



CEITEC



Central European Institute of Technology
BRNO | CZECH REPUBLIC

Vizualizace proteinů a ligandů



EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND
INVESTING IN YOUR FUTURE

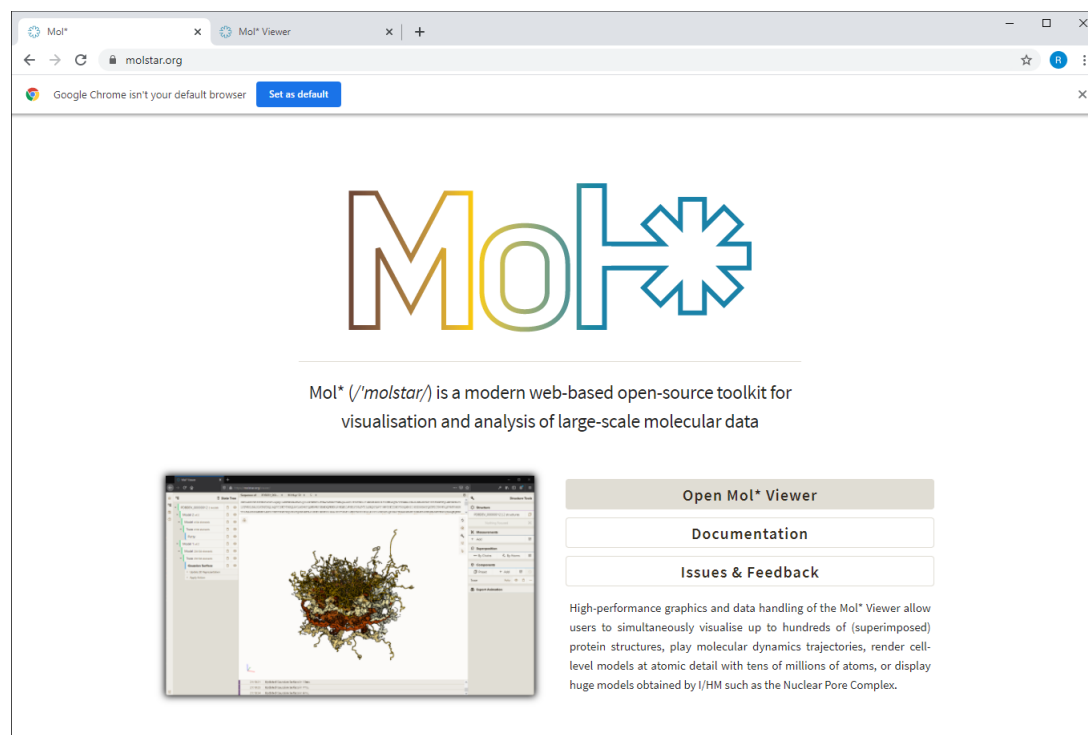


**OP Research and
Development for Innovation**



MolStar

- Webová aplikace pro vizualizaci proteinů a ligandů
- Zvládá i extrémně velké systémy
- Integrovaný v Protein Data Bank
- Vytvořený u nás v Národním centru pro výzkum biomolekul, ve spolupráci s EMBL EBI a RCSB PDB
- <https://molstar.org/>



Mol* (*molstar*) is a modern web-based open-source toolkit for visualisation and analysis of large-scale molecular data

[Open Mol* Viewer](#)

[Documentation](#)

[Issues & Feedback](#)

High-performance graphics and data handling of the Mol* Viewer allow users to simultaneously visualise up to hundreds of (superimposed) protein structures, play molecular dynamics trajectories, render cell-level models at atomic detail with tens of millions of atoms, or display huge models obtained by I/HM such as the Nuclear Pore Complex.

MolStar

The screenshot displays the MolStar web application interface. The browser address bar shows `molstar.org/viewer/`. The main content area is titled "Sequence" and indicates "No structure available".

The left sidebar is titled "Home" and contains several sections:

- Download Structure**: Includes a table with columns "Source" (PDB) and "PDB Id(s)" (1tqn). Below the table is an "Options" section with a refresh icon and a red-circled "Apply" button.
- Add Trajectory**
- Download Density**
- Download File**
- Open Files**
- Download**
- Load CellPack**
- Load Genome 3D (G3D)**

Below these is the "Remote States" section, which lists several states:

- Nuclear Pore Complex
- NPC-CIF
- 1RB8 Annotated Assembly
- Zika+EM
- Cytochromes Superposition
- AS
- ASX
- ASX-1 Something

At the bottom of the sidebar, there are two numbered items (1 and 2).

The right sidebar is titled "Structure Tools" and contains sections for:

- Structure**: "Nothing Loaded", "Nothing Focused"
- Measurements**: "+ Add"
- Components**: "Preset", "+ Add"
- Export Animation**

The bottom status bar shows the time "14:28:23" and the version "Mol* Plugin 1.2.7 [12/19/2020, 11:52:32 AM]". The MolStar logo is visible in the bottom right corner of the main area.

Vizualizace 3D souřadnic molekuly

Vizualizační model cartoon

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central 3D view shows the protein structure in a green cartoon representation, with a red ball-and-stick model of a ligand bound to it. The interface includes a state tree on the left, a sequence viewer at the top, and a structure tools panel on the right.

State Tree:

- 1TQN 1 model
- Model 1
 - Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell | 2 2 2

Sequence of 1TQN | Crystal... 1: cytochrome... A

```
MALYGIHSHGLFKLGI PGPTPLPFLGNILSYHKGFCMFDMECHKYKQKWFYDGOQFVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFMKSAI
122 132 142 152 162 172 182 192 202 212
SIAEDEEWKRLRSLLSPTFTSGKLEMPVPIIAQYGDVLRNLRREAETGKPVTLKDVFGAYSMDVITISFQVNIIDSLNNPQDFVENTKLLRFDF
222 232 242 252 262 272 282 292 302 312
LDPFFLSITVFPFLIPILEVLNLCVFPPEVINFLRKSVMKESRLEDTQKHRVDFLQMLIDSONSKETESHKALSDLELVAQSIIFIFAGYETTSS
322 332 342 352 362 372 382 392 402 412
```

Structure Tools:

- Structure**
 - 1TQN | Crystal Structure of Human ...
 - Type: Assembly
 - Asm Id: 1: Author Defined Asse...
 - Nothing Focused
- Measurements**
 - + Add
- Components** 1TQN
 - Preset + Add
 - Polymer: Cartoon
 - Ligand: Ball & Stick
 - Water: Ball & Stick
 - Unit Cell | 2 2 2
- Volume Streaming** 1TQN
 - Enable
- Assembly Symmetry** 1TQN
 - Enable
- Export Animation**

Log:

- 14:36:24 Created Ball & Stick in 19ms.
- 14:36:24 Created Ball & Stick in 19ms.
- 14:36:24 Updated Structure Focus Representation in 2ms.

