



CEITEC



Central European Institute of Technology
BRNO | CZECH REPUBLIC

Vizualizace proteinů a ligandů



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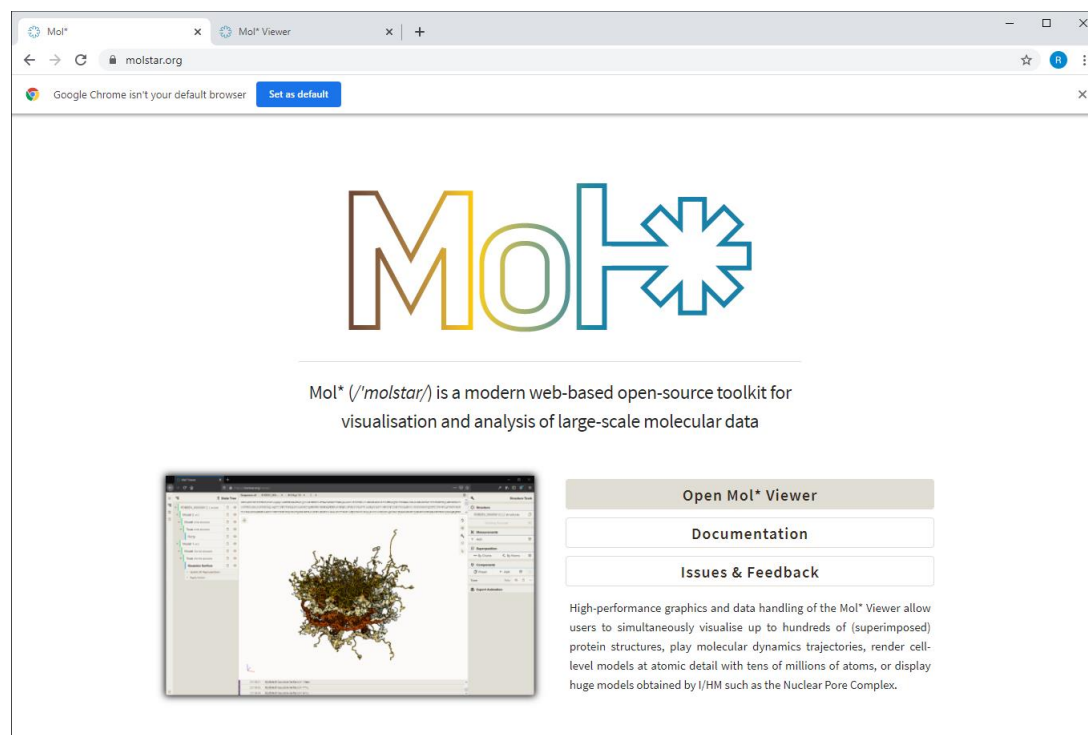


**OP Research and
Development for Innovation**



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 tabs at the top show 'Mol*' and 'Mol* Viewer'. The address bar contains 'molstar.org/viewer/'. The main interface is divided into three panels:

- Home (Left Sidebar):** Contains a 'Download Structure' section with a 'PDB' source and '1tqn' ID. Below this is an 'Options' section with a refresh icon and a red circle around the 'Apply' button. Further down are sections for 'Add Trajectory', 'Download Density', 'Download File', 'Open Files', 'Download', 'Load CellPack', and 'Load Genome 3D (G3D)'. At the bottom is a 'Remote States' table with entries like 'Nuclear Pore Complex', 'NPC-CIF', '1R88 Annotated Assembly', 'Zika+EM', 'Cytochromes Superposition', 'AS', 'ASX', 'ASX-1 Something', and two numbered rows.
- Sequence (Center Panel):** Displays 'No structure available'.
- Structure Tools (Right Panel):** Includes sections for 'Structure' (Nothing Loaded), 'Measurements' (+ Add), 'Components' (Preset, + Add), and 'Export Animation'.

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

Vizualizace 3D souřadnic molekuly

Vizualizační model cartoon

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows a 3D cartoon representation of the protein structure in green, with a ligand in blue and yellow, and water molecules as red spheres. The interface includes a state tree on the left, a sequence viewer at the top, and a structure tools panel on the right.

State Tree:

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

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

```
MALYGIHSHGLFKLGI32PGPTPLPFLGNILS42YHKGFCMFDME52CHKYKQWGF62YDQQPVLAITDPDMIKTVL72VKECYSV82FNRRPFGV92GVGFMKSAI102  
SIAEDEEWKRLRSLLSPTFTSGKLEMPV112IIAQYGDVLRNLR122REAE132TGKPVTLK142QVFGAYSMDV152ITIS162FGVNI172DSLNNPQD182PFVENT192KKLLR202DF212  
LDPFFLSITVFPFLIPILEVLN222ICV232FPREVINFLR242SKV252KRMKES262RLED272TQKHRVD282FLQ292LMD302SONSKETE312SHKALS322DLELVAQ332SI342IF352FAGYETT362SS372
```

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 green ribbon representation of the protein structure. The left sidebar contains a 'State Tree' with the following items:

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

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

- 1TQN | Crystal Structure of Human ...
- Type: Assembly
- Asm Id: 1: Author Defined Ass...
- Nothing Focused

The 'Measurements' section includes a '+ Add' button. The 'Components' section shows '1TQN' with a 'Preset' button and a '+ Add' button. The 'Polymer' section is expanded to show a list of representation options:

- Cartoon
- Ball & Stick** (highlighted with a red circle)
- Gaussian Surface
- Gaussian Volume
- Label
- Line
- Molecular Surface
- Orientation
- Point
- Putty
- Spacefill

The bottom status bar shows the following log entries:

- 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

```
MALYGIHSHGLFKLGI PGPTPLPFLGNILSYHKGF CMFDMECHKYGKVGWGFYDQQPFLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSR I  
SIAEDEEWKRLRSLLSPTFTSGKLEKMFIIAQYGDVLRNLRREARETGKPVTLKDVFGAYSMDVITSTSGVNIIDSLNPNQDFFVENTKGLLRDFD  
LDPFFLSIVVFPFLIPLEVLNICVFPREVINFLRKSVKRMKESRLEDIQKHRVDFLQMLMIDSONSKETESHKALSDELVAQSIIPFAGYETTSS
```

State Tree

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

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset + Add

Polymer	2 reprs	☐	⋮
Ligand	Ball & Stick	☐	⋮
Water	Ball & Stick	☐	⋮

Unit Cell | 2 2 2

Volume Streaming 1TQN

✓ Enable

Assembly Symmetry 1TQN

✓ Enable

Export Animation

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

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

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

Pozor, ostatní
módy je nutno
vypnout

Vizualizace 3D souřadic molekuly

Vizualizační model Line

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

- State Tree (Left):** A hierarchical tree showing the structure's components: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Cartoon, Ball & Stick, Line (selected), Ligand (49 elements), Water (190 elements), and Unit Cell (2 2 2).
- Sequence Viewer (Top):** Displays the amino acid sequence of the protein: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMCECHKKYGKWWGFYDQQQVLAITDPDMIKTVLVKECYSVFINRRRFGFVGFMKSAI... (with residue numbers 22, 42, 62, 82, 102, 112, 122, 142, 162, 182, 202, 212, 222, 242, 262, 282, 302, 322, 342, 362, 372, 382, 392, 402).
- Structure Tools (Right):** A panel for interacting with the structure, including options for Structure, Measurements, Components (Polymer, Ligand, Water), Volume Streaming, and Assembly Symmetry.
- Log (Bottom):** A timeline of user 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* web application interface. The central 3D view shows a protein structure (1TQN) rendered in a green 'Putty' style. The interface includes a 'State Tree' on the left, a 'Sequence of 1TQN | Crystal...' viewer at the top, and a 'Structure Tools' panel on the right. The 'Structure Tools' panel shows the structure name '1TQN | Crystal Structure of Human ...', type 'Assembly', and various settings. The 'Components' section lists 'Polymer' (4 reprs), 'Ligand' (Ball & Stick), and 'Water' (Ball & Stick). The 'Volume Streaming' and 'Assembly Symmetry' sections are also visible, both with 'Enable' checked. The 'Export Animation' section is at the bottom of the panel.

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

```
MALYGIHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMNECHKKYGKRWGFDGQQPVLAITDPMIKIVLVKECYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLSPFTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVTLKDVFGAYSMDVITSTSPGVNIDSLNPNQDPPVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNLCVFPREVINFLRKSVMKESRLEDTQKHRVDFLQMLIDSONSKETESHKALSDELVQAQSIIFAGYETTSS
```

State Tree

- 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

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	4 reprs		...
Ligand	Ball & Stick		...
Water	Ball & Stick		...

Volume Streaming 1TQN

Enable

Assembly Symmetry 1TQN

Enable

Export Animation

Log:

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

Vizualizace 3D souřadnic molekuly

Vizualizační model Spacefil

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

```
MLYGTSHSHGLFKKLGIPGPTLPLPFLGNILSYHKGFDMFCMECHKYKWKWGFYDGOQPVLAITDDPMIKIVLVKCYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLSPFTTSGKIKEMVPIIAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSGVNIIDSLNPDQDFEVENKGLLRDFD
LDPFFLSITVFFLIPILEVLNICVFFPREVINFLRKSVMKRESLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFAGAYETTSS
```

State Tree

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

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

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

Unit Cell | 2 2 2

Volume Streaming 1TQN

Enable

Assembly Symmetry 1TQN

Enable

Export Animation

14:53:35 Created Line in 53ms.

14:54:42 Created Putty in 90ms.

14:56:06 Created Spacefill in 26ms.

Vizualizace povrchu molekuly

Vizualizační model Molecular Surface

The screenshot displays the Mol* Viewer interface. The central 3D view shows a protein structure rendered as a green molecular surface. The left sidebar contains a 'State Tree' with a hierarchy: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), and various representations like Cartoon, Gaussian Surface, Gaussian Volume, Molecular Surface, Ligand (49 elements), Water (190 elements), and Unit Cell (2 2 2). The top center shows the protein sequence: MALYGT... SIAE... LD... with residue numbers 22, 42, 52, 62, 72, 82, 92, 102, 112, 122, 132, 142, 152, 162, 172, 182, 192, 202, 212, 222, 232, 242, 252, 262, 272, 282, 292, 302, 312. The right sidebar features 'Structure Tools' and a list of components including Molecular Surface, Orientation, Point, Putty, Spacefill, Non-covalent Interactions, Validation Clashes, Membrane Orientation, Set Coloring, Modify by Selection, Select This, and Edit Label. A bottom status bar shows log entries: 14:59:19 Created Gaussian Surface in 597ms., 14:59:36 Created Gaussian Volume in 64ms., and 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. The left sidebar contains a State Tree with the following structure:

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

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

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

The bottom status bar shows the following actions:

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

Vizualizace povrchu molekuly

Vizualizační model Gaussian Volume

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central 3D view shows the protein structure with a red Gaussian Volume representation overlaid. The left sidebar contains a State Tree with the following items:

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

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

The right sidebar contains the Structure Tools panel, which includes sections for Structure, Measurements, and Components. The Components section shows the polymer representation settings, including Molecular Surface, Orientation, Point, Putty, Spacefill, Non-covalent Interactions, Validation Clashes, Membrane Orientation, Set Coloring, Modify by Selection, Select This, and Edit Label.

The bottom of the interface shows a log of actions:

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

Vizualizace experimentálních dat

Elektronová hustota

molstar.org/viewer/

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

```

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

```

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset	+ Add	[icon]	[icon]
Polymer	Cartoon	[icon]	[icon]
Ligand	Ball & Stick	[icon]	[icon]
Water	Ball & Stick	[icon]	[icon]

Unit Cell I 2 2 2 [icon]

Volume Streaming 1TQN

[x] Enable

Assembly Symmetry 1TQN

[x] Enable

Export Animation

15:23:00 Created Ball & Stick in 26ms.

15:23:00 Created Ball & Stick in 12ms.

15:23:00 Updated Structure Focus Representation in 3ms.

Vizualizace experimentálních dat

Elektronová hustota

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows the protein structure in green ribbon representation, surrounded by electron density data points in red and yellow. The interface includes a state tree on the left, a sequence viewer at the top, and a structure tools panel on the right. The 'Volume Streaming' option is checked and highlighted with a red circle.

State Tree

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

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

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

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

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

Unit Cell | 2 2 2

Volume Streaming 1TQN

Enable

Assembly Symmetry 1TQN

Enable

Export Animation

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

Vizualizace experimentálních dat

Elektronová hustota

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows the protein structure in green cartoon representation, surrounded by electron density maps in red and blue. The interface is divided into several panels:

- State Tree (Left):** Lists the hierarchy of the model, including 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Ligand (49 elements), Water (190 elements), Volume Server 1tqn, Volume Streaming Selection, and Unit Cell I 2 2 2.
- Sequence (Top):** Shows the amino acid sequence of the protein: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVGWGFYDQQPVLAITDPDMIKTVLVKECYSVFINRRPFGVGFMKSAI... (with residue numbers 32, 42, 50, 62, 72, 82, 102, 112, 122, 132, 142, 152, 162, 172, 182, 192, 202, 212, 222, 232, 242, 252, 262, 272, 282, 292, 302, 312).
- Structure Tools (Right):** Provides controls for the structure, including Structure, Measurements, Components, Volume Streaming, and Assembly Symmetry.

The Volume Streaming panel on the right shows the following settings:

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

The bottom status bar shows the following updates:

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

Vizualizace experimentálních dat

Elektronová hustota

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows the protein structure in green cartoon representation, surrounded by electron density maps (Fo-Fc(+ve) and Fo-Fc(-ve)) shown as semi-transparent surfaces. A red arrow points to a specific atom in the structure, with the text "Kliknout na vybraný atom" (Click on the selected atom) next to it.

The interface includes a State Tree on the left, a Sequence of 1TQN | Crystal... at the top, and a Structure Tools panel on the right. The Structure Tools panel shows the current structure (1TQN | Crystal Structure of Human ...), assembly information, and various measurement and component settings.

The Structure Tools panel 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
 - Ligand: Ball & Stick
 - Water: Ball & Stick
 - 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

