



CEITEC



Central European Institute of Technology
BRNO | CZECH REPUBLIC

Vizualizace proteinů a ligandů



EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND
INVESTING IN YOUR FUTURE

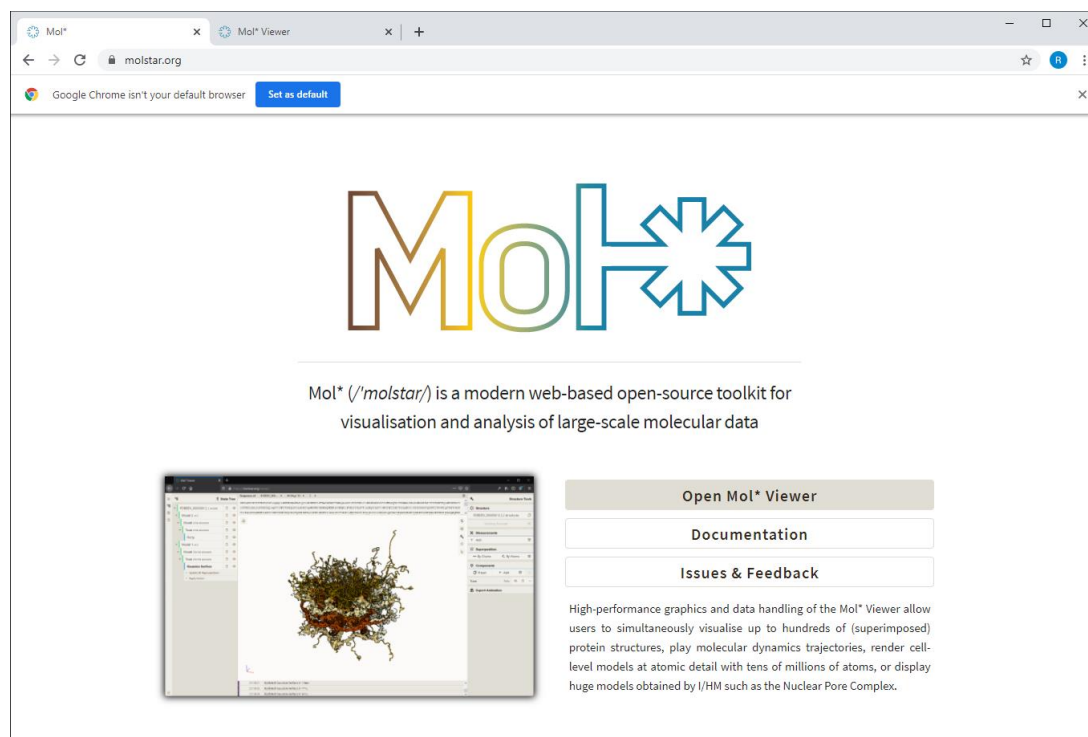


**OP Research and
Development for Innovation**



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 the "Download Structure" section 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

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 interface.

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, surrounded by red and blue spheres representing water molecules 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.

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

Structure Tools Panel:

- Structure:** 1TQN | Crystal Structure of Human ...
- Type: Assembly
- Asm Id: 1: Author Defined Asse...
- Nothing Focused
- Measurements:** + Add
- Components:** 1TQN
 - Preset: + Add
 - Polymer: Cartoon (visible)
 - Ligand: Ball & Stick (visible)
 - Water: Ball & Stick (visible)
 - Unit Cell | 2 2 2
- Volume Streaming:** 1TQN (Enabled)
- Assembly Symmetry:** 1TQN (Enabled)
- 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 view shows a 3D ribbon representation of the protein structure in green, with red spheres representing atoms. The left sidebar shows the State Tree with the following components:

- 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

The top of the interface shows the Sequence of 1TQN | Crystal... with the amino acid sequence: M A L Y G T H S H G L F K K L G I P G P T L P F L G N I L S Y H K G F C M F D M E C H K K Y G K W G F Y D G Q Q P V L A I T D P D M I K T V L V K E C Y S V F I N R R P F G F V G F M K S A I S I A E D E E W K R L R S L L S P T F T S G K L K E M V F I I A Q Y G D V L V R N L R R E A E T G K F V L K D V F G A Y S M D V I T T S T S F G V N I D S L N N F Q D P F V E N T K K L L R F D F L D P F F L S I T V F F L I P I L E V L N I C V F 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 P A G Y E T T S S.

