Stereozobrazování molekul

C9531 - Seminář k přednášce Strukturní biochemie

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24. září 2024

Úvodní slovo

Požadavky k udělení zápočtu

- nutno napsat **4 průběžné testy** (každý minimálně na 60 %)
- neúspěšný test lze opakovat na konci semestru
- úspěšné složení testů je potřebné pro udělení zápočtu, vstupenka na ústní zkoušku k C9530

Úvodní slovo

Datum	Náplň cvičení
25.9./27.9.	3D zobrazování molekul, stereozobrazování
2.10./4.10.	Určování torzních úhlů - peptidy, Ramachandranův diagram
9.10./11.10.	Určování torzních úhlů - nukleotidy, struktura sacharidů
16.10./18.10.	**Průběžný test 1: torzní úhly peptidů a nukleotidů**
23.10./25.10.	Sekvenace
30.10./1.11.	Optické metody
6.11./8.11.	**Průběžný test 2: sekvenace, optické metody**
13.11./15.11.	Rentgenová krystalografie
20.11./22.11.	Rentgenová krystalografie
27.11./29.11.	**Průběžný test 3: Rentgenová krystalografie**
4.12./6.12.	Nukleární magnetická rezonance
11.12./13.12.	Nukleární magnetická rezonance
18.12./20.12.	**Průběžný test 4: Nukleární magnetická rezonance**

Stereozobrazování

- zobrazení pohledu levého a pravého oka vedle sebe
- otočené o cca 5° kolem vertikální osy
- zaostřuje se mimo rovinu, ze dvou obrázků vzniknou čtyři
- prostřední dva se složí v pseudo-3D obraz

Varianty stereozobrazování

wall-eyed:

- oči zaostřují za rovinou obrázku
- vyžaduje přesnou vzdálenost mezi obrázky
- častější při zobrazení na papíře
- levé oko se dívá na levý obrázek, pravé na pravý
- **pomůcka: zaostřit na vzdálený bod (cca 3 metry)**

Varianty stereozobrazování

cross-eyed:

- oči zaostřují před rovinou obrázku
- vzdálenost mezi obrázky není tak důležitá
- častější při zobrazení na monitorech
- levé oko se dívá na pravý obrázek, pravé na levý
- **pomůcka: zaostřit na bližší předmět, např. tužku**

PDB databáze: stereo zobrazení (cross-eyed)

https://www.rcsb.org/

209,957 Structures from the PDB

1,068,577 Computed Structure Models (CSM)

New: More Computed Structure Models (CSM) available

RCSB Protein Data Bank (RCSB PDB) enables breakthroughs in science and education by providing access and tools for exploration, visualization, and analysis of:

- Experimentally-determined 3D structures from the **Protein Data Bank (PDB)** archive
- **Computed Structure Models (CSM)** from AlphaFold DB and ModelArchive

These data can be explored in context of external annotations providing a structural view of biology.

Virtual Crash Course
Leveraging RCSB PDB APIs for Bioinformatics Analyses and Machine Learning
October 12 | Register Now!

September **Molecule of the Month**

Histone Deacetylases

Latest Entries *As of Tue Sep 19 2023*

8AXE

Small molecule stabilizer for ERalpha and 14-3-3 (1074210)

Features & Highlights

Register Now for October Virtual Crash Courses on RCSB PDB APIs

Learn about *Leveraging RCSB PDB APIs for Bioinformatics Analyses and Machine Learning*. Part 1 will introduce the Data and Search APIs. Part 2 will offer hands-on exercises.

```
_chem
_comp.id
BB87Q
```

Coming Soon: PDB Entries with Novel Ligands Distributed Only in PDBx/mmCIF and PDBML File Formats

PDB will run out of 3-character CCD IDs before the end of 2023. Afterwards, PDB entries with novel ligands will not be

News

Poster Prize Awarded at ACA 2023

Congratulations to Alexander Paredes for *Biophysical characterization of the* Pseudomonas aeruginosa *BqsR/BqsS two-component system*

