Modifications to the Protein Data Bank: A new PDB format, Data Deposition, and Validation

Genji Kurisu

Institute for Protein Research

http://pdbj.org/

http://wwpdb.org/

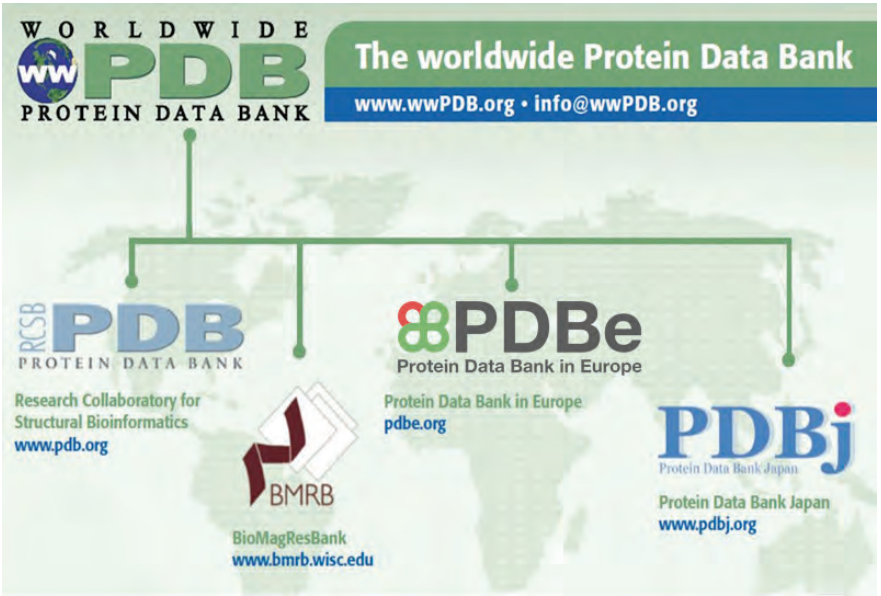
Protein Data Bank Japan

http://pdbj.org/

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

PDBj staffs (April 2014)

wwPDB.org



wwPDB members and their heads

PDBj Protein Data Bank Japan

WORLDWIDE PDB PROTEIN DATA BANK

RUTGERS THE STATE UNIVERSITY OF NEW JERSEY

Center for Integrative PROTEOMICS Research

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Stephen K. Burley, M.D., D.Phil.

Director, Center for Integrative Proteomics Research
Associate Director, RCSB-PDB
Distinguished Professor, Department of Chemistry and Chemical Biology
Member, Cancer Institute of New Jersey

A new director of the RCSB-PDB

(Helen M. Berman is going to be a chair of the wwPDB)

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, common archive as the ftp site and the characteristic services by each wwPDB member**

