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

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The PDB format: Design



- 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 metadata

| 1 | N | ASP | А | 46 | -12.862 | -28.141 | 34.844 | 1.00 31.64 |
|----|-----|-----|---|----|---------|---------|--------|------------|
| 2 | CA | ASP | А | 46 | -13.701 | -27.257 | 34.048 | 1.00 28.41 |
| 3 | С | ASP | Α | 46 | -13.154 | -27.089 | 32.633 | 1.00 30.93 |
| 4 | 0 | ASP | Α | 46 | -11.971 | -27.311 | 32.373 | 1.00 27.41 |
| 5 | CB | ASP | Α | 46 | -13.837 | -25.893 | 34.721 | 1.00 33.80 |
| 6 | CG | ASP | А | 46 | -14.503 | -25.981 | 36.080 | 1.00 52.37 |
| 7 | 0D1 | ASP | Α | 46 | -15.236 | -26.965 | 36.321 | 1.00 50.37 |
| 8 | OD2 | ASP | А | 46 | -14.293 | -25.067 | 36.907 | 1.00 49.04 |
| 9 | N | ASN | А | 47 | -14.035 | -26.784 | 31.720 | 1.00 24.71 |
| 10 | CA | ASN | Α | 47 | -13.654 | -26.384 | 30.350 | 1.00 18.63 |
| 11 | C | ASN | А | 47 | -13.165 | -24.947 | 30.262 | 1.00 15.54 |
| 12 | 0 | ASN | Α | 47 | -13.934 | -24.018 | 30.489 | 1.00 17.48 |
| 13 | CB | ASN | А | 47 | -14.849 | -26.614 | 29.422 | 1.00 16.02 |
| 14 | CG | ASN | А | 47 | -14.563 | -26.259 | 27.974 | 1.00 16.44 |
| 15 | 0D1 | ASN | Α | 47 | -13.467 | -25.814 | 27.614 | 1.00 16.28 |
| 16 | ND2 | ASN | А | 47 | -15.565 | -26.466 | 27.124 | 1.00 16.83 |
| 17 | N | PRO | Α | 48 | -11.880 | -24.754 | 29.928 | 1.00 14.95 |
| 18 | CA | PRO | Α | 48 | -11.293 | -23.489 | 29.917 | 1.00 14.40 |
| 19 | C | PRO | А | 48 | -11.842 | -22.508 | 28.811 | 1.00 17.57 |
| 20 | 0 | PRO | Α | 48 | -11.606 | -21.299 | 28.837 | 1.00 17.19 |
| 21 | CB | PRO | А | 48 | -9.801 | -23.683 | 29.699 | 1.00 21.37 |
| 22 | CG | PRO | Α | 48 | -9.759 | -25.006 | 29.000 | 1.00 23.14 |
| 23 | CD | PRO | А | 48 | -10.888 | -25.795 | 29.599 | 1.00 17.37 |
| 24 | N | TYR | Α | 49 | -12.572 | -23.088 | 27.863 | 1.00 16.03 |
| 25 | CA | TYR | Α | 49 | -13.070 | -22.336 | 26.716 | 1.00 14.59 |
| 26 | C | TYR | А | 49 | -14.525 | -21.881 | 26.842 | 1.00 16.63 |
| 27 | 0 | TYR | А | 49 | -15.048 | -21.229 | 25.936 | 1.00 14.89 |
| 28 | CB | TYR | Α | 49 | -12.912 | -23.172 | 25.444 | 1.00 15.50 |
| 29 | CG | TYR | Α | 49 | -11.521 | -23.749 | 25.285 | 1.00 14.95 |
| 30 | CD1 | TYR | Α | 49 | -10.393 | -22.959 | 25.494 | 1.00 17.86 |
| 31 | CD2 | TYR | А | 49 | -11.336 | -25.078 | 24.955 | 1.00 18.35 |
| 32 | CE1 | TYR | А | 49 | -9.122 | -23.481 | 25.361 | 1.00 15.32 |
| 33 | CE2 | TYR | А | 49 | -10.064 | -25.614 | 24.818 | 1.00 21.68 |
| 34 | CZ | TYR | Α | 49 | -8.963 | -24.809 | 25.030 | 1.00 24.11 |
| 35 | OH | TYR | Α | 49 | -7.692 | -25.323 | 24.898 | 1.00 26.68 |
| | | | | | | | | |



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



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_5ZNO | | |
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| audit_conform.dict_location | | |
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| '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 ? | | |
| # | | |
| _citation.country | US | |
| citation.id | primary | |
| citation.journal_abbrev | Biochemistry | |
| _citation.journal_id_ASTM | BICHAW | |
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| Structural Dynamics of the PET-Deg | rading Cutinase-li | ke Enzyme from |
| Saccharomonospora viridis AHK190 in | Substrate-Bound S | tates Elucidates th |
| Ca2+-Driven Catalytic Cycle. | | |
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| | 2018 | 01-00-004 |
| citation.pdbx_database_id_DOI | 10.1021/acs.bioch | em.8bUU624 |
| citation.pdbx database id PubMed | 30110540 | |

data item = name + value

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 webenvironment
- 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/cifparsers)
- 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 pdbbundle 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)

