Editing PDBx/mmCIF files via a web-based CIF editor

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The PDB format: Design

PDB format (full): 5zno

```
HEADER    HYDROLASE                               10-APR-18   5ZNO
TITLE     CRYSTAL STRUCTURE OF PET-DEGRADING CUTINASE CUT190 S176A/S226P/R228S/
TITLE    2 MUTANT IN CA(2+)-BOUND STATE
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: ALPHA/BETA HYDROLASE FAMILY PROTEIN;
COMPND   3 CHAIN: A, B;
COMPND   4 SYNONYM: CUTINASE;
COMPND   5 EC: 3.1.1.74;
COMPND   6 ENGINEERED: YES;
COMPND   7 MUTATION: YES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: SACCHAROMONOSPORA VIRIDIS;
SOURCE   3 ORGANISM_TAXID: 1852;
SOURCE   4 STRAIN: AHK190;
SOURCE   5 GENE: CUT190, SAMN02982918_2340;
SOURCE   6 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE   7 EXPRESSION_SYSTEM_TAXID: 562;
SOURCE   8 EXPRESSION_SYSTEM_STRAIN: ROSETTA-GAMI B (DE3);
SOURCE   9 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE  10 EXPRESSION_SYSTEM_PLASMID: PQE80L
KEYWDS    POLYESTERASE, ALPHA/BETA-HYDROLASE FOLD, PROTEIN ENGINEERING,
KEYWDS   2 THERMOSTABILITY, HYDROLASE
EXPDTA    X-RAY DIFFRACTION
AUTHOR    N.NUMOTO,S.INABA,Y.YAMAGAMI,N.KAMIYA,G.J.BEKKER,K.ISHII,S.UCHIYAMA,
AUTHOR   2 F.KAWAI,N.ITO,M.ODA
REVDAT    2   26-SEP-18 5ZNO    1       JRNL
REVDAT    1   12-SEP-18 5ZNO    0
JRNL        AUTH   N.NUMOTO,N.KAMIYA,G.J.BEKKER,Y.YAMAGAMI,S.INABA,K.ISHII,
JRNL       AUTH 2 S.UCHIYAMA,F.KAWAI,N.ITO,M.ODA
JRNL        TITL   STRUCTURAL DYNAMICS OF THE PET-DEGRADING CUTINASE-LIKE
JRNL        TITL 2 ENZYME FROM SACCHAROMONOSPORA VIRIDIS AHK190 IN
JRNL        TITL 3 SUBSTRATE-BOUND STATES ELUCIDATES THE CA2+-DRIVEN CATALYTIC
JRNL        TITL 4 CYCLE.
JRNL        REF    BIOCHEMISTRY                  V.  57  5289 2018
JRNL        REFN                   ISSN 1520-4995
JRNL        PMID   30110540
JRNL        DOI    10.1021/ACS.BIOCHEM.8B00624
REMARK   2
REMARK   2 RESOLUTION.    1.60 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : PHENIX 1.9_1692
REMARK   3   AUTHORS     : PAUL ADAMS,PAVEL AFONINE,VINCENT CHEN,IAN
REMARK   3                : DAVIS,KRESHNA GOPAL,RALF GROSSE-KUNSTLEVE,
REMARK   3                : LI-WEI HUNG,ROBERT IMMORMINO,TOM IOERGER,
REMARK   3                : AIRLIE MCCOY,ERIK MCKEE,NIGEL MORIARTY,
REMARK   3                : REETAL PAI,RANDY READ,JANE RICHARDSON,
REMARK   3                : DAVID RICHARDSON,TOD ROMO,JIN SACCHETTINI,
REMARK   3                : NICHOLAS SAUTER,JACOB SMITH,LAURENT
REMARK   3                : STORONI,TOM TERWILLIGER,PETER ZWART
REMARK   3
REMARK   3    REFINEMENT TARGET : NULL
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 1.60
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 47.72
REMARK   3   MIN(FOBS/SIGMA_FOBS)              : 1.347
REMARK   3   COMPLETENESS FOR RANGE        (%) : 99.3
REMARK   3   NUMBER OF REFLECTIONS             : 75047
```

- Designed in an age where scientists still used punched cards instead of digital files (right) in a keyword-value type of file
- Afterwards ported to a digital format (ASCII flat file), but still using a fixed-width column format (left)
- ATOM/HETATM records used for storing atomic data, other records for meta-data

```
ATOM      1  N   ASP A  46     -12.862 -28.141  34.844  1.00 31.64           N
ATOM      2  CA  ASP A  46     -13.701 -27.257  34.048  1.00 28.41           C
ATOM      3  C   ASP A  46     -13.154 -27.009  32.633  1.00 30.93           C
ATOM      4  O   ASP A  46     -11.971 -27.311  32.373  1.00 27.41           O
ATOM      5  CB  ASP A  46     -13.837 -25.893  34.721  1.00 33.80           C
ATOM      6  CG  ASP A  46     -14.503 -25.981  36.080  1.00 52.37           C
ATOM      7  OD1 ASP A  46     -15.236 -26.965  36.321  1.00 50.37           O
ATOM      8  OD2 ASP A  46     -14.293 -25.067  36.907  1.00 49.04           O
ATOM      9  N   ASN A  47     -14.035 -26.704  31.720  1.00 24.71           N
ATOM     10  CA  ASN A  47     -13.654 -26.384  30.350  1.00 18.63           C
ATOM     11  C   ASN A  47     -13.165 -24.947  30.262  1.00 15.54           C
ATOM     12  O   ASN A  47     -13.934 -24.018  30.489  1.00 17.48           O
ATOM     13  CB  ASN A  47     -14.849 -26.614  29.422  1.00 16.02           C
ATOM     14  CG  ASN A  47     -14.563 -26.259  27.974  1.00 16.44           C
ATOM     15  OD1 ASN A  47     -13.467 -25.814  27.614  1.00 16.28           O
ATOM     16  ND2 ASN A  47     -15.565 -26.466  27.124  1.00 16.83           N
ATOM     17  N   PRO A  48     -11.880 -24.754  29.928  1.00 14.95           N
ATOM     18  CA  PRO A  48     -11.293 -23.409  29.917  1.00 14.40           C
ATOM     19  C   PRO A  48     -11.842 -22.508  28.811  1.00 17.57           C
ATOM     20  O   PRO A  48     -11.606 -21.299  28.837  1.00 17.19           O
ATOM     21  CB  PRO A  48      -9.801 -23.683  29.699  1.00 21.37           C
ATOM     22  CG  PRO A  48      -9.759 -25.006  29.000  1.00 23.14           C
ATOM     23  CD  PRO A  48     -10.888 -25.795  29.599  1.00 17.37           C
ATOM     24  N   TYR A  49     -12.572 -23.088  27.863  1.00 16.03           N
ATOM     25  CA  TYR A  49     -13.070 -22.336  26.716  1.00 14.59           C
ATOM     26  C   TYR A  49     -14.525 -21.881  26.842  1.00 16.63           C
ATOM     27  O   TYR A  49     -15.048 -21.229  25.936  1.00 14.89           O
ATOM     28  CB  TYR A  49     -12.912 -23.172  25.444  1.00 15.50           C
ATOM     29  CG  TYR A  49     -11.521 -23.749  25.285  1.00 14.95           C
ATOM     30  CD1 TYR A  49     -10.393 -22.959  25.494  1.00 17.86           C
ATOM     31  CD2 TYR A  49     -11.336 -25.078  24.955  1.00 18.35           C
ATOM     32  CE1 TYR A  49      -9.122 -23.481  25.361  1.00 15.32           C
ATOM     33  CE2 TYR A  49     -10.064 -25.614  24.818  1.00 21.68           C
ATOM     34  CZ  TYR A  49      -8.963 -24.809  25.030  1.00 24.11           C
ATOM     35  OH  TYR A  49      -7.692 -25.323  24.898  1.00 26.68           O
```

