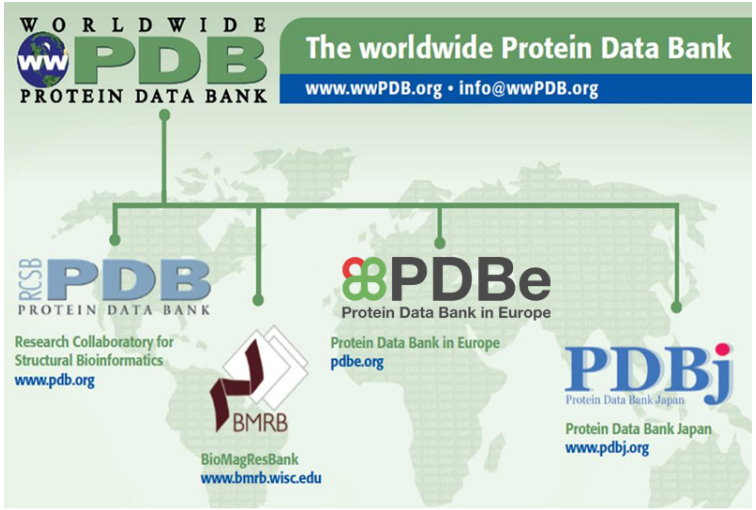
PDBj
Protein Data Bank Japan

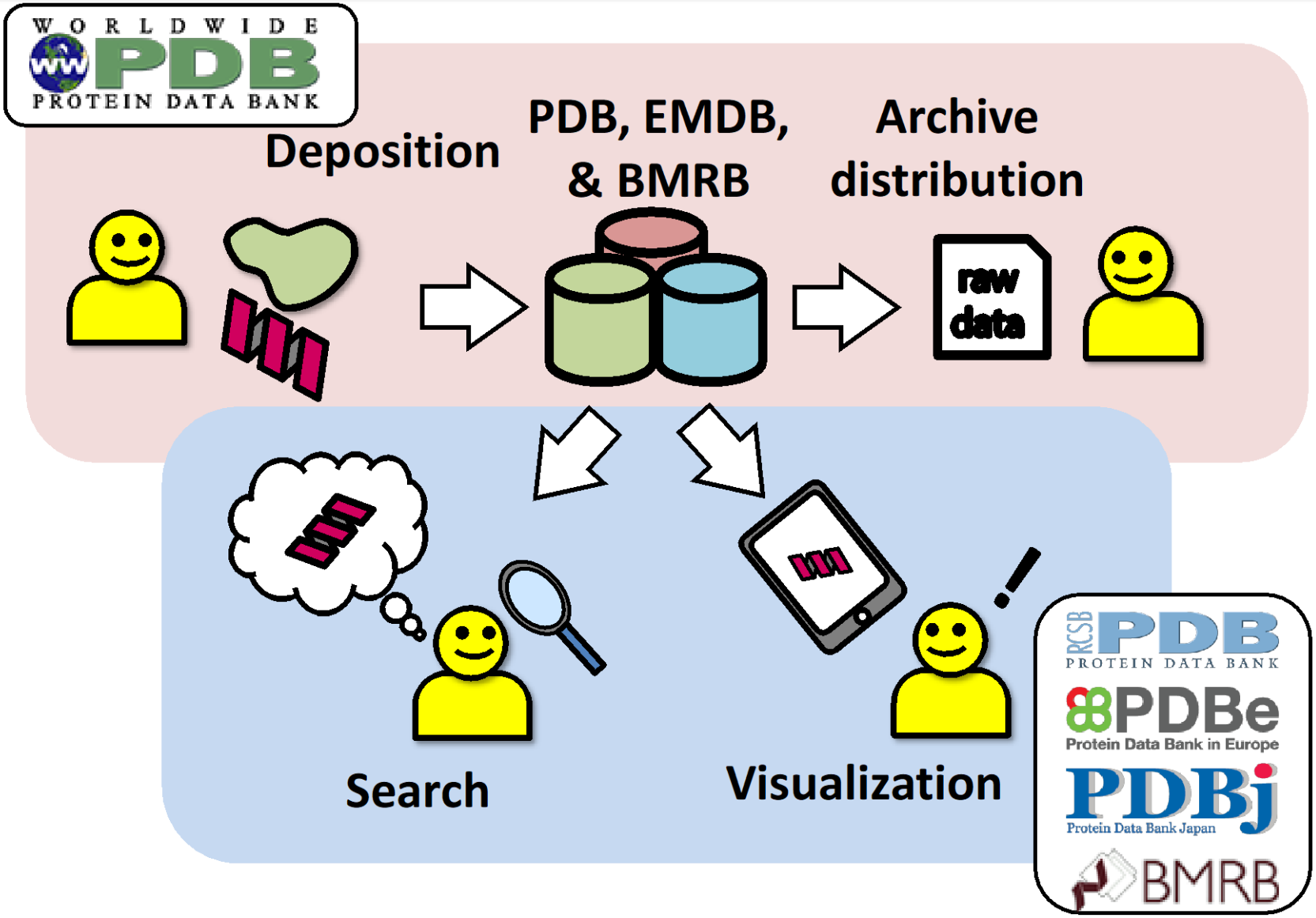
Protein Data Bank Japan

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.



wwPDB collaboration



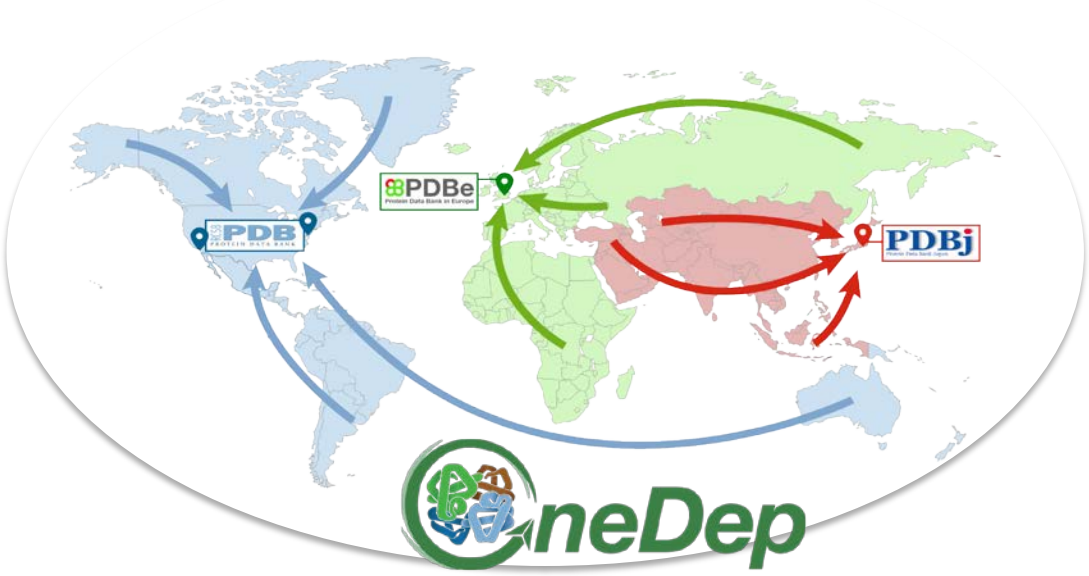
Activities/Services of each member of the wwPDB

