



CEITEC



Central European Institute of Technology
BRNO | CZECH REPUBLIC

Vizualizace proteinů a ligandů



EUROPEAN UNION
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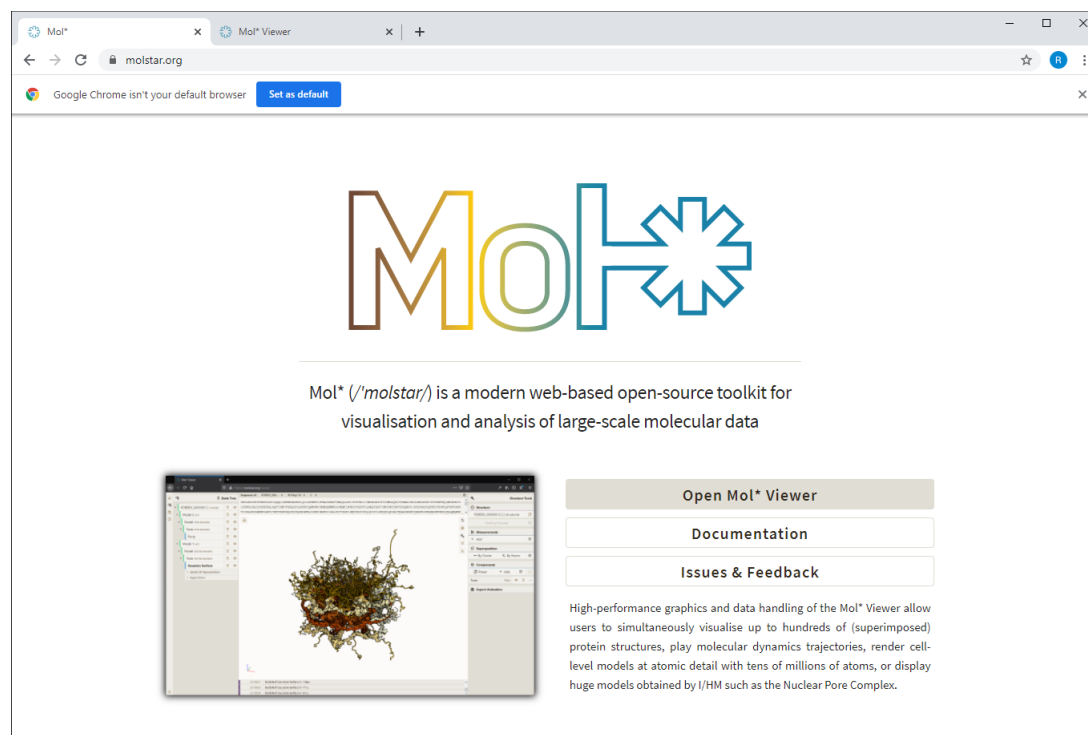


OP Research and
Development for Innovation



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'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**: A section with a table for inputting PDB information. The table has columns for "Source" (set to "PDB") and "PDB Id(s)" (set to "1tqn"). Below the table is an "Options" section and a green "Apply" button, which is circled in red in the image.
- 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) and a status bar showing the time "14:28:23" and the version "Mol* Plugin 1.2.7 [12/19/2020, 11:52:32 AM]".

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

- Structure**: Currently 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 MolStar logo is visible in the bottom right corner of the main content 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 backbone in a green cartoon representation, with red spheres representing water molecules. 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 view shows a 3D representation of the protein structure as a green cartoon with red dots representing atoms. 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 'Ball & Stick' representation selected for the polymer component.

