PDBj
Protein Data Bank Japan

PDBjとwwPDBの活動方針について

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栗栖源嗣

PDBj
Protein Data Bank Japan

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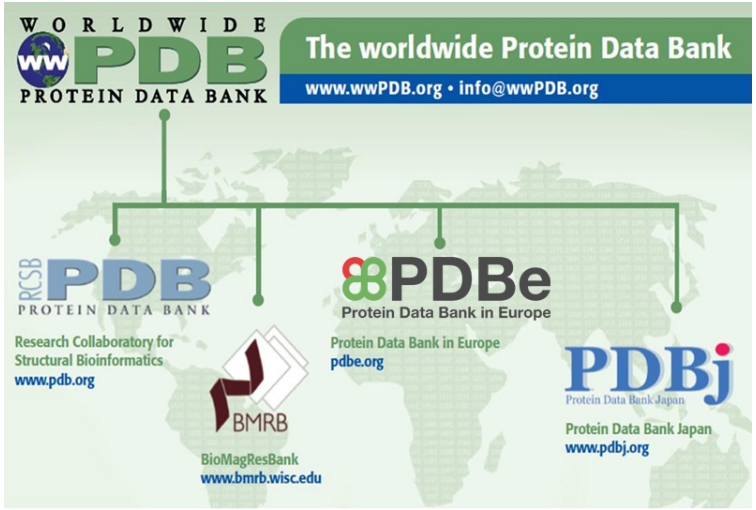
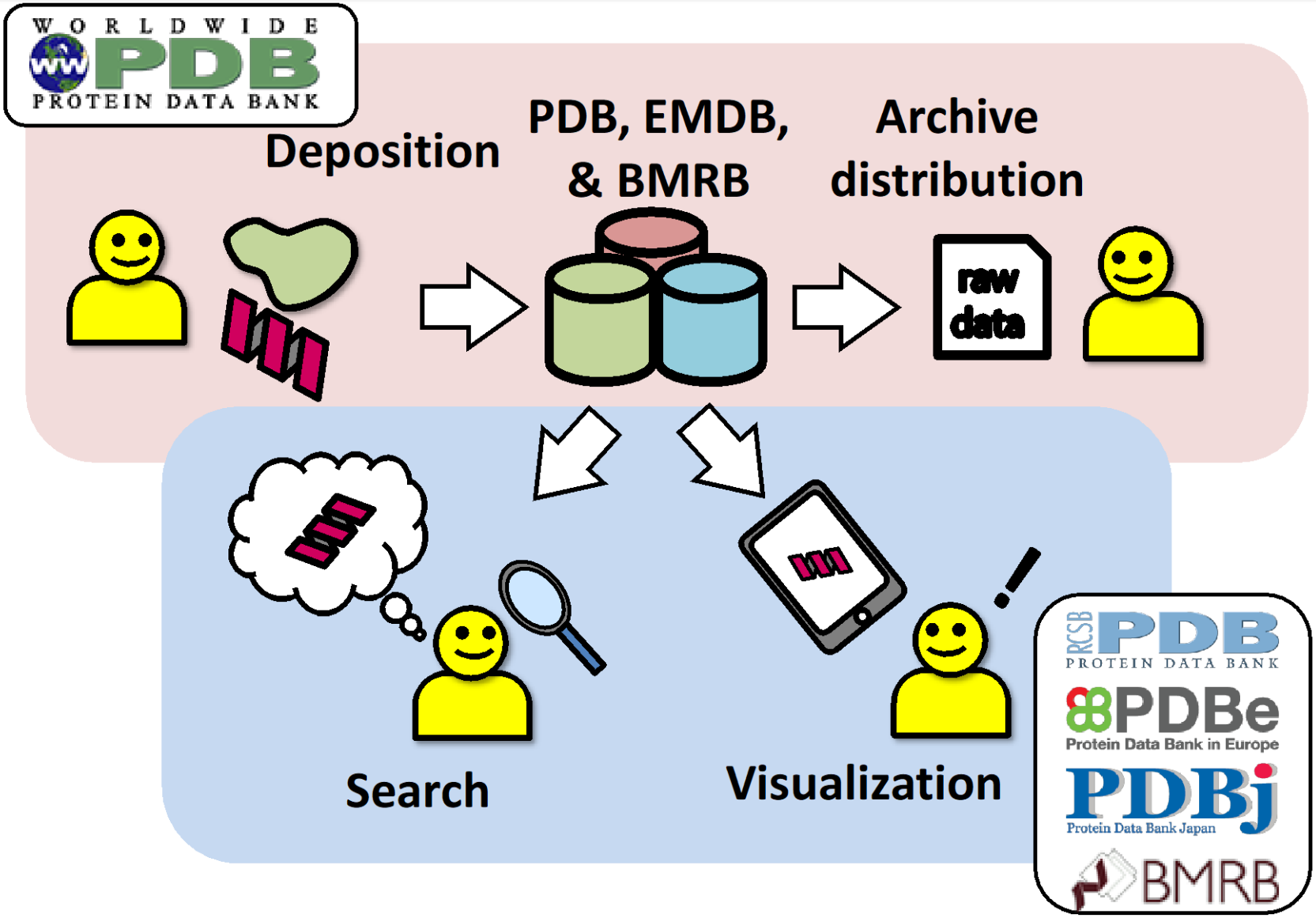
http://pdbj.org/

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



Atomic coordinates

```
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_atom_site.Cartn_z
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_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
```

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:

