



KATEDRA FYZIKÁLNÍ CHEMIE
UNIVERZITY PALACKÉHO V OLOMOUCI



Univerzita Palackého
v Olomouci

KFC/STBI

Strukturní bioinformatika

Cvičení – databáze

Karel Berka



Zadání



Základní PDB databáze

- PDBe - <https://www.ebi.ac.uk/pdbe/>
- RCSB – <https://www.rcsb.org/>

Souhrnné databáze

- PDBe-KB - <https://www.ebi.ac.uk/pdbe/pdbe-kb/>
- PDBSum - <http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/>

Modely

- AlphaFoldDB - <https://alphafold.ebi.ac.uk/>
- ESMAtlas - <https://esmatlas.com/>

Sekundární databáze – proteinové rodiny

- CATH - <https://www.cathdb.info/>
- SCOP - <https://scop.mrc-lmb.cam.ac.uk/>



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Základní databáze

- PDBe - <https://www.ebi.ac.uk/pdbe/>
- RCSB – <https://www.rcsb.org/>



Zadání PDBe vz RCSB

- 1) Porovnejte, jaké informace Vám poskytne RCSB a PDBe pro jedno PDBID (např. 2HI4), co má PDBe či RCSB navíc? (v analýze sekvencí, ligandů, vizualizace struktury, interakce s membránou)
- 2) Zjistěte, co vše se ví o zeatinu – kolik je struktur se zeatinem?
- 3) Které proteiny se strukturně nejvíce podobají PDBID 2HI4, případně 3T4T.
- 4) Jak vypadá kvartérní struktura proteinu 1stm? Z kolika podjednotek je složena?
- 5) Pomocí EMDB si prohlédněte struktury virů. Která struktura viru má nejlepší rozlišení?



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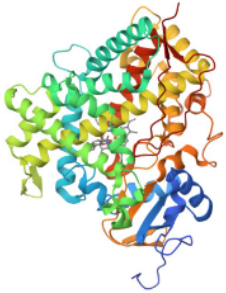
1) 2HI4



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Structure Summary 3D View Annotations Experiment **Sequence** Genome Ligands Versions

Biological Assembly 1 ?



3D View: [Structure](#) | [1D-3D View](#) | [Electron Density](#) | [Validation Report](#) | [Ligand Interaction](#) | [Predict Membrane](#)

Global Symmetry: Asymmetric - C1
Global Stoichiometry: Monomer - A1

[Find Similar Assemblies](#)

Biological assembly 1 assigned by authors.

2HI4

Crystal Structure of Human Microsomal P450 1A2 in complex with alpha-naphthoflavone

PDB DOI: <https://doi.org/10.2210/pdb2HI4/pdb>

Classification: **OXIDOREDUCTASE**

Organism(s): *Homo sapiens*

Expression System: *Escherichia coli*

Mutation(s): No

Membrane Protein: Yes **OPM**

Deposited: 2006-06-29 Released: 2007-02-20

Deposition Author(s): Sansen, S., Yano, J.K., Reynald, R.L., Schoch, G.S., Stout, C.D., Johnson, E.F.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

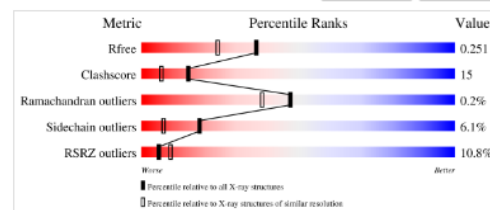
Resolution: 1.95 Å

R-Value Free: 0.267

R-Value Work: 0.226

R-Value Observed: 0.223

wwPDB Validation



Ligand Structure Quality Assessment



This is version 1.4 of the entry. See complete [history](#).