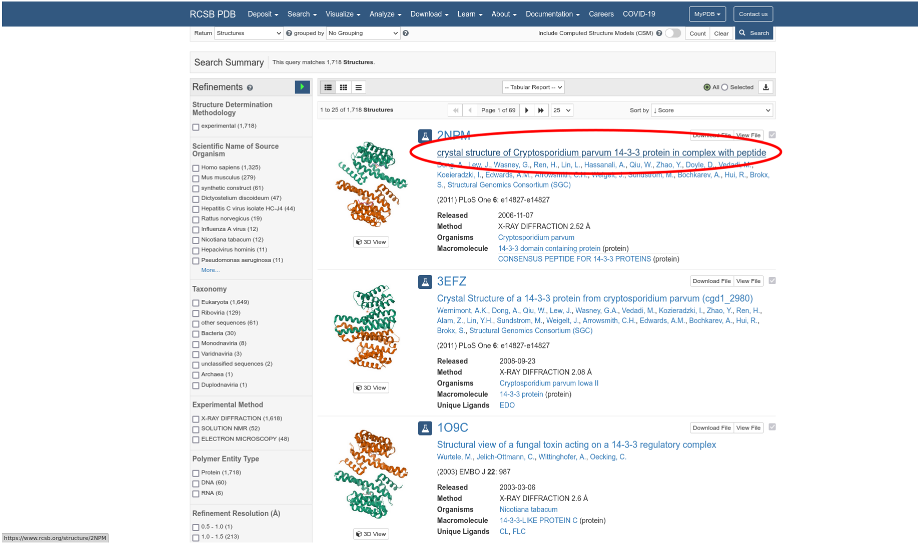
» 09/19/2023

September 19: DNS name changes for PDB archive downloads from RCSB PDB

Programmatic users (ftp, rsync or https) should update scripts

» 09/15/2023

PDB databáze: stereo zobrazení (cross-eyed)



Return: Structures; grouped by: No Grouping

Include Computed Structure Models (CSM)

Search Summary This query matches 1,718 **Structures**.

Refinements

Structure Determination Methodology

- ☐ experimental (1,718)

Scientific Name of Source Organism

- ☐ Homo sapiens (1,325)
- ☐ Mus musculus (279)
- ☐ synthetic construct (61)
- ☐ Dictyostelium discoideum (47)
- ☐ Hepatitis C virus isolate HC-J4 (44)
- ☐ Rattus norvegicus (19)
- ☐ Influenza A virus (12)
- ☐ Nicotiana tabacum (12)
- ☐ Hepacivirus hominis (11)
- ☐ Pseudomonas aeruginosa (11)
- More...

Taxonomy

- ☐ Eukaryota (1,649)
- ☐ Riboviria (129)
- ☐ other sequences (61)
- ☐ Bacteria (30)
- ☐ Monodnaviria (8)
- ☐ Varidnaviria (3)
- ☐ unclassified sequences (2)
- ☐ Archaea (1)
- ☐ Duplodnaviria (1)

Experimental Method

- ☐ X-RAY DIFFRACTION (1,618)
- ☐ SOLUTION NMR (52)
- ☐ ELECTRON MICROSCOPY (48)

Polymer Entity Type

- ☐ Protein (1,718)
- ☐ DNA (60)
- ☐ RNA (6)

Refinement Resolution (Å)

- ☐ 0.5 - 1.0 (1)
- ☐ 1.0 - 1.5 (213)

● All ○ Selected

1 to 25 of 1,718 **Structures**   Page 1 of 69   25   Sort by ↓ Score

2NPM

crystal structure of Cryptosporidium parvum 14-3-3 protein in complex with peptide

Dong, A., Lew, J., Wasney, G., Ren, H., Lin, L., Hassanali, A., Qiu, W., Zhao, Y., Doyle, D., Vedadi, M., Koeieradzki, I., Edwards, A.M., Arrowsmith, C.H., Weigelt, J., Sundstrom, M., Bochkarev, A., Hui, R., Brokx, S., Structural Genomics Consortium (SGC)