The right sidebar shows the Structure Tools panel with the following sections:

- Structure
 - 1TQN | Crystal Structure of Human ...
 - Type: Assembly
 - Asm Id: 1: Author Defined Ass...
 - Nothing Focused
- Measurements
 - + Add
- Components
 - 1TQN
 - Preset + Add
 - Polymer
 - Cartoon
 - Ball & Stick (highlighted with a red circle)
 - Gaussian Surface
 - Gaussian Volume
 - Label
 - Line
 - Molecular Surface
 - Orientation
 - Point
 - Putty
 - Spacefill
 - Cartoon Representation
- Ligand
 - Ball & Stick
- Water
 - Ball & Stick
- Unit Cell | 2 2 2

The bottom of the interface shows a log of 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

```
MALYGTSHGGLFKLGI PGPTPLPFLGNILSYHKGFDMCHCKYKGVWGFYDQQPVLAITDPDMIKTVLVKCEYSVPTNRRPFVGFVGMKSR I  
SIAEDEEWKRLRSLLSPTFTSGKLEKMFIIAQYGDVLVRLNRREAEITGKPVTLKDVFGAYSMDVITSTSGVNIIDSLNPNQDFFVENTKLLRDFD  
LDPFFLSIVFPFLIPILEVNIICVFPREVINFLRKSVKRMKESRLEDTQKHRVDFLQMLMIDSONSKETESHKALSDELVAQSIIPFAGYETTSS
```

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* web interface for the protein structure 1TQN. The central 3D view shows the protein backbone as a green line representation. The left sidebar (State Tree) lists the hierarchy: 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). The top sequence viewer shows the amino acid sequence: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKWWGFYDQQPVLAITDPDMIKTVLKECYSVFINRRPFGVGFMKSAI... The right sidebar (Structure Tools) shows the current structure is 1TQN | Crystal Structure of Human ... and lists components: Polymer (3 reprs), Ligand (Ball & Stick), Water (Ball & Stick), and Unit Cell (2 2 2). The bottom log shows: 14:36:24 Updated Structure Focus Representation in 2ms. 14:41:17 Created Ball & Stick in 255ms. 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 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 right of the interface shows the Sequence of 1TQN | Crystal... with the following amino acid sequence:

```
MALYGIHSHGLFKKLGIPGPTFLPFLGNILSYHMGFCMFDMECHKKYKGVWGFYDQQPVLAITDPMIKIVLVKECYSVFTNRRPFGVGFMKSAI  
SIAEDEEWKRLRSLSPFTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSPGVNIDSLNPNQDPPFVENTKLLRDFD  
LDPFFLSITVFPFLIPILEVNIQVFPREVINFLRKSVMKESRLEDTQKHRVDFLQMLIDSQNSKETESHKALSDELVQAQSIIFAGYETTS
```

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

Preset	+ Add	☰	🔄
Polymer	4 reprs	👁	🗑
Ligand	Ball & Stick	👁	🗑
Water	Ball & Stick	👁	🗑

The bottom status bar shows the following log entries:

- 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

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

```
MLYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFCMECHKYKWKWGFYDGOQPVLAITDDPMIKIVLVKCYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLSPFTTSGKIKEMVPIIAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSFVNIIDSLNPDQDFVENTKGLLRDFD
LDPFFLSITVFFFLIPILEVLNICVFFPREVINFLRKSVMKRESLEDTQKHRVDFLQMLIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

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

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 with a green molecular surface 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 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 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 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 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 representation is a Gaussian Surface. The bottom of the interface displays a log of actions performed, such as creating the Gaussian Surface, Gaussian Volume, and Molecular Surface representations.

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

```
MALYGTSHSHGLFYKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVGWGFYDQQQVLAITDPDMIKTVLVKECVSVFTNRRPFGVGFMSAI  
SIAEDEEWKRLRSLLSPTFTSGKLEMPVILIAQYGDVLRNLRREAEITGKPVILKQVFGAYSMQVITSTSGVNIIDSLNPNQDFFVENTKLLRDF  
LDPFFLSITVFPFLIPILEVNLICVFPREVINFRLKSVKRMKESRLEDITQKHRVDFLQMLMIDSQNSKETESHKALSDELEVAQSIIFIFAGYETTSS
```

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

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`

