



CEITEC



Central European Institute of Technology
BRNO | CZECH REPUBLIC

Vizualizace proteinů a ligandů



EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND
INVESTING IN YOUR FUTURE

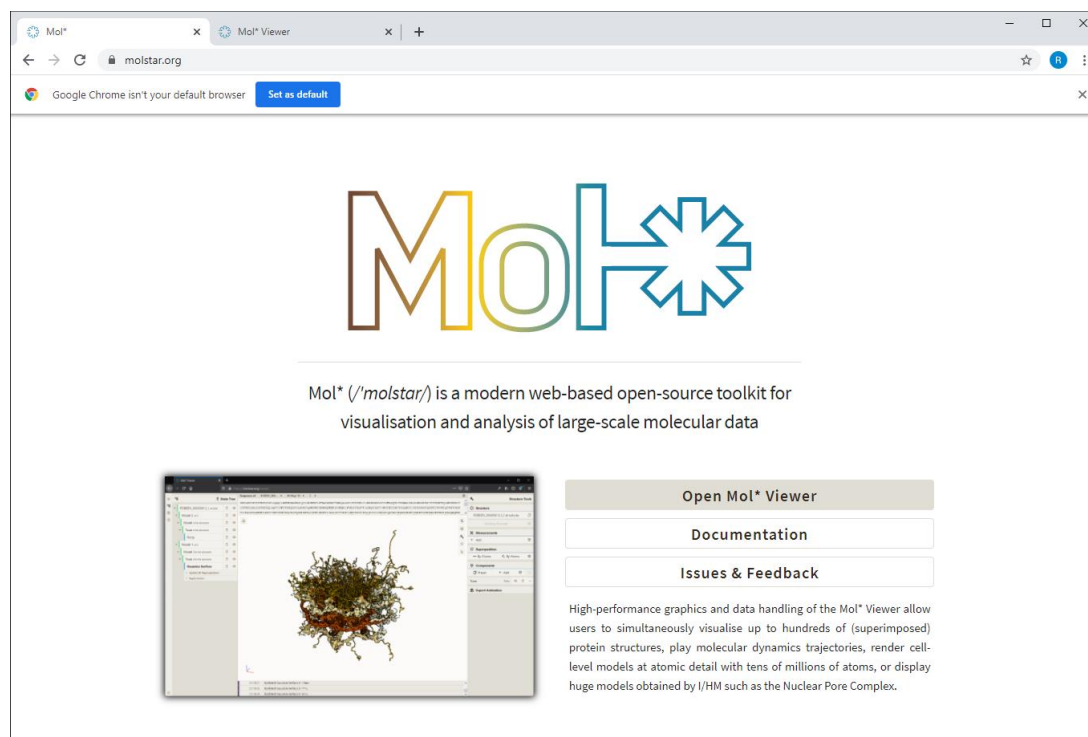


**OP Research and
Development for Innovation**



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.

The screenshot displays the MolStar web application interface. The browser's address bar shows the URL `molstar.org/viewer/`. The main content area is currently empty, displaying the text "Sequence No structure available".

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

- Download Structure**: Includes a "Source" dropdown set to "PDB" and a "PDB Id(s)" input field containing "1tqn". Below this is an "Options" section with a refresh icon and a green checkmark next to the word "Apply", which is circled in red.
- Add Trajectory**
- Download Density**
- Download File**
- Open Files**
- Download**
- Load CellPack**
- Load Genome 3D (G3D)**

Below these sections is a "Remote States" section with a list of 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) with a green vertical bar next to item 1.

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

- Structure**: Shows "Nothing Loaded" and "Nothing Focused".
- Measurements**: Includes a "+ Add" button.
- Components**: Includes a "Preset" button, a "+ Add" button, and a refresh icon.
- Export Animation**

The bottom status bar shows the time "14:28:23" and the version information "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 1TQN. The central 3D view shows the protein structure in a green cartoon representation, surrounded by red and blue spheres representing water and ligands. The interface includes a state tree on the left, a sequence viewer at the top, and a structure tools panel on the right.

Sequence of 1TQN | Crystal...

