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

Gert-Jan Bekker

Osaka University

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

Select display language

Omni search: search everything (Japanese OK)

Main menu

Search which service best fits your goal

Select by category

Service keyword search

COVID-19 structures

Links to other databases by PDBj
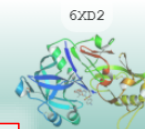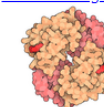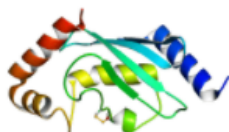
ubiquitin

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

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

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

1 2 3 4 >

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

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)

— Annotation callouts —

Query parameters

Modify keyword search query (Japanese OK)

Download arbitrary results for all (84) matches

Visualize entry using Molmil

Batch download files for all (84) matches
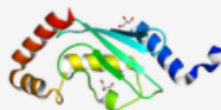
Download entry's mmCIF file

Return to filter page

Show entry page

Results pages

Quick search & filtering

- 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")

Batch download files & results

- For the search results, the corresponding files (mmCIF, mmJSON (all, header, plus), PDBML (all, header), RDF, structure factors and legacy PDB flatfile) can be downloaded in batches (left)

- For the search results, arbitrary data can be fetched from the Mine 2 RDB and returned in mmJSON, mmCIF or JSON (row- or column major) (right)

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

Batch file & data download is also supported

Add additional keywords

Return to RDB builder

- RDB implementation docs: https://pdbj.org/rdb/docs
- RDB builder: https://pdbj.org/rdb/build
- Local install: https://gitlab.com/pdbjapan/mine2updater

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)

Options

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

Category
- chem_comp
- chem_comp_atom
- chem_link
- *citation*
- citation_author
- citation_author_pdbmlplus

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

Filter
- *text*

Add Filter

Type

Search

Execute search

Help pages:

Show RDB documentation

RDB Query Builder help

1: select the schema

2: select the category

3: select the data-item to filter by

4: filter type

Help | Contact us | Terms and Conditions | Privacy policy

RDB docs

SQL query based search:

SQL Query search

Mine 2 RDB Documentation

PDBj's Mine 2 RDB interactive documentation. The Mine 2 RDB consists of the common data in each PDB parter "PDBx/mmCIF" and PDBj'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.
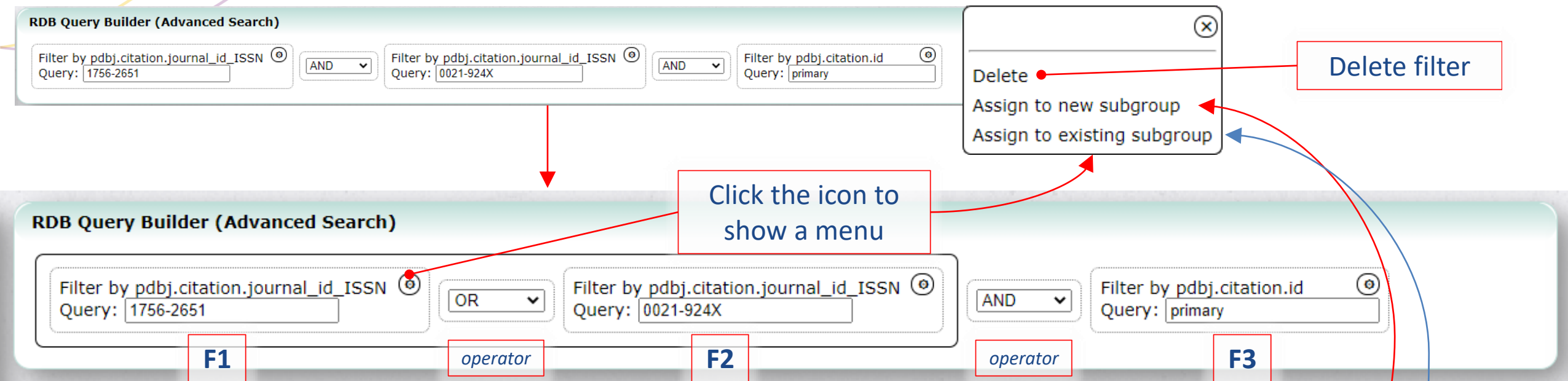
Search: category name, data name or keyword

The Mine 2 RDB holds 247 tables:

Manually input SQL query

Can be used to manually refine a query

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RDB builder: query example

RDB Query Builder (Advanced Search)

Filter by pdbj.citation.journal_id_ISSN
Query: 1756-2651 | AND | Filter by pdbj.citation.journal_id_ISSN
Query: 0021-924X | AND | Filter by pdbj.citation.id
Query: primary

Delete
Assign to new subgroup
Assign to existing subgroup

Delete filter

Click the icon to show a menu

RDB Query Builder (Advanced Search)

Filter by pdbj.citation.journal_id_ISSN
Query: 1756-2651 | OR | Filter by pdbj.citation.journal_id_ISSN
Query: 0021-924X | AND | Filter by pdbj.citation.id
Query: primary

F1 | *operator* | **F2** | *operator* | **F3**

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

Higher resolution structure (1st entity)

Structure Validation summary

View AU

Links to other databases

Molmil eF-site viewer

Molmil EDMap viewer

BSM-Arc link

Promode Elastic link

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

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

Style menu
- Structure
- EDMap
- Sites
- Alignment
- Miscellaneous
- Hide

BU selection/visualization

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

Biological unit styling options

Unit selection: [Biological unit 1 (240)]
Unit repr.: [Coarse surface, colored by each asymmetric chain]