- **“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**

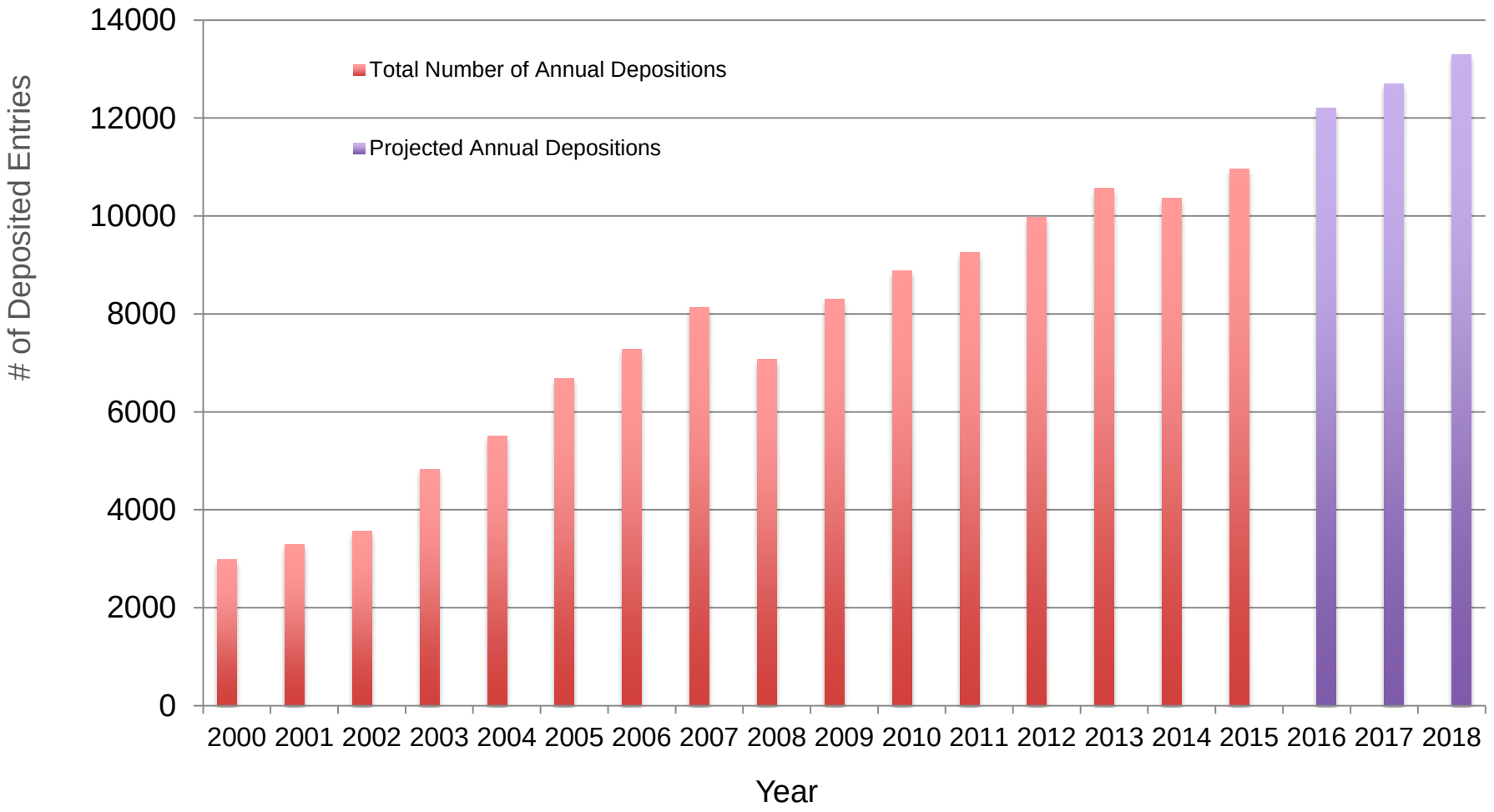
PDBj is the Data Center in Asia

- As of 2016 region-based processing of D&A-deposited entries:
  - RCSB PDB: Americas & Oceania
  - PDBe: Europe & Africa
  - PDBj: Asia & Middle east



Year	Total Depositions	Processed By		
		RCSB PDB	PDBj	PDBe
2000	2983	2297	158	528
2001	3287	2408	383	496
2002	3565	2401	657	507
2003	4830	3135	1026	669
2004	5508	3082	1614	812
2005	6678	3563	2110	1005
2006	7282	4252	1945	1085
2007	8130	4703	2299	1128
2008	7073	4106	1994	973
2009	8300	5069	2173	1058
2010	8878	5464	2041	1373
2011	9250	5938	1816	1496
2012	9972	6408	1888	1676
2013	10566	6652	2128	1786
2014	10364	6038	1781	2545
2015	10958	4845	2100	4013
2016	11614	5326	2238	4050
2017	2577	1579	394	604
TOTAL	131815	77266	28745	25804
		132K	**77K**	**29K**	**26K**

Growing Number of Depositions



Official wwPDB Validation Report is requested for peer review

WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 04:13 AM GMT

PDB ID	:	3WDZ
Title	:	Crystal Structure of Keap1 in Complex with phosphorylated p62
Authors	:	Fukutomi, T.; Takagi, K.; Mizushima, T.; Tanaka, K.; Komatsu, M.; Yamamoto, M.
Deposited on	:	2013-06-26
Resolution	:	2.60 Å(reported)

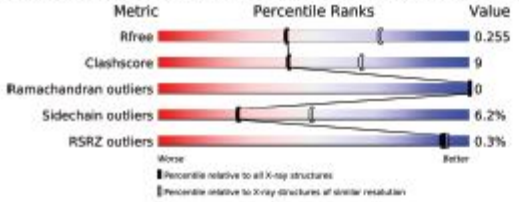
This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

Example of Validation report

1 Overall quality at a glance (i)

The reported resolution of this entry is 2.60 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.

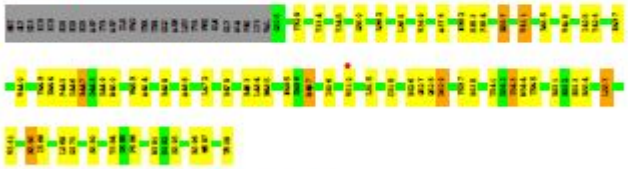


3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Kelch-like ECH-associated protein 1

Chain A:



- Molecule 2: Peptide from Sequestosome-1

Chain B:

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**

File Versioning: Planning Process

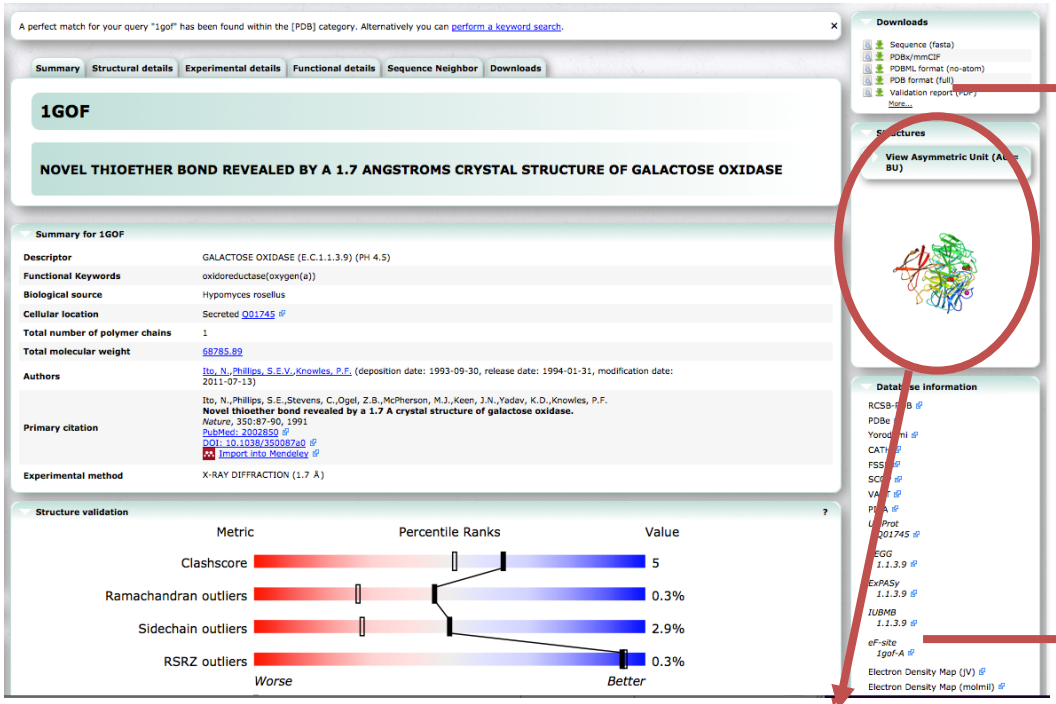
Current Issues:

- Loss of connection between PDB ID and Publication under current wwPDB Obsolete/Supersede Policy

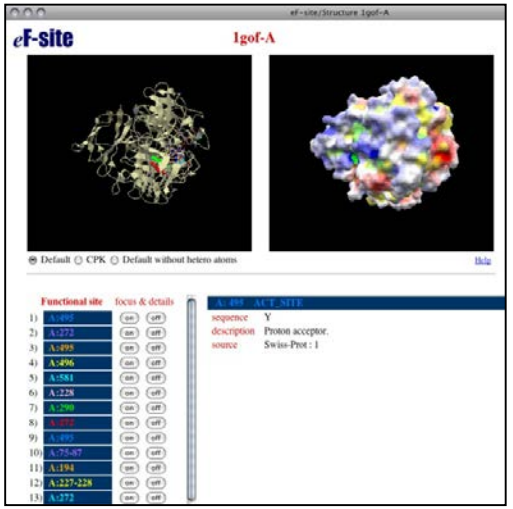
- Enable revisions to entries updated by the Depositor of Record (e.g., Version 1-0 → 1-1; 1-0 → 2-0)
  - wwPDB will NOT assign a new PDB ID going forward (for Depositor of Record revision only)
- Introduce new PDB ID code format
  - With PDB prefix and extension of 4 characters (e.g., from “1ABC” to “**PDB_00001ABC**”)
- Example: PDB_00001ABC_XYZ_V2-2.cif.gz