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

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKYKRWGFGYDQQPVLAIITDPDMIKTVLVKECYSVFTNRRPFGVGFPMKSAI
SIAEDEEWKRLRSLSLSPFTTSGKLEKMPVPIIAQYGVPLVRNLRREARETGKPVTKDVFVGAYSMVITSTSFVGNVDSLNNPQDPFVENTKLLRPF
LDPFFLSITVFFFLIPILEVLNI CVFPREVINFLRKSVKRMKESRLDETQKHRVDFLQMLIDSONSKETESHKALSDELVAQSIIFIFAGYETISS
```

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Ass...

HEM 508 | B [auth A]

Measurements

+ Add

Components 1TQN

Preset	+ Add		
Polymer	Cartoon	<input type="checkbox"/>	<input type="checkbox"/>
Ligand	Ball & Stick	<input type="checkbox"/>	<input type="checkbox"/>
Water	Ball & Stick	<input type="checkbox"/>	<input type="checkbox"/>
[Focus] Target	Ball & Stick	<input type="checkbox"/>	<input type="checkbox"/>
[Focus] Surroundings (5 Å)		<input type="checkbox"/>	<input type="checkbox"/>
Unit Cell 2 2 2		<input type="checkbox"/>	<input type="checkbox"/>

Volume Streaming 1TQN

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

Entry 1tqn

View Around Focus

Nothing to Update

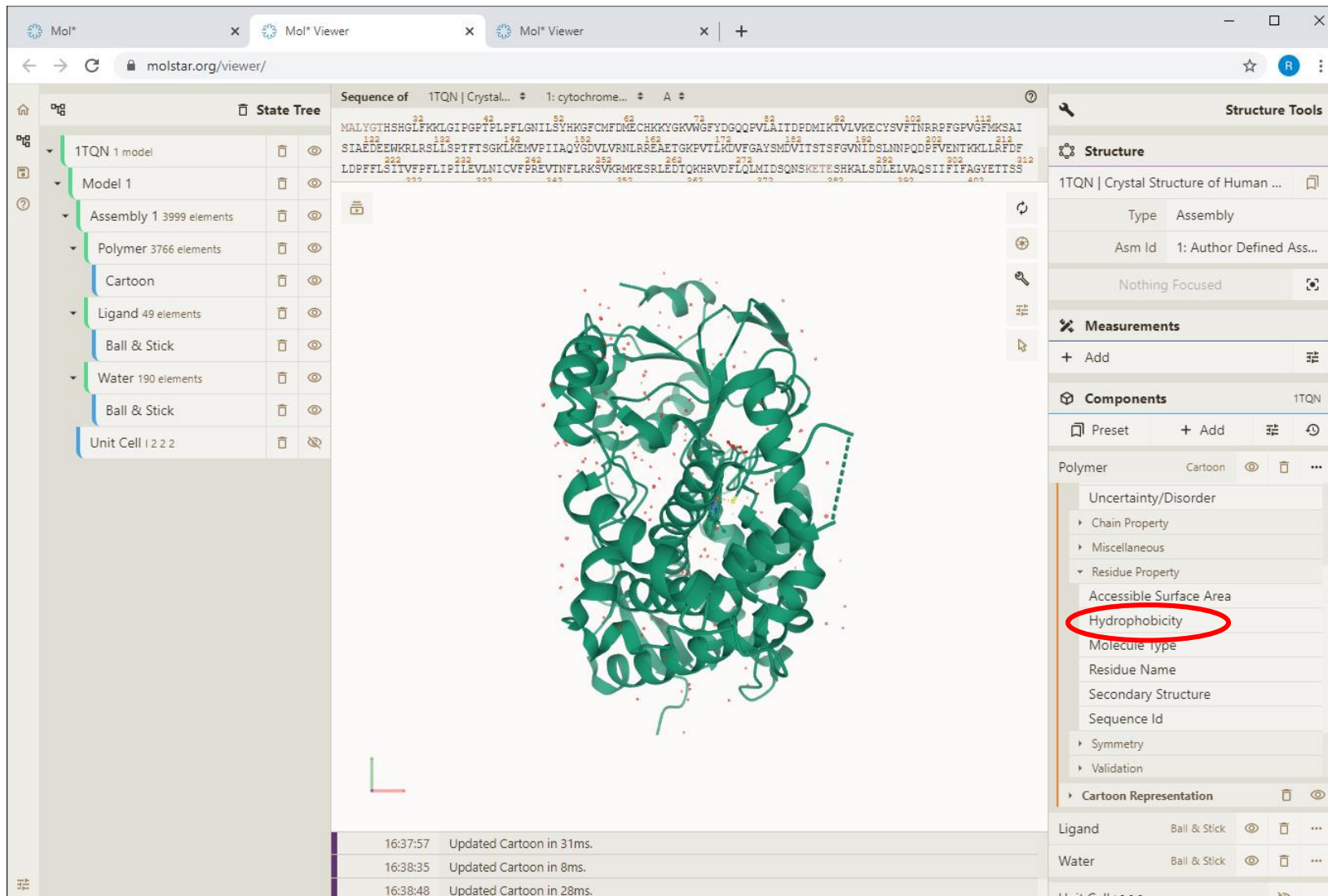
15:28:06 Updated 1.5 σ [2fo-fc] in 72ms.

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

15:28:06 Updated -3 σ [fo-fc(-ve)] in 32ms.

Vizualizace anotací

Obarvení podle vlastností



The screenshot displays the Mol* web interface for the protein 1TQN. The central view shows a green ribbon representation of the protein structure, with red dots indicating specific residues or atoms. The left sidebar contains a 'State Tree' with a hierarchical view of the model, including '1TQN 1 model', 'Model 1', 'Assembly 1', 'Polymer', 'Ligand', 'Water', and 'Unit Cell'. The top right panel, 'Structure Tools', shows the 'Structure' tab with details for '1TQN | Crystal Structure of Human ...'. The 'Measurements' section is expanded, and 'Hydrophobicity' is highlighted with a red circle. The 'Components' section shows the 'Polymer' component selected. The bottom status bar shows recent updates to the cartoon representation.

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

MALYGTSHSHGLFKLGI PGPTLPLPFLGNILSYHKGFCMFDMECHKKYGKWVFDGQQVLAITDPPMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEENKRLRSLLSPTFTSGKLRKEMWPIIAQYGDVLRNLRREAETGKPVILKDVFGAYSMDVITSTISFGVNISSLNPNQDFFVENTKLLRFDF
LDPFFLSITVFPFLIPILVNLNLCVFPREVINFLRKSVMKMKESRLSDTKQHRVDFLQMLIDSQNSKETESHKALSDELVAQSIIIFAGYETISS

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Ass...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset + Add

Polymer Cartoon

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

Ligand Ball & Stick

Water Ball & Stick

Unit Cell 1 2 2

16:37:57 Updated Cartoon in 31ms.

16:38:35 Updated Cartoon in 8ms.

16:38:48 Updated Cartoon in 28ms.

Vizualizace anotací

Obarvení podle vlastností - hydrofobicita

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central view shows the protein structure colored by hydrophobicity, with a color scale from blue (hydrophilic) to red (hydrophobic). The interface includes a State Tree on the left, a sequence viewer at the top, and a Structure Tools panel on the right. A log at the bottom shows update times for the cartoon representation.

State Tree:

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

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

