



CEITEC



Central European Institute of Technology  
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# Vizualizace proteinů a ligandů



EUROPEAN UNION  
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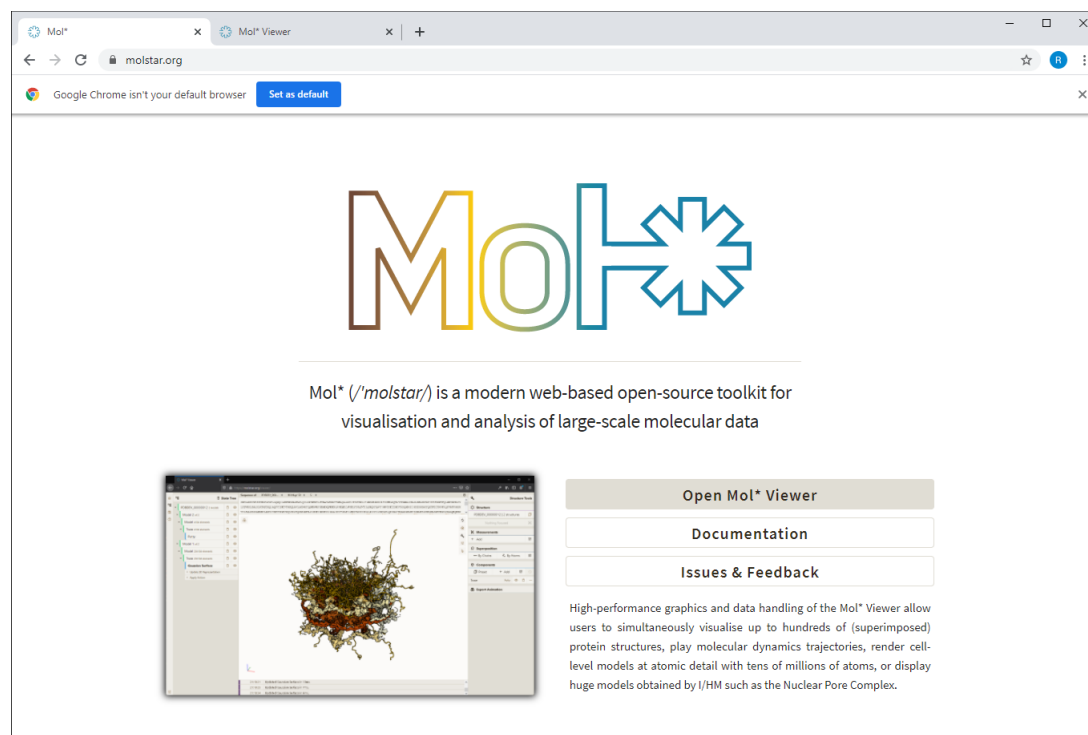


**OP Research and  
Development for Innovation**



# MolStar

- Webová aplikace pro vizualizaci proteinů a ligandů
- Zvládá i extrémně velké systémy
- Integrovaný v Protein Data Bank
- Vytvořený u nás v Národním centru pro výzkum biomolekul, ve spolupráci s EMBL EBI a RCSB PDB
- <https://molstar.org/>



Mol\* (*molstar*) is a modern web-based open-source toolkit for visualisation and analysis of large-scale molecular data

Open Mol\* Viewer

Documentation

Issues & Feedback

High-performance graphics and data handling of the Mol\* Viewer allow users to simultaneously visualise up to hundreds of (superimposed) protein structures, play molecular dynamics trajectories, render cell-level models at atomic detail with tens of millions of atoms, or display huge models obtained by I/HM such as the Nuclear Pore Complex.

# MolStar

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

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

- Download Structure**: Includes a table with columns "Source" (PDB) and "PDB Id(s)" (1tqn). Below the table is an "Options" section with a refresh icon and a red circle highlighting the "Apply" button.
- Add Trajectory**
- Download Density**
- Download File**
- Open Files**
- Download**
- Load CellPack**
- Load Genome 3D (G3D)**

Below these sections is a "Remote States" list with the following entries:

- Nuclear Pore Complex
- NPC-CIF
- 1RB8 Annotated Assembly
- Zika+EM
- Cytochromes Superposition
- AS
- ASX
- ASX-1 Something

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

# Vizualizace 3D souřadnic molekuly

## Vizualizační model cartoon

The screenshot displays the Mol\* Viewer interface for the protein structure 1TQN. The central 3D view shows the protein structure in a green cartoon representation, with a red ball-and-stick model of a ligand bound to 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.