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...:

```
MLALYGTSHSHGLFKKLGIPGPTLPLPFLGNILSYHKGFDMCECHKKYGKWNWGFYDGOQVLAITDPPMIKIVLVKECYSVFINRRPFGVGFMKSAI  
SIAEDEEWKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVIVRNLRREARETGKQVTLKDVFGAYSMDVITTSISFGVNIDSLNPFQDPFVENTKGLLRDFD  
LDPFFLSITVFPFLIPFILEVLNICVFRREVINFLRKSVKRMKESRLDTPKQHRVDFLQMLMDSQNSKETESHKALSDELVAQSIIFIPAGYETTSS
```

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
 - Ball & Stick (selected)
 - 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

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 souřadic molekuly

Vizualizační model Ball & Stick

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

```
MALYGTSHGGLFKLGI PGPTPLPFLGNILSYHKGFDMFMECHKYKGVWGFYDQQPVLAITDPDMIKTVLVKECYSVPTNRRPFGVGFYKSR I  
SIAEDEEWKRLASLLSPTFTSGKLEKMPV IIAQYGDVLVRLNRREAEETGKPVTLKDVFGAYSMDVITSTSGVNIIDSLNPNQDFFVENTKLLRDF  
LDPFFLSIVFPFLIPFILEVNI CVPREVINFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSONSKETESHKALSDELVAQSIIPFAGYETTS
```

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 structure 1TQN. The central 3D view shows the protein backbone as a green line with red and blue atoms. 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: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKWWGFYDQQPVLAITDPDMIKTVLVKECYSVFINRRPFGVGFMKSAI... The right panel (Structure Tools) shows the structure name, type (Assembly), and various tool options like Measurements, Components, Volume Streaming, and Assembly Symmetry. A log at the bottom indicates 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 right panel shows the Sequence of 1TQN | Crystal... with the following amino acid sequence:

```
MALYGTHTSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYKRWGFDYDQQPVLAITDPMIKIVLVKECYSVFTNRRPFGVGFMKSAI  
SIAEDEEWKRLRSLSPFTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVTLKDVFGAYSMDVITSTSPGVNIDSLNPNQDPPFVENTKLLRDFD  
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLRKSVMKESRLEDTQKHRVDFLQMLIDSONSKETESHKALSDELVAQSIIIFAGYETTSS
```

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

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

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 1 2 2 2

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

```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKKYGKWFYDGOQPVLAITDPMIKIVLVKCYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLSPFTTSGKIKEMVPIIAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSGVNIIDSLNPNQDPEVENTKGLLRDFD
LDPFFLSITVFFFLIPILEVLNLCVFFPREVINFLRKSVMKRESLEDTQKHRVDFLQMLIDSONSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

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 1 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 window shows a 3D molecular surface model of a protein, colored in a vibrant green. The surface is highly detailed, showing the complex folds and pockets of the protein. The background is a light gray, and the interface includes various toolbars and panels.

State Tree (Left Panel):

- 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

Sequence (Top Center):

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

```
MALYGTHTSHGLFKKLSIPGPTLPFLGNILSYHKGFDMFMECHHKYKQWGFYDSQQVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFMSAI  
SIAEDEEWKRLRSLLSPTFTSGKLEKMPVIAQYGDVLRNLRREAEATGKPFVILKDFVFGAYSMQVITSTSGVGNIDSLNPPQDFVENTKLLRDF  
LDPFFLSITVFPFLIPILEVLNICVFPREVINFRLKRSVKRMKESRLEDTQKHRVDFLQLMIDSSQNSKETESHKALSDELVAQSIIFIFAGYETISS
```

Structure Tools (Right Panel):

- 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

Log (Bottom):

- 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 viewer at the top, and a Structure Tools panel on the right. The State Tree shows the hierarchy of the model, including the protein assembly, polymer, and various representations. The Structure Tools panel provides options for different representations and measurements.

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 2

Sequence of 1TQN | Crystal...