Style menu
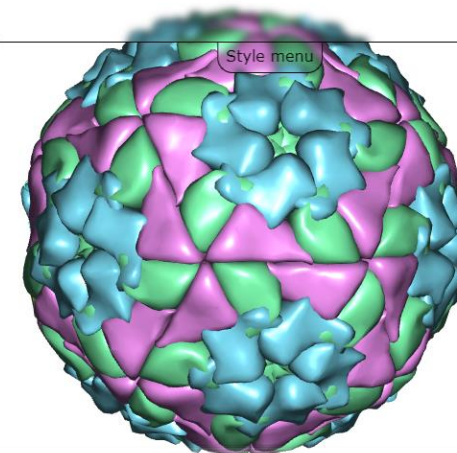
Molmil AU/BU viewer

Visualization of Biological Unit using Molmil

eF-site Molmil viewer

5zrr-A.mpbf ⚙

5ZRR

☐ A: 105, A: 1   4, A: 254, A: 540, A: 645
  Sequence:
  Description:

☐ A: 118, A: 2
  Sequence:
  Description:

☐ A: 57, A: 155, A: 547, A: 603
  Sequence: E, E, ,
  Description: binding site for residue ZN A 403

☐ A: 204, A: 206, A: 550, A: 574, A: 672, A: 729

Mesh options for 5zrr-A.mpbf

○ Wireframe ● Solid
Transparency: ▬▬▬○▬▬▬
[Close]

Style menu

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

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

Toggle sites
(stick model)
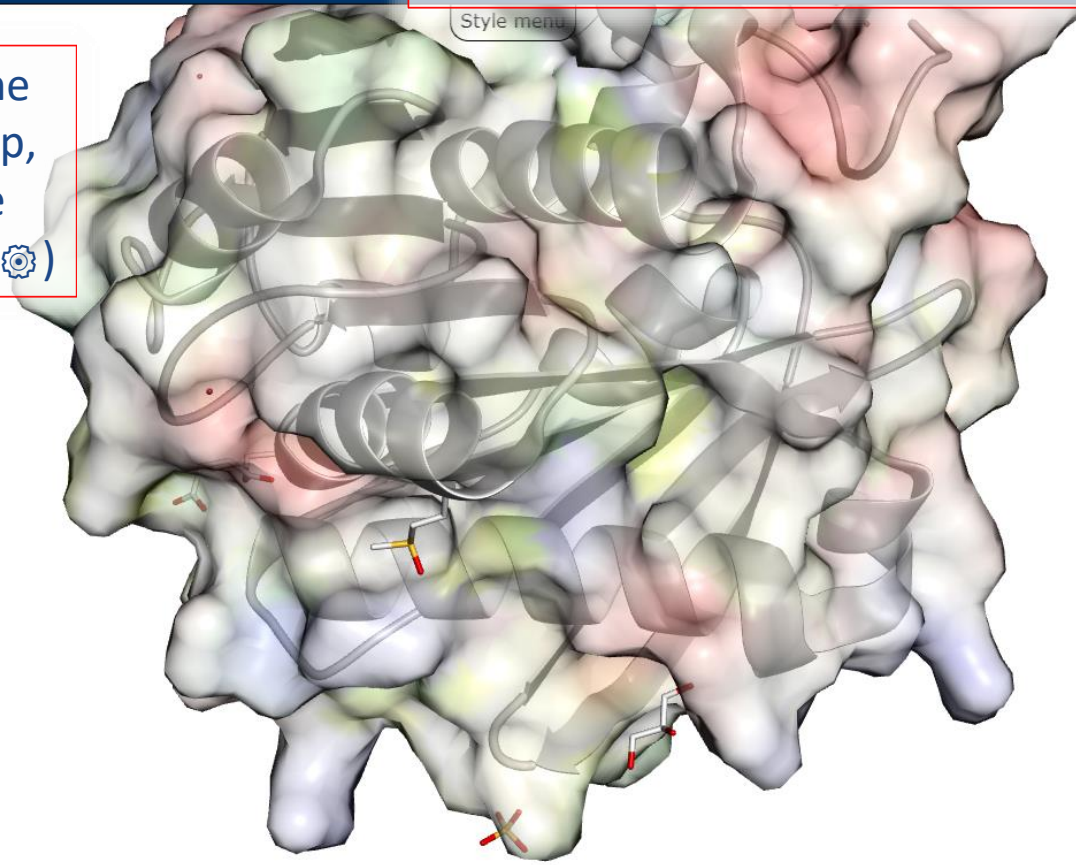
EDMap

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
[Create map]

Downloads: <u>Structure factors</u> <u>2fo-fc map (cif)</u> <u>fo-fc map (cif)</u> <u>2fo-fc map (mtz)</u> <u>fo-fc map (mtz)</u> <u>2fo-fc map (ccp4)</u> <u>fo-fc map (ccp4)</u>   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
[Delete] [Close]

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 ID

Asym ID

Clustering:

Find homologues

PDB entry | Custom sequence

No 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)

Superposition excludes flexible loops (to optimize superposition)

Sequence Neighbor

Chains

Entity | Asym IDs
1 | A

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.

