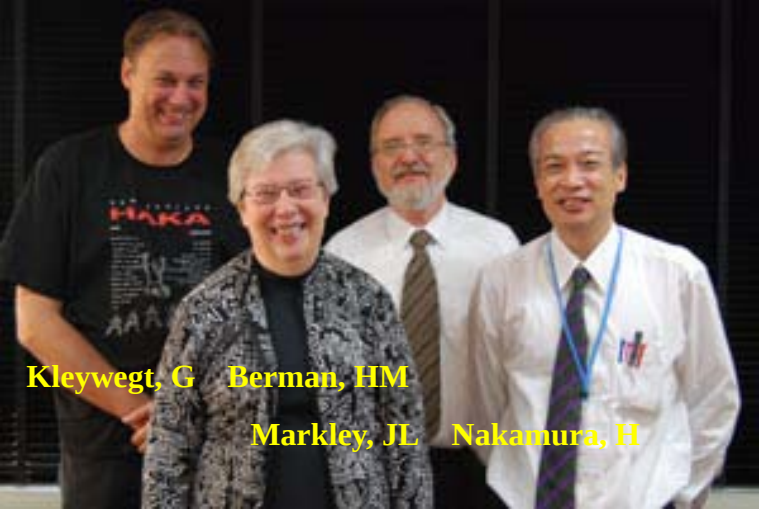
EMBL-EBI **PDB^e**
PROTEIN DATA BANK EUROPE

Protein Data Bank in Europe
pdbe.org

EMBL-EBI,
Wellcome Trust,
BBSRC, NIGMS, EU

PDBj
Protein Data Bank Japan

Protein Data Bank Japan
www.pdbj.org
NRDC-JST



Kleywegt, G Berman, HM
Markley, JL Nakamura, H



wwPDB and wwPDBAC members
at Rutgers Univ. on 1 Oct. 2010

International collaboration in wwPDB

- 1) Curation, data processing, and registration are made by all the members, collaborating with each other.
- 2) We have a single data archive, which is looked after by one “archive keeper (RCSB)”.
- 3) Data format and new descriptions are discussed among the members.
- 4) Members are encouraged to develop their own browsers, viewers, and other APIs and services.

(Berman, Henrick & Nakamura (2003) Nat. Struct. Biol. 10, 980)

PDB FTP Traffic (July 2009 - June 2010)



219 M files were downloaded from three wwPDB members (PDBj, RCSB-PDB, PDBe) during a year.

Protein Data Bank Japan (PDBj)

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

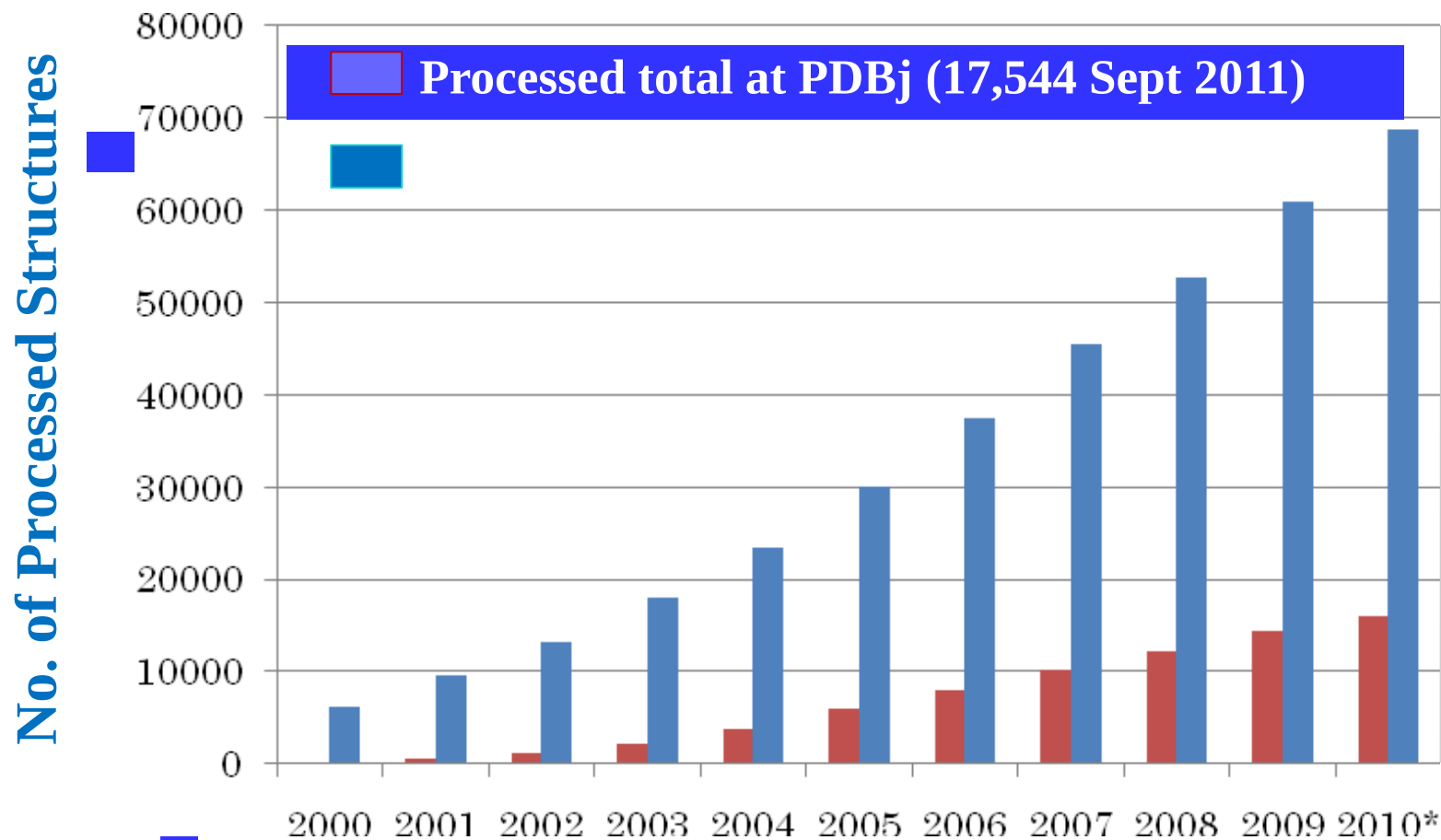
At Institute for Protein Research,
Osaka Univ. since 2001.
Supported by the Institute for
Bioinformatics Research and
Development, Japan Science and
Technology Agency (BIRD-JST).

