



PDBj tools and services for analyzing, editing and registering structural data.

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PDBj Luncheon Seminar – PSSJ 2021

PDBj website renewed

- Alongside transitioning to a new server, the software side was also renewed
 - New client-side implementation (<https://pdbj.org/>)
 - New REST interface (<https://pdbj.org/help/rest-interface>)
- New/improved services:
 - RDB query builder (basic interface around SQL search)
 - Batch data fetch & file download
 - Improved interfacing with Molmil
 - New sequence navigator interface
 - New Promode Elastic interface
 - New Data Archive (<https://data.pdbj.org/>)
 - New RDF site design (<https://rdf.wwpdb.org/>)

PDBj Top page & omni search

178938

PDB entries from 2021-06-16



PDBj
Protein Data Bank Japan



Worldwide Protein Data Bank Foundation

English 日本語 简体中文 繁體中文 한국어

Search pdbj.org

Select display language

Main menu

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Top Page
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Data deposition (OneDep)

Help
Deposition to PDB, EMDB or BMRB

Download

Download PDB archive / snapshot archive

Standard format

PDBx/mmCIF Resources
Format Conversion
PDBx/mmCIF editor

Quick links

Help
non-PDB format compatible
Group Depositions
Chemical Component entries
Latest entries

Search services

Help
Search PDB (PDBj Mine)
Search PDBj RDB
Chemie search

About PDBj

PDBj (Protein Data Bank Japan) is a national research project of the Institute for Protein Research, Osaka University. We maintain the single global PDB/BMRB/EMDB archives of macromolecular structures and provide integrated tools, in collaboration with RCSB PDB and BMRB in the USA, and PDBj in the EU. PDBj is now providing a new omni search service that incorporates cytochrome c (PDBID: 1cyc), which was the first structure determined in Japan.

Omni search: search everything (Japanese OK)

Find the service you need

Choose a keyword listed below or input keywords into the textbox at the right of the keyword list. The brief explanation of the matched services will be displayed.

- PDB
- BMRB
- EMDB
- search
- deposition
- viewer
- education/dictionary
- NMR
- electron microscopy
- secondary structure
- sequence
- similarity
- function prediction
- chemical component
- structure prediction
- binding site
- surface structure
- 3D structure
- genome
- RDF
- SPARQL
- gene
- disease
- drug

Select by category

Search which service best fits your goal

Show all services

e.g. motif molecular surf

Reset

Service keyword search

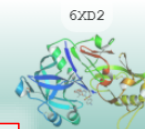
Latest news

- 2021-06-16 [195 new PDB entries have been released on 2021-06-16.](#)
- 2021-06-09 [\[wwPDB\] Congratulations to Poster Prize Winners](#)
- 2021-06-02 [\[wwPDB\] Consistent Format for Validation and Coordinate Data](#)
- 2021-05-27 [PDBj website update](#)
- 2021-05-23 [2021 PDBj web server transition](#)
- 2021-04-21 [\[wwPDB\] Future Planning: Entries with extended PDB and CCD ID codes will be distributed in PDBx/mmCIF format only](#)
- 2021-04-10 [\[wwPDB\] New pdb-l Bulletin Board](#)
- 2021-04-07 [\[wwPDB\] Biocurator Milestone: >10,000 Depositions Processed](#)
- 2021-04-01 [\[wwPDB\] Improved support for extended PDBx/mmCIF structure factor files](#)
- 2021-03-30 [\[wwPDB\] OneDep highlights curated assemblies for review in Mol*](#)

All news

COVID-19 structures

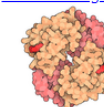
Links to other databases by PDBj



Latest new entries

Molecule of the Month

Fetal Hemoglobin



Article List



Hot Structural News on COVID-19

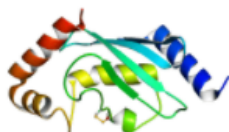


大阪大学
OSAKA UNIVERSITY

ubiquitin

Query parameters

2YB6



Native human Rad6

Descriptor: BETA-MERCAPTOETHANOL, CHLORIDE ION, UBIQUITIN-CONJUGATING ENZYME E2 B
Authors: [Hibbert, R.G.](#), [Sixma, T.K.](#)
Deposit date: 2011-03-02
Release date: 2011-04-20
Last modified: 2011-07-13
Method: X-RAY DIFFRACTION (1.5 Å)
Cite: **E3 Ligase Rad18 Promotes Monoubiquitination Rather Than Ubiquitin Chain Formation by E2 Enzyme Rad6.**
Proc.Natl.Acad.Sci.USA, 108, 2011

Modify keyword search query (Japanese OK)

Download arbitrary results for all (84) matches

Visualize entry using Molmil

Search results info

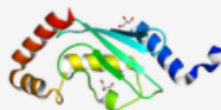
Total results: 84
Displayed results: 25
Sorted by: Hit score (from highest)
Query: ubiquitin
Deposition date: 2010-01-01 -
Number of Chains: - 1
Resolution: - 1.5
Source: homo sapiens

Download results

Download files

Filter results

5LBN



High-resolution crystal structure of the UBC core domain of UBE2E1/UbcH6

Descriptor: GLYCEROL, Ubiquitin-conjugating enzyme E2 E1
Authors: [Anandapadamanaban, M.](#), [Moche, M.](#), [Sunnerhagen, M.](#)
Deposit date: 2016-06-16
Release date: 2018-02-14
Method: X-RAY DIFFRACTION (1.42 Å)
Cite: **Structure of a TRIM21 - UBE2E1 complex reveals the specificity of E2 and ubiquitin recognition by TRIM E3 RINGS**
To Be Published

Batch download files for all (84) matches

Download entry's mmCIF file

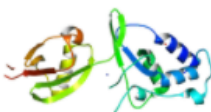
Return to filter page

Sort by

Hit score (from highest)

- PDBID ascending
- PDBID descending
- Deposition date (from oldest)
- Deposition date (from newest)
- Release date (from oldest)
- Release date (from newest)
- Resolution (from highest)

4A3P



Structure of USP15 DUSP-UBL deletion mutant

Descriptor: ACETATE ION, IODIDE ION, UBIQUITIN CARBOXYL-TERMINAL HYDROLASE 15
Authors: [Elliott, P.R.](#), [Liu, H.](#), [Pastok, M.W.](#), [Grossmann, G.J.](#), [Rigden, D.J.](#), [Clague, M.J.](#), [Urbe, S.](#), [Barsukov, I.L.](#)
Deposit date: 2011-10-03
Release date: 2011-11-16
Method: X-RAY DIFFRACTION (1.4 Å)
Cite: **Structural Variability of the Ubiquitin Specific Protease Dusp-Ubl Double Domains.**
FEBS Lett., 585, 2011

Show entry page

Results pages

Quick search & filtering

PDB filters

Query:

Title:

Release date: -

Deposition date: -

Last modification date: -

Deposition authors:

Citation authors:

Publication title:

Journal name:

Publication year:

Publication volume:

primary:

Contains Chain Type:

- ▶ polypeptide(D): Ignore
- ▶ polypeptide(L): Ignore
- ▶ polydeoxyribonucleotide: Ignore
- ▶ polyribonucleotide: Ignore
- ▶ polydeoxyribonucleotide/polyribonucleotide hybrid: Ignore
- ▶ cyclic-pseudo-peptide: Ignore
- ▶ other: Ignore
- ▶ peptide nucleic acid: Ignore

Descriptor:

Other DB:

Ligands and Prosthetic groups:

Number of Chains: -

Chain length: -

Method:

Resolution: -

Source:

Host species:

Options
Results: 84

Show results

Reset filters

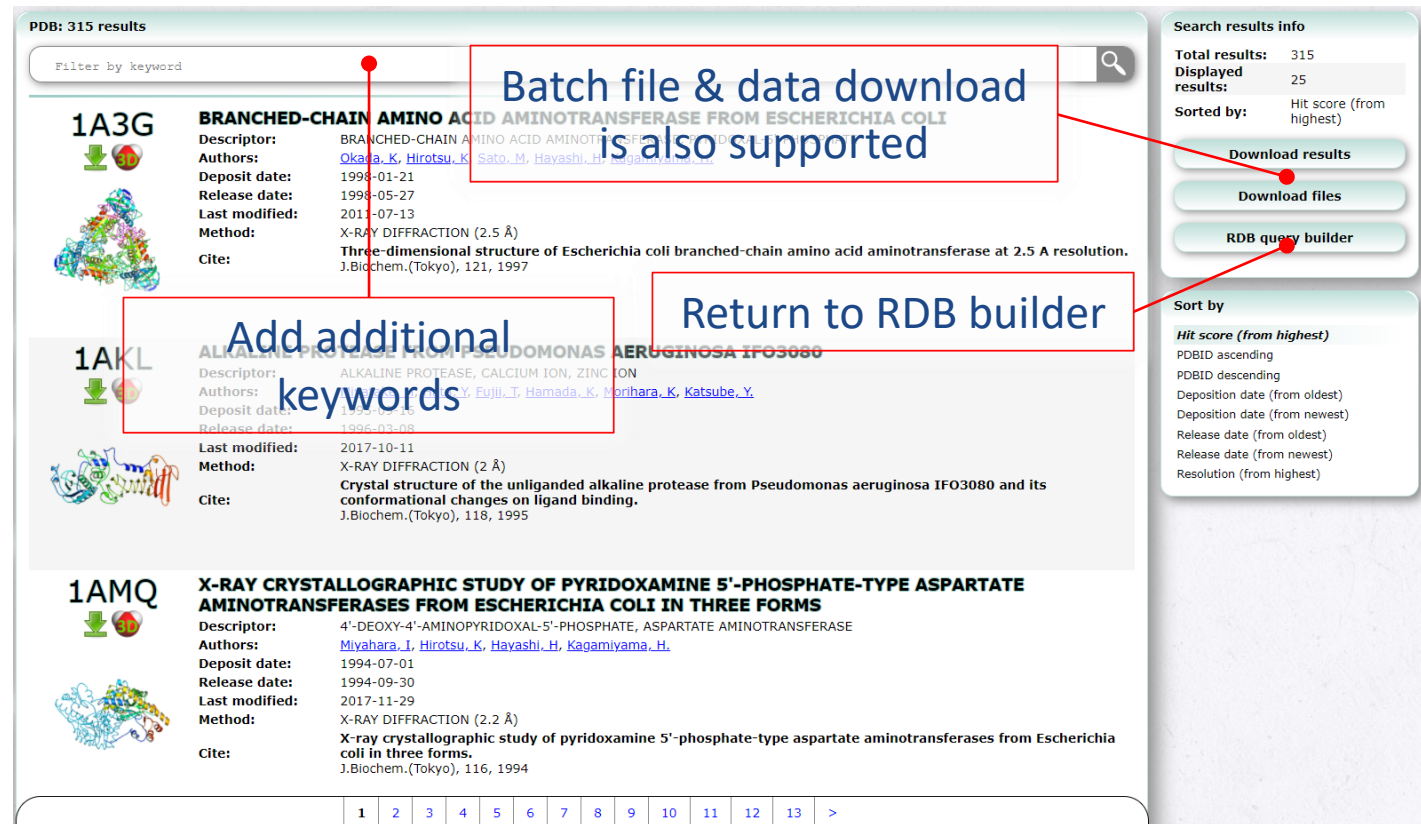
Number of matches is automatically updated