(2011) PLoS One **6**: e14827-e14827

Released	2006-11-07
Method	X-RAY DIFFRACTION 2.52 Å
Organisms	Cryptosporidium parvum
Macromolecule	14-3-3 domain containing protein (protein) CONSENSUS PEPTIDE FOR 14-3-3 PROTEINS (protein)

3EFZ

Crystal Structure of a 14-3-3 protein from cryptosporidium parvum (cgd1_2980)

Wernimont, A.K., Dong, A., Qiu, W., Lew, J., Wasney, G.A., Vedadi, M., Kozieradzki, I., Zhao, Y., Ren, H., Alam, Z., Lin, Y.H., Sundstrom, M., Weigelt, J., Arrowsmith, C.H., Edwards, A.M., Bochkarev, A., Hui, R., Brokx, S., Structural Genomics Consortium (SGC)

(2011) PLoS One **6**: e14827-e14827

Released	2008-09-23
Method	X-RAY DIFFRACTION 2.08 Å
Organisms	Cryptosporidium parvum Iowa II
Macromolecule	14-3-3 protein (protein)
Unique Ligands	EDO

1O9C

Structural view of a fungal toxin acting on a 14-3-3 regulatory complex

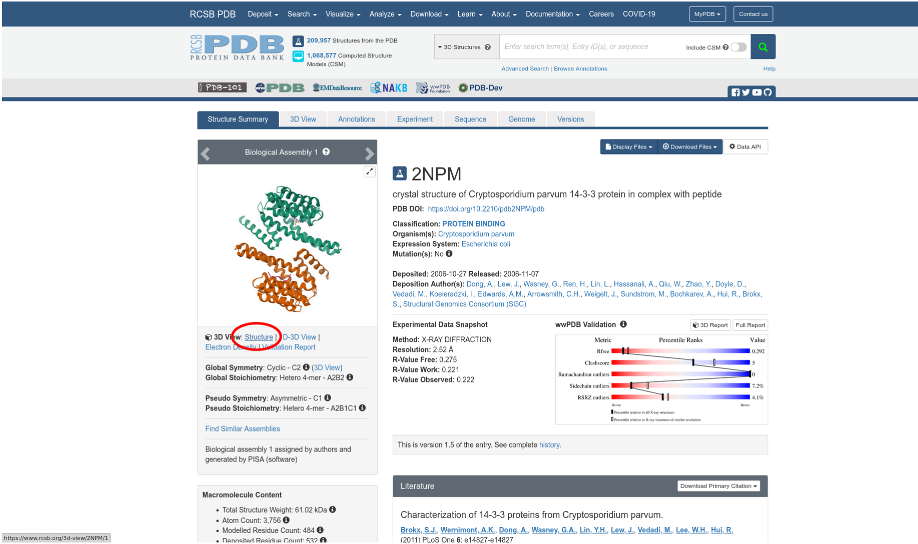
Wurtele, M., Jelich-Ottmann, C., Wittinghofer, A., Oecking, C.

(2003) EMBO J **22**: 987

Released	2003-03-06
Method	X-RAY DIFFRACTION 2.6 Å
Organisms	Nicotiana tabacum
Macromolecule	14-3-3-LIKE PROTEIN C (protein)
Unique Ligands	CL, FLC

https://www.rcsb.org/structure/2NPM

PDB databáze: stereo zobrazení (cross-eyed)



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2NPM

crystal structure of Cryptosporidium parvum 14-3-3 protein in complex with peptide

PDB DOI: https://doi.org/10.2210/pdb2NPM/pdb

Classification: PROTEIN BINDING
Organism(s): Cryptosporidium parvum
Expression System: Escherichia coli
Mutation(s): No

Deposited: 2006-10-27 **Released:** 2006-11-07
Deposition Author(s): Dong, A., Lew, J., Wasney, G., Ren, H., Lin, L., Hassanali, A., Qiu, W., Zhao, Y., Doyle, D., Vedadi, M., Koeieradzki, I., Edwards, A.M., Arrowsmith, C.H., Weigelt, J., Sundstrom, M., Bochkarev, A., Hui, R., Brokx, S., Structural Genomics Consortium (SGC)

