



CEITEC



Central European Institute of Technology
BRNO | CZECH REPUBLIC

Vizualizace proteinů a ligandů



EUROPEAN UNION
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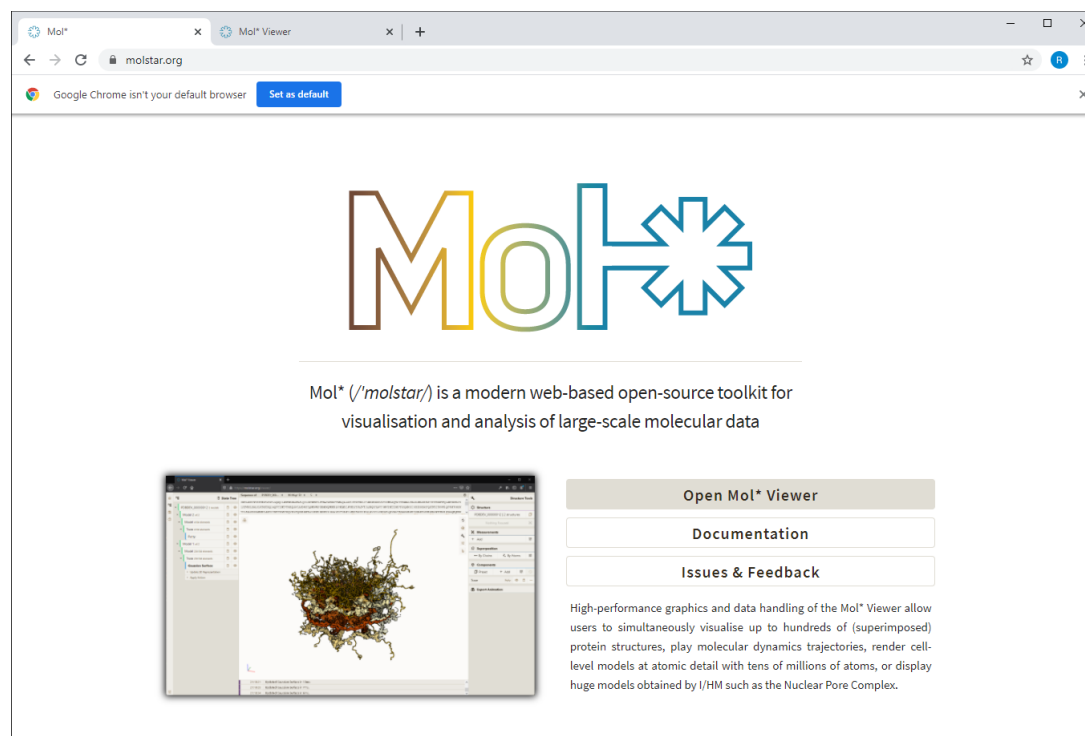


OP Research and
Development for Innovation



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.

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

The left sidebar, titled "Home", contains a "Download Structure" section with a table for inputting source information:

Source	PDB
PDB Id(s)	1tqn

Below the table, there is an "Options" section with a refresh icon and a button labeled "Apply" which is circled in red. Other options include "Add Trajectory", "Download Density", "Download File", "Open Files", "Download", "Load CellPack", and "Load Genome 3D (G3D)".

The right sidebar, titled "Structure Tools", includes sections for "Structure" (Nothing Loaded), "Measurements" (+ Add), "Components" (Preset, + Add), and "Export Animation".

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

Vizualizace 3D souřadnic molekuly

Vizualizační model cartoon

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central view shows a green cartoon representation of the protein structure, surrounded by red dots 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

```
MALYGTSHSHGLFKKLGIPGFTPLPFLGNILSYHKGFCMFDMECHKKYGKVGWGFYDGGQPVLAITDPDMIKIVLVKCEYSVFTNRRPFGVGPMSAI
SIAEDEEMKRLRSLLSPTFTSGKLEKMFIIAQYGDVLRNLRREAETGKPVTLKDVFGAYSMDVITSTSGVNI DSLNFPQDPFVENTKGLLRDFD
LDPFFLSITIVVFFLIPILEVLMNICVFPREVINFLRKSVMKMKRESLEDITQKHRVDFLQMLMIDSQNSKETESHKALSDLELVAQSTIIFAGYETTSS
```

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
 - 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* web application interface. The central 3D viewer shows a protein structure (1TQN) rendered as a green cartoon model, surrounded by red spheres representing water molecules. The left sidebar contains a 'State Tree' with a hierarchy: 1TQN 1 model > Model 1 > Assembly 1 3999 elements > Polymer 3766 elements > Cartoon. The top right panel, 'Structure Tools', is open to the 'Structure' section, showing details for '1TQN | Crystal Structure of Human ...'. Below this, the 'Measurements' and 'Components' sections are visible. In the 'Components' section, the 'Add Representation' button is circled in red. The 'Add Representation' dropdown menu is open, listing various representation styles: Cartoon, Ball & Stick, Gaussian Surface, Gaussian Volume, Label, Line, Molecular Surface, Orientation, Point, Putty, and Spacefill. The 'Cartoon Representation' option is currently selected. The bottom status bar shows recent actions: 'Created Ball & Stick in 19ms.' and 'Updated Structure Focus Representation in 2ms.'

Vizualizace 3D souřadnic molekuly

Volba vizualizačních modelů - Ball & Stick

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central 3D view shows the protein structure in green, with atoms represented as small red spheres. The interface includes a 'State Tree' on the left, a 'Sequence of' panel at the top with the amino acid sequence, and a 'Structure Tools' panel on the right. The 'Structure Tools' panel is currently set to 'Ball & Stick' representation, which is highlighted with a red circle. The 'Components' section shows the protein as a 'Polymer' with a 'Cartoon' representation selected. The 'Ligand' and 'Water' components are also visible, both set to 'Ball & Stick' representation. A log at the bottom shows recent actions: 'Created Ball & Stick in 19ms.' and 'Updated Structure Focus Representation in 2ms.'