https://swift.cmbi.umcn.nl/teach/B1M/BIOINF_4.html

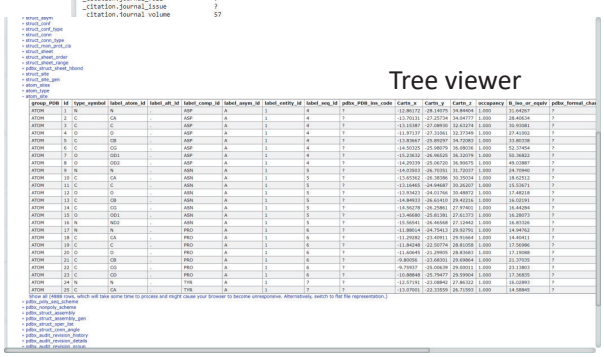
The PDB format: Fallen out of grace

- Over time, the REMARK records started to be used for many different items → messy, difficult to parse (computers) and understand (humans)
- Limited annotation capabilities (REMARK records are already overloaded)
- Fixed width introduced more and more problems as larger, more complex structures were solved (99999 atoms, 62 chains maximum)
- Limited number of 4-character PDB IDs & 3-character chem_comp IDs
- Alternative formats have been developed to deal with these issues

The successor format: mmCIF

- Format is based on the Self-defining Text Archive and Retrieval, developed by Hall et al. 1991 (DOI: 10.1021/ci00002a020)
- No more fixed-width columns
- Still uses a keyword-value based format, but one that is very extensible
- Comes with a dictionary

Raw mmCIF



Tree viewer

mmCIF format

- All-in-all: a very structured format suitable for proper annotation of the meta-data and extensible to allow now only large structures, but also many different experimental sources

data item = name + value

```
data_5ZNO
#
_entry.id   5ZNO
#
_audit_conform.dict_name       mmcif_pdbx.dic
_audit_conform.dict_version    5.296
_audit_conform.dict_location
http://mmcif.pdb.org/dictionaries/ascii/mmcif_pdbx.dic
#
loop_
_database_2.database_id
_database_2.database_code
PDB   5ZNO
WWPDB D_1300007412
#
_pdbx_database_status.status_code                     REL
_pdbx_database_status.status_code_sf                  REL
_pdbx_database_status.entry_id                        5ZNO
_pdbx_database_status.recvd_initial_deposition_date   2018-04-10
_pdbx_database_status.SG_entry                        N
_pdbx_database_status.deposit_site                    PDBJ
_pdbx_database_status.process_site                    PDBJ
_pdbx_database_status.pdb_format_compatible           Y
#
loop_
_audit_author.name
_audit_author.pdbx_ordinal
_audit_author.identifier_ORCID
'Numoto, N.'    1  ?
'Inaba, S.'     2  ?
'Yamagami, Y.'  3  ?
'Kamiya, N.'    4  ?
'Bekker, G.J.'  5  ?
'Ishii, K.'     6  ?
'Uchiyama, S.'  7  ?
'Kawai, F.'     8  ?
'Ito, N.'       9  ?
'Oda, M.'       10 ?
#
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_citation.id                        primary
_citation.journal_abbrev            Biochemistry
_citation.journal_id_ASTM           BICHAW
_citation.journal_id_CSD            0033
_citation.journal_id_ISSN           1520-4995
_citation.journal_volume            57
_citation.page_first                5289
_citation.page_last                 5300
_citation.title
;Structural Dynamics of the PET-Degrading Cutinase-like Enzyme from
Saccharomonospora viridis AHK190 in Substrate-Bound States Elucidates the
Ca2+-Driven Catalytic Cycle.
;
_citation.year                      2018
_citation.pdbx_database_id_DOI      10.1021/acs.biochem.8b00624
_citation.pdbx_database_id_PubMed   30110540
#
```
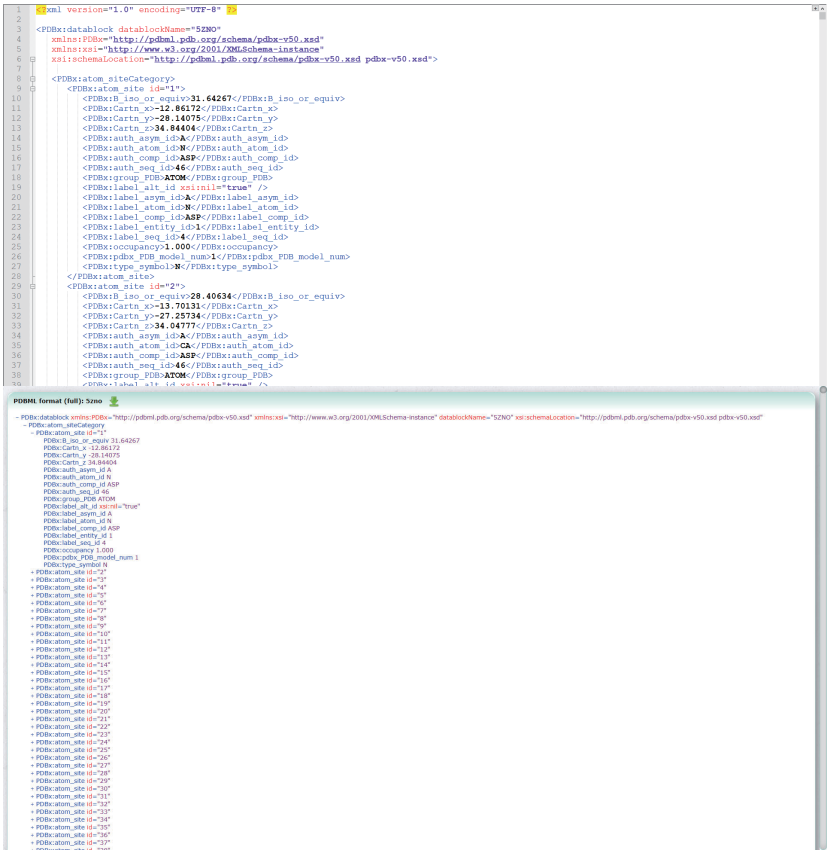