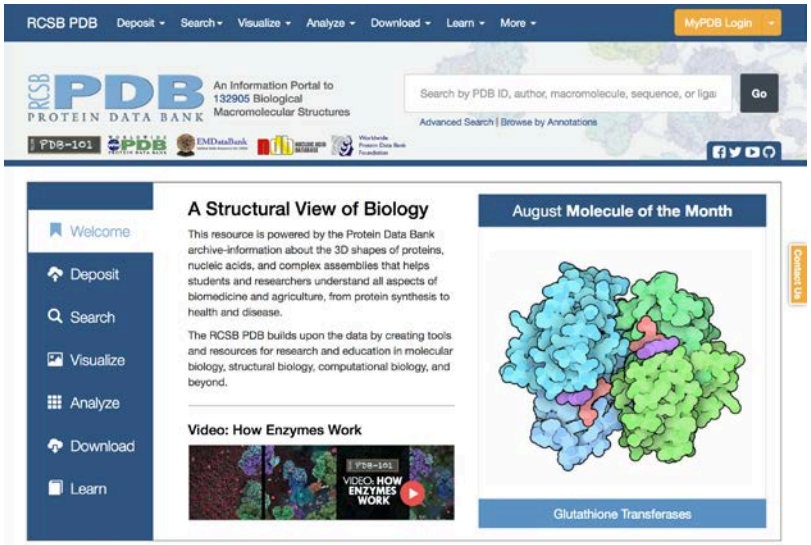
- Loss of connection between PDB ID and Publication under current wwPDB Obsolete/Supersede Policy

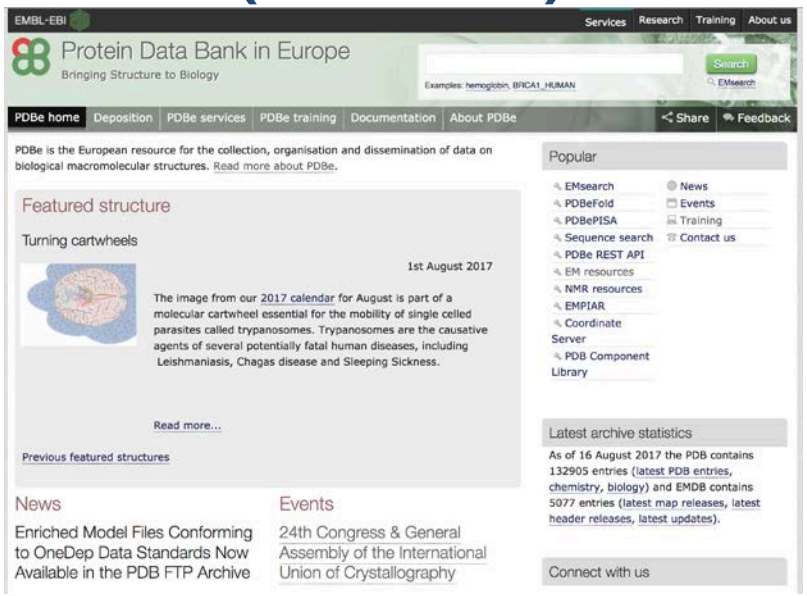
- Enable revisions to entries updated by the Depositor of Record (e.g., Version 1-0 → 1-1; 1-0 → 2-0)
  - wwPDB will NOT assign a new PDB ID going forward (for Depositor of Record revision only)
- Introduce new PDB ID code format
  - With PDB prefix and extension of 4 characters (e.g., from “1ABC” to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

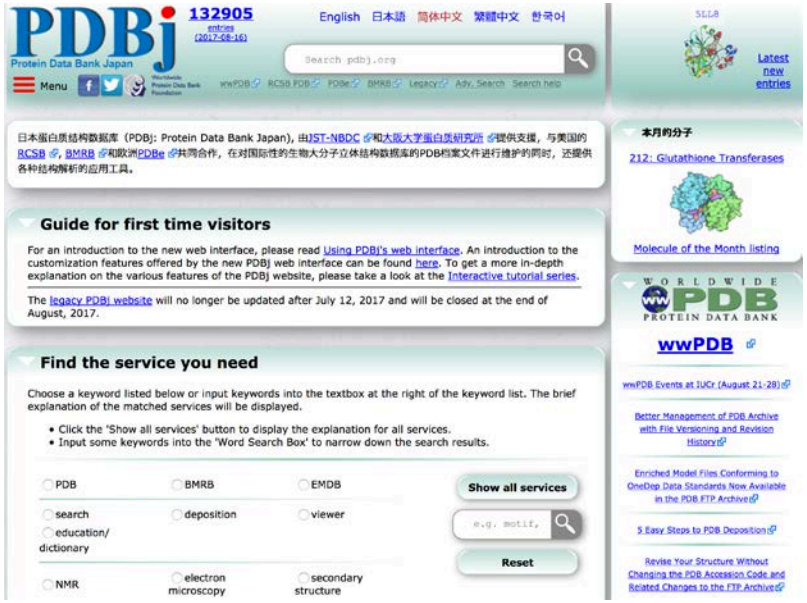
DOI Landing Page Layout (Planned)

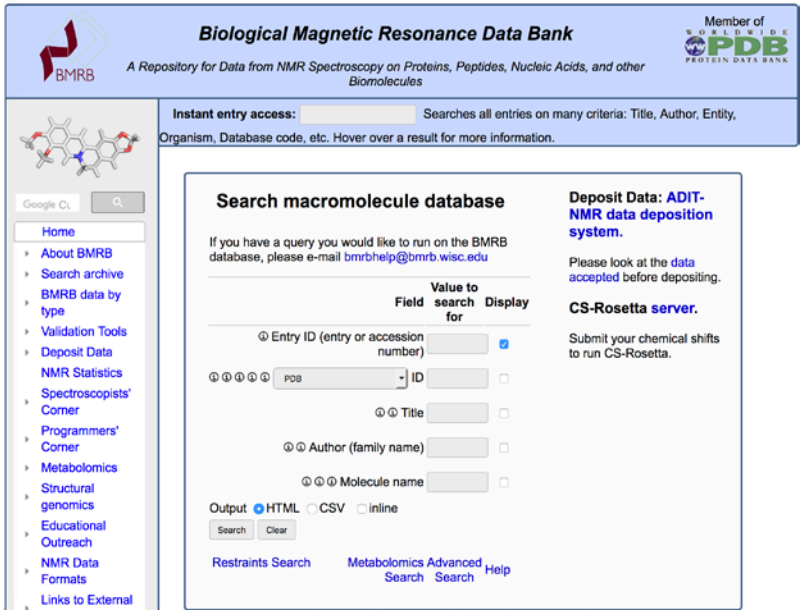
Worldwide Protein Data Bank (wwPDB)