Macromolecule Content

- Total Structure Weight: 57.18 kDa
- Atom Count: 4,069
- Modelled Residue Count: 480
- Deposited Residue Count: 495
- Unique protein chains: 1

EMBL-EBI Protein Data Bank in Europe
Bringing Structure to Biology

Services Research Training About us

Examples: [hemoglobin](#), [BRCA1_HUMAN](#)

Search

Feedback

PDBe > 2hi4

Crystal Structure of Human Microsomal P450 1A2 in complex with alpha-naphthoflavone

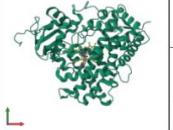
Source organism: *Homo sapiens*

Primary publication:
[Adaptations for the oxidation of polycyclic aromatic hydrocarbons exhibited by the structure of human P450 1A2.](#)
Sansen S, Yano JK, Reynald RL, Schoch GA, Griffin KJ, Stout CD, Johnson EF
J Biol Chem **282** 14348-55 (2007)
PMID: 17311915

X-ray diffraction
1,95Å resolution

Released: 20 Feb 2007
DOI: [10.2210/pdb2hi4/pdb](https://doi.org/10.2210/pdb2hi4/pdb)

Model geometry
Fit model/data



Quick links

- 2hi4 overview
- Citations
- Structure analysis
- Function and Biology
- Ligands and Environments
- Experiments and Validation

View
Downloads
3D Visualisation

Function and Biology

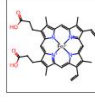
Reactions catalysed:

RH + [reduced NADPH--hemoprotein reductase] + O(2) = ROH + [oxidized NADPH--hemoprotein reductase] + H(2)O

A hydroperoxy icosatetraenoate = an oxoicosatetraenoate + H(2)O

Ligands and Environments

Cofactor:



1 x HEM

1 bound ligand:



Biochemical function:

- hydroperoxy icosatetraenoate dehydratase activity

Biological process:

- omega-hydroxylase P450 pathway

Cellular component:

- intracellular membrane-bounded organelle

Citations

49 review citations

Cytochrome P450 enzymes in drug metabolism: regulation of gene expression, enzyme activities, and impact of genetic variation.
Zanger et al. (2013)

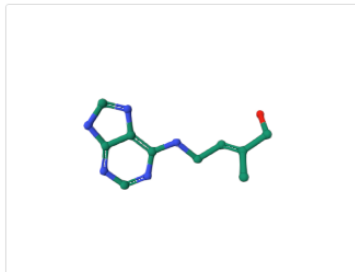
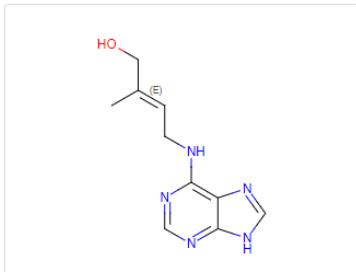
118 mentions without citation

Insights into the substrate specificity, inhibitors, regulation, and polymorphisms and the clinical impact of human cytochrome P450 1A2.
Zhou et al. (2009)



2) Zeatin

- <https://www.rcsb.org/ligand/ZEA>
- <https://www.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/ZEA>



Toggle Hydrogen Toggle Labels

Display Files Download Files Data API

ZEA

(2E)-2-methyl-4-(9H-purin-6-ylamino)but-2-en-1-ol

Find entries where: ZEA

☒ is present as a standalone ligand in 10 entries

search

Find related ligands:

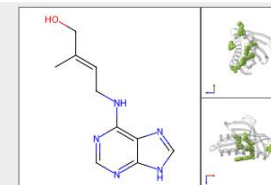
- Similar Ligands (Stereospecific)
- Similar Ligands (including Stereoisomers)
- Similar Ligands (Quick Screen)
- Similar Ligands (Substructure Stereospecific)
- Similar Ligands (Substructure including Stereoisomers)

