



Databáze

KFC/CHS



Typy databází

- Databáze odborné literatury (Web of science **WOS**, PubMed, Google scholar Reaserchgate)
- Databáze sekvencí biomolekul (GenBank, European Nucleotide Archive **ENA**)
- Strukturální databáze
- Proteinové databáze
- Databáze interakcí biomolekul
- Genomové databáze

Strukturní databáze

- **PDBe** doplnění PDB z BMRB (NMR) a EMDB (EM)
- **PDBsum** shromažďuje další informace o struktuře
- **PDBwiki** wikipedie zabývající se PDB strukturami
- **NDB** databáze nukleových struktur
- **CSD** databáze krystalů malých molekul – placená
- **MODBASE** databáze modelů proteinů

Klasifikace struktur proteinů

- **SCOP** hledání strukturních rodin proteinů
- **CATH** hledání strukturních rodin proteinů
- **GENE3D** strukturní genomika
- **3Dee** databáze zabývající se doménami proteinů

Protein Data Bank - PDB (www.pdb.org)

WORLDWIDE PDB PROTEIN DATA BANK

VALIDATION ▾ DEPOSITION ▾ DATA DICTIONARIES ▾ DOCUMENTATION ▾ TASK FORCES ▾ STATISTICS ▾ ABOUT ▾ wwPDB Foundation

Since 1971, the Protein Data Bank archive (PDB) has served as the single repository of information about the 3D structures of proteins, nucleic acids, and complex assemblies.

The Worldwide PDB (wwPDB) organization manages the PDB archive and ensures that the PDB is freely and publicly available to the global community.

Learn more about PDB HISTORY and FUTURE.

Validate Structure
or View validation reports

Deposit Structure
All Deposition Resources

Download Archive
Instructions

wwPDB Members

wwPDB data centers serve as deposition, annotation, and distribution sites of the PDB archive. Each site offers tools for searching, visualizing, and analyzing PDB data.

PDBe
Protein Data Bank in Europe

Rich information about all PDB entries, multiple search and browse facilities, advanced services including PDBePISA, PDBeFold and PDBeMotif, advanced visualisation and validation of NMR and EM structures, tools for bioinformaticians.

PDBj
Protein Data Bank Japan

Supports browsing in multiple languages such as Japanese, Chinese, and Korean; SeSAW identifies functionally or evolutionarily conserved motifs by locating and annotating sequence and structural similarities, tools for bioinformaticians, and more.

RCSB PDB
Research Collaboratory for Structural Bioinformatics Protein Data Bank

Simple and advanced searching for macromolecules and ligands, tabular reports, specialized visualization tools, sequence-structure comparisons, RCSB PDB Mobile, Molecule of the Month and other educational resources at PDB-101, and more.

BMRB

wwPDB Resources

Data Dictionaries

- Macromolecular Dictionary (PDBx/mmCIF)
- Small Molecule Dictionary (CCD)
- Peptide-like antibiotic and inhibitor molecules (BIRD)

Annotation

- Procedures and policies
- Improvements for consistency and accuracy

Community Input: Task Forces and Working Groups

- Validation Task Forces (X-ray, NMR, 3DEM)
- Small Angle Scattering Task Force
- PDB/mmCIF Working Group
- Hybrid/Integrative Methods Task Force
- Ligand Validation Workshop

PDB Data Growth & Usage Statistics

- Depositions: by data center, by year, and by depositor location
- Downloads: by year for all entries

Workshops & Symposia

- Summaries and presentations from past meetings and events

Information for Journals

- Policies, procedures, coordination with publishers, and preferred *Instructions to Authors*

News & Announcements

03/22/2017

- Archival PDBx/mmCIF Version V4 to V5 Update in the Protein Data Bank

The wwPDB is preparing the update of PDBx/mmCIF model files for all entries in the PDB archive to V5 version of the PDBx/mmCIF dictionary. When completed, all PDB model files will have better organized content and will conform to the revised data model used within the wwPDB OneDep System.

[Read more](#)

03/15/2017

- Updated Validation Reports for Archived PDB Structures Now Available

The wwPDB partners are pleased to announce that updated validation reports for all X-ray, NMR, and 3DEM structures deposited in the PDB archive are now available on March 15, 2017.

The updates include new percentile statistics reflecting the state of the PDB archive on December 31st 2016 and updated versions of the Mogul software (2017) and CSD archive (as538be).

[Read more](#)

03/14/2017

- Data Management: A global coalition to sustain core data

PDBe
Protein Data Bank in Europe

PDBj
Protein Data Bank Japan

RCSB PDB
PROTEIN DATA BANK

PDB - vyhledávání

<https://www.rcsb.org>

jednoduché vyhledávání
(PDB ID, jméno autora, druh makromolekuly, ligand)

The screenshot shows the top navigation bar of the PDB website. On the left is the PDB logo and the text 'An Information Portal to 128330 Biological Macromolecular Structures'. In the center is a search bar with the placeholder text 'Search by PDB ID, author, macromolecule, sequence, or ligands' and a 'Go' button. Below the search bar are links for 'Advanced Search' and 'Browse by Annotations'. On the right are social media icons for Facebook, Twitter, and YouTube.