Show results for filters

- Performs fuzzy search
- Old “Advanced search” has been integrated with Quick Search
- Filters can be used to filter the results based on a small set of criteria:
 - Main menu: “Search PDB (PDBj Mine)” / “PDB検索 (PDBj Mine)”
 - During search: “Filter results” / “結果フィルタ”

SQL search: RDB builder & query based

- Quick search uses fuzzy searching over a subset of PDB data
- SQL search enables very niche searches, but is difficult to use:
 - Requires knowledge of mmCIF dictionary structure
 - Requires knowledge of SQL syntax
- RDB builder provides a basic GUI to enable filtering by any data item in the Mine 2 RDB (PDB metadata & pdbjplus data)
- “Search PDBj RDB” / “PDB詳細検索” from the menu



PDB: 315 results

Filter by keyword

1A3G BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE FROM ESCHERICHIA COLI
 Descriptor: BRANCHED-CHAIN AMINO ACID AMINOTRANSFERASE FROM ESCHERICHIA COLI
 Authors: Okada, K, Hirotsu, K, Sato, M, Hayashi, H, Kagamiyama, H
 Deposit date: 1998-01-21
 Release date: 1998-05-27
 Last modified: 2011-07-13
 Method: X-RAY DIFFRACTION (2.5 Å)
 Cite: Three-dimensional structure of Escherichia coli branched-chain amino acid aminotransferase at 2.5 Å resolution. J.Biochem.(Tokyo), 121, 1997

1AKL ALKALINE PROTEASE FROM PSEUDOMONAS AERUGINOSA IFO3080
 Descriptor: ALKALINE PROTEASE, CALCIUM ION, ZINC ION
 Authors: Fujii, T, Hamada, K, Morihara, K, Katsube, Y
 Deposit date: 1995-03-15
 Release date: 1995-03-08
 Last modified: 2017-10-11
 Method: X-RAY DIFFRACTION (2 Å)
 Cite: Crystal structure of the unliganded alkaline protease from Pseudomonas aeruginosa IFO3080 and its conformational changes on ligand binding. J.Biochem.(Tokyo), 118, 1995

1AMQ X-RAY CRYSTALLOGRAPHIC STUDY OF PYRIDOXAMINE 5'-PHOSPHATE-TYPE ASPARTATE AMINOTRANSFERASES FROM ESCHERICHIA COLI IN THREE FORMS
 Descriptor: 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE, ASPARTATE AMINOTRANSFERASE
 Authors: Miyahara, J, Hirotsu, K, Hayashi, H, Kagamiyama, H
 Deposit date: 1994-07-01
 Release date: 1994-09-30
 Last modified: 2017-11-29
 Method: X-RAY DIFFRACTION (2.2 Å)
 Cite: X-ray crystallographic study of pyridoxamine 5'-phosphate-type aspartate aminotransferases from Escherichia coli in three forms. J.Biochem.(Tokyo), 116, 1994

Batch file & data download is also supported

Add additional keywords

Return to RDB builder

Search results info

Total results: 315
 Displayed results: 25
 Sorted by: Hit score (from highest)

Download results
 Download files
 RDB query builder

Sort by

Hit score (from highest)
 PDBID ascending
 PDBID descending
 Deposition date (from oldest)
 Deposition date (from newest)
 Release date (from oldest)
 Release date (from newest)
 Resolution (from highest)

- RDB implementation docs: <https://pd bj.org/rdb/docs>
- RDB builder: <https://pd bj.org/rdb/build>
- Local install: <https://gitlab.com/pdbjapan/mine2update>

RDB builder: create filters

Results type (PDB/Chemie/BIRD for pretty, General for SQL Query search)

Add new filter

5: add filter

RDB Query Builder (Advanced Search)

Schema

- ccmodel
- prd
- pdbj**
- vrpt
- cc
- sifts
- misc

1: select the schema

Category

- chem_comp
- chem_comp_atom
- chem_link
- citation**
- citation_author
- citation_author_pdbmplus

2: select the category

Item

- journal_abbrev
- journal_id_ASTM
- journal_id_CSD
- journal_id_ISSN**
- journal_issue
- journal_volume
- language

3: select the data-item to filter by

Filter

- text

4: filter type

Options

- Add Filter
- Type
- Search
- Execute search**
- Show RDB documentation
- RDB Query Builder help
- SQL query based search:
- SQL Query search**

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WORLDWIDE PDB and BIRD
PROTEIN DATA BANK

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RDB docs

SQL Search

Search query: `select distinct pdbj_extern.pdbid from pdbj_extern where (pdbj_extern."journal_id_ISSN" LIKE '1194-2051' OR pdbj_extern."journal_id_ISSN" LIKE '10021-9240') AND pdbj_extern.id code "protein"`

Total number of results: 315

Download options:
Download data
Download SQL results as csv
Download SQL results as xml
Download SQL results as json

Can be used to manually refine a query

Manually input SQL query

Mine 2 RDB Documentation - Protein Data Bank Japan - Google Chrome

pd bj | cc | ccmodel | prd | vrpt | emdb

Mine 2 RDB Documentation

PDB's Mine 2 RDB interactive documentation. The Mine 2 RDB consists of the common data in each PDB partner "PDB/mmCIF" and PDB's additional annotations "PDBjplus".

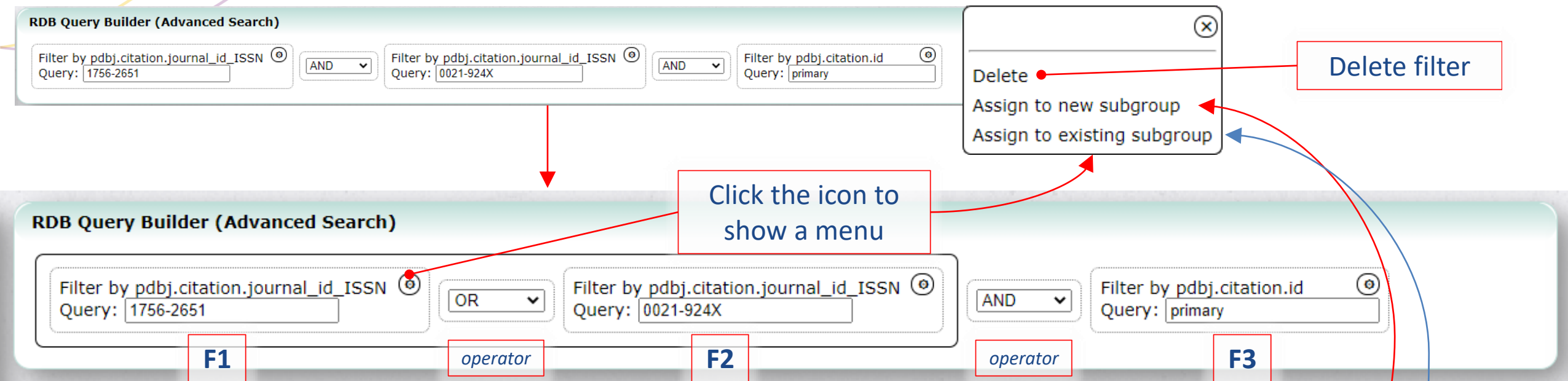
Browse through the categories or use the search bar to search and filter the results. For details regarding querying to the database see our [SQL Search service](#) and the corresponding [SQL Search help page](#).