PDBj Protein Data Bank Japan

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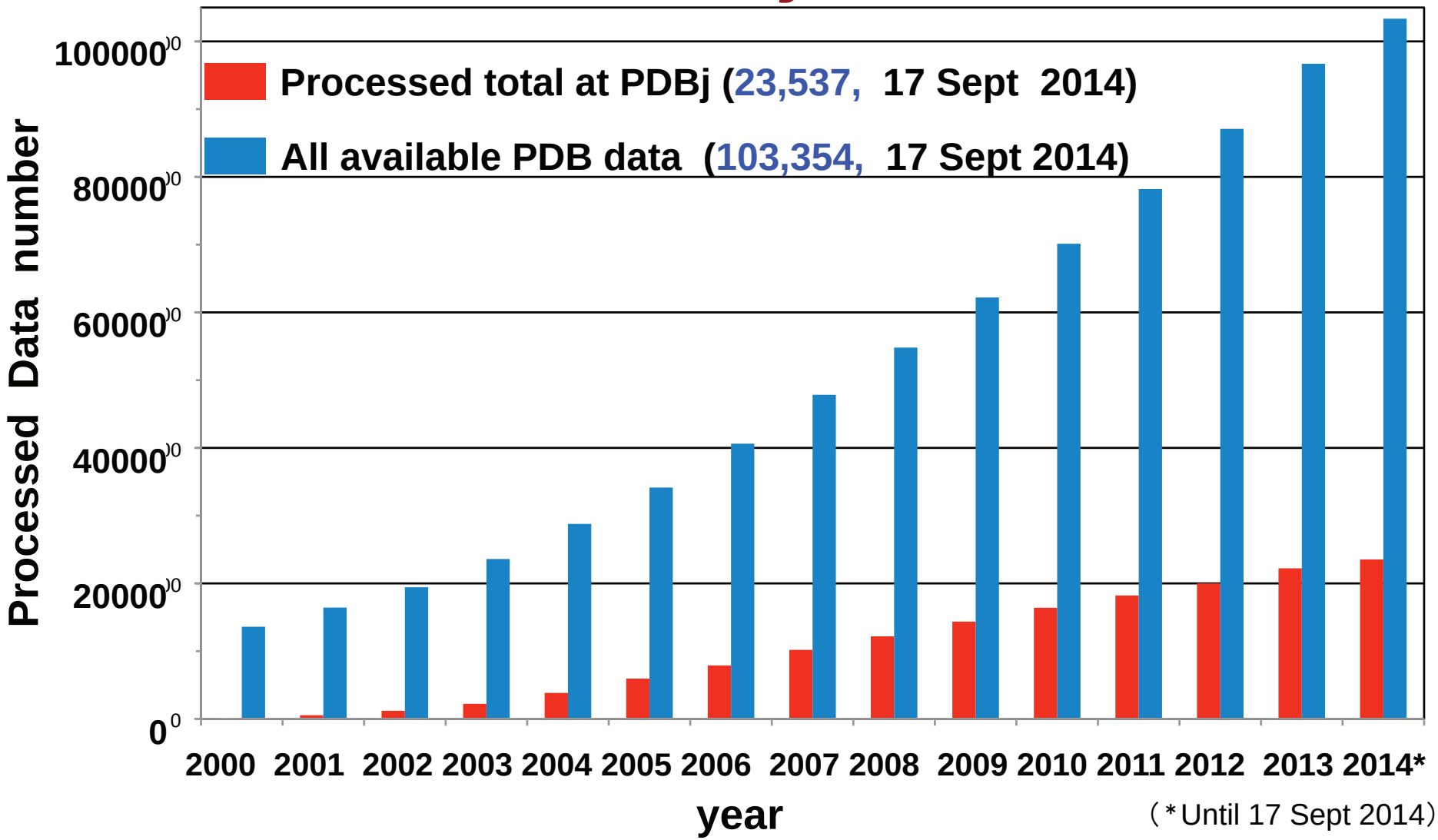
Data–in at PDBj and wwPDB



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

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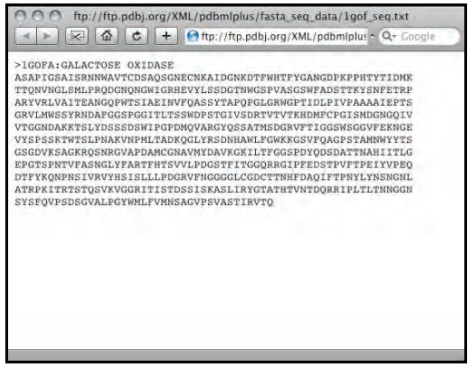
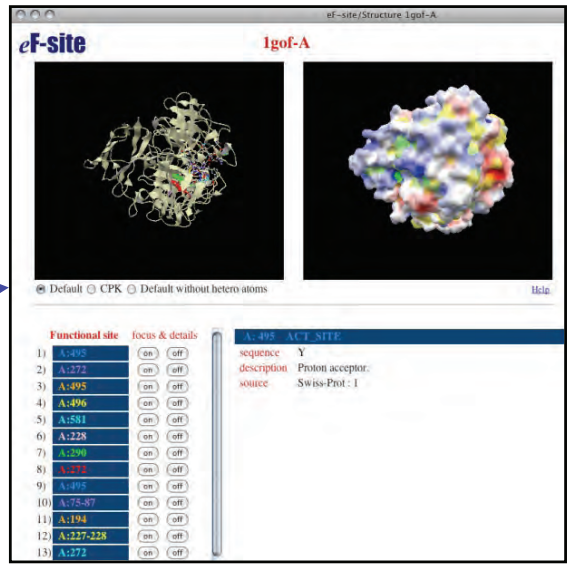
Data–out from PDBj

http://pdbj.org/

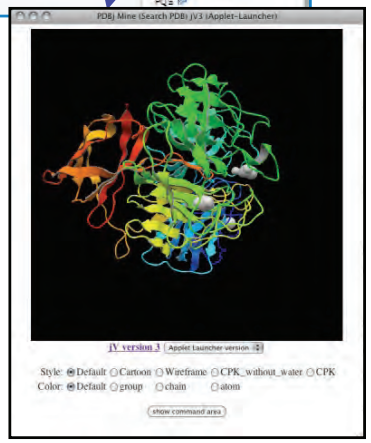
Data viewer at PDBj

Amino acid sequence (FASTA)