The screenshot shows the main content area of the PDB website. On the left is a vertical navigation menu with links for 'Welcome', 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', and 'Learn'. The main content area features two articles: 'A Structural View of Biology' and 'A Molecular View of HIV Therapy'. Below the HIV article is a 3D molecular model of a protein, labeled 'Photoactive Yellow Protein', which is the 'March Molecule of the Month'. The model is shown in a yellow surface representation with a blue ligand bound to it.

rozšířené vyhledávání

The screenshot shows the search filters sidebar on the PDB website. It is organized into several sections:

- Choose a Query Type:** Includes 'Quick Search' (All/Experimental Type/Molecule Type), 'ID(s) and Keywords' (PDB ID(s), Entity ID(s), Chain ID(s), PubMed ID(s), UniProtKB Accession Number(s), Text Search, mmCIF Keyword Search (Classification), Pfam Accession Number(s), UniProt Gene Name, Sequence Cluster Name), 'Structure Annotation' (Structure Title, Structure Description, Macromolecule Name, Pathway Reaction Name, Large Structures), 'Deposition' (Author Name, Deposit Date, Release Date, Revision Date, Latest Released Structures, Latest Modified Structures, Structural Genomics Project), and 'Structure Features' (Macromolecule Type, Number of Chains (Asymmetric Unit), Number of Chains (Biological Assembly), Number of Entities, Protein Stoichiometry, Protein Symmetry, Protein Symmetry Browser (opens popup), Number of Models, Number of Disulfide Bonds, Link records, Molecular Weight (Structure), Secondary Structure Content, Secondary Structure Length, SCOP Classification Browser (opens popup), CATH Classification Browser (opens popup), Taxonomy Browser (opens popup)).
- Sequence Features:** Includes Sequence (BLAST/FASTA/PSI-BLAST), Wild Type Protein, Mutation, Translated Nucleotide Sequence (BLASTX), Sequence Motif, Chain Length, Protein Modifications, Protein Modification Browser (opens popup), and Genome Location Browser (opens popup).
- Chemical Components:** Includes Chemical Name, Chemical ID(s), InChI Descriptor, Chemical structure (SMILES), Molecular Weight (Chemical component), Chemical Formula, Chemical Component Type, Binding Affinity, Has Ligand(s), Has Modified Residue(s), and Sub-components.
- Biologically Interesting Molecules:** Includes Biologically Interesting Molecules (from BIRD).
- Biology:** Includes Source Organism Browser (NCBI) (opens popup), Expression Organism, Enzyme Classification Browser (opens popup), Enzyme Classification, Biological Process Browser (GO) (opens popup), Cell Component Browser (GO) (opens popup), Molecular Function Browser (GO) (opens popup), and Transporter Classification Browser (opens popup).
- Methods:** Includes Experimental Method, X-ray Resolution, X-ray Average B Factor, Refinement R Factors, Diffraction Source, Structure Determination Method, Reflections, Cell Dimensions, and Software.
- Publication:** Includes Citation, Medical Subject Headings Browser (opens popup), and PubMed Abstract.

PDB - vyhledávání

vyhledejte: cytochrome p450

vyhledané struktury

vyhledávaný výraz

Search Parameter:
Text Search for: cytochrome p450

třídění dle organismu

Refinements

ORGANISM

- Homo sapiens (167)
- Pseudomonas putida (119)
- Bacillus megaterium (94)
- Mycobacterium tuberculosis (70)
- Saccharomyces cerevisiae (54)
- Oryctolagus cuniculus (24)
- Rattus norvegicus (19)
- Other (302)

třídění dle taxonomického zařazení

UNIPROT MOLECULE NAME

- Camphor 5-monooxygenase (119)
- Bifunctional cytochrome P ... (87)
- Cytochrome P450 (44)
- Lanosterol 14-alpha demet ... (38)
- Mycocyclosin synthase (31)
- 40S ribosomal protein S18-A (30)
- 60S ribosomal protein L18-A (30)
- Refine Query

třídění dle experimentální metody

TAXONOMY

- Bacteria (492)
- Eukaryota (341)
- Viruses (16)
- Archaea (14)
- Other (1)

třídění dle rozlišení

EXPERIMENTAL METHOD

- X-ray (835)
- Electron Microscopy (6)
- Solution NMR (6)

X-RAY RESOLUTION

- less than 1.5 Å (40)
- 1.5 - 2.0 Å (264)
- 2.0 - 2.5 Å (305)
- 2.5 - 3.0 Å (156)

Currently showing 1 - 25 of 847 Page: 1 of 34

View: Detailed Reports: Select a Report Sort: Release Date Newest to Oldest Download Files

5FSA
Crystal structure of sterol 14-alpha demethylase (CYP51) from a pathogenic yeast *Candida albicans* in complex with the antifungal drug posaconazole
Hargrove, T.Y., Friggeri, L., Wawrzak, Z., Qi, A., Hoekstra, W.J., Schotzinger, R.J., York, J.D., Guengerich, F.P., Lepesheva, G.I.
(2017) J Biol Chem
Released: 3/15/2017
Method: X-ray Diffraction
Resolution: 2.86 Å
Residue Count: 980
Macromolecule: CYP51 VARIANT1 (protein)
Unique Ligands: HEM, X2N