Search:

The Mine 2 RDB holds 247 tables:

- + atom
- + audit
- + brief
- + cell
- + chem
- + citation
- + database
- + diffrr
- + em
- + entity
- + entry
- + exptl
- + gene
- + history
- + link
- + ndb
- + pdbx
- + phasing
- + publ
- + refine
- + refin
- + refs

RDB builder: query example



The image shows two screenshots of the RDB Query Builder (Advanced Search) interface. The top screenshot shows three filters: 'Filter by pdbj.citation.journal_id_ISSN' with value '1756-2651', 'Filter by pdbj.citation.journal_id_ISSN' with value '0021-924X', and 'Filter by pdbj.citation.id' with value 'primary'. The operators between them are 'AND'. A red arrow points from the first filter to the second screenshot. The second screenshot shows the same three filters, but the operator between the first and second filters is now 'OR'. A red box labeled 'F1' is under the first filter, 'operator' is under the 'OR' dropdown, 'F2' is under the second filter, 'operator' is under the 'AND' dropdown, and 'F3' is under the third filter. A red box labeled 'Click the icon to show a menu' points to a small circular icon with a plus sign on the first filter. A red box labeled 'Delete filter' points to a red dot on the same icon. A dropdown menu is shown to the right of the first filter with options: 'Delete', 'Assign to new subgroup', and 'Assign to existing subgroup'. Red arrows point from the 'Delete filter' box to the 'Delete' option, and from the 'Click the icon to show a menu' box to the 'Assign to new subgroup' option. A blue arrow points from the 'Assign to existing subgroup' option to the 'AND' operator dropdown in the second screenshot.

How to formulate the above query (F1 OR F2) AND F3

- 1: create each individual filter F1, F2, F3 → F1 AND F2 AND F3
- 2: assign F1 to new subgroup → (F1) AND F2 AND F3
- 3: assign F2 to existing subgroup: select F1 → (F1 AND F2) AND F3
- 4: change operator → (F1 OR F2) and F3

Same query editor interface as used by the filtering function in our CIF Editor

Mine PDB entry pages

Versioned files

5ZRR
Higher resolution structure (1st entity)

Crystal structure of PET-degrading cutinase Cut190 S176A/S226P/R228S mutant in monoethyl succinate bound state

Summary for 5ZRR

Related: 5ZNO 5ZRO 5ZRS

Descriptor: Alpha/beta-hydrolase family protein, 4-ethoxy-4-oxobutanoic acid, ZINC ION, ... (6 entities in total)

Functional Keywords: beta-hydrolase, alpha/beta-hydrolase fold, protein engineering, thermostability, hydrolase

Total number of polymer chains: 1

Total formula weight: 29805.59

Authors: Numoto, N., Kamiya, N., Bekker, G.J., Yamagami, Y., Inaba, S., Ishii, K., Uchiyama, S., Kawai, F., Ito, N., Oda, M., Bekker, G.J., Inaba, S., Ishii, K., Ito, N., Kamiya, N., Kawai, F., Numoto, N., Oda, M., Uchiyama, S., Yamagami, Y.

Primary citation: Structural Dynamics of the PET-Degrading Cutinase-Like Enzyme from *Saccharomonospora viridis* AHK190 in Substrate-Bound States Elucidates the Ca²⁺-Driven Catalytic Cycle. *Biochemistry*, 57:5289-5300, 2018. DOI: 10.1021/acs.biochem.8b00624

Experimental method: X-RAY DIFFRACTION (1.34 Å)

Structure validation

Metric	Percentile Ranks	Value
Rfree	0.185	0.185
Clashscore	0	0
Ramachandran outliers	0	0
Sidechain outliers	0.9%	0.9%
RSRZ outliers	3.4%	3.4%

Database information: wwPDB DOI Landing Page, Torodumi, CATH, VAST, PISA, eF-site, 5zrr-A, BindingMOAD, 5zrr, Electron Density Map, wwPDB/RDF, BSM-Arc, BSM00004, UniProt, Pfam, PF03403, Promode Elastic, 5zrr

History

Please read more about PDB versioning on [our help page](#).

Version	Date	Type
1-0	2018-09-12	Initial release
1-1	2018-09-26	Data collection, Database references

Resources (version 1-1)

File format	File name (file size)	Display
PDBx/mmCIF	pdb_0005zrr_xyz_v1-1.cif.gz (85.51 KB)	Display
all	pdb_0005zrr_xyz_v1-1.xml.gz (106.78 KB)	Display
PDBML	pdb_0005zrr_xyz-no-atom_v1-1.xml.gz (23.89 KB)	Display
ext-atom	pdb_0005zrr_xyz-ext-atom_v1-1.xml.gz (64.94 KB)	Display

Structure Validation summary

View AU

Links to other databases

Molmil eF-site viewer

Molmil EDMap viewer

Download/ダウンロード lists available files for an entry (latest version)

File format	File name (file size)	Display
PDBx/mmCIF	5zrr.cif.gz (85.51 KB)	Display
all	5zrr.xml.gz (106.78 KB)	Display (Tree)
PDBx/mmJSON	5zrr-noatom.json.gz (15.91 KB)	Display (Header)
add only	5zrr-ext-atom.json.gz (421.00 B)	Display
PDBML	5zrr-no-atom.xml.gz (23.89 KB)	Display
ext-atom	5zrr-ext-atom.xml.gz (64.94 KB)	Display
PDB	5zrr.ent.gz (53.64 KB)	Display
RDF	5zrr.rdf.gz (51.77 KB)	Visualize
Structure factors	5zrr-structure-factors.gz (1.83 MB)	Display
Biological unit (PDB format)	5zrr-bu.xml.gz (48.56 KB) (A)	Display
PDF	5zrr-validation-edf.gz (568.65 KB)	Display
PDF-full	5zrr-full-validation-edf.gz (569.39 KB)	Display
Validation reports	5zrr-validation.xml.gz (14.86 KB)	Display
PNC	5zrr-validation-percentile-validation-pnc.gz (441.35 KB)	Display
SVC	5zrr-validation-percentile-validation-svc.gz (931.00 B)	Display
Zfo-fc (PDB/mmCIF)	5zrr-validation-zfo-fc-mao-coef.cif.gz (515.60 KB)	Display
fo-fc (PDB/mmCIF)	5zrr-validation-fo-fc-mao-coef.cif.gz (486.58 KB)	Display
Zfo-fc (MTZ)	5zrr-validation-zfo-fc-mao-coef.mtz (1.22 MB)	Visualize
fo-fc (MTZ)	5zrr-validation-fo-fc-mao-coef.mtz (1.22 MB)	Visualize

Structure styling options

Quick styling options:

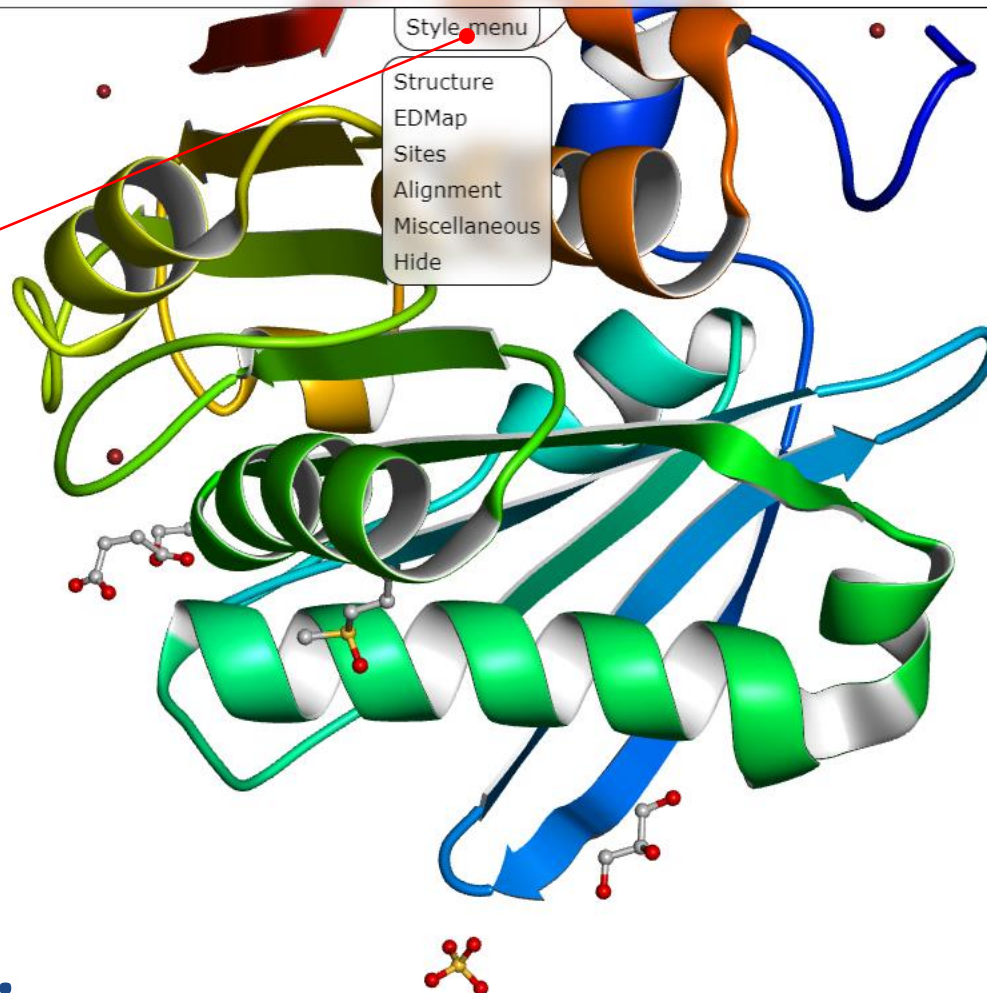
Default Default with sidechains Cartoon Cartoon with sidechains Cartoon, colored by chain Cartoon, color by chain with sidechains Sticks (CPK) Sticks (CPK), colored by chain Wireframe (CPK) Wireframe (CPK), colored by chain

For more advanced styling, please use the command line (bottom of the page), the structure menu (right-side of the page) or right-click on an atom/cartoon to show a context menu with styling options.

Visualization of Asymmetric Unit using Molmil

Click these buttons to quickly change the style

Click here to show the new styling menu, to style the structure (AU), BU (if available), EMap interface, show special sites, show alignments (e.g. seqnavi), or to hide the panel.

