Biophysical Society of Japan, Kyoto
Luncheon Seminar on 28 October 2013

Activities of PDBj and wwPDB: A new PDB format, Data Deposition, Validation, and Data Integration

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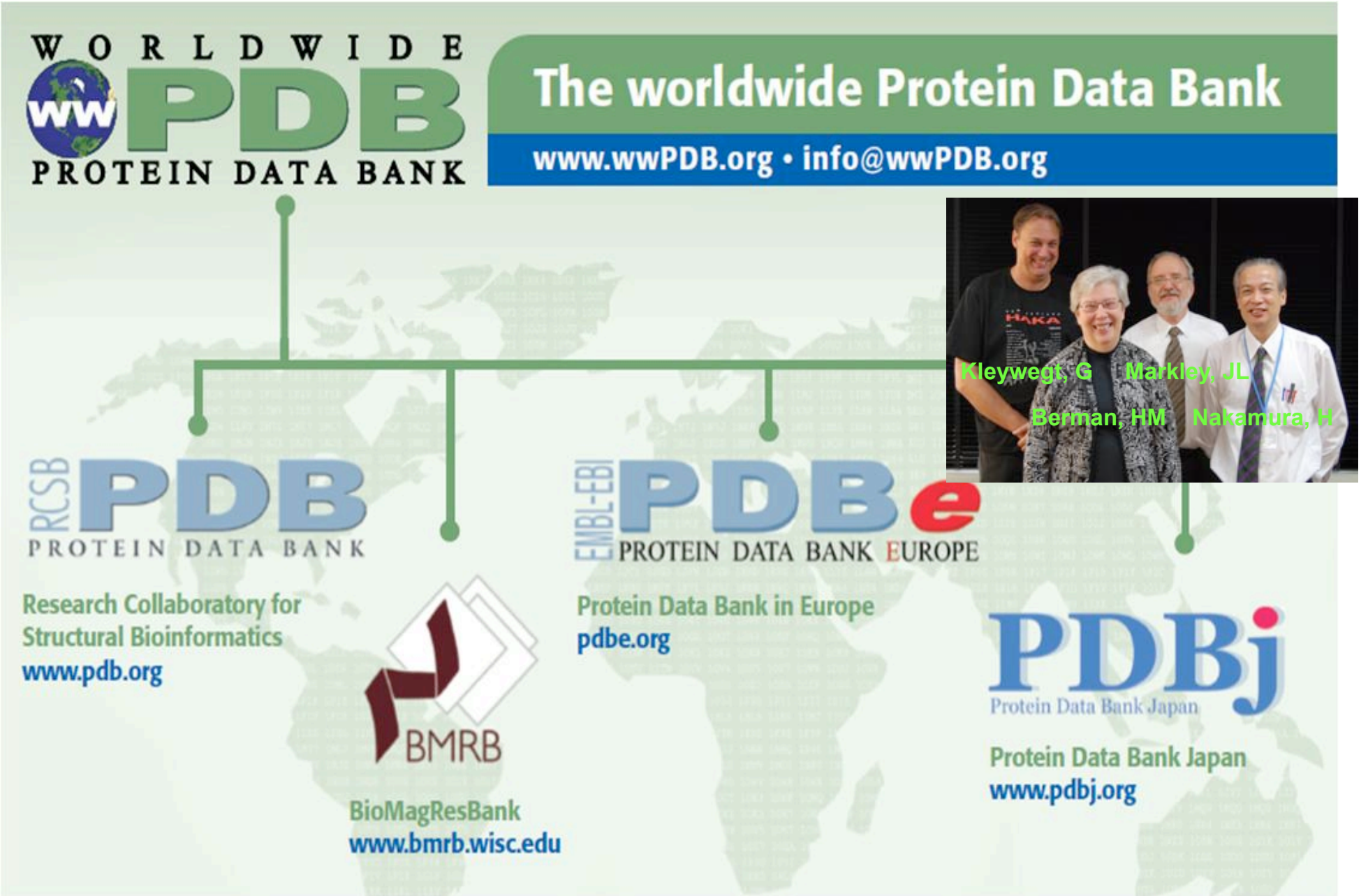
Institute for Protein Research

http://pdbj.org/
http://wwpdb.org/

wwPDB


WORLDWIDE PDB
PROTEIN DATA BANK
The worldwide Protein Data Bank
www.wwPDB.org • info@wwPDB.org
Kleywegt, G
Markley, JL
Berman, HM
Nakamura, H
RCSB PDB
PROTEIN DATA BANK
Research Collaboratory for Structural Bioinformatics
www.pdb.org
BMRB
BioMagResBank
www.bmrb.wisc.edu
EMBL-EBI PDBe
PROTEIN DATA BANK EUROPE
Protein Data Bank in Europe
pdbe.org
PDBj
Protein Data Bank Japan
Protein Data Bank Japan
www.pdbj.org

wwPDB Advisory Committee on Sept 27, 2013 Rutgers Univ.

PDBj Protein Data Bank Japan

WORLDWIDE PDB PROTEIN DATA BANK

Protein Data Bank Japan

http://pdbj.org/

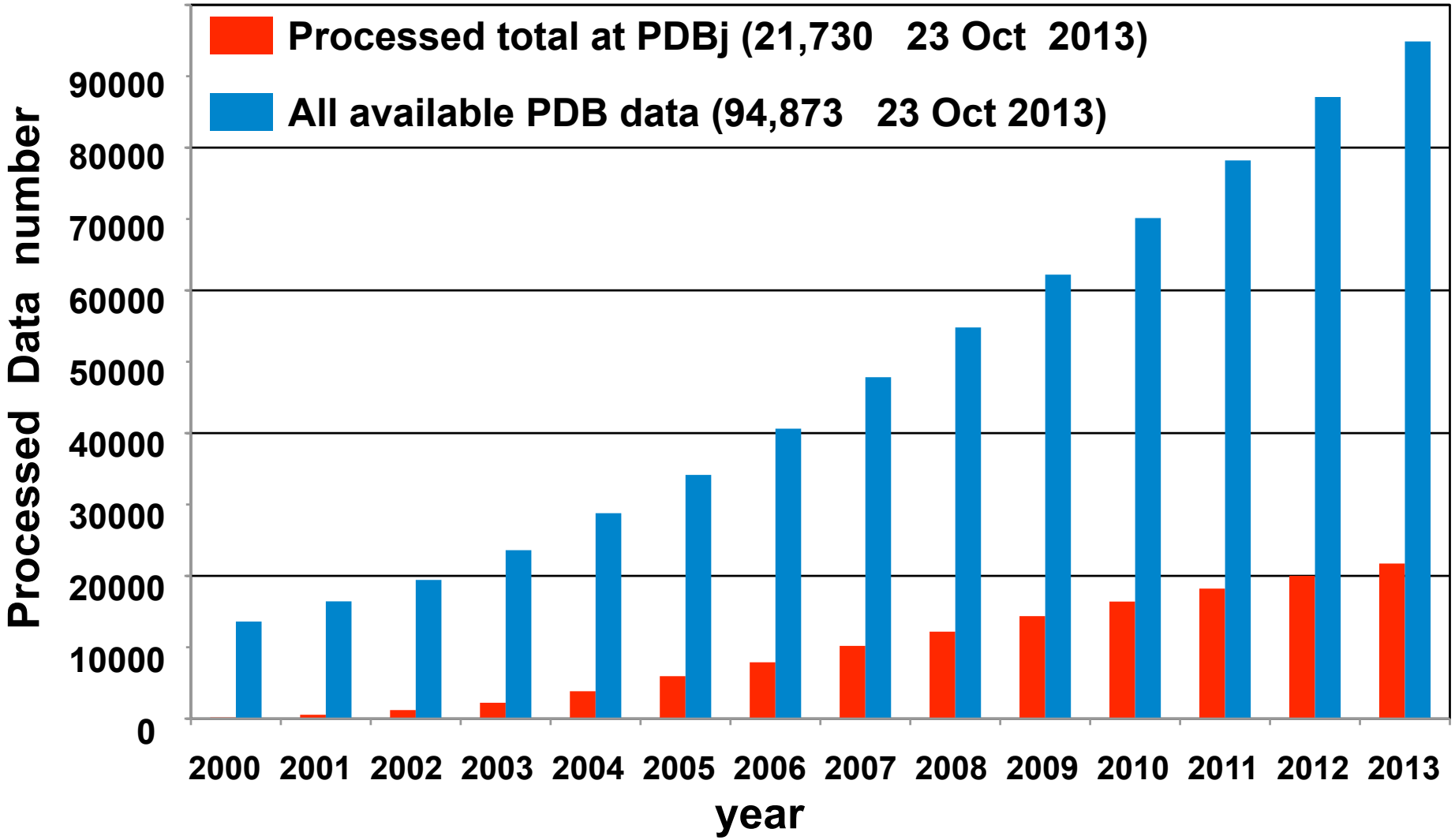
Since 2001, PDBj has been managed at Institute for Protein Research, Osaka University as a member of the wwPDB, to curate, edit and process the deposited data for an open, public, and single archive of the wwPDB.