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

MALYGTSHSHGLPKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKYKQWGFYDQGPVLAITDPDMIKTVLVKCYSVFTNRRPFGVPVGMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEKMFIIAQYGDVLRNLRREAETGKPKVLKDFVFGAYSMDVITSTSGVNI DSLNNPQDPFVENTKGLLRDFD
LDPFFLSITVVFFLIPILEVLIICVFPREVINFRLKSVKRMKESRLEDTQKHRVDFLQMLIDSONSKETESHKALSDLELVAQSIIFIFAGYETTSS

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Ass...

Nothing Focused

Measurements

Components 1TQN

Polymer Cartoon

Add Representation

Cartoon

Ball & Stick

Gaussian Surface

Gaussian Volume

Label

Line

Molecular Surface

Orientation

Point

Putty

Spacefill

Cartoon Representation

Ligand Ball & Stick

Water Ball & Stick

Unit Cell 1 2 2

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

MALYGTSHSHGLPKKLGIPGPTPLPFLGNILSYHKGFDMFCMECHKYKGVWGFYDQQPVLAITDPMIKTVLVKECYSVFTNRRPFGVPVGMKSAI
SIAEDEEWKRLRSLSPFTTSGKLEKEMVPIIAQYGDVLVNRNRREAEETGKQVILKDVFGAYSMDEVITSTSGVNIIDSLNPNQDPFVENTKLLRDFD
LDPFFLSITVFFFLIPILEVLNLCVFPREVINFLRKSVMKESRLEDITQRHRVDFLQMLIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTS

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 application interface for visualizing the 3D coordinates of the protein 1TQN. The main window shows the protein structure in a line representation, with the backbone colored in green and red. The interface is divided into several panels:

- State Tree (Left):** A hierarchical list of the structure's components, including 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Cartoon, Ball & Stick, Line (selected), Ligand (49 elements), Water (190 elements), and Unit Cell (2 2 2).
- Sequence Viewer (Top):** A text-based representation of the protein sequence, with amino acid residues and their corresponding positions (e.g., 22, 42, 55, 62, 72, 82, 102, 112, 122, 132, 142, 152, 162, 172, 182, 202, 212, 222, 232, 242, 252, 262, 272, 282, 292, 302, 312, 322, 332, 342, 352, 362, 372, 382, 392, 402) displayed below the sequence.
- Structure Tools (Right):** A panel for managing the structure, including options for Structure, Measurements, Components, Volume Streaming, and Assembly Symmetry. The Components section shows the structure is composed of 3 polymer repeats, 1 ligand, and 190 water molecules.

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

- 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 souřadnic molekuly

Vizualizační model Putty

The screenshot displays the Mol* Viewer interface. The central 3D view shows a protein structure rendered in a green Putty 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
 - Ball & Stick
 - Line
 - Putty
- Ligand 49 elements
 - Ball & Stick
- Water 190 elements
 - Ball & Stick
- Unit Cell 1 2 2 2

The top right panel shows the Sequence of 1TQN | Crystal... 1: cytochrome... A. The sequence is:

```
MALYGT HSHGLFKLGI PGFTPL PFLGNILSYHKGF CMFDMECHKGYK GWGFDGQQVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGPMKSAI  
SIAEDEEWKRLRSLSPITFTSGKLEKMPV IIAQYGDVLRNLRREAEATGKPVILKDVFGAYSMDVITSTSGVNI DSNLPQDPFVENTKGLLRDFD  
LDPFFLSITVFFFLIPILEV LNICVFFREVINFLRKSVMKRESRLDTQKRHVDVFLQMLIDSONSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

The right sidebar contains 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: 4 reprs
 - Ligand: Ball & Stick
 - Water: Ball & Stick
 - Unit Cell 1 2 2 2
- Volume Streaming** (1TQN)
 - Enable
- Assembly Symmetry** (1TQN)
 - Enable
- Export Animation

The bottom status bar 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 structure 1TQN. The central view shows a 3D space-filling model of the protein, with atoms represented by colored spheres (red, blue, green, yellow). The interface is divided into several panels:

- State Tree (Left):** A hierarchical tree showing the structure's components: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Ligand (49 elements), and Water (190 elements). The 'Spacefill' option is selected under the Polymer component.
- Sequence Viewer (Top):** Shows the amino acid sequence of the protein: MALYGTSHSHGLPKLGI... SIAEDEEWKRLRSLSPFT... LDPFFLSITVFFFLIPI... with residue numbers 1-312.
- Structure Tools (Right):** A panel with various tool options: Structure (1TQN | Crystal Structure of Human...), Measurements, Components (1TQN), Volume Streaming (1TQN), and Assembly Symmetry (1TQN). The 'Spacefill' option is selected under the Polymer component.
- Log (Bottom):** A log of user actions: 14:53:35 Created Line in 53ms, 14:54:42 Created Putty in 90ms, 14:56:06 Created Spacefill in 26ms.

Vizualizace povrchu molekuly

Vizualizační model Molecular Surface

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central view shows a green molecular surface representation of the protein. 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 creation of the molecular surface representation.

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

```
MLYGT22HSHGL42FKLGI55PGFT62PLPFLGNIL72SVYHKG82FCMFD92MECHK102KYK112GWG122FYD132GQQ142PVLA152ITD162PDMIK172IVL182VKE192CYS202VFT212NR222RP232FG242V252GM262K272SAI282  
SIA122E132DE142EW152K162RL172RS182LL192SPT202FT212SG222KL232EM242VF252IIA262Q272Y282GD292VL302VR312NL322RR332E342ET352GK362P372VL382K392D402V412FG422AY432S442MD452V462IT472ST482S492FG502V512NI522DS532L542NN552Q562DD572F582V592ENT602K612GL622LR632FD642  
L222DP232FF242L252SI262TV272FF282FL292I302PI312LEV322L332NI342CV352FP362REV372IN382FL392R402K412SV422K432RM442K452ES462RL472ET482Q492K502HR512VD522FL532Q542LM552IDS562Q572SK582ET592ESH602K612ALS622D632LE642L652V662A672Q682SI692IF702F712AG722Y732ET742TS752
```

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

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 Surface

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central 3D view shows a green Gaussian Surface representation of the protein. The interface includes a State Tree on the left, a sequence viewer at the top, and a Structure Tools panel on the right. The Structure Tools panel shows the current representation is 'Gaussian Surface' and lists other available representations like 'Molecular Surface', 'Cartoon', and 'Ball & Stick'. A log at the bottom shows the creation of the Gaussian Surface in 597ms.

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