Chain list

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  DNPYERGPDPTEDSIEAIRGPFSVATERVSSFASGFGGGTIYYPRETDEGTFGAVAVAPG 102
46  DNPYERGPDPTEDSIEAIRGPFSVATERVSSFASGFGGGTIYYPRETDEGTFGAVAVAPG 105
103 FTASQGSMSWYGERVASQGFIVFTIDTNTRLDQPGQRGRQLLAALDYLVERSDRKVRERL 162
106 FTASQGSMSWYGERVASQGFIVFTIDTNTRLDQPGQRGRQLLAALDYLVERSDRKVRERL 165
163 DPNRLAVMGHAMGGGGSLEATV*RPSLKASIPLTPWNLDKTWGQVQVPTFIIGAELDTIA 222
166 DPNRLAVMGHAMGGGGSLEATVMRPSLKASIPLTPWNLDKTWGQVQVPTFIIGAELDTIA 225
223 PVSTHAKPFYESLPSSLPKAYMELDGATHFAPNIPNTTIAKYVISWLKRFVDEDTRYSQF 282
```

Sequence Navigator for 5zrr_A

Exact matches to 5zrr_A: 5zno_A ▾ 5zno_B ▾ 5zrg_A ▾ 5zrs_A ▾ 7ceh_A ▾

Click on the ID to show a menu

Options

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

Clustering

Hit: 5zno_A ▾
Sequence identity: 100%
Sequence positives: 100%
E-value: 0
Score: 1410
Query coverage: 100%
Compound: Alpha/beta ... UM ION, GLYCEROL, water

5zno_A ⊗
Superpose with 5zrr_A
Search homologues of 5zno_A
View PDB entry page of 5zno

Alignment:
```
5zrr_A1   GPQDNPYERGPDPTEDSIEAIRGPFSVATERVSSFASGFGGGTIYYPRETDEGTFGAVAV 60
5zno_A1   GPQDNPYERGPDPTEDSIEAIRGPFSVATERVSSFASGFGGGTIYYPRETDEGTFGAVAV 60
5zrr_A61  APGFTASQGSMSWYGERVASQGFIVFTIDTNTRLDQPGQRGRQLLAALDYLVERSDRKVR 120
5zno_A61  APGFTASQGSMSWYGERVASQGFIVFTIDTNTRLDQPGQRGRQLLAALDYLVERSDRKVR 120
5zrr_A121 ERLDPNRLAVMGHAMGGGGSLEATVMRPSLKASIPLTPWNLDKTWGQVQVPTFIIGAELD 180
5zno_A121 ERLDPNRLAVMGHAMGGGGSLEATVMRPSLKASIPLTPWNLDKTWGQVQVPTFIIGAELD 180
5zrr_A181 TIAPVSTHAKPFYESLPSSLPKAYMELDGATHFAPNIPNTTIAKYVISWLKRFVDEDTRY 240
5zno_A181 TIAPVSTHAKPFYESLPSSLPKAYMELDGATHFAPNIPNTTIAKYVISWLKRFVDEDTRY 240
5zrr_A241 SQFLCPNPTDRAIEEYRSTCPYKLN 265
5zno_A241 SQFLCPNPTDRAIEEYRSTCPYKLN 265
```

Exact matches to 5zno_A: 5zno_B ▾ 5zrg_A ▾ 5zrr_A ▾ 5zrs_A ▾ 7ceh_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   GPQDNPYERGPDPTEDSIEAIRGPFSVATERVSSFASGFGGGTIYYPRETDEGTFGAVAV 60
7cef_A1   GPQDNPYERGPDPTEDSIEAIRGPFSVATERVSSFASGFGGGTIYYPRETDEGTFGAVAV 60
5zrr_A61  APGFTASQGSMSWYGERVASQGFIVFTIDTNTRLDQPGQRGRQLLAALDYLVERSDRKVR 120
7cef_A61  APGFTASQGSMSWYGERVASQGFIVFTIDTNTRLDQPGQRGRQLLAALDYLVERSDRKVR 120
5zrr_A121 ERLDPNRLAVMGHAMGGGGSLEATVMRPSLKASIPLTPWNLDKTWGQVQVPTFIIGAELD 180
7cef_A121 ERLDPNRLAVMGHSMGGGGSLEATVMRPSLKASIPLTPWNLDKTWGQVQVPTFIIGAELD 180
5zrr_A181 TIAPVSTHAKPFYESLPSSLPKAYMELDGATHFAPNIPNTTIAKYVISWLKRFVDEDTRY 240
7cef_A181 TIAPVSTHAKPFYESLPSSLPKAYMELDGATHFAPNIPNTTIAKYVISWLKRFVDEDTRY 240
5zrr_A241 SQFLCPNPTDRAIEEYRSTCPY 262
7cef_A241 SQFLCPNPTDR... 
```

Exact matches to 7cef_A: 7cef_B ▾

Sequence homologues in the PDB

Molmil performs sequence alignment & structure superposition

Style menu

OSAKA UNIVERSITY

Promode Elastic

Statistics

Statistics: Fluctuation of

Select graph

Fluctuation of atoms (Modes 1, 2, 3)

Interactive 3D visualization

Select mode

Select visualization

Mode: Mode 1

Visualization: All displacement vectors

Mouse-over graph to see values

0.0442195 Mode 3
0.009361734 Mode 1
0.002828427 Mode 2
A 65

— Mode 1 — Mode 2 — Mode 3

Fluctuation (Å)

Residue number

Fluctuation of atoms (Time average)

Left-click and drag to select a zoom window

Fluctuation (Å)

Residue number

— All atoms — Backbone atoms — Temperature factor (all atoms)