PDBj
Protein Data Bank Japan



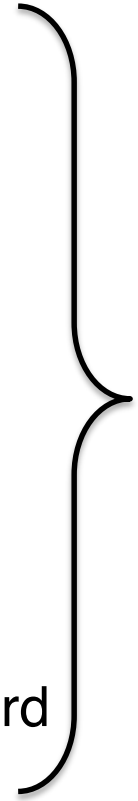






File Formats provided by PDBj

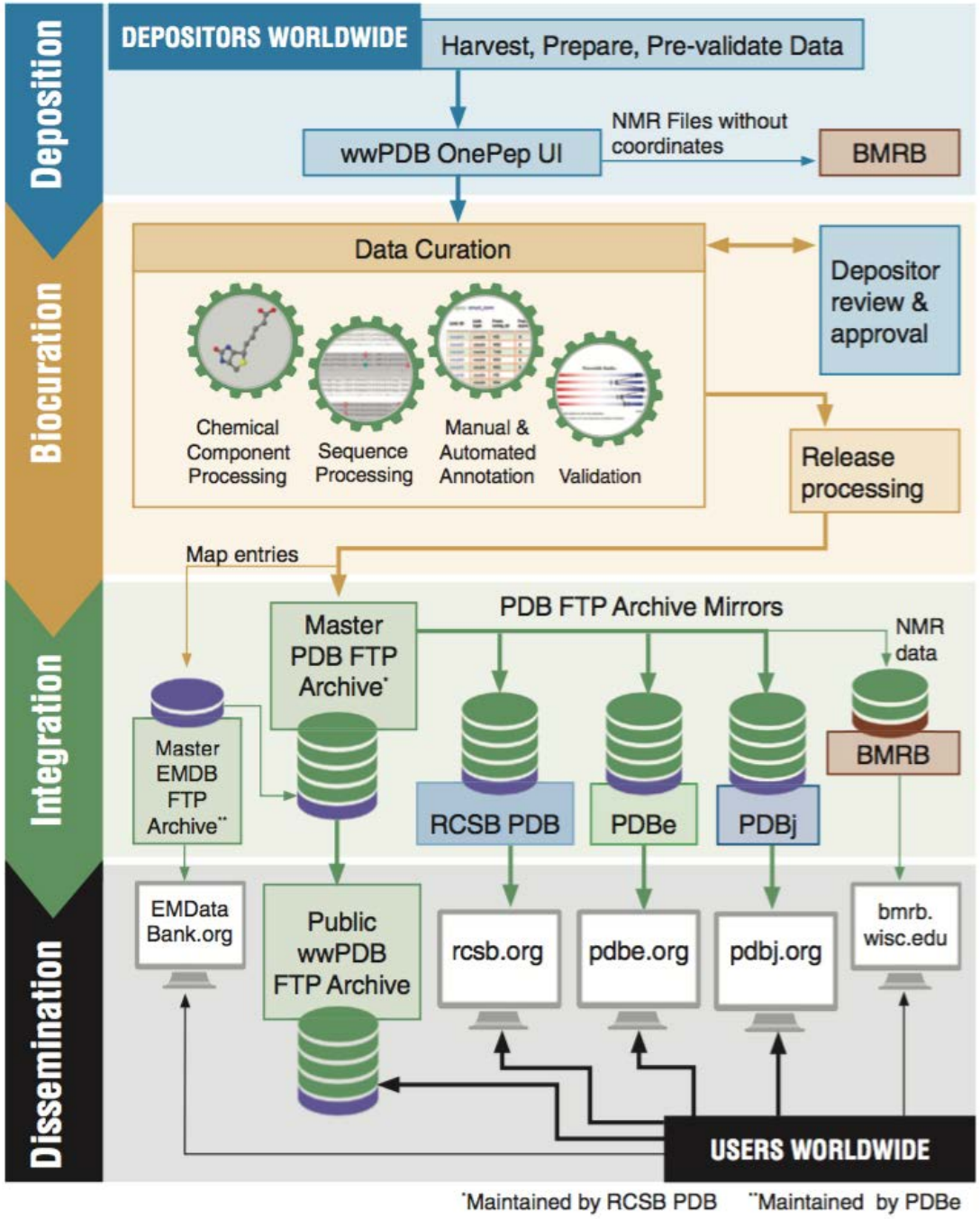
- mmCIF
  - The canonical format of the wwPDB.
  - Ver. 5 released this year!
- PDBML
  - “direct translation” of mmCIF into XML.
- (Legacy) PDB format
  - *NOT RECOMMENDED!*
- PDB/RDF
  - Translation of PDBML into RDF/XML (the standard format for the Semantic Web).



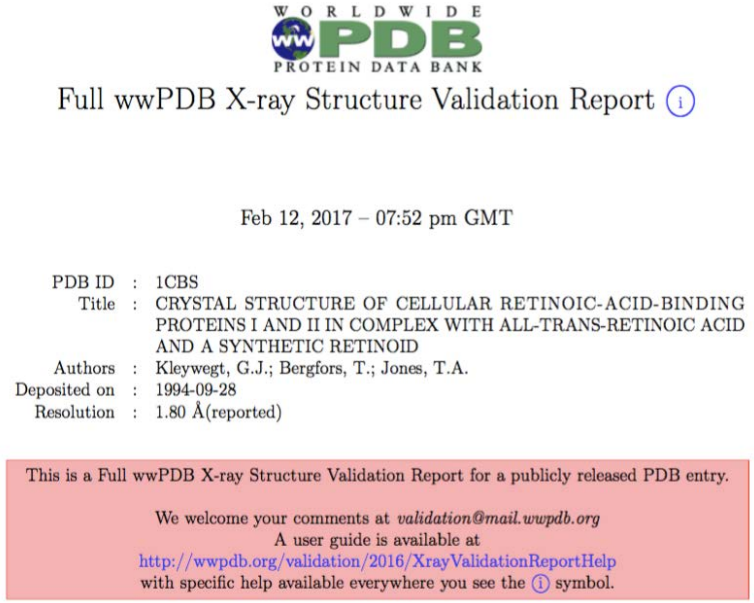
- Experimental Data (X-ray, NMR, 3DEM=EMDB)
- Validation Report (PDF, XML, RDF)