Data-out from PDBj

http://pdbj.org/



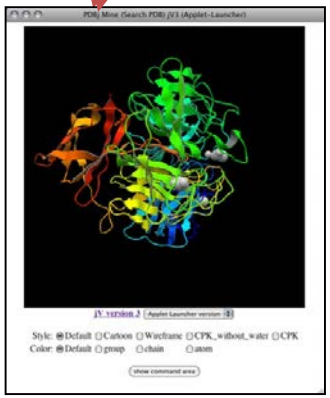
Amino acid sequence (FASTA)



Molecular surface DB: *eF-site*

http://ef-site.hgc.jp/eF-site/

Data viewer at PDBj



Graphic viewer: *jV* and *Molmil*

http://pdbj.org/jV/

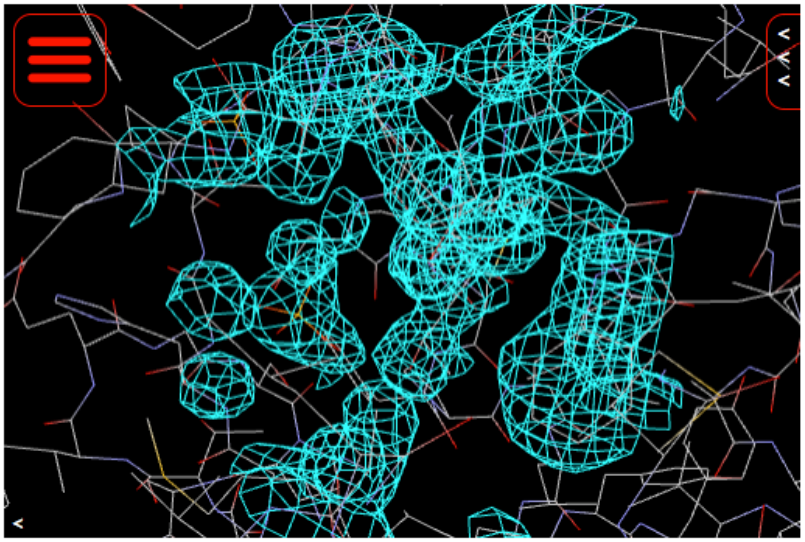
Kinjo et al. NAR 40, D453 (2012)

ED map viewer

PDBj
Protein Data Bank Japan

EDmap (Molmil): 2xvy

Style: Wireframe Color: Atom



Parameters for Electron Density Map

About the PDBj Electron Density Map Viewer

Type of the map:
(•) contour mesh ( ) iso surface

Map position:
(•) atom nearest to the center of the map
( ) Atom ID: [ ] , [ ] , [ ]
you can select "Atom ID" by clicking in the viewer)
( ) coordinates (x: [ ] y: [ ] z: [ ])

mapped area: [10] Å
(this is the length of edge of a cube)

contour level: [1] σ

color: R: [0.0] **G:** [1.0] **B:** [1.0]

isosurface transparency level: [0.5]

Create map Reset

Electron Density Map Download/Delete

file format	filename		
structure factor	r2xvysf.ent.gz		Download
refinement file	2xvy_ref.tar.gz		Download
ccp4 file	2xvy.ccp4.gz		Download
edmap file	2016518184431_2xvy.c.xml.gz	Delete	Download

PDBj Publication

Nucleic Acids Research Advance Access published October 26, 2016

Nucleic Acids Research, 2016 1
doi: 10.1093/nar/gkw962

Protein Data Bank Japan (PDBj): updated user interfaces, resource description framework, analysis tools for large structures

Akira R. Kinjo*, Gert-Jan Bekker, Hirofumi Suzuki, Yuko Tsuchiya, Takeshi Kawabata, Yasuyo Ikegawa and Haruki Nakamura

Institute for Protein Research, Osaka University, 3-2 Yamadaoka, Suita, Osaka 565-0871, Japan

Received September 15, 2016; Revised October 06, 2016; Editorial Decision October 07, 2016; Accepted October 11, 2016

ABSTRACT

The Protein Data Bank Japan (PDBj, http://pdbj.org), a member of the worldwide Protein Data Bank (wwPDB), accepts and processes the deposited data of experimentally determined macromolecular structures. While maintaining the archive in collaboration with other wwPDB partners, PDBj also provides a wide range of services and tools for analyzing structures and functions of proteins. We herein outline the updated web user interfaces together with RESTful web services and the backend relational database that support the former. To enhance the interoperability of the PDB data, we have previously developed PDB/RDF, PDB data in the Resource Description Framework (RDF) format, which is now a wwPDB standard called wwPDB/RDF. We have enhanced the connectivity of the wwPDB/RDF data by incorporating various external data resources. Services for searching, comparing and analyzing the ever-increasing large structures determined by hybrid methods are also described.

major changes regarding user interfaces and analysis tools as well as additional data provided. The previously described Resource Description Framework (RDF) format, PDB/RDF, is now one of the wwPDB standard formats called wwPDB/RDF and is enhanced with supplementary information in order to connect PDB data with other biological data resources.

USER INTERFACES

User interfaces include interactive (and graphical) web interfaces for humans and RESTful web services for computer programs. We also expose our backend database in the forms of web services or dump files for enabling very complex queries. These are described in turn.

Web interface

The web interface of PDBj was updated to provide a uniform integrated interface for the available services as well as to provide a scalable interface for devices ranging from smartphones to workstations. This update incorporates several innovative/renovative features as described below.

We have implemented various functionalities to ease

PROTEIN SCIENCE

Explore this journal >

Tools for Protein Science

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

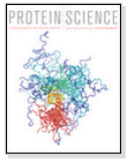
Akira R. Kinjo, Gert-Jan Bekker, Hiroshi Wako, Shigeru Endo, Yuko Tsuchiya, Hiromu Sato, Hafumi Nishi, Kengo Kinoshita, Hirofumi Suzuki, Takeshi Kawabata, Masashi Yokochi, Takeshi Iwata, Naohiro Kobayashi, Toshimichi Fujiwara, Genji Kurisu, Haruki Nakamura

Accepted manuscript online: 17 August 2017 Full publication history

DOI: 10.1002/pro.3273 View/save citation

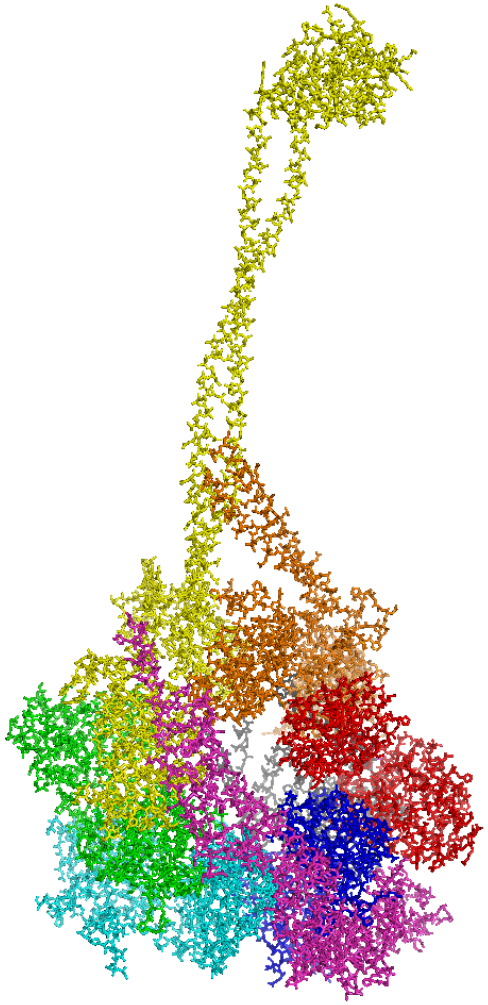
Cited by (CrossRef): 0 articles Check for updates Citation tools

Accepted Articles



Browse Accepted Articles
Accepted, unedited articles published online and citable. The final edited and typeset version of record will appear in future.