```
MALYGT HSHGLFKLGI PGFTL PFLGNILSYHKGFCMFDMECHKYKGVWGFYDGOQPVLAITDPDMIKIVLVKCEYSVFTNRRPFGVGFMSAI
SIAEDEEMKRLRSLLSPTFTISGKLEKMFIIAQYGDVLRNLRREAETGKPVTLKDVFGAYSMDVITSTSGVNI DSLNNQDFFVENTKGLLRDFD
LDPFFLSITIVFFLIPILEVLNLCVFPREVINFLRKSVMKRESRLDTQKHRVDFLQMLIDSQSKETESHKALSDLELVAQSTIIFIFAGYETTSS
```

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Ass...

Nothing Focused

Measurements

Components 1TQN

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 1TQN. The central view shows a protein structure with a red Gaussian Volume representation. 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 is 1TQN | Crystal Structure of Human ... and includes sections for Measurements, Components, and Polymer. The Components section lists various representations, including 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, and Molecular Surface Representation. The Polymer section shows 4 representations. The bottom status bar indicates the creation of the Gaussian Surface, Gaussian Volume, and Molecular Surface representations.

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

MALYGTSHSHGLPKKLGIPGPTPLPFLGNILSYHKGFDMFCMFDMECHKKYGKWGFYDQGPVLAITDPDMIKTVLVKECYSVFTNRRPFGVPVGMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEKMFVIAAQYGDVLVRNLRREAEATGKPVILKQVFGAYSMDVITSTSGVNI D SLNNPQDPFVENTKGLLRDFD
LDPFFLSITVFFFLIPILEVLNICVFFREVINFLRKSVMKRESRLDITQKRVDFLQIMIDSONSKETESHKALSDLELVAQSIIFIFAGYETTSS

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

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

```
MLYGTGHSGLFKKLGIPGFTLPLFLGNILSYHGKFCMFDMECHKYKGVWGFYDQGPVLAITDPDMIKIVLVKCEYSVFTNRRPFGVGPMSAI
SIAEDEEMKRLRSLLSPTFTSGKLEKMFIIAQYGDVLRNLRREAETGKPVTLKDVFGAYSMVDVITSTSGVNI DSLNFPQDPFVENTKGLLRDFD
LDPFFLSITIVFFFLIPILEVLMNICVFPREVINFLRKSVMKMKRESLEDTQKHRVDFLQMLMIDSQSKETESHKALSDLELVAQSTIIFAGYETTSS
```

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

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 a green ribbon representation of the protein structure, with red dots representing electron density. The left sidebar shows 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

The top panel shows the sequence of 1TQN | Crystal... and 1: cytochrome... with amino acid residues and their corresponding positions. 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...
- Measurements: + Add
- Components: 1TQN
 - Polymer: Cartoon
 - Ligand: Ball & Stick
 - Water: Ball & Stick
 - Unit Cell 1 2 2
- Volume Streaming: Enable
- Assembly Symmetry: Enable
- Export Animation

The bottom status bar shows the following log entries:

- 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* web application interface. The central view shows a 3D model of the protein 1TQN in a green cartoon representation, surrounded by a red mesh representing the electron density. The interface is divided into several panels:

- State Tree (Left):** A hierarchical list of the model's components, including 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Ligand (49 elements), Water (190 elements), and Unit Cell (1 2 2 2).
- Sequence Viewer (Top):** Shows the amino acid sequence of the protein: MALYGT HSHGLFKLGI PGFTL PFLGNILSYHKGF CMFDM ECHKYKGVWGFYD GQQPVLAITDPDMIKIVLVKECYSVFTNRRPFGVGFPMKSAI SIAEDEEMKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVLRNLRREAETGKPVTLKDVFGAYSM DVIITSTSGVNI DSNLNNQDQDFVENTKGLLRDFD LDPFFLSITVFFFLIPILEVLNLCVFPREVINFLRKSVMKRMKRESLEDTQKHRVDFLQMLMIDSNQSKETESHKALSDLELVAQSIIFIFAGYETTSS.
- Structure Tools (Right):** A control panel for the structure, including sections for Structure (1TQN | Crystal Structure of Human ...), Measurements, Components (1TQN), and Volume Streaming (1TQN). The Volume Streaming section shows sliders for 2Fo-Fc σ (1.5), Fo-Fc(+ve) σ (3), and Fo-Fc(-ve) σ (-3).
- Log (Bottom):** A log of recent updates: 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 image shows a screenshot of the Mol* web viewer interface. The central view displays a protein structure (1TQN) in a green cartoon representation, surrounded by red electron density mesh. A red arrow points to a specific atom within 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 structure name, type (Assembly), and various settings for the polymer, ligand, and water components. The Volume Streaming section is also visible, showing settings for 2Fo-Fc σ , Fo-Fc(+ve) σ , and Fo-Fc(-ve) σ .

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

MALYGTSHSHGLFKLGI PGPTPLPFLGNILSYHKGFCMFDMECHKYKQWGFYDQQPVLAITDPDMIKTVLKECYSVFTNRRPFGVGFPMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEKMFIIAQQYGDVLRNLRREAEATGKPVILKQVFGAYSMDVITSTSGVNI DLSLNNFQDPPEVENTKGLLRDFD
LDPFFLSITVFFFLIPILEVNLICVFFREVINFLRKSVKRMKESRLEDTQKHRVDFLQMLIDSONSKETESHKALSDLELVAQSIIFIFAGYETTSS

Kliknout na vybraný atom

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Ass...

Nothing Focused

Measurements

Components 1TQN

Polymer Cartoon

Ligand Ball & Stick

Water Ball & Stick

Unit Cell 1 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

Assembly Symmetry 1TQN

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