The screenshot shows the PDBj website with a header in English, Japanese, Chinese, and Korean. The main navigation menu includes Home, Data Deposition, Search, Service and Software, Derived database, Download, and Links. The Search section features a search bar with a dropdown for 'PDB ID or Keyword' and a 'Go' button. There are also links for 'Search PDB Mine' and 'Search NMR Data'. The 'What's new' section contains several announcements: a weekly data update on October 14, 2009, at 9:00 AM (JST); the introduction of a new data viewer, PDBj Mine, on October 14, 2009; changes to the wwPDB FTP site announced on September 25, 2009; the release of PDB Archive Version 3.15 on March 18, 2009; and the release of PDB Archive Version 3.15 on February 13, 2009. The right sidebar displays statistics (60756 entries available on 14 Oct. 2009) and logos for various databases and organizations, including eProts, Protein Globe, and DBCLS.

Protein Data Bank Japan: PDJ

1. The **wwPDB** management as one of the members
 2. **Curation and data processing** for the deposited data (PDB and BMRB)
 3. Data **remediation** and development of the **format** for correct description
 4. Addition of **experimental information** from literatures
 5. Development of **query tools and derived databases** as the web service
-

Data Processed at PDBj and wwPDB



PDBj curaa Quarter of the deposited data, mainly from Asian and Oceania regions.

Japanese

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日本蛋白質構造データバンク (PDB; 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の利用はできません。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)

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Encyclopedia of Protein Structures

Protein Globe

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日本蛋白质结构数据库 (PDB; Protein Data Bank Japan), 由JST-BIRD提供支援, 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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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)

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한국 단백질 구조 데이터뱅크 (PDB; Protein Data Bank Korea)는 미국의 구조 생물학 정보학 연구 공동체(RCSB)와 유럽 생물 정보학 연구소(PDBe)의 협력하에 고분자 입체구조의 구조 해석 등을 제공하고 있습니다. PDB는 독립 행정법인 과학기술 진흥기구 생물 정보학 추진센터(JST-BIRD)의 후원을 받고 있습니다.

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Quick Tour of How to Deposit (X-ray) Structures with ADIT

Before deposition, please check;

- Is it the **final** structure?
 - Coordinates **and structure factors** (raw images in the future?)
 - You have a sequence file? (**real** sequence used in the experiment, one-letter code, database ID... If it's a new protein, sequence deposition is also required)
 - Ligand information (IUPAC name, images...)
-

To make the procedure easier

- Have various log files ready
(crystallisation note, data collection, scaling...)
 - Run preprocessing programs (pdb_extract, deposit_mmcif, CCP4 data harvesting...)
-

Welcome to PDBj - Home - Windows Internet Explorer

http://www.pdbj.org/

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Links

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

Deposition

Data Deposition Information >>

PDB Deposition  Auto Dep Input Tool

NMR Data Deposition 

Search

Search PDB 

PDB ID or Keyword

Advanced Search >>

Search NMR Data 

☐ Accession number
☐ Deposition code

What's new

6-Oct-2010
Effective December 6, 2010, deposition of chemical shift data will be mandatory when submitting NMR entries to the PDB. ([more...](#))

19-Aug-2010
Validation Report PDFs ([more...](#))

13-Jul-2010
The latest version of jV (jV3.8), the molecular graphics viewer developed by PDBj, has been released. A new functional command "displayatom on/off" has been added, which provides various display methods easily. Please download the newest version from [here](#).

30-Jun-2010
Version 2 NMR restrain files have been released. ([more...](#))

19-May-2010
The latest version of jV (jV3.7.1) has been released.

7-May-2010
The IP address of PDBj ftp server (ftp.pdbj.org) has been changed to 133.1.158.142. If you access to the PDBj ftp using the IP address directly, please replace the IP address with the new one. The IP address of PDBj Web server has

68998
[entries available on 3 Nov., 2010](#)
00:00(UTC) / 09:00(JST)

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http://pdbdep.protein.osaka-u.ac.jp/en/

お気に入り PDBj Validation & Deposition Portal

PDBj Protein Data Bank, Japan

A member of the **WORLDWIDE PDB** PROTEIN DATA BANK

Last update: 2009-04-24

Languages: en | [ja](#) | [ko](#) | [zh-cn](#) | [zh-tw](#)

[News](#) | [Deposition Tutorial](#) (en, ja, ko, zh-cn, zh-tw) | [Validation and Deposition](#) | [Policies and Procedures](#) | [Contact Us](#)

PDBj Validation & Deposition Portal

Welcome to the PDBj validation/deposition portal.

Need help?

If you have any questions, please read "[Deposition tutorial](#)" first. If you still need help, please [contact us](#). Questions, comments, and suggestions in validation/deposition service and tutorial are welcome.

Data Deposition Tools

Search

You may search HET groups using [Ligand Expo](#). If your HET groups are **NOT new**, you should use the existent ones.

Check sequence database references for proteins or nucleic acids in your structure at [UniProtKB](#). The author is encouraged to submit their sequence information via [SPIN](#) (the UniProtKB submission tool) for directly sequenced proteins, or via submission tools provided by [INSDC](#) members ([SAKURA at DDBJ](#), [Webin at EMBL](#), [BankIt at GenBank](#)) if the nucleotide sequence is available.

Validate

Before you deposit the structure data, validate your structure using the [validation server at PDBj](#).

» **ADIT!** Validation Server [ADIT Validation Server](#)

Deposit

After you validate your structure data, deposit your structure using the structure deposition tool [ADIT at PDBj](#), [beta-ADIT](#) or [ADIT-NMR at PDBj](#) (for NMR studies). For other deposition servers at wwPDB member sites, please visit from the [wwPDB](#) web site.