5IRQ
Human cytochrome P450 17A1 bound to inhibitors (R)- and (S)- orteronel
Petrunak, E.M., Rogers, S.A., Aube, J., Scott, E.E.
PubMed ID is not available.
Released: 3/15/2017
Method: X-ray Diffraction
Resolution: 2.2 Å
Residue Count: 1976
Macromolecule: Steroid 17-alpha-hydroxylase/17,20 ... (protein)
Unique Ligands: 6D7, 7D6, HEM

5IRV
Human cytochrome P450 17A1 bound to inhibitor VT-464
Petrunak, E.M., Rogers, S.A., Aube, J., Scott, E.E.
PubMed ID is not available.
Released: 3/15/2017
Method: X-ray Diffraction
Resolution: 3.1 Å
Macromolecule: Steroid 17-alpha-hydroxylase/17,20 ... (protein)
Unique Ligands: 6D8, HEM

název struktury/publikace

autoři

zkratka struktury + obsažené ligandy

popis použité expt. metody a rozlišení struktury

PDB vyhledávání

PDB ID

náhled

Structure Summary 3D View Annotations Sequence Sequence Similarity Structure Similarity Experiment Literature

Biological Assembly 1 ?

3QE2

Crystal Structure of Human NADPH-Cytochrome P450 Reductase

DOI: 10.2210/pdb3qe2/pdb

Classification: **OXIDOREDUCTASE**

Deposited: 2011-01-19 Released: 2011-08-03

Deposition author(s): [Xia, C.](#), [Marohnic, C.](#), [Panda, S.P.](#), [Masters, B.S.](#), [Kim, J.-J.P.](#)

Organism: [Homo sapiens](#)

Expression System: Escherichia coli

Mutation(s): 2

Structural Biology Knowledgebase: [3QE2 \(>22 annotations\)](#) [SSKB.org](#)

Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 1.75 Å

R-Value Free: 0.239

R-Value Work: 0.211

wwPDB Validation

Metric	Percentile Ranks	Value
Rfree		0.239
Clashscore		9
Ramachandran outliers		0.3%
Sidechain outliers		2.1%
RSRZ outliers		5.5%

Water Percentile relative to all X-ray structures
 Percentile relative to X-ray structures of similar resolution

Literature

Structural basis for human NADPH-cytochrome P450 oxidoreductase deficiency.

[Xia, C.](#), [Panda, S.P.](#), [Marohnic, C.C.](#), [Martasek, P.](#), [Masters, B.S.](#), [Kim, J.J.](#)

(2011) Proc.Natl.Acad.Sci.USA **108**: 13486-13491

PubMed: 21808038

PubMedCentral: PMC3158178

DOI: 10.1073/pnas.1106632108

Primary Citation of Related Structures: [3QE2](#) [3QFC](#) [3QFR](#) [3QFS](#) [3QFT](#)

PubMed Abstract:

NADPH-cytochrome P450 oxidoreductase (CYPOR) is essential for electron donation to microsomal cytochrome P450-mediated monooxygenation in such diverse physiological processes as drug metabolism (approximately 85-90% of therapeutic drugs), steroid biosynthesis, and bioactive metabolite production (vitamin D and retinoic acid

- FASTA Sequence
- PDB Format
- PDB Format (gz)
- PDBx/mmCIF Format
- PDBx/mmCIF Format (gz)
- PDBML/XML Format (gz)
- Structure Factors (CIF)
- Structure Factors (CIF - gz)
- Biological Assembly 1 (PDB Format - gz) (A+S)
- Biological Assembly 2 (PDB Format - gz) (A+S)

publikace, ve které byla struktura popsána

PDB vyhledávání

klasifikace proteinu

řetězce proteinu

délka AMK sekvence

organismus

rozlišení sekundárních strukturních prvků

název molekuly

sekvence z UniProtu

topologie výskytu segmentu (lumen/TMD/cytosol)

Macromolecules

Classification: [OXIDOREDUCTASE](#) Sequence Display for 3QE2

Total Structure Weight: 144272.03 ⓘ

Macromolecule Entities Toggle Protein Feature View

Molecule	Chains	Length	Organism	Details
NADPH--cytochrome P450 reductase	A, B	618	Homo sapiens	EC#: 1.6.2.4 IUBMB Fragment: UNP residues 64-677 Mutation: P228L, A503V POR Gene View CYPOR Full Protein Feature View for P16435 Find similar proteins by: Sequence Structure

Protein Feature View - UniProtKB AC: [P16435](#) UniProt

UniProtKB

P16435

Molec. Processing Motif

Lum **Red** Cytoplasmic

Flavodoxin-like

FAD-binding FR-type

1.6.2.4: NADPH--hemoprotein reductase

UniProt Sites

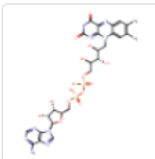

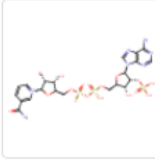
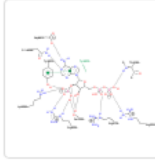
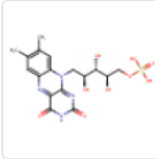
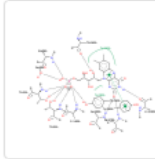
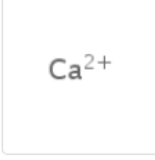
Secstruc