```
MALYGTSHSLFKLGI PGP TLPFLGNILSYHKGF CMFDM ECHKKYKGVNGFYD GQQVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI  
SIAEDEEWKRLRSLLSPTFTSGKLEMPV IIAQYGDVLRNLRREAE T GKFVTLKQVFGAYSMOVITSTSFGVNI D SLNNPQD SFVENTKLLRDF  
LDPFFLSITVFPFLIPILEV LNICVFPREVINFLRKS VKRMKESRLEDTQKHRVDFLQLMID SQNSKETESHKALS DLELVAQSIIFIFAGYEITSS
```

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

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

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

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central view shows the protein as green ribbons with red dots representing electron density. The left sidebar shows the State Tree with the following components:

- 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: MALYGT HSHGLFKKLGIPGFTL PFLGNILSYHKGFCMPDMECHKKYGKWWGFDGQQPVLAITDPDMIKTVLVEKCYSVFTNRRPFGVGFMSAI SIAEDEEWKRLRSLLSPTFTISGKLEKMFIIAQYGDVLRNLRREAEATGKPVILKDFGAYSMQVITSTSGVNDISLNNPQDPFVENTKLLRDFD LDPFFLSITIVFFLIPILEVLNLCVFPREVINF LRKSVKRMKESRLEDIQGRVDFLQLMIDSQNSKETESHKALSDELVAQSIIFIFAGYETTSS

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 (visible)
 - Ligand: Ball & Stick (visible)
 - Water: Ball & Stick (visible)
 - Unit Cell 1 2 2 2 (hidden)
- Volume Streaming
 - 1TQN
 - Enable (checked)
- Assembly Symmetry
 - 1TQN
 - Enable (checked)
- 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 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 1 2 2 2

The top panel shows the sequence of 1TQN | Crystal... | 1: cytochrome... | A. The sequence is: MALYGT HSHGLFKKLGIPGFTPLPFLGNILSYHKGF C MFDMECHKKYGKWWGFDGQQPVLAITD PDMIKITLVKECYSVFTNRRRPF GFGVGMKSAI SIAEDEEWKRLRSLLSPTFTSGKLEKMPV IIAQYGDVLRNLRREAEATGKPVILKDVFGAYSM DVIITSTSFGVNI D S L N N P 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 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

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 (visible)
 - Ligand: Ball & Stick (visible)
 - Water: Ball & Stick (visible)
 - Unit Cell 1 2 2 2
- Volume Streaming: 1TQN
 - Enable
- Assembly Symmetry: 1TQN
 - 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 red dots representing electron density. 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
 - Volume Server 1tqn
 - Volume Streaming Selec...
 - Unit Cell | 2 2 2

The top of the interface shows the sequence of the protein:

```
Sequence of 1TQN | Crystal... 1: cytochrome... A
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFDMCHKKYKGVWGFYDQQQVLAITDPDMIKIVLVKECYSVFINRRPFGVGFVGMKSAI
SIAEDEENKRLRSLSPFTFTSGKLEKEMVPIIAQYGVVLRNLRREAEATGKPVILKDFVFGAYSMDVITSTISFGVNIIDSLNPNQDFPVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNLCVFPREVINFRLKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDELEVAQSIIFIFAGYETTSS
```

The right sidebar contains the Structure Tools panel, which includes 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 (visible)
 - Ligand: Ball & Stick (visible)
 - Water: Ball & Stick (visible)
 - 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
- 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 left sidebar with a State Tree, a top navigation bar, and a right sidebar with Structure Tools and a detailed view of the selected structure.

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

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHGKFCMFDMECHKKYKQWGFYDQQPVLAITDPDMIKIVLKECYSVFINRRPFGVGFVGMKSAI
122 132 142 152 162 172 182 192 202 212
SIAEDEENKRLRSLSPFTFTSGKLKEMVPIIAQYGVLVLRNLRREAETGKPVILKDFVFGAYSMDVITSTISFGVNIIDSLNNPQDFVENTKLLRDFD
222 232 242 252 262 272 282 292 302 312
LDPFFLSITVFPFLIPILEVLNLCVFPREVINFLRKSVMKRESRLDITQKHRVDFLQLMIDSQNSKETESHKALSDELELVAQSIIFIFAGYETTSS
222 232 242 252 262 272 282 292 302 312
```