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プロテインデータバンクへの構造解析データ登録のご案内 - Windows Internet Explorer

http://pdbdep.protein.osaka-u.ac.jp/tutorial/ja/

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PDBj A member of the PDB WORLDWIDE PROTEIN DATA BANK

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プロテインデータバンクへの構造解析データ登録のご案内

PDB (Protein Data Bank) への登録は、ウェブブラウザを利用して対話的に登録を行うことができるADIT (Auto Deposition Input Tool)を使用して行います。また、pdb_extractを使用すると、ADITで手動入力する項目を減らすことができます。このページでは登録の手順、必要なデータ類とその書式や注意事項などについてご案内いたします。

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- [登録前の確認事項](#)
- [原子座標ファイルの準備](#)
- [構造因子ファイルの準備](#)
- [各種プログラムのログファイルの準備](#)
- [登録情報の抽出](#)
- [登録データの検証](#)
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- [本チュートリアルについて](#) (ご利用前に必ずご覧ください)
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本チュートリアルは、wwPDBに構造解析データを登録する際の手引きを、日本語を用いる登録者の便宜のためにPDBjが日本語で解説するものです。PDBで公開するファイルの書式およびwwPDBへのデータ登録に関する公式文書は、“[Annotation Documentation](#)”です。また、PDBおよびRCSB PDBによる登録データの編集方針に関する公式文書は“[Data Processing and Annotation Procedures Manual](#)”です。本チュートリアルでは公式文書に忠実に解説するよう努めていますが、万一、本チュートリアルと公式文書の間に相違が生じた場合は、公式文書の記述が優先されます。

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PDBj ADIT Deposition Tool - Windows Internet Explorer

http://pdbdep.protein.osaka-u.ac.jp/adit/en/

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お気に入り PDBj ADIT Deposition Tool ページ(P) セーフティ(S)

ADIT Deposition Tool

Need help?

If you have any questions, please read "[Deposition tutorial](#)" first. If you still need help, please [contact us](#). Questions, comments, and suggestions in validation/deposition service and tutorial are welcome.

If your question is about a particular entry, please include the RCSB ID in your message.

Announcements

- If TLS is involved in refinement, Please read "[Depositors for using TLS](#)" document.**
- Please make sure that your depositing coordinate meets wwPDB policy. wwPDB annotation polices document is available from [wwPDB web site](#) in [HTML](#) or [PDF](#) format.
- Structure factor amplitudes/intensities (for crystal structures) and restraints (for NMR structures) are a mandatory requirement for PDB deposition. This policy is published at [wwPDB news](#).
- Structures solved by Electron Microscopy should deposit their maps to the EMDB (at [PDBe](#) or [RCSB](#)) first, and should supply the EMD-id as an associated entry with their ADIT deposition.

Files and information required to deposit [X-ray](#), [NMR](#), and [Electron Microscopy](#), or [other methods](#) structures.

Start New Session

To **start a new** ADIT session, select the experimental method and the molecular structure type. Then press the **BEGIN** button.

Method: X-ray Structure Type: Protein **BEGIN**

Continue Previous ADIT Session

To **continue** a session from an earlier date, Enter your session restart ID and press the **CONTINUE SESSION** button.

Session Restart ID: **CONTINUE SESSION**
(example: 2006-07-01.serverhostname.9999.12345678)

If you have started an ADIT-NMR session, you can continue at [ADIT-NMR](#).

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An Information Portal to Biological Macromolecular Structures

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ADIT! Auto Dep Input Tool

Running an ADIT Session

1. Please review the [format requirements](#) before starting the session.
2. You may wish to use [pdb_extract](#) to process log files for deposition.
3. Check ligands with [Ligand Expo](#).

Upload coordinate file 参照...
Compress (.gz or .Z files) first.

Upload structure factor file 参照...
Compress (.gz or .Z files) first.

Choose Operation: ☐ Precheck ☐ Validate ☐ Deposit

Select file type: ☐ PDB ☐ mmCIF
☐ mmCIF ☐ mtz ☐ Other ASCII

BEGIN

Coordinates

Structure Factors

“Precheck” “Validate” “Deposit”

About ADIT

An ADIT session involves three steps:

1. A data format precheck
2. A validation check
3. The actual deposition of the structural data to the database

Precheck confirms that the data files you enter are in a format that can be automatically processed by our software. The format and required data items for coordinate files are described for the [PDB](#) and [mmCIF](#) formats. The required mmCIF data items for [structure factor data](#) are also described. The precheck identifies any changes that need to be made in your data files in order to obtain a validation report or to deposit your structure.

The **validation check** creates a validation report for the structure which includes an RCSB PDB Atlas page, a validation report with stereochemical checks, and, depending on the type and content of the files uploaded, produces Procheck, Molprobity, NUCheck and SFCheck reports. The validation may take a few minutes depending on the size of your

Data Syntax Check - Windows Internet Explorer

http://pdbprotein.osaka-u.ac.jp/cgi-bin/adit/adit-operation-driver

ファイル(E) 編集(E) 表示(V) お気に入り(A) ツール(T) ヘルプ(H)

Google 検索 ブックマーク プロック数: 10 チェック 翻訳 次へ送信

お気に入り PDBj Data Syntax Check

設定

PDBj
Protein Data Bank Japan

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An Information Portal to Biological Macromolecular Structures

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Validation and Deposition Services Home

Deposition Top | Tutorial | ADIT FAQ | Deposition FAQ | pdb_extract | Ligand Expo

ADIT!

Auto Dep Input Tool

Data Syntax Check

Click here to e-mail the session restart ID

Coordinate format is OK!

Sequence information:

One polymer chain was extracted from the coordinate section. The detailed residue information of each chain is listed below. Standard residues are listed as one letter code sequence. Non-standard residues are included in parenthesis. Please check the sequence information carefully. If you think it was incorrectly extracted, please check if TER cards were added correctly. PDB format requires all polymer chains should have a TER card at the end and no TER cards should be included at the end of non-polymer residues (such as ions, ligands, waters).