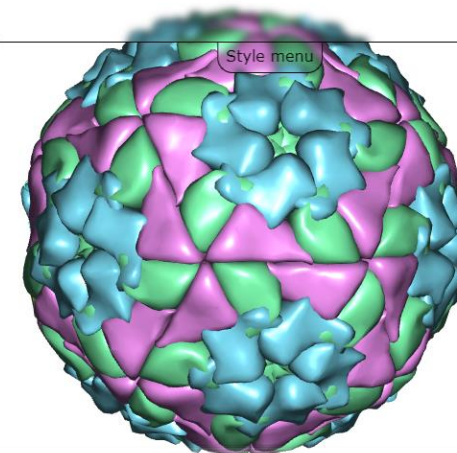


BU selection/visualization

Biological unit styling options

Unit selection:

Unit repr.:




Visualization of Biological Unit using Molmil

Molmil AU/BU viewer

eF-site Molmil viewer



5zrr-A.mpbf  Mesh options for 5zrr-A.mpbf

A: 105, A: 118, A: 155, A: 547, A: 603, A: 254, A: 540, A: 645

Sequence: E, E, ,

Description: binding site for residue ZN A 403

Wireframe Solid

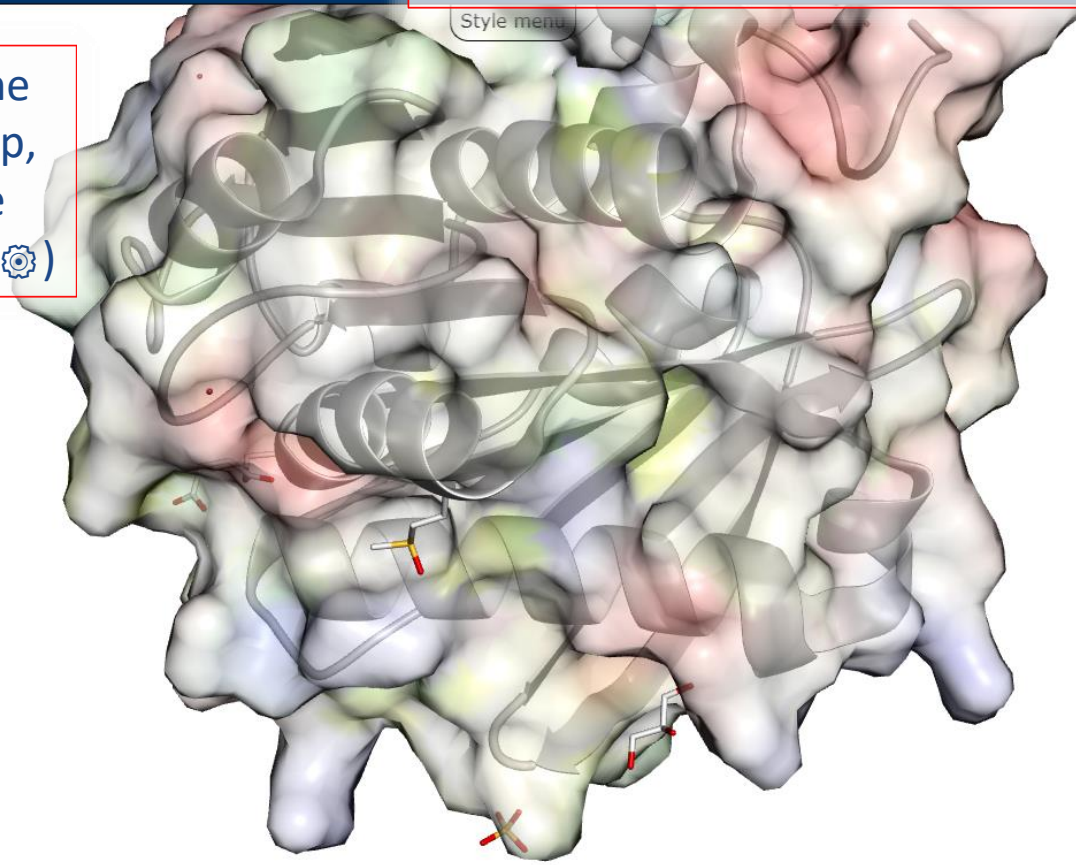
Transparency:

Close

Change representation (wireframe/solid) and transparency (solid mode) of surface.

Toggle sites (stick model)

To change the style of a map, click on the options icon (⚙)



EDMap

EDMap options

Type of map: Both 2fo-fc fo-fc
 Map size: 25 Å
 Contour level (2fo-fc): 1 σ
 Contour level (fo-fc): 2 σ

Downloads: [Structure factors](#) [2fo-fc map \(cif\)](#) [fo-fc map \(cif\)](#) [2fo-fc map \(mtz\)](#) [fo-fc map \(mtz\)](#) [2fo-fc map \(ccp4\)](#) [fo-fc map \(ccp4\)](#)

Download edmap_2fo-fc_0.ccp4

Download edmap_fo-fc_0.ccp4

Mesh options for edmap_2fo-fc_0.ccp4

Wireframe Solid

Transparency:

Contour level 1 σ

To change the style of a map, click on the options icon (⚙)

Click on an atom, then click on the button to generate the map (by default both 2fo-fc & fo-fc maps are generated at 25 Å around the selected atom)

Delete the map

Change representation (wireframe/solid), color, transparency (solid mode) and modify the contour level σ .

```
Pymol-like command interface bound.
fetch 5zrr
repr lines
style-if edmap, both
Clicked on atom: C (1148) - ALA 194 - Chain A
```


Sequence Neighbor (Navigator)

Sequence Navigator

Mode: PDB entry Custom sequence

PDB ID:

Asym ID:

Clustering:

Alignment of **5zrr_A** vs **5zno_A**
 Initial RMSD: 1.32 Å (over all matched residues)
 Optimized RMSD: 0.34 Å (over all green matched residues)

Sequence Neighbor

Chains

Entity	Asym IDs
1	5zrr_A

Chain list

Click on a chain to show homologues chains within the PDB.
 Click on an exact match to show the superposition between a chain and a match.

100% sequence identity matching chains

Number of Exact matches: 5

Alignment of **5zrr_A** vs **5zno_A**
 Initial RMSD: 1.32 Å (over all matched residues)
 Optimized RMSD: 0.34 Å (over all green matched residues)

```

43  DNPYERGGPOPTEDSIEAIRGPFVSATERVSSFASGFGGGTIYYPRETDEGTFGAVAVAPG 142
46  DNPYERGGPOPTEDSIEAIRGPFVSATERVSSFASGFGGGTIYYPRETDEGTFGAVAVAPG 105
103 FTASQGSMSWYGERVASQGFIVFTIDNTRLDQPGQRQLLAALDYLVERSDRKYRERL 162
106 FTASQGSMSWYGERVASQGFIVFTIDNTRLDQPGQRQLLAALDYLVERSDRKYRERL 165
163 DPNRLAVMGHAMGGGSLKATV*RPFLKASIPLPWNLKDTWQVQVPTFIIGAEIDTIA 222
166 DPNRLAVMGHAMGGGSLKATV*MRPFLKASIPLPWNLKDTWQVQVPTFIIGAEIDTIA 225
223 PVSTHAKPFYELPSSLPKAYMELDGATHFAPNIPNTTIARVI*SWLKRFDVDETRY 262
  
```

Superposition excludes flexible loops (to optimize superposition)

Sequence Navigator for 5zrr_A

Exact matches to 5zrr_A: 5zno_A * 5zno_B * 5zrq_A * 5zrs_A * 7cef_A *

Click on the ID to show a menu

Hit:	5zno_A *
Sequence identity:	100%
Sequence positives:	100%
E-value:	0
Score:	1410
Query coverage:	100%
Compound:	Alpha/beta View PDB entry page of 5zno

Alignment:

```

5zrr_A1  GFQDNFYERGGPDPEDSIEAIRGPFVSATERVSSFASGFGGGTIYYPRETDEGTFGAVAV 60
5zno_A1  GFQDNFYERGGPDPEDSIEAIRGPFVSATERVSSFASGFGGGTIYYPRETDEGTFGAVAV 60
5zrr_A61  APGFTASQGSMSWYGERVASQGFIVFTIDNTRLDQPGQRQLLAALDYLVERSDRKYR 120
5zno_A61  APGFTASQGSMSWYGERVASQGFIVFTIDNTRLDQPGQRQLLAALDYLVERSDRKYR 120
5zrr_A121 ERLDPNRLAVMGHAMGGGSLKATV*MRPFLKASIPLPWNLKDTWQVQVPTFIIGAE 180
5zno_A121 ERLDPNRLAVMGHAMGGGSLKATV*MRPFLKASIPLPWNLKDTWQVQVPTFIIGAE 180
5zrr_A181 TIAFVSTHAKPFYELPSSLPKAYMELDGATHFAPNIPNTTIARVI*SWLKRFDVDE 240
5zno_A181 TIAFVSTHAKPFYELPSSLPKAYMELDGATHFAPNIPNTTIARVI*SWLKRFDVDE 240
5zrr_A241 SQFLCPNPTDRAIEEVRSTCKRLN 265
5zno_A241 SQFLCPNPTDRAIEEVRSTCKRLN 265
  
```

Exact matches to 5zno_A: 5zno_B * 5zrq_A * 5zrr_A * 5zrs_A * 7cef_A *

Hit:	7cef_A *
Sequence identity:	100%
Sequence positives:	100%
E-value:	0
Score:	1391
Query coverage:	99%
Compound:	Alpha/beta hydrolase family protein, CALCIUM ION, ZINC ION, water

Alignment:

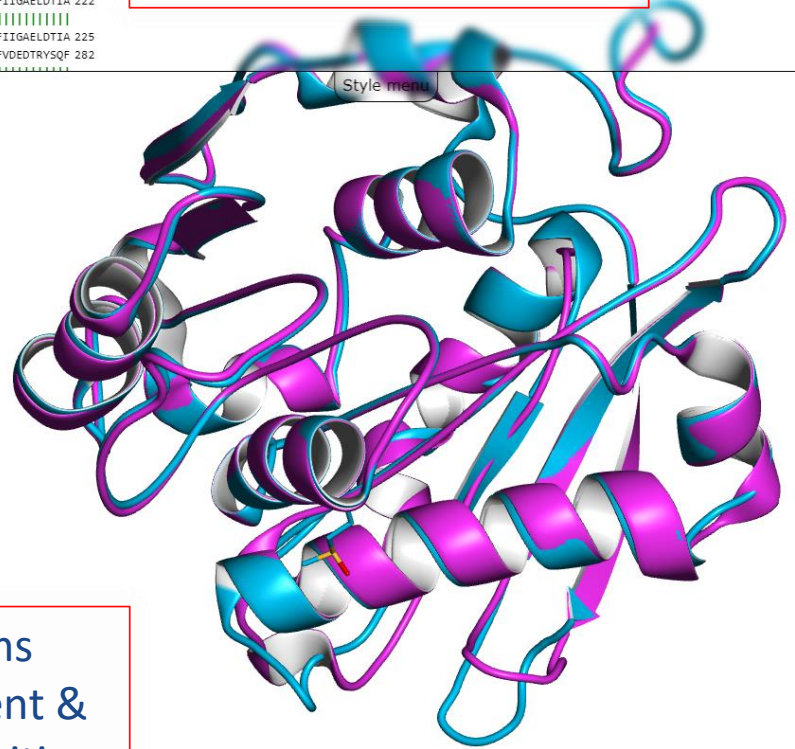
```

5zrr_A1  GFQDNFYERGGPDPEDSIEAIRGPFVSATERVSSFASGFGGGTIYYPRETDEGTFGAVAV 60
7cef_A1  GFQDNFYERGGPDPEDSIEAIRGPFVSATERVSSFASGFGGGTIYYPRETDEGTFGAVAV 60
5zrr_A61  APGFTASQGSMSWYGERVASQGFIVFTIDNTRLDQPGQRQLLAALDYLVERSDRKYR 120
7cef_A61  APGFTASQGSMSWYGERVASQGFIVFTIDNTRLDQPGQRQLLAALDYLVERSDRKYR 120
5zrr_A121 ERLDPNRLAVMGHAMGGGSLKATV*MRPFLKASIPLPWNLKDTWQVQVPTFIIGAE 180
7cef_A121 ERLDPNRLAVMGHAMGGGSLKATV*MRPFLKASIPLPWNLKDTWQVQVPTFIIGAE 180
5zrr_A181 TIAFVSTHAKPFYELPSSLPKAYMELDGATHFAPNIPNTTIARVI*SWLKRFDVDE 240
7cef_A181 TIAFVSTHAKPFYELPSSLPKAYMELDGATHFAPNIPNTTIARVI*SWLKRFDVDE 240
5zrr_A241 SQFLCPNPTDRAIEEVRSTCKRLN 265
7cef_A241 SQFLCPNPTDRAIEEVRSTCKRLN 265
  
```

Sequence homologues in the PDB

Options

Query ID: 5zrr
 Chain ID: A
 Clustering: 100 %
 Results: 43



Molmil performs sequence alignment & structure superposition

Promode Elastic

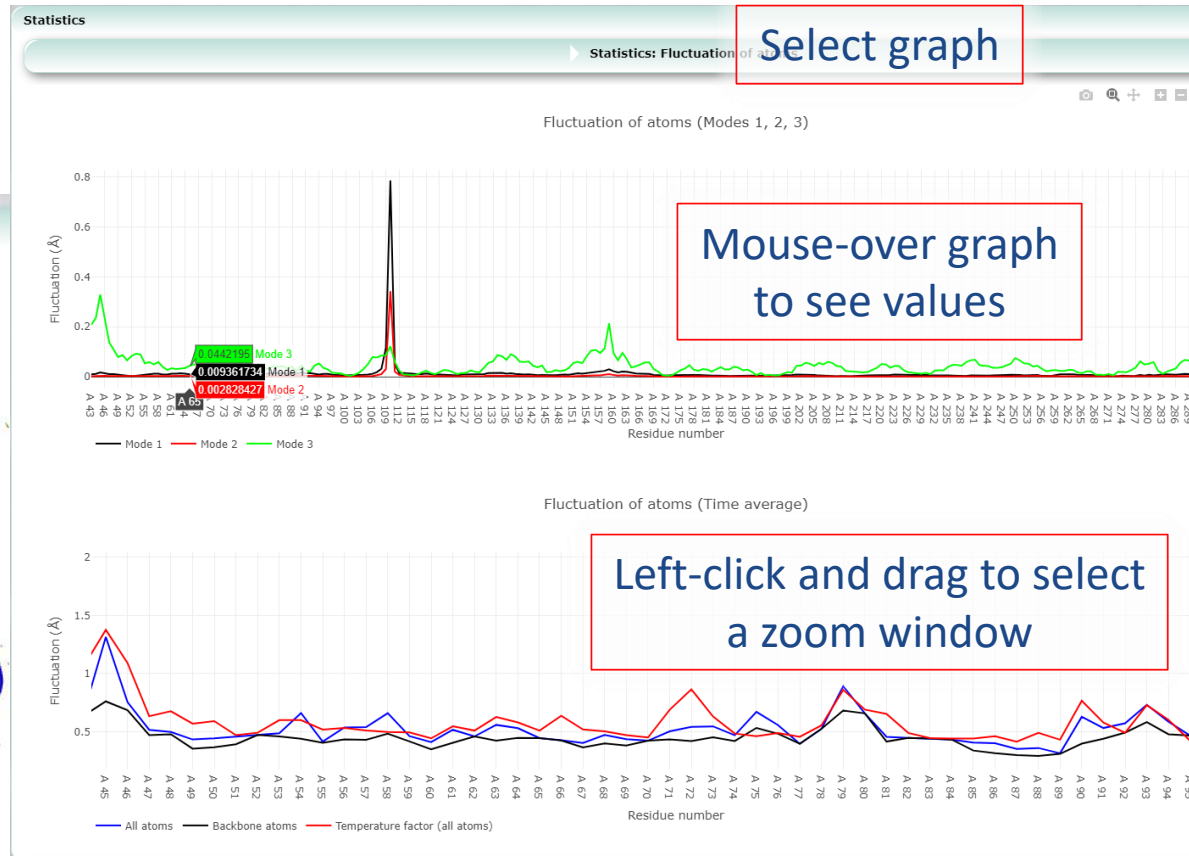
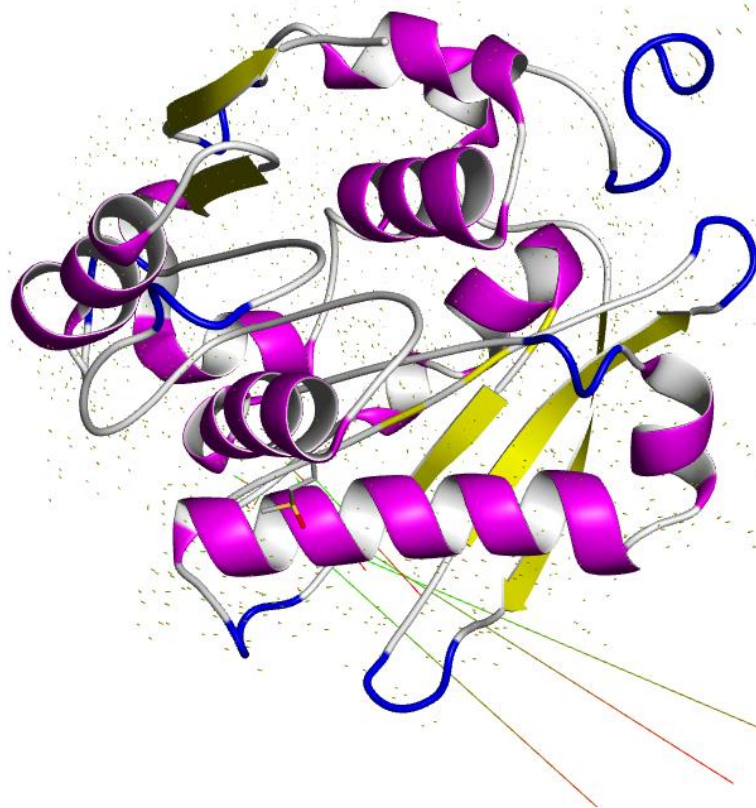
Interactive 3D visualization

Select mode

Select visualization

Mode: Mode 1

Visualization: All displacement vectors



Biological Structure Model Archive

BSM-Arc English 日本語

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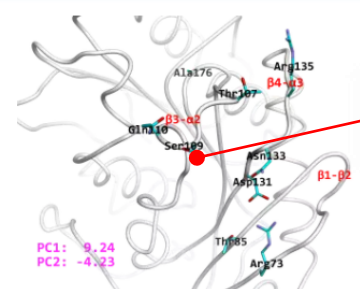
BSM00004: Structural Dynamics of the PET-Degrading Cutinase-like Enzyme from *Saccharomonospora viridis* AHK190 in Substrate-Bound States Elucidates the Ca²⁺-Driven Catalytic Cycle.