**State Tree:**

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

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

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

**Structure Tools:**

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

**Log:**

- 14:36:24 Created Ball & Stick in 19ms.
- 14:36:24 Created Ball & Stick in 19ms.
- 14:36:24 Updated Structure Focus Representation in 2ms.

# Vizualizace 3D souřadnic molekuly

## Volba vizualizačních modelů

The screenshot displays the Mol\* Viewer interface for the protein 1TQN. The central 3D view shows the protein structure in a green cartoon representation. The left sidebar (State Tree) lists the hierarchy: 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 top panel shows the sequence of the protein: MALYGTSHSHGLFKKLGIPGPTLPLPFLGNILSYHKGFDMCECHKKYGKWNQFYDGOQVLAITDPPMIKIVLVKECYSVFNRRPFGVGFMSAI SIAEDEEWKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVIVRNLRREARETGKQVTLKDVFGAYSMDVITTSISFGVNIDSLNPFQDPFVENTKGLLRDFD LDPFFLSITVFPFLIPFILEVLNICVFRREVINFLRKSVKRMKESRLDTPKQHRVDFLQMLMDSQNSKETESHKALSDELVAQSIIFIPAGYETTSS. The right sidebar (Structure Tools) shows the 'Structure' panel with the protein name '1TQN | Crystal Structure of Human ...'. Below it, the 'Measurements' and 'Components' panels are visible. The 'Components' panel shows the 'Polymer' component selected, and the 'Ball & Stick' representation is highlighted in red. The bottom status bar shows the following actions: 14:36:24 Created Ball & Stick in 19ms., 14:36:24 Created Ball & Stick in 19ms., and 14:36:24 Updated Structure Focus Representation in 2ms.

# Vizualizace 3D souřadnic molekuly

## Vizualizační model Ball & Stick

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

```
MALYGTSHGGLFKLGI PGPTPLPFLGNILSYHKGFDMFDMCHCKYKGVWGFYDQQPVLAITDPDMIKTVLVKECYSVPTNRRPFGVGFYKSR I
SIAEDEEWKRLRSLSPFTTSGKLEKMPV IIAQYGDVLRNLRREAEETGKPVTLKDVFGAYSMDVITSTSGVNIIDSLNPNQDFFVENTKLLRDFD
LDPFFLSIIVFPFLIPFILEVNI CVPREVINFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSONSKETESHKALSDELVAQSIIPFAGYETTSS
```

State Tree

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

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset	+ Add		
Polymer	2 reprs		...
Ligand	Ball & Stick		...
Water	Ball & Stick		...

Unit Cell | 2 2 2

Volume Streaming 1TQN

✓ Enable

Assembly Symmetry 1TQN

✓ Enable

Export Animation

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

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

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

Pozor, ostatní  
módy je nutno  
vypnout

# Vizualizace 3D souřadic molekuly

## Vizualizační model Line

The screenshot displays the Mol\* Viewer interface for the protein structure 1TQN. The central 3D view shows the protein backbone as a green line with red and blue atoms. The left sidebar (State Tree) lists the hierarchy: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), Cartoon, Ball & Stick, Line (selected), Ligand (49 elements), Water (190 elements), and Unit Cell (2 2 2). The top sequence viewer shows the amino acid sequence: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKWWGFYDQQPVLAITDPDMIKTVLVKECYSVFINRRPFGVGFMKSAI SIAEDEEWKRLRSLSPFTSGKLEKEMVPIIAQYGDVLRNLRREAEETGKPVILKDVFGAYSMDVITSTSGVNIIDSLNPNQDFFVENTIKLLRDFD LDFPFLSITVFPFLIPIILEVLNICVFPREVINFLRKSVKRMKESRLÉDTQKHRVDFLQMLMIDSONSKETESHKALSDELVAQSIIIFAGYETTSS. The right panel (Structure Tools) shows the structure name '1TQN | Crystal Structure of Human ...', assembly type, and a list of components: Polymer (3 reprs), Ligand (Ball & Stick), Water (Ball & Stick), and Unit Cell (2 2 2). The bottom log shows: 14:36:24 Updated Structure Focus Representation in 2ms. 14:41:17 Created Ball & Stick in 255ms. 14:53:35 Created Line in 53ms.