Vizualizace 3D souřadnic molekuly

Volba vizualizačních modelů

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central 3D view shows the protein structure in a green cartoon representation, with a dashed green box highlighting a specific region. The left sidebar shows the 'State Tree' with a tree view of the structure's components, including '1TQN 1 model', 'Model 1', 'Assembly 1 3999 elements', 'Polymer 3766 elements', 'Ligand 49 elements', and 'Water 190 elements'. The top right panel, 'Structure Tools', is open, showing the 'Structure' section with the protein name '1TQN | Crystal Structure of Human ...'. Below this, the 'Measurements' section is empty. The 'Components' section shows '1TQN' with a 'Preset' button and a '+ Add' button. The 'Polymer' section is expanded, showing a list of representation options: 'Add Representation', 'Cartoon', 'Ball & Stick' (circled in red), 'Gaussian Surface', 'Gaussian Volume', 'Label', 'Line', 'Molecular Surface', 'Orientation', 'Point', 'Putty', and 'Spacefill'. The 'Cartoon Representation' section is also expanded, showing 'Ligand' and 'Water' with their respective representations: 'Ball & Stick' and 'Ball & Stick'. The bottom status bar shows a log of actions: '14:36:24 Created Ball & Stick in 19ms.', '14:36:24 Created Ball & Stick in 19ms.', and '14:36:24 Updated Structure Focus Representation in 2ms.'

Vizualizace 3D souřadic molekuly

Vizualizační model Ball & Stick

Sequence of 1TQN | Crystal... 1: cytochrome... A #

```
MALYGTSHGSLFKLGI PGPTPLPFLGNILSYHKGFDMFDCHECKYKGVWGFYDQQPVLAITDPDMIKTVLVKECYSVPTNRRPFGVGFYKSR I  
SIAEDEEWKRLRSLSPFTTSGLKEMVPIIAQYGDVLRNLRREAEETGKPVTLKDVFGAYSMDVITSTSGVNIIDSLNPNQDFFVENTKLLRDFD  
LDPFFLSIVVFPFLIPILEVNI CVPREVINFLRKSVKRMKESRLEDTQKHRVDFLQMLMIDSONSKETESHKALSDELVAQSIIPFAGYETTS S
```

State Tree

- 1TQN 1 model
- Model 1
- Assembly 1 3999 elements
- Polymer 3766 elements
 - Cartoon
 - Ball & Stick**
- Ligand 49 elements
 - Ball & Stick
- Water 190 elements
 - Ball & Stick
- Unit Cell | 2 2 2

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset	+ Add		
Polymer	2 reprs		...
Ligand	Ball & Stick		...
Water	Ball & Stick		...
Unit Cell 2 2 2			...

Volume Streaming 1TQN

✓ Enable

Assembly Symmetry 1TQN

✓ Enable

Export Animation

14:36:24 Created Ball & Stick in 19ms.

14:36:24 Updated Structure Focus Representation in 2ms.

14:41:17 Created Ball & Stick in 255ms.

Pozor, ostatní módy je nutno vypnout

Vizualizace 3D souřadnic molekuly

Vizualizační model Line

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central 3D view shows the protein backbone in a 'Line' representation, with atoms colored by element (carbon in green, oxygen in red, nitrogen in blue). The interface is divided into several panels:

- State Tree (Left):** A hierarchical tree showing the structure's components: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Cartoon, Ball & Stick, Line (selected), Ligand (49 elements), Water (190 elements), and Unit Cell (2 2 2).
- Sequence Viewer (Top):** Displays the amino acid sequence of the protein: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKWWGFYDQQPVLAITDPDMIKTVLVKECYSVFINRRPFGVGFMKSAI... (with residue numbers 1-312 indicated).
- Structure Tools (Right):** A panel for managing the structure, including sections for Structure, Measurements, Components, Volume Streaming, and Assembly Symmetry. The 'Line' representation is selected in the Structure section.
- Log (Bottom):** A log of recent actions: 14:36:24 Updated Structure Focus Representation in 2ms, 14:41:17 Created Ball & Stick in 255ms, and 14:53:35 Created Line in 53ms.

Vizualizace 3D souřadic molekuly

Vizualizační model Putty

The screenshot displays the Mol* Viewer interface. The central 3D view shows a protein structure (1TQN) rendered in a green Putty style. The left sidebar contains a State Tree with the following items:

- 1TQN 1 model
 - Model 1
 - Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Ball & Stick
 - Line
 - Putty
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell | 2 2 2

The top of the interface shows the sequence of the protein: 1TQN | Crystal... 1: cytochrome... A

```
MALYGTHTSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYKRWGFDYDQQPVLAITDPMIKIVLVKECYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLSPFTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVTLKDVFGAYSMDVITSTSPGVNIDSLNPNQDPPFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLRKSVMKESRLEDTQKHRVDFLQMLIDSONSKETESHKALSDELVQAQSIIFAGYETTSS
```

The right sidebar contains the Structure Tools panel, which includes sections for Structure, Measurements, Components, Volume Streaming, Assembly Symmetry, and Export Animation.

At the bottom of the interface, a log shows the following actions:

- 14:41:17 Created Ball & Stick in 255ms.
- 14:53:35 Created Line in 53ms.
- 14:54:42 Created Putty in 90ms.

Vizualizace 3D souřadnic molekuly

Vizualizační model Spacefil

Mol* Mol* Viewer Mol* Viewer

molstar.org/viewer/

State Tree

- 1TQN 1 model
 - Model 1
 - Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Ball & Stick
 - Line
 - Putty
 - Spacefill
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell | 2 2 2