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

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

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"/>	...
Ligand	Ball & Stick	<input type="checkbox"/>	...
Water	Ball & Stick	<input type="checkbox"/>	...

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 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 view shows a 3D ribbon representation of the protein structure in green. The left sidebar contains a State Tree with the following elements:

- 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

The top of the interface shows the sequence of the protein: 1TQN | Crystal... 1: cytochrome... A. The sequence is displayed with residue numbers and corresponding amino acid codes.

The right sidebar contains the Structure Tools panel, which includes the following sections:

- Structure**: 1TQN | Crystal Structure of Human ...
- Measurements**: + Add
- Components**: 1TQN
 - Preset + Add
 - Polymer
 - Cartoon
 - Ball & Stick** (highlighted in red)
 - Gaussian Surface
 - Gaussian Volume
 - Label
 - Line
 - Molecular Surface
 - Orientation
 - Point
 - Putty
 - Spacefill

The bottom of the interface shows a log of recent actions:

- 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

Vizualizační model Ball & Stick

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

```
MALYGTSHGSLFKLGI PGPTPLPFLGNILSYHKGFDMCECHKYKGVWGFYDQQPVLAITDPDMIKTVLVKCEYSVPTNRRPFVGFVGMKSR I  
SIAEDEEWKRLRSLLSPTFTSGKLEKMFIIAQYGDVLRNLRREAEITGKPVTLKDVFGAYSMDVITSTSFVGNIDSLNPNQDFFVENTKLLRDFD  
LDPFFLSIVFPFLIPILEVNICVFPREVINFLRKSVKRMKESRLEDITQKHRVDFLQMLMIDSONSKETESHKALSDELVAQSIIPFAGYETTSS
```

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 souřadic molekuly

Vizualizační model Line

The screenshot displays the Mol* Viewer interface for the protein 1TQN (Cytochrome c). The central 3D view shows the protein backbone in a green 'Line' representation. The left 'State Tree' lists the hierarchy: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), and its sub-representations: Cartoon, Ball & Stick, and Line. Other components include Ligand (49 elements), Water (190 elements), and Unit Cell (2 2 2). The top sequence viewer shows the amino acid sequence: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKWWGFYDQQPVLAITDPDMIKTVLKECYSVFINRRPFGVGFMKSAISIAEDEEWKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVLRNLRREARETGKPVILKDVFGAYSMDVITSTSGVNIIDSLNNPQDFPVENTIKGLRFDLDFPFLSITVFPFLIPIILEVLNICVFPREVINFLRKSVKRMKESRLDTOKHRVDFLQMLIDSONSKETE SHKALSDELVAQSIIIFAGYETTSS. The right 'Structure Tools' panel shows the current structure, assembly details, and options for measurements, components, volume streaming, and assembly symmetry. A log at the bottom indicates recent actions: 'Updated Structure Focus Representation in 2ms.', 'Created Ball & Stick in 255ms.', and 'Created Line in 53ms.'

Vizualizace 3D souřadic molekuly

Vizualizační model Putty

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central 3D view shows the protein in a green 'Putty' representation. The left 'State Tree' lists the hierarchy: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements) with sub-styles Cartoon, Ball & Stick, Line, and Putty, Ligand (49 elements) with Ball & Stick, Water (190 elements) with Ball & Stick, and Unit Cell (2 2 2). The top sequence viewer shows the amino acid sequence: MALYGIHSHGLFKKLGIPGPTFLPFLGNILSYHMGFCMFDMECHKKYKGVWGFYDQQPVLAITDPDMIKIVLVKECYSVFTNRRPFGVGFMKSAI... The right 'Structure Tools' panel shows settings for the 'Structure' (1TQN | Crystal Structure of Human ...), 'Measurements', 'Components' (Polymer, Ligand, Water, Unit Cell), 'Volume Streaming', and 'Assembly Symmetry'. A log at the bottom indicates: 14:41:17 Created Ball & Stick in 255ms, 14:53:35 Created Line in 53ms, and 14:54:42 Created Putty in 90ms.