```
MALYGIHSHGLFKLGIIPGPTLPFLGNILSYHKGFDMCECHKYGRWGFYDGGQPVLAITDPDMIKTVLVKECYSVETNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLRKEMVPIIAQYGDVLRNLRREAETGKPVTLKQVFGAYSMVDVITSTSGVNI DLSLNNPQDPFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNICVFPREVTFNFLRKSVMKESRLEDTQKHRVDFLQLMIDSQNSKETE SHKALSDLELVAQSIIFTFAGYETTS
```

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset + Add

Polymer Cartoon

Ligand Ball & Stick

Water Ball & Stick

Unit Cell | 2 2 2

Volume Streaming 1TQN

Enable

Assembly Symmetry 1TQN

Enable

Export Animation

16:38:35 Updated Cartoon in 8ms.

16:38:48 Updated Cartoon in 28ms.

16:40:29 Updated Cartoon in 32ms.

Vizualizace anotací

Obarvení podle vlastností – kvalita

The screenshot displays the Mol* Viewer interface for the protein structure 1TQN. The central view shows the protein as a green cartoon ribbon. The left sidebar contains a 'State Tree' with the following items:

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

The top of the interface shows the sequence of the protein: 1TQN | Crystal... 1: cytochrome... A. The sequence is displayed in a multi-line format with residue numbers 32, 42, 52, 62, 72, 82, 92, 102, 112, 122, 132, 142, 152, 162, 172, 182, 192, 202, 212, 222, 232, 242, 252, 262, 272, 282, 292, 302, 312, 322.

The right sidebar contains the 'Structure Tools' panel. The 'Structure' section shows the protein name '1TQN | Crystal Structure of Human ...'. The 'Measurements' section has a '+ Add' button. The 'Components' section shows '1TQN' with a 'Preset' button and '+ Add' and '⌵' icons. The 'Polymer' section is expanded to show 'Cartoon' representation. Under 'Uncertainty/Disorder', the 'Structure Quality Report' is highlighted with a red circle. Other options include 'Chain Property', 'Miscellaneous', 'Residue Property', 'Symmetry', 'Validation', 'Density Fit', 'Geometry Quality', 'Modify by Selection', 'Select This', and 'Edit Label'. The 'Cartoon Representation' section has a trash icon and an eye icon. The 'Ligand' and 'Water' sections show 'Ball & Stick' representation with eye and trash icons.

The bottom of the interface shows a timeline of updates:

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

Vizualizace anotací

Obarvení podle vlastností - kvalita

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

```
MALYGTSHGFLFKLGI PGPTLPFLGNILSYHKGF C MFDMECHKKYGK WGFYD GQQPVLAI TDPDMIKT VLVKECYSVPTNRRPFGVGF M KSAI
SIAEDEEWKRLRSLLSPTFTSGK LKEMVPI IAQYGDV LVRNLRREAETGKPV LKDVFGAYSMDVITSTSGVWNIDSLNNPQDFFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNLCVFPREVINFLAKSVKRMKRESRLDITQRHRVDFLQMLIDISQNSKETESHKALSDELVAQSIIIFAGYETTSS
```

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset	+ Add	☰	↻
Polymer	Cartoon	☑	🗑
Ligand	Ball & Stick	☑	🗑
Water	Ball & Stick	☑	🗑
Unit Cell 2 2 2		🗑	...

Volume Streaming 1TQN

☑ Enable ☰

Assembly Symmetry 1TQN

☑ Enable

Export Animation

16:47:43 Updated Cartoon in 9ms.

16:47:52 Updated Cartoon in 11ms.

16:51:37 Updated Cartoon in 25ms.

Vizualizace proteinových assemblies

The screenshot displays the Mol* web application interface. The main window shows a 3D visualization of a protein assembly (3J3Q) with a Gaussian surface representation. 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 and update of the polymer and Gaussian surface.

State Tree:

- 3J3Q 1 model
 - Model 1
 - Assembly 1 2440800 elements
 - Polymer 2440800 elements
 - Gaussian Surface

Sequence of 3J3Q | Atomic-level structure of the ...