Where is the detailed validation data?

https://pdbj.org



Overview of OneDep system



WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report

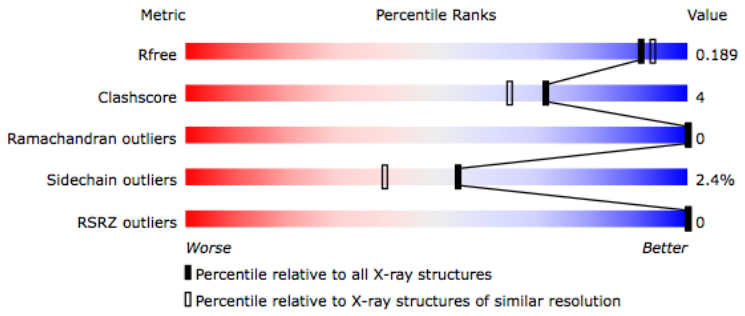
Feb 12, 2017 – 07:52 pm GMT

PDB ID : 1CBS
Title : CRYSTAL STRUCTURE OF CELLULAR RETINOIC-ACID-BINDING PROTEINS 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)

This is a Full wwPDB X-ray Structure Validation 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

wwPDB validation report (PDF)

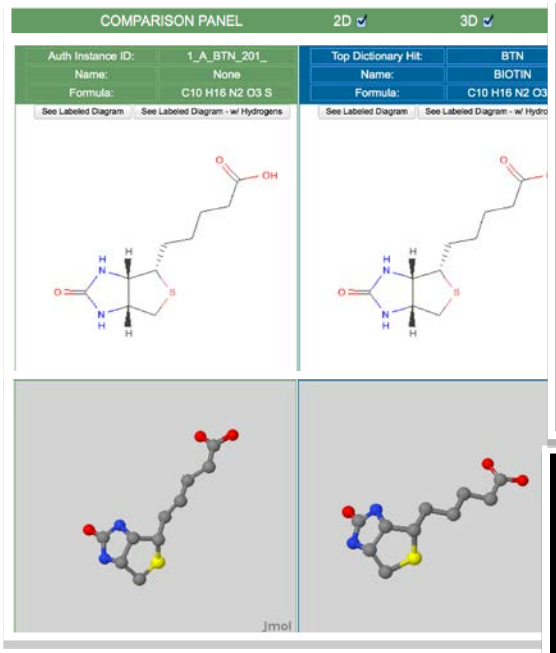


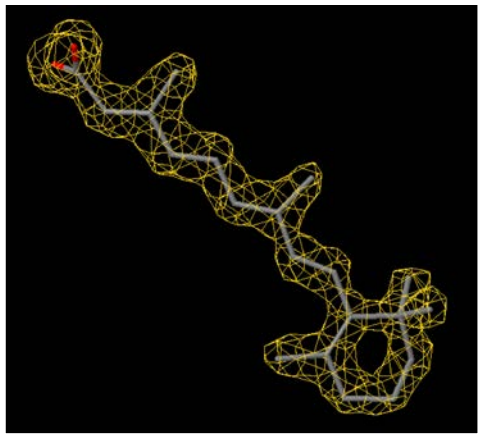
Percentile view of validation report

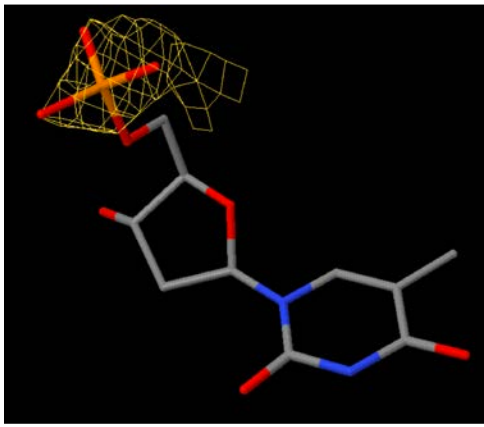
Young, JY et al., Structure, 25(3), 536–545, 2017

Improved Ligand Validation

- Batch search against Chemical Component Dictionary with automated CCD ID assignment
- Captures and displays author-provided chemical information
- Comparison panel
  - 2D and 3D views of ligand for review
  - ID assignment
- Display of local ligand electron density fit