PDB Validation

3QE2.B

3QE2.A

PDB vyhledávání

Small Molecules					
Ligands 4 Unique					
ID	Chains	Name / Formula / InChI Key	2D Diagram & Interactions		3D Interactions
FAD Query on FAD Download SDF File Download CCD File	A, B	FLAVIN-ADENINE DINUCLEOTIDE C ₂₇ H ₃₃ N ₉ O ₁₅ P ₂ VWWQXMAJTJZDQX-UYBVJOGSSA-N			Ligand Explorer NGL Binding Pocket (JSmol) Electron Density (JSmol)
NAP Query on NAP Download SDF File Download CCD File	A, B	NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE 2'-MONOPHOSPHOADENOSINE 5'-DIPHOSPHORIBOSE (<i>Synonym</i>) C ₂₁ H ₂₈ N ₇ O ₁₇ P ₃ XJLXINKUBYWONI-NNYOXOHSSA-N			Ligand Explorer NGL Binding Pocket (JSmol) Electron Density (JSmol)
FMN Query on FMN Download SDF File Download CCD File	A, B	FLAVIN MONONUCLEOTIDE RIBOFLAVIN MONOPHOSPHATE (<i>Synonym</i>) C ₁₇ H ₂₁ N ₄ O ₉ P FVTCRASFADXXNN-SCRDCRAPSA-N			Ligand Explorer NGL Binding Pocket (JSmol) Electron Density (JSmol)
CA Query on CA Download SDF File Download CCD File	A	CALCIUM ION Ca BHPQYMZQTCNFJ-UHFFFAOYSA-N			Ligand Explorer NGL Binding Pocket (JSmol)

Výčet molekul neproteinového charakteru – převážně malé organické molekuly (kofaktory, léčiva) či ionty

PDB vyhledávání – anotace

Structure Summary 3D View **Annotations** Sequence Sequence Similarity Structure Similarity Experiment Literature

3QE2

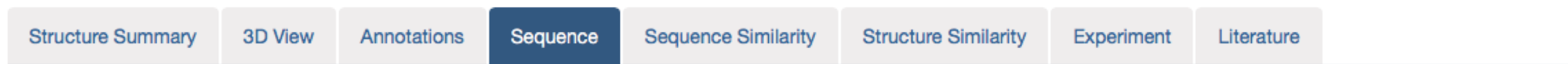
Display Files Download Files

Crystal Structure of Human NADPH-Cytochrome P450 Reductase

Macromolecule Annotations for the Entities in PDB 3QE2

Chains	Polymer	Molecular Function	Biological Process	Cellular Component
A,B	NADPH--cytochrome P450 reductase (3QE2:A,B)	<ul style="list-style-type: none">Nadph Hemoprotein Reductase ActivityCytochrome B5 Reductase Activity Acting On Nad(p)hProtein BindingNitric Oxide Dioxygenase ActivityElectron Carrier ActivityFmn BindingOxidoreductase ActivityHydrolase ActivityEnzyme BindingIron Cytochrome C Reductase ActivityFlavin Adenine Dinucleotide BindingNadp Binding	<ul style="list-style-type: none">Regulation of Growth Plate Cartilage Chondrocyte ProliferationXenobiotic Metabolic ProcessResponse to NutrientCarnitine Metabolic ProcessFlavonoid Metabolic ProcessInternal Peptidyl Lysine AcetylationFatty Acid OxidationPositive Regulation of Chondrocyte DifferentiationPositive Regulation of Monooxygenase ActivityResponse to DrugNegative Regulation of Apoptotic ProcessNegative Regulation of Cysteine Type Endopeptidase Activity Involved in Apoptotic ProcessNitrate Catabolic ProcessPositive Regulation of Cholesterol Biosynthetic ProcessPositive Regulation of Smoothened Signaling PathwayNitric Oxide Catabolic ProcessOxidation Reduction ProcessNegative Regulation of Lipase ActivityDemethylationCellular Response to Gonadotropin StimulusCellular Response to Follicle Stimulating Hormone StimulusCellular Response to Peptide Hormone StimulusPositive Regulation of Steroid Hormone Biosynthetic ProcessRegulation of Cholesterol Metabolic ProcessCellular Organofluorine Metabolic Process	<ul style="list-style-type: none">MitochondrionEndoplasmic ReticulumEndoplasmic Reticulum MembraneMembraneIntegral Component of MembraneIntracellular Membrane Bounded Organelle

PDB vyhledávání – sekvence



Chain A: NADPH--cytochrome P450 reductase

Chain Downloadable Files

[Download FASTA File](#)

[View Sequence & DSSP Image](#)

[Download Sequence Chain Image](#)