PDBj staffs (April 2013)

Activities/Services of each member of the wwPDB

- "Data-in" activity, common in all the wwPDB members with high quality control. For that purpose, new format, data deposition, and validation system are developed
- "Data-out" services, characteristic at each wwPDB member site except common ftp-site data.

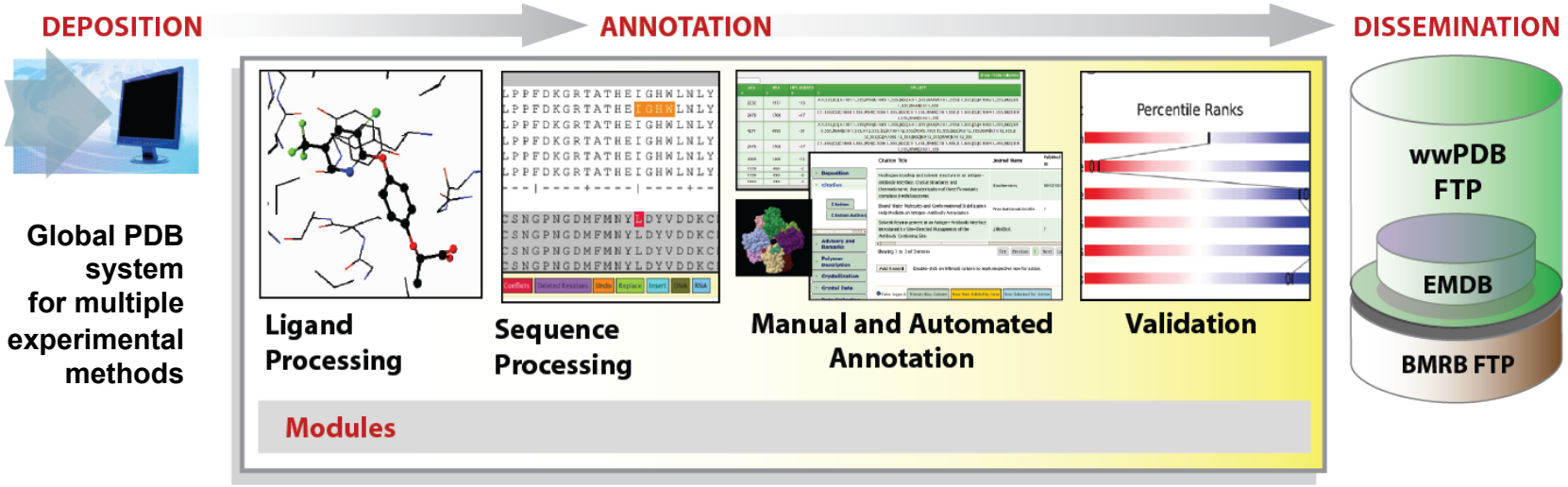
Data–in at PDBj and wwPDB



PDBj curates and processes about a Quarter of the deposited data, mainly from Asian and Oceania regions

New Annotation System

For data increase and high quality data management



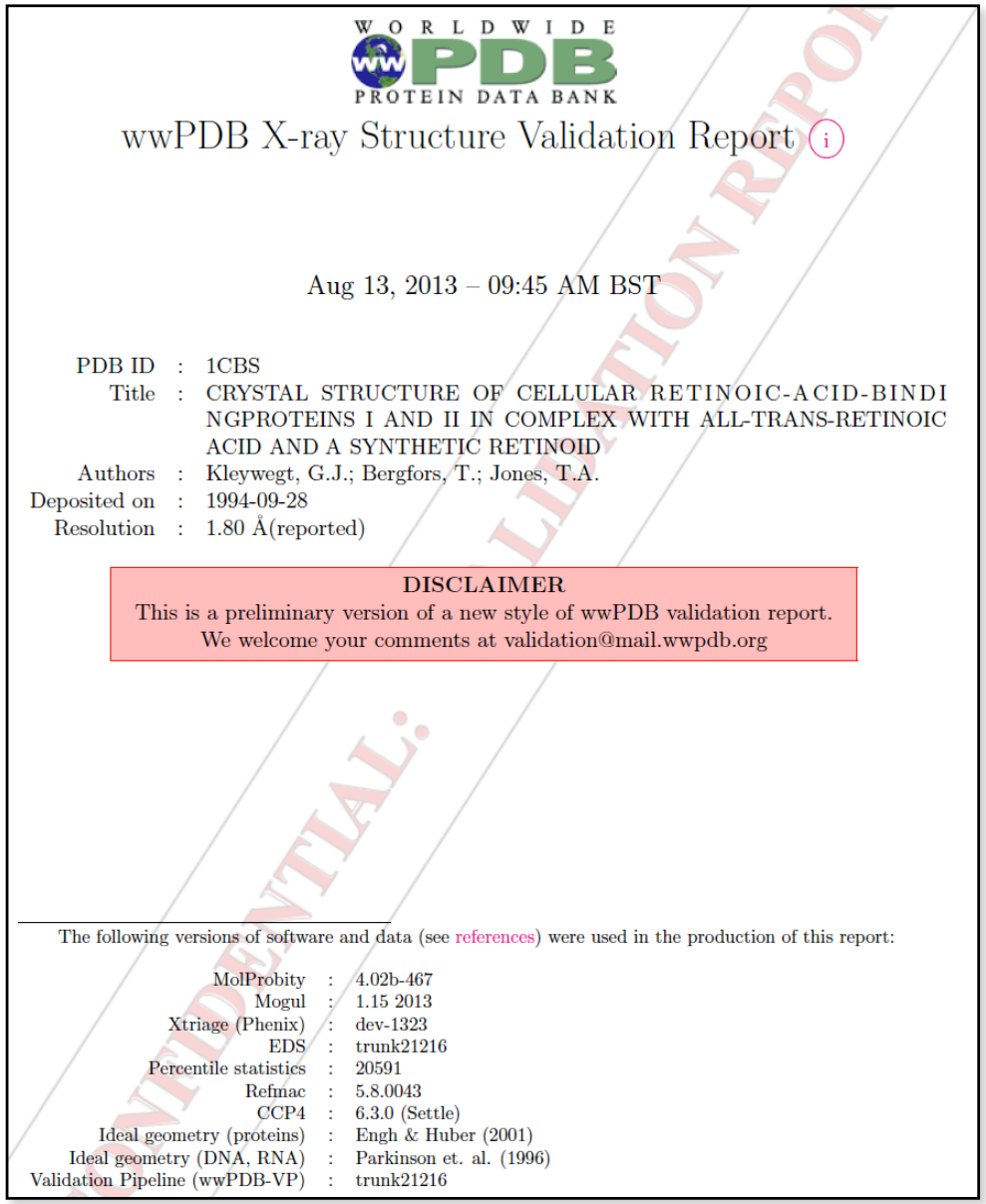
- Enables workload balancing and increased productivity
- Better quality assurance of **ligand chemistry and polymer sequences**
- **PDBx/mmCIF** is the master file format
- Validation suites based on recommendations from expert task forces; **X-ray validation pipeline** is available as a stand-alone server
- System will support all accepted experimental methods