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

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKYKWKWGFYDQQPVLAITDPDMIKTVLVEKCYSVFTNRRPFGVGFPMKSAI
SIAEDEEWKRLRSLSLSPFTTSGKLEKLVPIIAQYGVVLRNLRREARETGKQVTLKQVFGAYSMQVITSTSFQVNISSLNPPQDFVENTKLLRDF
LDPFFLSITVFFFLIPILEVLNLCVFFREVINFLRKSVKRMKESRLLEDTQKHRVDFLQMLIDSONSKETESHKALSDELVAQSIIIFIFAGYETISS
```

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 for the protein structure 1TQN. The central view shows the protein in a green cartoon representation, with red dots indicating specific residues. The interface is divided into several panels:

- State Tree (Left):** A hierarchical tree showing the structure components: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Cartoon, Ligand (49 elements), Water (190 elements), and Unit Cell (2 2 2).
- Sequence Viewer (Top):** Shows 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 'Components' section is expanded to show the 'Hydrophobicity' property, which is circled in red.
- Log (Bottom):** A log of recent actions, such as 'Updated Cartoon in 31ms'.

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 and white spheres.

State Tree (Left Panel):

- 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... (Top Panel):

```
MALYGIHSHGLFKKLGIPGPTLPFLGNILSYHKGFCEMFKKYGKVGFDGQPVLAITDPDMIKITVLVKECYSVETNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLSPFTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVITLQVFGAYSMDVITSTISFGVNI DLSLNNPQDPFVENTKLLRFD
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLLRKSVMKESRLEDYQKHRVDFLQLMIDSQNSKETE SHKALSDELVQAQSIITPFGYVETTS
```

Structure Tools (Right Panel):

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

Log (Bottom Panel):

- 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 several panels:

- State Tree:** A hierarchical tree on the left 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:** A sequence viewer at the top showing the amino acid sequence of 1TQN: MALYGTSHSHGLFKKLGIPGPTLPFLGNILSYHKGFCMFDMECHKRYGKVGWGYDQQVLAITDPDMIKTVLVKECYSVFINRRPFGVGVGFMKSAI... (with residue numbers 32, 42, 52, 62, 72, 82, 92, 102, 112).
- Structure Tools:** A panel on the right with tabs for Structure, Measurements, and Components. The Structure tab is active, showing details for 1TQN | Crystal Structure of Human ...
- Components:** A list of components for 1TQN, including Polymer, Cartoon, and Unit Cell. The Polymer component is expanded to show various properties, with "Structure Quality Report" circled in red.
- Log:** A log at the bottom showing recent updates: "Updated Cartoon in 557ms.", "Updated Cartoon in 9ms.", and "Updated Cartoon in 11ms."

Vizualizace anotací

Obarvení podle vlastností - kvalita

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central 3D view shows the protein as a ribbon, colored by quality, with a color gradient from green (high quality) to red (low quality). 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... A

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMCHKKYKGVWGFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFMKSAI
SIAEDEWKRRLRSLLSPTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVILKDVFGAYSMVDVITSTSGVNIIDSLNNPQDFFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLAKSVKRMKRESRLDTQKRHVDVFLQMLMIDSQNSKETESHKALSDELVAQSIIIFAGYETTSS
```

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

Log:

- 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 browser address bar shows `molstar.org/viewer/`. The main window contains several panels:

- State Tree (Left):** A hierarchical tree showing the loaded data: `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 BIVNLOGQMVHQAI SPRTLNANVVKVVEEKAFSPVEIPMFSALSSEGATPODLNTMLNTVGGHQAAQMQLKETINEEAAEWDRLHPVHAGPIEPGQMR
EPRGSDIAGTTSTLQEQIGWMTNHPPIPVGGEIYKRWII LGLNKKIVMYSPTSIDIRQGPKEPFRDYVDRFYKTLRAEQASQEVKQWMMTETLLVQNA
NPDCKTILKALGPAATLEEMMTACQGVGGPGHKARVL`
- 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` (3J3Q | Atomic-level structure of the ...), `Measurements` (Add), `Components` (3J3Q), `Volume Streaming` (3J3Q, Enable), and `Assembly Symmetry` (3J3Q, Enable).
- Log (Bottom):** A list of recent 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* Viewer interface for a protein structure. The central view shows a green ball-and-stick model of a protein chain. 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 sequence of the protein: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKWWGFYDGOQFVLAITDPMIKTVLVKECVSVFTNRRPFGVPGFMKSAI SIAEDEENKRLRSLLSPTFTSGKLEMPVPIIAQYGDVLRNLRREAEETGKPEVTLKDVFGAYSMDVITSTSGVNIIDSLNPNQDPPEVENTKKLLRDFD LDPFFLSITVFPFLIPILEVLNICVFPREVTFNLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS. 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, Unit Cell (2 2 2), and Measurements (Distance 2 source(s), 49 elements). The right sidebar shows Structure Tools, 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), and Export Animation.