4ryv > ZEA

(2E)-2-methyl-4-(9H-purin-6-ylamino)but-2-en-1-ol

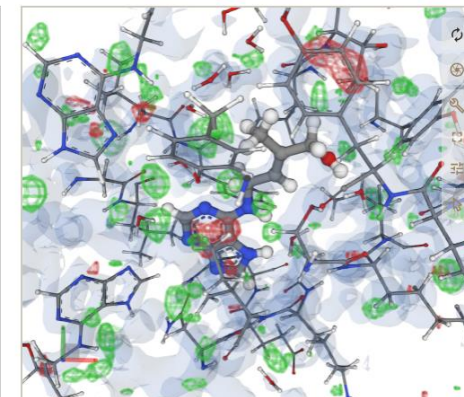
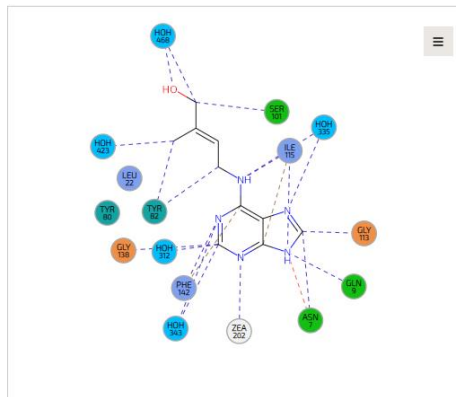
Formula: C₁₀ H₁₃ N₅ O

Molecular weight: 219 Da



Environment details NEW

ZEA 201 bound to chain A



Quick links

- 4ryv overview
- Citations
- Structure analysis
- Function and Biology
- Ligands and Environments**
- Experiments and Validation

Downloads

Search similar ligands

- Contain substructure (ChEBI)
- Similar structures (ChEBI)

EBI resources (ZEA)

- ZEA in PDBeChem
- Bioassay data (ChEMBL)

External mappings

- DrugBank -

Chemical Component Summary	
Name	(2E)-2-methyl-4-(9H-purin-6-ylamino)but-2-en-1-ol
Synonyms	TRANS-ZEATIN
Identifiers	(E)-2-methyl-4-(9H-purin-6-ylamino)but-2-en-1-ol
Formula	C ₁₀ H ₁₃ N ₅ O
Molecular Weight	219.243
Type	NON-POLYMER
Isomeric SMILES	C/C(=C/CNc1c2c([nH]cn2)ncn1)/CO
InChI	InChI=1S/C10H13N5O/c1-7(4-16)2-3-11-9-8-10(13-5-12-8)15-6-14-9/h2,5-6,16H,3-4H2,1H3,(H2,11,12,13,14,15)/b7-2+
InChIKey	UZKQTCBAMSWPJD-FARCUNLSSA-N

Chemical Details	
Formal Charge	0
Atom Count	29
Chiral Atom Count	0
Bond Count	30
Aromatic Bond Count	10



3) Strukturní podobnost

- RCSB

Macromolecules

Find similar proteins by: **Sequence** (by identity cutoff) | 3D Structure

Entity ID: 1	100%	
Molecule	95%	
Cytochrome P450 1A2	90%	Sequence Length
	80%	495
	70%	
	60%	
	50%	
UniProt & NIH Comm	40%	
Find proteins for P0517	30%	

PHAROS: **P05177**

PDBeFold

Molecule details >

Download

Search similar proteins

- Similar 3D structures (PDBeFold)
- Similar sequences

BLAST P05177 (UniProt)



3b) Strukturní podobnost



RCSB

PDBeFold

Refinements  -- Tabular Report --  All ☐ Selected 

Structure Determination Methodology

☐ experimental (411)

Scientific Name of Source Organism

☐ Homo sapiens (154)

☐ Priestia megaterium (124)

☐ Priestia megaterium NBRC 15308 = ATCC 14581 (24)

☐ Oryctolagus cuniculus (22)

☐ Trypanosoma cruzi (7)

☐ Arabidopsis thaliana (6)

☐ Escherichia coli K-12 (6)

☐ Pseudomonas fluorescens (5)