Validation Report

- **Version 1.0** in production use since August 2013
  - **http://www.wwpdb.org/validation.html**
  - Fixing occasional bugs
  - Collecting feedback to inform possible changes

    validation@mail.wwpdb.org

- January 2014 – validation data for all X-ray structures will be made publicly available through the wwPDB ftp sites



WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Report (i)

Aug 13, 2013 – 09:45 AM BST

PDB ID	:	1CBS
Title	:	CRYSTAL STRUCTURE OF CELLULAR RETINOIC-ACID-BINDINGPROTEINS I AND II IN COMPLEX WITH ALL-TRANS-RETINOIC ACID AND A SYNTHETIC RETINOID
Authors	:	Kleywegt, G.J.; Bergfors, T.; Jones, T.A.
Deposited on	:	1994-09-28
Resolution	:	1.80 Å(reported)

DISCLAIMER
This is a preliminary version of a new style of wwPDB validation report.
We welcome your comments at validation@mail.wwpdb.org

The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	trunk21216
Percentile statistics	:	20591
Refmac	:	5.8.0043
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk21216

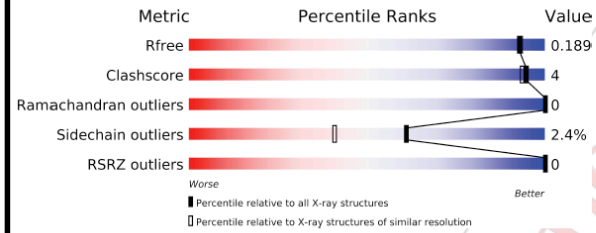
Validation Report

- **Summary**
  - **Quality vs. all PDB X-ray**
  - **Quality vs. entries at similar resolution**
  - **Overview of residue-based quality for every polymer**
  - **Table of ligands that may need attention**

1 Overall quality at a glance

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	65580	5522 (1.84-1.76)
Clashscore	76988	5040 (1.82-1.78)
Ramachandran outliers	75395	6528 (1.84-1.76)
Sidechain outliers	75377	6529 (1.84-1.76)
RSRZ outliers	65576	5522 (1.84-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	137	

Mol	Chain	Length	Quality of chain
1	A	371	
1	C	371	

The following table lists non-polymeric compounds that contain outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	401	-	X
2	NAG	C	401	-	X

Validation Report

- **Residue quality**

  Red dots: poor density (RSR-Z > 2, as in EDS)

- **Model/data fit ligands etc.**
  - **"*LLDF*" –*Local Ligand Density Fit* = Z-score of ligand RSR relative to nearby polymeric residues**

3 Residue-property plots

The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence annotated by issues in geometry and electron density. Residues are color-coded according to the number of different types of geometric errors found. Green signifies no errors, yellow, orange and red 1, 2, and 3 or more errors respectively. A red dot above a residue indicates a problem with electron density. Regions of sequence for which no errors are detected are indicated by a green connector.

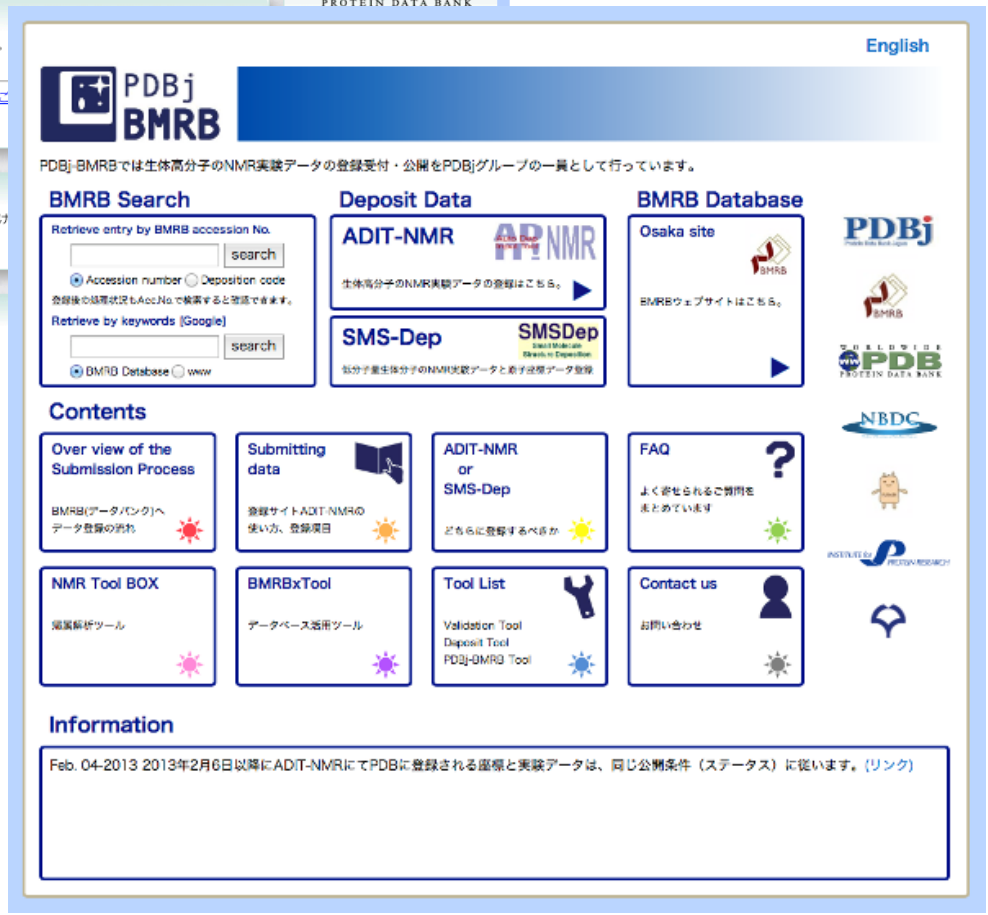
• Molecule 1: Jumonji domain-containing protein 2A