# Vizualizace 3D souřadic molekuly

## Vizualizační model Putty

The screenshot displays the Mol\* Viewer interface. The central 3D view shows a protein structure (1TQN) rendered in a green Putty style. The left sidebar contains a State Tree with the following items:

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

The top of the interface shows the sequence of the protein: 1TQN | Crystal... 1: cytochrome... A. The sequence is: `MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYKGVWGFYDQQPVLAITDPMIKIVLVKECYSVFTNRRPFGVGFMKSAI`  
`SIAEDEEWKRLRSLSPFTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSPGVNIDSLNPNQDPPFVENTKLLRDFD`  
`LDPPFLSITVFPFLIPILEVLNICVFPREVINFLRKSVMKESRLEDTQKHRVDFLQMLIDSONSKETESHKALSDELVAQSIIIFAGYETTSS`

The right sidebar contains the Structure Tools panel, which includes sections for Structure, Measurements, Components, Volume Streaming, Assembly Symmetry, and Export Animation. The Components section lists: Polymer (4 reprs), Ligand (Ball & Stick), Water (Ball & Stick), and Unit Cell | 2 2 2.

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

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



# Vizualizace 3D souřadnic molekuly

## Vizualizační model Spacefil

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

```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKKYGKWFYDGOQPVLAITDDPMIKIVLVKCYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLSPFTTSGKIKEMVPIIAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSGVNIIDSLNPNQDPEVENTKGLLRDFD
LDPFFLSITVFFFLIPILEVLNICVFFPREVINFLRKSVMKRESLEDTQKHRVDFLQMLIDSONSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

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 for the protein 1TQN. The central view shows a green molecular surface representation of the protein. 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: MALYGT HSHGLFKKLSIPGPTLPFLGNILSYHKGF C MFDMECHHKYKQWGFYDSQQVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFMSAI SIAEDEEWKRLRSLLSPTFTSGKLEKMPVIAQYGDVLRNLRREAEATGKPVILKDVFGAYSMQVITSTSGVGNIDSLNPPQDFVENTKLLRDF LDPFFLSITVFPFLIPILEVLNICVFPREVINF LRKSVKRMKESRLDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETITSS.

The right sidebar contains the Structure Tools panel, which includes sections for Structure, Measurements, and Components. The Components section shows the Molecular Surface representation selected.

The bottom log 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 Surface

The screenshot displays the Mol\* Viewer interface for the protein 1TQN. The central view shows a green Gaussian Surface representation of the protein structure. The left sidebar contains a State Tree with the following items:

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

The top of the interface shows the sequence of the protein: MALYGTSHGLFKLGI... The right sidebar contains the Structure Tools panel, which includes sections for Structure, Measurements, and Components. The Components section shows the following items:

- 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

# Vizualizace povrchu molekuly

## Vizualizační model Gaussian Volume

The screenshot displays the Mol\* Viewer interface for the protein structure 1TQN. The central 3D view shows the protein backbone in a stick representation, surrounded by a red, semi-transparent Gaussian Volume mesh. The interface includes a State Tree on the left, a Structure Tools panel on the right, and a log at the bottom.

**State Tree:**

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

**Structure Tools:**

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

**Log:**

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

# Vizualizace experimentálních dat

## Elektronová hustota

The screenshot displays the Mol\* Viewer interface for the protein 1TQN. The central view shows the protein structure in green cartoon representation, surrounded by red dots representing electron density. 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

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

```
MALYGTSHSHGLFKKLGIPGFTPLPFLGNILSYHKGFCDMECHKKYKQWVFDGQQPVLAITDPMIKITVLVKECYSVFTNRRPFVGFVGMKSAI
123 132 142 152 162 172 182 192 202 212
SIAEDEEWKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVLRNLRREAEATGKPVILKDVFGAYSMDVITSTSGVNVDSLNNPQDPFVENTKLLRDF
222 232 242 252 262 272 282 292 302 312
LDPFFLSITIVFFFLIPILEVLMNICVFPREVINFLRKSVMKESRLEDIQKRVDFLQLMIDSQNSKETESHKALSDELVAQSIIFIFAGYETTSS
322 332 342 352 362 372 382 392 402
```

**Structure Tools:**

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

**Activity Log:**

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

# Vizualizace experimentálních dat

## Elektronová hustota

The screenshot displays the Mol\* Viewer interface for the protein 1TQN. The central 3D view shows the protein structure in green cartoon representation, surrounded by a red electron density map. The left sidebar shows the State Tree with the following items:

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

The right-hand panel shows the Structure Tools section, with the following options:

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

The 'Enable' checkbox under 'Volume Streaming' is highlighted with a red circle.

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