X-ray crystal structure



Experimental Data

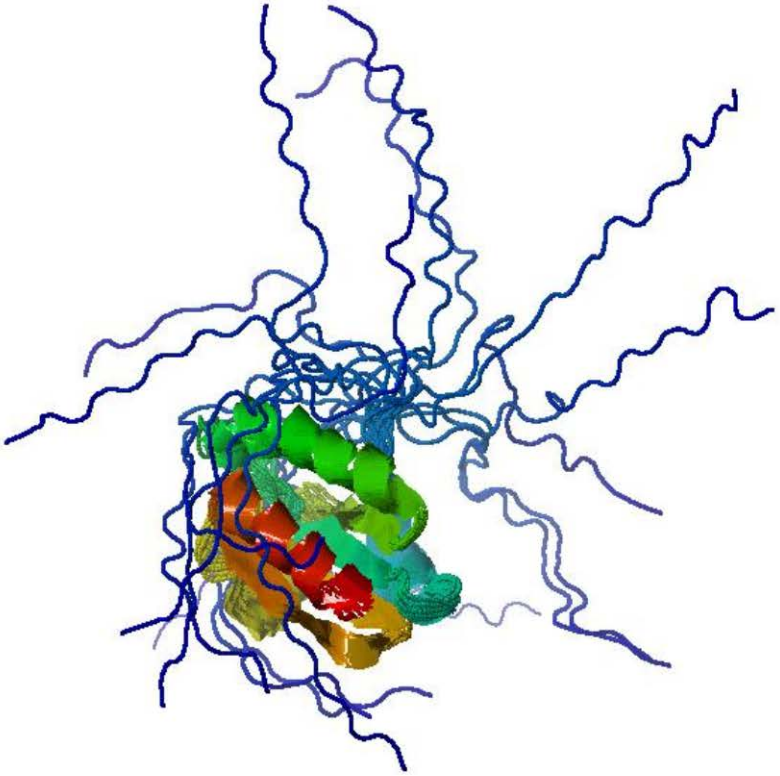
One set of Structure factors

Deposition

One coordinates file

PDB-3vkh
Cytoplasmic Dynein

Structure Ensembles by NMR



Experiment

1 sample condition

100 conformers

Deposition

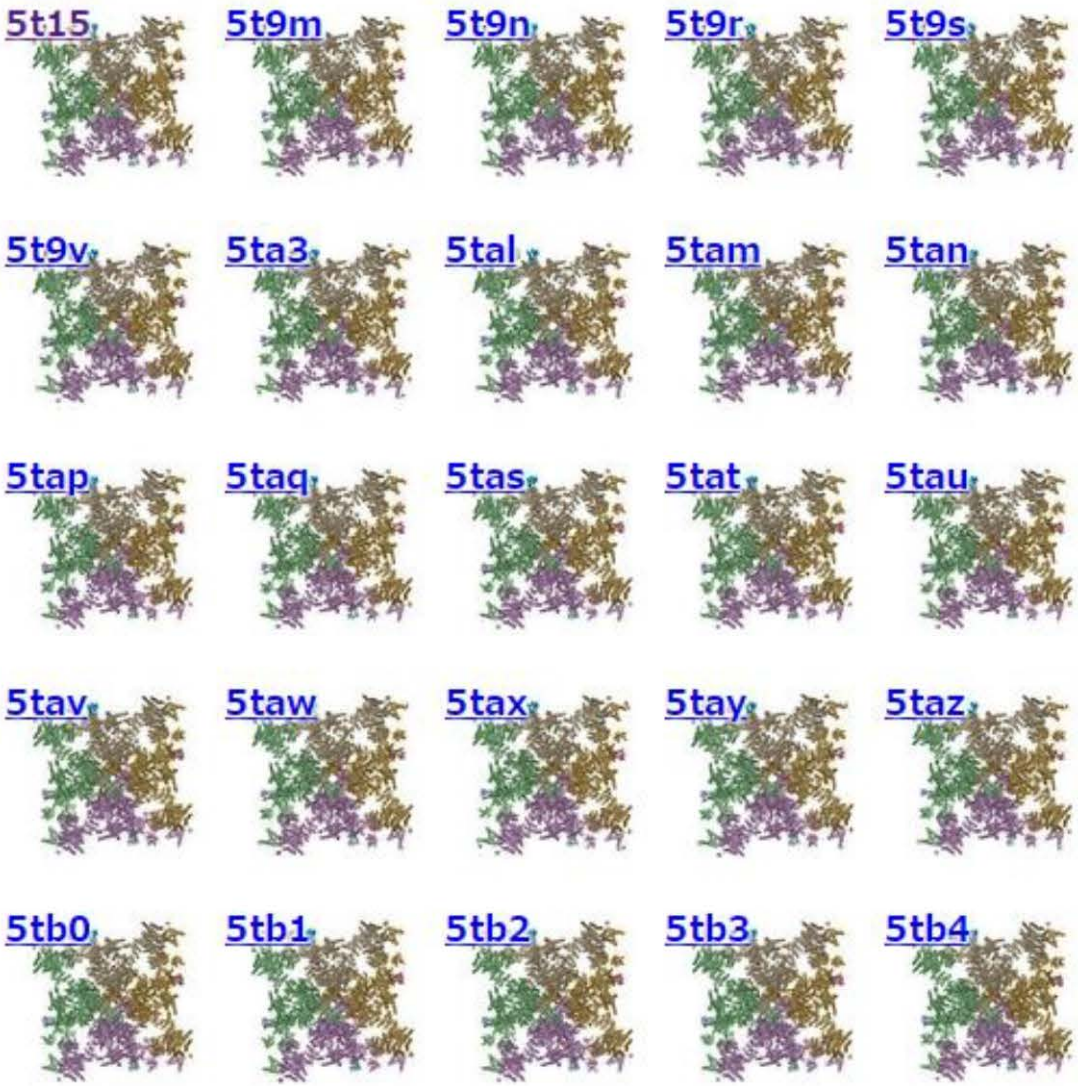
20 conformers

1 entry

PDB-6ali

putative thioredoxin

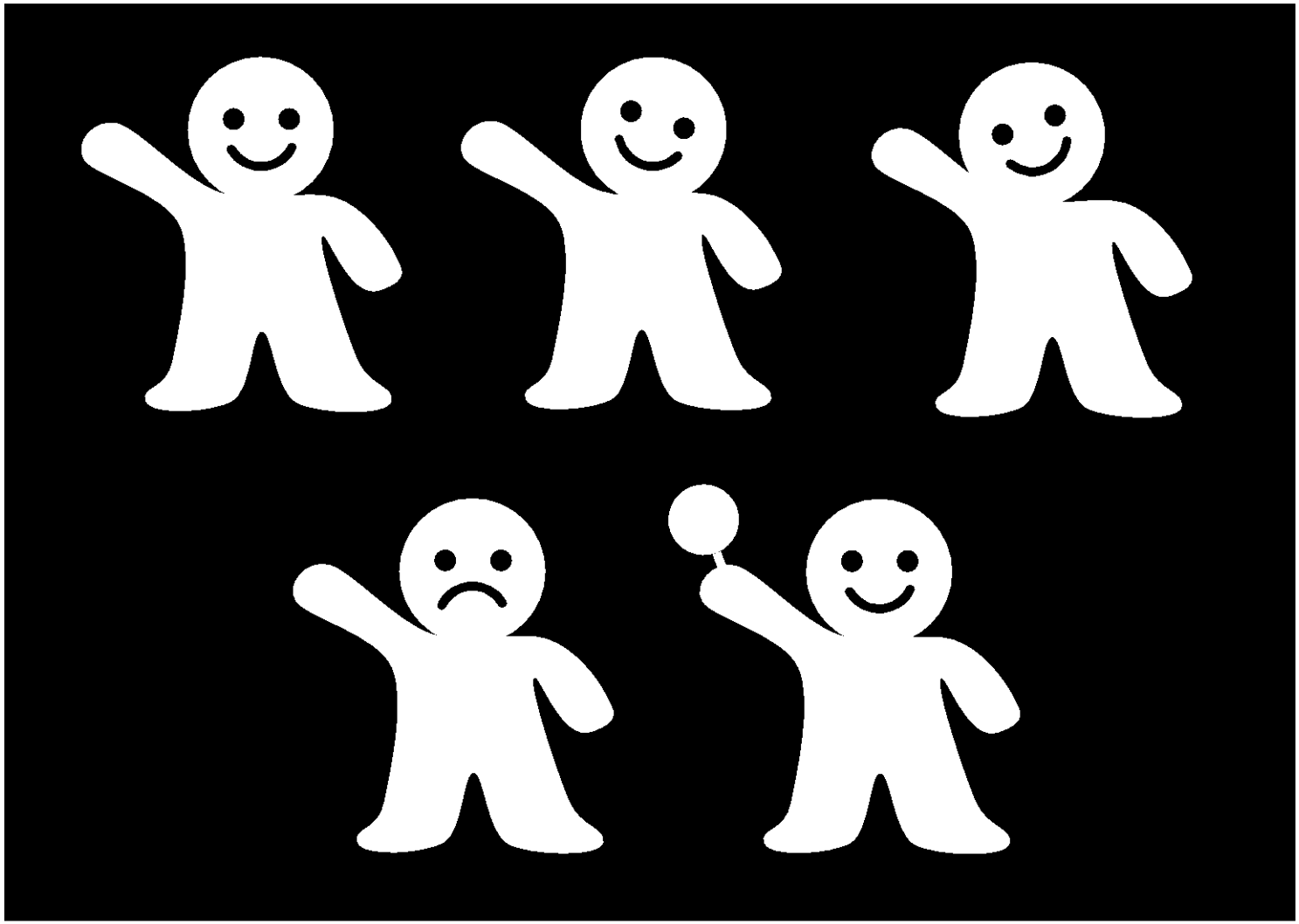
Structure Ensembles by 3DEM



5 samples
x (1 all + 4 classes)
= 25 PDB entries

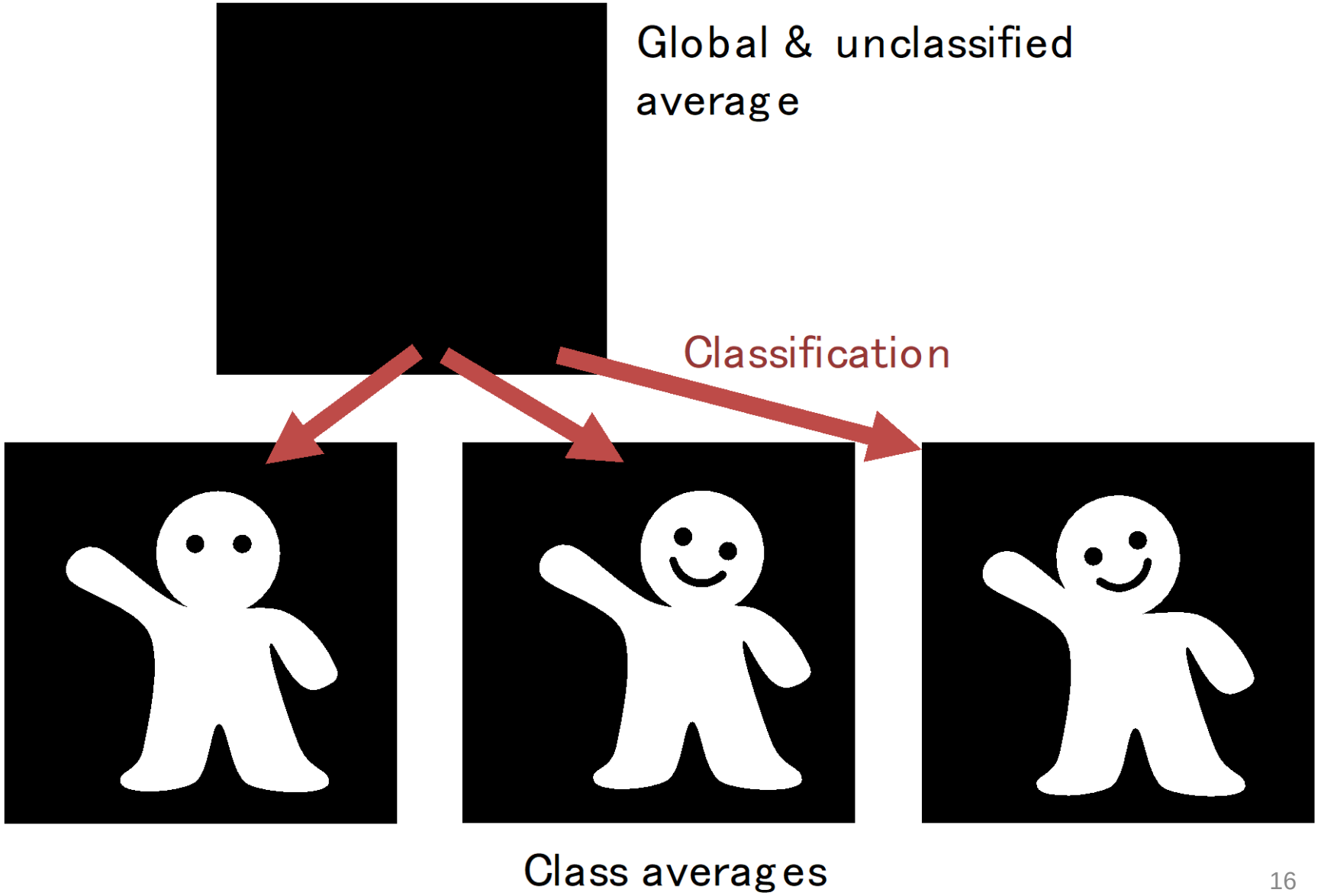
