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/

Základní databáze

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

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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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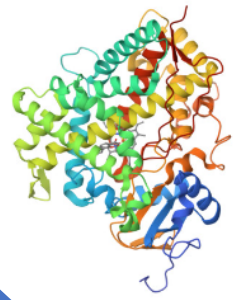
1) 2HI4

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

Biological Assembly 1



3D View: S ure | 1D-3D View | Electron Density alidation Report | Ligand Interaction | Predict Membrane

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

Find Similar Assemblies

Biological assembly 1 assigned by authors.

Macromolecule Content

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

Display Files | Download Files | Data API

2HI4

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

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

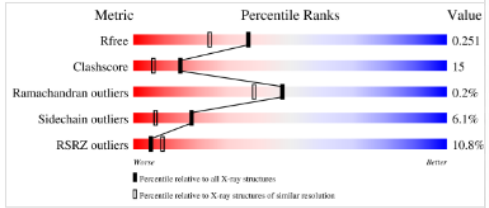
Classification: OXIDOREDUCTASE
Organism(s): Homo sapiens
Expression System: Escherichia coli
Mutation(s): No
Membrane Protein: Yes OPM

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 3D Report | Full Report



Ligand Structure Quality Assessment

This is version 1.4 of the entry. See complete history.

EMBL-EBI | Services | Research | Training | About us

Protein Data Bank in Europe
Bringing Structure to Biology

Search | Advanced search | Examples: hemoglobin, BRCA1_HUMAN | Feedback

PDBe › 2hi4

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

Source organism: *Homo sapiens*

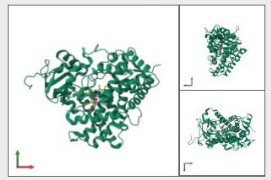
Primary publication:
Adaptations for the oxidation of polycyclic aromatic hydrocarbons exhibited by the structure of human P450 1A2.

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

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 Details

Reactions catalysed:

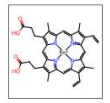
RH + [reduced NADPH--hemoprotein reductase] + O(2) = ROH + [oxidized NADPH--hemoprotein reductase] + H(2)O

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

Biochemical function: hydroperoxy icosatetraenoate dehydratase activity
Biological process: omega-hydroxylase P450 pathway
Cellular component: intracellular membrane-bounded organelle

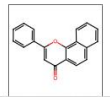
Ligands and Environments

Cofactor:



1 x HEM

1 bound ligand:



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)

48 more

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)

117 more

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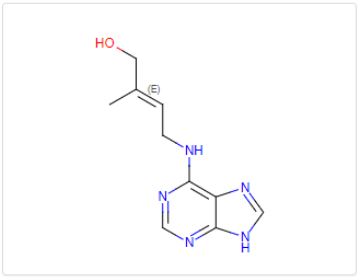
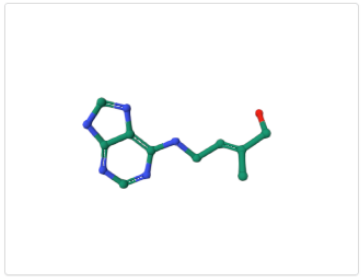
2) Zeatin

- 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

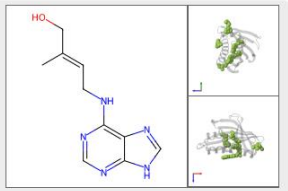
Find related ligands:
Similar Ligands (Stereospecific)
Similar Ligands (including Stereoisomers)
Similar Ligands (Quick Screen)
Similar Ligands (Substructure Stereospecific)
Similar Ligands (Substructure including Stereoisomers)