Sequence of 1TQN | Crystal... 1: cytochrome... A

```
MALYGHSHGLFKLGI PGPTLPFLGNILSYHKGF CMFDMECHKKGKYGKWFYDGOQPVLAITDPDMIKIVLVKCYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLSPFTTSGKIKEMVPIIAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSGVNI DLSLNNPQDFEVENKGLLRDFD
LDPFFLSITVFFFLIPILEVLNICVFFPREVINFLRKSVMKRESLEDTQKHRVDFLQMLIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

Components 1TQN

Preset	Add	...
Polymer	5 reprs	...
Ligand	Ball & Stick	...
Water	Ball & Stick	...

Unit Cell | 2 2 2

Volume Streaming 1TQN

Enable

Assembly Symmetry 1TQN

Enable

Export Animation

14:53:35 Created Line in 53ms.

14:54:42 Created Putty in 90ms.

14:56:06 Created Spacefill in 26ms.

Vizualizace povrchu molekuly

Vizualizační model Molecular Surface

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows a green molecular surface representation of the protein. The left sidebar contains a 'State Tree' with the following items:

- 1TQN 1 model
 - Model 1
 - Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Gaussian Surface
 - Gaussian Volume
 - Molecular Surface
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell 1 2 2 2

The top of the interface shows the sequence of the protein: 1TQN | Crystal... 1: cytochrome... A. The sequence is: MALYGT HSHGLFKKLSIPGPTLPFLGNILSYHKGF C MFDMECHHKYKQWGFYDSQQVLAITDPDMIKT VLVKECYSVFTNRRPFGVGFMSAI SIAEDEEWKRLRSLLSPTFTSGKLEKMPV IIAQYGDVLRNLRREAEATGKPFVILKDFVFGAYSMQVITSTSGVGNIDSLNPPQDFVENTKLLRDF LDPFFLSITVFPFLIPILEVLNICVFPREVINF LRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETITSS.

The right sidebar contains the 'Structure Tools' panel, which includes sections for Structure, Measurements, and Components. The 'Components' section shows the 'Molecular Surface' representation selected.

The bottom log shows the following actions:

- 14:59:19 Created Gaussian Surface in 597ms.
- 14:59:36 Created Gaussian Volume in 64ms.
- 14:59:47 Created Molecular Surface in 1.749s.

Vizualizace povrchu molekuly

Vizualizační model Gaussian Surface

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows a green Gaussian Surface representation of the protein structure. The left sidebar contains a State Tree with the following items:

- 1TQN 1 model
 - Model 1
 - Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Gaussian Surface
 - Gaussian Volume
 - Molecular Surface
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell 1 2 2 2

The top of the interface shows the sequence of the protein: `MALYGTSHGLFKLGI... 1: cytochrome...`. The right sidebar contains the Structure Tools panel, which includes sections for Structure, Measurements, and Components. The Components section shows the following items:

- Polymer 4 reprs
 - Molecular Surface
 - Orientation
 - Point
 - Putty
 - Spacefill
 - Non-covalent Interactions
 - Validation Clashes
 - Membrane Orientation
 - Set Coloring
 - Modify by Selection
 - Select This
 - Edit Label
 - Cartoon Representation
 - Gaussian Surface Representation
 - Gaussian Volume Representation
 - Molecular Surface Representation

Vizualizace povrchu molekuly

Vizualizační model Gaussian Volume

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central 3D view shows the protein backbone in a stick representation, surrounded by a red, semi-transparent Gaussian Volume mesh. The interface includes a State Tree on the left, a Structure Tools panel on the right, and a log at the bottom.

State Tree:

- 1TQN 1 model
 - Model 1
 - Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Gaussian Surface
 - Gaussian Volume
 - Molecular Surface
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell 1 2 2

Structure Tools:

- Structure
 - 1TQN | Crystal Structure of Human ...
 - Type Assembly
 - Asm Id 1: Author Defined Ass...
 - Nothing Focused
- Measurements
 - + Add
- Components
 - 1TQN
 - Preset + Add
 - Polymer 4 reprs
 - Molecular Surface
 - Orientation
 - Point
 - Putty
 - Spacefill
 - Non-covalent Interactions
 - Validation Clashes
 - Membrane Orientation
 - Set Coloring
 - Modify by Selection
 - Select This
 - Edit Label

Log:

- 14:59:19 Created Gaussian Surface in 597ms.
- 14:59:36 Created Gaussian Volume in 64ms.
- 14:59:47 Created Molecular Surface in 1.749s.

Vizualizace experimentálních dat

Elektronová hustota

molstar.org/viewer/

Sequence of 1TQN | Crystal... 1: cytochrome... A

MALYGTSHSHGLFKKLGIPGFTPLPFLGNILSYHKGFCDMECHKYKQWVFDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFMSAI
SIAEDEEWKRLRSLLSPTFTSGKLEMVPIIAQYGDVLRNLRREAEATGKPVILKDVFGAYSMDEVITSTSGVNIIDSLNPNQDPFVENTKLLRDF
LDPFFLSITVFFFLIPILEVLMICVFPREVINFLRKSVMKESRLEDTQKRVDFLQLMIDSQNSKETESHKALSDELVAQSIIFIFAGYETTSS

1TQN 1 model
Model 1
Assembly 1 3999 elements
Polymer 3766 elements
Cartoon
Ligand 49 elements
Ball & Stick
Water 190 elements
Ball & Stick
Unit Cell | 2 2 2

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset + Add

Polymer Cartoon

Ligand Ball & Stick

Water Ball & Stick

Unit Cell | 2 2 2

Volume Streaming 1TQN

Enable

Assembly Symmetry 1TQN

Enable

Export Animation

15:23:00 Created Ball & Stick in 26ms.
15:23:00 Created Ball & Stick in 12ms.
15:23:00 Updated Structure Focus Representation in 3ms.

Vizualizace experimentálních dat

Elektronová hustota

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows the protein structure in green cartoon representation, surrounded by a red electron density map. The interface includes a State Tree on the left, a central 3D view, and a Structure Tools panel on the right. The 'Volume Streaming' option is highlighted with a red circle.

State Tree

- 1TQN 1 model
 - Model 1
 - Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Ball & Stick
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell | 2 2 2

Sequence of 1TQN | Crystal... 1: cytochrome... A