```
1  EIVONLQGMVHQAI11SPRILN21AWVKVVEEKAF31SPEVIMF41SALSEGAT51POD61INTMLNT71VGGHQ81AAMQMLKET91INEEA101AEW111DR121LHPVHAG131PIEPGQMR  
E101PRGSDIAGT111TSTLQE121QIGW131MTHN141PP151IPVGE161IYK171RW181IILGLN191KIV201MYSP211TSILD221IRQ231GPK241EP251FRDY261VDR271FYK281TLRAEQ291ASQEV301IGNW311MTET321LLV331ONA  
NP201DCK211TIL221KALG231PAAT241LEEM251TAC261QGV271GG281PG291H301K311AR321VL
```

Structure Tools:

- Structure**
 - 3J3Q | Atomic-level structure of the ...
 - Type: Assembly
 - Asm Id: 1: Author Defined Asse...
 - Nothing Focused
- Measurements**
 - + Add
- Components** (3J3Q)
 - Preset + Add
 - Polymer Gaussian Surface
- Volume Streaming** (3J3Q)
 - Enable
- Assembly Symmetry** (3J3Q)
 - Enable
- Export Animation**

Log:

- 16:54:29 Created Polymer in 110ms.
- 16:54:34 Created Gaussian Surface in 4.661s.
- 16:54:34 Updated Structure Focus Representation in 2ms.

Měření

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows a green ball-and-stick model of the protein structure. 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 protein sequence: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKAVGFDGQPVLAITDPDMIKTVLVKECVSVETNRRPFGPVGFMKSAI SIAEDEENKRLRSLLSPTFTSGKLEMPVPIIAQYGDVLRNLRREAEETGKPVTLKDFGAYSMDEVITSTSEGVNIDSLNPNQDPPEVENTKKLLRDFD LDPFFLSITVFPFLIPILEVLNICVFPREVTFNLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS. The left sidebar contains a State Tree with categories like 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Ligand (49 elements), Water (190 elements), and Measurements. The right sidebar shows Structure Tools and a list of components including Polymer, Ligand, Water, and Unit Cell. A log at the bottom shows recent actions: 'Created Ball & Stick in 23ms', 'Created Ball & Stick in 11ms', and 'Updated Structure Focus Representation in 2ms'.

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

MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKAVGFDGQPVLAITDPDMIKTVLVKECVSVETNRRPFGPVGFMKSAI
SIAEDEENKRLRSLLSPTFTSGKLEMPVPIIAQYGDVLRNLRREAEETGKPVTLKDFGAYSMDEVITSTSEGVNIDSLNPNQDPPEVENTKKLLRDFD
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 1TQN. The central 3D view shows the protein structure in a green cartoon representation, with red dots indicating hydrophobic residues. 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 1 2 2 2

Příkládání struktur

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

On the left side, the "Home" menu is open, showing the "Download Structure" section. The "PDB Id(s)" field contains the text "2h7s 2rfc", which is circled in red. Below this field, there is an "Apply" button with a checkmark icon. Other options in the menu include "Add Trajectory", "Download Density", "Download File", "Open Files", "Download", "Load CellPack", and "Load Genome 3D (G3D)".

At the bottom of the left sidebar, there is a "Remote States" section with a list of entries: "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", "Measurements", "Components", and "Export Animation". The "Structure" section shows "Nothing Loaded" and "Nothing Focused".

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

Příkládání struktur

The screenshot displays the Mol* Viewer interface. The central 3D view shows a protein structure with two chains: one in green and one in purple. The structure is rendered as a ribbon with ball-and-stick representations of atoms. A red circle highlights the 'Focus' icon in the right-hand toolbar. The left sidebar contains a 'State Tree' with a hierarchical view of the loaded data, including two models (2H7S and 2RFC) and their respective assemblies, polymers, ligands, and water molecules. The top of the interface shows the sequence of the protein, '1: Cytochrome...', with residue numbers and amino acid codes. The bottom status bar shows a log of recent actions, such as 'Created Ball & Stick in 18ms.' and 'Updated Structure Focus Representation in 2ms.'

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

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

Příkladání struktur

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

- State Tree (Left):** A hierarchical tree view showing the loaded structures: 2H7S 1 model, Model 1, Assembly 1 (3355 elements), Polymer (3201 elements), Ligand (49 elements), Water (111 elements), and Unit Cell P 1 21 1. Below this, 2RFC 1 model and its components are also listed.
- Sequence Viewer (Top):** Shows the amino acid sequence for Cytochrome c (P1: 214A). The sequence is: `TTETIQSNANLAPLPPHVPHELVDFDMYNFNSLSAGVQEAMAVLQESNVDFLWTRCNGGHWIATRGQLIREAYEDYRHFSSSECFPIPREAGEAYD` (with some residues highlighted in yellow). Below the sequence is a toolbar with icons for 'Residue', 'Cartoon', 'Ball & Stick', 'Water', 'Ligand', 'Unit Cell', and 'Focus'.
- 3D View (Center):** A 3D ribbon representation of the protein structure, colored in shades of green and purple. A red circle highlights the 'Residue' button in the toolbar above the view.
- Structure Tools (Right):** A panel with various tools and settings:
 - Structure:** Shows 2 structures, with 'Nothing Focused' selected.
 - Measurements:** Includes an 'Add' button.
 - Superposition:** Options for 'By Chains' and 'By Atoms'.
 - Components:** Lists 'Polymer' (Cartoon), 'Ligand' (Ball & Stick), and 'Water' (Ball & Stick). It also shows '2 Unit Cells'.
 - Export Animation:** A section for exporting the structure.

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

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

Příkládání struktur

The screenshot displays the Mol* web application interface. The main window shows a protein structure (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. The right sidebar contains 'Structure Tools' and a 'Structure' panel showing 2 structures. The bottom panel shows a log of actions.

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