4ryv › ZEA

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

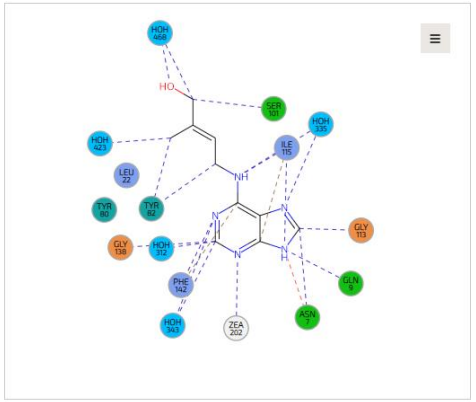
Formula: $C_{10}\ H_{13}\ N_5\ O$

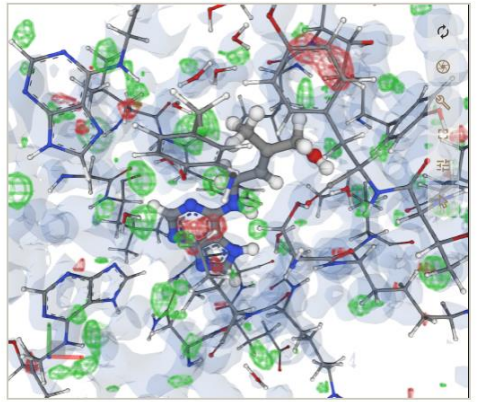
Molecular weight: 219 Da



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

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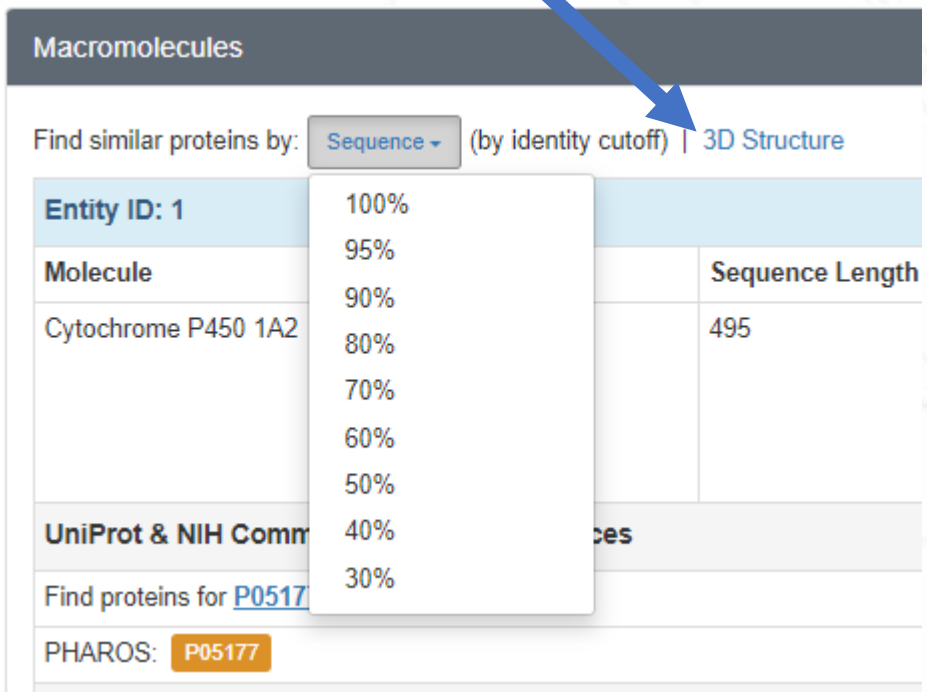
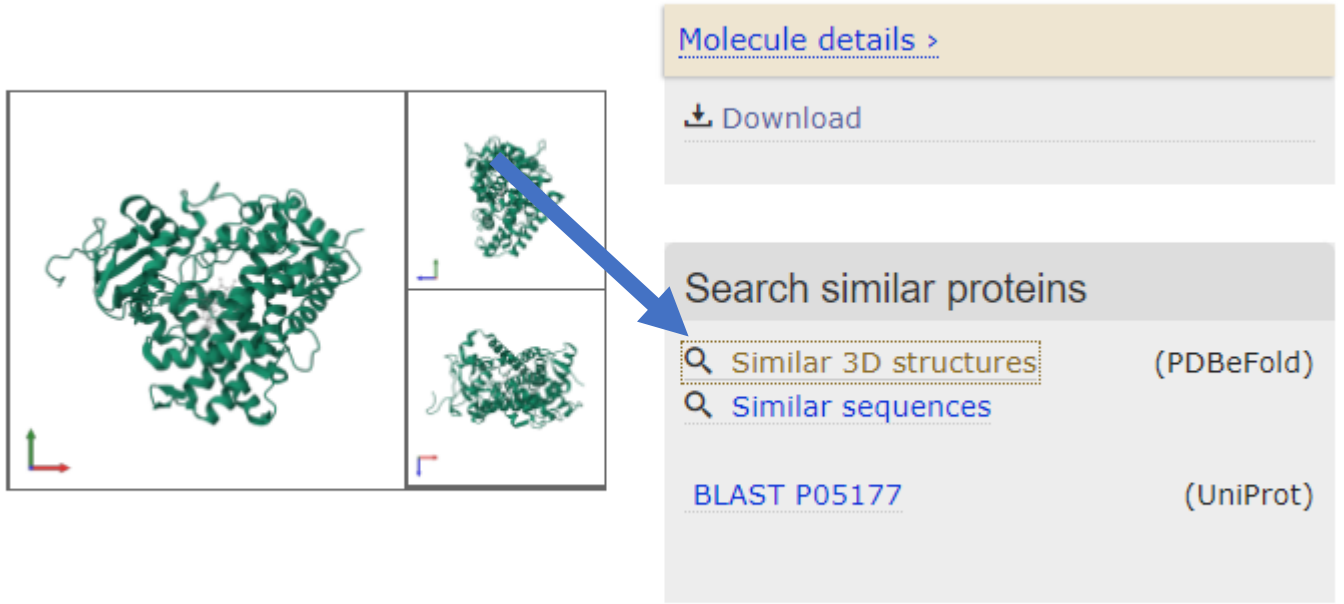
3) Strukturní podobnost