```
MALYGT HSHGLFKKLGIPGFTPLPFLGNILSYHKGFCDMECHKYKQWVFDGQQPVLAITDPMIKITLVKECYSVFTNRRPFGVGFMSAI  
123 132 142 152 162 172 182 192 202 212  
SIAEDEEWKRLRSLSPFTISGKLEKMPV IIAQYGDVLRNLRREAEATGKPVILKDVFGAYSMQVITSTSGVNI DLSLNPQDPFVENTKLLRDF  
222 232 242 252 262 272 282 292 302 312  
LDPFFLSITVFFFLIPILEV LNICVFPREVINFLRKSVMKESRLEDTQKRVDFLQLMID SQNSKETESHKALSDELVAQSIIFIFAGYETTSS  
222 232 242 252 262 272 282 292 302 312
```

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset	+ Add		
Polymer	Cartoon	<input type="checkbox"/>	<input type="checkbox"/>
Ligand	Ball & Stick	<input type="checkbox"/>	<input type="checkbox"/>
Water	Ball & Stick	<input type="checkbox"/>	<input type="checkbox"/>

Unit Cell | 2 2 2

Volume Streaming 1TQN

Enable

Assembly Symmetry 1TQN

Enable

Export Animation

15:23:00 Created Ball & Stick in 26ms.
15:23:00 Created Ball & Stick in 12ms.
15:23:00 Updated Structure Focus Representation in 3ms.

Vizualizace experimentálních dat

Elektronová hustota

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central view shows the protein backbone in a green cartoon representation, surrounded by red electron density maps. The interface includes a State Tree on the left, a sequence viewer at the top, and a right-hand panel with various toolbars and settings.

State Tree:

- 1TQN 1 model
 - Model 1
 - Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Volume Server 1tqn
 - Volume Streaming Selec...
 - Unit Cell | 2 2 2

15:24:41 Updated 1.5 σ [2fo-fc] in 1ms.
15:24:41 Updated 3 σ [fo-fc(+ve)] in 0ms.
15:24:41 Updated -3 σ [fo-fc(-ve)] in 0ms.

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Ass...

Nothing Focused

Measurements

+ Add

Components

Preset + Add

Polymer Cartoon

Ligand Ball & Stick

Water Ball & Stick

Unit Cell | 2 2 2

Volume Streaming

+ 2Fo-Fc σ 1.5

+ Fo-Fc(+ve) σ 3

+ Fo-Fc(-ve) σ -3

Entry 1tqn

View Around Focus

Nothing to Update

Controls Help

Assembly Symmetry

1TQN

Vizualizace experimentálních dat

Elektronová hustota

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows the protein structure in green cartoon representation, surrounded by electron density maps (2Fo-Fc, Fo-Fc(+ve), and Fo-Fc(-ve)) shown as semi-transparent surfaces. A red arrow points to a specific atom in the structure, with the text "Kliknout na vybraný atom" (Click on the selected atom) next to it. The interface includes a State Tree on the left, a Sequence of 1TQN | Crystal... at the top, and a Structure Tools panel on the right. The bottom status bar shows update times and actions like "Updated 1.5 σ [2fo-fc] in 1ms."

Volume Streaming	1TQN
+ 2Fo-Fc σ	1.5
+ Fo-Fc(+ve) σ	3
+ Fo-Fc(-ve) σ	-3

Assembly Symmetry	1TQN
Entry	1tqn
View	Around Focus

Vizualizace experimentálních dat

Elektronová hustota

Sequence of 1TQN | Crystal... 1: cytochrome... A

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKYKWKWGFYDQQPVLAITDPDMIKTVLVEKCYSVFTNRRPFGVGFPMKSAI
SIAEDEEWKRLRSLSLSPFTTSGKLELMPVPIIAQYGVVLRNLRREARETGKQVTLKQVFGAYSMQVITSTSFQVNISSLNPPQDFVENTKLLRDFD
LDPFFLSITVFFFLIPILEVLNLCVFFREVINFLRKSVKRMKESRLQEDTQKHRVDFLQMLIDSONSKETESHKALSDELVAQSIIIFIFAGYETISS
```

15:28:06 Updated 1.5 σ [2fo-fc] in 72ms.
15:28:06 Updated 3 σ [fo-fc(+ve)] in 30ms.
15:28:06 Updated -3 σ [fo-fc(-ve)] in 32ms.

Structure Tools	
Structure	
1TQN Crystal Structure of Human ...	
Type	Assembly
Asm Id	1: Author Defined Ass...
HEM 508 B [auth A]	
Measurements	
+ Add	
Components 1TQN	
Preset	+ Add
Polymer	Cartoon
Ligand	Ball & Stick
Water	Ball & Stick
[Focus] Target	Ball & Stick
[Focus] Surroundings (5 Å)	
Unit Cell 2 2 2	
Volume Streaming 1TQN	
+ 2Fo-Fc σ	1.5
+ Fo-Fc(+ve) σ	3
+ Fo-Fc(-ve) σ	-3
Entry	1tqn
View	Around Focus
Nothing to Update	

Vizualizace anotací

Obarvení podle vlastností

The screenshot displays the Mol* web application interface. The central part shows a 3D ribbon representation of a protein structure (1TQN) in green, with red dots indicating specific annotations. The left sidebar contains a 'State Tree' with a hierarchy: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Cartoon, Ligand (49 elements), Ball & Stick, Water (190 elements), Ball & Stick, and Unit Cell (2 2 2). The top right shows the 'Structure Tools' panel with sections for Structure, Measurements, and Components. The 'Components' section is expanded to show 'Polymer' with 'Cartoon' representation. Under 'Polymer', the 'Hydrophobicity' property is circled in red. The bottom status bar shows recent updates: 'Updated Cartoon in 31ms.', 'Updated Cartoon in 8ms.', and 'Updated Cartoon in 28ms.'

Vizualizace anotací

Obarvení podle vlastností - hydrofobicita

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows a ribbon representation of the protein structure, colored according to its hydrophobicity. The color scale ranges from green (low hydrophobicity) to red (high hydrophobicity). The protein is surrounded by water molecules, shown as small red spheres. The interface includes a state tree on the left, a sequence viewer at the top, and a structure tools panel on the right.

State Tree

- 1TQN 1 model
- Model 1
- Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
- Unit Cell | 2 2 2

Sequence of 1TQN | Crystal...

```
MALYGIHSHGLFKKLGIPGPTLPFLGNILSYHKGFCEMDECHKYKGVWGFYDQQPVLAITDPDMIKITVLVKECYSVETNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLSPFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTISFGVNI DLSLNNPQDPFVENTKLLRFD
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLLRKSVMKESRLEDYQKHRVDFLQLMIDSQNSKETE SHKALSDLELVAQSIIFPAGYETTS
```

Structure Tools

- Structure
 - 1TQN | Crystal Structure of Human ...
 - Type Assembly
 - Asm Id 1: Author Defined Asse...
 - Nothing Focused
- Measurements
 - + Add
- Components 1TQN
 - Preset + Add
 - Polymer Cartoon
 - Ligand Ball & Stick
 - Water Ball & Stick
 - Unit Cell | 2 2 2
- Volume Streaming 1TQN
 - Enable
- Assembly Symmetry 1TQN
 - Enable
- Export Animation

Log

- 16:38:35 Updated Cartoon in 8ms.
- 16:38:48 Updated Cartoon in 28ms.
- 16:40:29 Updated Cartoon in 32ms.

Vizualizace anotací

Obarvení podle vlastností – kvalita

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central 3D view shows the protein structure in a green cartoon representation, surrounded by red dots representing water molecules. The interface includes a 'State Tree' on the left, a 'Sequence of' panel at the top with the amino acid sequence, and a 'Structure Tools' panel on the right. The 'Structure Tools' panel is currently open to the 'Components' section, where the 'Structure Quality Report' option is highlighted with a red circle. A log at the bottom shows recent updates to the cartoon representation.