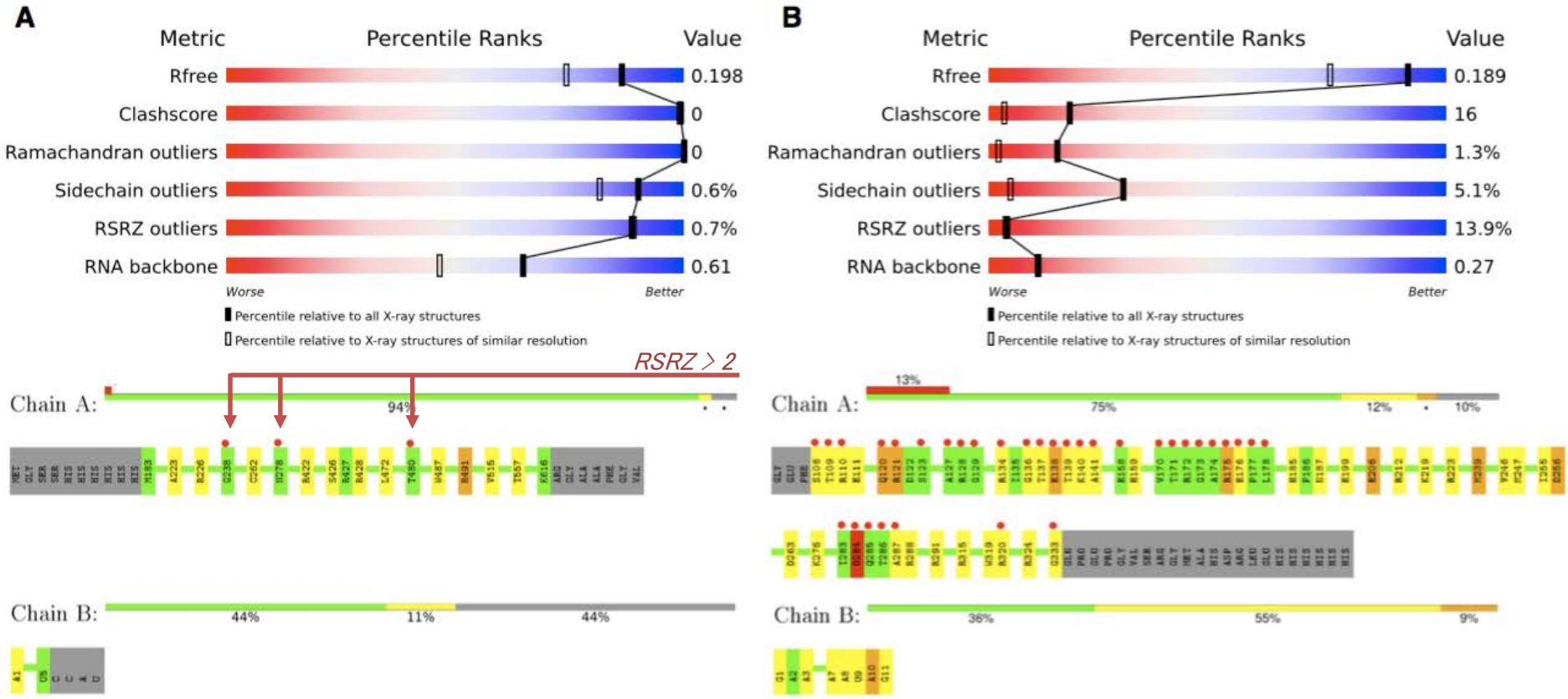


Deposited instance from coordinates (left) and the closest match in the dictionary (right)

Local ligand density display (1.5 sigma omit map)
Top: REA in entry 1CBS with LLDF=1.31 (RSR=0.10, CC=0.95)
Bottom: TMP in entry 3HW4 with LLDF=6.77 (RSR=0.41, CC=0.70)

wwPDB validation report PDFs

Summary quality metrics in wwPDB validation reports



wwPDB validation PDFs are easily reviewed and shared an assessment of structure quality.

Structure 25, 1916–1927, 2017

Validation metrics in wwPDB validation reports

X-ray/EM/NMR

- Geometric & conformational
  - bond, angle, planarity
  - protein backbone conformation
  - protein side-chain conformation
- Atomic & molecular interaction
  - all-atom contacts
  - under packing
  - hydrogen bond quality
- Non-protein
  - nucleic acids (RNA pucker, suite)
  - carbohydrates (N-glycan core)
  - ligands (CSD)
  - ions & other solvent
- Incomplete model (e.g. CA_ONLY)

X-ray

- Structure factor & electron density
  - Wilson plot, outliers, tNCS
  - wrong symmetry
  - twinning
  - agreement (R_{free}, RSR, RSCC)

NMR

- Chemical shifts
  - completeness
  - outliers
  - estimated reference error
  - random coil index
- Structure ensembles
  - representative model (medoid)
  - domain detection

Caveat:

LLDF (Local Ligand Density Fit) has been replaced by a combination of RSR (Real-space R factor) > 0.4 and RSCC (Real-space correlations coefficient) < 0.8 since this March.

wwPDB validation report PDFs

- **Standard geometry**

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.47	0/1107	0.71	0/1491

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

- **Too close contacts**

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1091	0	1106	7	0
2	A	22	0	27	2	0
3	A	100	0	0	2	0
All	All	1213	0	1133	9	0

- **Protein backbones**

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	135/137 (98%)	132 (98%)	3 (2%)	0	100	100

- **Protein sidechains**

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	123/123 (100%)	120 (98%)	3 (2%)	52	38

- **Ligand geometry**

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	REA	A	200	-	19,22,22	1.05	1 (5%)	26,30,30	1.02	2 (7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	200	REA	C1-C6	2.25	1.56	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	200	REA	C11-C10-C9	-2.40	123.89	127.31
2	A	200	REA	C18-C5-C6	2.08	126.83	124.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	200	REA	2	0