```
MLYGTHTSHGLPKKLGIPGPTPLPFLGNILSYHKGFDMFDMCHKKYKWKWGFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFVGVGPKMSAI
122 132 142 152 162 172 182 192 202 212
SIAEDEEWKRLRSLSPFTTSGKLRKEMVPIIAQYGDVLRNLRREAETGKPVLRKDFGAYSDVITSTSEFVNIIDSLNPPQFPFVENTKLLRDF
222 232 242 252 262 272 282 292 302 312
LDPFFLSITVFFFLIPILEVLNLCVFPREVINFLRKSVKRMKESRLEDTQKHRVDFLQMLMDSQNSKETESHKALSDELVAQSIIIFAGYETTSS
222 232 242 252 262 272 282 292 302 312
```

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

- 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

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 1TQN. The central view shows the protein structure in green ribbon representation, with a red mesh representing the electron density map. 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
 - 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 HSHGLFKKLGIPGFTPLPFLGNILSYHKGF C MFDMECHKKYGKWWGFDGQQPVLAITD DPMIKITVLVKECYSVFTNRRPFGVGFMSAI  
123 132 142 152 162 172 182 192 202 212  
SIAEDEEMKRLRSLLSPTFTISGKLEKMFIIAQYGDVLRNLRREAETGKPVILKDVFGAYSM DVI TSTSFGVNI 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  
L D P F F L S I T V F P F L I P I L E V 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
```

Structure Tools Panel:

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

Activity Log:

- 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 a red electron density map. The left sidebar shows the 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 | 2 2 2

The right sidebar shows the Structure Tools panel with the following sections:

- 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
 - Enable
- Assembly Symmetry
 - Enable
- Export Animation

The bottom status bar shows the following actions:

- 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 electron density maps in red and blue. The interface is divided into several panels:

- State Tree (Left):** Lists the hierarchy of the model, including 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Cartoon, Ligand (49 elements), Water (190 elements), Volume Server 1tqn, Volume Streaming Selection, and Unit Cell (2 2 2).
- Sequence (Top):** Shows the amino acid sequence of the protein: `MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVGFGYDQQVLAITDDPMIKTVLVKECYSVFINRRPFGVGFMKSAI`
`SIAEDEENKRLRSLSPFTFTSGKLEKMPVPIIAQYGVLVLRNLRREAEATGKPVTLKQVFGAYSMQVITSTISFGVNIIDSLNPNQDPEFVENTKLLRDFD`
`LDPFFLSITVFPFLIPILEVNLICVFPREVINFLRKSVMKRESRLDTQKRVDFLQLMIDSONSKETE SHKALSDELVAQSIIFIFAGYETTSS`
- Structure Tools (Right):** Provides controls for the structure, including Type (Assembly), Asm Id (1: Author Defined Ass...), and Nothing Focused.
- Measurements (Right):** Includes an Add button and a list of components.
- Components (Right):** Lists the components of the structure: Polymer (Cartoon), Ligand (Ball & Stick), Water (Ball & Stick), and Unit Cell (2 2 2).
- Volume Streaming (Right):** Controls the electron density maps with sliders for 2Fo-Fc σ (1.5), Fo-Fc(+ve) σ (3), and Fo-Fc(-ve) σ (-3).
- Assembly Symmetry (Right):** Shows the symmetry of the assembly (1TQN).
- Log (Bottom):** Displays system messages: `15:24:41 Updated 1.5 σ [2fo-fc] in 1ms.`, `15:24:41 Updated 3 σ [fo-fc(+ve)] in 0ms.`, and `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 in various colors (red, green, blue). 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 different density maps.