```
MALYGTSHSHGLPKKLGIPGFTPLPFLGNILSYHKGFDMFCMECHKYKQWGFYDQGPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGMKSAI
SIAEDEEWKRLRSLSPTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVILKQVFGAYSMDVITSTSGVNI DSLNPNQDPFVENTKLLRDFD
LDPFFLSITVFFFLIPILEVLNLCVFPREVINFLRKSVMKRESLEDIQKHRVDVFLQMLIDSONSKETESHKALSDELEVAQSIIFIFAGYETTSS
```

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

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

Vizualizace anotací

Obarvení podle vlastností

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows a green cartoon representation of the protein structure, with red dots indicating specific residues. The left sidebar shows the State Tree with a hierarchy: 1TQN 1 model > Model 1 > Assembly 1 3999 elements > Polymer 3766 elements > Cartoon. The top right shows the Sequence of 1TQN | Crystal... with the amino acid sequence: MALYGT HSHGLFKKLGIPGFTL PFLGNILSYHKGFCMFDMECHKYKGVKWFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFPMKSAI SIAEDEEMKRLRLSLLSPTFTISGKLEKMFIIAQYGDVLRNLRREAETGKPVILKDVFGAYSMDVITSTSGVNI DSNLNNQDPPFVENTKGLLRFDL LDPFFLSITVFFFLIPILEVLNLCVFPREVINFLRKSVMKRESRLDTQKHRVDFLQMLMIDSNQSKETESHKALSDLELVAQSTIIFIFAGYETTSS. The right sidebar shows the Structure Tools panel with the Structure section expanded to show the 'Residue Property' menu, which is circled in red. The menu items include: Chain Property, Miscellaneous, Residue Property (circled), Accessible Surface Area, Hydrophobicity, Molecule Type, Residue Name, Secondary Structure, Sequence Id, Symmetry, and Validation. Below the menu, the 'Cartoon Representation' section is visible, showing 'Ligand' set to 'Ball & Stick' and 'Water' set to 'Ball & Stick'. The bottom status bar shows update times: 16:37:57 Updated Cartoon in 31ms, 16:38:35 Updated Cartoon in 8ms, and 16:38:48 Updated Cartoon in 28ms.

Vizualizace anotací

Obarvení podle vlastností - hydrofobicita

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central 3D view shows the protein structure as a ribbon, colored according to its hydrophobicity. The structure is composed of several alpha-helices and beta-strands, with a color gradient ranging from green (low hydrophobicity) to red (high hydrophobicity). The interface includes a state tree on the left, a sequence viewer at the top, and a structure tools panel on the right.

Sequence of 1TQN | Crystal Structure of Human Cytochrome c

```
1  MALYGT HSHGLFKLGI PGFTPL PFLGNILSYHKGF CDFMECHKKYGVKWFYDQQVLAITDPDMIKTVLVKCEYSVFTNRRPFGVGFPMKSAI
2  SIAEDEEMKRLRSLLSPTFTISGKLEKMFIIAQYGDVLRNLRREAETGKPVILKDVFGAYSDVITSTSGVNI DLSLNNQDQDFVENTKGLLRDFD
3  LDPFFLSITVVFPLIPILEVLMICVFPREVINFLRKSVMKRESRLDITQKHRVDFLQMLMIDSQNSKETESHKALSDLELVAQSTIIFAGYETTSS
```

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

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

Vizualizace anotací

Obarvení podle vlastností – kvalita

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central view shows a green ribbon representation of the protein structure, with red dots indicating specific residues or annotations. The left sidebar shows the State Tree with a hierarchy: 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). The top right panel shows the Structure Tools menu, with the Structure Quality Report option highlighted by a red circle. The bottom status bar shows update times for the cartoon representation.

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

MALYGTHTSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKYKGVWGFYDQGPVLAITDPDMIKTVLVKCYSVFTNRRPFGVPVGMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEKMFIIAQYGDVLRNLRREAETGKPVILKQVFGAYSMDVITSTSGVNIIDSLNNPQDPFVENTKGLLRDFD
LDPFFLSITVVFPLIPILEVLNICVFFREVINFLRKSVMKESRLEDITQKHRVDFLQMLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Ass...

Nothing Focused

Measurements

Components 1TQN

Polymer

Cartoon

Structure Quality Report

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

Vizualizace anotací

Obarvení podle vlastností - kvalita

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central 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 control 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

```
MALYGTHTSHGLPKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKYKQWGFYDQQPVLAITDPDMIKTVLVKECVYSVTNRRPFGPVGPMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEKMFIIAQYGDVLRNLRREAETGKPVILKQVFGAYSMDVITSTISFGVNI DLSLNNPQDPFVENTKGLLRDFD
LDPFFLSITVVFPLIPILEVLIICVFFREVINFLRKSVMKRESRLDITQKHRVDFLQMLIDSONSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

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.