Alternative: PDBML

- Attempt to make something more computer friendly: PDBML (XML version of mmCIF)
- The good: many programming languages have an XML parser, structured & easier to parse then the flat-file,
- The bad: very bloated, slow to parse & requires a dictionary to properly parse, not very human friendly



Alternative: mmJSON

- PDBML is not really that computer-friendly, especially in a web-environment
- The JSON (JavaScript Object Notation) is an alternative to XML, especially for the web
- The good: many programming languages have a JSON parser, structured, easier to parse than the other formats, lightweight (uncompressed smaller than uncompressed XML, compressed smaller than compressed mmCIF), fast to parse, numbers are pre-parsed (no dictionary or additional work required)
- The bad: not very human friendly

Alternative: mmJSON

- Simply a JSON serialized version of parsed mmCIF data (https://gitlab.com/pdbjapan/cif-parsers)
- Initially developed for Molmil (pdbj.org/molmil2), afterwards also used for PDBj Mine (entry pages on the web, loading of SQL RDB for searching) and available on the ftp (pdbj.org/help/mmjson)

The demise of the flat-file

- 2013: the release of PDBID: 3j3q, an entry with over 2 million atoms that is incompatible with the PDB format
- 2014: Consolidation of previously split entries into a single large entry that are incompatible with the PDB format, introduced the pdb-bundle format (a best-effort approximation of the data split over multiple PDB flat files)
- 2019: MX deposition requires mmCIF files instead of PDB flat files
- 2021: Potentially full retirement of PDB flat files

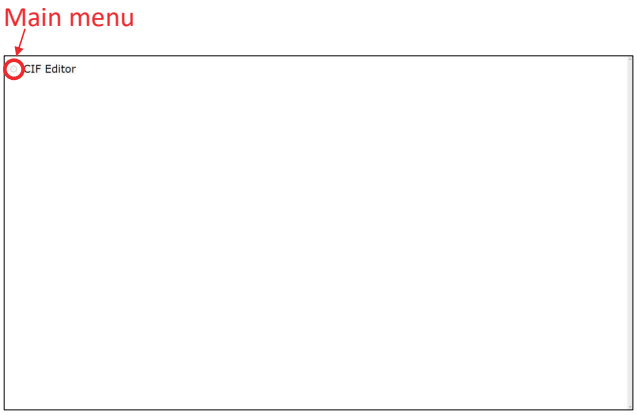
(Adams et al. 2019, DOI: 10.1107/S2059798319004522)

Development of a new mmCIF editor

- It's not easy to edit mmCIF files, especially when used to PDB flat files
- PDBj has developed an mmCIF editor:
  - Available at: https://pdbj.org/cif-editor/
  - Help page: https://gitlab.com/pdbjapan/cif-editor/wikis/home
  - Bekker et al. 2019, DOI: 10.5940/jcrsj.61.159
- Multiple methods to edit are supported
- Development however hasn't finished and new features will be added in the future
  - If you have any requests, please contact us at https://pdbj.org/contact
  - Or create an issue at https://gitlab.com/pdbjapan/cif-editor/issues