☐ Sphingobium sp. SYK-6 (5)

☐ Cryptosporidium parvum Iowa II (4)

[More...](#)

Taxonomy

☐ Eukaryota (226)

☐ Bacteria (183)

☐ Duplodnaviria (3)

☐ other sequences (2)

☐ Archaea (1)

Experimental Method

☐ X-RAY DIFFRACTION (405)

☐ ELECTRON MICROSCOPY (6)

Polymer Entity Type

☐ Protein (411)

Refinement Resolution (Å)

☐ 1.0 - 1.5 (16)

1 to 25 of 411 Polymer Entities

Page 1 of 17

Sort by

2HI4_1

4I8V_1

6UDL_1

6O5Y_1

6DWN_1

6DWM_1

6UDM_1

3C6G_1

3CZH_1

3DL9_1

4RSN_1

4DVQ_1

3V8D_1

3DAX_1

3MZS_1

3KW4_1

Structure Alignment Results. 

Query: pdb entry 2hi4:A , 480 residues

CRYSTAL STRUCTURE OF HUMAN MICROSOMAL P450 1A2 IN COMPLEX WITH ALPHA- NAPHTHOFLAVONE

Examined 187732 entries (530702 chains). Displaying Matches 1-20 of 621.

[Back to query](#) [next](#) [last page](#) Sort by arrange by SCOP family ☐ match [jump](#)

##	Scoring 			RMSD	Nalign	Ng	%se	Query				Target (PDB entry)			
	Q	P	Z					Match	%sse	Nres	x	Title			
1	1.00	122.1	33.4	0.00	480	0	100	100	2hi4:A	100	480	☐	CRYSTAL STRUCTURE OF HUMAN MICROSOMAL P450 1A2 IN COMPLEX WITH ALPHA-NAPHTHOFL		
2	0.87	55.4	22.4	0.87	459	4	76	97	6ud1:C	93	466	☐	STRUCTURE OF HUMAN CYTOCHROME P450 1A1 WITH DUOCARMYCIN PRODRUG (S) ICT-2700		
3	0.87	54.7	22.3	0.84	457	5	76	97	6udm:D	90	465	☐	STRUCTURE OF HUMAN CYTOCHROME P450 1A1 WITH DUOCARMYCIN PRODRUG (S) ICT-2726		
4	0.87	55.4	22.4	0.85	458	5	76	93	6udm:A	87	467	☐	STRUCTURE OF HUMAN CYTOCHROME P450 1A1 WITH DUOCARMYCIN PRODRUG (S) ICT-2726		
5	0.87	51.5	21.6	0.91	461	5	75	90	6udm:C	84	468	☐	STRUCTURE OF HUMAN CYTOCHROME P450 1A1 WITH DUOCARMYCIN PRODRUG (S) ICT-2726		
6	0.86	57.9	22.9	0.80	454	5	76	100	6dvm:D	94	464	☐	STRUCTURE OF HUMAN CYTOCHROME P450 1A1 WITH BERGAMOTTIN		
7	0.86	49.6	21.2	0.88	459	5	75	86	4i8v:C	96	468	☐	HUMAN CYTOCHROME P450 1A1 IN COMPLEX WITH ALPHA-NAPHTHOFLAVONE		
8	0.86	58.8	23.1	0.83	455	5	76	100	6dvm:C	94	464	☐	STRUCTURE OF HUMAN CYTOCHROME P450 1A1 WITH BERGAMOTTIN		
9	0.86	59.5	23.2	0.85	458	4	76	100	6ud1:A	94	469	☐	STRUCTURE OF HUMAN CYTOCHROME P450 1A1 WITH DUOCARMYCIN PRODRUG (S) ICT-2700		
10	0.86	54.1	22.1	0.92	461	4	75	97	6dvm:A	90	470	☐	STRUCTURE OF HUMAN CYTOCHROME P450 1A1 WITH BERGAMOTTIN		
11	0.86	47.7	20.9	0.81	455	5	76	86	4i8v:D	83	467	☐	HUMAN CYTOCHROME P450 1A1 IN COMPLEX WITH ALPHA-NAPHTHOFLAVONE		
12	0.86	57.0	22.7	0.89	455	5	76	100	6dvm:C	94	462	☐	STRUCTURE OF HUMAN CYTOCHROME P450 1A1 WITH ERLOTINIB		
13	0.85	54.4	22.2	0.86	458	6	75	97	4i8v:B	93	472	☐	HUMAN CYTOCHROME P450 1A1 IN COMPLEX WITH ALPHA-NAPHTHOFLAVONE		