Chain Info

Polymer: 1
 Length: 618 residues
 Chain Type: polypeptide(L)
 Reference: [UniProtKB \(P16435\)](#)
 Up-to-date UniProt Ids are provided by the [SIFTS project](#)

Protein Modification Legend

* calcium ion

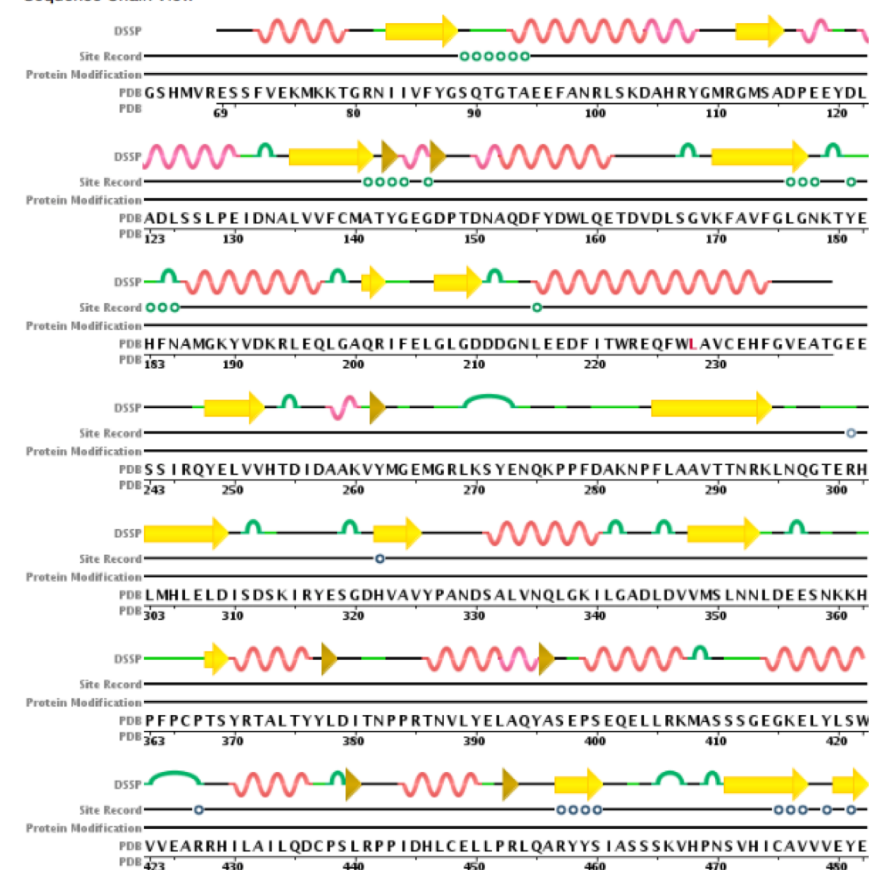
Site Record Legend

- BINDING SITE FOR RESIDUE NAP A 753 (SOFTWARE)
- BINDING SITE FOR RESIDUE CA A 762 (SOFTWARE)
- BINDING SITE FOR RESIDUE FMN A 751 (SOFTWARE)
- BINDING SITE FOR RESIDUE FAD A 752 (SOFTWARE)

DSSP Legend

- E: beta strand
- T: turn
- empty: no secondary structure assigned
- G: 3/10-helix
- B: beta bridge
- S: bend
- H: alpha helix