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)

New standard PDB format: PDBx/mmCIF

- Current 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
- PDBML (XML) and RDF format files are available.
- Start in 2014 and the current PDB format will be phased out in 2016.

```
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
```

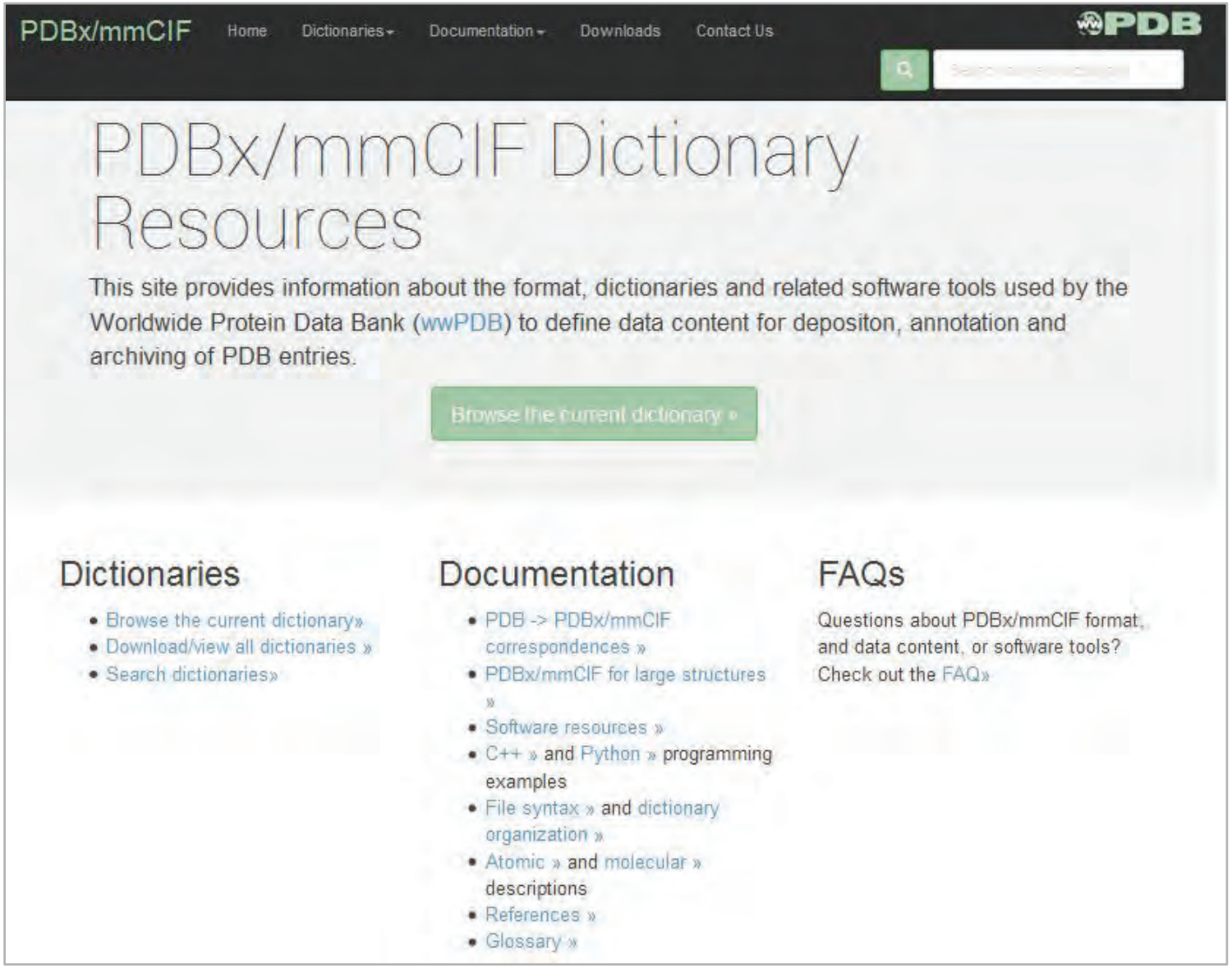
PDB

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
```

wwPDB Service site for a new format

http://mmcif.wwpdb.org/



wwPDB Service site for a new format

http://mmcif.pdbj.org/

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** - **UCSF Chimera**, **Jmol**, **OpenRasMol, jV, molmil**

PDB actively working with community developers to help fill in missing functionalities.

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.