Chain A:

Data-out from PDBj

http://pdbj.org/ and http://legacy.pdbj.org/

PDBj-BMRB

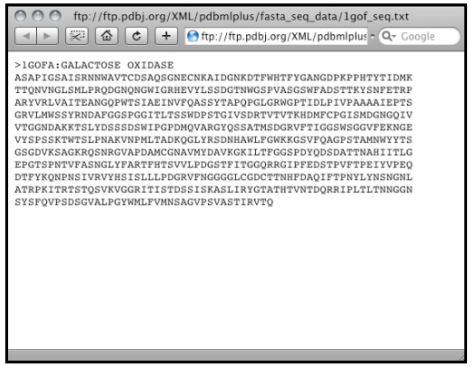


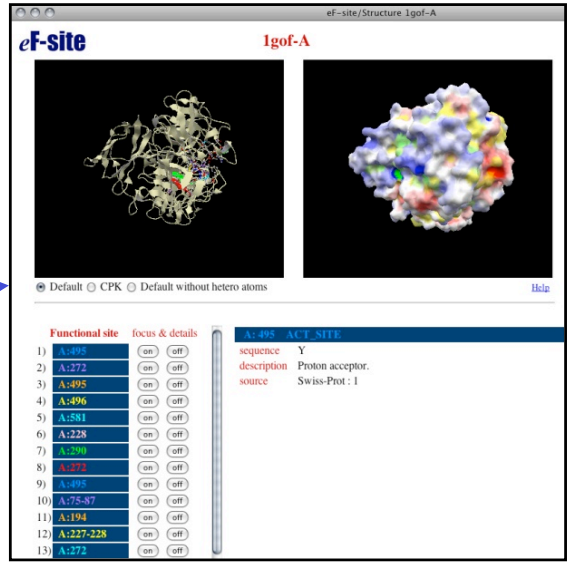
Duplicated portal

Summary page

http://pdbj.org/

Amino acid sequence (FASTA)





Data viewer at PDBj

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

Graphic viewer: *jV*
http://pdbj.org/jV/

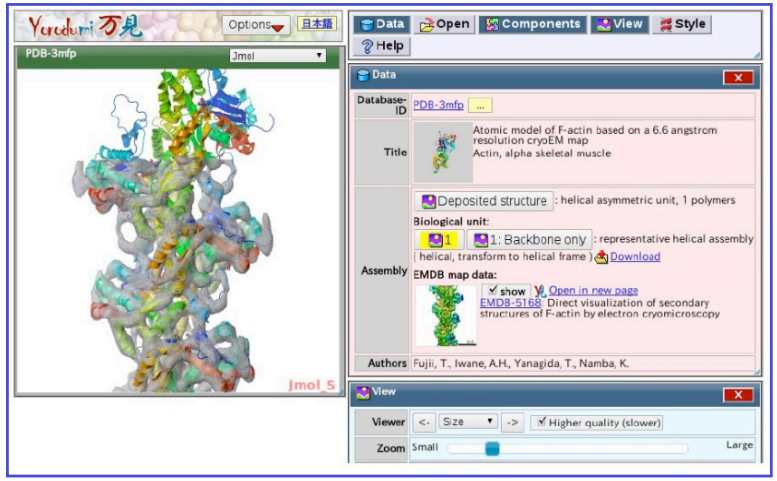
Kinjo et al. NAR 40, D453 (2012)

PDBj Protein Data Bank Japan

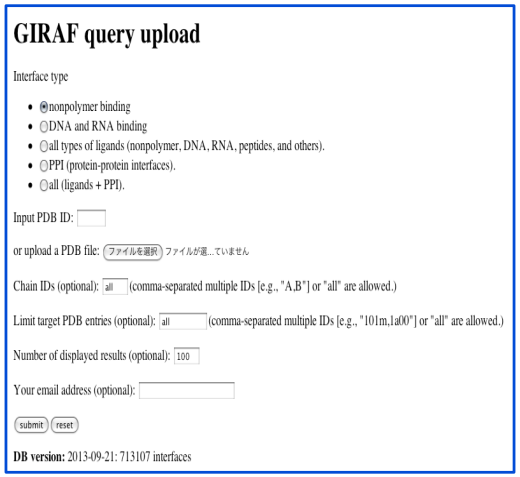
WORLDWIDE PDB PROTEIN DATA BANK

PDBj services

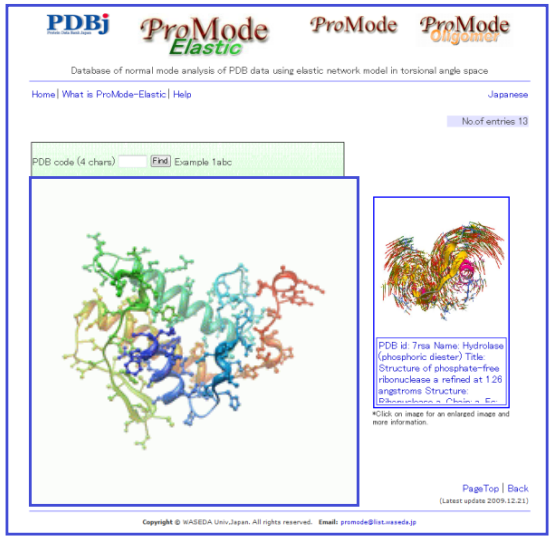
***EM Navi*: EMDB browser**



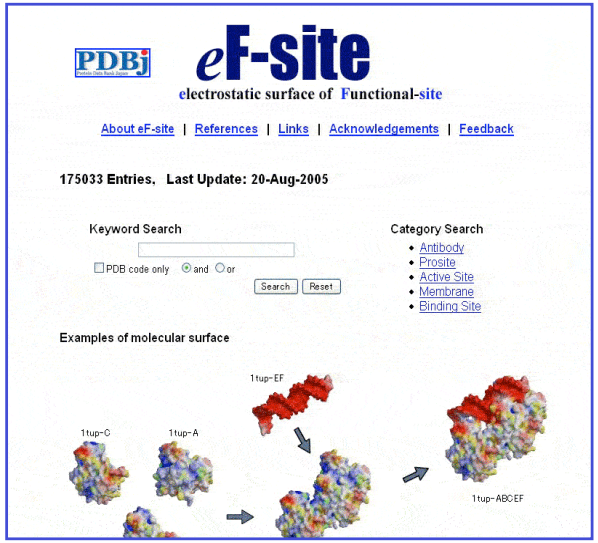
***Yorodumi*: PDB & EMDB**



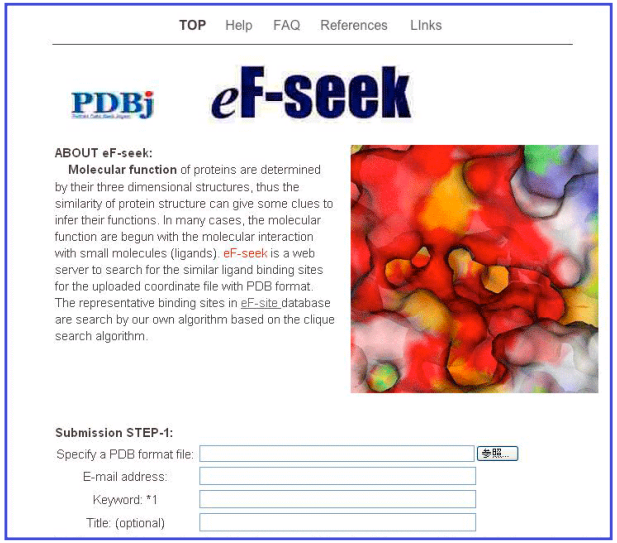
***GIRAF*: Similar binding site**



***ProMode*: Normal Mode**



***e*F-site: Mol. SurfaceDB**



***e*F-seek: Similar surface**

PDBj Protein Data Bank Japan　WORLDWIDE PDB PROTEIN DATA BANK

EM Navigator

3次元電子顕微鏡データナビゲーター [English / 日本語]