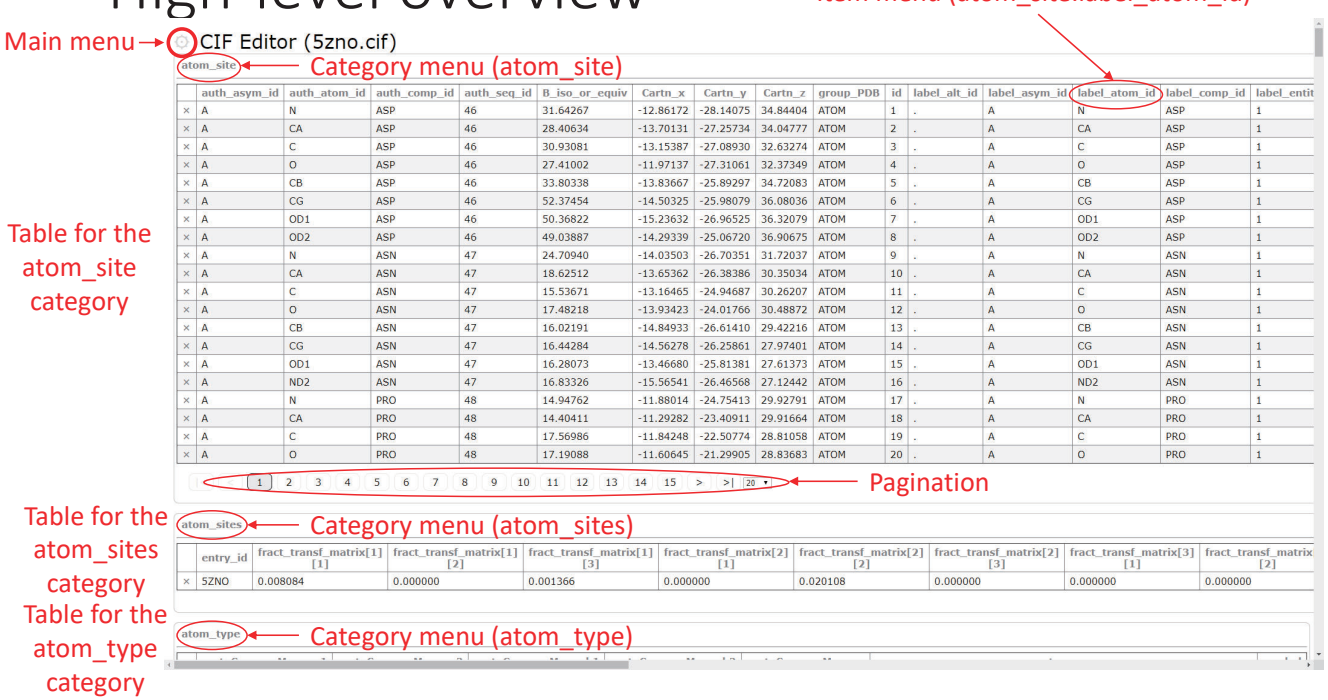
How-to: Load a file

- Looks very plain on first load (right)



- Three options:
  - Main menu (⚙) → Open mmCIF file → Select file in dialogue
  - Drag file from local file system into the CIF Editor and drop the file
  - Load a publicly available file via URL:
    https://pdbj.org/cif-editor/#https://pdbj.org/rest/displayPDBfile?format=mmcif&id=1crn

High-level overview



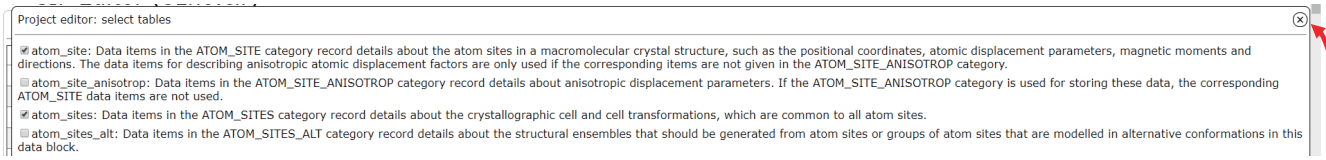
	auth_asym_id	auth_atom_id	auth_comp_id	auth_seq_id	B_iso_or_equiv	Cartn_x	Cartn_y	Cartn_z	group_PDB	id	label_alt_id	label_asym_id	label_atom_id	label_comp_id	label_entit
×	A	N	ASP	46	31.64267	-12.86172	-28.14075	34.84404	ATOM	1	.	A	N	ASP	1
×	A	CA	ASP	46	28.40634	-13.70131	-27.25734	34.04777	ATOM	2	.	A	CA	ASP	1
×	A	C	ASP	46	30.93081	-13.15387	-27.08930	32.63274	ATOM	3	.	A	C	ASP	1
×	A	O	ASP	46	27.41002	-11.97137	-27.31061	32.37349	ATOM	4	.	A	O	ASP	1
×	A	CB	ASP	46	33.80338	-13.83667	-25.89297	34.72083	ATOM	5	.	A	CB	ASP	1
×	A	CG	ASP	46	52.37454	-14.50325	-25.98079	36.08036	ATOM	6	.	A	CG	ASP	1
×	A	OD1	ASP	46	50.36822	-15.23632	-26.96525	36.32079	ATOM	7	.	A	OD1	ASP	1
×	A	OD2	ASP	46	49.03887	-14.29339	-25.06720	36.90675	ATOM	8	.	A	OD2	ASP	1
×	A	N	ASN	47	24.70940	-14.03503	-26.70351	31.72037	ATOM	9	.	A	N	ASN	1
×	A	CA	ASN	47	18.62512	-13.65362	-26.38386	30.35034	ATOM	10	.	A	CA	ASN	1
×	A	C	ASN	47	15.53671	-13.16465	-24.94687	30.26207	ATOM	11	.	A	C	ASN	1
×	A	O	ASN	47	17.48218	-13.93423	-24.01766	30.48872	ATOM	12	.	A	O	ASN	1
×	A	CB	ASN	47	16.02191	-14.84933	-26.61410	29.42216	ATOM	13	.	A	CB	ASN	1
×	A	CG	ASN	47	16.44284	-14.56278	-26.25861	27.97401	ATOM	14	.	A	CG	ASN	1
×	A	OD1	ASN	47	16.28073	-13.46680	-25.81381	27.61373	ATOM	15	.	A	OD1	ASN	1
×	A	ND2	ASN	47	16.83326	-15.56541	-26.46568	27.12442	ATOM	16	.	A	ND2	ASN	1
×	A	N	PRO	48	14.94762	-11.88014	-24.75413	29.92791	ATOM	17	.	A	N	PRO	1
×	A	CA	PRO	48	14.40411	-11.29282	-23.40911	29.91664	ATOM	18	.	A	CA	PRO	1
×	A	C	PRO	48	17.56986	-11.84248	-22.50774	28.81058	ATOM	19	.	A	C	PRO	1
×	A	O	PRO	48	17.19088	-11.60645	-21.29905	28.83683	ATOM	20	.	A	O	PRO	1

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 > >| 20

	entry_id	fract_transf_matrix[1][1]	fract_transf_matrix[1][2]	fract_transf_matrix[1][3]	fract_transf_matrix[2][1]	fract_transf_matrix[2][2]	fract_transf_matrix[2][3]	fract_transf_matrix[3][1]	fract_transf_matrix[3][2]
×	5ZNO	0.008084	0.000000	0.001366	0.000000	0.020108	0.000000	0.000000	0.000000

How-to: Showing/hiding categories

- By default, only the categories part of the loaded mmCIF file are shown
- To add data to non-existing categories, first the category has to be toggled.
- Main menu → Toggle tables:



- Check the categories to show in the above menu
- To close, click on the close button

How-to: Adding new data

- To add data to a category, click on the corresponding category menu, then select “Add new row”
- Enter the mandatory items (click on the corresponding table cell to show an input field) and click on the (+) icon to add the item
- The editor only shows the mandatory data items and those included in the loaded file
- To show more, click on the Category menu → Toggle columns
- Like the category toggler, select the columns (data items) to show and click on the close button (x)
- While editing the content, the user inputted values are checked against the dictionary
- To delete rows, simply click on the x button in front of the row

How-to: Search & filter

- To quickly search or filter the data items, the editor supports the following filter mechanisms:
  - Filter by number (>, <, ==, <=, >= filters for int/float)
  - Filter by value (select a specific value from a list)
  - Search by value (free text search)
- Multiple operations can also be combined using AND and OR operators
- To add an operation, click on the Item menu and select one of the above filter/search options

How-to: Batch operations

- This can be used in combination with the filtering
- Delete shown rows (only available after filtering):
  - Category menu → Delete

- Item specific operations from Item menu → Batch Operations:
  - Add/subtract value (int/float items only): Adds the user-inputted value to each shown item
  - Renumber (int items only): Renumber all shown items starting from the user-inputted value
  - Set value: Sets a specific value for all shown items

How-to: Raw editor

- To perform complex operations that are either not possible with the UI of the editor, or are otherwise challenging, the editor also supports a raw mode (category independent)
- Category menu → Raw editor
- To check the validity of the content, click on the Category menu → Validate CIF.
- After completing the modifications, click on the Category menu → Validate CIF & update. → This is required to load the modified content back into the main memory structure

How-to: merging CIF files

- Main menu → Merge additional mmCIF file → Select file to merge in
- Will only perform a simply merge (similar to copy-and-past of the data)
- Then, the merged file is checked against the dictionary and issues caused by the merger are reported
- Changes to the data (e.g. chain/entity IDs) can be made afterwards, but it is probably easier to do those before merging

How-to: Saving an entry

- After the editing has finished, the data can be saved to a file:
  - Main menu → Save mmCIF
- Alternatively, it is also possible to save the content as mmJSON (as they are equivalent in terms of the editor)

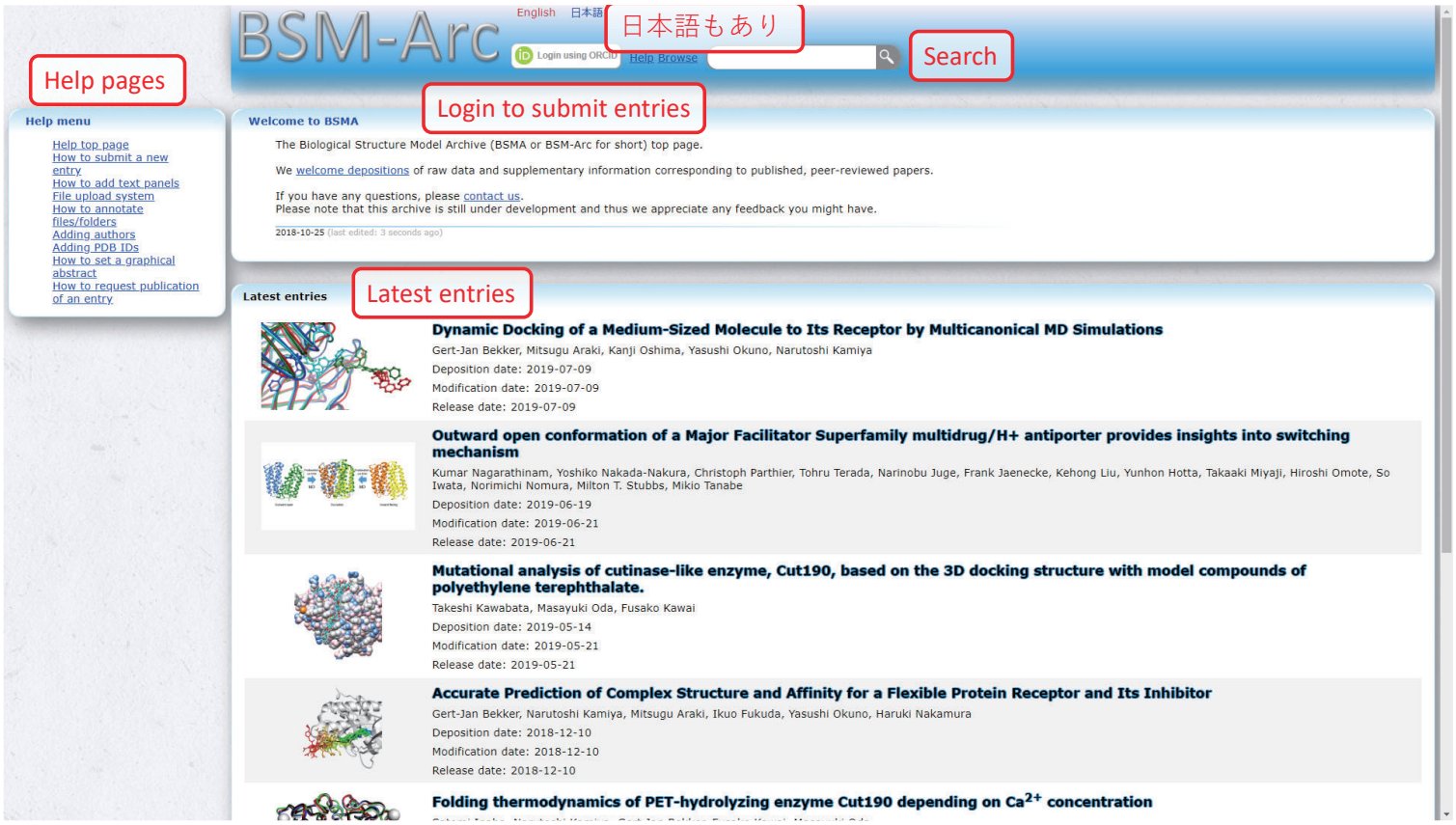
- Finally, the mmCIF editor can also be used to load non-mmCIF data, e.g. NMR-STAR & BSMA-STAR.