Authors: Nobutaka Numoto; Narutoshi Kamiya; [Gert-Jan Bekker](#); Yuri Yamagami; Satomi Inaba; Kentaro Ishii; Susumu Uchiyama; Fusako Kawai; Nobutoshi Ito; Masayuki Oda

DOI: [10.1021/acs.biochem.8b00624](https://doi.org/10.1021/acs.biochem.8b00624)

PDB: [5zno](#) [5zrq](#) [5zrr](#) [5zrs](#)

Entry: [Download](#) (12.07 GB)



PC1: 9.24
PC2: -4.23

File manager

Path: /

Name	Description	Size	Changed
data			
fig6C.mjs		678 B	12/10/2018, 4:20:02 PM
fig6D.mjs		497 B	12/10/2018, 4:20:02 PM
figS1.mjs		2.05 KB	12/10/2018, 4:20:02 PM
ga.webp		169.5 KB	12/10/2018, 4:39:22 PM

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Options
[Tree view](#)

Links back to PDB entries

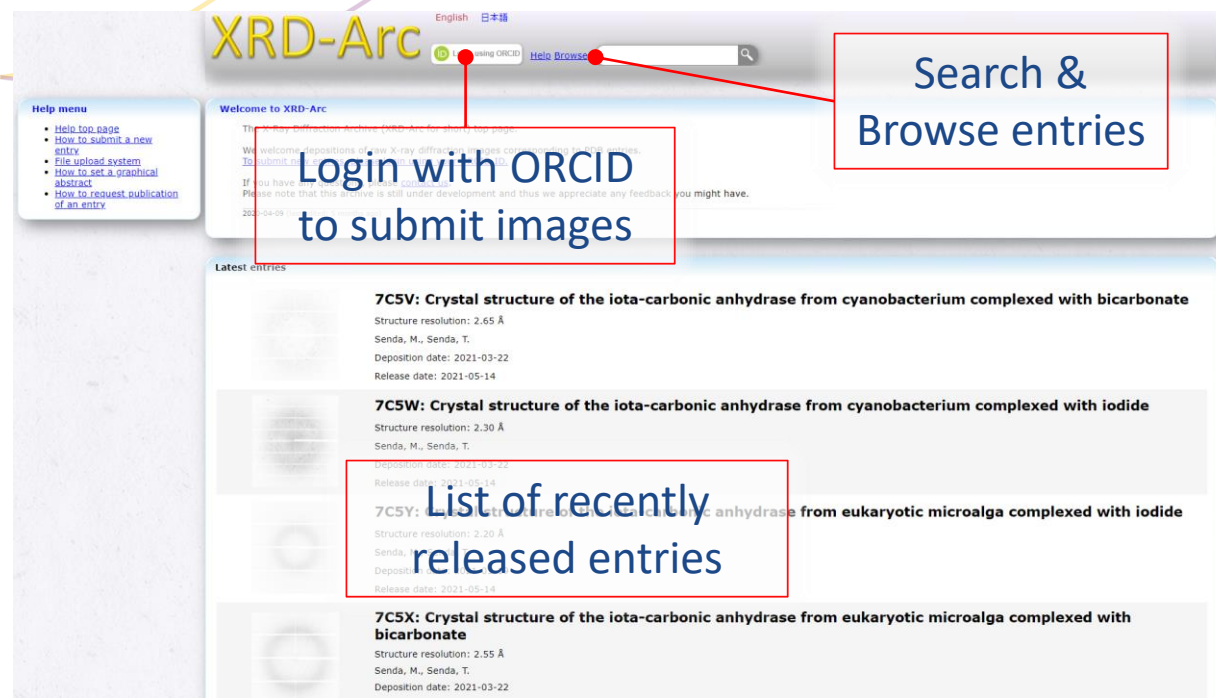
Double click to open folders

Double click to visualize files (e.g. pdb, gro, mol2, mjs, etc)

Graphical abstract

File list

X-Ray Diffraction Archive



XRDArc English 日本語

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- [How to request publication of an entry](#)

Welcome to XRD-Arc

We welcome depositions of new X-ray diffraction images corresponding to PDB entries. To submit your images, please refer to the following pages.

If you have any comments or suggestions, please contact us.

Please note that this archive is still under development and thus we appreciate any feedback you might have.

2020-04-09

Latest entries

7c5V: Crystal structure of the iota-carbonic anhydrase from cyanobacterium complexed with bicarbonate
Structure resolution: 2.65 Å
Senda, M., Senda, T.
Deposition date: 2021-03-22
Release date: 2021-05-14

7c5W: Crystal structure of the iota-carbonic anhydrase from cyanobacterium complexed with iodide
Structure resolution: 2.30 Å
Senda, M., Senda, T.
Deposition date: 2021-03-22
Release date: 2021-05-14

7c5Y: Crystal structure of the iota-carbonic anhydrase from eukaryotic microalga complexed with iodide
Structure resolution: 2.20 Å
Senda, M., Senda, T.
Deposition date: 2021-03-22
Release date: 2021-05-14

7c5X: Crystal structure of the iota-carbonic anhydrase from eukaryotic microalga complexed with bicarbonate
Structure resolution: 2.55 Å
Senda, M., Senda, T.
Deposition date: 2021-03-22

Search & Browse entries

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List of recently released entries

7c5V: Crystal structure of the iota-carbonic anhydrase from cyanobacterium complexed with bicarbonate

Authors: Senda, M., Senda, T.

R-work: 0.20710

R-free: 0.26310

Unit cell edges (Å): 52.841 x 83.734 x 87.267

Unit cell angles (°): 90, 90, 90

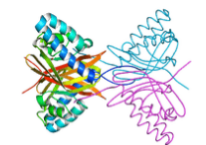
Resolution: 45.2 Å - 2.65 Å

Space group: P 21 21 2

[Primary citation](#)

[PDBj website for 7c5V](#)

[Download everything](#)



Dataset Carbonic anhydrase from all2909

Number of frames: 1440

Distance (mm): 84

Oscillation width (°): 0.5

Wavelength (Å): 1.9

Equipment: DECTRIS EIGER2 X 4M

Beamline: PHOTON FACTORY BEAMLINE BL-1A

Data: [Download](#)

File manager

Path: /

Name	Description	Size
data	full data set from a s	

Database information

- wwPDB DOI Landing Page
- Yorodumi
- CATH
- VAST
- PISA
- Electron Density Map
- wwPDB/RDF
- XRDArc**
- 7c5V**
- UniProt

Links from PDB to XRDA

After depositing your structure to OneDep, head to <https://xrda.pdbj.org/> to deposit your raw images (PDB entries registered to your ORCID ID in OneDep will automatically be linked in XRDA, for older entries, contact us at <https://xrda.pdbj.org/contact>)

Click to open main menu

Click on a category name to open a menu

Select which columns (data items) to show

Adds new row to the table

Text-edit category

Select which tables (categories) to show

CIF Editor

Merge file into loaded one

Save file

Interactive mmCIF file editor

Access

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

Load a file that is accessible via the web

<https://pdbj.org/cif-editor/#https://data.pdbj.org/pub/pdb/data/structures/divided/mmCIF/cr/1crn.cif>

Load a file from your local HDD

- Drag & drop the file into the window
- Click on the icon --> Open STAR file

Save the final STAR/JSON file

- Click on the icon --> Save STAR
- Click on the icon --> Save JSON

Hide or show categories (tables) after loading a CIF file

1. Click on the icon
2. Click on "Toggle tables"
3. Select the tables to show
4. Click on the icon to hide the menu

Hide or show data names (columns) after loading a CIF file

1. Click on the category name (top-left corner of each box)
2. Click on "Toggle columns"
3. Select the columns to show
4. Click again on the category name to hide the menu

Add new entry (set of data-values, or a single row in the table) after loading a CIF file

1. Click on the category name (top-left corner of each box)
2. Click on "Add new row"
3. Enter the mandatory items
4. Click on the (+) icon to add the row

Modify a data value (single column) after loading a CIF file

1. Click on the value to modify
2. Update the value using the input field
3. Defocus from the input field (e.g. click somewhere else)

Show only rows with specific value (from list) for this data item

Free-text search for rows with value

Batch operations to manipulate values (set/increment/decrement) of shown rows

Drag-and-drop a CIF (.gz OK) into the browser window to open it

NOTE: data is not sent to any server, and any unsaved data will be lost upon closing

Main menu

- View dictionary
- Toggle tables
- Merge additional mmCIF file
- Save mmCIF
- Save mmJSON
- Help

Category: atom_site

- Description
- Toggle columns
- Add new row
- Raw editor

Click on a cell to edit it

Click on an item name to open a menu

Item: auth_asym_id*

- Description
- Filter by value
- Search by value
- Batch operations

CIF Editor (1crn.cif)