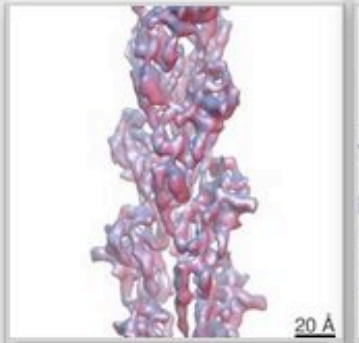
トップ | ギャラリー | リスト | 分布図 | 統計情報 | ビューア | 解説

PDBj > EM Navigator

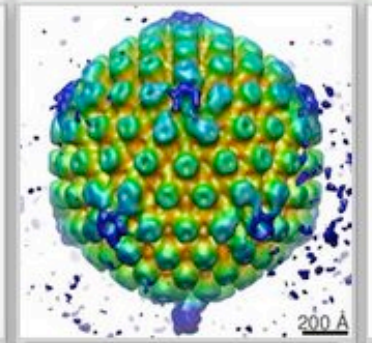
データを見る　詳しく

- **さがす**：(キーワード / EMDB ID / PDB ID)　EMDBかPDBのID、あるいはキーワードを入力　実行
- **眺める**：ギャラリー リスト 表

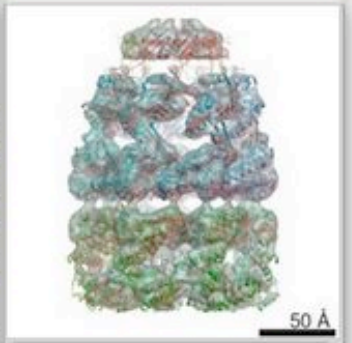
ムービースロット　再生　方向　シャッフル



EMDB-1980



EMDB-5452



EMDB-2325

情報

EM Navigatorとは？

- 生体分子や生体組織の3次元電子顕微鏡データを、**気軽にわかりやすく**眺めるためのウェブサイトです。
- EMDB と PDB のデータを利用しています (統計情報)
- 分子・構造生物学の専門家にも、初心者や専門外のかたにも利用していただけるサイトを目指しています。
- PDBjが運営しています。

詳しくはこちら

お知らせ

- 2013-09-11: 公開データ

その他の最新データ: EMDB付随情報, EMDB更新, PDB更新

- 2013-09-04: 公開データ

New format PDB: PDBx/mmCIF

- PDB format is almost 40 years old and does not support today's science.
- PDB Record format limitations
  - Max. 62 chains
  - Max. 99,999 atoms
  - No bond orders or chirality specified for ligands
  - No support for NMR, EM, hybrid methods, …
  - Meta-data specification cumbersome and inflexible

↓

- Preserve backward compatibility where possible
- web service to create PDB format data files
- Start in early 2014

Current Supported Archival Formats
protein structure format universe

PDB (*ca.* 1974)

PDBx/mmCIF (*ca.* 1997)

PDBML (*ca.* 2005)

RDF (*ca.* 2011)

In managing the formats, PDBx is the master format.

PDB Format Example

```
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.57
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 23.00
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 0.000
REMARK   3   COMPLETENESS FOR RANGE        (%) : NULL
REMARK   3   NUMBER OF REFLECTIONS             : 43316
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD          : NULL
REMARK   3   FREE
REMARK   3   R VA
REMARK   3   R VA
REMARK   3   FREE
REMARK   3   FREE
REMARK   3   FREE
REMARK   3
```

- Record-oriented with fixed column format
- Metadata in semi-structured remarks
- Documentation by example
- Most widely used and supported archival format

```
ATOM      1  N   VAL A 363      22.741   1.397  11.729  1.00 33.32           N
ATOM      2  CA  VAL A 363      21.557  -0.831  11.024  1.00 32.13           C
ATOM      3  C   VAL A 363      20.954  -1.757   9.943  1.00 31.73           C
ATOM      4  O   VAL A 363      19.737  -1.906   9.845  1.00 30.94           O
ATOM      5  CB  VAL A 363      21.883   0.552  10.391  1.00 33.45           C
```

PDBx/mmCIF Format Example

- Name – value pairs

```
_exptl.entry_id          1XBB
_exptl.method            'X-RAY DIFFRACTION'
_exptl.crystals_number   1
```

- Tabl

```
 loop
_data
_data
_data
_data
_database_PDB_rev.replaces
_database_PDB_rev.status
1 2004-11-02 2004-08-30 0 1XBB ?
2 2005-03-22 ?          1 1XBB ?
3 2009-02-24 ?          1 1XBB ?
```

- Simple syntax
- Named data items
- Data semantics defined in the PDBx data dictionary
- Software support in most popular languages

PDBML Example

```
<PDBx:entity_polyCategory>
     <PDBx:entity_poly entity_id="1">
        <PDBx:type>polypeptide(L)</PDBx:type>
        <PDBx:nstd_linkage>no</PDBx:nstd_linkage>
        <PDBx:nstd_monomer>no</PDBx:nstd_monomer>
        <PDBx:pdbx_seq_one_letter_code>
         DIVLTQSPASLSASVGETVTITCRASGNIHNYLAWYQQKQGKSPQLLVYYTTTLADG
```

- Three flavors of XML files:
  - fully marked-up files
  - files without atom records
  - files with a more space efficient encoding of atom records
- Follows naming and semantics of the PDBx data dictionary

RDF Example

```
<?xml version="1.0" encoding="UTF-8"?>
<?xml-stylesheet type="text/xml" href="http://pdbj.org/rdf-supp/pdbj-rdf.xsl" ?>
<rdf:RDF xmlns:PDBo="http://pdbj.org/schema/pdbx-v40.owl#"
         xmlns:rdfs="http://www.w3.org/2000/01/rdf-schema#"
         xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#">
  <PDBo:PDBID rdf:about="http://pdbj.org/pdb/1GOF">
    <rdfs:label>1GOF</rdfs:label>
  </PDBo:PDBI
  <rdf:Des
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo
    <PDBo:re
    <rdf:type rdf:resource="http://pdbj.org/schema/pdbx-v40.owl#entity"/>
  </rdf:Description>
</rdf:RDF>
```