Měření

The screenshot displays a molecular visualization software interface. The central view shows a protein structure in a green cartoon representation. A context menu is open over the structure, with the option "Atom/Coarse Element" highlighted in red. 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 50 elements
 - Ball & Stick
 - Water 190 elements
 - Ball & Stick
 - Unit Cell 1 2 2 2

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

MALYGHSHGLFKKLGIPGTPFLPFLGNILSYHKGFCMFDMECHKYKGVWGFYDGGQVFLAITDDPMIKTVLVKECVSFTNRRPFGVGFMSAISIAEDEWKRRLSLLSPTFTSGKLEKEMVPIIAQYGDVLRNLRREAEYTKPK
172 182 192 202 212 222 232 242 252 262 272 282 292 302 312
VTLKDVFGAYSMDVITSTSGVNIIDSLNPDQFVNTKLLRFDFLDPFELSITVFPFLIILEVLNICVPREVNTFLRKSVMKESLLEDTQKRVDFLQIMIDSQNSKETESHKALSDELLEVAQSIIFIFAGYETTSSVLSFI
322 332 342 352 362 372 382 392 402 412 422 432 442 452 462
MYELATHPDVQQKLEIDEAVLENRAPPTDYTVLQMEYLDVVNTELRLLFFIARLRELVCKDVEINGMFIKGVVMIPISYALHRDPKYWTEPEKFLPERFSSKNKNDIDPYIYTPFGSGPRNCIGMRFALMNMKLLALIRVLQNFSP

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Dynamic Bonds X Off

Nothing Focused

Measurements

+ Add

Quick Styles

Apply Representation

Default Cartoon Spacefill Surface

Apply Style

Default Illustrative

Components 1TQN

Preset + Add

Polymer Cartoon

Ligand Ball & Stick

Water Ball & Stick

Unit Cell 1 2 2 2

Volume Streaming 1TQN

Enable

Assembly Symmetry 1TQN

19:07:36 Created Ball & Stick in 8ms.

19:07:36 Created Ball & Stick in 4ms.

19:07:36 Updated Structure Focus Representation in 1ms.

Měření

The screenshot displays the Mol* web application interface. The central view shows a protein structure in green cartoon representation. A specific distance of 2.92 Å is highlighted between two atoms, with a dashed line and a label '2.92 Å' overlaid on the structure. The top of the interface shows the browser tabs and the URL 'molstar.org/viewer/'. Below the browser, the 'State Tree' on the left lists the hierarchy of the model: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Ligand (49 elements), Water (190 elements), and Unit Cell (2 2 2). The 'Measurements' section is expanded to show 'Distance 2 source(s), 49 elements...' and 'Distance'. The top right shows the 'Sequence of 1TQN | Crystal...' with the amino acid sequence: MALYGT HSHGLFKKLGIPGFTLPLFLGNILSYHKGFCMFDMECHKKYGKVGWGFYDGOQPVLAITDPDMIKTVLVKCEYSVFTNRRPFGVGFPMKSAI SIAEDEEMKRLRSLSPFTISGKLEKMFIIAQYGDVLRNLRREAETGKPVILKDVFGAYSDVITSTSGVNI DSNLPQDFVENTKGLRFDL LDPFFLSITVFFFLIPILEV LNICVFPREVINFLRKSVKRMKRESLEDTQKHRVDFLQMLIDSNQSKETESHKALSDLELVAQSIIFIFAGYETTSS. The right sidebar contains the 'Structure Tools' panel, which includes 'Structure' (1TQN | Crystal Structure of Human ...), 'Measurements' (2.92 Å | HEM 508 — CYS ...), 'Components' (1TQN), 'Volume Streaming' (1TQN), and 'Assembly Symmetry' (1TQN). The bottom status bar shows recent actions: 'Created Ball & Stick in 23ms.', 'Created Ball & Stick in 11ms.', and 'Updated Structure Focus Representation in 2ms.'

Příkládání struktur

The screenshot displays the Mol* Viewer web application interface. The browser address bar shows the URL `molstar.org/viewer/`. The main content area is titled "Sequence" and indicates "No structure available". On the left sidebar, under the "Home" section, the "Download Structure" menu is expanded. The "Source" is set to "PDB" and the "PDB Id(s)" field contains the text "2h7s 2rfc", which is circled in red. Below this, there is an "Options" section with an "Apply" button. Further down, there are several expandable menu items: "Add Trajectory", "Download Density", "Download File", "Open Files", "Download", "Load CellPack", and "Load Genome 3D (G3D)". At the bottom of the sidebar, there is a "Remote States" section with a list of items: "Nuclear Pore Complex", "NPC-CIF", "1RB8 Annotated Assembly", "Zika+EM", "Cytochromes Superposition", "AS", "ASX", "ASX-1 Something", "1", and "2". On the right side, the "Structure Tools" panel is visible, containing sections for "Structure" (Nothing Loaded), "Measurements" (+ Add), "Components" (Preset, + Add), and "Export Animation". The bottom status bar shows the time "21:28:55" and the version information "Mol* Plugin 1.2.7 [12/19/2020, 11:52:32 AM]".

Přikládání 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. The top of the interface features a browser window with the URL molstar.org/viewer/. Below the browser, a sequence viewer displays the amino acid sequence of Cytochrome, with residue numbers 1 to 291. On the left side, a 'State Tree' panel lists the loaded models and their components, including '2H7S 1 model', 'Model 1', 'Assembly 1 3355 elements', 'Polymer 3201 elements', 'Ligand 49 elements', 'Water 111 elements', 'Unit Cell P 1 21 1', '2RFC 1 model', and another 'Model 1' with its own assembly and components. On the right side, the 'Structure Tools' panel is visible, with the 'Superposition' tool highlighted by a red circle. The 'Superposition' tool is currently set to 'By Chains' and 'By Atoms'. Below the 3D view, a log shows 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* Viewer interface. On the left, the State Tree shows a hierarchy of models and assemblies. The top bar shows the sequence of the protein, 2H7S | L244A ... 1: Cytochrome... A. The central 3D view shows a protein structure in green cartoon representation. The right panel contains the Structure Tools, including Structure, Measurements, Superposition, and Components. A red circle highlights the 'Residue' button in the toolbar.

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

Residue

Structure Tools

Structure

2 structures

Nothing Focused

Measurements

+ Add

Superposition

By Chains By Atoms

Components

2 structures

Preset + Add

Polymer Cartoon

Ligand Ball & Stick

Water Ball & Stick

2 Unit Cells

Export Animation

21:31:10 Created Ball & Stick in 18ms.

21:31:10 Created Ball & Stick in 4ms.

21:31:10 Updated Structure Focus Representation in 2ms.