State Tree

- 1TQN 1 model
 - Model 1
 - Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell 1 2 2 2

Sequence of 1TQN | Crystal... 1: cytochrome... A

MALYGTSHSHGLFKKLGIPGPTLPFLGNILSYHKGFCMFDMECHKRYGKWWGFYDQQPVLAITDPDMIKTVLVKECYSVFINRRPFGVGVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVLRNLRREARETKGFVTLKDVFGAYSMDEVITSTISFGVNIIDSLNPNQDPPVENTKKLLRDFD
LDPFFLSITVFPFLIPLEVLNLCVFPREVINFLRKSVKRMKESRLEDTQKHRVDFIQLMIDSQNSKETESHKALSDLELVAQSIITFFAGYETTSS

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Ass...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset + Add

Polymer Cartoon

- Uncertainty/Disorder
 - Chain Property
 - Miscellaneous
 - Residue Property
 - Symmetry
 - Validation
 - Density Fit
 - Geometry Quality
 - Structure Quality Report**
 - Modify by Selection
 - Select This
 - Edit Label
- Cartoon Representation

Ligand Ball & Stick

Water Ball & Stick

Unit Cell 1 2 2 2

16:46:40 Updated Cartoon in 557ms.
16:47:43 Updated Cartoon in 9ms.
16:47:52 Updated Cartoon in 11ms.

Vizualizace anotací

Obarvení podle vlastností - kvalita

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central view shows a 3D ribbon representation of the protein, colored by quality. The ribbon is primarily green and yellow, with some orange and red segments, indicating different quality levels. The protein is surrounded by water molecules represented as small red spheres.

The interface includes a State Tree on the left, a sequence viewer at the top, and a Structure Tools panel on the right. The sequence viewer shows the amino acid sequence of the protein, with residue numbers indicated above the sequence. The Structure Tools panel provides various options for viewing and interacting with the structure, including a list of components and their properties.

Sequence of 1TQN | Crystal... 1: cytochrome... A

```
MALYGTSHSHGLFKKLGIPGPTLPFLGNILSYHKGFDMCHKKYKGVWGFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVILKDVFGAYSMVDVITSTSGVWNIDSLNPNQDFFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLAKSVKRMKRESRLDTQKRHVDVFLQMLMIDSQNSKETESHKALSDELVAQSIIIFAGYETTSS
```

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset	+ Add	☰	🔄
Polymer	Cartoon	👁	🗑
Ligand	Ball & Stick	👁	🗑
Water	Ball & Stick	👁	🗑

Unit Cell | 2 2 2

Volume Streaming 1TQN

✓ Enable

Assembly Symmetry 1TQN

✓ Enable

Export Animation

16:47:43 Updated Cartoon in 9ms.

16:47:52 Updated Cartoon in 11ms.

16:51:37 Updated Cartoon in 25ms.

Vizualizace proteinových assemblies

The screenshot displays the Mol* Viewer interface for the protein assembly 3J3Q. The main view shows a 3D representation of the protein structure with a multi-colored Gaussian surface overlay. The interface is divided into several panels:

- State Tree (Left):** Shows the hierarchy of the model, including "3J3Q 1 model", "Model 1", "Assembly 1 2440800 elements", "Polymer 2440800 elements", and "Gaussian Surface".
- Sequence (Top):** Displays the amino acid sequence of the protein: `1 BIVNLOGQMVHQAI SPRTLNANVVKVVEEKAFSPVEIPMFSALSSEGATPODLNTMLNTVGGHQAAOMQLKETINEEAAEWDRLHPVHAGPIEPGQMR
EPRGSDIAGTTSTLQEQIGWMTNHPPIPVGGEIYKRWII LGLNKKIVMYSPTSILDIRQGPKEPRFRDYDRFYKTLRAEQASQEVKQWMMTETLLVQNA
NPDCKTILKALGPAATLEEMMTACQGVGGPGHKARVL`
- Structure Tools (Right):** Provides controls for the structure, including "Structure" (3J3Q | Atomic-level structure of the ...), "Measurements", "Components" (3J3Q), "Volume Streaming" (3J3Q), and "Assembly Symmetry" (3J3Q).
- Log (Bottom):** Shows a timeline of actions: "16:54:29 Created Polymer in 110ms.", "16:54:34 Created Gaussian Surface in 4.661s.", and "16:54:34 Updated Structure Focus Representation in 2ms."

Měření

The screenshot displays the Mol* web application interface. The central window shows a protein structure in green ball-and-stick representation. A specific distance of 2.92 Å is highlighted between two atoms, with a dashed line and a label indicating the measurement. The top of the interface shows the browser address bar with the URL `molstar.org/viewer/` and several tabs labeled "Mol*" and "Mol* Viewer".

On the left side, there is a "State Tree" panel with a hierarchical view of the structure:

- 1TQN 1 model
- Model 1
- Assembly 1 3999 elements
- Polymer 3766 elements
 - Cartoon
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell | 2 2 2
- Measurements
 - Distance 2 source(s), 49 elemen...
 - Distance

At the top of the main view, the "Sequence of 1TQN | Crystal..." is displayed with amino acid residues and their corresponding positions. Below the sequence is a toolbar with various interaction tools like "Residue", "Ball & Stick", and "Unit Cell".

On the right side, there is a "Structure Tools" panel with several sections:

- Structure**: 1TQN | Crystal Structure of Human ...
- Type: Assembly
- Asm Id: 1: Author Defined Asse...
- Nothing Focused
- 1 Chain + 1 Residue Selected
- Measurements**: + Add
- Distances: 2.92 Å | HEM 508 — CYS ...
- Components**: 1TQN
 - Polymer: Cartoon
 - Ligand: Ball & Stick
 - Water: Ball & Stick
 - Unit Cell | 2 2 2
- Volume Streaming**: 1TQN
 - Enable
- Assembly Symmetry**: 1TQN
 - Enable
- Export Animation**

At the bottom of the interface, a log shows recent actions:

- 1:20:48 Created Ball & Stick in 23ms.
- 1:20:48 Created Ball & Stick in 11ms.
- 1:20:48 Updated Structure Focus Representation in 2ms.

Vizualizace anotací

Obarvení podle vlastností - hydrofobicita

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows a green ribbon representation of the protein structure, with red dots indicating specific annotations or residues. The interface includes a top navigation bar, a left sidebar with a State Tree, a central sequence viewer, and a right sidebar with Structure Tools and a detailed component panel.

State Tree

- 1TQN 1 model
 - Model 1
 - Assembly 1 3999 elements
 - Polymer 3766 elements
 - Cartoon
 - Ligand 49 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell 1 2 2 2

Sequence of 1TQN | Crystal... 1: cytochrome... A

```
MALYGTSHSHGLFKLGI PGPTLPFLGNILSYHKGFCMFDMECHKKYGKVGWGFYDQQVLAITDPMIKTVLWKECVSVFTNRRPFGVGFMSAI  
SIAEDEEWKRLRSLLSPTFTSGKLEKMPVILIAQYGDVLRNLRRAEATGKPVILKDFGAYSMQVITSTSGVWNISSLNPPDFFVENTKLLRDF  
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLRKSVKRMKESRLDITQKRRVDFLQMLIDSQNSKETE SHKALSDELEVAQSIIFIFAGYEITTS
```

16:46:40 Updated Cartoon in 557ms.
16:47:43 Updated Cartoon in 9ms.
16:47:52 Updated Cartoon in 11ms.