```
MALYGTHTSHGLFKKLGIPGFTPLPFLGNILSYHKGFCDPMECHKKYKQWVFDGQQPVLAITDPMIKITLVKECYSVFTNRRPFGVGFMSAI
123 132 142 152 162 172 182 192 202 212
SIAEDEEWKRLRSLLSPTFTSGKLEKMPVIIAQYGDVLRNLRREAEATGKPVILKDVFGAYSMQVITSTSGVNIIDSLNPNQDPFVENTKLLRDF
222 232 242 252 262 272 282 292 302 312
LDPFFLSITVFPFLIPILEVLMNICVFPREVINFLRKSVKRMKESRLEDTQKRVDFLQLMIDSQNSKETESHKALSDELVAQSIIFIFAGYETTSS
222 232 242 252 262 272 282 292 302 312
```

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 a green cartoon representation, surrounded by red dots representing electron density. 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), Ligand (49 elements), Water (190 elements), Volume Server 1tqn, Volume Streaming Selection, and Unit Cell I 2 2 2.
- Sequence Viewer (Top):** Shows the amino acid sequence of the protein with residue numbers (e.g., 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) and the corresponding sequence: `MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFCMDECHKKYGKVMGFYDQQQVLAITDPPMIKIVLVKECYSVFINRRPFGVGFVGMKSAI`
- Structure Tools (Right):** A control panel for the structure, including sections for Structure, Measurements, Components, Volume Streaming, and Assembly Symmetry.

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

Component	Value	Visibility
2Fo-Fc $\sigma$	1.5	Visible
Fo-Fc(+ve) $\sigma$	3	Visible
Fo-Fc(-ve) $\sigma$	-3	Visible

The bottom status bar shows the following updates:

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

# Vizualizace experimentálních dat

## Elektronová hustota

The screenshot displays the Mol\* Viewer interface for the protein structure 1TQN. The main view shows the protein in a green cartoon representation with electron density maps (Fo-Fc(+ve) and Fo-Fc(-ve)) shown as red and blue mesh 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 various toolbars and panels on the right. The Structure Tools panel on the right shows the Structure section with the following information:

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 $\sigma$	1.5
+ Fo-Fc(+ve) $\sigma$	3
+ Fo-Fc(-ve) $\sigma$	-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

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKYKWKWGFYDQQPVLAITDPDMIKTVLVEKCYSVFTNRRPFGVGFPMKSAI
SIAEDEEWKRLRSLSLSPFTTSGKLELMPVPIIAQYGVVLRNLRREARETGKQVTLKQVFGAYSMQVITSTSFQVNISSLNPPQDFVENTKLLRDF
LDPFFLSITVFFFLIPILEVLNLCVFFREVINFLRKSVKRMKESRLQEDTQKRVDFLQMLIDSONSKETESHKALSDELVAQSIIIFIFAGYETISS
```

15:28:06 Updated 1.5  $\sigma$  [2fo-fc] in 72ms.  
15:28:06 Updated 3  $\sigma$  [fo-fc(+ve)] in 30ms.  
15:28:06 Updated -3  $\sigma$  [fo-fc(-ve)] in 32ms.

Structure Tools	
<b>Structure</b>	
1TQN   Crystal Structure of Human ...	
Type	Assembly
Asm Id	1: Author Defined Ass...
HEM 508   B [auth A]	
<b>Measurements</b>	
+ Add	
<b>Components</b> 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
<b>Volume Streaming</b> 1TQN	
+ 2Fo-Fc $\sigma$	1.5
+ Fo-Fc(+ve) $\sigma$	3
+ Fo-Fc(-ve) $\sigma$	-3
Entry	1tqn
View	Around Focus
Nothing to Update	

# Vizualizace anotací

## Obarvení podle vlastností

The screenshot displays the Mol\* web application interface. The central 3D view shows a protein structure (1TQN) rendered in a green cartoon representation, with red dots indicating specific 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), Ball & Stick, Water (190 elements), Ball & Stick, and Unit Cell (2 2 2). The top panel shows the protein sequence: MALYGTSHSHGLFKLGI... The right sidebar, titled 'Structure Tools', contains a 'Structure' section for '1TQN | Crystal Structure of Human ...', a 'Measurements' section with an 'Add' button, and a 'Components' section for '1TQN'. The 'Hydrophobicity' property is circled in red in the 'Components' list. A log at the bottom shows updates to the cartoon representation.

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

# Vizualizace anotací

## Obarvení podle vlastností - hydrofobicita

The screenshot displays the Mol\* Viewer interface for the protein structure 1TQN. The central view shows a 3D ribbon representation of the protein, colored by hydrophobicity. The interface includes a State Tree on the left, a sequence viewer at the top, and a Structure Tools panel on the right.