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

MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKWWGFYDGOQFVLAITDPMIKTVLVKECVSVFTNRRPFGVPGFMKSAI
SIAEDEENKRLRSLLSPTFTSGKLEMPVPIIAQYGDVLRNLRREAEETGKPEVTLKDVFGAYSMDVITSTSGVNIIDSLNPNQDPPEVENTKKLLRDFD
LDPFFLSITVFPFLIPILEVLNICVFPREVTFNLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS

2.92 Å

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 structure 1TQN. The central view shows the protein in a green cartoon representation, with a color scale at the bottom left indicating hydrophobicity. The State Tree on the left lists the following components:

- 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 Sequence of 1TQN | Crystal... is shown as:

```
MALYGTSHSHGLFKLGI PGPTLPFLGNILSYHKGFCMFDMECHKKYGKVGWGFYDQQVLAITDPMIKTVLWKECVSVFTNRRPFGVGFMSAI  
SIAEDEEWKRLRSLLSPTFTSGKLEKMPVILIAQYGDVLRNLRRAEATGKPVILKDFGAYSMQVITSTSGVWNISSLNPPQDFVENTKLLRDF  
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLRKSVMKRESLEDTQKRRVDFLQMLIDQNSKETE SHKALSDELEVAQSIIFIFAGYEITTS
```

The Structure Tools panel on the right shows the following settings:

- 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

The bottom status bar 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.

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.

Příkladání struktur

The screenshot displays the Mol* Viewer interface. The central window shows a 3D ribbon representation of a protein structure, colored in shades of green and purple, with a central ligand and water molecules. The left sidebar contains a 'State Tree' listing various components: 2H7S 1 model (Model 1, Assembly 1 with 3355 elements, Polymer with 3201 elements, Cartoon, Ligand with 49 elements, Water with 111 elements, 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, Water with 5 elements, Unit Cell P 1 21 1). The top right panel shows the 'Structure Tools' menu with options like Structure, Measurements, Superposition, and Components. The 'Superposition' option is highlighted with a red circle. 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* web application interface. The browser address bar shows `molstar.org/viewer/`. The main window is divided into several panels:

- Left Panel (State Tree):** 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 water molecules, along with unit cell information.
- Top Panel (Sequence):** Displays the amino acid sequence of the protein, with residue numbers and corresponding letters (e.g., 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 F S N L S A G V Q E A M A V L Q E S N V F 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).
- Top Center Panel (Toolbar):** A set of interactive tools for the 3D view, including buttons for 'Residue', 'Ball & Stick', 'Cartoon', 'Ribbon', 'Surface', 'Focus', 'Zoom', and 'Reset'. The 'Residue' button is highlighted with a red circle.
- Right Panel (Structure Tools):** A sidebar with various tool categories: Structure (2 structures), Measurements (Add), Superposition (By Chains, By Atoms), Components (2 structures), and Export Animation.
- Bottom Panel (Status Bar):** A log of recent actions, such as 'Created Ball & Stick in 18ms' and 'Updated Structure Focus Representation in 2ms'.

Příkládání struktur

The screenshot displays the Mol* web application interface. The main window shows a protein structure visualization of Cytochrome c (1: Cytochrome...) with a sequence viewer at the top. The left sidebar contains a 'State Tree' with a hierarchical view of the structure, including models, assemblies, polymers, and ligands. A context menu is open over the structure, listing various selection options. The 'Structure Property' option is highlighted with a red circle. The right sidebar contains 'Structure Tools' and a 'Structure' panel showing 2 structures. The bottom status bar displays recent actions.