Příkládání struktur

The screenshot displays the Mol* Viewer interface with a protein structure loaded. The main window shows a ribbon representation of the protein in green and purple. A context menu is open over the structure, with the 'Structure Property' option highlighted by a red circle. The menu includes options like 'All', 'Polymer/Carbohydrate Entities', 'Ligand/Non-standard Residue', 'Type', 'Bond Property', 'Residue Property', 'Manipulate Selection', 'Amino Acid', 'Nucleic Base', and 'Element Symbol'. The left sidebar shows a 'State Tree' with a hierarchical view of the loaded models and their components. The right sidebar contains various tool panels such as 'Structure Tools', 'Measurements', 'Superposition', 'Components', and 'Export Animation'. The top of the browser window shows the URL 'molstar.org/viewer/' and the sequence of the protein: 'Sequence of 2H7S | L244A ... 1: Cytochrome...'. The bottom status bar shows recent actions like 'Created Ball & Stick in 18ms'.

Příkládání struktur

The screenshot displays the Mol* Viewer interface. On the left is a 'State Tree' panel showing a hierarchical view of the loaded data, including '2H7S 1 model', 'Model 1', 'Assembly 1 3355 elements', 'Polymer 3201 elements', 'Ligand 49 elements', 'Water 111 elements', 'Unit Cell P 1 21 1', '2RFC 1 model', 'Model 1', 'Assembly 1 2811 elements', 'Polymer 2752 elements', 'Ligand 60 elements', 'Water 5 elements', and 'Unit Cell P 1 21 1'. The main window shows a protein structure in a cartoon representation. A context menu is open over the structure, listing various selection options: 'Residue', 'Add/Union Selection', 'All', 'Polymer/Carbohydrate Entities', 'Ligand/Non-standard Residue', 'Type', 'Structure Property', 'Trace', 'Sidechain', 'Sidechain with Trace', 'Helix', 'Beta Strand/Sheet', and 'Bond Property'. The 'Backbone' option under 'Trace' is highlighted with a red circle. At the top, the sequence of the protein is displayed: 'Sequence of 2H7S | L244A ... 1: Cytochrome...'. The right sidebar contains 'Structure Tools' and a list of components: 'Polymer' (Cartoon), 'Ligand' (Ball & Stick), 'Water' (Ball & Stick), and '2 Unit Cells'. A log at the bottom shows recent actions: 'Created Ball & Stick in 18ms.', 'Created Ball & Stick in 4ms.', and 'Updated Structure Focus Representation in 2ms.'

Přikládání struktur

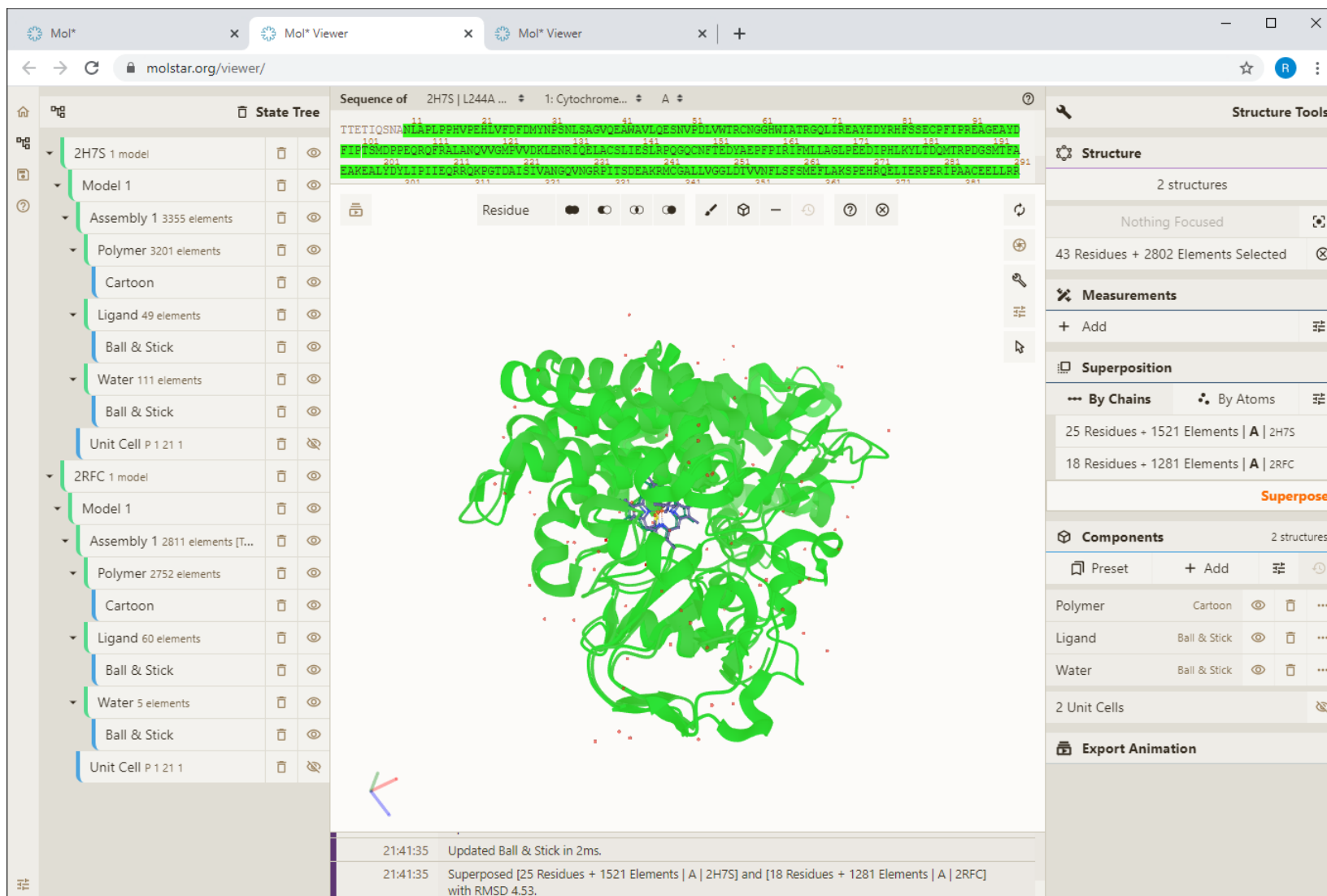
The screenshot displays the Mol* Viewer interface. On the left, the State Tree shows a hierarchy of models and assemblies. The top center shows the protein sequence for Cytochrome c, with a segment highlighted in green. The main view shows the protein structure in green cartoon representation. The right panel, titled 'Structure Tools', contains several sections: 'Structure' (2 structures), 'Measurements' (+ Add), 'Superposition' (By Chains selected and circled in red, and By Atoms), and 'Components' (2 structures). The Components section lists Polymer (Cartoon), Ligand (Ball & Stick), and Water (Ball & Stick). At the bottom, a log shows recent actions: 'Created Ball & Stick in 18ms.', 'Created Ball & Stick in 4ms.', and 'Updated Structure Focus Representation in 2ms.'