Ryanodine receptor
(calcium channel)
des Georges *et al.*,
Cell, 2016

Flexibility in Biomolecule

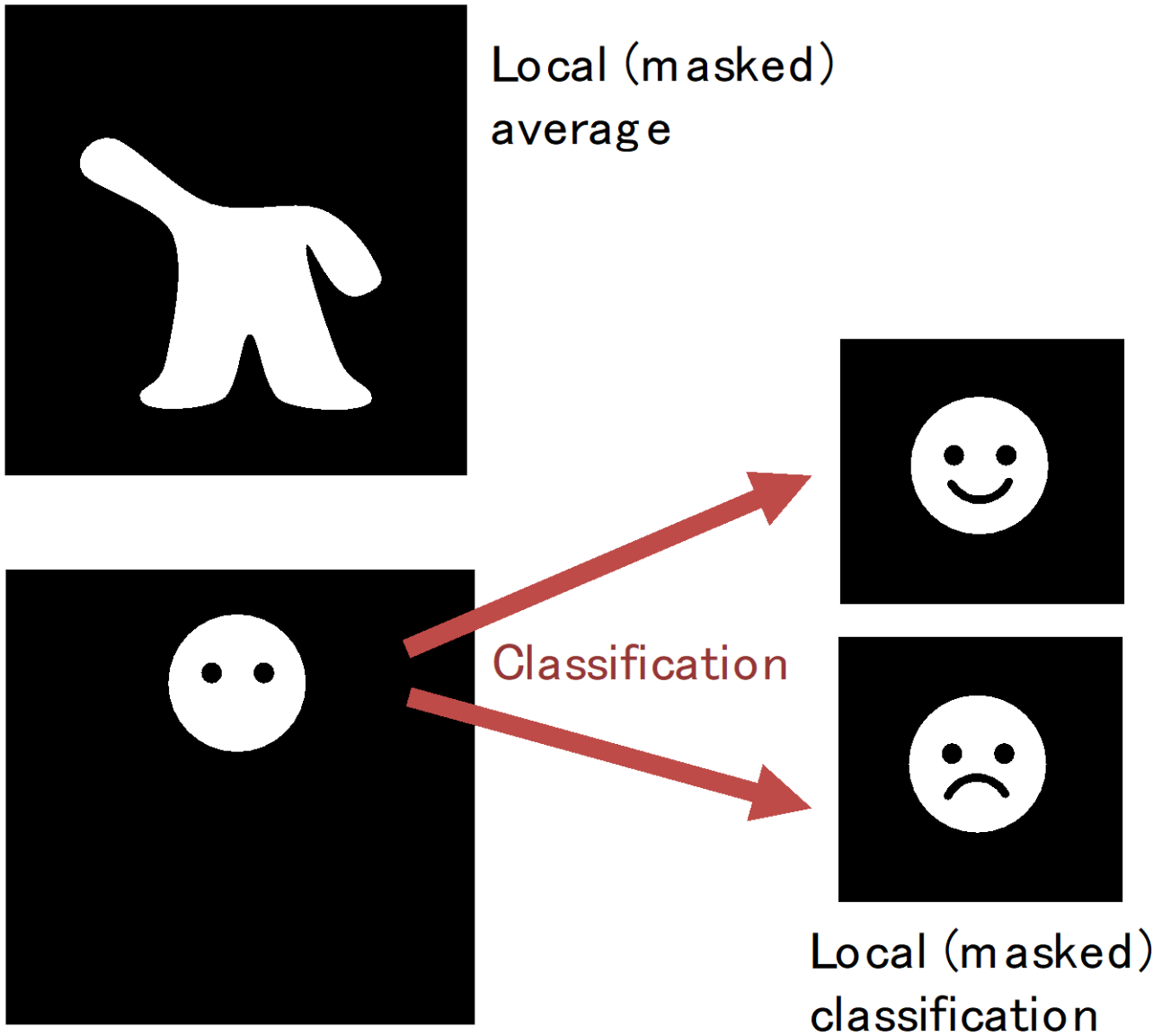


flexibility, heterogeneity & inoccupancy

Classification



Local averaging & classification



File Formats

- mmCIF
  - The canonical format of the wwPDB.
  - Ver. 5 released this year!
- PDBML
  - “direct translation” of mmCIF into XML.
- (Legacy) PDB format
  - *NOT RECOMMENDED!*
- PDB/RDF
  - Translation of PDBML into RDF/XML (the standard format for the Semantic Web).