<
* To zoom using the mousewheel, please hold the CTRL button.
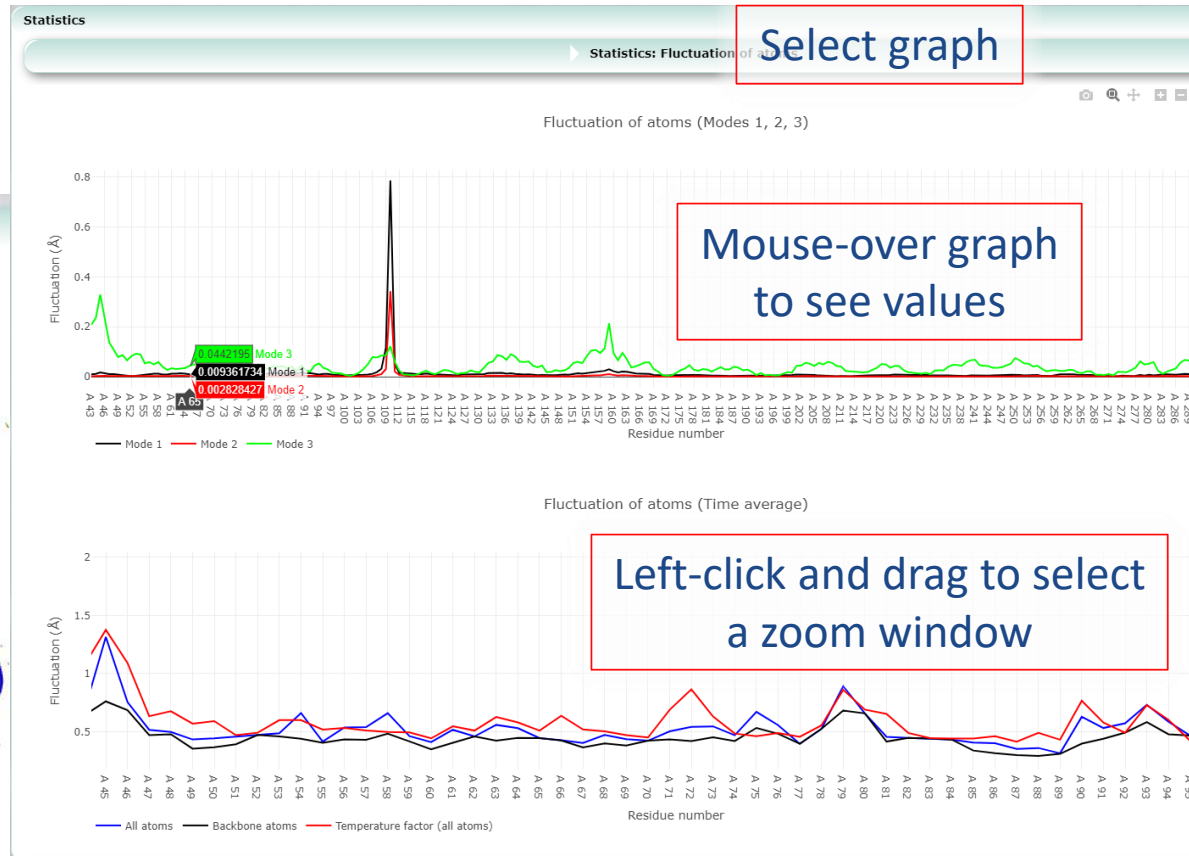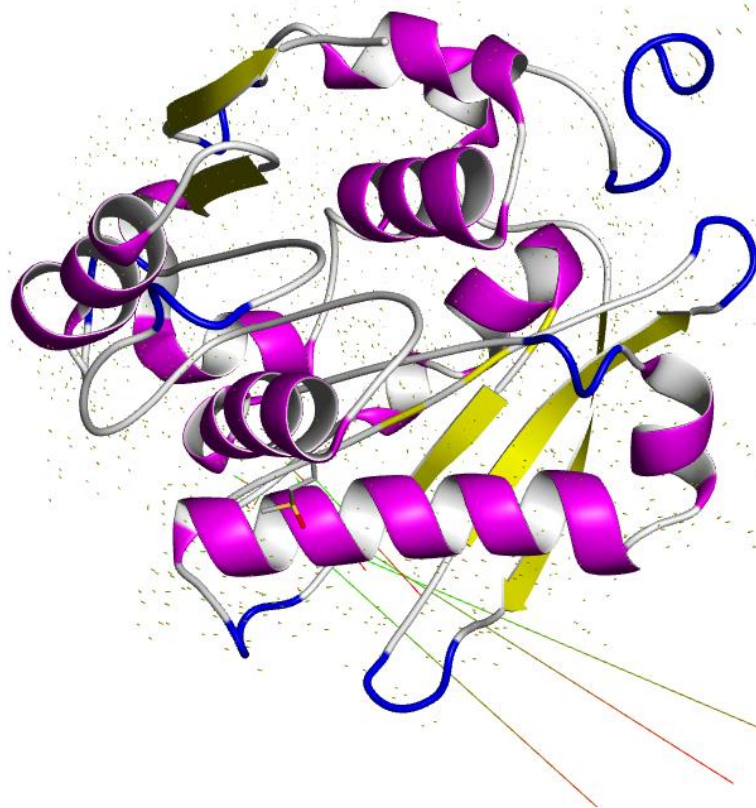
Biological Structure Model Archive
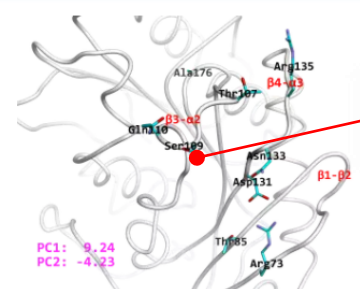
Graphical abstract