Detailed wwPDB validation reports (XML)


```
<?xml version="1.0" ?>
<wwPDB-validation-information xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:noNamespaceSchemaLocation="http://wwpdb.org/validation/schema/
    wwpdb_validation_v002.xsd">
    <Entry B_factor_type="FULL" CCP4version="7.0 (Gargrove)" DCC_R="0.18" DCC_Rfree="0.19" DCC_refinement_program="CNS" DataAnisotropy="0.434"
        DataCompleteness="90.54" EDS_R="0.18" EDS_resolution="1.80" EDS_resolution_low="14.93" Fo_Fc_correlation="0.956" IoverSigma="3.77(1.79A)" PDB-R="0.20"
        PDB-Rfree="0.24" PDB-deposition-date="1994-09-28" PDB-resolution="1.80" PDB-resolution-low="8.00" PDB-revision-date="2011-07-13" PDB-revision-number="3"
        RefmacVersion="5.8.0158" RestypesNotcheckedForBondAngleGeometry="REA" TransNCS="The largest off-origin peak in the Patterson function is 9.26% of the
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        WilsonBaniso="[16.802,17.606,11.032,0.000,0.000,0.000]" WilsonBestimate="14.785" XMLcreationDate="Mar 10, 2018 -- 04:41 pm GMT" absolute-percentile-
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        validation-pack,xtriage,eds,percentiles.writexml" babinet_b="141.456" babinet_k="0.156" bonds_rmsz="0.47" bulk_solvent_b="72.956" bulk_solvent_k="0.401"
        centric_outliers="0" clashscore                                                                                                    high-resol-
        relative-percentile-percent-RSR                                                                                                    tile-percent-rota-
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        outliers="1.8" low-resol-relati                                                                                                    m-H-reduce="1133"
        num-free-reflections="1496" num                                                                                                    lashscore="122126"
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        outliers="0.00" percent-rota-outliers="2.44" percentilebins="all,1.8,xray" protein-DNA-RNA-entities="1" relative-percentile-DCC_Rfree="92.5" relative-
        percentile-clashscore="62.5" relative-percentile-percent-RSRZ-outliers="100.0" relative-percentile-percent-rama-outliers="100.0" relative-percentile-
        percent-rota-outliers="38.4" xtriage_input_columns="F_meas_au,F_meas_sigma_au"/>
    <ModelledSubgroup NatomsEDS="7" altcode=" " avgoccu="1.000" chain="A" ent="1" icode=" " model="1" num-H-reduce="9" owab="28.790" resname="PRO" resnum="1"
        rota="Cg_endo" rscc="0.908" rsr="0.143" rsrz="0.706" said="A" seq="1">
        <clash atom="HB2" cid="4" clashmag="0.47" dist="1.97"/>
    </ModelledSubgroup>
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        rama="Favored" resname="ASN" resnum="2" rota="t30" rscc="0.906" rsr="0.144" rsrz="0.485" said="A" seq="2"/>
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        rama="Favored" resname="SER" re
    <ModelledSubgroup NatomsEDS="4" alt
        rama="Favored" resname="GLY" re
```


Entry-level validation information:
Percentiles, overall validation metrics (e.g. Rfree), statistics.

Residue-level validation information:
Geometric outliers, torsion angles, RSR, RSRZ, clash score, occupancy

validation report of modeled subgroups (residues) repeat…


```
    <ModelledEntityInstance absolute_RSRZ_percentile="100.00" absolute_rama_percentile="100.00" absolute_sidechain_percentile="51.82" angles_rmsz="0.71"
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        relative_rama_percentile="100.00" relative_sidechain_percentile="38.37" said="A"/>
```


Entity-level validation information: Percentiles

validation report of modeled entities repeat…


```
</wwPDB-validation-information>
```

PDBML-validation and wwPDB/RDF-validation

PDBML-validation:

Note that PDBML-validation is an experimental archive and may be changed or replaced in the future.

```
% rsync -av --delete rsync://bmrbpub.pdbj.org/pdbml-valid .
```

wwPDB/RDF-validation:

Note that wwPDB/RDF-validation is an experimental archive and may be changed or replaced in the future.

```
% rsync -av --delete rsync://bmrbpub.pdbj.org/wwpdb-rdf-valid .
```

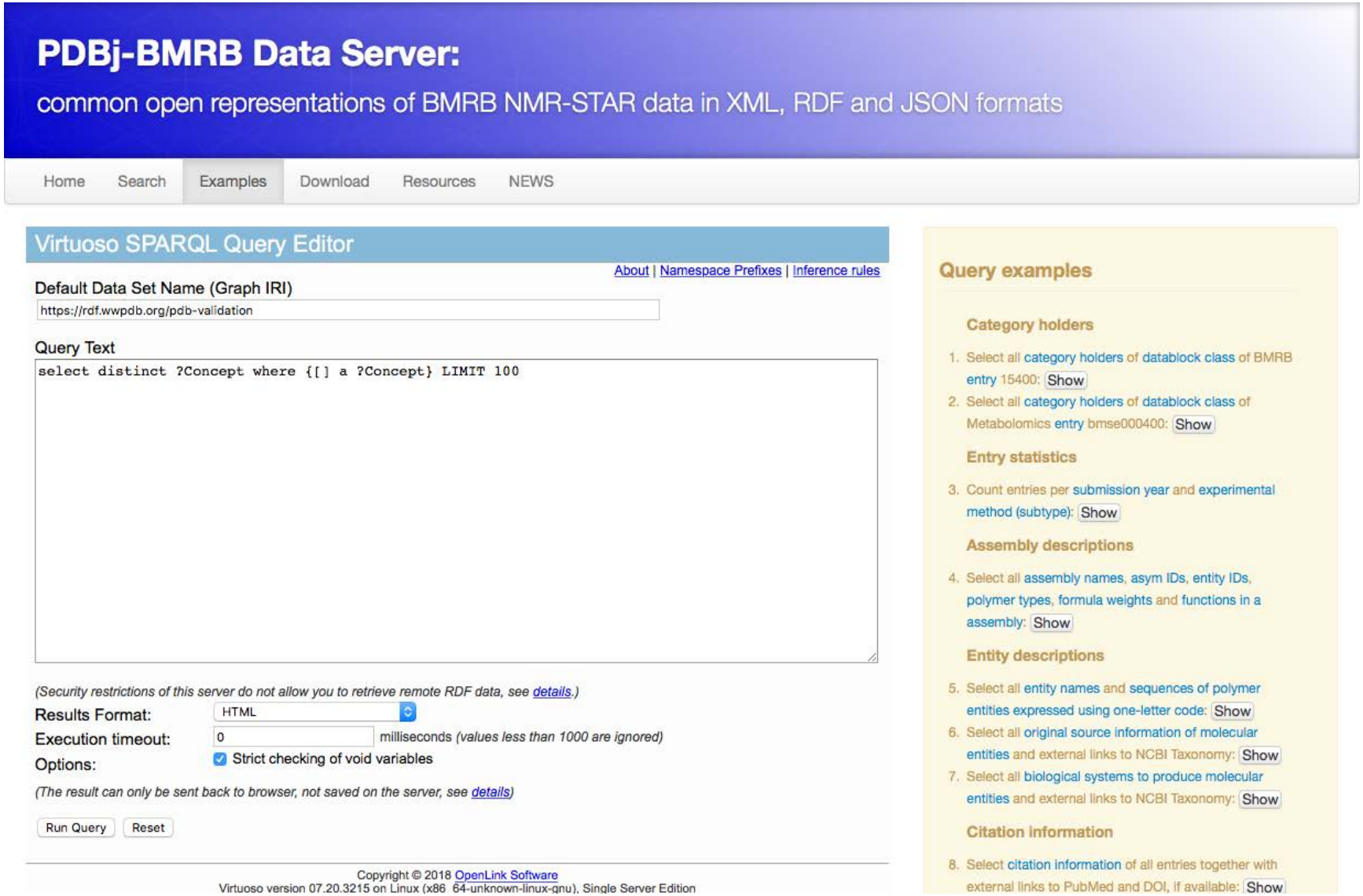
PostgreSQL dump image:

category	description	size (GB)
pdbx_dcc_map	output of MAPMAN used by DCC (RSR, RSCC, LLDF)	10
pdbx_poly_seq_scheme	residue nomenclature mapping for polymer entities	8
struct_mon_prot	structure properties of a protein	6
entity_poly_seq	sequence of monomers in a polymer	2
pdbx_validate_close_contact	close contact with regard to the distance expected	2

https://bmrbpub.pdbj.org

SPARQL endpoint contains wwPDB/RDF-validation graph

https://bmrbpub.pdbj.org



Example #1: Search wwPDB/RDF-validation with SPARQL

Search all enzyme–ligand complexes of which real space R–factor (RSR) of ligand is less than 10%. (showing only essential part of about 30 line–SPARQL query)

```
PREFIX PDBov: <https://rdf.wwpdb.org/schema/pdbx-validation-v1.owl#>
SELECT ?PDB_ID ?enzyme ?ligand ?comp_id MIN(?RSR AS ?minRSR)
FROM <http://rdf.wwpdb.org/pdb-validation>
WHERE {
 ?entity PDBov:link_to_enzyme ?link_to_enzyme ;
        PDBov:entity.pdbx_description ?enzyme ;
        PDBov:of_datablock ?datablock .

 BIND (SUBSTR(STR(?datablock),38,4) AS ?PDB_ID)

…

 FILTER (?ligand != "water" && !STRENDS(?ligand, "ION"))

…

 ?dcc_map PDBov:pdbx_dcc_map.auth_asym_id ?asym_id ;
         PDBov:pdbx_dcc_map.auth_comp_id ?comp_id ;
         PDBov:pdbx_dcc_map.RSR ?RSR .

 FILTER (xsd:float(?RSR) < 0.1)

} GROUP BY ?PDB_ID ?enzyme ?ligand ?comp_id
```

✍ selection of enzyme

✍ ligand selection: non–polymer, not water, not ion

✍ RSR < 0.1

Example #1: Search wwPDB/RDF-validation with SPARQL

Found 15k pairs of enzyme–ligand complexes of which real space R–factor (RSR) of ligand is less than 10%.

PDB ID, enzyme name, ligand name, ligand (3–letters code), minimum RSR value of the ligand

"4CK1","INTEGRASE","(4-CARBOXY-1,3-BENZODIOXOL-5-YL)METHYL-[[2-[(4-METHOXYPHENYL)METHYLCARBAMOYL]PHENYL]METHYL]AZANIUM","OM1","0.081"
"2IOD","Dihydroflavonol 4-reductase","NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE","NAP","0.091"
"5BYR","Iron hydrogenase 1","FE2/S2 (INORGANIC) CLUSTER","FES","0.096"
"2PU0","Enolase","PHOSPHONOACETOHYDROXAMIC ACID","PAH","0.075"
"4LV2","Beta-lactamase","[1-(6-chloropyrimidin-4-yl)-1H-pyrazol-4-yl]boronic acid","N95","0.083"
"3OLE","Pancreatic alpha-amylase","ALPHA-D-GLUCOSE","GLC","0.084"
"4MOR","Pyranose 2-oxidase","DODECAETHYLENE GLYCOL","12P","0.093"
"4FKX","Nucleoside diphosphate kinase","CYTIDINE-5'-DIPHOSPHATE","CDP","0.073"
"4JPU","Cytochrome c peroxidase","PROTOPORPHYRIN IX CONTAINING FE","HEM","0.094"
"1GTV","THYMIDYLATE KINASE","THYMIDINE-5'-DIPHOSPHATE","TYD","0.090"
"5IA2","7-(5-hydroxy-2-methylphenyl)-8-(2-methoxyphenyl)-1-methyl-1H-imidazo[2,1-f]purine-2,4(3H,8H)-dione","7-(5-hydroxy-2-methylphenyl)-8-(2-methoxyphenyl)-1-methyl-1H-imidazo[2,1-f]purine-2,4(3H,8H)-dione","L66","0.077"
"1NFQ","Putative oxidoreductase Rv2002","1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE","NAI","0.090”

Example #2: Search wwPDB/RDF-validation with SPARQL

Search all enzyme-ligand complexes of which percentage of outlier in real space R-factor, defined by Z-score (RSRZ) is larger than 2, of enzyme is less than 1%. (showing only essential part of about 20 line-SPARQL query)

```
PREFIX PDBov: <https://rdf.wwpdb.org/schema/pdbx-validation-v1.owl#>
SELECT ?PDB_ID ?Enzyme (GROUP_CONCAT(?Ligand; SEPARATOR=",") AS ?Ligands)
?RSRZ_outliers_percent
FROM <http://rdf.wwpdb.org/pdb-validation>
WHERE {
 ?map_overall PDBov:pdbx_dcc_map_overall.entry_id ?PDB_ID ;
          PDBov:pdbx_dcc_map_overall.RSRZ_outliers_percent ?RSRZ_outliers_percent .

 FILTER (xsd:float(?RSRZ_outliers_percent) < 0.01)
                                                    ✍ % of outliers in RSRZ < 1%
 BIND (IRI(CONCAT("https://rdf.wwpdb.org/pdb-validation/", ?PDB_ID, "/entityCategory")) AS
?entity_category)

 ?entity_category PDBov:has_entity ?entity .

 ?entity PDBov:link_to_enzyme ?link_to_enzume ;
       PDBov:entity.pdbx_description ?Enzyme .
                                                    ✍selection of enzyme
...

}                                                   ✍ligand selection (omission)
```

Example #2: Search wwPDB/RDF-validation with SPARQL

Found 5k pairs of enzyme–ligand complexes of which percentage of outlier in real space R-factor (RSRZ) of enzyme is less than 1%, 1k pairs for 0%.