4) Assembly 1stm

60 podjednotek

1stm > Structure analysis

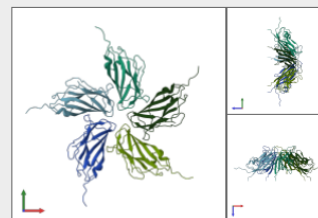
SATELLITE PANICUM MOSAIC VIRUS

Source organism: *Panicum mosaic satellite virus*

Assembly composition: homo 60-mer (preferred)

Entry contents: 1 distinct polypeptide molecule

X-ray diffraction
1,9Å resolution



Quick links

[1stm overview](#)

[Citations](#)

[Structure analysis](#)

[Function and Biology](#)

[Ligands and Environments](#)

[Experiments and Validation](#)

[Downloads](#)

Assemblies

Assembly 1 (preferred) [Download](#) [3D Visualisation](#)

Assembly Name: Coat protein

Multimeric state: homo 60-mer

Accessible surface area: 240781.71 Å²

Buried surface area: 222091.91 Å²

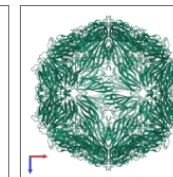
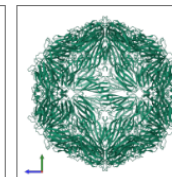
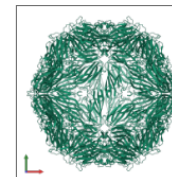
Dissociation area: 75 049,63 Å²

Dissociation energy (ΔG^{dis}): 978,18 kcal/mol

Dissociation entropy ($T\Delta S^{dis}$): 184,92 kcal/mol

Symmetry number: 60

PDBe Complex ID: PDB-CPX-183111



Macromolecules

Coat protein

Chains: A, B, C, D, E

Length: 157 amino acids

Theoretical weight: 16,98 KDa

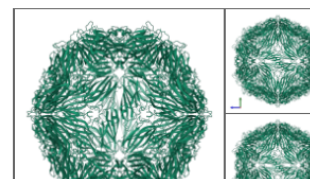
Source organism: *Panicum mosaic satellite virus*

UniProt:

◦ Canonical: [Q86993](#) (Residues: 1-157; Coverage: 100%)

Pfam: [Potexvirus coat protein](#)

Tatena



Molecule details >

[Download](#)

Search similar proteins

[Similar 3D structures](#) (PDBeFold)

[Similar sequences](#)



5) Best resolution EM virů



EMDB
Electron Microscopy Data Bank

Enter your search term(s) in the box below or [build an advanced search query](#)

Search EMDB...

Examples: 1001, Apoferritin, Tomography, Rossmann MG, 5A1A

Home | Deposition | Documentation | Resources | FTP Archive | REST API | About | Feedback | Share

Edit your search query here and hit Return to execute it:

database:EMDB AND current_status:[* TO *] AND resolution:[0 TO 2] AND sample_type:"virus"

Filter By

Current Database

- EMDB [7]

Current status

- REL [7]

Sample type

- Virus [7]
- Ligand [5]
- Protein [5]
- RNA [1]

Organism

- Tobacco mosaic virus [2]
- Adeno-associated dependoparvovirus a [1]
- Enterovirus c [1]
- Tobacco mosaic virus [1]