Příkládání struktur

The screenshot displays the Mol* Viewer web application interface. The browser tabs at the top show 'Mol*' and 'Mol* Viewer'. The address bar contains 'molstar.org/viewer/'. The main interface is divided into several panels:

- Home Panel (Left):** Contains a 'Download Structure' section with a 'Source' dropdown set to 'PDB'. Below it, a search bar contains 'PDB Id (s) 2h7s 2rfc', which is circled in red. There is an 'Apply' button and a list of 'Remote States' including 'Nuclear Pore Complex', 'NPC-CIF', '1RB8 Annotated Assembly', 'Zika+EM', 'Cytochromes Superposition', 'AS', 'ASX', and 'ASX-1 Something'.
- Sequence Panel (Top Center):** Displays 'No structure available'.
- Structure Tools Panel (Right):** Includes sections for 'Structure' (Nothing Loaded), 'Measurements' (+ Add), 'Components' (Preset, + Add), and 'Export Animation'.

The status bar at the bottom shows the time '21:28:55' and the version 'Mol* Plugin 1.2.7 [12/19/2020, 11:52:32 AM]'. The Mol* logo is visible in the bottom right corner of the viewer area.

Příkládání struktur

The screenshot displays the Mol* web viewer interface. The central window shows a 3D ribbon representation of a protein structure, colored in shades of green and purple. The interface is divided into several panels:

- Left Panel (State Tree):** A hierarchical tree view showing the structure's components. It includes:
 - 2H7S 1 model
 - Model 1
 - Assembly 1 3355 elements
 - Polymer 3201 elements
 - Cartoon
 - Ligand 49 elements
 - Ball & Stick
 - Water 111 elements
 - Ball & Stick
 - Unit Cell P 1 21 1
 - 2RFC 1 model
 - Model 1
 - Assembly 1 2811 elements
 - Polymer 2752 elements
 - Cartoon
 - Ligand 60 elements
 - Ball & Stick
 - Water 5 elements
 - Ball & Stick
 - Unit Cell P 1 21 1

- Top Panel (Sequence):** Displays the amino acid sequence for two chains: "2H7S | L244A ..." and "1: Cytochrome...".
- Right Panel (Structure Tools):** A sidebar with various tool options:
- Structure: 2 structures, Nothing Focused.
- Measurements: + Add.
- Superposition: By Chains, By Atoms.
- Components: 2 structures, with a table for Polymer, Ligand, and Water.
- Export Animation.
- Bottom Panel (Log):** A timeline of actions:
- 21:31:10 Created Ball & Stick in 18ms.
- 21:31:10 Created Ball & Stick in 4ms.
- 21:31:10 Updated Structure Focus Representation in 2ms.

Příkládání struktur

The screenshot displays the Mol* Viewer interface with the following components:

- Browser:** molstar.org/viewer/
- Sequence:** 2H7S | L244A ... 1: Cytochrome... A
- State Tree:**
 - 2H7S 1 model
 - Model 1
 - Assembly 1 3355 elements
 - Polymer 3201 elements
 - Cartoon
 - Ligand 49 elements
 - Ball & Stick
 - Water 111 elements
 - Ball & Stick
 - Unit Cell P 1 21 1
 - 2RFC 1 model
 - Model 1
 - Assembly 1 2811 elements
 - Polymer 2752 elements
 - Cartoon
 - Ligand 60 elements
 - Ball & Stick
 - Water 5 elements
 - Ball & Stick
 - Unit Cell P 1 21 1

The central visualization shows two protein structures, one in green and one in purple, with a ligand in yellow and red sticks. A red circle highlights the 'Residue' button in the toolbar.

Structure Tools Panel:

- Structure: 2 structures, Nothing Focused
- Measurements: + Add
- Superposition: By Chains, By Atoms
- Components: 2 structures
 - Polymer: Cartoon
 - Ligand: Ball & Stick
 - Water: Ball & Stick
- 2 Unit Cells
- Export Animation

Log:

- 21:31:10 Created Ball & Stick in 18ms.
- 21:31:10 Created Ball & Stick in 4ms.
- 21:31:10 Updated Structure Focus Representation in 2ms.

Příkladání struktur

The screenshot displays the Mol* web application interface. On the left, a "State Tree" lists the loaded components: 2H7S 1 model (Model 1, Assembly 1 3355 elements, Polymer 3201 elements, Cartoon, Ligand 49 elements, Water 111 elements, Unit Cell P 1 21 1), 2RFC 1 model (Model 1, Assembly 1 2811 elements, Polymer 2752 elements, Cartoon, Ligand 60 elements, Water 5 elements, Unit Cell P 1 21 1). The top panel shows the "Sequence of 2H7S | L244A ..." and the amino acid sequence: `TTETIQSNANLAPLPHPVPEHLVDFDMYNFNSLGSAGVQEAVALQESNVFDLWVTRCNGGHWIATRGQLIREAYEDYRHSSECFPIPREAGEAYD
FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRPOGQCNTEDYAEPPPIRIFMLLAGLFEEDIPHLKYLTDQMTRPDGSMTFA
EAKEALYDYLPIIEQRRQKPGTDAISIVANGQVNGRPITSDEAKRMCGALLVGGLDIVVNFSLFSMEFLAKSPEHRQELIERPERIPACEELLR`. A context menu is open over a green ribbon structure, with "Structure Property" highlighted in red. The right panel shows "Structure Tools" with "Structure" selected, displaying "2 structures" and "Nothing Focused". Below are sections for "Measurements", "Superposition", "Components" (listing Polymer, Ligand, Water, and 2 Unit Cells), and "Export Animation". The bottom status bar shows logs: "21:31:10 Created Ball & Stick in 18ms.", "21:31:10 Created Ball & Stick in 4ms.", and "21:31:10 Updated Structure Focus Representation in 2ms."

Příkládání struktur

The screenshot displays the Mol* Viewer interface. The main window shows a protein structure in a cartoon representation, colored in shades of green and purple. A context menu is open over the structure, listing various selection options. The 'Backbone' option is highlighted with a red circle. The left sidebar contains a 'State Tree' with a hierarchical view of the structure's components, including '2H7S 1 model', 'Model 1', 'Assembly 1', 'Polymer', 'Cartoon', 'Ligand', 'Water', and 'Unit Cell'. The top of the browser window shows the URL 'molstar.org/viewer/' and the title 'Mol* Viewer'. The right sidebar contains 'Structure Tools' and a list of components including 'Structure', 'Measurements', 'Superposition', 'Components', and 'Export Animation'. A log at the bottom shows recent actions like 'Created Ball & Stick in 18ms.' and 'Updated Structure Focus Representation in 2ms.'