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

MALYGTSHSGLFKGLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYKGVWGFYDGOQFVLAITDIPDMIKTVLVKECYSVFINRRPFGVGVGFMKSAI
SIAEDEENKRLRSLSPFTFTSGKLEMPVPIIAQYGDVLRNLRREAEATGKPVTLKDFVFGAYSMDEVITSTISFGVNIIDSLNPNQDFEVNTKLLRDFD
LDPFFLSITVFPFLIPILEVNLICVFPREVINFLRKSVMKRESRLDTQKRVDFLQLMIDSONSKETE 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

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFMFDMCECHKYKWKWGFYDQQPVLAIITDPMIKITVLVKECYSVFTNRRFPFGVGFMKSAI
SIAEDEEWKRLRSLSLSPFTSGKLEAVPIIAQYGVVLRNLRREAEITGKEVTLKQVFGAYSMDVITSTSFQVNISSLNPPQDFVENTKLLRDF
LDPFFLSITVFFFLIPILEVLNICVFFREVINFLRKSVKRMKESRLÉDTQKHRVDFLQMLIDSONSKETE SHKALSDELVAQSII FIFAGYETISS
```

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	<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 viewer interface. The central window shows a protein structure (1TQN) rendered in 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 of the interface shows the sequence of the protein: 1TQN | Crystal... 1: cytochrome... A. The sequence is: MALYGTSHSHGLFKLGI PGPTLP LFLGNILSYHKGFCMFDMECHKKYGKWWFYDQQQVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI SIAEDEENKRLRSLLSPTFTSGKLRKEMWPIIAQYGDVLRNLRREAETGKPVILKDVFGAYSMDEVITSTISFGVNISSLNPFQDFVENTKLLRDF LDPFFLSITVFPFLIPILEVLNICVFPREVINFLLRSVKRMKESRLEDTKQHRVDFLQMLIDSQNSKETESHKALSDELVAQSIIIFAGVETISS. The right sidebar contains 'Structure Tools' and a 'Properties' panel for the selected polymer. The 'Hydrophobicity' property is circled in red.

Properties panel (selected Polymer):

- Uncertainty/Disorder
- Chain Property
- Miscellaneous
- Residue Property
 - Accessible Surface Area
 - Hydrophobicity**
 - Molecule type
 - Residue Name
 - Secondary Structure
 - Sequence Id
- Symmetry
- Validation
- Cartoon Representation

Bottom status bar:

- 16:37:57 Updated Cartoon in 31ms.
- 16:38:35 Updated Cartoon in 8ms.
- 16:38:48 Updated Cartoon in 28ms.

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.

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

```
MALYGIHSHGLFKLGIIPGPTLPFLGNILSYHKGFCEMDECHKYGRWGFYDGGQPVLAITDPDMIKTVLVKECYSVETNRRPFGPVGFMKSAI  
SIAEDEEWKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVLVNLRRAEATGKPVTLKQVFGAYSMVDVITSTSGVNI 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 1TQN. The central 3D view shows the protein structure in a green cartoon representation, with red dots indicating specific residues. The top panel shows the amino acid sequence: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFQCFMDECHKKYGKWWGFYDQQPVLAITDPDMIKTVLVKECVSVFINRRPFGVGFMKSAI SIAEDEEWKRLRSLLSPTFTSGKLRKEMVPIIAQYGDVLRNLRREARETGKFTVLKDVFGAYSMDVITSTSTSGVNISSLNPNQDPPFVENTKLLRDFD LDPFFLSITVFFLIPLEVLNLCVFPREVINFLRKSVMKMKESRLEDTQKHRVDFIQLMIDSQNSKETESHKALSDEELVAQSIIIFFGYETTSS. The left sidebar shows a state tree with categories like Model 1, Assembly 1, Polymer, Ligand, and Water. The right sidebar contains structure tools and a components panel where 'Structure Quality Report' is highlighted with a red circle. A log at the bottom shows update times for the cartoon representation.

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

MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFQCFMDECHKKYGKWWGFYDQQPVLAITDPDMIKTVLVKECVSVFINRRPFGVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLRKEMVPIIAQYGDVLRNLRREARETGKFTVLKDVFGAYSMDVITSTSTSGVNISSLNPNQDPPFVENTKLLRDFD
LDPFFLSITVFFLIPLEVLNLCVFPREVINFLRKSVMKMKESRLEDTQKHRVDFIQLMIDSQNSKETESHKALSDEELVAQSIIIFFGYETTSS

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Ass...