CHAIN A: Total 353 residues, first residue (6 ALA), last residue (358 SER)

AAGPEMVRGQVFDVGPFRYTNLSYIGEGAYGMVCSAYDNLNKKVRVAIKKISPFHQTYCQRTLREIKILLR
FRHENIIGINDIIRAPTIEQMKDVYIVQDLMETDLYKLLKTQHLSDNHICYFLYQILRGLKYIHSANVLH
RDLKPSNLLNTTCDLKICDFGLARVADPDHDTGFL (TPO) E (PTR) VATRWYRAPEIMLSKGYTKSI
DIWSVGCILAEMLSNRPIFFGKHYLDQLNHILGILGSPSQEDLNCIINLKARNYLLSLPHKNKVPWNRLE
FNADSKALDLDKMLTFNPHKRIEVEQALAHFYLEQYYDPSDEPIAEAPFKFDMELDDLPKEKLKELIFE
ETARFQPGYRS

If a sequence above has missing residues, correct the sequence later during deposition.

ページが表示されました

インターネット 100%



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Validation and Deposition Services Home

[Deposition Top](#) | [Tutorial](#) | [ADIT FAQ](#) | [Deposition FAQ](#) | [pdb_extract](#) | [Ligand Expo](#)



Validation Report

[Click here to e-mail the session restart ID](#)

Please review the Validation Report carefully. If there are any outstanding issues such as sequence link problem, geometry errors, chirality errors etc., please make sure you fix the problem(s) and start a fresh session with corrected file.

Please note that the geometry errors shown in the Validation Report will also appear in the processed PDB file.

For ligands, please make sure the three letter codes are correct. Both extra and missing atoms may appear in the Validation Report if incorrect ligand three letter code was used. If only missing atoms are listed in the Validation Report, either incorrect ligand three letter code was used or part of ligand is missing coordinates (see [Ligand Expo](#)).

Thank you for using PDB. The following geometrical and stereochemical features have been calculated for your structure:

CLOSE CONTACTS

==> Close contacts in same asymmetric unit. Distances smaller than 2.2 Angstroms are considered as close contacts.

Chain	Atom	Res	Seq	Chain	Atom	Res	Seq	Symm_Code	Distance
	O	HOH	542 -	O	HOH	543	(1, 5, 5, 5)	Dist = 0.69	
	O	HOH	534 -	O	HOH	537	(1, 5, 5, 5)	Dist = 1.00	
	O	HOH	551 -	O	HOH	557	(1, 5, 5, 5)	Dist = 1.00	
	O	HOH	552 -	O	HOH	554	(1, 5, 5, 5)	Dist = 1.00	
	O	HOH	585 -	O	HOH	586	(1, 5, 5, 5)	Dist = 1.00	
	O	HOH	587 -	O	HOH	588	(1, 5, 5, 5)	Dist = 1.00	

==> Close contacts based on crystal symmetry. Distances smaller than 2.2 Angstroms are considered as close contacts.

ADIT! Auto Dep Input Tool

Please input sequence(s):

Only sequences for proteins, peptides, and nucleic acids should be entered in the boxes below.

- Please enter the sequence of each macromolecular polymer. The sequence should include all residues in the experiment including uncleaved expression tags (like his tags), as well as residues missing due to disorder.
- If a sequence applies to more than one chain, enter the sequence once and specify the chain IDs with spaces or commas in between each chain ID.
- N- and C-terminal tags can be entered in the "uncleaved N-/C-terminal HIS-tag or cloning artifact" boxes. The N- and C-terminal boxes should be left blank if no tags were used or if they are already listed in the sequence.
- To indicate a modified or non-standard residue like selenomethionine, use parenthesis: (MSE). Three letter codes can be found at [Ligand Expo](#).
- The polymer type must be selected.
- If the sequence database reference exists, please select the database name and enter the accession code (GB (GeneBank) for nucleic acids and UNP (UniProt) protein sequence).
- For Structure Genomics, if the sequence has been or will be deposited to [TargetDB](#), please indicate the Target ID in the "Target identifiers" box. This is for structural genomics project only.
- One-letter code for polymer sequence INCLUDING THE RESIDUES MISSING IN THE COORDINATES (mandatory). Do not repeat terminal tags if already provided in the boxes above or below.

[Click here to e-mail the session restart ID](#)

[Save Sequence](#)

1st sequence	
Uncleaved N-terminal HIS-tag or cloning artifact <i>If none, leave the box blank</i>	
One-letter code for polymer sequence INCLUDING THE RESIDUES MISSING IN THE COORDINATES <i>(mandatory)</i>	AHHHHHHMAAAAAGPEMVRGQVFDVGPRTNLSYIGEGA

ADIT V12.812 ***** Your Session Restart ID is 2010-Nov-09.21.16.59.5209.Session.11011 - Windows Internet Explorer

http://pdb.dep.protein.osaka-u.ac.jp/cgi-bin/adit/mk-top-interface-screen-view?ufid=2010-Nov-09.21.16.59.5209.Session.11011&blockid=2ERK&context=deposit

ファイル(E) 編集(E) 表示(V) お気に入り(A) ツール(T) ヘルプ(H)

Google 検索 ブックマーク プロック数: 10 チェック 翻訳 次へ送信

お気に入り ADIT V12.812 ***** Your Session Restart ID is 2...