Links back to PDB entries
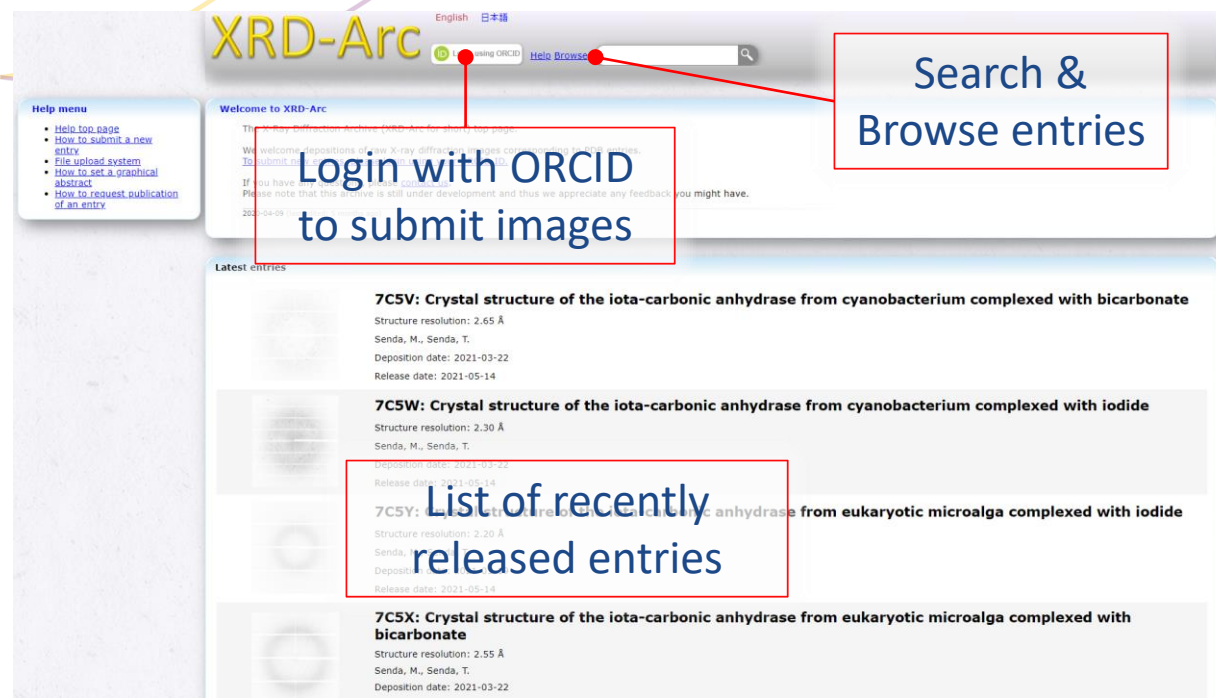
Double click to open folders

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

File list

X-Ray Diffraction Archive

Search & Browse entries

Login with ORCID to submit images

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
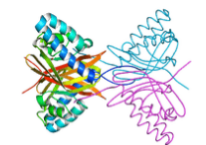
Primary citation
PDBj website for 7c5v
Download everything

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
- *XRD-Arc*
  - 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)

CIF editor

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

Category: atom_site ⊗
- Description
- Toggle columns
- Add new row
- Raw editor

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

Select which tables (categories) to show

Merge file into loaded one

Save file

CIF Editor

Interactive mmCIF-f...

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 lo...
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)

Change d...

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

CIF Editor (1crn.cif)