Přikládání struktur

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

- State Tree (Left):** A hierarchical tree showing the loaded models and their components. The selected model is 2H7S, which includes a polymer (3201 elements) in cartoon representation, a ligand (49 elements) in ball & stick representation, and water molecules (111 elements) in ball & stick representation.
- Sequence Viewer (Top):** Shows the amino acid sequence of the protein. The sequence is: `TIETIQSNL...LPLPFRVFERLVDFDMYNS...LSAGVQV...EAMVNLQENVFDLWTRCNGSHNIATRGQLIPEAYEDYRFRFSSECFPIFPLAGEAV...
...SMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRFQGCNFTEDVAEPFIRIFMLLAGLPEDIPHLKYLIDQMTRPDQSMIT...
...AREALDYVIFITEQRQNPSTDAISIVANGVNGRPTISDEAKRNGALLVGGLDIVNFLSFSMEFLAKSPERRQLTERPERIPACCELLAR...`
- Structure Tools Panel (Right):** Contains various tool options. The 'Superpose' button is highlighted with a red circle. Other options include 'Structure', 'Measurements', and 'Components'.
- Structure Tools Panel (Bottom):** Shows the current selection: '43 Residues + 2802 Elements Selected'. It also displays the 'Superpose' button and a list of components: Polymer (Cartoon), Ligand (Ball & Stick), and Water (Ball & Stick).
- Log (Bottom):** Shows a list of recent actions: 'Created Ball & Stick in 18ms.', 'Created Ball & Stick in 4ms.', and 'Updated Structure Focus Representation in 2ms.'

Přikládání struktur



Mol* Viewer interface showing a protein structure (green cartoon) and a ligand (blue ball & stick) superposed. The interface includes a State Tree on the left, a Sequence of 2H7S | L244A ... 1: Cytochrome... A at the top, and a Structure Tools panel on the right. The Structure Tools panel shows 2 structures selected, with 43 Residues + 2802 Elements Selected. The Components panel lists Polymer (Cartoon), Ligand (Ball & Stick), and Water (Ball & Stick). The bottom status bar shows a log of 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.

Přikládání struktur

The screenshot displays the Mol* Viewer interface. On the left is the State Tree, showing a hierarchy of models and assemblies. The top center shows the sequence of the protein: "Sequence of 2H7S | L244A ... 1: Cytochrome...". The central 3D view shows a protein structure in green and purple cartoon representation. The right-hand panel contains the Structure Tools, including Structure, Measurements, Superposition, and Components. The Components panel shows 2 structures: Polymer (Cartoon), Ligand (Ball & Stick), and Water (Ball & Stick). The bottom status bar shows the current structure: "Cytochrome P450-cam 2H7S | Model 1 | Instance ASM_1 | A | ARG 290". A log at the bottom indicates updates to the Ball & Stick representation and a superposition of two structures with an RMSD of 4.53.

State Tree

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

Residue

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

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

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.

Vizualizace proteinových assemblies

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

- State Tree (Left):** Lists the loaded components: 3J3Q 1 model, Model 1, Assembly 1 (2440800 elements), Polymer (2440800 elements), and Gaussian Surface.
- Sequence Viewer (Top):** Shows the amino acid sequence of the protein: PIVQN... EPRGS... NPDCK... with residue numbers 1-221.
- Structure Tools (Right):** Provides configuration options for the assembly, including Type (Assembly), Asm Id (1: Author Defined Asse...), and various settings like Volume Streaming and Assembly Symmetry.
- Log (Bottom):** Records recent actions: Created Polymer in 110ms, Created Gaussian Surface in 4.661s, and Updated Structure Focus Representation in 2ms.

Molstar Integrace

- **RCSB PDB (Protein Data Bank) a PDBe** – k vizualizaci molekulárních struktur přímo v databázi PDB
- **AlphaFold DB** – k vizualizaci predikci struktur proteinů z AlphaFold
- **EMDB (Electron Microscopy Data Bank)** – pro vizualizaci map elektronové hustoty
- **MOLEonline** – k vizualizace interaktivní analýzy kanálů
- ...