Home RSS Print ページ(P) セーフティ(S)

ADIT!
Auto Dep Input Tool

HELP PREVIEW ENTRY DEPOSIT DEPOSITION HOME

Categories

- Deposition
 - [Contact Authors](#)
 - [Structural Genomics](#)
 - [Release Status](#)
 - [Title](#)
 - [Related Entries](#)
- Authors
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- Chemical/Biological Features
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 - [Molecule Details](#)
 - [Sequence](#)
 - [Genetically Manipulated Source](#)
 - [Natural Source](#)
 - [Synthetic Source](#)
- Structure Features
 - [Keywords](#)
 - [Biological Assembly](#)
- Crystallization
 - [Methods and Conditions](#)
- Crystal Data
 - [Unit Cell](#)
 - [Space Group](#)
- Data Collection
 - [Crystals](#)
 - [Radiation Source](#)
 - [Radiation Detector](#)
 - [Collection Temperature](#)
 - [Collection Protocol](#)
 - [Reflections](#)

Data Items

DISPLAY AS TABLE

How to use the AUTO DEP INPUT TOOL

- BEGIN ENTERING DATA:** For each category, a set of instructions and places to enter data will be displayed in this frame. Fill in any relevant missing information.
- RESTART:** if you want to restart your session at a later time, record the restart ID for this session: **2010-Nov-09.21.16.59.5209.Session.11011** ([Click here to e-mail the session restart ID](#)). This ID is also displayed in the title bar of your browser. When you are ready to continue, enter this code in the appropriate box at the bottom of the ADIT HOME page.
- HELP:** An explanation for any item can be obtained by selecting the Help button within the table. This information will appear in the bottom frame. Pressing the Help button in the top frame will display these instructions.
- EXAMPLE:** An example for any item can be obtained by selecting the Example button within the table. This information will appear in the bottom frame.
- SAVING YOUR DATA:** You must press the Save button in each category after entering data. Switching to another category without saving your data will erase the information that you have entered.

This is the HELP frame

This frame is used to display dictionary descriptions, examples, tables and diagnostic information.

For Data Items:

- Press the **HELP** button for advice about how to enter data in the item.
- Press the **EXAMPLE** button in the item frame to view examples of the item.

ページが表示されました

インターネット 100%

ADIT V12.812 *** Your Session Restart ID is 2010-Nov-09.21.16.59.5209.Session.11011 - Windows Internet Explorer

http://pdbdep.protein.osaka-u.ac.jp/cgi-bin/adit/mk-top-interface-screen-view?ufid=2010-Nov-09.21.16.59.5209.Session.11011&blockid=2ERK&context=deposit

ファイル(E) 編集(E) 表示(V) お気に入り(A) ツール(T) ヘルプ(H)

Google 検索 ブックマーク プロック数: 10 ABC チェック 翻訳 次送信 設定

お気に入り ADIT V12.812 *** Your Session Restart ID is 2...

Auto Dep Input Tool

HELP PREVIEW ENTRY DEPOSIT DEPOSITION HOME

Categories

- Deposition
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 - Structural Genomics
 - Release Status
 - Title
 - Related Entries
- Authors
 - Entry Authors
 - Citation Authors
 - Citation
- Chemical/Biological Features
 - Molecule Names
 - Molecule Details
 - Sequence
 - Genetically Manipulated Source
 - Natural Source
 - Synthetic Source
- Structure Features
 - Keywords
 - Biological Assembly
- Crystallization
 - Methods and Conditions
- Crystal Data
 - Unit Cell
 - Space Group
- Data Collection
 - Crystals
 - Radiation Source
 - Radiation Detector
 - Collection Temperature
 - Collection Protocol
 - Reflections

Data Items

DISPLAY AS TABLE

Enter Data in Category Unit Cell

Enter the crystallographic cell parameters for this structure.

Save Unit Cell

Unit Cell			
Length a	Help	Example	92.500
Length b	Help	Example	92.500
Length c	Help	Example	103.000
Angle alpha	Help	Example	90.00
Angle beta	Help	Example	90.00
Angle gamma	Help	Example	90.00

Examples of Angle gamma

(mmCIF item _cell.angle_gamma)

Example 1:

90.00

Example 2:

72.96

Required Information

Deposition

Contact Authors
Structural Genomics
Release Status
Title
Related Entries

Authors

Entry Authors
Contact Authors
Citation

Chemical/Biological Features

Molecule Names
Molecule Details
Sequence
Genetically Manipulated Source
Natural Source
Synthetic Source

Structure Features

Keywords
Biological Assembly

Crystallization

Methods and Conditions

Crystal Data

Unit Cell

Space Group

Data Collection

Crystals

Radiation Source

Radiation Detector

Collection Temperature

Collection Protocol

Reflections

Reflection Shells

Refinement

Refinement Statistics

Resolution Shells

RMS Deviations

Coordinates Error

Software

Programs

Biological Assembly

Upload Supplemental Information

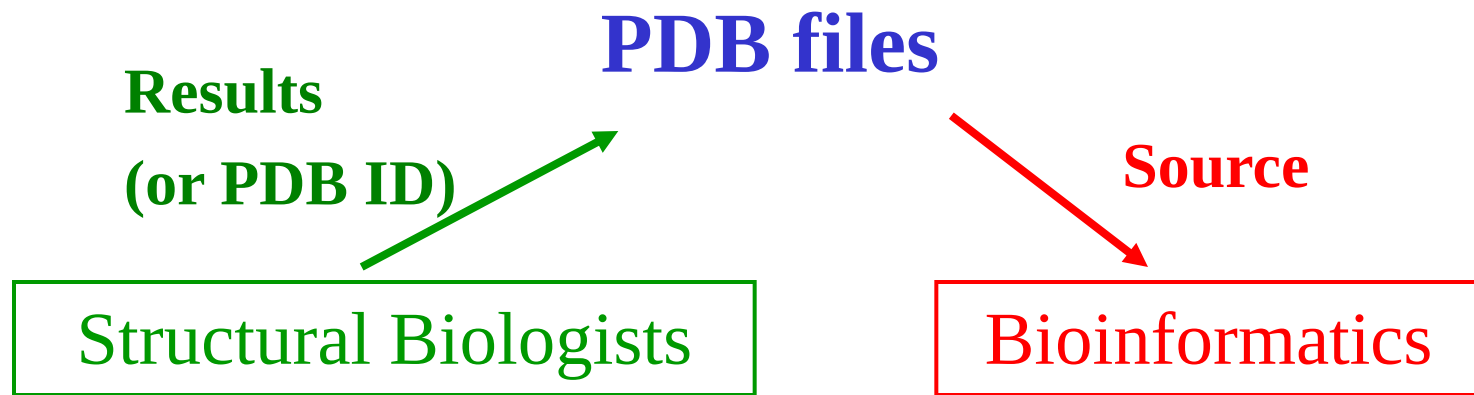
Supersede/Obsolete Information

Ligand Information

Virus Matrices

Quantity and Quality of PDB data

Differences of views



Data Quantity

- Fill in as many data items as possible (various small tools available)
 - Notify us when the paper gets published so that we can release the entry
-

Data Quality

It is up to depositors (you!!)...

but we have done about our
part of it.