Number of entries released by year

Year	EMDB entries	EMPIAR entries
2002	0	0
2004	0	0
2006	0	0
2008	0	0
2010	0	0
2012	0	0
2014	0	0
2016	0	0
2018	1	0
2019	2	0
2020	2	0
2021	1	0
2022	1	0

Sort by: Resolution | Download | Showing 1 - 7 of 7. Page 1 of 1 | Display 10 | Statistics

EMD-22854

Download Map | 3D View | data

Adeno-Associated Virus (AAV-DJ) - cryo-EM structure at 1.56 Angstrom Resolution

Release date: Dec. 16, 2020 | Fitted PDBs: 7kfr | Resolution: 1.56 Å | Q-score: 0.838 | EM Method: Single-particle

Xie Q, Yoshioka CK, Chapman MS



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Souhrnné databáze

- PDBe-KB - <https://www.ebi.ac.uk/pdbe/pdbe-kb/>
- PDBSum - <http://www.ebi.ac.uk/thornton-srv/databases/pdbsum/>



Zadání PDBe-KB a PDBSum



- **PDBe-KB**

1) Najděte si cytochrom P450 3A4

a. kolik je známo struktur?

b. Jaké části struktur jsou pokryty? Jak se liší jejich sekundární struktury

c. S jakými ligandy byly cytochromy P450 3A4 vykrystalizovány? Rozlište mezi nimi kofaktory, substráty, inhibitory, krystalizační činidla a ionty

- **PDBSum**

1) Zjistěte, jak spolu interagují jednotlivé domény v Na/K – ATPase.

2) Který cleft (záhyb) je pravděpodobně aktivním místem cytochromu P450 ve struktuře 2HI4?

3) Zjistěte, které aminokyseliny a jak interagují s ligandy ve strukturách cytokininových receptorů. (LIGPLOT)



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PDBe-KB



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**PDBe-KB**
Protein Data Bank in Europe Knowledge Base

Aggregated Views of Proteins
Režim celé obrazovky ukončíte stisknutím klávesy **F11**

Home Documentation

Search in PDBe

Summary Structures Ligands Interactions Annotations Similarity Publications Feedback

What's new?

Cytochrome P450 3A4

Gene: CYP3A4 Enzyme: EC 1.14.14.1 Disease

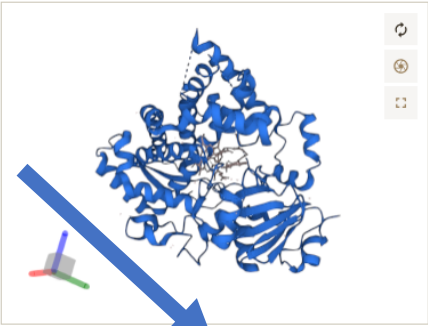
Organism: *Homo sapiens (Human)*

Synonyms: CYP3A3

Uniprot: **P08684** [go to UniProt](#)

Biological function: A cytochrome P450 monooxygenase involved in the metabolism of sterols, steroid hormones, retinoids and fatty acids ([PubMed:10681376](#), [PubMed:11093772](#), [PubMed:11555828](#), [PubMed:14559847](#), [PubMed:12865317](#), [PubMed:15373842](#), [PubMed:15764715](#), [PubMed:20702771](#), [PubMed:19965576](#), [PubMed:21490593](#), [PubMed:21576599](#)). ... [+ \[show more\]](#) [go to UniProt](#)

Representative structure for UniProt P08684
PDB chain with highest data quality, coverage and best resolution



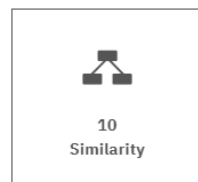
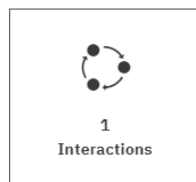
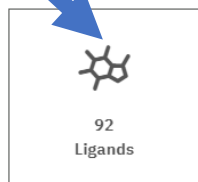
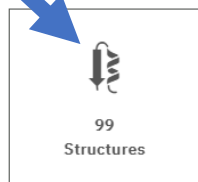
PDB chain shown: 6ung A [go to PDBe](#)