Nothing Focused

Measurements

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* web viewer interface for the protein structure 1TQN. The central view shows a 3D ribbon representation of the protein, colored by quality. The interface includes a state tree on the left, a sequence viewer at the top, and a control panel on the right. A log at the bottom shows update times for the cartoon representation.

Sequence of 1TQN | Crystal...

```
MALYGTSHGFLFKLGI PGPTLPFLGNILSYHKGF C MFDMECHKKYGKWG F YDQQPVLAI TDPDMIKT VLVKECYSVPTNRRPFGVGF M KSAI  
SIAEDEWKRRLRSLLSPTFTSGKLEKMPV I IAQYGDVLRNLRREAETGKPVILKDVFGAYSM D VITSTSGVWNIDSLNPNQDFFVENTKLLRDFD  
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLAKSVKRMKRESRLDITQRHRVDFLQMLIDISQNSKETESHKALS DLELVAQSIIIFAGYETTSS
```

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	👁	🗑
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* web application interface for visualizing protein assemblies. The main window shows a 3D representation of a protein assembly, colored by residue type, with a semi-transparent Gaussian surface overlaid. The interface is divided into several panels:

- State Tree (Left):** A hierarchical view of the loaded models, including "3J3Q 1 model", "Model 1", "Assembly 1 2440800 elements", "Polymer 2440800 elements", and "Gaussian Surface".
- Sequence Viewer (Top):** Displays the amino acid sequence for the protein 3J3Q, with residue numbers 1 through 231 indicated above the sequence.
- Structure Tools (Right):** A control panel for the visualization, including sections for Structure, Measurements, Components, Volume Streaming, Assembly Symmetry, and Export Animation.
- Log (Bottom):** A timeline of recent actions, such as "Created Polymer in 110ms" and "Created Gaussian Surface in 4.661s".

Měření

The screenshot displays the Mol* web application interface. The browser address bar shows `molstar.org/viewer/`. The main window features a central 3D molecular model of a protein structure, rendered in green ball-and-stick representation. A specific distance of **2.92 Å** is highlighted between two atoms, indicated by a dashed line and a label. Above the model, the amino acid sequence is displayed with residue numbers 32 through 312. The left sidebar contains a 'State Tree' with a hierarchical view of the structure, including '1TQN 1 model', 'Model 1', 'Assembly 1 3999 elements', 'Polymer 3766 elements', 'Cartoon', 'Ligand 49 elements', 'Water 190 elements', 'Unit Cell 1 2 2 2', and 'Measurements'. The right sidebar, titled 'Structure Tools', includes sections for 'Structure', 'Measurements', 'Components', 'Volume Streaming', and 'Assembly Symmetry'. The 'Measurements' section shows a list of distances, with the selected one being '2.92 Å | HEM 508 — CYS ...'. The 'Components' section lists 'Polymer', 'Ligand', and 'Water'. The 'Volume Streaming' section is checked and set to '1TQN'. The 'Assembly Symmetry' section is also checked and set to '1TQN'. At the bottom of the interface, a log shows recent actions: 'Created Ball & Stick in 23ms.', 'Created Ball & Stick in 11ms.', and '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 as a green cartoon representation. The left sidebar (State Tree) lists the 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 sequence viewer shows the amino acid sequence: MALYGTGTHSHGLFKLGI... The right sidebar (Structure Tools) includes sections for Structure (1TQN | Crystal Structure of Human ...), Measurements (Add), Components (1TQN), and Polymer (Cartoon). The bottom status bar shows update logs for the cartoon representation.

Time	Action
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.

Přikládání struktur

The screenshot displays the Mol* Viewer interface. The main window shows a protein structure rendered in a green cartoon representation, with a purple ribbon structure overlaid. The structure is surrounded by red spheres representing water molecules. The interface includes a 'State Tree' on the left, a 'Sequence of' panel at the top, and a 'Structure Tools' panel on the right. The 'Structure Tools' panel has a red circle around the 'Superposition' icon. The 'Superposition' panel shows options for 'By Chains' and 'By Atoms'. The 'Components' panel shows a list of components: Polymer (Cartoon), Ligand (Ball & Stick), and Water (Ball & Stick). The 'Export Animation' panel is also visible.