Vizualizace 3D souřadnic molekuly

Vizualizační model Spacefil

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central 3D view shows a space-filling model of the protein, with atoms represented by semi-transparent spheres in green, red, and blue. The interface includes a left-hand 'State Tree' for navigation, a top sequence viewer, and a right-hand 'Structure Tools' panel with various visualization options.

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

```
MLYGTGHSGLFKLGI PGPTL PFLGNILSYHKGF CMFDM ECHKYKWKWGFYD GQOPVLA ITDPDMIKIVLVK ECVSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLSPFTTSGKIKEMVPIIAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSFVNI DSNLPQDPEVENTKGLLRDFD
LDPFFLSITVFFLIPILEVLNICVFFPREVINFLRKSVMKRESLEDTQKHRVDFLQLMIDSNQSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

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

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 5 reprs
 - Ligand Ball & Stick
 - Water Ball & Stick
 - Unit Cell | 2 2 2
- Volume Streaming 1TQN
 - Enable
- Assembly Symmetry 1TQN
 - Enable
- Export Animation

Log

- 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. The central 3D view shows a protein structure rendered as a green molecular surface. The left sidebar contains a 'State Tree' with a hierarchy: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), and various representations like Cartoon, Gaussian Surface, Gaussian Volume, Molecular Surface, Ligand (49 elements), Water (190 elements), and Unit Cell (2 2 2). The top right shows the 'Structure Tools' panel with 'Structure' selected, displaying '1TQN | Crystal Structure of Human ...'. The bottom right panel shows 'Components' for '1TQN' with a list of representations including Molecular Surface, Orientation, Point, Putty, Spacefill, Non-covalent Interactions, Validation Clashes, Membrane Orientation, Set Coloring, Modify by Selection, Select This, and Edit Label. A log at the bottom shows actions like 'Created Gaussian Surface in 597ms.' and '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 | 2 2 2

The top right panel shows the Structure Tools section with the following details:

- 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
 - Cartoon Representation
 - Gaussian Surface Representation
 - Gaussian Volume Representation
 - Molecular Surface Representation

The bottom status bar 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 Volume

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows a protein structure with a red Gaussian Volume representation. 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 panel shows the protein sequence: `Sequence of 1TQN | Crystal... 1: cytochrome... A`