atom_site

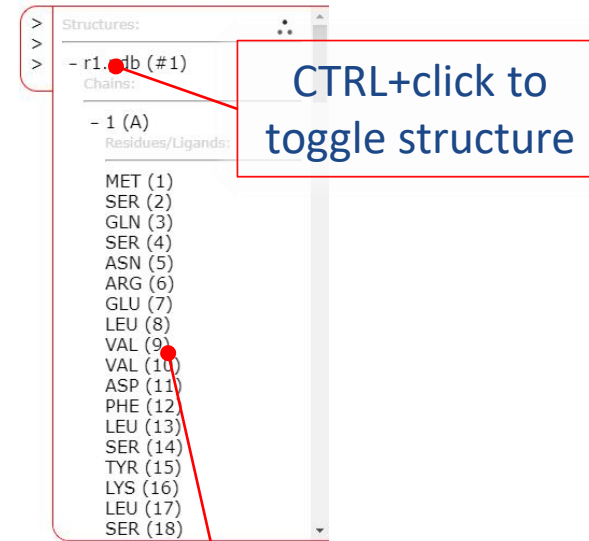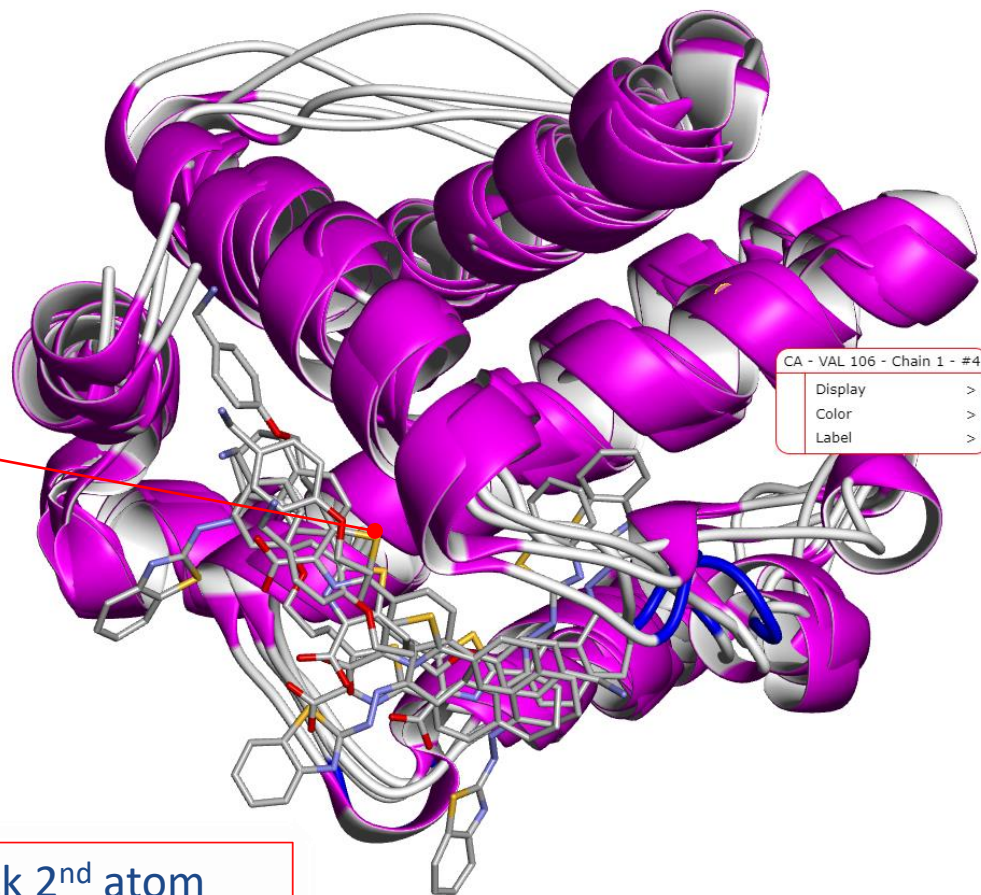|	auth_asym_id*	auth_atom_id	auth_comp_id	auth_seq_id	B_iso_or_equiv	Cartn_x	Cartn_y	Cartn_z	group_PDB	id*	label_alt_id*	label_asym_id	label_atom_id*	label_comp_id*	label_en
×	A	N	THR	1	13.79	17.047	14.099	3.625	ATOM	1	.	A	N	THR	1
×	A	CA	THR	1	10.80	16.967	12.784	4.338	ATOM	2	.	A	CA	THR	1
×	A	C	THR	1	9.19	15.685	12.755	5.133	ATOM	3	.	A	C	THR	1
×	A	O	THR	1	9.85	15.268	13.825	5.594	ATOM	4	.	A	O	THR	1
×	A	CB	THR	1	13.02	18.170	12.703	5.337	ATOM	5	.	A	CB	THR	1
×	A	OG1	THR	1	15.06	19.334	12.829	4.463	ATOM	6	.	A	OG1	THR	1
×	A	CG2	THR	1	14.23	18.150	11.546	6.304	ATOM	7	.	A	CG2	THR	1
×	A	N	THR	2	7.81	15.115	11.555	5.263	ATOM	8	.	A	N	THR	1
×	A	CA	THR	2	8.31	13.856	11.469	6.000	ATOM				CA	THR	1
×	A	C	THR	2	6.94	14.993	9.862	7.443	ATOM				C	THR	1
×	A	O	THR	2	6.94	14.993	9.862	7.443	ATOM				O	THR	1
×	A	CB	THR	2	10.32	12.732	10.711	5.261	ATOM	12	.	A	CB	THR	1
×	A	OG1	THR	2	12.81	13.308	9.439	4.926	ATOM	13	.	A	OG1	THR	1
×	A	CG2	THR	2	11.90	12.484	11.442	3.895	ATOM	14	.	A	CG2	THR	1
×	A	N	CYS	3	5.24	13.488	11.241	8.417	ATOM	15	.	A	N	CYS	1
×	A	CA	CYS	3	5.39	13.660	10.707	9.787	ATOM	16	.	A	CA	CYS	1
×	A	C	CYS	3	4.45	12.269	10.431	10.323	ATOM	17	.	A	C	CYS	1
×	A	O	CYS	3	6.54	11.393	11.308	10.185	ATOM	18	.	A	O	CYS	1
×	A	CB	CYS	3	5.99	14.368	11.748	10.691	ATOM	19	.	A	CB	CYS	1
×	A	SG	CYS	3	7.01	15.885	12.426	10.016	ATOM	20	.	A	SG	CYS	1

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

Click on a cell to edit it

atom_sites

	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_matri[2]
×	1CRN	0.024414	0.000000	0.000328	0.000000	0.053619	0.000000	0.000000	0.000000

...om_type

Item: auth_asym_id* ⊗
- Description
- Filter by value
- Search by value
- Batch operations

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

Click on an item name to open a menu

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

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Molmil as a general viewer

Open >
Save >

Settings
View >
Enable full-screen
Toggle CLI
Clear

Help
Manual

Structures:
- r1.db (#1)
Chains:
- 1 (A)
Residues/Ligands:
MET (1)
SER (2)
GLN (3)
SER (4)
ASN (5)
ARG (6)
GLU (7)
LEU (8)
VAL (9)
VAL (10)
ASP (11)
PHE (12)
LEU (13)
SER (14)
TYR (15)
LYS (16)
LEU (17)
SER (18)

CTRL+click to toggle structure

Double click to jump to residue

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

CA - VAL 106 - Chain 1 - #4
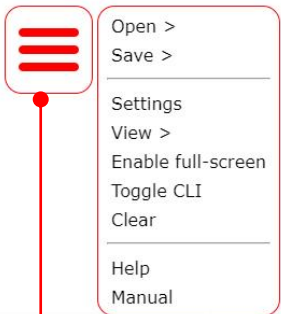Display >
Color >
Label >