- RCSB



PDBeFold



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3b) Strukturní podobnost

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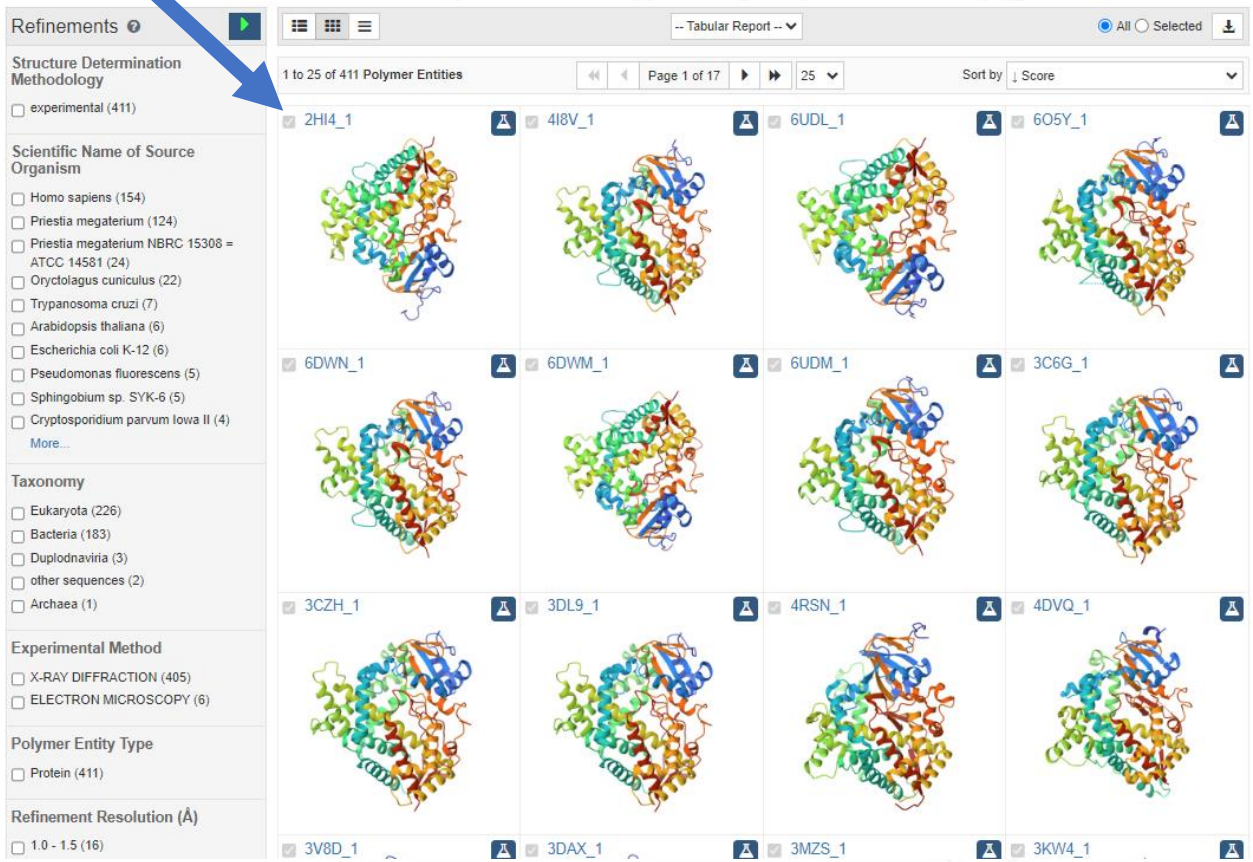
RCSB



PDBeFold

Structure Alignment Results.