```
MLYGTHTSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFDMCHKKYKWKWGFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFPMKSAI
122 132 142 152 162 172 182 192 202 212
SIAEDEEWKRLRSLSPFTTSGKLRKEMVPIIAQYGDVLRNLRREAETGKPVLRKDFGAYSDMVIITSTSEFGVNIIDSLNPPQDFVENTKLLRDF
222 232 242 252 262 272 282 292 302 312
LDPFFLSITVFFFLIPILEVLNLCVFPREVINFLRKSVKRMKESRLEDTQKHRVDFLQMLMDSQNSKETESHKALSDELVAQSIIIFAGAYETSS
```

The right sidebar contains the Structure Tools panel, showing the Structure section with the following items:

- 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
 - Cartoon Representation
 - Gaussian Surface Representation
 - Gaussian Volume Representation
 - Molecular Surface Representation

The bottom status bar shows the following log entries:

- 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

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central view shows the protein backbone in green cartoon representation, surrounded by a red electron density mesh. The interface includes a state tree on the left, a sequence viewer at the top, and a right-hand panel with various tool options. The 'Volume Streaming' option is highlighted with a red circle.

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

MALYGT HSHGLFKKLGIPGFTPLPFLGNILSYHKGF C MFDMECHKKYGKWWF YDQQPVLAITD PDMIKITLVKECYSVFTNRRPFGVGFMSAI
123 132 142 152 162 172 182 192 202 212
SIAEDEEMKRLRSLSPFTISGKLEMVPIIAQYGDVLRNLRREAETGKPVILKDVFGAYSMDVITSTSGVNI D S L N N P Q D P F V E N T K K L L R F D F
222 232 242 252 262 272 282 292 302 312
LDPFFLSITVFFFLIPILEV L N I C V F P R E V I N F L R K S V K R M K E S R L E D T Q K H R V D F L Q L M I D S Q N S K E T E S H K A L S D L E L V A Q S I I F I F A G Y E T T S S
322 332 342 352 362 372 382 392 402

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 I 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 3D view shows the protein structure in green cartoon representation, surrounded by electron density maps shown as red and yellow spheres. The interface is divided into several panels:

- State Tree (Left):** A hierarchical tree showing the structure's components, including 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Ligand (49 elements), Water (190 elements), Volume Server 1tqn, Volume Streaming Selection, and Unit Cell (2 2 2).
- Sequence (Top):** A sequence viewer showing the amino acid sequence of the protein, with residue numbers and corresponding amino acid codes.
- Structure Tools (Right):** A panel for managing the structure, including options for Type (Assembly), Asm Id (1: Author Defined Ass...), and Nothing Focused.
- Measurements (Right):** A panel for adding and managing measurements, including a + Add button and a list of components.
- Components (Right):** A table listing the components of the structure, including Polymer, Ligand, Water, and Unit Cell.
- Volume Streaming (Right):** A panel for managing volume streaming, including a + Add button and a list of volume maps (2Fo-Fc σ , Fo-Fc(+ve) σ , Fo-Fc(-ve) σ).
- Assembly Symmetry (Right):** A panel for managing assembly symmetry, including a + Add button and a list of assembly types (Entry, View).

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

- 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.

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 sigma, Fo-Fc(+ve) sigma, and Fo-Fc(-ve) sigma) 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 Structure Tools panel shows the current structure (1TQN | Crystal Structure of Human ...), its type (Assembly), and various measurement and component settings. The bottom status bar shows the time and update status for the density maps.

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

MALYGTSHSGLFKKLGI PGPTLP LFGNLSYHKGF CMFDMCHKKYKGVWGFYDGGQFVLAITDPDMIKTVLVKECYSVFINRRPFGVGVGFMKSAI
SIAEDEENKRLRSLSPFTFTSGKLEMPVPIIAQYGDVLRNLRREAEATGKPVTLKDFVFGAYSMDEVITSTISFGVNI DLSLNPQDFEVNTKLLRFDF
LDPFFLSITVFPFLIPILEVLNLCVFPREVINFLRKSVMKRESRLDTQKRVDFLQLMIDSONSKETE SHKALSDELELVAQSIIFIFAGYETTSS

Kliknout na vybraný atom

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.

Vizualizace experimentálních dat

Elektronová hustota

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

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKYKWKWGFYDQQPVLAITDPMIKITVLVKECYSVFTNRRFPFVGVGFMKSAI
SIAEDEEWKRLRSLSPTFTSGKLEAVPIIAQYGVVLRNLRREAEITGKEVTLKQVFGAYSMDVITSTSFVGNIDSLNNPQDFVENTKLLRDF
LDPFFLSITVFFFLIPILEVNI CVFPRVFNFLRKSVKRMKESRLÉDTQKHRVDFLQMLIDSONSKETE SHKALSDELVAQSII FIFAGYETISS
```

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Ass...

HEM 508 | B [auth A]

Measurements

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"/>
[Focus] Target	Ball & Stick	<input type="checkbox"/>	<input type="checkbox"/>
[Focus] Surroundings (5 Å)		<input type="checkbox"/>	<input type="checkbox"/>
Unit Cell 2 2 2		<input type="checkbox"/>	<input type="checkbox"/>

Volume Streaming 1TQN

+ 2Fo-Fc σ	<input type="checkbox"/>	1.5	<input type="checkbox"/>
+ Fo-Fc(+ve) σ	<input type="checkbox"/>	3	<input type="checkbox"/>
+ Fo-Fc(-ve) σ	<input type="checkbox"/>	-3	<input type="checkbox"/>

Entry 1tqn

View Around Focus

Nothing to Update

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.