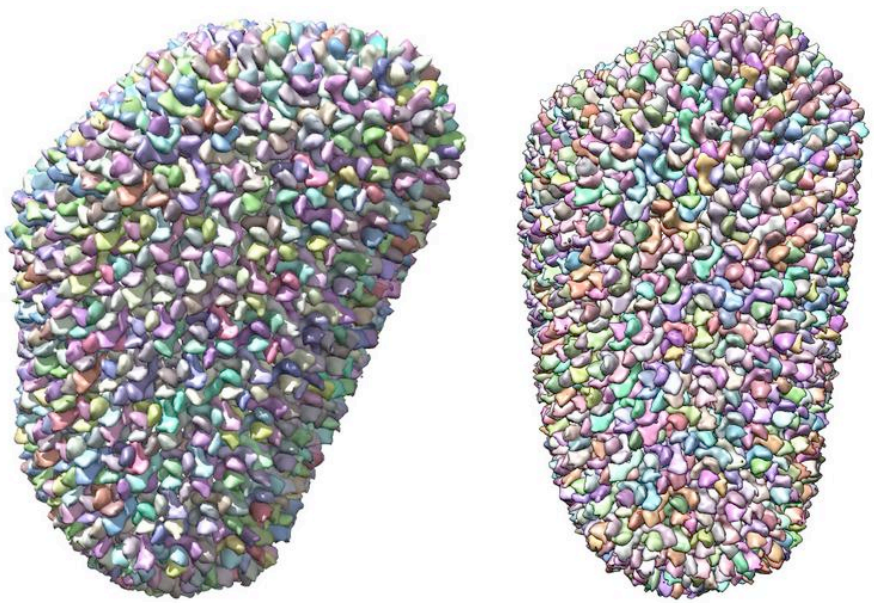
- Entry point for semantic web and reasoning systems
- Translates data items in PDBx/mmCIF schema into triples with URL identifiers
- Follows naming and semantics of the PDBx data dictionary
- http://pdbj.org/rdf/<pdbID>/<categoryName>/<pkey1>,…
- For example, http://pdbj.org/rdf/1GOF/entity/1

Transitional Home for Large Structures

Large single entries are now stored separately on the wwPDB ftp site, and PDB internally produces *divided/split* PDB format files.

ftp://ftp.wwpdb.org/pub/pdb/data/large_structures/mmCIF/
ftp://ftp.wwpdb.org/pub/pdb/data/large_structures/XML/

HIV-1 Capsid 3J3Q –
- 1356 chains
- >2M atoms
- 25 – PDB format entries



3J3Y 3J3Q

Providing Format Compatibility

- Adopt a *PDB friendly* mmCIF/PDBx style -
  - All records on a single text line
  - Columns presented in standard column order.
  - Tabular presentation with leading record names (*e.g.* ATOM, CELL, REFINE)
  - Method independent features in left-most columns (*e.g.* identifiers & coordinates)
  - Method specific features in the right-most columns (*e.g.* ADPs, NMR order/disorder parameters)
  - Continue to support PDB nomenclature semantics (*e.g*. PDB style chains, residue numbering, and insertion codes)
- Large entries will be internally converted to divided/split PDB format files.

```
ATOM      1  N   GLN A  39      24.690 -27.754  24.275  1.00 60.76          N
ATOM      2  CA  GLN A  39      23.581 -26.768  24.416  1.00 60.98          C
ATOM      3  C   GLN A  39      23.990 -25.379  23.905  1.00 59.98          C
ATOM      4  O   GLN A  39      25.070 -25.209  23.330  1.00 60.25          O
ATOM      5  CB  GLN A  39      23.136 -26.685  25.878  1.00 60.69          C
ATOM      6  N   VAL A  40      23.115 -24.395  24.122  1.00 59.58          N
ATOM      7  CA  VAL A  40      23.342 -23.010  23.690  1.00 57.26          C
ATOM      8  C   VAL A  40      24.000 -22.152  24.778  1.00 56.00          C
ATOM      9  O   VAL A  40      23.992 -20.920  24.692  1.00 55.53          O
ATOM     10  CB  VAL A  40      22.015 -22.337  23.275  1.00 57.32          C
```

PDB

PDBx/mmCIF

```
loop_
_atom_site.group_PDB
_atom_site.id
_atom_site.auth_atom_id
_atom_site.type_symbol
_atom_site.auth_comp_id
_atom_site.auth_asym_id
_atom_site.auth_seq_id
_atom_site.Cartn_x
_atom_site.Cartn_y
_atom_site.Cartn_z
_atom_site.pdbx_PDB_model_num
_atom_site.occupancy
_atom_site.pdbx_auth_alt_id
_atom_site.B_iso_or_equiv
ATOM      1  N    N  GLN  A   39   24.690  -27.754   24.275  1  1.000  .  60.760
ATOM      2  CA   C  GLN  A   39   23.581  -26.768   24.416  1  1.000  .  60.980
ATOM      3  C    C  GLN  A   39   23.990  -25.379   23.905  1  1.000  .  59.980
ATOM      4  O    O  GLN  A   39   25.070  -25.209   23.330  1  1.000  .  60.250
ATOM      5  CB   C  GLN  A   39   23.136  -26.685   25.878  1  1.000  .  60.690
ATOM      6  N    N  VAL  A   40   23.115  -24.395   24.122  1  1.000  .  59.580
ATOM      7  CA   C  VAL  A   40   23.342  -23.010   23.690  1  1.000  .  57.260
ATOM      8  C    C  VAL  A   40   24.000  -22.152   24.778  1  1.000  .  56.000
ATOM      9  O    O  VAL  A   40   23.992  -20.920   24.692  1  1.000  .  55.530
ATOM     10  CB   C  VAL  A   40   22.015  -22.337   23.275  1  1.000  .  57.320
ATOM     11  N    N  ALA  A   41   24.560  -22.804   25.797  1  1.000  .  54.570
```

PDBx/mmCIF Software Support

- **Phenix and Refmac – produce native PDBx files for deposition**
- **MMDB** - macromolecular object library in CCP4
- **iotbx.cif/ucif** - CCTBx C++/Python IO library with dictionary validation
- **CCIF** – CCP4 C++ library with FORTRAN support and dictionary validation
- **CBFLib** - ANSI-C library for CIF & imgCIF files
- **mmLIB** - Python toolkit supporting CIF & mmCIF
- **BioPython** - Python toolkit for computational biology
- **PyCifRW** - Python CIF/mmCIF parsing tools
- **BioJava** - Java mmCIF IO package
- **STAR::Parser** – Perl mmCIF parser and molecular object library
- **RCSBTools** - C++/Python parsing and dictionary validation tools plus many other supporting format conversion and data management applications
- **Visualization** - **Chimera**, **Jmol**, **OpenRasMol**

PDB actively working with community developers to help fill in missing functionalities. Two workshops scheduled in Fall 2013 …

Converter Program: CIFTr

http://mmcif.pdb.org

RCSB PDB PROTEIN DATA BANK

A MEMBER OF THE WWPDB

An Information Portal to Biological Macromolecular Structures

PDB Home | Contact Us

Dictionary Home | PDBML Home | Software Tools Home Search: PDB Exchange Dictionary Go

Dictionary Resources

The Protein Data Bank (PDB) uses macromolecular Crystallographic Information File (mmCIF) data dictionaries to describe the information content of PDB entries. The PDB Exchange data dictionary consolidates content from a variety of crystallographic dictionaries including: the IUCr Core, mmCIF, Image and symmetry dictionaries. The PDB Exchange Dictionary also includes extensions describing NMR, Cryo-EM, and protein production data. PDB data processing, data exchange, annotation, and database management operations all make heavy use of the data format and the content of the PDB Exchange Dictionary. Software tools are used to convert mmCIF data files to the older PDB format and to PDBML/XML.