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

```
TTETIQSNANLAPLPPHVPEHLVDFDMYNFSNLSAGVQEAWAVLQESNVFDLWVTRCNGGHWIATRQQLIREAYEDYRHFSSSECFIPREAGEAYD
FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRAPOGQCNTEDYAEPPPIRIFMLLAGLFEEDIPHLKYLTDQMTRPDGSMIFA
EAKEALDYLIPIIEQRQKPGTDAISIVANGQVNGRPITSDAQRKMGALLVGGLDIVVNFSLFSMEFLAKSPEHRQELIERPERIPACEELLRR
```

Residue [Icons]

Add/Union Selection X

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

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. The top navigation bar shows three tabs for 'Mol*' and 'Mol* Viewer'. The address bar indicates the URL 'molstar.org/viewer/'. The main window is divided into several panels:

- State Tree (Left):** A hierarchical tree view of the loaded structure. It includes entries for '2H7S 1 model', 'Model 1', 'Assembly 1 3355 elements', 'Polymer 3201 elements' (with sub-entries for 'Cartoon' and 'Ball & Stick'), 'Ligand 49 elements' (with sub-entries for 'Ball & Stick'), 'Water 111 elements' (with sub-entries for 'Ball & Stick'), 'Unit Cell P 1 21 1', '2RFC 1 model', 'Model 1', 'Assembly 1 2811 elements', 'Polymer 2752 elements' (with sub-entries for 'Cartoon', 'Ligand 60 elements', and 'Water 5 elements'), and another 'Unit Cell P 1 21 1'.
- Sequence of 2H7S | L244A ... (Top):** A protein sequence viewer showing the amino acid sequence: `TTETIQSNANLAPLPHPVHEHLVDFDMYNFNSLSAGVQEAWAVLQESNVFDLWVTRCNGGHWIATRGQLIREAYEDYRHFSSSECFPIPREAGEAYD` (truncated). Residue numbers are indicated above the sequence.
- Structure (Center):** A 3D ribbon representation of the protein structure, colored in shades of green and purple. A context menu is open over the structure, listing selection options. The 'Backbone' option is circled in red.
- Structure Tools (Right):** A panel with various tool icons for structure manipulation.
- Measurements (Right):** A panel with a '+ Add' button.
- Superposition (Right):** A panel with options for 'By Chains' and 'By Atoms'.
- Components (Right):** A panel showing a list of components: 'Polymer' (Cartoon), 'Ligand' (Ball & Stick), and 'Water' (Ball & Stick). It also shows '2 Unit Cells'.
- Export Animation (Right):** A panel with an 'Export Animation' button.
- Log (Bottom):** A log window showing recent 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 with the following components:

- State Tree (Left):** A hierarchical tree showing the loaded structure. It includes models for 2H7S and 2RFC, each with an assembly, polymer, ligand, and water components, and unit cells.
- Sequence Viewer (Top):** Shows the amino acid sequence of Cytochrome P-450 2H7S. A segment of the sequence is highlighted in green: `TTETIQSNALAPLPPHVFHILVDFDMYNFNSLSAGVQEAVALQESNVPDLVWTRCNGGHWIATRGQLIREAYEDYRHFSSSECPFIPREAGEAYLFIETSMQPPPEQRFPRALANQVVGMPVVDKLENRIQELACSLIESLNPPQQCNFTEDYAEPPFIRIFMLLAGLPEEDIPHLKYLTDQMTIRPDGSMIFEAKEALYDYLFIITEQRRCRPGIDALSIVANGQVNGRPITSDAKPMCGALLVGGLDIVVNFLSFSMEFLAKSFEHRQELIETPERIPACEELLER`
- Structure Tools (Right):** A panel with various options for interacting with the structure. The 'Superposition' section has the 'By Chains' option selected and highlighted with a red circle.
- Structure (Center):** A 3D representation of the protein structure in green cartoon style, with a blue ligand and red water molecules.
- Log (Bottom):** A log of recent actions, such as 'Created Ball & Stick in 18ms' and 'Updated Structure Focus Representation in 2ms'.