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](#)

Přikládání struktur – PDB a AlphaFold

Pairwise Structure Alignment

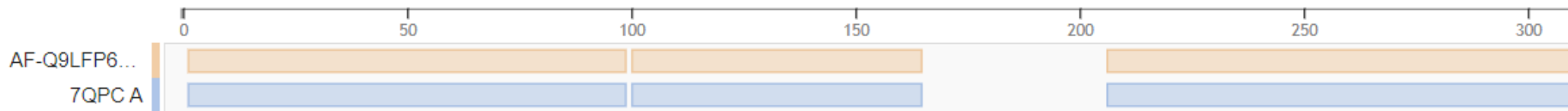
[Help](#)

▸ 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

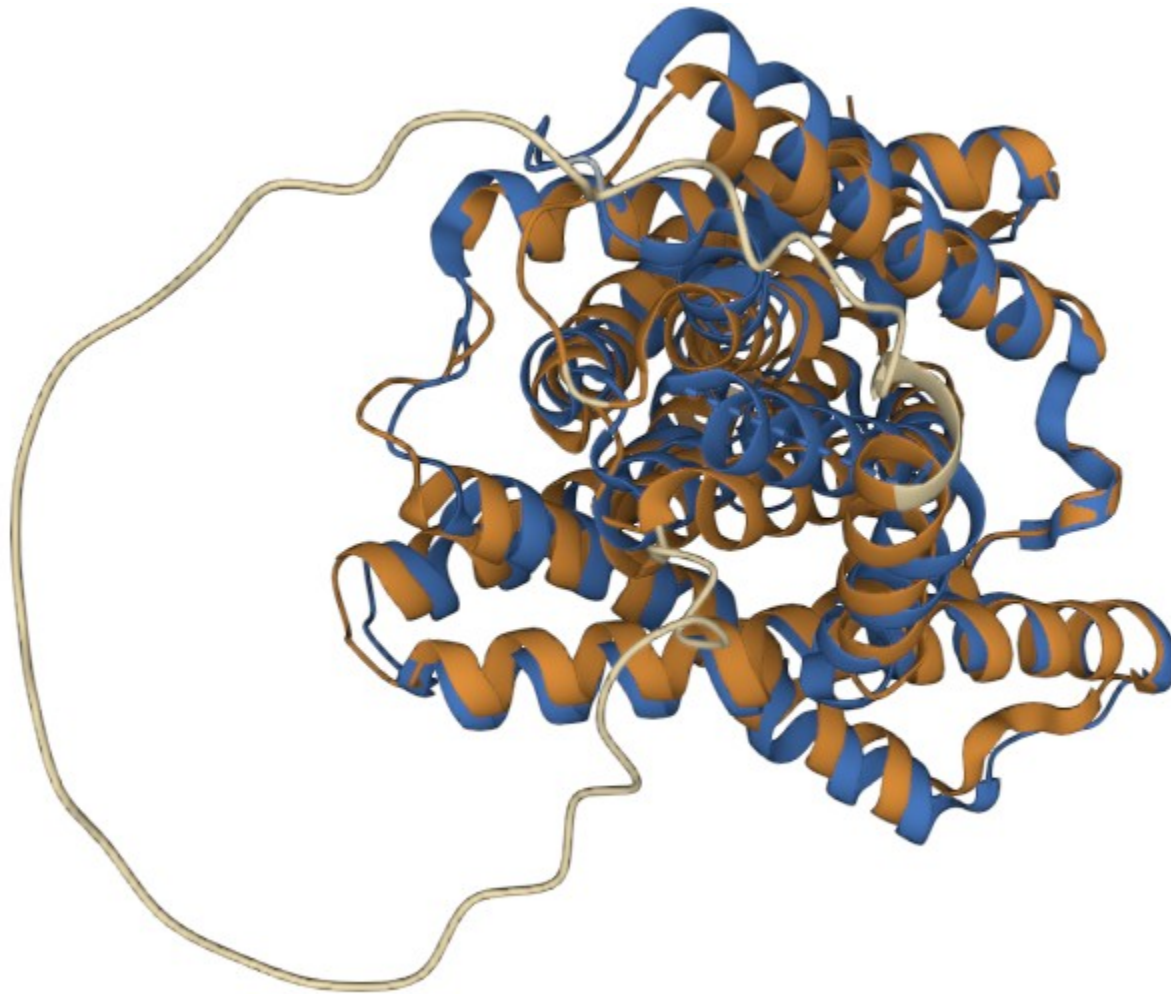
SEQUENCE ALIGNMENT

SCORES



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

Přikládání struktur – PDB a AlphaFold



Molstar Rozšíření

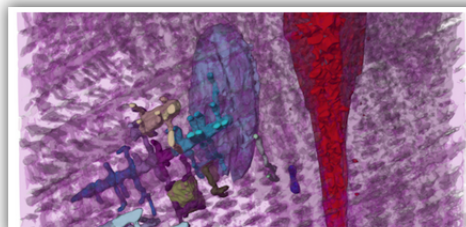
Extensions

MolViewSpec

```
builder = create_builder()
(
  builder.download(url=url_for_mmcif(id))
  .parse(format="mmcif")
  .model_structure()
  .component()
  .representation()
  .color(color="blue")
)
```

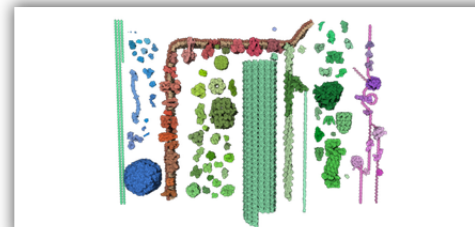
MolViewSpec provides a generic mechanism for describing visual scenes or views that are used in molecular visualizations. It adopts declarative data-driven approach to describe, load, render, and visually deliver molecular structures, along with 3D representations, coloring schemes, and associated structural, biological, or functional annotations.

Volumes and Segmentations



Volumes and Segmentations extension adds support for large scale volumetric data & their segmentations. Building on the existing Mol* ecosystem, this extension allows seamless integration of biomolecular data from cellular to atomic scale. It provides the means to visualize large-scale volumetric and segmentation data from cryo-EM, light microscopy, volume-EM, and other imaging experiments together with related 3D model data and biological annotations.

Mesoscale Explorer



The advent of cryo-EM and cryo-ET, coupled with computational modeling, has enabled the creation of integrative 3D models of viruses, bacteria, and cellular organelles. Based on these models, the **Mesoscale Explorer** provides unprecedented access and insight into the molecular fabric of life, enhancing perception, streamlining exploration, and simplifying visualization of diverse data types, showcasing the intricate details with unparalleled clarity. See the [interactive tours and examples](#).