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 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 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 V 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 with the following components:

- State Tree (Left):** A hierarchical tree showing the loaded 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. A second structure, 2RFC 1 model, is also visible with its own 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 for Cytochrome c (1: Cytochrome...). The sequence is: TTETIQSNANLÄPLPPHVEHLVDFDMYNFNSNLGAVQEAHVAVLQESNVFDLWTRCNGGHWIATRGQLIREAYEDYRHSSECFPIPREAGEAYD... (with residue numbers 1-104 indicated).
- Toolbar (Top Center):** A toolbar with various icons. The 'Residue' button, which is circled in red, is used to focus on a specific residue in the structure.
- 3D View (Center):** A 3D representation of the protein structure in cartoon mode, colored in shades of green and purple. A small 3D coordinate system is visible at the bottom left of the view.
- Structure Tools Panel (Right):** A panel with sections for Structure (2 structures), Measurements (Add), Superposition (By Chains, By Atoms), Components (2 structures), and Export Animation.
- Log (Bottom):** A log showing recent actions: 'Created Ball & Stick in 18ms.', 'Created Ball & Stick in 4ms.', and 'Updated Structure Focus Representation in 2ms.'

Příkládání struktur

The screenshot displays the Mol* web application interface. The main window shows a protein structure (Cytochrome) with a sequence of 281 amino acids. The structure is rendered in a cartoon style, with green and purple ribbons. A context menu is open over the structure, listing various selection options, with "Structure Property" highlighted in red. The left sidebar shows a "State Tree" with a hierarchical view of the structure, including models, assemblies, polymers, and ligands. The right sidebar contains "Structure Tools" and "Components" panels. The "Components" panel shows a list of components: Polymer (Cartoon), Ligand (Ball & Stick), Water (Ball & Stick), and 2 Unit Cells. The bottom status bar shows a log of recent actions.

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

```
TTETIQSNANLAPLPPHVPHEHLVDFDFMYNPSNLSAGVQEAWAVLQESNVFDLWVTRCGNGGHWIATRGQLIREAYEDYRHFSSSECFIPREAGEAYD
FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRAPOGQCNTEDYAEPPPIRIFMLLAGLPEEDIIPHLKYLTDQMTRPDGSMITFA
EAKAELYDYLIPITIEQRQKPGTDAISIVANGQVNGRPIITSDAKRMCGALLVGGDLTVVNFSLFSMEFLAKSPEHRQELIERPERIPRACEELLR
```

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

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.

Příkladání 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 top of the interface shows the sequence of the protein: `TTEIIQSNANLAPLPPHVEHLVDFDMYNFNSNLGAVQEAVALQESNVDPDLVWTRCNGGHWIATRGQLIREAYEDYRHFSSSECFPIPREAGEAYD`. The left sidebar contains a 'State Tree' with a hierarchical view of the structure, including '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', and 'Unit Cell P 1 21 1'. The right sidebar contains 'Structure Tools', 'Structure' (2 structures), 'Measurements', 'Superposition', 'Components' (2 structures), and 'Export Animation'. 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.'

Příkladání struktur

The screenshot displays the Mol* Viewer interface. On the left, the State Tree shows a hierarchy of models and assemblies. The main view shows a protein structure in green cartoon representation. The top panel displays the sequence of the protein, with residues 1-281 highlighted in green. The right panel, Structure Tools, includes sections for Structure, Measurements, Superposition, and Components. The 'Superposition' section is highlighted with a red circle, showing 'By Chains' selected. The 'Components' section shows 2 structures: Polymer (Cartoon), Ligand (Ball & Stick), and Water (Ball & Stick). The bottom panel shows a log of actions performed, such as 'Created Ball & Stick in 18ms' and 'Updated Structure Focus Representation in 2ms'.