Common troubles observed...

- Wrong or missing data items
(“to be published,” species, R-factors etc)
 - Redundant definition
(“human” or “homo sapience”)
 - Ligand structure and definition
-

mmCIF-specific troubles

- Lack of validation program of contents
(`_phasing.method` 'MAGIC')
- (Inconsistent) redundancy of data items



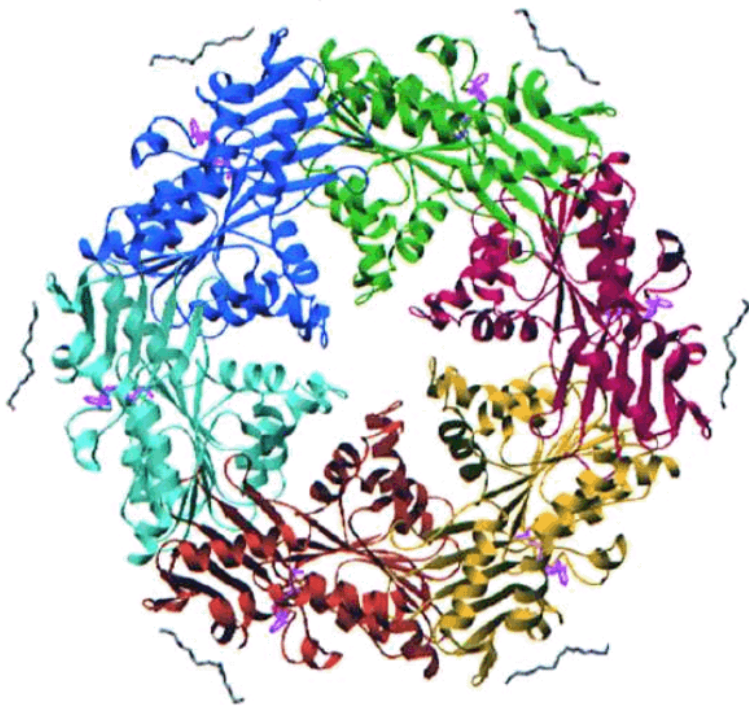
PDB Remediation Project

Thorough check of the PDB contents by all
wwPDB members.

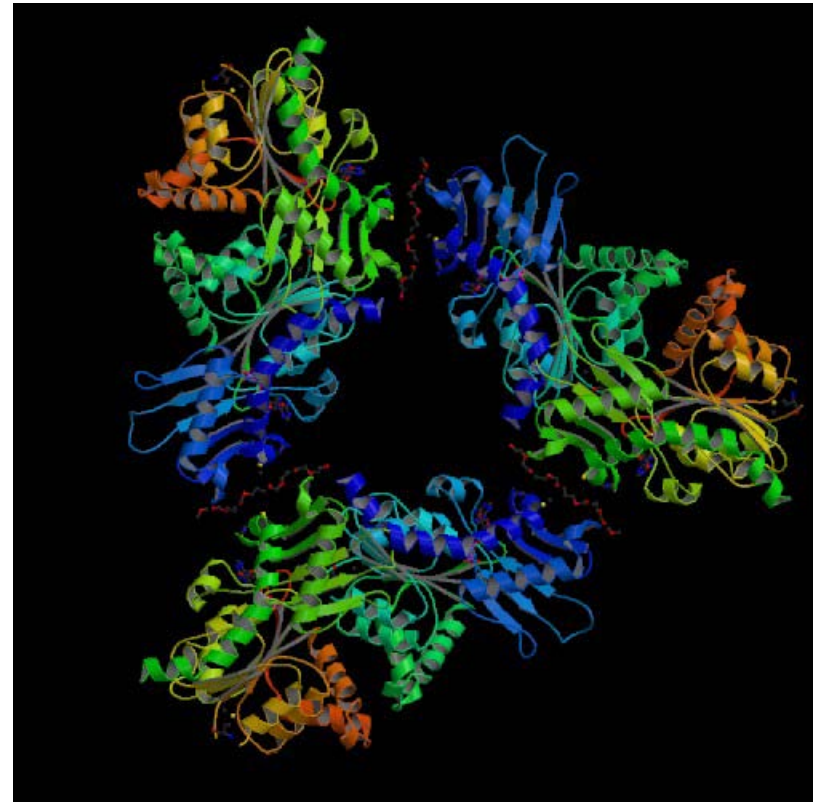
New dataset was released on 1 August 2007.

Henrick K, *et.al.*, *Nucleic Acid Res.*, **36**, D426-433 (2008)

What went wrong?



Paper



PDB

Related Database/Services at PDBj

PDBj Mine

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JV: Graphic Viewer
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CPNBPED

PDBj (Protein Data Bank Japan) maintains a centralized 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-BIRD](#).

Deposition

[Data Deposition Information >>](#)

[PDB Deposition](#)  Auto Dep Input Tool [NMR Data Deposition](#) 

Search

[Search PDB](#) 

[Advanced Search >>](#)

[Search NMR Data](#) 
☒ **Accession number**
☐ **Deposition code**

What's new

6-Oct-2010
Effective December 6, 2010, deposition of chemical shift data will be mandatory when submitting NMR entries to the PDB. ([more...](#))

69162
entries available
on 10 Nov., 2010
00:00(UTC) / 09:00(JST)

WORLDWIDE

PROTEIN DATA BANK


Encyclopedia of
Protein Structures


Protein
Globe


Database Center for Life Science



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[Search NMR Data
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[Status Search](#)[Service and Software
>>](#)[jV: Graphic Viewer](#)
[Protein Globe](#)
[ASH](#)
[MAFFTash](#)
[SEALA](#)

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Mine**Summary [12as]**[About PDBj Mine](#)
[Update Information](#)**Summary**[Structural Details](#)[Experimental Details](#)[Functional Details](#)[Sequence Neighbor](#)[Download/Display](#)[External DB](#) PDB ID or Keyword