Query: pdb entry 2hi4:A , 480 residues

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

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

Back to query | next | last page | Sor | Q-score | arrange by SCOP family | match 1 | jump

##	Scoring			RMSD	N_{align}	N_g	%	Query		Target (PDB entry)				
	Q	P	Z						Match	$\%_{sse}$	N_{res}	×	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	6udl: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	6dwm: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	6dwm:C	94	464	☐	STRUCTURE OF HUMAN CYTOCHROME P450 1A1 WITH BERGAMOTTIN
9	0.86	59.5	23.2	0.85	458	4	76	100	6udl: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	6dwm: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	6dwm: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

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4) Assembly 1stm

60 podjednotek

1stm › Structure analysis

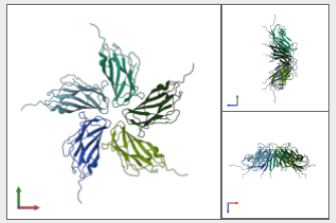
SATELLITE PANICUM MOSAIC VIRUS

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

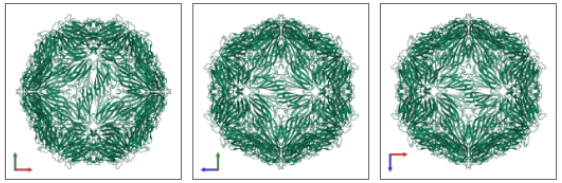
Downloads

Assemblies

Assembly 1 (preferred) Download 3D Visualisation

Assembly Name: Coat protein

Multimeric state:	homo 60-mer	**Dissociation energy (ΔG^{diss}):**	978,18 kcal/mol
Accessible surface area:	240781.71 Å^2	**Dissociation entropy ($T\Delta S^{diss}$):**	184,92 kcal/mol
Buried surface area:	222091.91 Å^2	**Symmetry number:**	60
Dissociation area:	75 049,63 Å^2	**PDBe Complex ID:**	PDB-CPX-183111

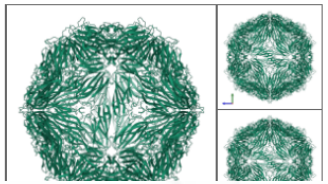


Macromolecules

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



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

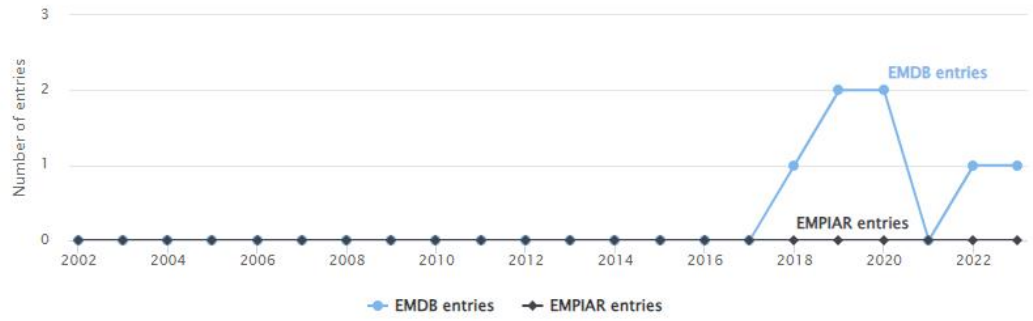
Current Database
- EMDB [7]

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]

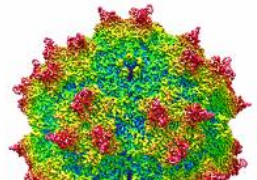
Number of entries released by year



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
Resolution: 1.56 Å
EM Method: Single-particle