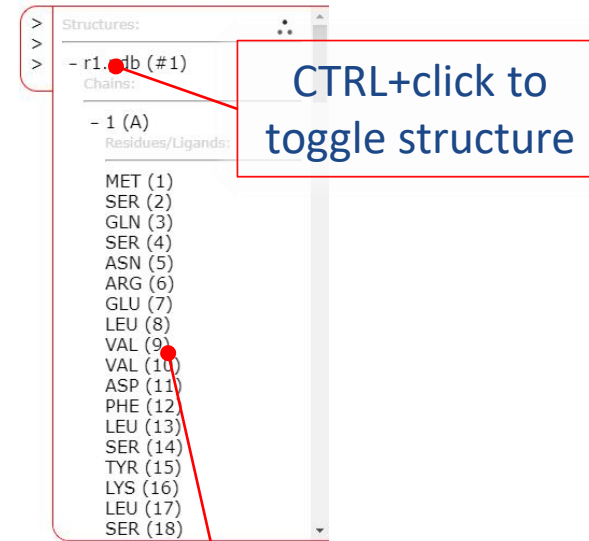
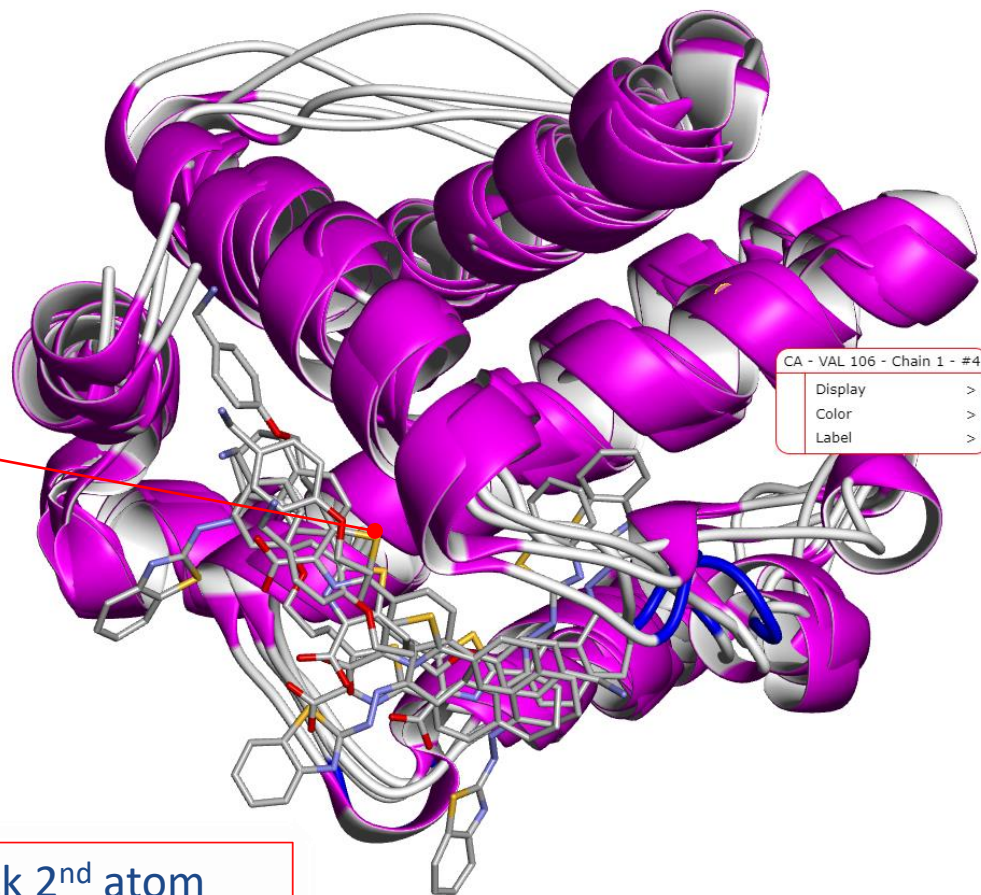
auth_asym_id*	auth_asym_id	auth_comp_id	auth_seq_id	B_iso_or_equiv	Cartn_x	Cartn_y	Cartn_z	group_PDB	id*	label_alt_id*	label_asym_id*	label_atom_id*	label_comp_id*	label_element_symbol	
x	A	N	THR	1	13.79	17.047	14.099	3.625	ATOM	1	.	A	N	THR	1
x	A	CA	THR	1	10.80	16.967	12.784	4.338	ATOM	2	.	A	CA	THR	1
x	A	C	THR	1	9.19	15.685	12.755	5.133	ATOM	3	.	A	C	THR	1
x	A	O	THR	1	9.85	15.268	13.825	5.594	ATOM	4	.	A	O	THR	1
x	A	CB	THR	1	13.02	18.170	12.703	5.337	ATOM	5	.	A	CB	THR	1
x	A	OG1	THR	1	15.06	19.334	12.829	4.463	ATOM	6	.	A	OG1	THR	1
x	A	CG2	THR	1	14.23	18.150	11.546	6.304	ATOM	7	.	A	CG2	THR	1
x	A	N	THR	2	7.81	13.115	11.555	3.285	ATOM	8	.	A	N	THR	1
x	A	CA	THR	2	8.21	13.856	11.469	6.064	ATOM	9	.	A	CA	THR	1
x	A	C	THR	2	5.94	14.993	9.862	7.443	ATOM	10	.	A	C	THR	1
x	A	O	THR	2	6.94	14.993	9.862	7.443	ATOM	11	.	A	O	THR	1
x	A	CB	THR	2	10.32	12.732	10.711	5.261	ATOM	12	.	A	CB	THR	1
x	A	OG1	THR	2	12.81	13.308	9.439	4.926	ATOM	13	.	A	OG1	THR	1
x	A	CG2	THR	2	11.90	12.484	11.442	3.895	ATOM	14	.	A	CG2	THR	1
x	A	N	CYS	3	5.24	13.488	11.241	8.417	ATOM	15	.	A	N	CYS	1
x	A	CA	CYS	3	5.39	13.660	10.707	9.787	ATOM	16	.	A	CA	CYS	1
x	A	C	CYS	3	4.45	12.269	10.431	10.323	ATOM	17	.	A	C	CYS	1
x	A	O	CYS	3	6.54	11.393	11.308	10.185	ATOM	18	.	A	O	CYS	1
x	A	CB	CYS	3	5.99	14.368	11.748	10.691	ATOM	19	.	A	CB	CYS	1
x	A	SG	CYS	3	7.01	15.885	12.426	10.016	ATOM	20	.	A	SG	CYS	1

CIF editor

Molmil as a general viewer



Temporarily place atom at rotation center: left-click on atom → hold CTRL while rotating
 Permanently: use *origin* CLI command

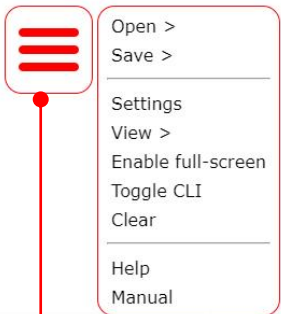


CTRL+click to toggle structure

Double click to jump to residue

Distance: click 1st atom, Ctrl+click 2nd atom
 Angle: click 1st atom, Ctrl+click 2nd, 3rd, atoms
 Angle: click 1st atom, Ctrl+click 2nd, 3rd, 4th atoms

Molmil as a general viewer



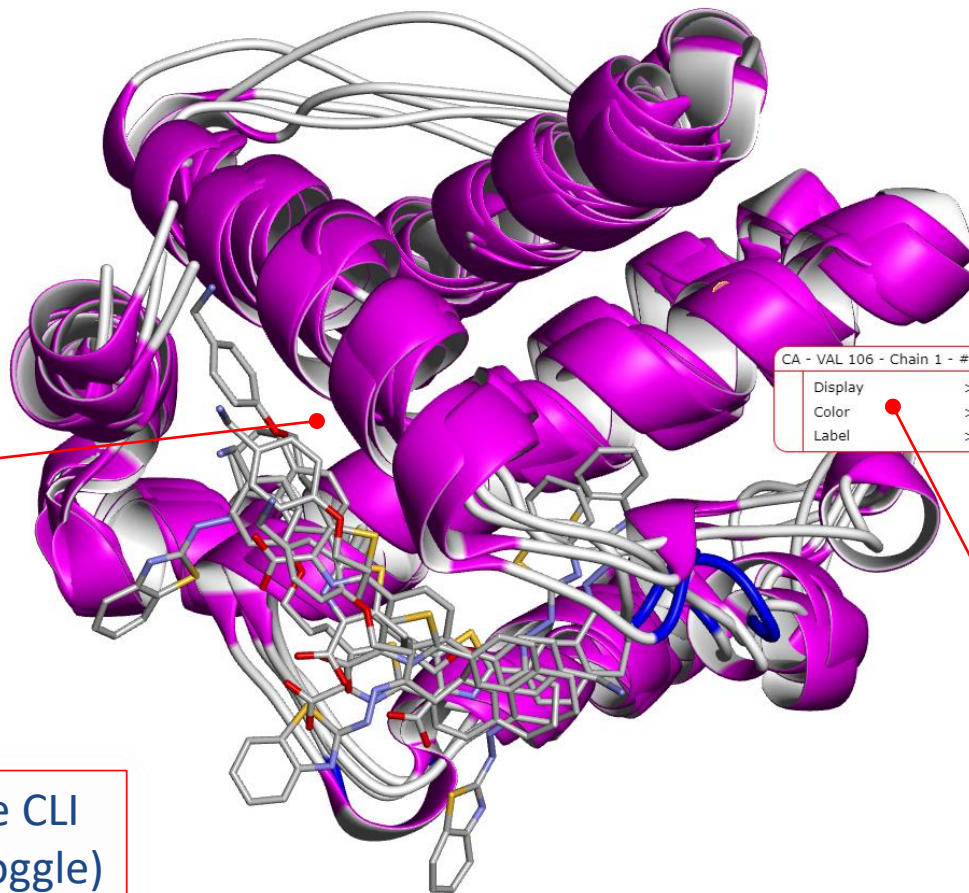
Main menu
(click to show)

Multiple files
can be drag-
and-dropped in

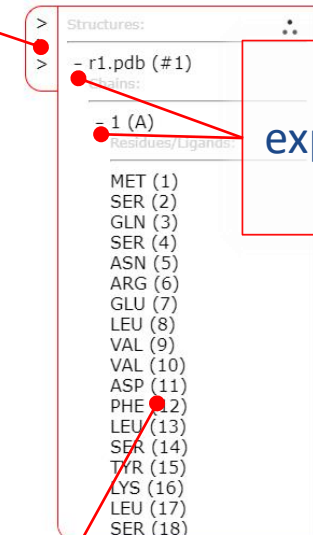
Click on “<” to show, “>” to hide CLI
(or double press ESC button to toggle)

Pymol-like command interface bound.
Clicked on atom: CA (4490) - VAL 106 - Chain 1
>

Commands can also be added to the URL



Structures menu
(click to show)