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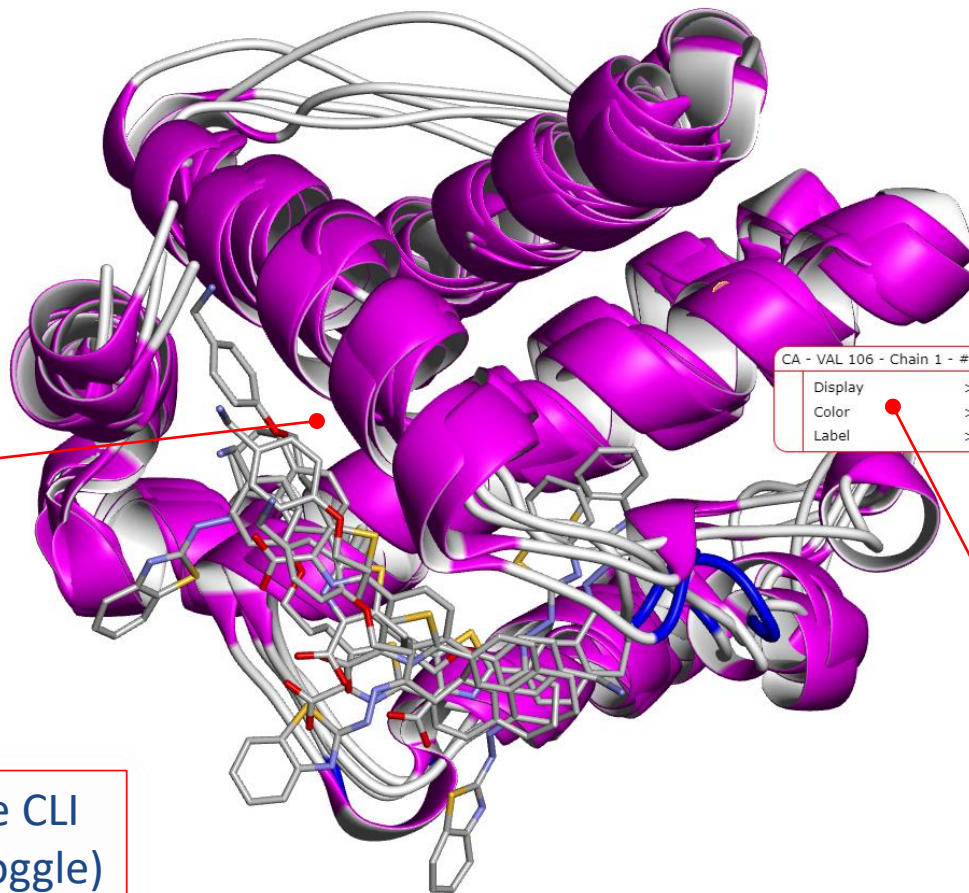Angle: click 1st atom, Ctrl+click 2nd, 3rd, 4th atoms

Clicked on atom: CA (4490) - VAL 106 - Chain 1

https://pdbj.org/molmil2/

Molmil as a general viewer

Open >
Save >

Settings
View >
Enable full-screen
Toggle CLI
Clear

Help
Manual

**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)**

**Structures menu
(click to show)**

Structures:
- r1.pdb (#1)
Chains:
- 1 (A)
Residues/Ligands

MET (1)
SER (2)
GLN (3)
SER (4)
ASN (5)
ARG (6)
GLU (7)
LEU (8)
VAL (9)
VAL (10)
ASP (11)
PHE (12)
LEU (13)
SER (14)
TYR (15)
LYS (16)
LEU (17)
SER (18)
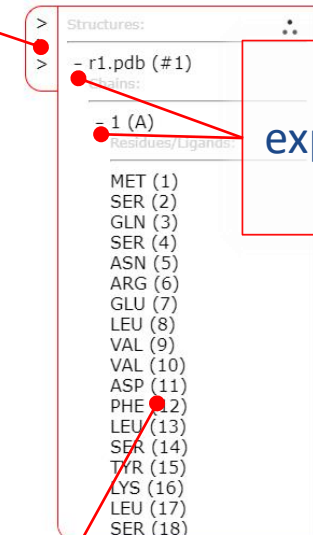
**Click +/- to
expand/contract
menu**