Příkladání struktur

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

```

TTETIQSN11...21...31...41...51...61...71...81...91
NLAPLPPHVPEHLVDFDMY101NF111S121N131L141S151AGVQEAMAVLQESN161VDLW171TRC181NG191GH201IA211TR221Q231L241REAYED251VR261FS271SEC281PF291I301PREAGEAY311
EIT321F331SM341DP351PE361Q371R381Q391F401ALAN411Q421V431GV441WG451F461V471V481DK491LEN501RI511Q521EL531AC541SL551IES561L571R581F591GG601QN611F621ED631Y641AE651PP661IR671IP681ML691L701AG711L721PE731DI741PH751L761K771YL781TD791OM801IR811PD821GS831M841TF851
ENPEAL861Y871VD881YL891PI901TE911QR921R931Q941PG951TD961ALS971IV981ANG991Q1001V1011NR1021P1031ITS1041DEAK1051RM1061CG1071ALL1081V1091GG1101LD1111V1121V1131N1141FL1151S1161F1171S1181M1191E1201F1211L1221AK1231S1241PE1251H1261R1271Q1281EL1291I1301ER1311PER1321I1331PAACE1341ELL1351EE1361

```

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

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.

Structure Tools

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

Superpose

Components 2 structures

Preset	Add	Close	Delete
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 in green cartoon representation with a blue ligand. 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 the superposition of two structures with an RMSD of 4.53.

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 [T...]
 - Polymer 2752 elements
 - Cartoon
 - Ligand 60 elements
 - Ball & Stick
 - Water 5 elements
 - Ball & Stick
 - Unit Cell P 1 21 1

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 N 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 L A G E A N Y 81  
101 F I F T S M D P P E Q R Q P A L A N Q V 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 151  
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 251
```

Structure Tools:

- 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
- Superpose
- Components: 2 structures
- Presets: + Add
- Polymer: Cartoon
- Ligand: Ball & Stick
- Water: Ball & Stick
- 2 Unit Cells
- Export Animation

Log:

- 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.

Přikládání struktur

The screenshot displays the Mol* web interface for a protein structure. The main view shows a ribbon representation of the protein in green and purple, with a sequence viewer at the top. The sequence viewer shows the amino acid sequence: `TTETIQSNANLAPLPPHVPHEHLVDFDMYNFNSLSAGVQEAQAVLQESNVDFLWVTRCNGGHWIATRGQLIREAYEDYRHFSSSECFPIPREAGEAYD` (residues 1-100) and `FIPTSMDFPEQRFALANQVWGMFVVDKLENRIQELACSLIESLRPQGCNFTEDYAEFPPIRIFMLLAGLPEDIPHLKYLTDQMTRPDGSMTFA` (residues 101-200). The structure is shown in a ribbon representation, with the main chain in green and the side chains in purple. The interface includes a state tree on the left, a structure tools panel on the right, and a log at the bottom.

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 [T...]
 - 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
 - Add 2 or more selections (toggle mode) from separate structures. Selections must be limited to single polymer chains or residues therein.
- Components
 - 2 structures
 - Preset + Add
 - Polymer: Cartoon
 - Ligand: Ball & Stick
 - Water: Ball & Stick
 - 2 Unit Cells
- Export Animation

Log

- 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.

Cytochrome P450-cam
2H7S | Model 1 | Instance ASM_1 | A | ARG 290

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

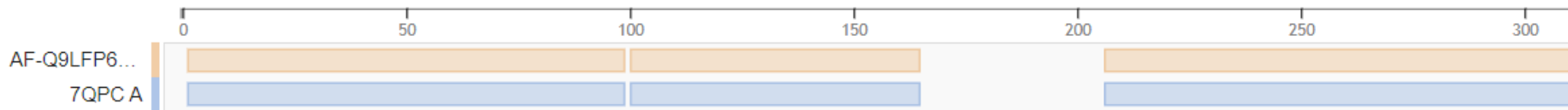
[Help](#)

▸ 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