Fitted PDBs: 7kfr
Q-score: 0.838

Xie Q, Yoshioka CK, Chapman MS

Souhrnné databáze

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

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Zadání PDBe-KB a PDBSum

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- **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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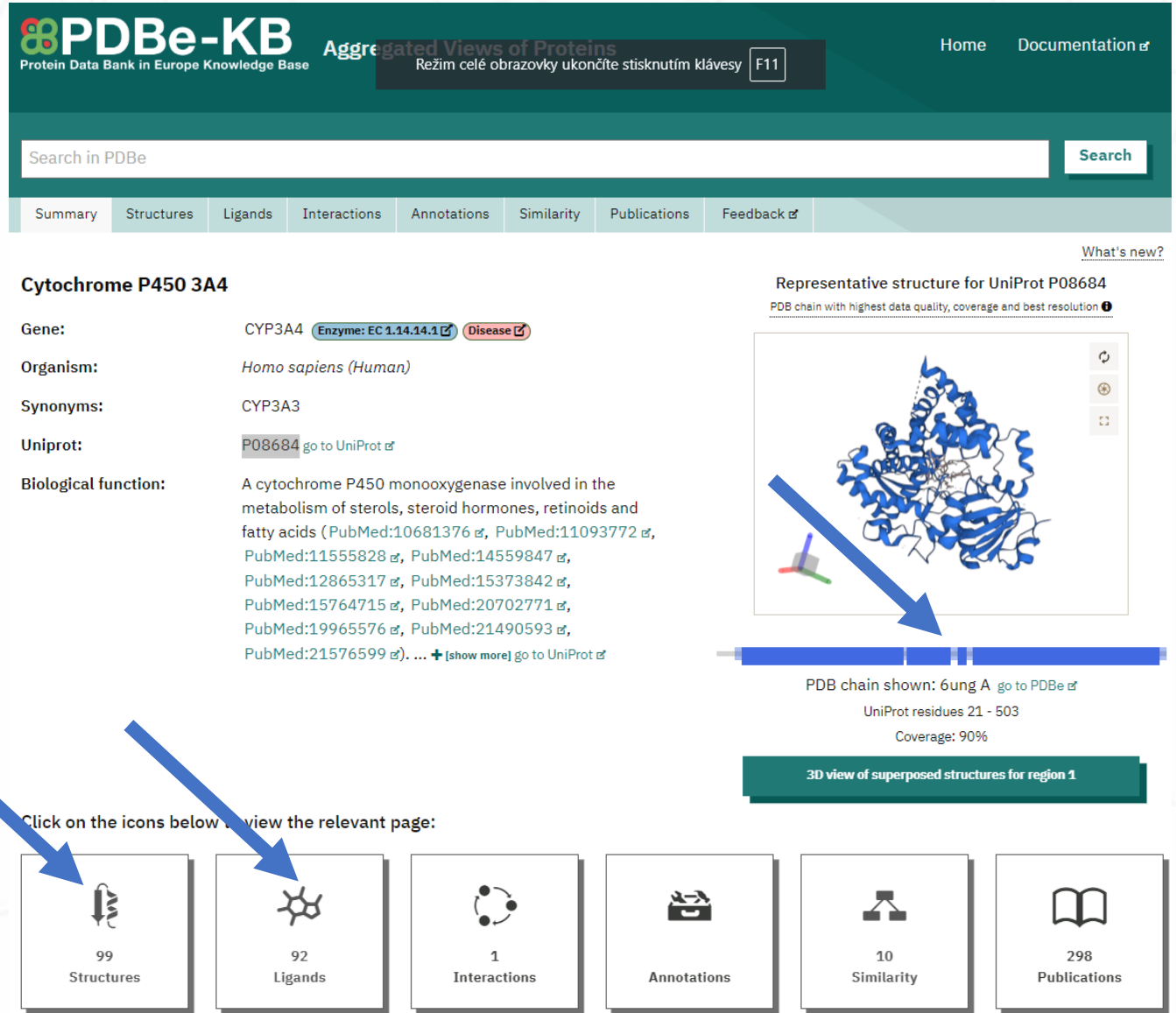
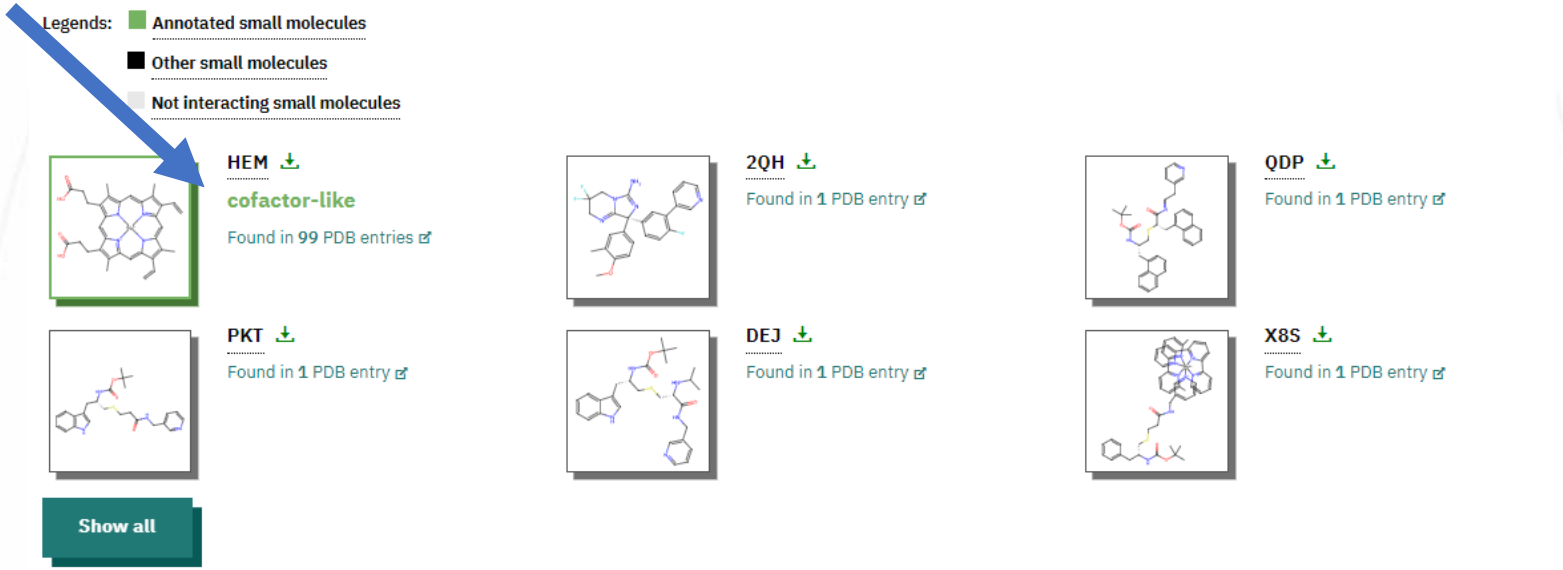
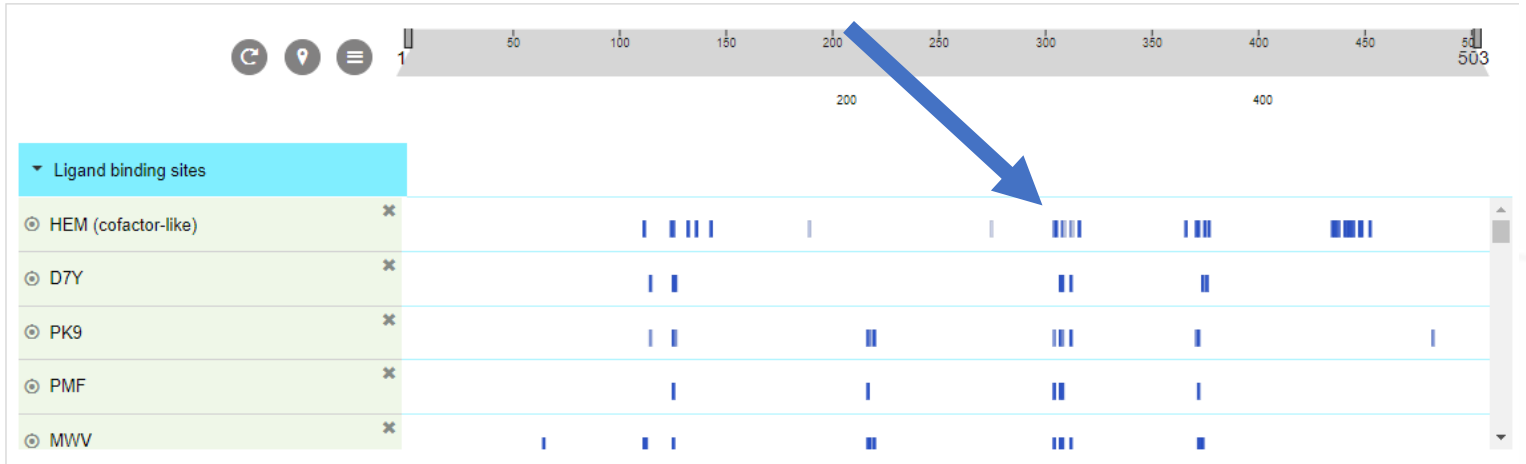
PDBe-KB



PDBe-KB ligands





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PDBsum

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Děkuji za pozornost