```
TTETIQSNANLAPLPPHVPHEHLVDFDMDYNFNSLGSAGVQEAWAVLQESNVFDLWVTRCNGGHWIATRGQLIREAYEDYRHFSSSECFIPREAGEAYD  
FIPTSMDFPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRAPOGQCNTEDYAEPPPIRIFMLLAGLPEEDIHPLKYLTDQMTRPDGSMITFA  
EAKREALYDYLPIIEIQRKQPGTDAISIVANGQVNGRPIITSDEAKRMCGALLVGGDLTVVNFSLFSMEFLAKSPEHRQELIERPERIPRACEELLR
```

Structure Tools

- Structure (2 structures)
- Measurements (+ Add)
- Superposition (By Chains, By Atoms)
- Components (2 structures)
- Export Animation

Log:

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

Příkladání struktur

The screenshot displays the Mol* Viewer interface with a protein structure loaded. The main window shows a ribbon representation of the protein in green. A context menu is open over the structure, with the 'Backbone' option highlighted by a red circle. The menu includes options for 'Residue', 'Add/Union Selection', 'All', 'Polymer/Carbohydrate Entities', 'Ligand/Non-standard Residue', 'Type', 'Structure Property', 'Trace', 'Backbone', 'Sidechain', 'Sidechain with Trace', 'Helix', 'Beta Strand/Sheet', and 'Bond Property'. The left sidebar shows a 'State Tree' with a hierarchy of models and assemblies. The right sidebar contains 'Structure Tools' and a list of components including 'Polymer', 'Ligand', and 'Water'. The top of the browser window shows the URL 'molstar.org/viewer/' and the protein sequence: 'Sequence of 2H7S | L244A ... 1: Cytochrome...'. The bottom status bar shows recent actions: 'Created Ball & Stick in 18ms.', 'Created Ball & Stick in 4ms.', and 'Updated Structure Focus Representation in 2ms.'

Příkladání struktur

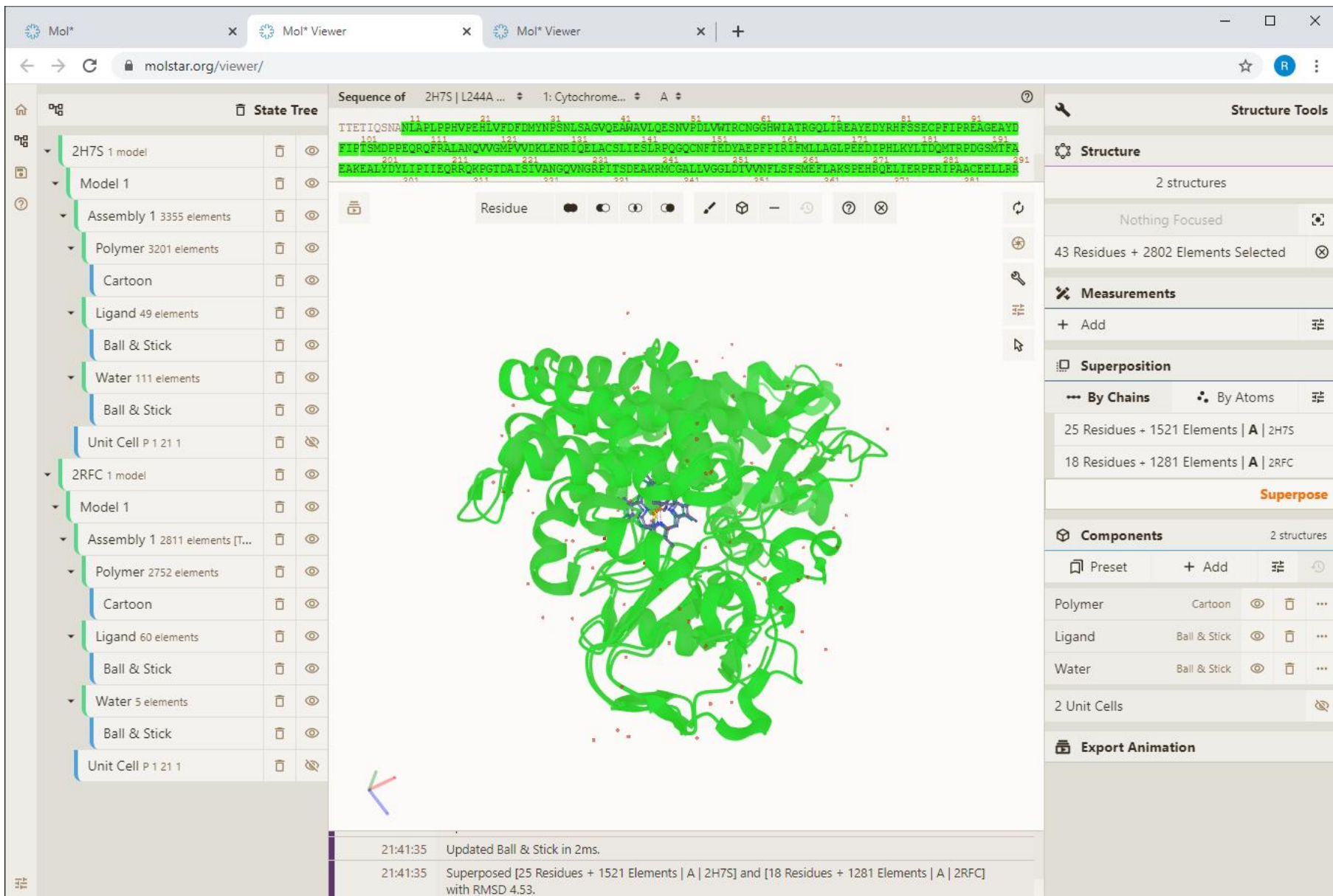
The screenshot displays the Mol* Viewer interface. On the left is the State Tree, listing models and their components. The top center shows the protein sequence: `TTETIQSN...NIAPLPPHVF...FD...DMYNP...NSAGV...QEA...AVLQES...NVP...DLVW...TRC...NGGHWI...TRG...QLI...REAYEDY...RHF...SSEC...PFIP...REAGEAYD...FIPTSM...DPPE...QRQ...FRALAN...QV...GMF...VVD...KLEN...RI...QELAC...SL...IES...LAP...QGC...NF...TEDY...AEP...PPI...RIF...EM...LAG...LPE...EDI...SH...LKY...LTD...QM...TR...PD...GSM...TF...EAK...EAL...DY...LIL...E...ITE...QR...R...K...PG...T...DAI...SIV...ANG...QV...N...GR...P...ITS...DE...AK...RM...OG...ALL...V...GG...LDI...V...VN...FL...S...F...S...ME...FL...AK...S...PE...HR...Q...EL...I...ER...PER...I...PA...ACE...ELL...AR`. The central view shows a green cartoon protein structure with a blue ligand. The right panel shows 'Structure Tools' with 'Structure' selected, displaying '2 structures' and '43 Residues + 2802 Elements Selected'. The 'Superposition' panel has 'By Chains' selected and circled in red. The 'Components' panel lists 'Polymer', 'Ligand', and 'Water'. A log at the bottom shows: '21:31:10 Created Ball & Stick in 18ms.', '21:31:10 Created Ball & Stick in 4ms.', and '21:31:10 Updated Structure Focus Representation in 2ms.'

Příkládání struktur

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

- State Tree (Left):** A hierarchical tree showing the structure's components, including 2H7S 1 model, Model 1, Assembly 1 (3355 elements), Polymer (3201 elements), Ligand (49 elements), Water (111 elements), and Unit Cell P 1 21 1.
- Sequence Viewer (Top):** Shows the amino acid sequence of the protein, with a green highlight on a specific segment: `TTETIQSN...NLAFLPPHVPEHLVDFDMYNF...SAGVQERMAV...LQESN...VFDLVMTRCNGGHWIATRGQLREAYEDYRHF...SSECFFIPREAGEAY...FIFISMDPPPEQRQFRALANQVVGMPVWIKLENRIQELACSLIESLRPQGQCNFTEDYAEPPFIRAF...MILLAGLPEDIPHLKYLTDQMTIRPDGSMIF...EMPEALYDYLPIITEORROKPGTDAISIVANGQVNGRPI...TSDAQRMGOGALLVGGLDIVVNF...LFSFMEFLAKSPEHQELIERPERIPACEELLER`
- Structure Tools (Right):** A panel with various tools for interacting with the structure. The 'Superposition' section is highlighted with a red circle around the 'Superpose' button.
- Structure Panel (Right):** Shows the current structure (2 structures) and provides details for the selected structure (43 Residues + 2802 Elements Selected).
- Components Panel (Right):** Lists the components of the structure, including Polymer (Cartoon), Ligand (Ball & Stick), Water (Ball & Stick), and 2 Unit Cells.
- Log (Bottom):** A log of recent actions, such as 'Created Ball & Stick in 18ms.' and 'Updated Structure Focus Representation in 2ms.'

Příkládání struktur



Mol* Mol* Viewer Mol* Viewer

molstar.org/viewer/

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 D 11 N L A P L P P H V P E R L V F D F D M Y N F S N L S A G V Q E A P 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 R H F S S E G P F I P R E A G E A Y D 21
101 F I F T S M D P P E Q R Q F R A L A N Q V G M F V V D K L E N R I Q E L A C S L T E S L R P Q S C N F T E D Y A E P F I R I F M L L A G L P R E E D I P H L K V L I D Q M T R P D G S M T E 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 E 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 P L A K S P E H R Q E L T E R P E R I P A A C E E L L R R 251
```