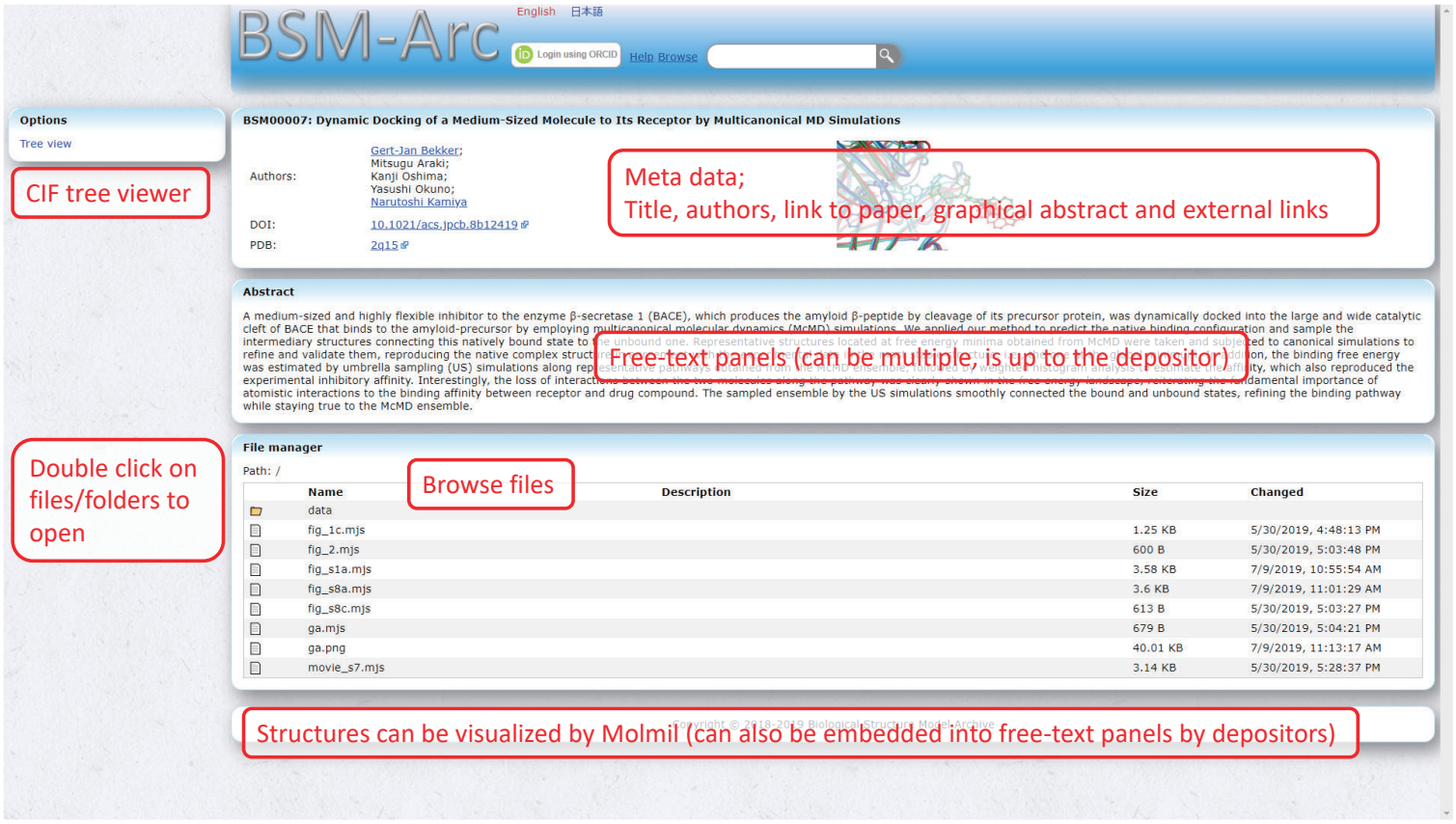
What's BSMA?

- A new archive for computationally derived data
- A BINDS project (創薬等先端技術支援基盤プラットフォーム)
- Because of it's difficult name, people tend to simply call it "MD-database", but other computational data is also accepted
- Uses BSMA-STAR data format, where its editor forms the basis of the CIF-editor

- Data of released entries can be downloaded freely
- New entries can be submitted after logging in using your ORCID-ID
  - Computational work
  - Peer-reviewed paper is required (DOI)
  - Related to protein structures

  (https://bsma.pdbj.org/articles/bsma-terms-of-service)


BSM-Arc
English
日本語
日本語もあり
Login using ORCID
Help Browse
Search
Help pages
Login to submit entries
Help menu
Help top page
How to submit a new entry
How to add text panels
File upload system
How to annotate files/folders
Adding authors
Adding PDB IDs
How to set a graphical abstract
How to request publication of an entry
Welcome to BSMA
The Biological Structure Model Archive (BSMA or BSM-Arc for short) top page.
We welcome depositions of raw data and supplementary information corresponding to published, peer-reviewed papers.
If you have any questions, please contact us.
Please note that this archive is still under development and thus we appreciate any feedback you might have.
2018-10-25 (last edited: 3 seconds ago)
Latest entries
Latest entries
Dynamic Docking of a Medium-Sized Molecule to Its Receptor by Multicanonical MD Simulations
Gert-Jan Bekker, Mitsugu Araki, Kanji Oshima, Yasushi Okuno, Narutoshi Kamiya
Deposition date: 2019-07-09
Modification date: 2019-07-09
Release date: 2019-07-09
Outward open conformation of a Major Facilitator Superfamily multidrug/H+ antiporter provides insights into switching mechanism
Kumar Nagarathinam, Yoshiko Nakada-Nakura, Christoph Parthier, Tohru Terada, Narinobu Juge, Frank Jaenecke, Kehong Liu, Yunhon Hotta, Takaaki Miyaji, Hiroshi Omote, So Iwata, Norimichi Nomura, Milton T. Stubbs, Mikio Tanabe
Deposition date: 2019-06-19
Modification date: 2019-06-21
Release date: 2019-06-21
Mutational analysis of cutinase-like enzyme, Cut190, based on the 3D docking structure with model compounds of polyethylene terephthalate.
Takeshi Kawabata, Masayuki Oda, Fusako Kawai
Deposition date: 2019-05-14
Modification date: 2019-05-21
Release date: 2019-05-21
Accurate Prediction of Complex Structure and Affinity for a Flexible Protein Receptor and Its Inhibitor
Gert-Jan Bekker, Narutoshi Kamiya, Mitsugu Araki, Ikuo Fukuda, Yasushi Okuno, Haruki Nakamura
Deposition date: 2018-12-10
Modification date: 2018-12-10
Release date: 2018-12-10
Folding thermodynamics of PET-hydrolyzing enzyme Cut190 depending on Ca^{2+} concentration