PDB ID, enzyme name, ligand name, percentage of outliers in RSR value of the enzyme

"1BUL","NMC-A BETA-LACTAMASE","2-(1-CARBOXY-2-HYDROXY-2-METHYL-PROPYL)-5,5-DIMETHYL-THIAZOLIDINE-4-CARBOXYLIC ACID,2-(N-MORPHOLINO)-ETHANESULFONIC ACID","0.00"
"5A1G","S-ADENOSYLMETHIONINE SYNTHASE ISOFORM TYPE-2","(DIPHOSPHONO)AMINOPHOSPHONIC ACID,[(3S)-3-amino-3-carboxypropyl]{[(2S,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl}ethylsulfonium,(4S)-2-METHYL-2,4-PENTANEDIOL,IMIDAZOLE","0.00"
"2DRS","Xylanase Y","GLYCEROL","0.00"
"2AS1","Cytochrome c peroxidase, mitochondrial","PROTOPORPHYRIN IX CONTAINING FE,THIOPHENE-3-CARBOXIMIDAMIDE","0.00"
"1H4W","TRYPSIN IVA","BENZAMIDINE","0.00"
"142L","T4 LYSOZYME","BETA-MERCAPTOETHANOL","0.00"
"4CIK","PLASMINOGEN","5-[(2R,4S)-2-(phenylmethyl)piperidin-4-yl]-1,2-oxazol-3-one","0.00"
"4L4O","Endo-1,4-beta-xylanase","TRIS-HYDROXYMETHYL-METHYL-AMMONIUM","0.00"
"4G5P","Epidermal growth factor receptor","N-{4-[(3-chloro-4-fluorophenyl)amino]-7-[(3S)-tetrahydrofuran-3-yloxy]quinazolin-6-yl}-4-(dimethylamino)butanamide","0.00"
"3GA6","Exodeoxyribonuclease","GLYCEROL","0.00"

SIFTS: Structure Integration with Function, Taxonomy and Sequences resource

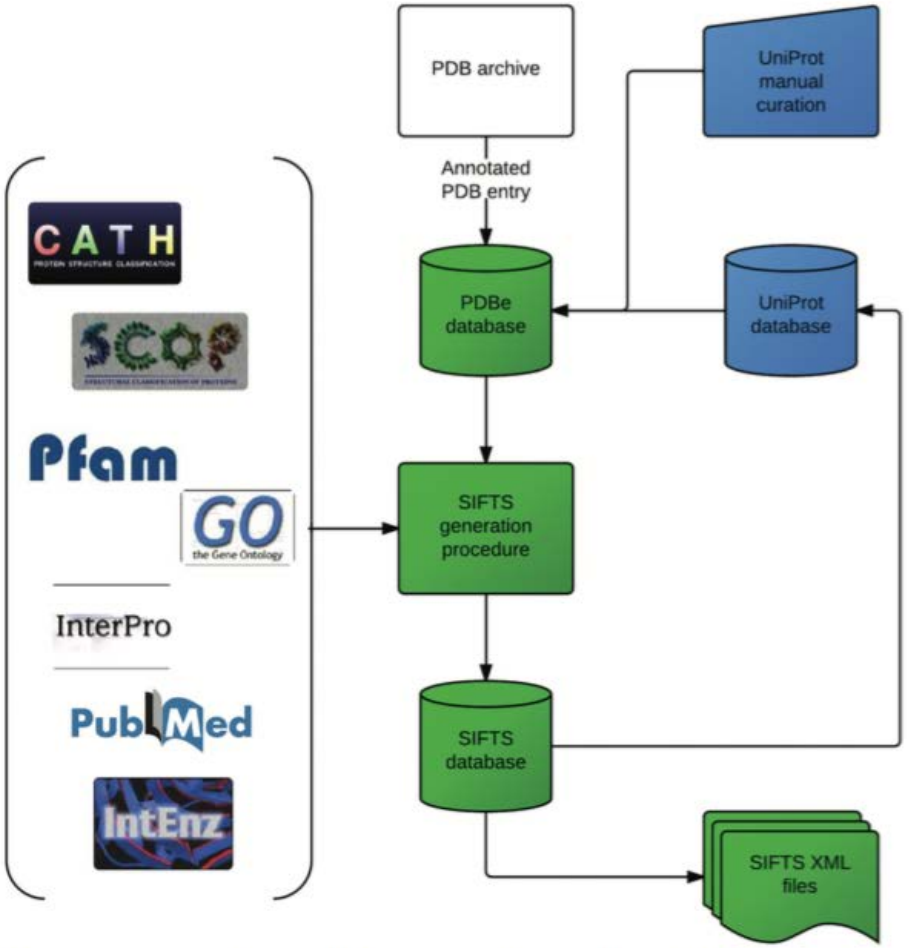


Figure 1. The SIFTS pipeline combines manual and automated processes to produce up-to-date residue-level mappings between proteins in the PDB and their corresponding UniProtKB entry. The pipeline also enriches the annotations of proteins in the PDB by adding data from other biological resources. The SIFTS data are distributed in XML format.

Nucleic Acids Research, 2013, Vol. 41, D483–D489
Nucleic Acids Research, 2017, Vol. 45, D282–D288

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