Sequence of 2H7S | L244A ... 1: Cytochrome... A

```
T T E T I Q S N A N L A P L P P H V E H L V F D F M Y N F S N L S A G V Q E A W A V L Q E S N V P D L V W T R C N G G H W I A T R G Q L I R E A Y E D Y R H F S S E C F F I P R E A G E A Y D  
F I P T S M D P P E Q R Q F R A L A N Q V W G M F V V D K L E N R I Q E L A C S L I E S L R P Q G C N F T E D Y A E P F P I R I F M L L A G L P E E D I P H L K Y L T D Q M T R P D G S M T F A  
E A K E A L Y D Y L I P I I E Q R R Q K P G T D A I S I V A N G Q V N G R P I T S D E A K R M C G A L L V G G L D T V V N F L S F S M E P L A K S P E H R Q E L I E R P E R I P A C E L L A R
```

Residue [toggle icons]

Add/Union Selection

- All
- Polymer/Carbohydrate Entities
- Ligand/Non-standard Residue
- Type
- Structure Property
- Trace
 - Backbone**
 - Sidechain
 - Sidechain with Trace
 - Helix
 - Beta Strand/Sheet
- Bond Property

21:31:10 Created Ball & Stick in 18ms.
21:31:10 Created Ball & Stick in 4ms.
21:31:10 Updated Structure Focus Representation in 2ms.

Příkladání struktur

The screenshot displays the Mol* Viewer interface with the following components:

- State Tree (Left):** A hierarchical tree showing the loaded models and their components. The first model is 2H7S (1 model), which includes Model 1, Assembly 1 (3355 elements), Polymer (3201 elements), Ligand (49 elements), Water (111 elements), and Unit Cell P 1 21 1. The second model is 2RFC (1 model), which includes Model 1, Assembly 1 (2811 elements), Polymer (2752 elements), Ligand (60 elements), Water (5 elements), and Unit Cell P 1 21 1.
- Sequence Viewer (Top):** Shows the amino acid sequence of the protein, with residues 11 to 291 highlighted in green. The sequence is: TTETIQSN¹¹NL²¹AP³¹PP⁴¹PH⁵¹VE⁶¹RL⁷¹VD⁸¹FD⁹¹MY¹⁰¹N¹¹¹FS¹²¹NL¹³¹S¹⁴¹AG¹⁵¹VO¹⁶¹EA¹⁷¹VL¹⁸¹Q¹⁹¹SN²⁰¹VP²¹¹DL²²¹W²³¹IR²⁴¹C²⁵¹NG²⁶¹GH²⁷¹WI²⁸¹AT²⁹¹RG³⁰¹L³¹¹IR³²¹E³³¹AY³⁴¹ED³⁵¹Y³⁶¹R³⁷¹HS³⁸¹SE³⁹¹CP⁴⁰¹FI⁴¹¹PR⁴²¹E⁴³¹AGE⁴⁴¹AY⁴⁵¹...
F¹⁰¹I¹¹¹S¹²¹MD¹³¹PP¹⁴¹EQ¹⁵¹RQ¹⁶¹FR¹⁷¹AL¹⁸¹AN¹⁹¹Q²⁰¹V²¹¹GM²²¹FV²³¹VD²⁴¹K²⁵¹LEN²⁶¹R²⁷¹I²⁸¹Q²⁹¹EL³⁰¹AG³¹¹SL³²¹IE³³¹SL³⁴¹NP³⁵¹Q³⁶¹Q³⁷¹C³⁸¹N³⁹¹F⁴⁰¹TE⁴¹¹D⁴²¹Y⁴³¹AE⁴⁴¹PP⁴⁵¹PI⁴⁶¹RI⁴⁷¹FM⁴⁸¹LL⁴⁹¹AG⁵⁰¹LP⁵¹¹ED⁵²¹IP⁵³¹HL⁵⁴¹K⁵⁵¹YL⁵⁶¹TD⁵⁷¹Q⁵⁸¹M⁵⁹¹IR⁶⁰¹PD⁶¹¹GS⁶²¹MT⁶³¹...
EA²⁰¹KE²¹¹AL²²¹Y²³¹D²⁴¹YL²⁵¹IL²⁶¹PI²⁷¹IE²⁸¹QR²⁹¹R³⁰¹CK³¹¹PG³²¹TD³³¹AI³⁴¹SI³⁵¹V³⁶¹ANG³⁷¹Q³⁸¹V³⁹¹NG⁴⁰¹R⁴¹¹PI⁴²¹TS⁴³¹DE⁴⁴¹AK⁴⁵¹K⁴⁶¹MG⁴⁷¹AL⁴⁸¹LV⁴⁹¹GG⁵⁰¹LD⁵¹¹V⁵²¹V⁵³¹N⁵⁴¹FL⁵⁵¹S⁵⁶¹F⁵⁷¹ME⁵⁸¹FL⁵⁹¹AK⁶⁰¹S⁶¹¹PE⁶²¹HR⁶³¹Q⁶⁴¹EL⁶⁵¹EA⁶⁶¹PE⁶⁷¹RI⁶⁸¹PA⁶⁹¹ACE⁷⁰¹ELL⁷¹¹ER

The Structure Tools panel on the right includes sections for Structure, Measurements, Superposition, and Components. The 'By Chains' option in the Superposition section is highlighted with a red circle. The Components section shows 2 structures: Polymer (Cartoon), Ligand (Ball & Stick), and Water (Ball & Stick).

At the bottom, a log shows the following actions:

- 21:31:10 Created Ball & Stick in 18ms.
- 21:31:10 Created Ball & Stick in 4ms.
- 21:31:10 Updated Structure Focus Representation in 2ms.