<Asymmetric unit>

(no rotation) [More images...](#)**Structure Viewers****jV3 / Jmol**(jV3 and Jmol require [Java](#)
(TM)Plug-in 1.5 or later.)**PDB ID**12as [sequence information \(FASTA format\)](#)[download PDB format file](#)**Descriptor**ASPARAGINE SYNTHETASE, L-ASPARAGINE,
ADENOSINE MONOPHOSPHATE**Title**ASPARAGINE SYNTHETASE MUTANT C51A, C315A
COMPLEXED WITH L-ASPARAGINE AND AMP**Functional Keywords**LIGASE, ASPARAGINE SYNTHETASE, NITROGEN
FIXATION**Biological source**

Escherichia coli K12

Cellular location[\[UNP - P00963\]](#) Cytoplasm**Total number of
polymer chains**

2

Total molecular weight74226 (the details in [Structural Details Page](#))**Authors**Nakatsu, T. , Kato, H. , Oda, J. (*deposition date* :
1997-12-02, *release date* : 1998-12-30)

Nakatsu, T. , Kato, H. , Oda, J.

Graphic viewer: jV version 3.8

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

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



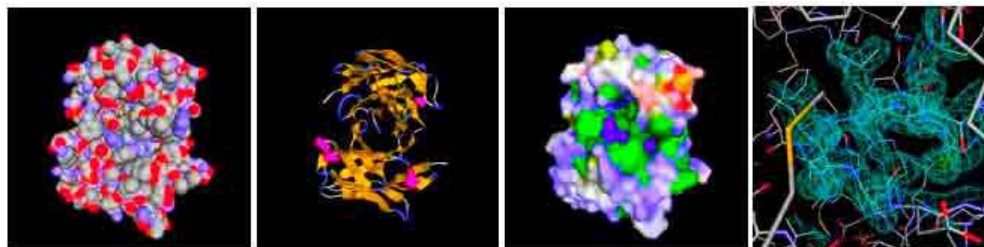
jV version 3



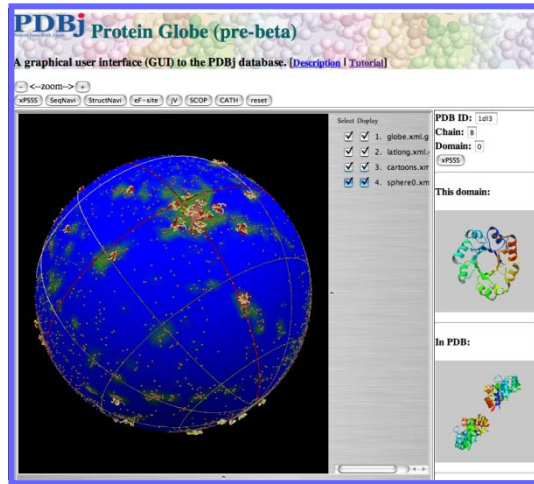
jV version 3 (formerly known as PDBjViewer) is a program to display molecular graphics of proteins and nucleic acids. jV supports the following features:

- 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.

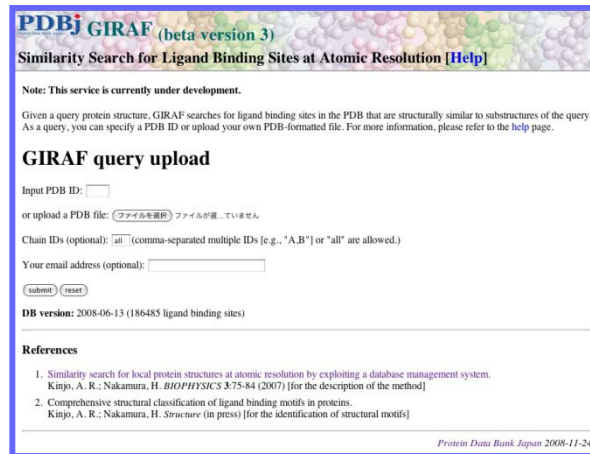
[Download](#)



Development of other Databases & Services



Protein Folds Browser,
Protein Globe (Kinjo & Standley)



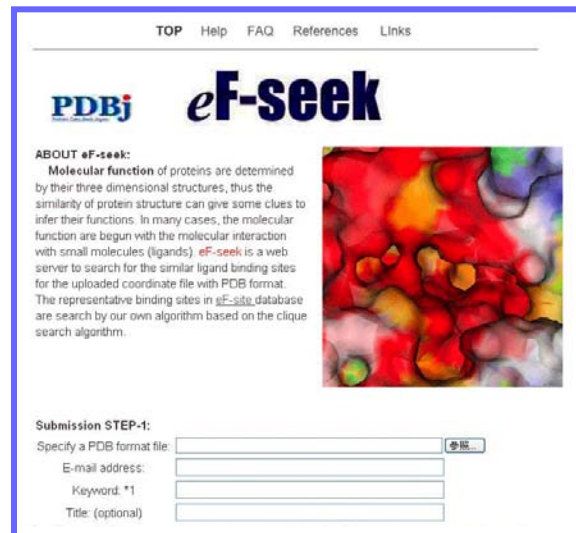
Ligand Binding Site Search,
GIRAF (Kinjo)



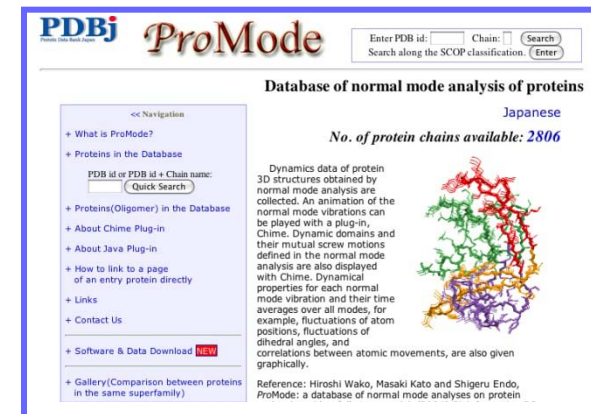
Electron Microscopy Navigator,
EM-Navi (Suzuki)