BSM-Arc
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BSM00007: Dynamic Docking of a Medium-Sized Molecule to Its Receptor by Multicanonical MD Simulations
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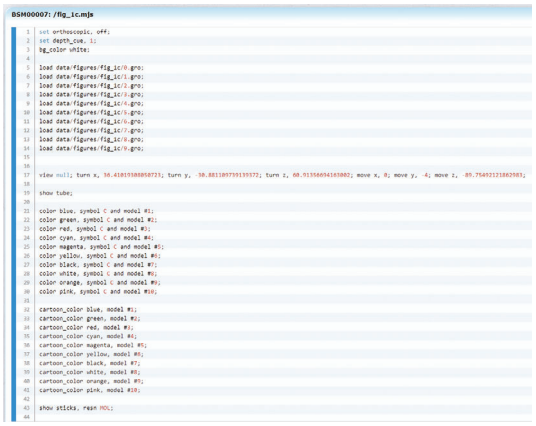
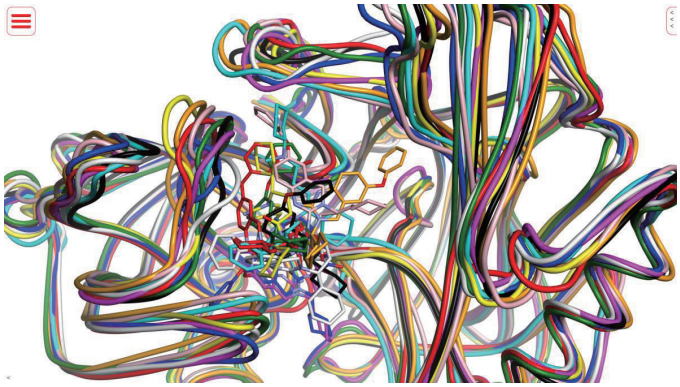
DOI:
10.1021/acs.jpcb.8b12419
PDB:
2q15
Meta data;
Title, authors, link to paper, graphical abstract and external links
Abstract
A medium-sized and highly flexible inhibitor to the enzyme β-secretase 1 (BACE), which produces the amyloid β-peptide by cleavage of its precursor protein, was dynamically docked into the large and wide catalytic cleft of BACE that binds to the amyloid-precursor by employing multicanonical molecular dynamics (McMD) simulations. We applied our method to predict the native binding configuration and sample the intermediary structures connecting this natively bound state to the unbound one. Representative structures located at free energy minima obtained from McMD were taken and subjected to canonical simulations to refine and validate them, reproducing the native complex structure with high accuracy. Furthermore, in addition, the binding free energy was estimated by umbrella sampling (US) simulations along representative pathways obtained from the McMD ensemble, aided by weighted histogram analysis. Estimate of affinity, which also reproduced the experimental inhibitory affinity. Interestingly, the loss of interactions between the molecules along the pathways most clearly shown in the free energy landscape, revealing the fundamental importance of atomistic interactions to the binding affinity between receptor and drug compound. The sampled ensemble by the US simulations smoothly connected the bound and unbound states, refining the binding pathway while staying true to the McMD ensemble.
Free-text panels (can be multiple, is up to the depositor)
File manager
Path: /
Browse files
Double click on files/folders to open
Name
Description
Size
Changed
data
fig_1c.mjs 1.25 KB 5/30/2019, 4:48:13 PM
fig_2.mjs 600 B 5/30/2019, 5:03:48 PM
fig_s1a.mjs 3.58 KB 7/9/2019, 10:55:54 AM
fig_s8a.mjs 3.6 KB 7/9/2019, 11:01:29 AM
fig_s8c.mjs 613 B 5/30/2019, 5:03:27 PM
ga.mjs 679 B 5/30/2019, 5:04:21 PM
ga.png 40.01 KB 7/9/2019, 11:13:17 AM
movie_s7.mjs 3.14 KB 5/30/2019, 5:28:37 PM
Structures can be visualized by Molmil (can also be embedded into free-text panels by depositors)

Visualization using Molmil (I)

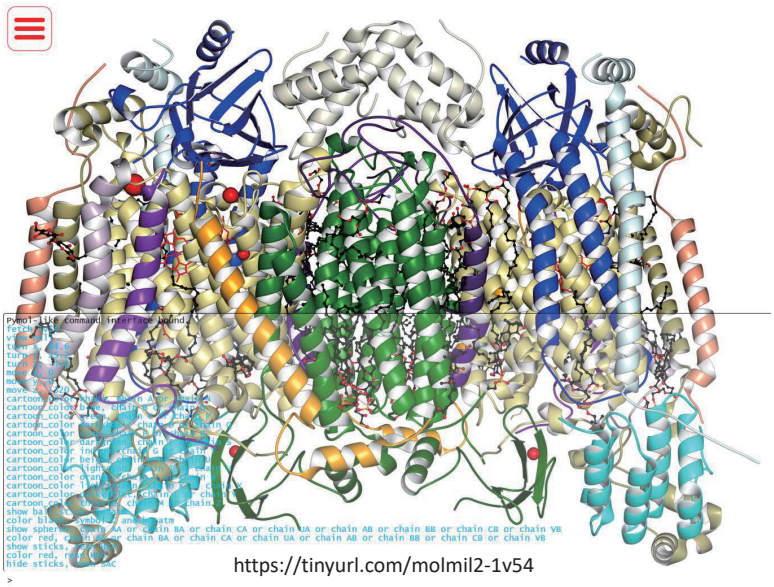
- 3D structures submitted to BMSA can be visualized by Molmil
- Files with known extensions can be simply opened by double clicking
- Alternatively, it is possible to store and load Molmil's .mjs files :