CA - VAL 106 - Chain 1 - #4
Display   >
Color   >
Label   >

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

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

Commands can also be added to the URL

**CLI supports a subset of pymol commands
(see https://pdbj.org/molmil2/manual.html)**

https://pdbj.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
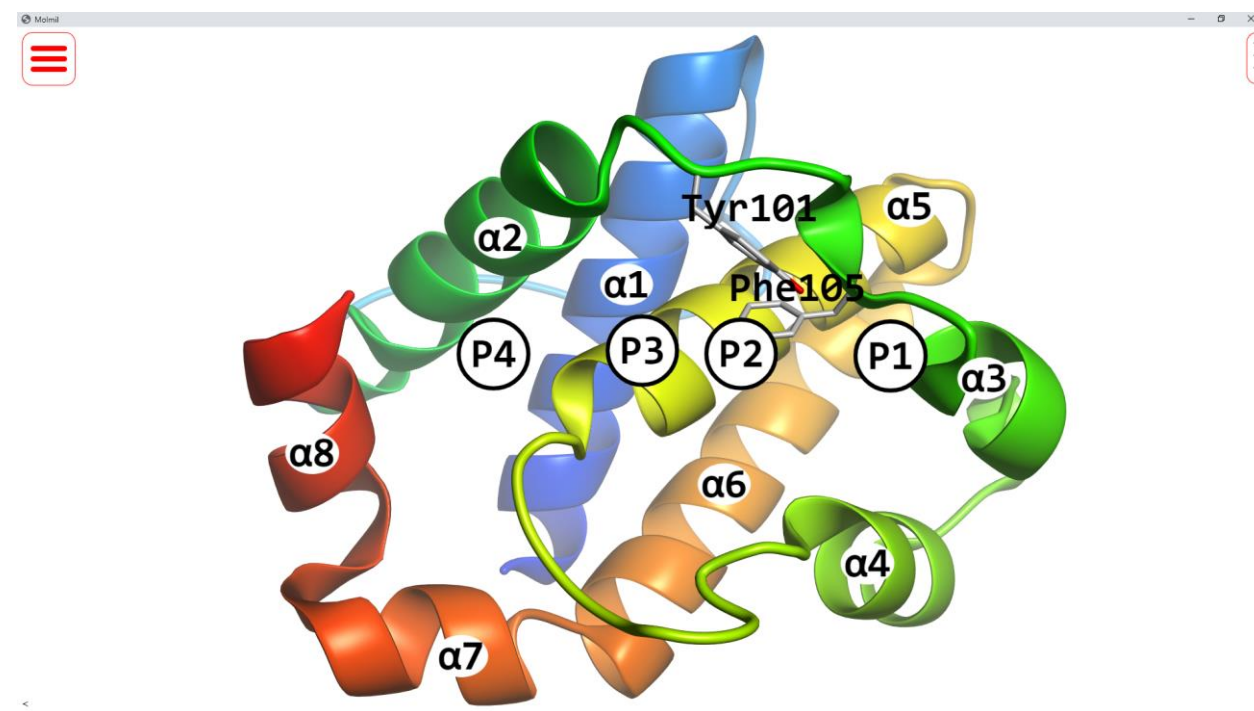
Example: generate images

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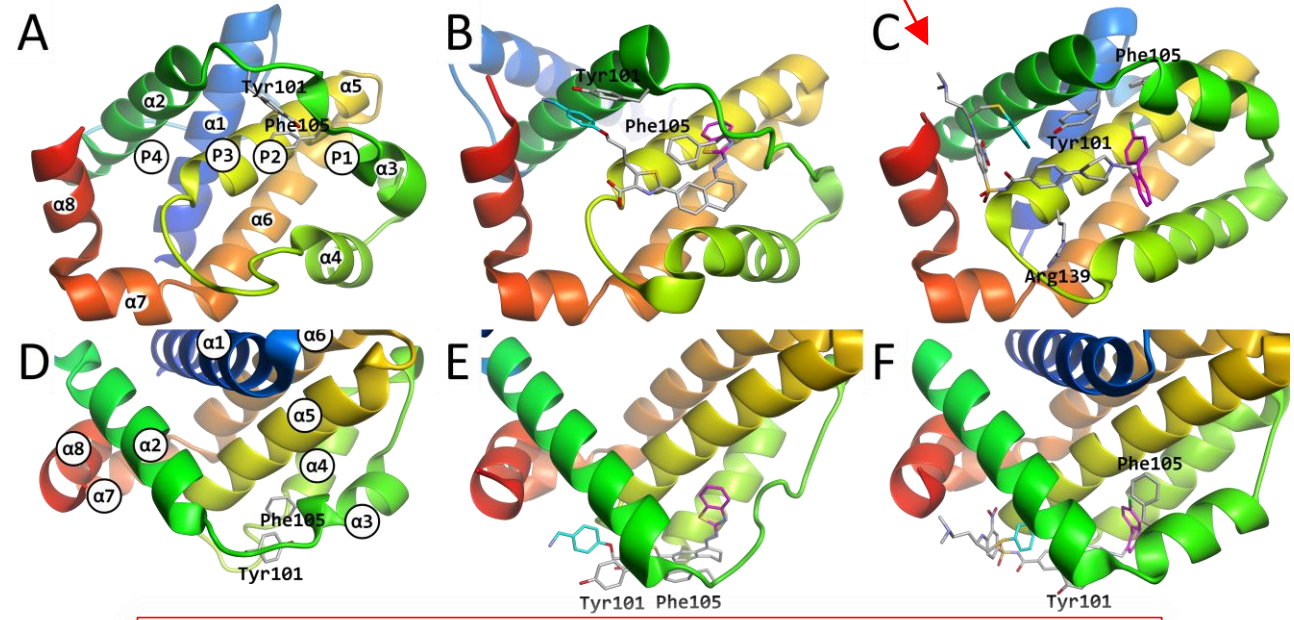
Set image size, high quality mesh, load subfigure script, save png and exit x6

Python script that combines all subfigures (A-F)

Molmil script A.mjs (for A subfigure)

```
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, α1;
40  label resi 90-94 and name Ca and model #1, α2;
41  set label_position, (5, 7, 0);
42  label resi 102-106 and name Ca and model #1, α3;
43  set label_position, (0, 0, 0);
44  label resi 123-127 and name Ca and model #1, α4;
45  set label_position, (5, -4, 0);
46  label resi 147-151 and name Ca and model #1, α5;
47  set label_position, (0, 0, 0);
48  label resi 167-171 and name Ca and model #1, α6;
49  label resi 179-183 and name Ca and model #1, α7;
50  label resi 188-192 and name Ca and model #1, α8;
```

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

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

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Questions?

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