UniProt residues 21 - 503

Coverage: 90%

3D view of superposed structures for region 1

Click on the icons below to view the relevant page:





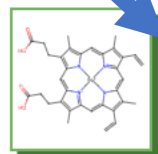
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PDBe-KB ligands

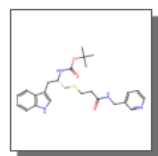


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Legends: ■ Annotated small molecules
■ Other small molecules
■ Not interacting small molecules

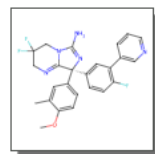


HEM
cofactor-like
Found in 99 PDB entries

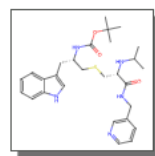


PKT
Found in 1 PDB entry

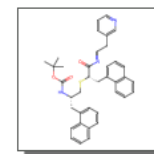
Show all



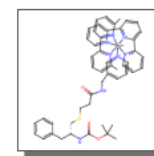
2QH
Found in 1 PDB entry



DEJ
Found in 1 PDB entry



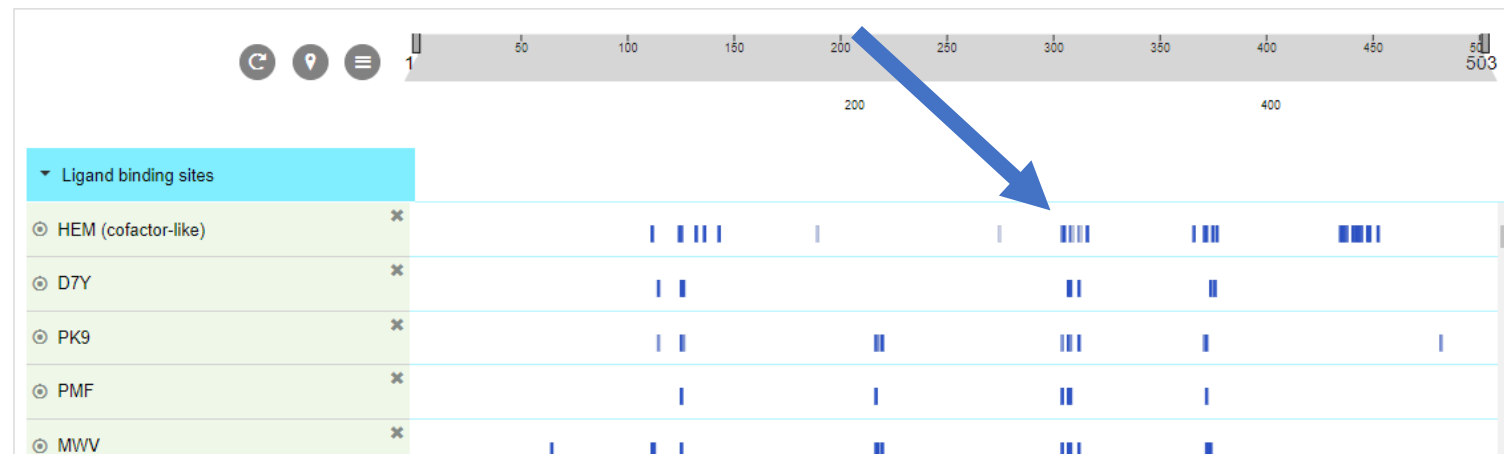
QDP
Found in 1 PDB entry



X8S
Found in 1 PDB entry

Ligand-binding Residues

The visualisation is using UniProt numbering for residues, not PDB numbering.





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PDBsum



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Děkuji za pozornost