Přikládání struktur

The screenshot displays the Mol* Viewer interface with the following components:

- State Tree (Left):** A hierarchical tree showing the loaded structure: 2H7S 1 model, Model 1, Assembly 1 (3355 elements), Polymer (3201 elements), Cartoon, Ligand (49 elements), Water (111 elements), Unit Cell P 1 21 1, 2RFC 1 model, Model 1, Assembly 1 (2811 elements), Polymer (2752 elements), Cartoon, Ligand (60 elements), Water (5 elements), and Unit Cell P 1 21 1.
- Sequence Viewer (Top):** Shows the amino acid sequence of Cytochrome c (2H7S | L244A ...). A segment of the sequence is highlighted in green: `TTETIQSN...NLAPLPPHVP...EHLVDFDMY...NFSNL...SAGVQ...EAMAVLQESNV...FDLVMTRCNGGHWIATR...GQLREAYEDVRRHFSSECFPIPREAGEAY...LIF...SMDFPEQRQ...FALANQV...GVPVVKLENRIQELACSLIESL...FPQQCNFTEDYAE...PPIRIPMLLAGLPEEDIPHLKYLTDOMIRPDGSMIP...EAKPEALYDYLPIITEQRORQ...FGTDAISIVANGQVNGRPIISDEAKRMCGALLVGGLDIVVNF...LFSMEEFLAKSPEHRQELIERPERIPAAACEELLR...`
- Structure Tools (Right):** A panel with various tools and panels:
 - Structure:** 2 structures loaded.
 - Measurements:** Nothing Focused.
 - Superposition:** Active panel showing two structures: 2H7S (25 Residues + 1521 Elements) and 2RFC (18 Residues + 1281 Elements). A **Superpose** button is circled in red.
 - Components:** Lists Polymer (Cartoon), Ligand (Ball & Stick), Water (Ball & Stick), and 2 Unit Cells.
 - Export Animation:** A section for exporting the animation.
- Log (Bottom):** A list of recent actions:
 - 21:31:10 Created Ball & Stick in 18ms.
 - 21:31:10 Created Ball & Stick in 4ms.
 - 21:31:10 Updated Structure Focus Representation in 2ms.

Příkládání struktur

Sequence of 2H7S | L244A ... 1: Cytochrome... A

```
T T E T I Q S N E 11 N I A L F P P H V P E H I V F D F D N Y N F S N L S A G V Q E A V L Q E S N V P D L V W T R C N G S H W I A T R G Q L I R E A Y E D Y A H F S S E C P F I P R E A G E A V N 81  
101 F I F T S M D P P E Q R Q F A L A N Q V G M P V V D K L E N R I Q E L A C S L I E S L R P Q S Q C N F T E D Y A E F F I R I F M L L A G L P E E D I P H L K V L I D Q M T R P D G S M T F A 181  
201 E A K E A L Y D V L I P I T E Q R R K P G T D A I S I V A N G Q V N G R P I T S D E A K R M C G A L L V G G L D I V V N F L S F S M E F L A K S P E H S Q E L I E R P E R I P A A C E E L L R R 291
```

Components	2 structures
Polymer	Cartoon
Ligand	Ball & Stick
Water	Ball & Stick
2 Unit Cells	

21:41:35 Updated Ball & Stick in 2ms.
21:41:35 Superposed [25 Residues + 1521 Elements | A | 2H7S] and [18 Residues + 1281 Elements | A | 2RFC] with RMSD 4.53.

Příkládání struktur

The screenshot displays the Mol* web interface for protein structure visualization. The main window shows a 3D ribbon representation of a protein structure, colored in shades of green and purple. The interface is divided into several panels:

- State Tree (Left):** A hierarchical tree view showing the loaded structures and their components. It includes entries for 2H7S (1 model, Model 1, Assembly 1 with 3355 elements, Polymer with 3201 elements, Cartoon, Ligand with 49 elements, Ball & Stick, Water with 111 elements, Ball & Stick, Unit Cell P 1 21 1), 2RFC (1 model, Model 1, Assembly 1 with 2811 elements, Polymer with 2752 elements, Cartoon, Ligand with 60 elements, Ball & Stick, Water with 5 elements, Ball & Stick, Unit Cell P 1 21 1).
- Sequence Viewer (Top):** Shows the amino acid sequence of the protein, with residue numbers 1 to 291. The sequence is: TTETIQSNANLAPLPPHVPHEHLVDFDMYNFNSNLSAGVQEAQAVLQESNVDFLWVTRCNGGHWIATRGQLIREAYEDYRHFSSSECFPIPREAGEAYD FIFPTSMDFPEQRFALANQVWGMFVVDKLENRIQELACSLIESLRPQGCNFTEDYAEPPFIRIFMLLAGLPEDIPHLKYLTDQMTRPDGSMTFA EAKEALYDYLIPIIEQRQKPGTDAISIVANGQVNGRPITSDEAKRMCQALLVGGLDIVNFLSFSMEFLAKSPEHRQELIERPERIPAAACEELLR.
- Structure Tools (Right):** A panel for interacting with the structure, including options for Structure (2 structures), Measurements, Superposition (By Chains, By Atoms), and Components (2 structures).
- Log (Bottom):** A log of recent actions, such as "Updated Ball & Stick in 2ms." and "Superposed [25 Residues + 1521 Elements | A | 2H7S] and [18 Residues + 1281 Elements | A | 2RFC] with RMSD 4.53."

2DProts: Integration of AlphaFoldDB

AlphaFold Protein Structure Database

Home About FAQs Downloads

AlphaFold Protein Structure Database

Developed by DeepMind and EMBL-EBI

Search for protein, gene, UniProt accession or organism BETA Search

Examples: Free fatty acid receptor 2 At1g58602 Q5VSL9 E. coli Help: AlphaFold DB search help

Feedback on structure: Contact DeepMind

2DProts: Integration of AlphaFoldDB

AlphaFold Protein Structure Database

Home About FAQs Downloads

AlphaFold DB provides open access to over 200 million protein structure predictions to accelerate scientific research.

Developed by DeepMind and EMBL-EBI

Search for protein, gene, UniProt accession or organism BETA Search

Examples: Free fatty acid receptor 2 At1g58602 Q5VSL9 E. coli Help: AlphaFold DB search help

Feedback on structure: Contact DeepMind

Přikládání struktur – PDB a AlphaFold

Pairwise Structure Alignment

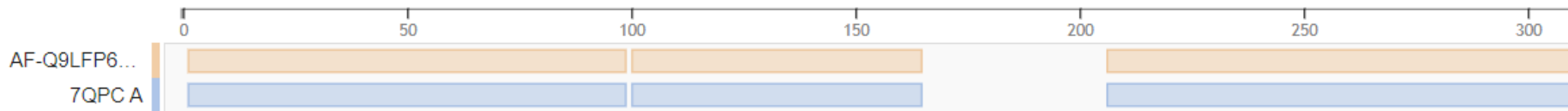
[Help](#)

▸ Compare Protein Structures

Entry ID	Chain ID	Description	Organism	Sequence Length	Modeled Residues
AF-Q9LFP6-F1	A	N/A	N/A	367	367
7QPC	A	Auxin efflux carrier component 8	Arabidopsis thaliana	376	327

SEQUENCE ALIGNMENT

SCORES



<https://www.rcsb.org/alignment/>

Přikládání struktur – PDB a AlphaFold