Vizualizace anotací

Obarvení podle vlastností

The screenshot displays the Mol* web application interface. The central view shows a protein structure (1TQN) rendered in a green cartoon representation, surrounded by small red spheres representing water molecules. 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, Ligand (49 elements), Ball & Stick, Water (190 elements), Ball & Stick, and Unit Cell (2.2.2).
- Sequence Viewer (Top):** Displays the amino acid sequence of the protein: MALYGTSHSHGLFKLGI... The sequence is color-coded by residue type and position.
- Structure Tools (Right):** A panel for interacting with the structure. It includes sections for Structure, Measurements, and Components. The 'Residue Property' section is expanded, and 'Hydrophobicity' is highlighted with a red circle.
- Log (Bottom):** A log of recent actions, such as 'Updated Cartoon in 31ms.' and 'Updated Cartoon in 8ms.'

Vizualizace anotací

Obarvení podle vlastností - hydrofobicita

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 hydrophobicity. The interface includes a State Tree on the left, a sequence viewer at the top, and a Structure Tools panel on the right. A log at the bottom shows update times for the cartoon representation.

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

```
MALYGIHSHGLFKLGIPIGPTLPFLGNILSYHKGFDMCKKYGKVGFDGQQPVLAITDPDMIKTVLVKECYSVETNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVLRNLRREAETGKPVTLKQVFGAYSMVDVITSTSGVNI DLSLNNPQDPFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNICVFPREVTFNFLRRSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETE SHKALSDLELVAQSIIFTFAGYETTS
```

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

16:38:35 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 structure 1TQN. The central view shows the protein as a green cartoon representation. The left sidebar contains a 'State Tree' with the following items:

- 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

The top panel shows the sequence of the protein: 1TQN | Crystal... 1: cytochrome... A. The sequence is: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMCHKKYKWKWGFYDQQPVLAITDPDMIKTVLVKECYSVFINRRPFGVGFMKSAI SIAEDEEWKRLRSLLSPTFTSGKLRKEMVPIIAQYGDVLRNLRREARETGKPFVTLKDVFGAYSMDVITSTSGVNIIDSLNPNQDPPFVENTKLLRDFD LDPFFLSITVFFLIPLEVLNLCVFPREVINFLRKSVKRMKESRLEDTQKHRVDFIQLMIDSNQSKETESHKALSDEELVAQSIIIFFGYETTSS.

The right sidebar contains the 'Structure Tools' panel. Under the 'Structure' section, the protein is identified as '1TQN | Crystal Structure of Human ...'. The 'Measurements' section is empty. The 'Components' section shows '1TQN' as a polymer. The 'Structure Quality Report' option is highlighted with a red circle.

The bottom log shows the following updates:

- 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 structure is surrounded by small red and blue spheres, likely representing water molecules or other atoms.

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 and quality scores 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.

Log entries at the bottom of the interface show the following update times for the cartoon representation:

- 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* web application interface. At the top, the browser address bar shows `molstar.org/viewer/`. The main window is divided into several sections:

- State Tree (Left):** A hierarchical list of loaded models and assemblies, including "3J3Q 1 model", "Model 1", "Assembly 1 2440800 elements", "Polymer 2440800 elements", and "Gaussian Surface".
- Sequence Viewer (Top):** Shows the amino acid sequence for protein 3J3Q: `1 BIVONLQGMVHQAI SPRTLNANVVKVVEEKAFSPVEVIMFSA LSEGATPODLNTMLNTVGGHQAA MQMLKETINEEA AEWDRLHPVHAGPIEPGQMR
101 EPRGSDIAGTTSTLQE QIGWMTNHPPIPVGGEIYKRWII LGLNKIVMYSPTSILDIRQGPKEPFRDYDRFYKTLRAEQASQEVKQWMMETLLVQNA
201 NPDKTILKALGPARTLEEMMTACQGVGGPGHKARVL`
- 3D Visualization (Center):** A large, colorful protein assembly is shown, overlaid with a semi-transparent Gaussian surface. The surface is rendered in various colors (red, yellow, green, blue, purple, orange) to represent different chemical environments or electrostatic potentials.
- Structure Tools (Right):** A panel with various controls for the visualization, including "Structure", "Measurements", "Components", "Volume Streaming", and "Assembly Symmetry".
- Log (Bottom):** A list of recent actions:
 - 16:54:29 Created Polymer in 110ms.
 - 16:54:34 Created Gaussian Surface in 4.661s.
 - 16:54:34 Updated Structure Focus Representation in 2ms.