- mmCIF/PDBx example files for PDB entries containing large structures
- PDBx/mmCIF tutorial for the protein structure modules of BioJava
- Data files in mmCIF format can be downloaded from the RCSB PDB website or by ftp.
- Software tools are available for preparing and editing depositions.
- Software tools are available for converting mmCIF data files to PDB and PDBML formats
- A complete list of PDB software tools for managing PDB data in mmCIF format can be found here.

Dictionary Content and Representation

- Background and Introduction about mmCIF
- Chapter 3.6. Classification and use of macromolecular data. (PDF) in *International Tables for Crystallography G.* Definition and exchange of crystallographic data, S.R. Hall and B. McMahon, Editors. 2005, Springer: Dordrecht, The Netherlands. p. 144-198.
  - Appendix 3.6.2 The Protein Data Bank exchange dictionary (PDF) in *International Tables for Crystallography G.* Definition and exchange of crystallographic data, S.R. Hall and B. McMahon, Editors. 2005, Springer: Dordrecht, The Netherlands. p. 195-198.

Converter Program: CIFTr

http://mmcif.pdb.org

RCSB PDB PROTEIN DATA BANK

A MEMBER OF THE PDB

An Information Portal to Biological Macromolecular Structures

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CIFTr

CIFTr is an application program for translating files in mmCIF format into files in PDB format. CIFTr is currently available in source form and binary form for several UNIX platforms.

CIFTr can be used to translate the files released that are in in mmCIF format at ftp://ftp.rcsb.org/pub/pdb/data/structures/.

Installation and usage notes for the source distribution of CIFTr

Click here to download source distribution of CIFTr.

Installation and usage notes for the binary distribution of CIFTr

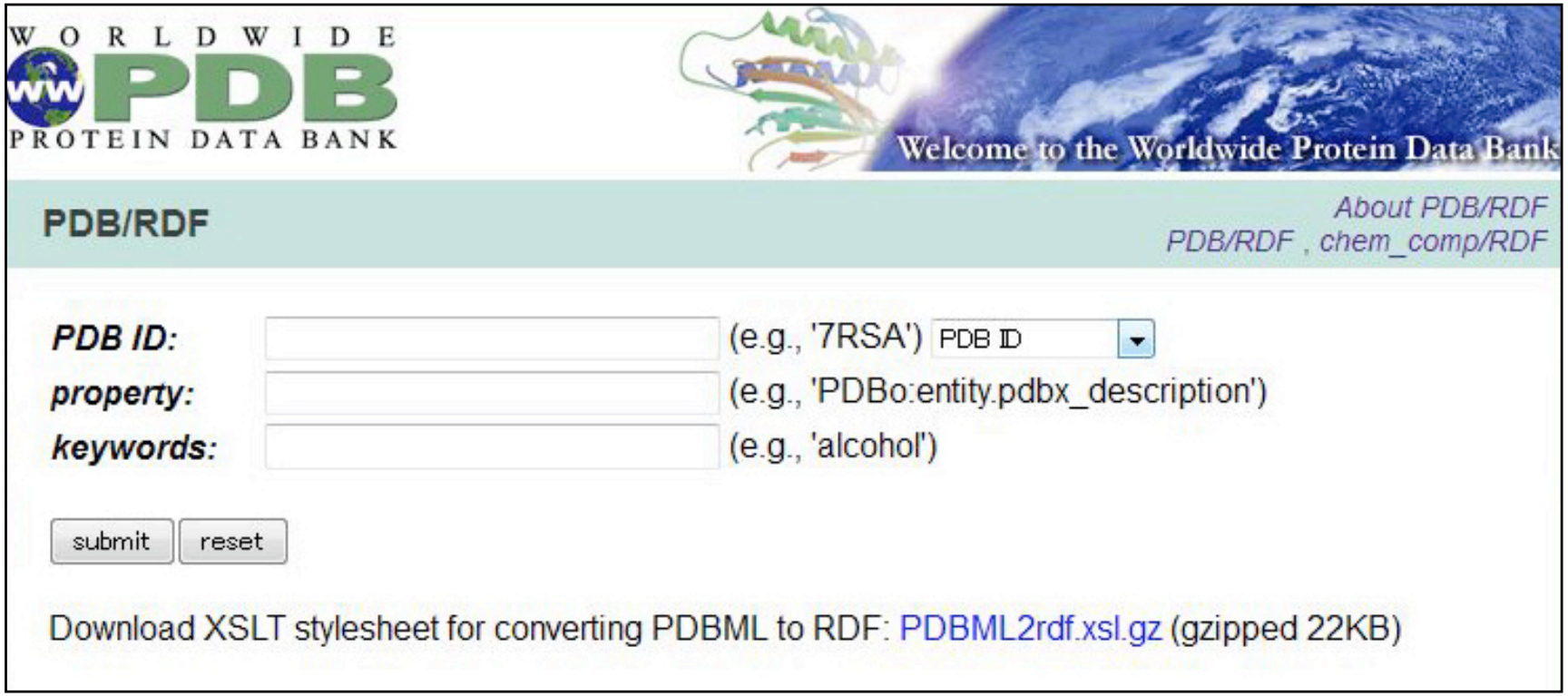
Click here to download binary (Linux, SGI, OSF, MACOSX, or SUN) distribution of CIFTr.

PDB/RDF format for Semantic Web

Service from wwPDB by Akira R. Kinjo (PDBj) & Tom Oldfield (PDBe)

http://rdf.wwpdb.org/

Kinjo et al. (2012) Nucl. Acids Res. 40, D453-D460.



In UniProt RDF:

```
<rdf:Description rdf:about="http://rdf.wwpdb.org/pdb/1BY4">
  <rdf:type rdf:resource="http://purl.uniprot.org/core/Structure_Resource"/>
  <database rdf:resource="http://purl.uniprot.org/database/PDB"/>
  <method rdf:resource="http://purl.uniprot.org/core/X-Ray_Crystallography"/>
  <resolution rdf:datatype="http://www.w3.org/2001/XMLSchema#float">2.10</resolution>
</rdf:Description>
```

BMRB/XML and /RDF for Semantic Web

(developed by PDBj and BMRB)