3D View: Structure | 1D-3D View | Electron Density | Validation Report

Global Symmetry: Cyclic - C2 (3D View)
Global Stoichiometry: Hetero 4-mer - A2B2

Pseudo Symmetry: Asymmetric - C1
Pseudo Stoichiometry: Hetero 4-mer - A2B1C1

Find Similar Assemblies

Biological assembly 1 assigned by authors and generated by PISA (software)

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 2.52 Å
R-Value Free: 0.275
R-Value Work: 0.221
R-Value Observed: 0.222

wwPDB Validation

Metric	Value
Rfree	0.292
Clashscore	5
Ramachandran outliers	0
Sidechain outliers	7.2%
RSRZ outliers	4.1%

This is version 1.5 of the entry. See complete history.

Macromolecule Content

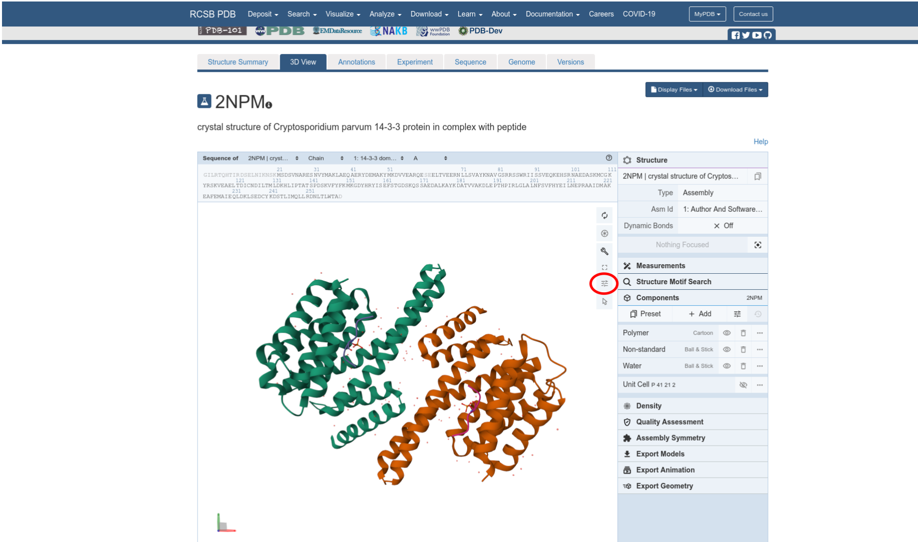
- Total Structure Weight: 61.02 kDa
- Atom Count: 3,756
- Modelled Residue Count: 484
- Deposited Residue Count: 532

Literature

Characterization of 14-3-3 proteins from Cryptosporidium parvum.

Brokx, S.J., Wernimont, A.K., Dong, A., Wasney, G.A., Lin, Y.H., Lew, J., Vedadi, M., Lee, W.H., Hui, R.
(2011) PLoS One **6**: e14827-e14827

PDB databáze: stereo zobrazení (cross-eyed)



2NPM

crystal structure of Cryptosporidium parvum 14-3-3 protein in complex with peptide