Click +/- to
expand/contract
menu

Right clicking
on an atom (or
cartoon), as
well as
residues in the
menu shows a
context menu

CLI supports a subset of pymol commands
(see <https://pd bj.org/molmil2/manual.html>)

<https://pd bj.org/molmil2/>

Molmil as a locally installed viewer

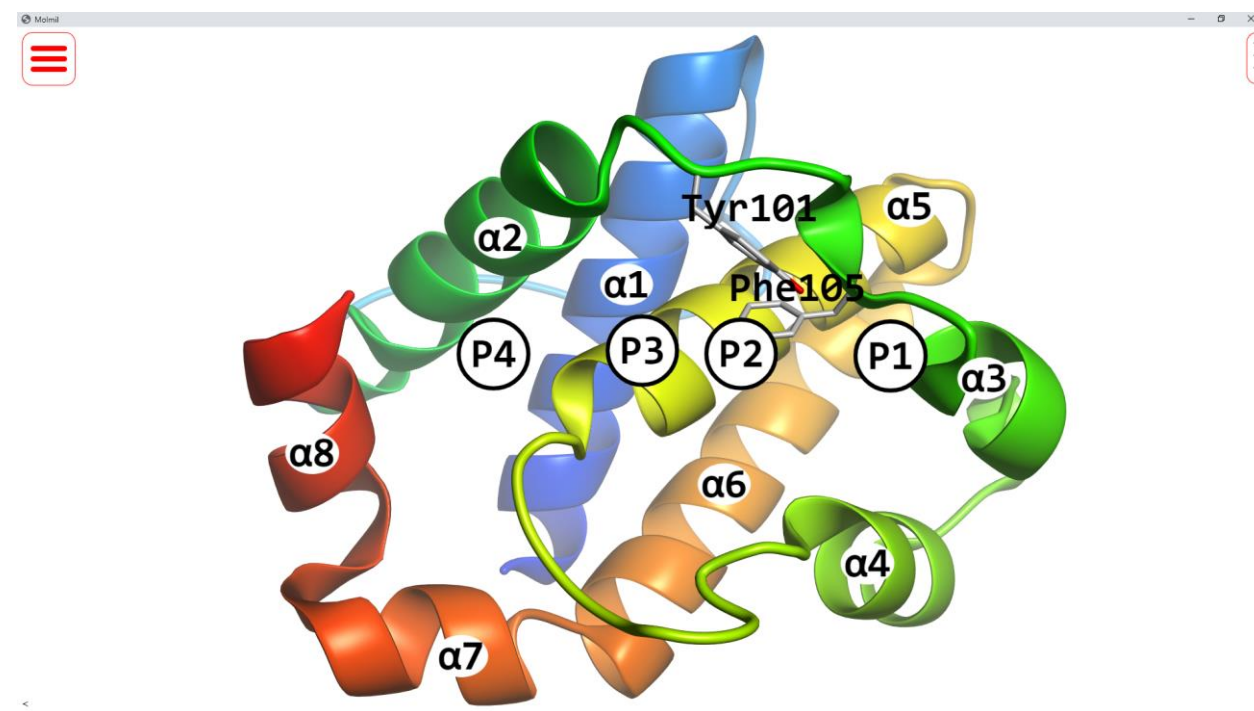
Install molmil-app as described on <https://gitlab.com/pdbjapan/molmil-app>

Then local files can be loaded directly like a native app

```
bekker@DESKTOP-FQPC05G: /mnt/c/Users/Gert-Jan/Desktop/research/bcl/figs/1
bekker@DESKTOP-FQPC05G:/mnt/c/Users/Gert-Jan/Desktop/research/bcl/figs/1$ molmil load ref.gro
```



```
bekker@DESKTOP-FQPC05G: /mnt/c/Users/Gert-Jan/Desktop/research/bcl/figs/1
bekker@DESKTOP-FQPC05G:/mnt/c/Users/Gert-Jan/Desktop/research/bcl/figs/1$ molmil load A.mjs
```



Example: generate images

Molmil script A.mjs (for A subfigure)

Bash script generate.sh

```

1 MOLMIL=/home/bekker/windesk/work/molmil-app/molmil.js
2
3 node $MOLMIL --headless \
4 "viewport 1400, 1080; molmil.configBox.strictDetailLV = 4; load A.mjs; png A.png; quit;" \
5 "viewport 1400, 1080; molmil.configBox.strictDetailLV = 4; load B.mjs; png B.png; quit;" \
6 "viewport 1400, 1080; molmil.configBox.strictDetailLV = 4; load C.mjs; png C.png; quit;" \
7 "viewport 1400, 1080; molmil.configBox.strictDetailLV = 4; load D.mjs; png D.png; quit;" \
8 "viewport 1400, 1080; molmil.configBox.strictDetailLV = 4; load E.mjs; png E.png; quit;" \
9 "viewport 1400, 1080; molmil.configBox.strictDetailLV = 4; load F.mjs; png F.png; quit;"
10
11 python combine.py

```

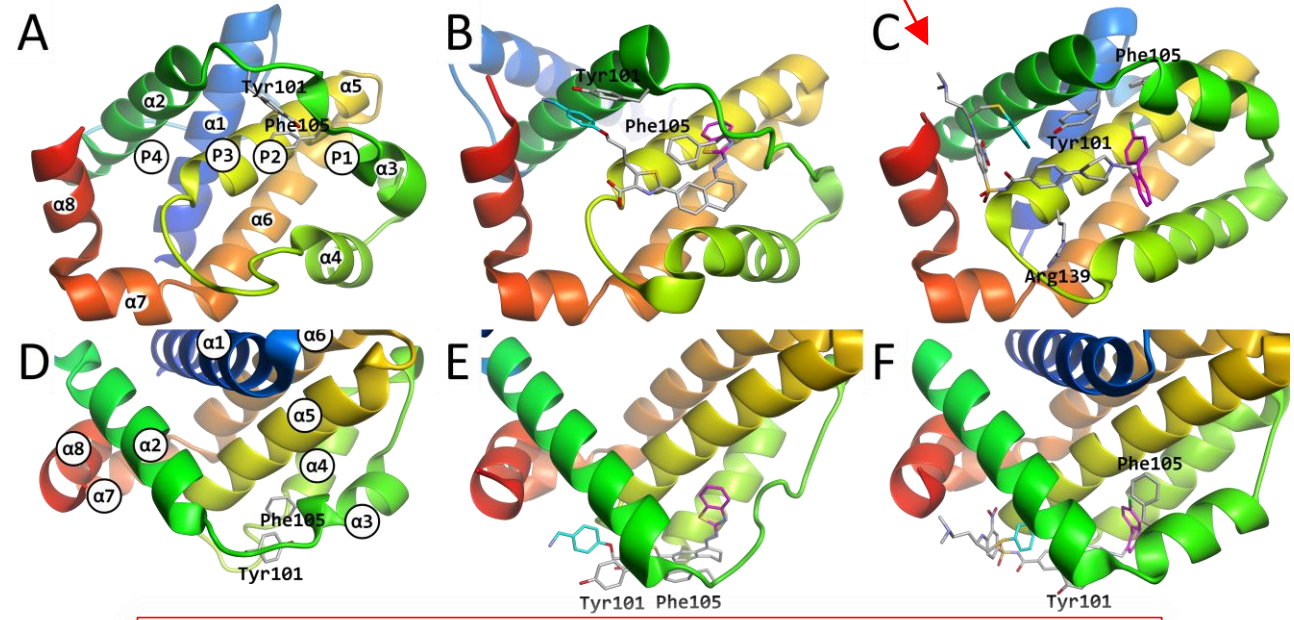
Set image size, high quality mesh, load subfigure script, save png and exit x6

Python script that combines all subfigures (A-F)

```

1 load base.mjs;
2 hide sticks, model #2 or model #3;
3 hide cartoon, model #2 or model #3;
4
5 cli_soup.skipCOGupdate = true;
6 load 4qvf.pdb;
7 hide cartoon, model #4;
8
9 show sticks, resi 101 and sidechain and model #1;
10 show sticks, resi 105 and sidechain and model #1;
11
12 set label_color, black;
13
14 set label_front, 1;
15
16 set label_position, (0, 0, 0);
17
18 set label_position, (0, -1, 0);
19 label resi 101 and sidechain and model #1, Tyr101;
20 label resi 105 and sidechain and model #1, Phe105;
21 set label_position, (0, 0, 0);
22
23 set label_border, on;
24
25 set label_bg_color, white;
26
27 label resi 58 and name CA and model #4, P1;
28 label resi 62 and name CA and model #4, P2;
29
30 set label_position, (0, 2, 0);
31
32 label resi 65 and name CA and model #4, P3;
33 label resi 69 and name CA and model #4, P4;
34
35 set label_position, (0, 0, 0);
36 set label_border, off;
37
38 set label_size, 40;
39 label resi 10-14 and name Ca and model #1, alpha1;
40 label resi 90-94 and name Ca and model #1, alpha2;
41 set label_position, (5, 7, 0);
42 label resi 102-106 and name Ca and model #1, alpha3;
43 set label_position, (0, 0, 0);
44 label resi 123-127 and name Ca and model #1, alpha4;
45 set label_position, (5, -4, 0);
46 label resi 147-151 and name Ca and model #1, alpha5;
47 set label_position, (0, 0, 0);
48 label resi 167-171 and name Ca and model #1, alpha6;
49 label resi 179-183 and name Ca and model #1, alpha7;
50 label resi 188-192 and name Ca and model #1, alpha8;

```



Final figure (Fig. 1, 10.1038/s41598-021-84488-z)

See <https://bsma.pdbj.org/entry/21>

Questions?

<https://pdbj.org/contact>

Contact us

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Name:

Email:

Subject:

Message:

Submit

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