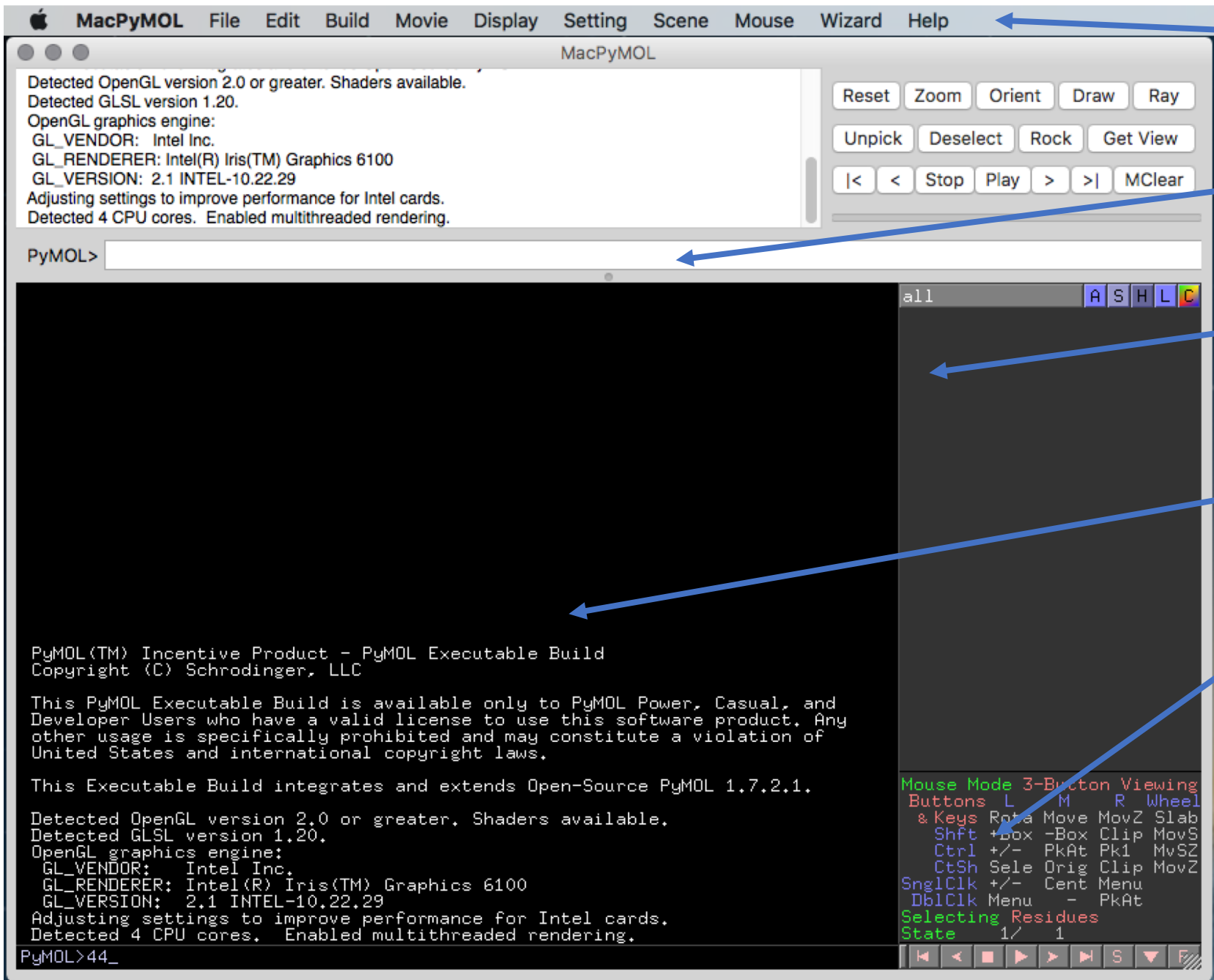
Sequence Chain View



PyMol

KFC/CHS





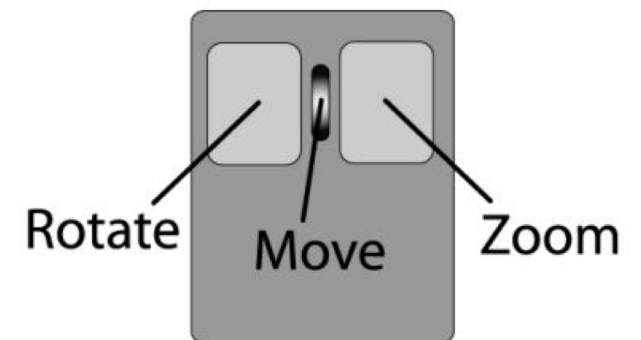
hlavní nabídka

příkazový řádek

nástroj práce s objekty

pracovní plocha

nástroj výběru objektů



Práce s objekty - akce

all

A S H L C

orientace objektu na pracovní ploše

pohyb objektu po pracovní ploše

přednastavené možnosti zobrazení

hledání (polárních kontaktů)

přeložení „align“ struktur

generování – matice symetrie, mapa elektrostatického potenciálu

práce s objektem (přejmenování, duplikace, kopírování)

přidat/odebrat - vodíkové atomy, solvent

výpočet zákl. vlastností (molekulová hmotnost, náboj)

```
Action:  
zoom  
orient  
center  
origin  
drag matrix  
reset matrix  
drag coordinates  
clean  
preset  
find  
align  
generate  
assign sec. struc.  
rename object  
duplicate object  
delete object  
hydrogens  
remove waters  
state  
masking  
sequence  
movement  
compute
```

Práce s objekty – možnosti zobrazení/skrytí

all A S H L C

možnost reprezentace objektu jako:

- lines
- sticks
- ribbon
- cartoon

zobrazení popisků

zobrazení nekov. vázaných (např. vody)

možnost zobrazení objektu teček/koulí

zobrazení buňky/povrchu objektu

zobrazení hlavního/postranního řetězce,
disulfidových můstků

zobrazení aromatických kruhů

zobrazení:

```
Show:  
as  
lines  
sticks  
ribbon  
cartoon  
label  
cell  
nonbonded  
dots  
spheres  
nb_spheres  
mesh  
surface  
organic  
main chain  
side chain  
disulfides  
valence
```

skrytí:

```
Hide:  
everything  
lines  
sticks  
ribbon  
cartoon  
label  
cell  
nonbonded  
dots  
spheres  
nb_spheres  
mesh  
surface  
main chain  
side chain  
waters  
hydrogens  
unselected  
valence
```


Práce s objekty – označení/možnosti vybarvení



vymazat veškeré označení

označení jednotlivých reziduí,
řetězců a segmentů

označení zákl. vlastností atomů
(název, značka atomu, název
rezidua ...)

```
Label:  
clear  
residues  
chains  
segments  
atom name  
element symbol  
residue name  
residue identifier  
chain identifier  
segment identifier  
b-factor  
occupancy  
vdw radius  
other properties  
atom identifiers  
user properties
```

```
Color:  
by element  
by chain  
by ss  
by rep  
spectrum  
auto  
reds  
greens  
blues  
yellows  
magentas  
cyans  
oranges  
tints  
grays
```