wwPDB/RDF for Semantic Web

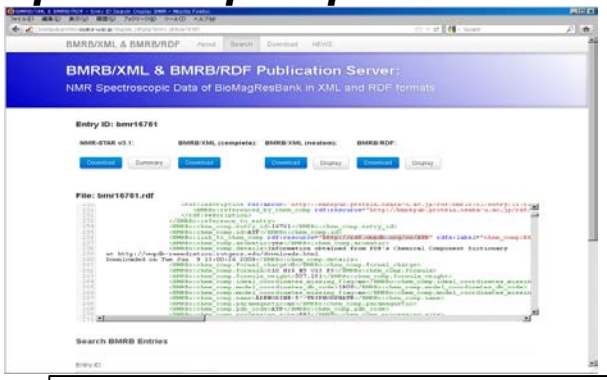
Kinjo et al. (2012) Nucl. Acids Res. 40, D453-D460.
Yokochi et al. (2016) J. Biomed. Semantics, 7:16.

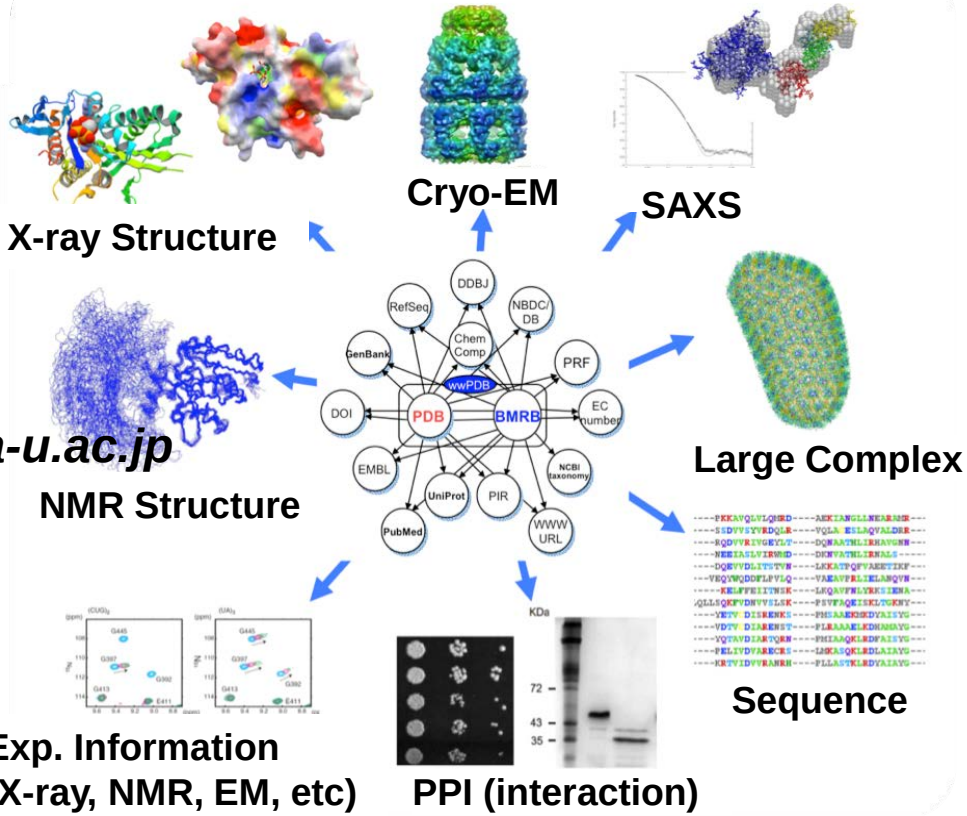
wwPDB/RDF

http://rdf.wwpdb.org/

BMRB/RDF

http://bmrbpub.protein.osaka-u.ac.jp

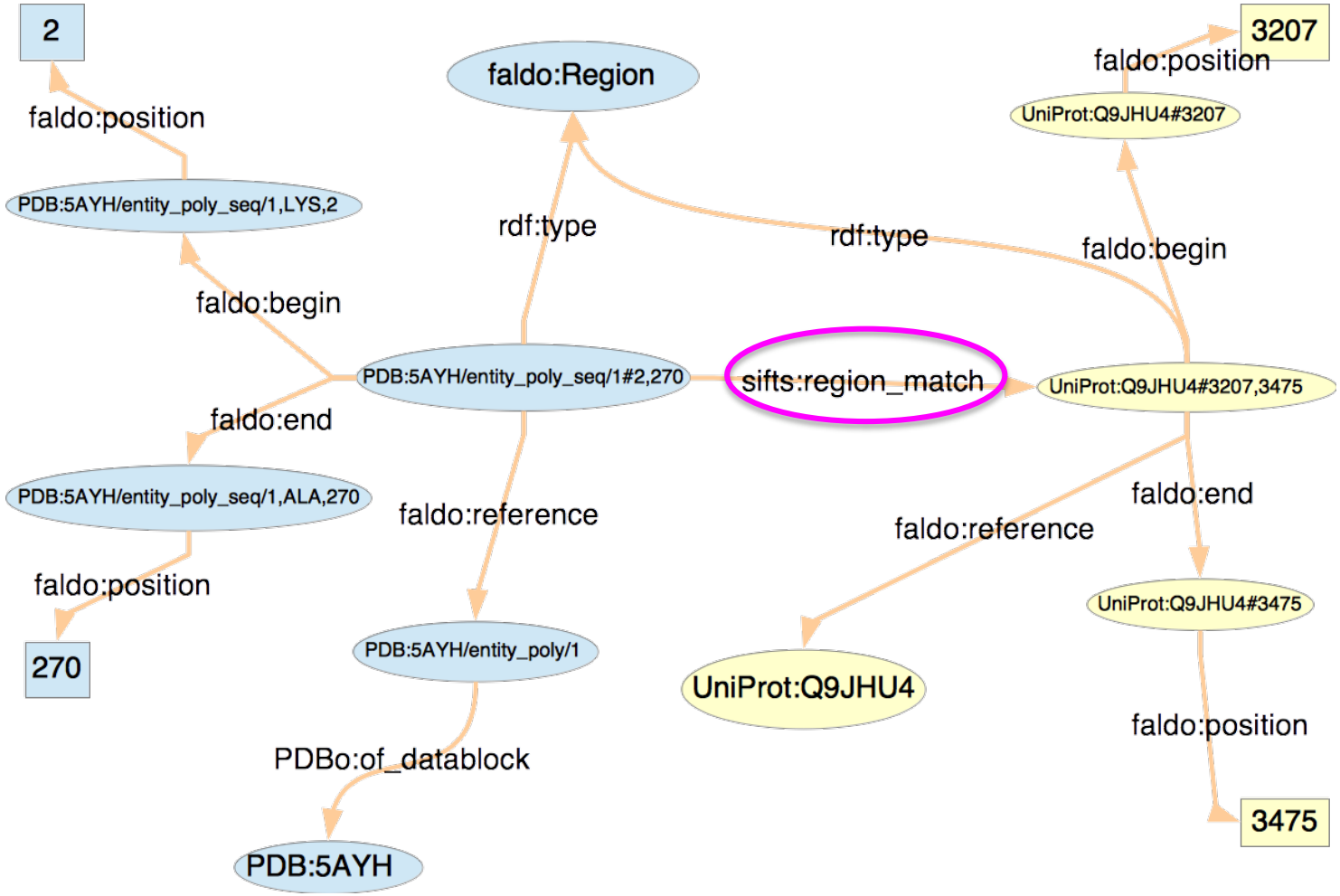





```
<rdf:Description rdf:about="http://rdf.wwpdb.org/pdb/1BY4">
  <rdf:type rdf:resource="http://purl.uniprot.org/core/Structure_Resource"/>
  <database rdf:resource="http://purl.uniprot.org/database/PDB"/>
  <method rdf:resource="http://purl.uniprot.org/core/X-Ray_Crystallography"/>
  <resolution rdf:datatype="http://www.w3.org/2001/XMLSchema#float">2.10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

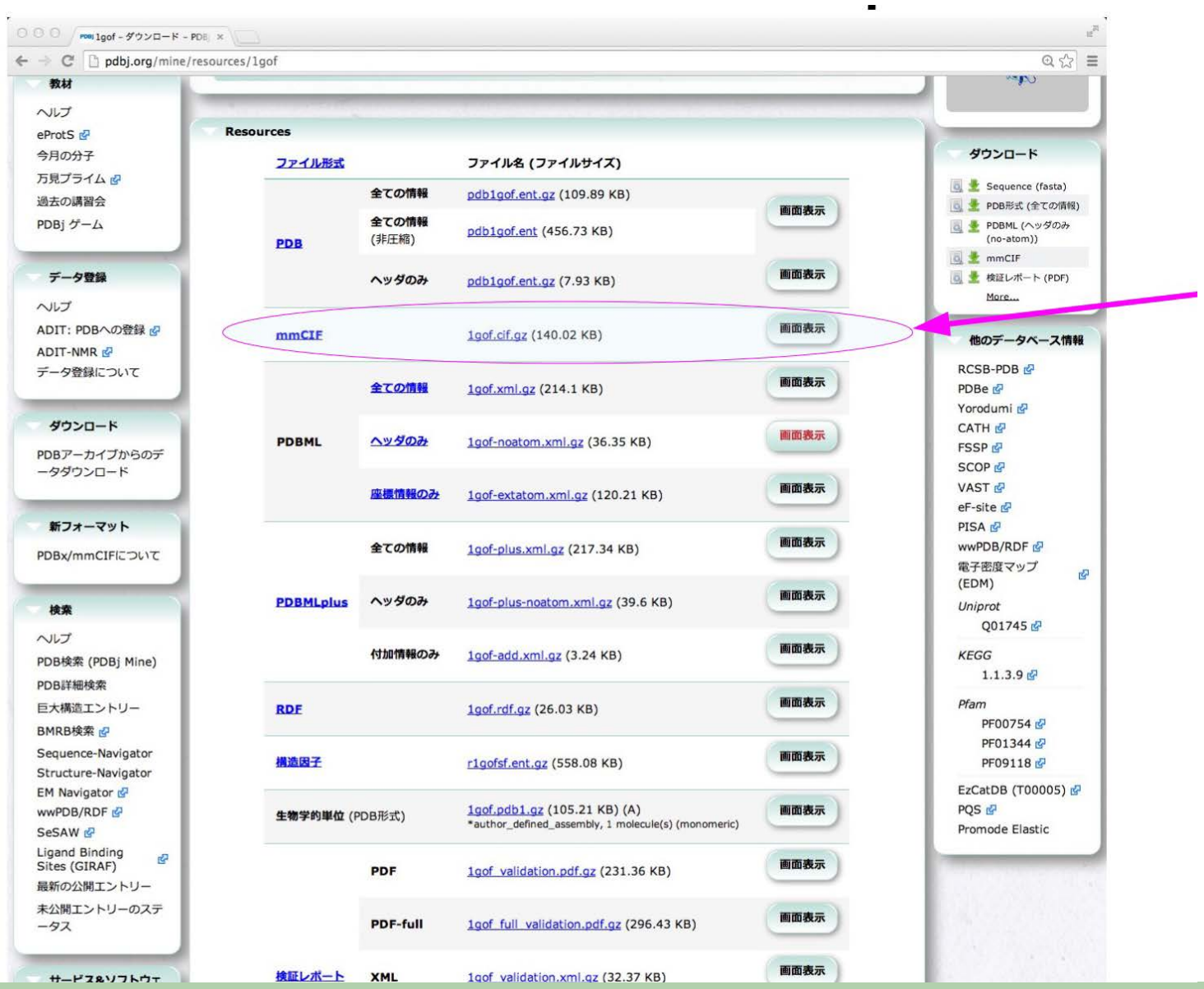
Usage of SIFTS information

(Structure integration with function, taxonomy and sequence)



SIFTS/RDF has been developed with EBI group : FALDO (Feature Annotation Location Description Ontology: Bolleman et al, 2016) is used at BioHackathon

mmCIF: an example

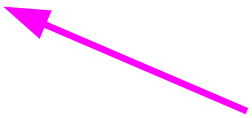


mmCIF basics

- Data are divided into “categories”.
  - *_category.item*
  - e.g., _entry.id “entry” is the category name, “id” is an item of the “entry” category.
  - “_entry.id 1GOF” The value of “id” item of “entry” category is “1GOF”.
- Two ways of presenting data.
  - key-value: if only one value exists for an item.
  - loop: if more than one item exists for an item.

Example of key-value pairs

```
_cell.entry_id                    1GOF
_cell.length_a                    98.000
_cell.length_b                    89.400
_cell.length_c                    86.700
_cell.angle_alpha                 90.00
_cell.angle_beta                  117.80
_cell.angle_gamma                 90.00
_cell.Z_PDB                       4
_cell.pdbx_unique_axis            ?
#
```



The last “#” is a convention to indicate the end of a category.

Example of “loop” structure