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

TTETIQSN¹¹NL²¹AP³¹PPH⁴¹VE⁵¹RL⁶¹VD⁷¹FD⁸¹MY⁹¹N¹⁰¹PS¹¹¹N¹²¹LS¹³¹AG¹⁴¹VO¹⁵¹EA¹⁶¹VL¹⁷¹Q¹⁸¹SN¹⁹¹VD²⁰¹L²¹¹W²²¹TR²³¹C²⁴¹NG²⁵¹GH²⁶¹WI²⁷¹AT²⁸¹RG²⁹¹LI³⁰¹RE³¹¹AY³²¹ED³³¹Y³⁴¹R³⁵¹HF³⁶¹SS³⁷¹EC³⁸¹PF³⁹¹IP⁴⁰¹RE⁴¹¹AGE⁴²¹AY⁴³¹D⁴⁴¹
F⁴⁵¹IP⁴⁶¹TS⁴⁷¹MD⁴⁸¹PP⁴⁹¹EQ⁵⁰¹Q⁵¹¹FR⁵²¹AL⁵³¹AN⁵⁴¹Q⁵⁵¹V⁵⁶¹GM⁵⁷¹F⁵⁸¹V⁵⁹¹VD⁶⁰¹K⁶¹¹LEN⁶²¹R⁶³¹I⁶⁴¹Q⁶⁵¹EL⁶⁶¹AC⁶⁷¹SL⁶⁸¹IE⁶⁹¹SL⁷⁰¹AP⁷¹¹Q⁷²¹G⁷³¹QC⁷⁴¹N⁷⁵¹F⁷⁶¹TE⁷⁷¹D⁷⁸¹Y⁷⁹¹AE⁸⁰¹PP⁸¹¹PI⁸²¹RI⁸³¹EM⁸⁴¹LL⁸⁵¹AG⁸⁶¹LP⁸⁷¹EE⁸⁸¹DI⁸⁹¹SH⁹⁰¹L⁹¹¹K⁹²¹YL⁹³¹TD⁹⁴¹Q⁹⁵¹MT⁹⁶¹RP⁹⁷¹D⁹⁸¹G⁹⁹¹SM¹⁰⁰¹TE¹⁰¹¹
E¹⁰²¹AK¹⁰³¹E¹⁰⁴¹AL¹⁰⁵¹Y¹⁰⁶¹D¹⁰⁷¹YL¹⁰⁸¹IL¹⁰⁹¹FI¹¹⁰¹TE¹¹¹¹QR¹¹²¹R¹¹³¹K¹¹⁴¹PG¹¹⁵¹TD¹¹⁶¹AI¹¹⁷¹SI¹¹⁸¹V¹¹⁹¹AN¹²⁰¹Q¹²¹¹V¹²²¹NG¹²³¹R¹²⁴¹PI¹²⁵¹TS¹²⁶¹DE¹²⁷¹AK¹²⁸¹RM¹²⁹¹CG¹³⁰¹AL¹³¹¹LV¹³²¹GG¹³³¹LD¹³⁴¹IV¹³⁵¹N¹³⁶¹FL¹³⁷¹S¹³⁸¹F¹³⁹¹S¹⁴⁰¹ME¹⁴¹¹FL¹⁴²¹AK¹⁴³¹SP¹⁴⁴¹EH¹⁴⁵¹R¹⁴⁶¹Q¹⁴⁷¹EL¹⁴⁸¹IE¹⁴⁹¹R¹⁵⁰¹PER¹⁵¹¹I¹⁵²¹PA¹⁵³¹ACE¹⁵⁴¹ELL¹⁵⁵¹LR¹⁵⁶¹

Residue

Structure Tools

Structure

2 structures

Nothing Focused

43 Residues + 2802 Elements Selected

Measurements

+ Add

Superposition

By Chains (highlighted)

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* 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 protein sequence for Cytochrome... with residues 11-291 highlighted in green. The sequence is: TTETIQSN...NLAPLPPHVP...EHLVDFD...MYPNSL...SAGVQ...EAWVLG...ESNV...DLVW...TRCNG...SHWI...ATRG...QLREAY...EDYR...HFS...ECP...FPI...REAGEAY...
FIF...TSM...DP...PE...QR...FR...AL...AN...QV...VG...MP...V...VD...K...LEN...RI...Q...E...L...A...G...S...L...I...E...S...L...R...P...Q...G...C...N...F...T...E...D...Y...A...E...P...F...I...R...A...P...M...L...L...A...G...L...P...E...E...D...I...P...H...K...Y...L...T...D...Q...M...I...R...P...D...G...S...M...I...F...
E...K...E...A...L...Y...D...Y...L...I...P...I...T...E...O...R...R...O...K...P...G...I...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...I...V...N...F...L...S...F...S...M...E...E...F...L...A...K...S...P...E...H...R...O...E...L...I...E...R...P...E...I...P...A...C...E...L...L...E...R...