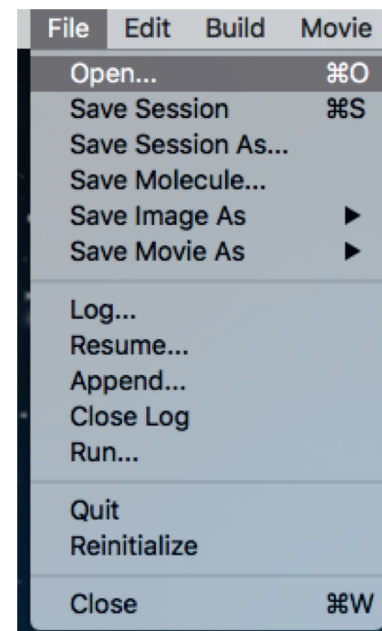
vybarvení na základě:

- prvku
- řetězce
- sekundární struktury
- reprezentace (sticks, lines, cartoons)
- spectrum (změna barvy dle pořadí v sekvenci)

barevná paleta

Import souborů

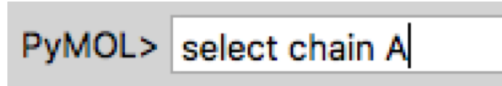
1. Soubor > Otevřít
2. Příkazem `fetch` + PDB ID
(např. `fetch 3QE2`)



```
PyMOL> fetch 3QE2
```

1. Odebrat vody: **3QE2 > Action > Remove waters**

2. Vybrat jeden z řetězců `select chain A`



```
PyMOL> select chain A
```

3. Přesuňte selekci do nového objektu a přejmenujte na CPR_chainA

**(sele) > Action > extract object
obj01 > Action > rename object**

a zobrazte v reprezentaci cartoon

**CPR_chainA > show > cartoon
CPR_chainA > hide > lines**

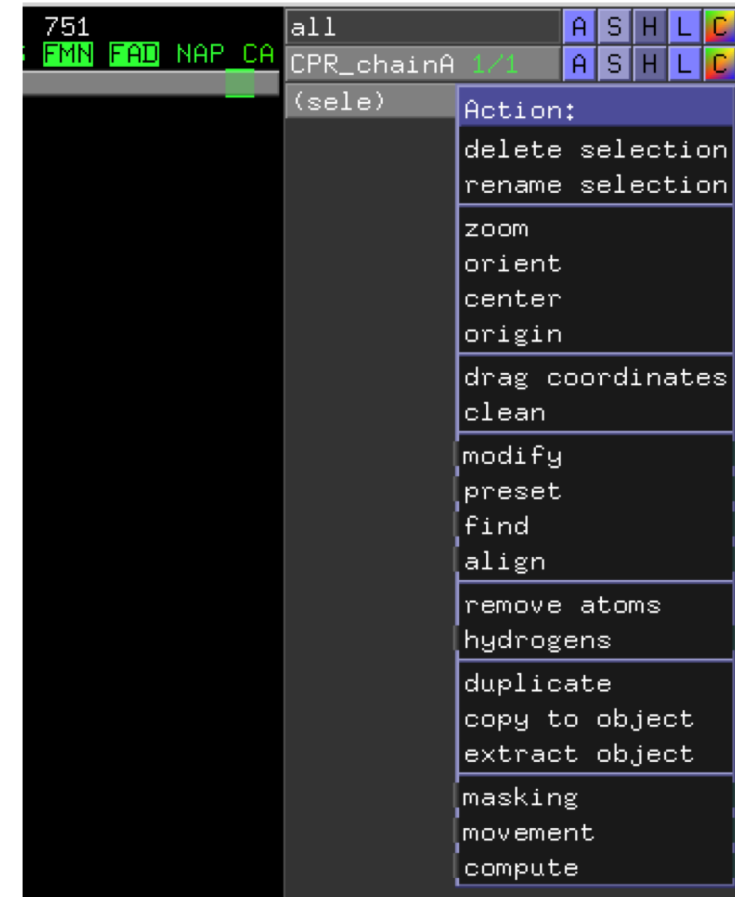
4. Pomocí hledání v sekvenci vyberte kofaktory FMN a FAD a přesuňte je do nového objektu a ten pojmenujete kofaktory



**(sele) > Action > extract object
obj01 > Action > rename object**

5. Kofaktory zobrazte v reprezentaci stick
kofaktory > show > sticks

Protein (Cytochrom P450 reduktáza) s PDB ID 3QE2
– 2 řetězce + kofaktory (NADP, FAD, FMN)