Vizualizace anotací

Obarvení podle vlastností - hydrofobicita

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central view shows the protein structure in a green cartoon representation. The interface includes a State Tree on the left, a sequence viewer at the top, and a Structure Tools panel on the right. The Structure Tools panel shows various measurement and component options.

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

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.

Přikládání struktur

The screenshot displays the Mol* Viewer interface. The main window shows a protein structure (Cytochrome c) with a green ribbon representation. The left sidebar contains a 'State Tree' listing the structure's 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), and Unit Cell P 1 21 1. The top right shows the 'Structure Tools' panel with sections for Structure, Measurements, Superposition, Components, and Export Animation. A red circle highlights the 'Superposition' icon in the Structure Tools panel. The bottom status bar shows a log of actions: 'Created Ball & Stick in 18ms.', 'Created Ball & Stick in 4ms.', 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 P E H L V F D F M Y N P S N L S A G V Q E A W A V L Q E S N V D L W 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 P 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 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 L I P 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 O G A L L V G G L D T V W N F L S F S M E F L A K S P E H R Q E L I E R P E R I F A A C E E L L R R

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. On the left, the State Tree shows a hierarchy of structures: 2H7S 1 model, Model 1, Assembly 1 (3355 elements), Polymer (3201 elements), Cartoon, Ligand (49 elements), Water (111 elements), and Unit Cell P 1 21 1. The central 3D view shows a protein structure in green cartoon representation. The top panel displays the sequence of 2H7S | L244A ... and 1: Cytochrome... with residue numbers. The right panel, Structure Tools, shows 2 structures, Nothing Focused, Measurements, Superposition, Components (2 structures), and Export Animation. A red circle highlights the 'Residue' button in the toolbar.

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

TTETIQSNANLÄPLPPHVEHLVDFDMYNFSLNSAGVQEAWVLQESNVFDLWTRCNGGHWIATRGQLIREAYEDYRHSSECFPIPREAGEAYD
FIPTSMDFPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRPQGQCNFTEDYAEFPPIRIFMLLAGLPEDIPHLKYLTDQMTRPDGSMTFA
EAKAELYDYLIPIIEQRQKPGTDAISIVANGQVNGRPITSDEAKRMOGALLVGGDLTVVNFSLFSMEFLAKSPEHRQELIERPERIPAAACELLAR

Residue

Structure Tools

Structure

2 structures

Nothing Focused

Measurements

Add

Superposition

By Chains By Atoms

Components 2 structures

Preset Add

Polymer Cartoon

Ligand Ball & Stick

Water Ball & Stick

2 Unit Cells

Export Animation

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* web application interface. The main window shows a protein structure (Cytochrome) in a cartoon representation. A context menu is open over the structure, with the "Structure Property" option highlighted in red. The left sidebar contains a "State Tree" with a hierarchical view of the structure's components, including models, assemblies, polymers, and ligands. The top of the interface shows the sequence of the protein, and the right sidebar contains various tool panels such as "Structure Tools", "Measurements", "Superposition", "Components", and "Export Animation".

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

```
TTETIQSNANLAPLPPHVP EHLVDFD MYNPSNLSAGVQEAWAVLQESNVFDLWVTRCGNGGHWIATRGQLIREAYEDYRHFSSSECFIPREAGEAYD
FIPTSM DPPEQRQFRALANQVGMFVVDKLENRIQELACSLIESLRAPOGQCNFTE DYAEPPPIRIFMLLAGLPEEDI PHLKYLTDQMTRPDGSMITFA
EAK EALYDYLIP IIEQRQKPGTDAISIVANGQVNGRPIITSDEAKRMCGLLVGGLDIVVNFLSFSEFLAKSPEHRQELIERPERIPRACEELLR
```

Residue [Icons]

Add/Union Selection

- All
- Polymer/Carbohydrate Entities
- Ligand/Non-standard Residue
- Type
- Structure Property**
- Bond Property
- Residue Property
- Manipulate Selection
- Amino Acid
- Nucleic Base
- Element Symbol

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

2:31:10 Created Ball & Stick in 18ms.