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

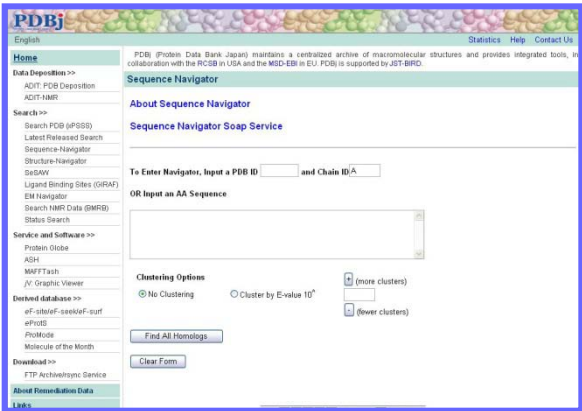


Search for Similar Surface, **eF-seek** (Kinoshita & Nakamura)

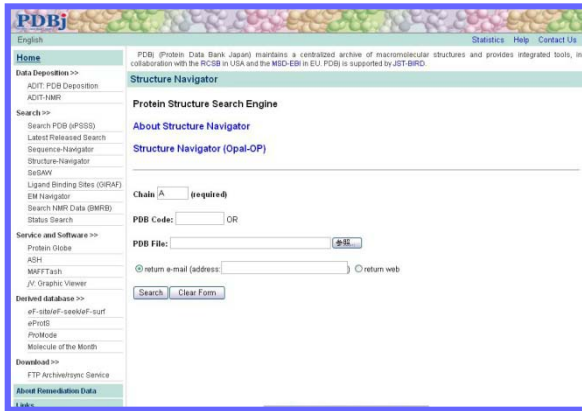


Protein Dynamics Database,
ProMode (Wako & Endo)

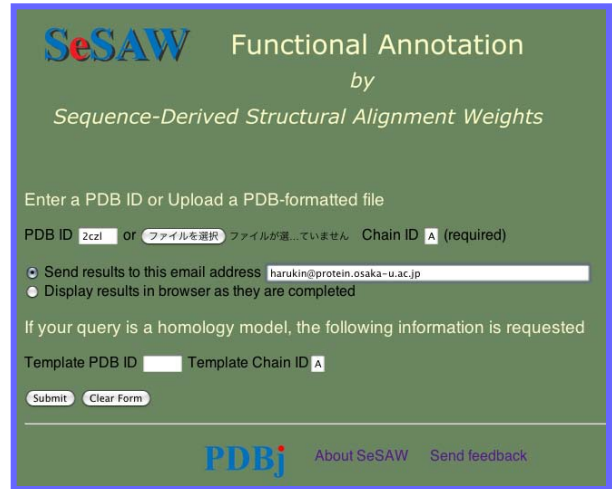
Development of other Databases & Services



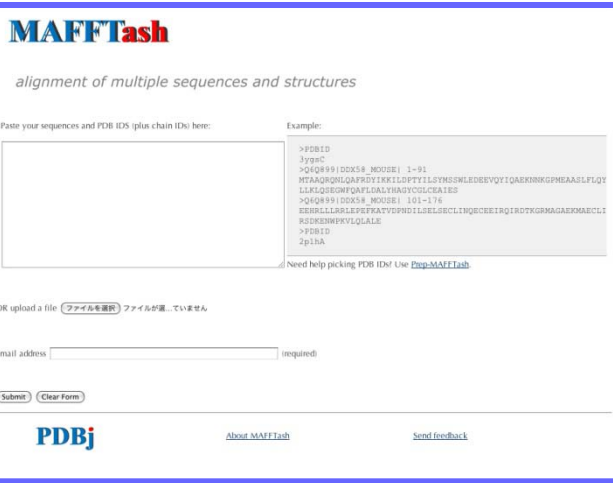
Homolog protein search, Sequence Navigator (Standley)



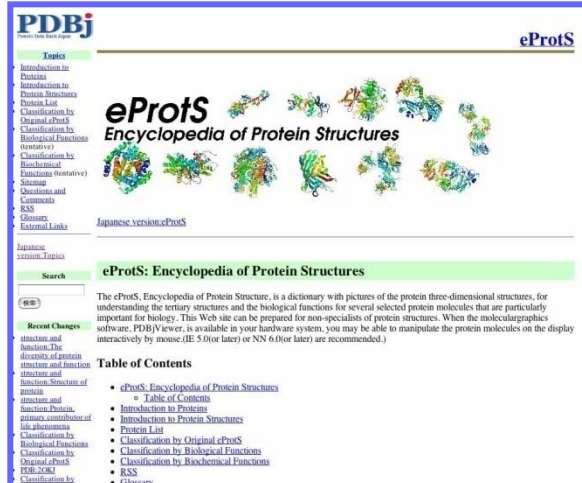
Similar fold search, Structure Navigator (Standley & Toh)



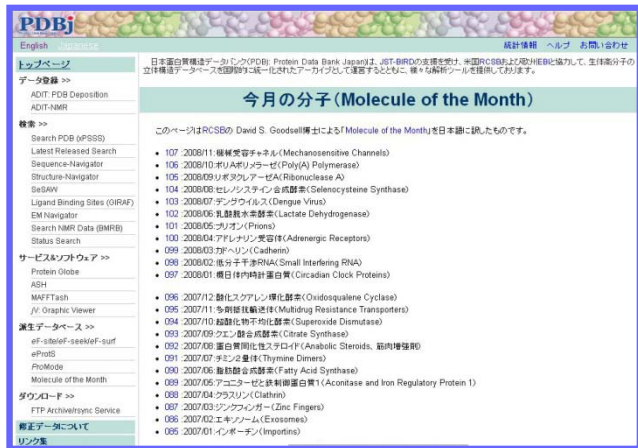
Function Annotation from Folds and Sequences, SeSAW (Standley)



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



Encyclopedia of Protein Structures, eProts (Kinjo, Kudo, & Ito)



Molecule of the Month, MoM (Goodsell & Kudo)