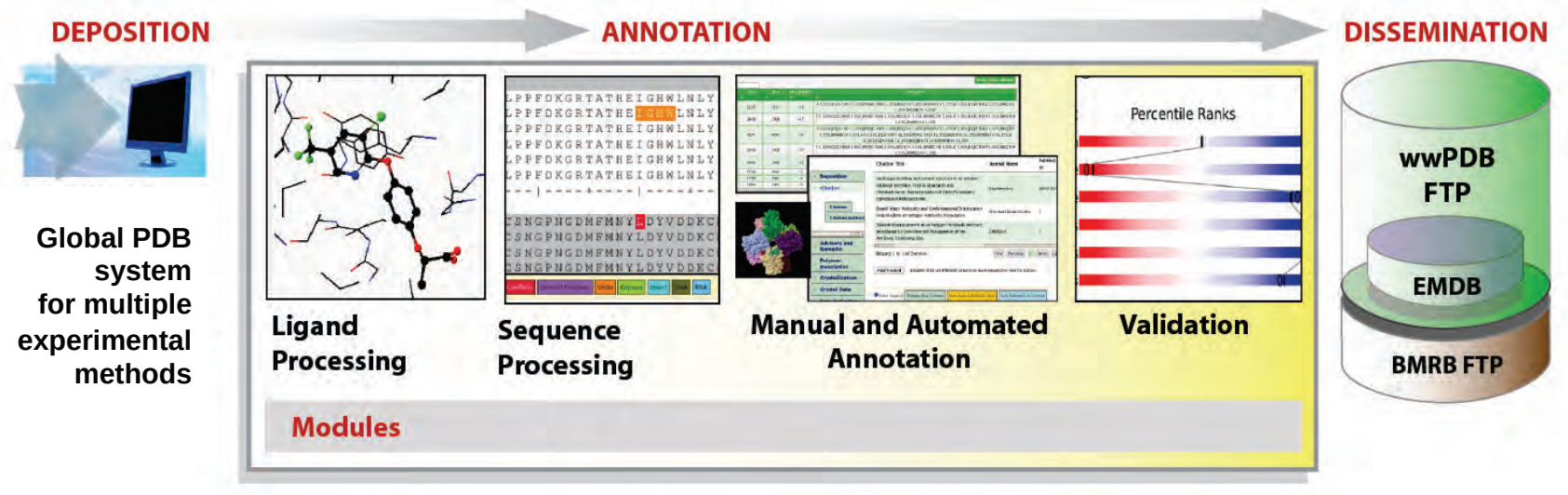
ftp://ftp.wwpdb.org/pub/pdb/data/large_structures/mmCIF/
ftp://ftp.wwpdb.org/pub/pdb/data/large_structures/XML/

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

PDBj Protein Data Bank Japan WORLDWIDE PDB PROTEIN DATA BANK

New Annotation System

For data increase and high quality data management



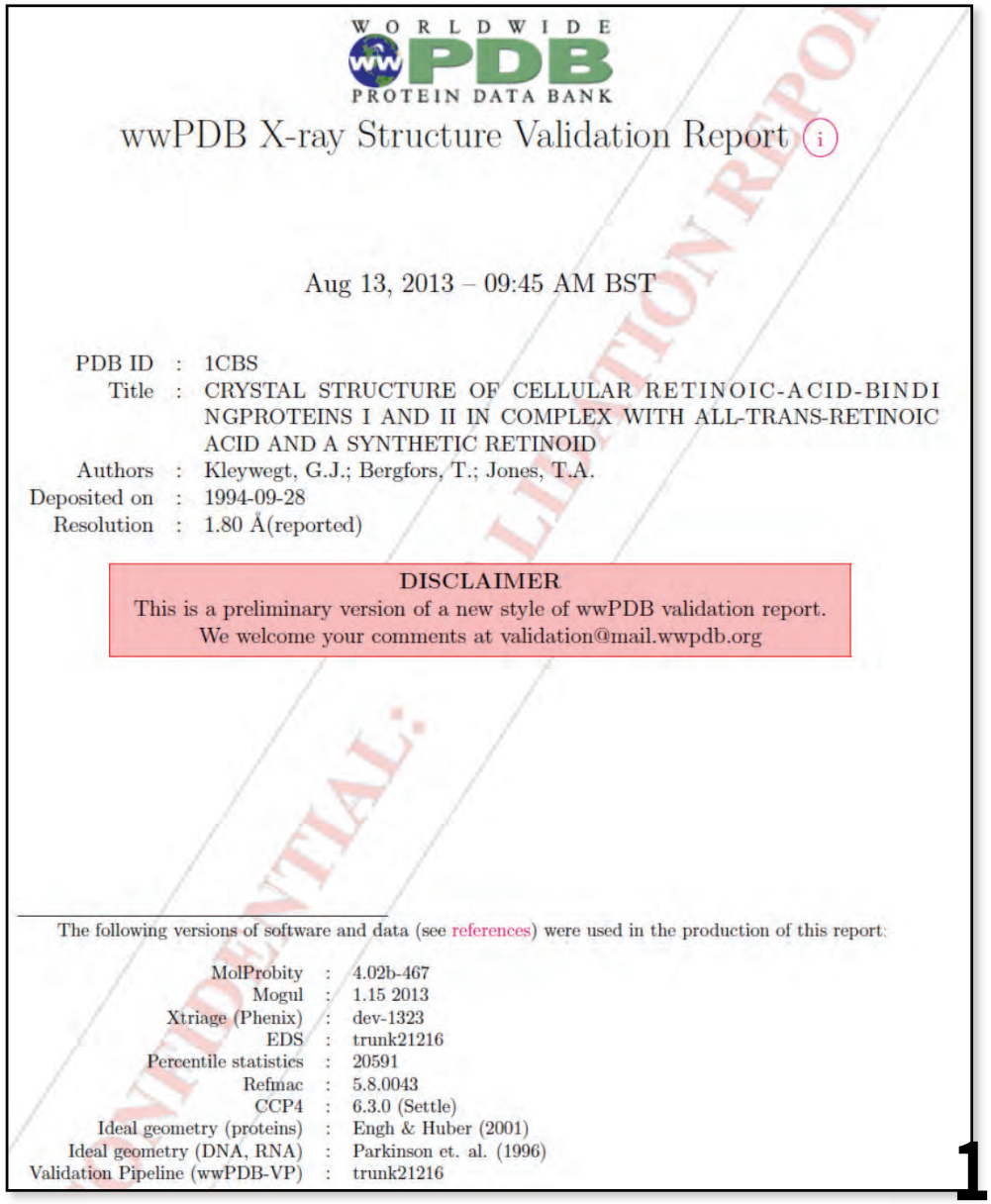
- Enables workload balancing and increased productivity
- Better quality assurance of **ligand chemistry and polymer sequences**
- **PDBx/mmCIF** is the master file format
- Validation suites based on recommendations from expert task forces; **X-ray validation pipeline** is available as a stand-alone 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-BINDI NGPROTEINS 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)

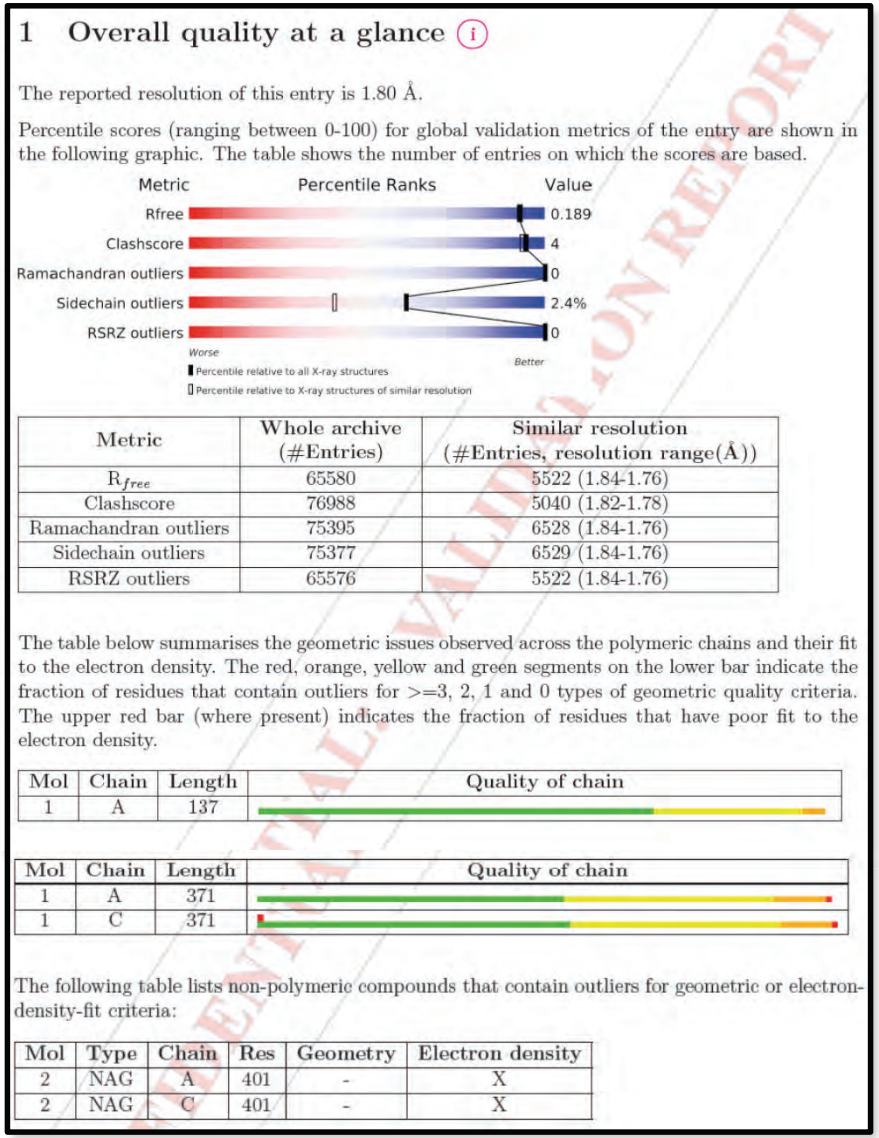
DISCLAIMER