Main menu

CIF Editor

- Three options:
 - Main menu (\bigcirc) \rightarrow Open mmCIF file \rightarrow 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

Item menu (atom_site.label_atom_id)

| Main menu→(| CIF Edito | or (5zno.) | cif) | eu (ete | na cita) | | | | | | | | | | ĺ |
|----------------|----------------|---------------------------|-----------------------|---------------|---------------------------|------------|-------------------|-----------|-------------------|--------|-------------|----------------------|------------------------|------------------|--------------------|
| | atom_site | | gory me | iu (ato | m_site) | | | | | | | | | | |
| | 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 la | abel_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. | | Α | N | ASP | 1 |
| | × A | CA | ASP | 46 | 28.40634 | -13.70131 | -27.25734 | 34.04777 | ATOM | 2. | | Α | CA | ASP | 1 |
| | × A | С | ASP | 46 | 30.93081 | -13.15387 | -27.08930 | 32.63274 | ATOM | 3. | | Α | С | ASP | 1 |
| | × A | 0 | ASP | 46 | 27.41002 | -11.97137 | -27.31061 | 32.37349 | ATOM | 4. | | Α | 0 | ASP | 1 |
| | × A | CB | ASP | 46 | 33.80338 | -13.83667 | -25.89297 | 34.72083 | ATOM | 5. | | Α | CB | ASP | 1 |
| | × A | CG | ASP | 46 | 52.37454 | -14.50325 | -25.98079 | 36.08036 | ATOM | 6. | | Α | CG | ASP | 1 |
| Table Constant | × A | OD1 | ASP | 46 | 50.36822 | -15.23632 | -26.96525 | 36.32079 | ATOM | 7. | | Α | OD1 | ASP | 1 |
| lable for the | × A | OD2 | ASP | 46 | 49.03887 | -14.29339 | -25.06720 | 36.90675 | ATOM | 8. | | Α | OD2 | ASP | 1 |
| atom cita | ×A | N | ASN | 47 | 24.70940 | -14.03503 | -26.70351 | 31.72037 | ATOM | 9. | | Α | N | ASN | 1 |
| atom_site | × A | CA | ASN | 47 | 18.62512 | -13.65362 | -26.38386 | 30.35034 | ATOM | 10 . | | Α | CA | ASN | 1 |
| catogory | × A | С | ASN | 47 | 15.53671 | -13.16465 | -24.94687 | 30.26207 | ATOM | 11 . | | Α | С | ASN | 1 |
| category | × A | 0 | ASN | 47 | 17.48218 | -13.93423 | -24.01766 | 30.48872 | ATOM | 12 . | | Α | 0 | ASN | 1 |
| | × A | CB | ASN | 47 | 16.02191 | -14.84933 | -26.61410 | 29.42216 | ATOM | 13 . | | Α | CB | ASN | 1 |
| | × A | CG | ASN | 47 | 16.44284 | -14.56278 | -26.25861 | 27.97401 | ATOM | 14 . | | Α | CG | ASN | 1 |
| | × A | OD1 | ASN | 47 | 16.28073 | -13.46680 | -25.81381 | 27.61373 | ATOM | 15 . | | Α | OD1 | ASN | 1 |
| | × A | ND2 | ASN | 47 | 16.83326 | -15.56541 | -26.46568 | 27.12442 | ATOM | 16 . | | Α | ND2 | ASN | 1 |
| | × A | N | PRO | 48 | 14.94762 | -11.88014 | -24.75413 | 29.92791 | ATOM | 17 . | | Α | N | PRO | 1 |
| | × A | CA | PRO | 48 | 14.40411 | -11.29282 | -23.40911 | 29.91664 | ATOM | 18 . | | Α | CA | PRO | 1 |
| | × A | С | PRO | 48 | 17.56986 | -11.84248 | -22.50774 | 28.81058 | ATOM | 19 . | | A | С | PRO | 1 |
| | × A | 0 | PRO | 48 | 17.19088 | -11.60645 | -21.29905 | 28.83683 | ATOM | 20 . | | А | 0 | PRO | 1 |
| Table for the | | 2 3 4 | 5 6 7 | 8 9 10 | 11 12 13 | 14 15 | > > 20 | • | — Pa | agi | natior | I | | | |
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| category | | | | | | | | | | | | | | | , |

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 \rightarrow 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 \rightarrow 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 \rightarrow Delete
- Item specific operations from Item menu \rightarrow 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 userinputted 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 \rightarrow 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 \rightarrow Merge additional mmCIF file \rightarrow 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 \rightarrow 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)

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| | Ŵ:Ø: <mark>%</mark> | 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 |
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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/



|--|

- select (select sc12, resi 12 and sidechain)
- COLOT (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)
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- move (move x, 90)
- fetch (fetch 1crn)
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- 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)
- **QUİT** (**) **) Only available for molmil-app, a local version of Molmil (https://gitlab.com/pdbjapan/molmil-app)

- 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



Questions

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| | | c | ASN | 47 | 15.53671 | -13.16462 | 5 -24.94587 | 30.26203 | ATOM 7 | 11 | | A | c | ASN | 1 |
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