2:31:10 Created Ball & Stick in 4ms.

2:31:10 Updated Structure Focus Representation in 2ms.

Structure Tools

Structure

2 structures

Nothing Focused

Measurements

+ Add

Superposition

By Chains By Atoms

Components 2 structures

Preset + Add

Polymer Cartoon

Ligand Ball & Stick

Water Ball & Stick

2 Unit Cells

Export Animation

Příkládání struktur

The screenshot displays the Mol* Viewer interface. The main window shows a protein structure rendered in a green cartoon representation. A context menu is open over the structure, with the 'Backbone' option highlighted in red. The menu includes options for 'Residue', 'Add/Union Selection', 'All', 'Polymer/Carbohydrate Entities', 'Ligand/Non-standard Residue', 'Type', 'Structure Property', 'Trace', 'Backbone', 'Sidechain', 'Sidechain with Trace', 'Helix', 'Beta Strand/Sheet', and 'Bond Property'. The left sidebar shows a 'State Tree' with a hierarchy of models and assemblies. The top right shows the 'Structure Tools' panel with options for 'Structure', 'Measurements', 'Superposition', 'Components', and 'Export Animation'. The bottom status bar shows a log of actions performed at 21:31:10.

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 P 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 V V N F L S F S M E F L A K S F E H R Q E L I E R P E R I P A C E L L R R
```

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

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* Viewer interface with the following components:

- State Tree (Left):** A hierarchical tree showing the loaded models and their components. For example, '2H7S 1 model' contains 'Model 1', 'Assembly 1 3355 elements', 'Polymer 3201 elements' (Cartoon), 'Ligand 49 elements' (Ball & Stick), and 'Water 111 elements' (Ball & Stick).
- Sequence Viewer (Top):** Shows the amino acid sequence of the protein, with residues 11 to 291 highlighted in green. The sequence is: TTETIQSN¹¹NL²¹AP³¹PP⁴¹VF⁵¹ER⁶¹LV⁷¹DF⁸¹DM⁹¹YN¹⁰¹PS¹¹¹NL¹²¹SAG¹³¹VOE¹⁴¹AW¹⁵¹VL¹⁶¹QES¹⁷¹NV¹⁸¹PD¹⁹¹LW²⁰¹TR²¹¹CG²²¹NG²³¹GH²⁴¹WI²⁵¹AT²⁶¹RG²⁷¹QL²⁸¹IR²⁹¹EAY³⁰¹ED³¹¹YR³²¹HFS³³¹SEC³⁴¹PF³⁵¹IP³⁶¹RE³⁷¹AGE³⁸¹AY³⁹¹D⁴⁰¹
F⁴¹¹IP⁴²¹SM⁴³¹DP⁴⁴¹PE⁴⁵¹QR⁴⁶¹Q⁴⁷¹FR⁴⁸¹ALAN⁴⁹¹QV⁵⁰¹GM⁵¹¹FV⁵²¹VD⁵³¹KLEN⁵⁴¹R⁵⁵¹I⁵⁶¹Q⁵⁷¹ELAC⁵⁸¹SL⁵⁹¹IES⁶⁰¹LAP⁶¹¹Q⁶²¹QC⁶³¹N⁶⁴¹F⁶⁵¹TE⁶⁶¹DY⁶⁷¹AE⁶⁸¹PP⁶⁹¹PI⁷⁰¹RI⁷¹¹EM⁷²¹L⁷³¹AG⁷⁴¹LP⁷⁵¹ED⁷⁶¹IS⁷⁷¹HL⁷⁸¹KY⁷⁹¹LD⁸⁰¹Q⁸¹¹M⁸²¹TR⁸³¹PD⁸⁴¹GS⁸⁵¹M⁸⁶¹TE⁸⁷¹
E⁸⁸¹AK⁸⁹¹EAL⁹⁰¹Y⁹¹¹DY⁹²¹IL⁹³¹EL⁹⁴¹TE⁹⁵¹QR⁹⁶¹R⁹⁷¹K⁹⁸¹PG⁹⁹¹IDA¹⁰⁰¹LS¹⁰¹¹IV¹⁰²¹ANG¹⁰³¹QV¹⁰⁴¹NG¹⁰⁵¹RP¹⁰⁶¹ITS¹⁰⁷¹DE¹⁰⁸¹AK¹⁰⁹¹RM¹¹⁰¹CG¹¹¹¹ALL¹¹²¹V¹¹³¹GG¹¹⁴¹LD¹¹⁵¹V¹¹⁶¹N¹¹⁷¹FL¹¹⁸¹S¹¹⁹¹FS¹²⁰¹ME¹²¹¹FL¹²²¹AK¹²³¹SP¹²⁴¹EH¹²⁵¹R¹²⁶¹Q¹²⁷¹EL¹²⁸¹ER¹²⁹¹PER¹³⁰¹I¹³¹¹PA¹³²¹ACE¹³³¹ELL¹³⁴¹LR¹³⁵¹

The central 3D view shows the protein structure in green cartoon representation. The 'Structure Tools' panel on the right includes sections for Structure, Measurements, Superposition (with 'By Chains' selected and circled in red), and Components. A log at the bottom shows 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

The screenshot displays the Mol* web interface with a protein structure visualization and a sequence alignment. The interface is divided into several panels:

- State Tree (Left):** A hierarchical tree view showing the structure's components, including models, assemblies, polymers, ligands, and water molecules.
- Sequence of (Top Center):** A sequence alignment for 2H7S | L244A ... and 1: Cytochrome... with residue numbers and a green highlight on a specific segment.
- Residue (Center):** A toolbar for interacting with the structure, including options for Residue, Ball & Stick, and other representations.
- Structure Tools (Right):** A panel with various tools for structure manipulation, including Structure, Measurements, Superposition, and Components.

The central visualization shows a protein structure in a green cartoon representation, with a blue and red ligand bound to it. The structure is surrounded by water molecules (red and white spheres). The sequence alignment shows the following residues highlighted in green:

```
TTETIQSN11NL11APLPPHVP21EHV21DF21DMY21NF21SNL21SAGV21QEL21AW21VL21GES21NV21DL21VW21IR21CNG21SH21WI21TR21QGL21RE21AY21ED21YR21H21FS21SEC21PF21IP21RE21GE21AY21  
F104I104P104T104S104M104D104P104PE104QR104FR104AL104AN104QV104VG104MP104VV104DK104LEN104RI104QEL104AG104SL104IE104SL104RP104QG104CN104FT104ED104YAE104PF104IR104IP104ML104LAG104LP104ED104IP104HL104KYL104T104Q104M104IR104PD104GS104MT104FA104  
E201NE201AL201Y201DL201PI201IE201QR201R201Q201PG201IDA201IS201V201ANG201QV201NG201RP201ITS201DE201AK201RM201OG201ALL201V201GG201L201DI201VN201FL201S201F201S201ME201FL201AK201SP201EH201RO201EL201IE201R201PE201RI201PA201ACE201ELL201ER
```


Příkládání struktur

The screenshot displays the Mol* web application interface. The top navigation bar shows the Mol* logo and three browser tabs. The address bar indicates the URL `molstar.org/viewer/`. The main 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, 2RFC, and their respective models, assemblies, polymers, ligands, and waters.
- Sequence Viewer (Top):** Displays the amino acid sequence of the protein, with residue numbers and a highlighted residue (ARG 290).
- 3D View (Center):** A 3D rendering of the protein structure, showing two superposed models. The structure is primarily green and purple, with red dots indicating specific residues.
- Structure Tools (Right):** A panel containing various tools and settings for the 3D view, including Structure Tools, Structure (2 structures), Measurements, Superposition (By Chains, By Atoms), and Components (2 structures).

At the bottom of the 3D view, a tooltip identifies the structure as **Cytochrome P450-cam** (2H7S | Model: 1 | Instance ASM_1 | A | ARG 290). A log at the bottom shows the following entries:

- 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.