6. Změňte barvu objektu CPR_chainA na modrou a u kofaktorů změňte barvu uhlíků na červenou

CPR_chainA > Color > blue

kofaktory > Color > red

7. Kofaktorům přidejte vodíkové atomy

kofaktory > Action > Hydrogens > Add

8. Změňte barvu pozadí na bílou

Display > Background > White

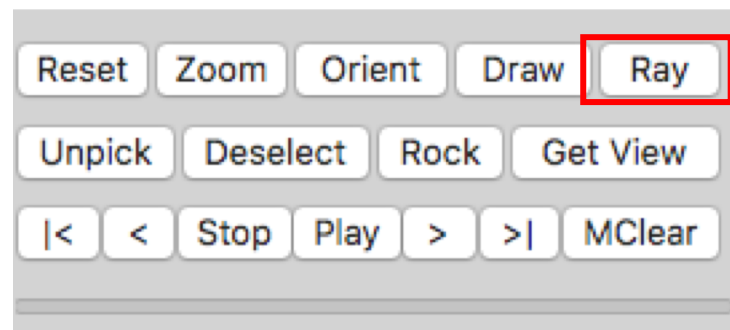
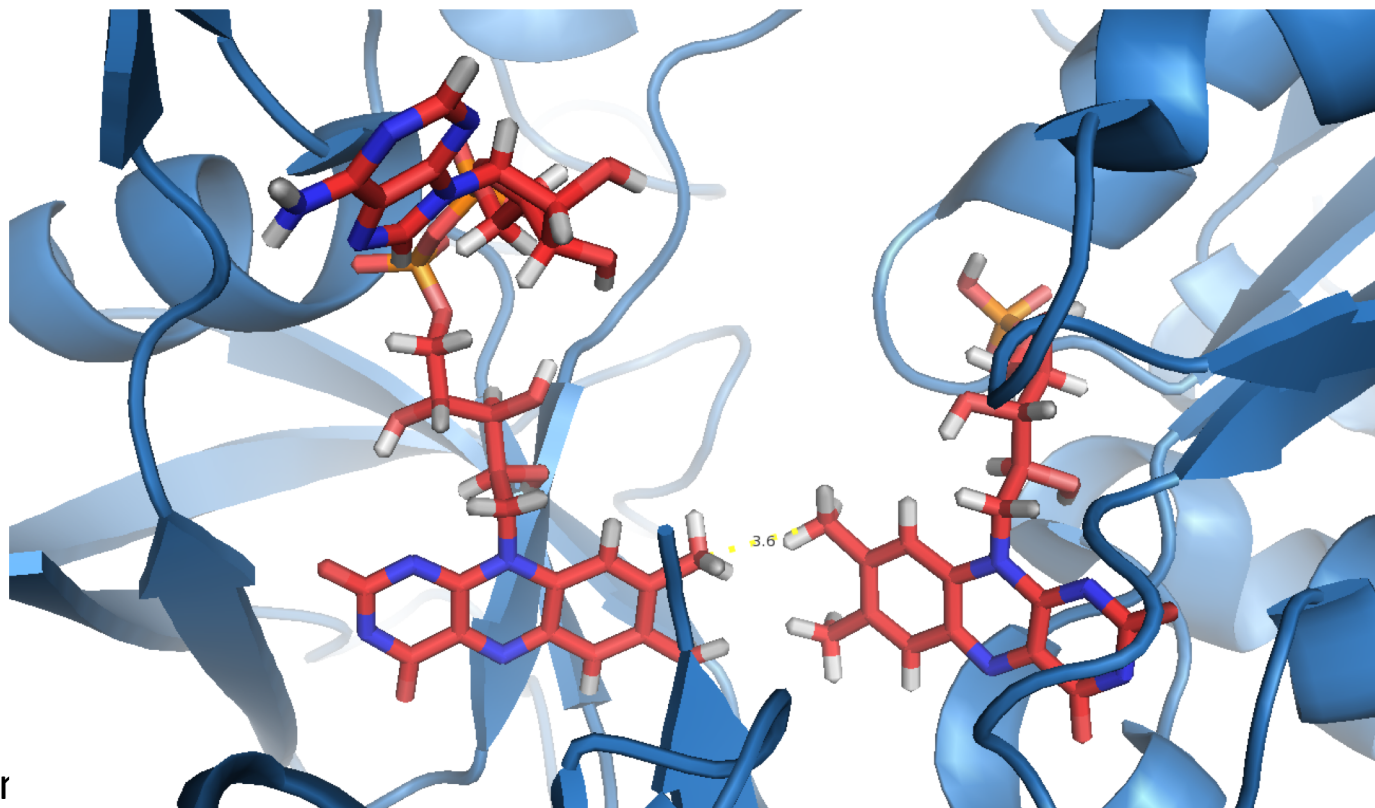
9. Vycentrujte pracovní plochu na kofaktory

kofaktory > Action > Orient

10. Pomocí nástroje Measurement změřte vzdálenost metylových skupin FAD a FMN kofaktorů

Wizard > Measurement

11. Pomocí nástroje **Ray** vyrenderujte strukturu a uložte jako obrázek ve formátu PNG



Cvičení (advance search)

- cytochrom P450
- metoda: X-ray
- od roku 2015
- obsahuje ligandy
- rozlišení přes 3.0 Å
- enzym. klasifikace:
1.14.14.19
- (5IRV)

- pouze chain A
- protein cartoon (zelená),
HEME sticks (modrá), droga
sticks (červená)
- bílé pozadí