Residue

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

Polymer Cartoon

Ligand Ball & Stick

Water Ball & Stick

2 Unit Cells

Export Animation

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 viewing and manipulating molecular structures. The main window shows a protein structure (Cytochrome P450) rendered as a ribbon. The left sidebar contains a 'State Tree' with the following items:

- 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

The top right of the interface shows the 'Structure Tools' panel with the following sections:

 - 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**

The bottom status bar shows the following information:

 - 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.

2DProts: Integration of AlphaFoldDB

AlphaFold Protein Structure Database

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AlphaFold Protein Structure Database

Developed by DeepMind and EMBL-EBI

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

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

Feedback on structure: Contact DeepMind

2DProts: Integration of AlphaFoldDB

AlphaFold Protein Structure Database

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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

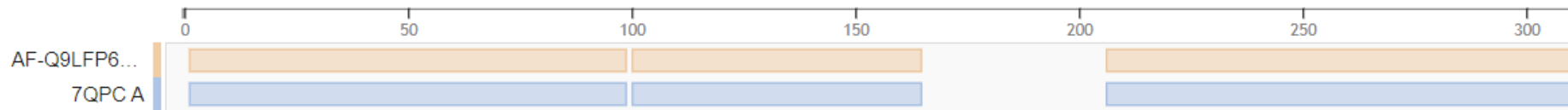
[Help](#)

▸ 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