The Structure Tools panel on the right includes the following sections:

- Structure:** 2 structures, Nothing Focused, 43 Residues + 2802 Elements Selected.
- Measurements:** + Add.
- Superposition:** By Chains, By Atoms, 25 Residues + 1521 Elements | A | 2H7S, 18 Residues + 1281 Elements | A | 2RFC. The **Superpose** button is highlighted with a red circle.
- Components:** 2 structures, Preset, + Add. Components include Polymer (Cartoon), Ligand (Ball & Stick), Water (Ball & Stick), and 2 Unit Cells.
- Export Animation:**

The bottom status bar shows the following log entries:

- 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* web interface for protein structure visualization. The main window shows a 3D ribbon representation of a protein structure in green, with a blue ligand molecule bound in the center. The interface is divided into several panels:

- State Tree (Left):** A hierarchical tree view showing the loaded structures: 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, and Unit Cell P 1 21 1.
- Sequence (Top):** A sequence viewer for Cytochrome... (A) showing the amino acid sequence with residue numbers. The sequence is: TTETIQSN... NIAPLPPHVP... FDFDMYNP... SAGVQEA... AVLQESN... VPDVWTRC... NGGHWIAT... RQGDI... REAYEDY... RHPSS... ECPPI... PR... EAGEAY... IIP... TSM... DP... PE... QR... QF... RALAN... QV... GMP... VVD... KLEN... RI... QEL... ACS... LIE... SL... RP... Q... C... NF... TED... YAE... P... F... P... I... R... I... E... M... L... LAG... LP... E... DI... P... H... L... K... V... L... D... Q... M... TR... PD... GS... M... TE... A... E... A... ME... AL... Y... DV... LI... PI... IE... QR... R... K... PG... TD... AI... SI... V... AN... G... V... NG... R... PI... TS... DE... AK... R... M... CG... ALL... V... GG... LD... TV... V... N... FL... S... F... S... ME... FL... AK... S... PE... H... Q... EL... I... ER... PE... RI... PA... ACE... ELL... RR... Residue numbers are indicated below the sequence.
- Structure Tools (Right):** A panel for managing the loaded structures. It shows 2 structures: 2H7S (25 Residues + 1521 Elements) and 2RFC (18 Residues + 1281 Elements). It includes options for Superposition (By Chains, By Atoms), Components (Polymer, Ligand, Water), and Export Animation.
- Log (Bottom):** A log of recent actions: 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.

Příkladání struktur

The screenshot displays the Mol* Viewer interface. The main window shows a protein structure (Cytochrome P450-cam) rendered in a ribbon representation, colored in shades of green and purple. The structure is superposed with another structure (2RFC). The left sidebar contains a 'State Tree' with a hierarchical view of the loaded structures, including 2H7S and 2RFC models and their respective assemblies and polymers. The top of the interface shows the sequence of the protein: 'Sequence of 2H7S | L244A ... 1: Cytochrome... A'. The right sidebar contains the 'Structure Tools' panel, which includes options for 'Structure', 'Measurements', 'Superposition', and 'Components'. The 'Superposition' section is currently active, showing options for 'By Chains' and 'By Atoms'. The 'Components' section shows the current structure is a 'Polymer' rendered as a 'Cartoon'. The bottom status bar shows the current view: '21:41:35 Updated Ball & Stick in 2ms.' and '21:41:35 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

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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](#)

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Přikládání struktur – PDB a AlphaFold

Pairwise Structure Alignment

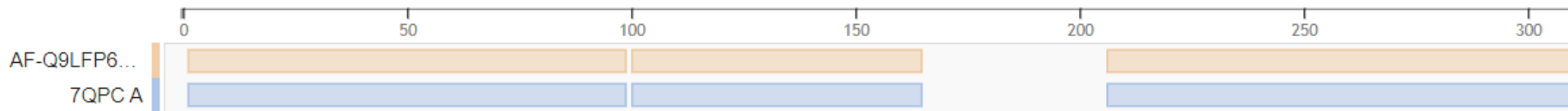
[Help](#)

▸ 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