Visualization using Molmil (II)

https://pdbj.org/molmil2/



https://tinyurl.com/molmil2-1v54

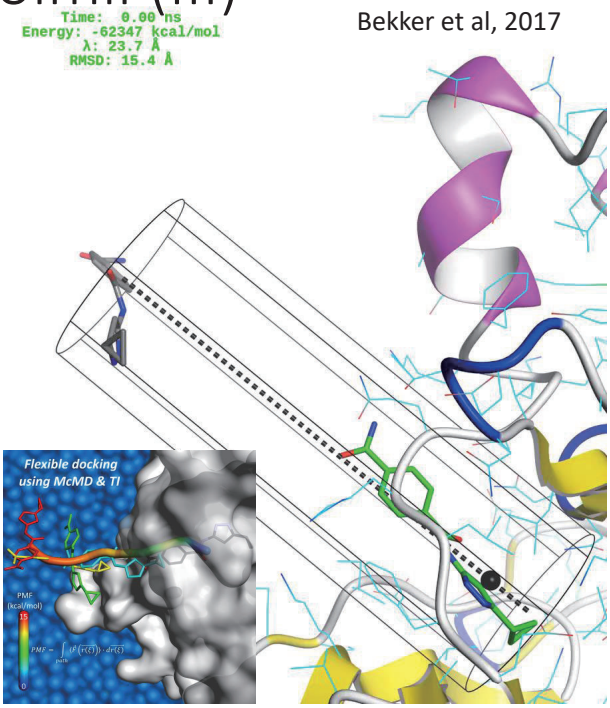
Pymol commands
- select (select sc12, resi 12 and sidechain)
- color (color cyan, model #1 and symbol C)
- cartoon_color (cartoon_color cyan, model #1)
- set_color (set_color mycolor 12 12 12)
- show (show sticks, sidechain)
- hide (hide cartoon, model #1)
- turn (turn x, 90)
- move (move x, 90)
- fetch (fetch 1crn)
- fetch-cc (fetch-cc hem)
- load (load https://pdbj.org/rest/displayPromodeEfile?format=anm&id=1ubq_1, format=pdb)
- mplay
- mstop
- origin (origin chain A)
- set (stick_radius f, depth_cue 1/0, orthoscopic on/off, cartoon_smooth_loops 0/2)
- bg_color (bg_color cyan)
- label (label resi 12 and sidechain, Res12)
- save (save filename.pdb, model #1 and name CA, 0, pdb)
- viewport (viewport 500, 500)
- view (view test, store)
- findseq (findseq ACDEF, model #1, my_seq)
- delete (delete chain A)
- edmap (edmap hetatm, 5)
- frame (frame 2)
- bond (bond resi 10 and name C, resi 1 and name N)
- stereo (stereo anaglyph)
- orient (orient chain A)
- indicate (indicate resi 32)
- quit (**)

**) Only available for molmil-app, a local version of Molmil (https://gitlab.com/pdbjapan/molmil-app)

Visualization using Molmil (III)

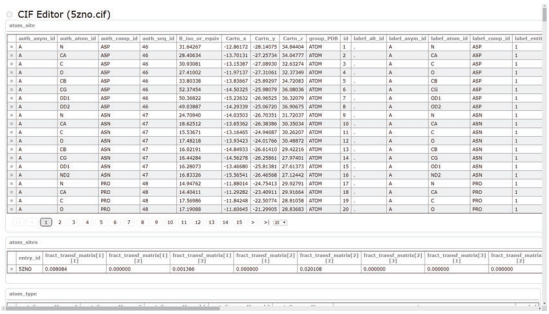
- Drag-and-drop multiple files
- Load in user-specified files of various formats:
  - PDB (**.pdb**/.ent)
  - mmCIF (.cif)
  - GROMACS (**.gro**, .trr, .xtc)
  - myPRESTO (.cod, .cor, .mnt)
  - CCP4 (.ccp4)
  - MOL MDL (.mdl, .mol, .sdl)
  - MOL2 (**.mol2**)
  - XYZ (.xyz)
  - efvet (.efvet)
  - MPBF (.mpbf)
  - MJS (**.mjs**)
- Embedding of Molmil
- Scripting of Molmil (.mjs & pymol-like commands)
- Embed commands in URLs:
- https://pdbj.org/molmil2/#fetch 3atg
- High quality image & movies

Extensions in bold are those that are automatically loaded by BSMA using Molmil when double clicking from the File manager

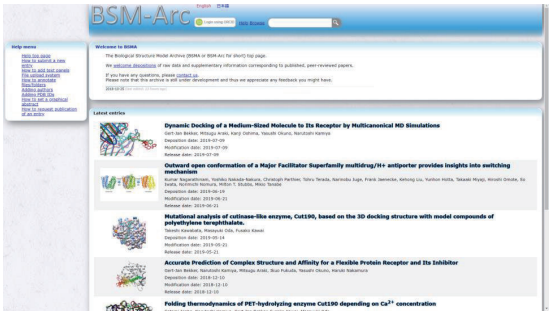


Bekker et al, 2017

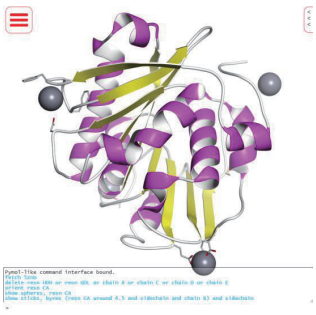
Questions



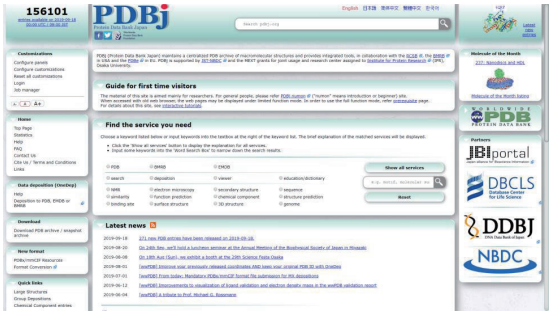
https://pdbj.org/cif-editor/



https://bsma.pdbj.org/



https://pdbj.org/molmil2/



https://pdbj.org/