```
loop_
_entity.id
_entity.type
_entity.src_method
_entity.pdbx_description
_entity.formula_weight
_entity.pdbx_number_of_molecules
_entity.details
_entity.pdbx_mutation
_entity.pdbx_fragment
_entity.pdbx_ec
1 polymer     man 'GALACTOSE OXIDASE' 68579.250 1   ? ? ? 1.1.3.9
2 non-polymer syn 'COPPER (II) ION'   63.546    1   ? ? ? ?
3 non-polymer syn 'SODIUM ION'        22.990    1   ? ? ? ?
4 non-polymer syn 'ACETIC ACID'       60.052    2   ? ? ? ?
5 water       nat water               18.015    316 ? ? ? ?
#
```

Start of a loop

A list of items.
“One item per line” is just a convention.

- Each item is whitespace-delimited.
- In the same order as the item list (above).
- Use quotes (') for data with whitespace.

The last “#” is a convention to indicate the end of a loop.

Atomic coordinates

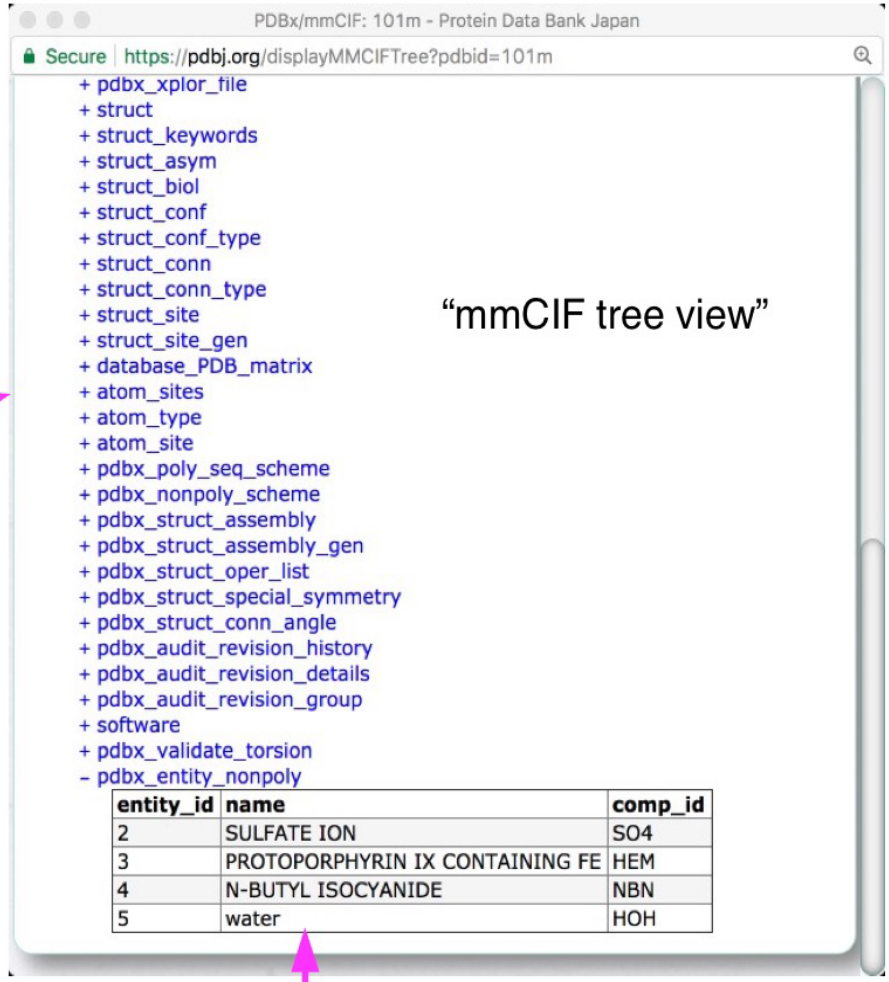
```
loop_
_atom_site.group_PDB
_atom_site.id
_atom_site.type_symbol
_atom_site.label_atom_id
_atom_site.label_alt_id
_atom_site.label_comp_id
_atom_site.label_asym_id
_atom_site.label_entity_id
_atom_site.label_seq_id
_atom_site.pdbx_PDB_ins_code
_atom_site.Cartn_x
_atom_site.Cartn_y
_atom_site.Cartn_z
_atom_site.occupancy
_atom_site.B_iso_or_equiv
_atom_site.Cartn_x_esd
_atom_site.Cartn_y_esd
_atom_site.Cartn_z_esd
_atom_site.occupancy_esd
_atom_site.B_iso_or_equiv_esd
_atom_site.pdbx_formal_charge
_atom_site.auth_seq_id
_atom_site.auth_comp_id
_atom_site.auth_asym_id
_atom_site.auth_atom_id
_atom_site.pdbx_PDB_model_num
ATOM   1    N  N   . ALA A 1 1   ? 38.840  0.236   1.012   1.00 34.65 ? ? ? ? ? ? 1    ALA A N   1
ATOM   2    C  CA  . ALA A 1 1   ? 38.356  -0.999  0.357   1.00 42.26 ? ? ? ? ? ? 1    ALA A CA  1
ATOM   3    C  C   . ALA A 1 1   ? 37.098  -1.547  1.056   1.00 41.25 ? ? ? ? ? ? 1    ALA A C   1
ATOM   4    O  O   . ALA A 1 1   ? 36.619  -0.946  2.028   1.00 29.44 ? ? ? ? ? ? 1    ALA A O   1
ATOM   5    C  CB  . ALA A 1 1   ? 39.398  -2.114  0.379   1.00 40.70 ? ? ? ? ? ? 1    ALA A CB  1
ATOM   6    N  N   . SER A 1 2   ? 36.610  -2.666  0.495   1.00 32.67 ? ? ? ? ? ? 2    SER A N   1
ATOM   7    C  CA  . SER A 1 2   ? 35.411  -3.244  1.202   1.00 34.90 ? ? ? ? ? ? 2    SER A CA  1
ATOM   8    C  C   . SER A 1 2   ? 35.683  -4.740  1.081   1.00 38.30 ? ? ? ? ? ? 2    SER A C   1
ATOM   9    O  O   . SER A 1 2   ? 36.827  -5.147  0.747   1.00 28.59 ? ? ? ? ? ? 2    SER A O   1
ATOM   10   C  CB  . SER A 1 2   ? 34.063  -2.660  0.823   1.00 24.49 ? ? ? ? ? ? 2    SER A CB  1
ATOM   11   O  OG  . SER A 1 2   ? 33.031  -3.308  1.686   1.00 20.37 ? ? ? ? ? ? 2    SER A OG  1
```

Main category groups

- _entity (Info about molecules)
  - entity, entity_poly, pdbx_entity_nonpoly, ...
- _atom (Info about atoms)
  - atom_site
- _struct (structural info)
  - struct, struct_conf, struct_sheet, struct_conn, pdbx_struct_assembly, ...
- _chem_comp (chemical components)
  - chem_comp
- _citation (literature info)
  - citation, citation_author, ...

Ex. PDB entries containing “HEM”

```
SELECT pdbid
FROM pdbx_entity_nonpoly
WHERE comp_id = 'HEM'
```

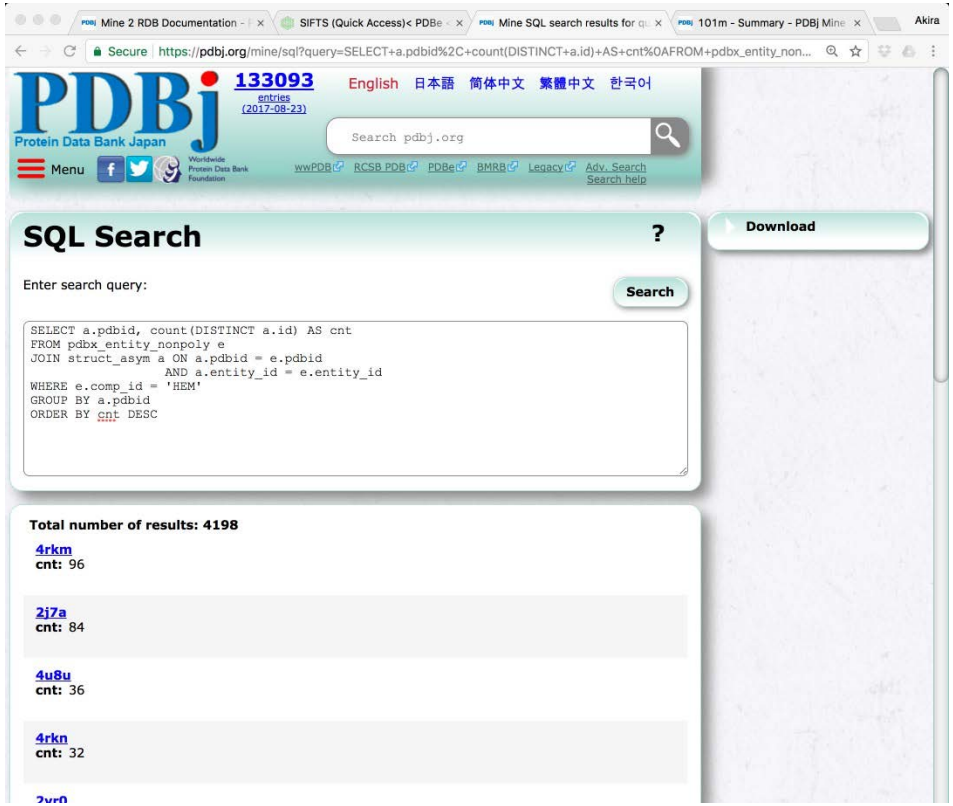


“mmCIF tree view”

“pdbx_entity_nonpoly” category

Ex. PDB entries containing “HEM” by the number of HEM’s in asymetric unit

```
SELECT a.pdbid, count(DISTINCT a.id) AS cnt
FROM pdbx_entity_nonpoly e
JOIN struct_asym a ON a.pdbid = e.pdbid
                    AND a.entity_id = e.entity_id
WHERE e.comp_id = 'HEM'
GROUP BY a.pdbid
ORDER BY cnt DESC
```



Retrieve PDB chain sequence matching to the Pfam accession “PF00046” (Homeobox) and having resolution better than 2.0 Angstrom and sequence length greater than or equal to 58 (residues)

```
SELECT s.*, r.ls_d_res_high as reso,
     LENGTH(p.pdbx_seq_one_letter_code_can) as len,
     ('>' || s.pdbid || s.chain) as header,
     p.pdbx_seq_one_letter_code_can as aaseq
FROM sifts.pdb_chain_pfam s
JOIN refine r on r.pdbid = s.pdbid
JOIN entity_poly p on p.pdbid = s.pdbid
     AND s.chain = ANY(regexp_split_to_array(p.pdbx_strand_id,','))
WHERE pfam_id = 'PF00046'
AND r.ls_d_res_high < 2.0
AND LENGTH(p.pdbx_seq_one_letter_code_can) >= 58
ORDER BY reso, len,s.chain
```

* “entity_poly.pdbx_seq_one_letter_code_can” contains AA seq in one-letter codes.

If you want to do complicated queries,
we may be able to help!
（質問はお気軽にPDBjまで）
Feel free to ask any questions at:
https://pdbj.org/contact?tab=PDBjmaster