This is a preliminary version of a new style of wwPDB validation report.
We welcome your comments at validation@mail.wwpdb.org

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:

PDBj members in 2014

- **Head**
  - Nakamura, Haruki, Ph. D. (Prof., IPR, Osaka Univ.)
- **Group for PDB Database Curation**
  - Nakagawa, Atsushi, Ph. D. (Group Leader, Prof., IPR, Osaka Univ.)
  - Matsuda, Makoto, Ph. D. (IPR, Osaka Univ.)
  - Igarashi, Reiko (IPR, Osaka Univ.)
  - Kengaku, Yumiko (IPR, Osaka Univ.)
  - Cho, Hasumi, Ph. D. (IPR, Osaka Univ.)
  - Ikegawa, Yasuyo (IPR, Osaka Univ.)
  - Sato, Junko (IPR, Osaka Univ.)
- **Group for Development of new tools and services**
  - Kinjo, Akira R., Ph. D. (IPR, Osaka Univ.)
  - Iwasaki, Kenji, Ph. D. (IPR, Osaka Univ.)
  - Suzuki, Hirofumi, Ph. D. (IPR, Osaka Univ.)
  - Yamashita, Reiko (IPR, Osaka Univ.)
  - Kudou, Takahiro (IPR, Osaka Univ.)
  - Bekker, Gert-Jan (IPR, Osaka Univ.)
- **Group for BMRB**
  - Fujiwara, Toshimichi, Ph. D. (Group Leader, Prof. Osaka Univ.)
  - Akutsu, Hideo, Ph. D. (Guest Prof., IPR, Osaka Univ.)
  - Kojima, Chojiro, Ph. D. (IPR, Osaka Univ.)
  - Kobayashi, Naohiro, Ph. D. (IPR, Osaka Univ.)
  - Iwata, Takeshi (IPR, Osaka Univ.)
  - Yokochi, Masashi (IPR, Osaka Univ.)
- **Collaboratory Researchers**
  - Wako, Hiroshi, Ph. D. (Prof., Waseda Univ.) (for Pro Mode)
  - Ito, Nobutoshi, Ph. D. (Prof., Tokyo Medical and Dental Univ.)
  - Kinoshita, Kengo, Ph.D. (Prof., Tohoku Univ.) (for *e* F-site)
  - Standley, Daron, Ph. D. (IFReC, Osaka Univ.) (for SeqNavi, StructNavi, SeSAW, and ASH)
  - Katoh, Kazutaka, Ph. D. (IFReC, Osaka Univ.) (for MAFFTash)
- **Secretary**
  - Haruki, Nahoko (IPR, Osaka Univ.)