2NPM | crystal structure of Cryptos…

Type Assembly

Asm Id 1: Author And Software…

Dynamic Bonds ✕ Off

Nothing Focused

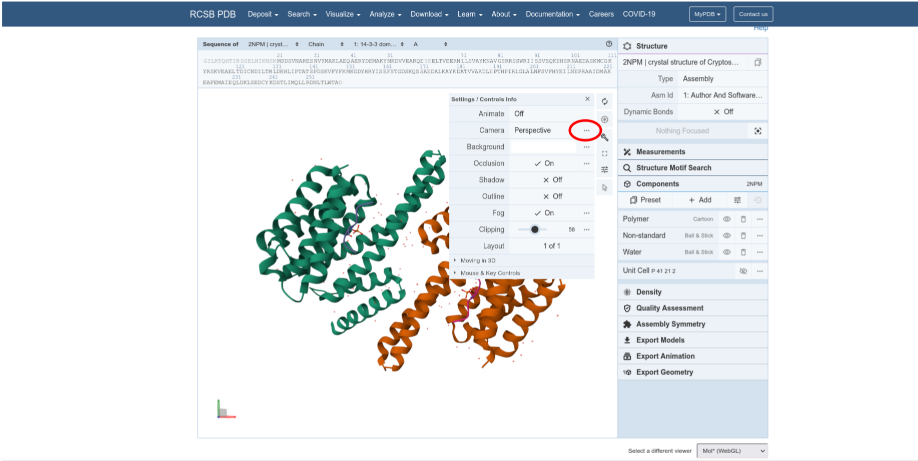
Polymer Cartoon

Non-standard Ball & Stick

Water Ball & Stick

Unit Cell P 41 21 2

PDB databáze: stereo zobrazení (cross-eyed)



Sequence of 2NPM | cryst… Chain 1: 14-3-3 dom… A

GILRTQHTIRDSELNIKNSKMSDSVNARES NVYMAKLAEQ AERYDEMAKY MKDVVEARQE SEELTVEERN LLSVAYKNAV GSRRSSWRII SSVEQKEHSR NAEDASKMCGK
YRSKVEAEL TDICNDILTM LDKHLIPTAT SPDSKVFYFK MKGDYHRYIS EFSTGDSKQS SAEDALKAYK DATVVAKDLE PTHPIRLGLA LNFSVFHYEI LNEPRAAIDMAK
EAFEMAIE QLDKLSEDCY KDSTLIMQLL RDNLTLWTAD

Settings / Controls Info

Animate	Off
Camera	Perspective
Background	
Occlusion	✓ On
Shadow	✕ Off
Outline	✕ Off
Fog	✓ On
Clipping	58
Layout	1 of 1

Structure

2NPM | crystal structure of Cryptos…

Type	Assembly
Asm Id	1: Author And Software…
Dynamic Bonds	✕ Off

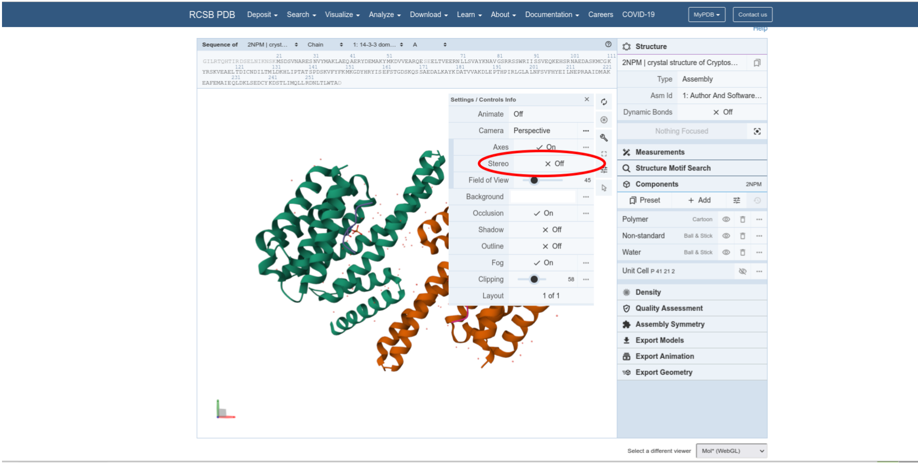
Nothing Focused

Components 2NPM

Polymer	Cartoon
Non-standard	Ball & Stick
Water	Ball & Stick
Unit Cell	P 41 21 2

Select a different viewer: Mol* (WebGL)

PDB databáze: stereo zobrazení (cross-eyed)