NMR-STAR v3

```
######################
#  Entry information  #
######################

save_entry_information
   _Entry.Sf_category                      entry_information
   _Entry.Sf_framecode                     entry_information
   _Entry.ID                               15400
   _Entry.Title
;
Backbone and side chain chemical shift assignments of the F1
53-to-5-flurotryptophan mutant of human cardiac troponin C
;
   _Entry.Version_type                     new
   _Entry.Submission_date                  2007-07-20
   _Entry.Accession_date                   2007-07-20
   _Entry.Last_release_date                .
   _Entry.Original_release_date            .
   _Entry.Origination                      author
   _Entry.NMR_STAR_version                 3.0.8.100
   _Entry.Original_NMR_STAR_version        3.0.8.100
   _Entry.Experimental_method              NMR
   _Entry.Experimental_method_subtype      solution
   _Entry.Details                          .
   _Entry.BMRB_internal_directory_name
```

bmr15400.str

BMRBxTool

BMRB/XML

```
<BMRBx:entryCategory>
  <BMRBx:entry id="15400">
    <BMRBx:accession_date>2006-12-07+09:00</BMRBx:accession_date>
    <BMRBx:bmrb_internal_directory_name xsi:nil="true"/>
    <BMRBx:details xsi:nil="true"/>
    <BMRBx:experimental_method>NMR</BMRBx:experimental_method>
    <BMRBx:experimental_method_subtype>SOLUTION</BMRBx:experimental_method_subtype>
    <BMRBx:last_release_date xsi:nil="true"/>
    <BMRBx:nmr_star_version>3.0.8.100</BMRBx:nmr_star_version>
    <BMRBx:original_nmr_star_version>3.0.8.100</BMRBx:original_nmr_star_version>
    <BMRBx:original_release_date xsi:nil="true"/>
    <BMRBx:origination>author</BMRBx:origination>
    <BMRBx:sf_category>entry_information</BMRBx:sf_category>
    <BMRBx:sf_framecode>entry_information</BMRBx:sf_framecode>
    <BMRBx:submission_date>2006-12-07+09:00</BMRBx:submission_date>
    <BMRBx:title>Backbone and side chain chemical shift assignments of the F153-to-
5-flurotryptophan mutant of human cardiac troponin C</BMRBx:title>
    <BMRBx:version_type>original</BMRBx:version_type>
  </BMRBx:entry>
</BMRBx:entryCategory>
```

bmr15400.xml

BMRB/RDF

BMRBoTool

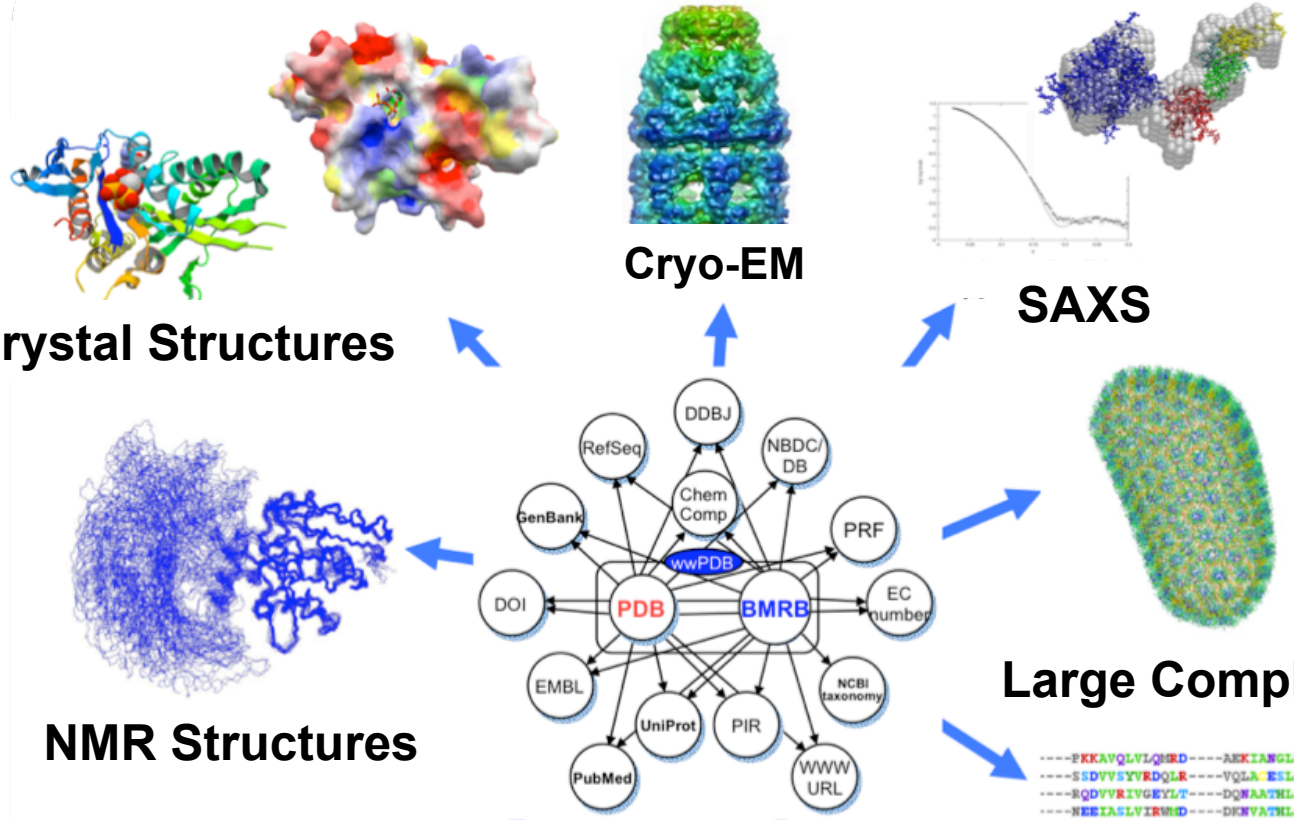
```
<BMRBo:has_entryCategory>
  <BMRBo:entryCategory rdf:about="http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr15400/entryCategory">
    <BMRBo:has_entry>
      <BMRBo:entry rdf:about="http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr15400/entry/15400">
        <BMRBo:of_datablock rdf:resource="http://bmrbpub.protein.osaka-u.ac.jp/rdf/bmr15400"/>
        <BMRBo:entry.id>15400</BMRBo:entry.id>
        <BMRBo:entry.accession_date>2006-12-07+09:00</BMRBo:entry.accession_date>
        <BMRBo:entry.experimental_method>NMR</BMRBo:entry.experimental_method>
        <BMRBo:entry.experimental_method_subtype>SOLUTION</BMRBo:entry.experimental_method_subtype>
        <BMRBo:entry.nmr_star_version>3.0.8.100</BMRBo:entry.nmr_star_version>
        <BMRBo:entry.original_nmr_star_version>3.0.8.100</BMRBo:entry.original_nmr_star_version>
        <BMRBo:entry.origination>author</BMRBo:entry.origination>
        <BMRBo:entry.sf_category>entry_information</BMRBo:entry.sf_category>
        <BMRBo:entry.sf_framecode>entry_information</BMRBo:entry.sf_framecode>
        <BMRBo:entry.submission_date>2006-12-07+09:00</BMRBo:entry.submission_date>
        <BMRBo:entry.title>Backbone and side chain chemical shift assignments of the F153-to-5-fluro
tryptophan mutant of human cardiac troponin C</BMRBo:entry.title>
        <BMRBo:entry.version_type>original</BMRBo:entry.version_type>
      </BMRBo:entry>
    </BMRBo:has_entry>
  </BMRBo:entryCategory>
</BMRBo:has_entryCategory>
```

bmr15400.rdf

Format	NMR-STAR v3	BMRB/XML	BMRB/RDF
Ontology	NMR-STAR v3 dictionary	BMRB/XML schema	BMRB/OWL
Validation	ADIT-NMR & manual	Schema validation	RDF validator
Data type	Text file (.str)	XML file (.xml)	RDF file (.rdf)

Yokochi, M. et al., in preparation

Links among PDB/RDF, BMRB/RDF and many other databases



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