Sequence of 2NPM | cryst… Chain 1: 14-3-3 dom… A

```
                    21        31        41        51                  71        81        91        101       111
GILRTQHTIRDSELNIKNSKMSDSVNARES NVYMAKLAEQ AERYDEMAKY MKDVVEARQE SEELTVEERN LLSVAYKNAV GSRRSSWRII SSVEQKEHSR NAEDASKMCG K
         121       131       141       151       161       171       181       191       201       211       221
YRSKVEAEL TDICNDILTM LDKHLIPTAT SPDSKVFYFK MKGDYHRYIS EFSTGDSKQS SAEDALKAYK DATVVAKDLE PTHPIRLGLA LNFSVFHYEI LNEPRAAIDMAK
        231       241       251
EAFEMAIE QLDKLSEDCY KDSTLIMQLL RDNLTLWTAD
```

Settings / Controls Info

Animate: Off
Camera: Perspective
Axes: ✓ On
Stereo: × Off
Field of View: 45
Background
Occlusion: ✓ On
Shadow: × Off
Outline: × Off
Fog: ✓ On
Clipping: 58
Layout: 1 of 1

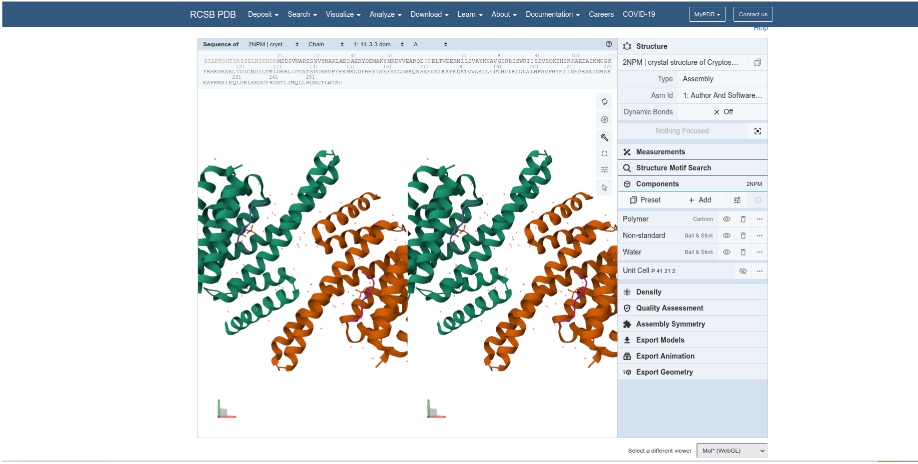
Structure

2NPM | crystal structure of Cryptos…
Type: Assembly
Asm Id: 1: Author And Software…
Dynamic Bonds: × Off
Nothing Focused

Polymer: Cartoon
Non-standard: Ball & Stick
Water: Ball & Stick
Unit Cell P 41 21 2

Select a different viewer: Mol* (WebGL)

PDB databáze: stereo zobrazení (cross-eyed)



Sequence of 2NPM | cryst… Chain 1: 14-3-3 dom… A

```
                   21        31        41        51                  71        81        91        101       111
GILRTQHTIRDSELNIKNSKMSDSVNARESNVYMAKLAEQAERYDEMAKYMKDVVEARQESEELTVEERNLLSVAYKNAVGSRRSSWRIISSVEQKEHSRNAEDASKMCGK
         121       131       141       151       161       171       181       191       201       211       221
YRSKVEAELTDICNDILTMLDKHLIPTATSPDSKVFYFKMKGDYHRYISEFSTGDSKQSSAEDALKAYKDATVVAKDLEPTHPIRLGLALNFSVFHYEILNEPRAAIDMAK
        231       241       251
EAFEMAIEQLDKLSEDCYKDSTLIMQLLRDNLTLWTAD
```

2NPM | crystal structure of Cryptos…

Type	Assembly
Asm Id	1: Author And Software…
Dynamic Bonds	Off

Nothing Focused

Components 2NPM

Polymer	Cartoon
Non-standard	Ball & Stick
Water	Ball & Stick
Unit Cell P 41 21 2	

Select a different viewer: Mol* (WebGL)

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