**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**

```
MALYGIHSHGLFKKLGIPGPTLPFLGNILSYHKGFCEMFKKYGKVGFDGQPVLAITDPDMIKTVLVKECYSVETNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLSPFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSGVNI DLSLNNPQDPFVENTKLLRDF
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLLRKSVMKESRLEDYQKHRVDFLQLMIDSQNSKETE SHKALSDLELVAQSIIFPAGYETTS
```

**Structure Tools**

**Structure**

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

**Measurements**

+ Add

**Components** 1TQN

Preset + Add

Polymer Cartoon

Ligand Ball & Stick

Water Ball & Stick

Unit Cell | 2 2 2

**Volume Streaming** 1TQN

Enable

**Assembly Symmetry** 1TQN

Enable

**Export Animation**

16:38:35 Updated Cartoon in 8ms.

16:38:48 Updated Cartoon in 28ms.

16:40:29 Updated Cartoon in 32ms.

# Vizualizace anotací

## Obarvení podle vlastností – kvalita

The screenshot displays the Mol\* Viewer interface for the protein 1TQN. The central view shows a green ribbon representation of the protein structure, surrounded by red dots representing water molecules. The left sidebar contains a 'State Tree' with a tree view of the assembly and its components. The top right shows the 'Structure Tools' panel, and the bottom right shows the 'Components' panel with a 'Structure Quality Report' sub-panel highlighted by a red circle. The 'Structure Quality Report' panel lists various properties such as Chain Property, Miscellaneous, Residue Property, Symmetry, Validation, Density Fit, Geometry Quality, and Structure Quality Report. The 'Structure Quality Report' item is circled in red. The bottom status bar shows a log of updates: '16:46:40 Updated Cartoon in 557ms.', '16:47:43 Updated Cartoon in 9ms.', and '16:47:52 Updated Cartoon in 11ms.'

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

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

1TQN | Crystal Structure of Human ...

Type	Assembly
Asm Id	1: Author Defined Ass...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset + Add

Polymer Cartoon

- Uncertainty/Disorder
- Chain Property
- Miscellaneous
- Residue Property
- Symmetry
- Validation
- Density Fit
- Geometry Quality
- Structure Quality Report**
- Modify by Selection
- Select This
- Edit Label
- Cartoon Representation

Ligand Ball & Stick

Water Ball & Stick

Unit Cell 1 2 2 2

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 various tool panels 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**

```
MALYGTSHSHGLFKKLGIPGPTLPFLGNILSYHKGFDMCHKKYKGVWGFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVILKDVFGAYSMVDVITSTSGVWNIDSLNPNQDFFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLAKSVKRMKRESRLDTQKRVDFLQMLMIDSQNSKETESHKALSDELVAQSIIIFAGYETTSS
```

**Structure Tools:**

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

**Log:**

- 16:47:43 Updated Cartoon in 9ms.
- 16:47:52 Updated Cartoon in 11ms.
- 16:51:37 Updated Cartoon in 25ms.

# Vizualizace proteinových assemblies

The screenshot displays the Mol\* web application interface for visualizing a protein assembly. The central 3D view shows a protein structure with a multi-colored Gaussian surface representation. The interface is divided into several panels:

- State Tree (Left):** A hierarchical tree showing the loaded models and components: 3J3Q 1 model, Model 1, Assembly 1 (2440800 elements), Polymer (2440800 elements), and Gaussian Surface.
- Sequence Viewer (Top):** Displays the amino acid sequence for 3J3Q: `1 BIVNLOGQMVHQAI SPRTLNANVVKVVEEKAFSPVEIPMFSALSSEGATPODLNTMLNTVGGHQAAQMQLKETINEEAAEWDRLHPVHAGPIEPGQMR  
EPRGSDIAGTTSTLQEQIGWMTNHPPIPVGGEIYKRWIIILGLNKIVMYSPTSILDIRQGPKEPFRDYVDRFYKTLRAEQASQEVKQWMMTETLLVQNA  
NPDCKTILKALGPAATLEEMMTACQGVGGPGHKARVL`
- Structure Tools (Right):** A control panel for the structure, including sections for Structure, Measurements, Components, Volume Streaming, Assembly Symmetry, and Export Animation.
- Log (Bottom):** A timeline of actions: 16:54:29 Created Polymer in 110ms, 16:54:34 Created Gaussian Surface in 4.661s, and 16:54:34 Updated Structure Focus Representation in 2ms.

# Měření

The screenshot displays the Mol\* Viewer interface for a protein structure. The central view shows a green ball-and-stick model of a protein chain. A specific distance of 2.92 Å is highlighted between two atoms, with a dashed line and a label indicating the measurement. The top of the interface shows the sequence of the protein: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKWWGFYDGOQFVLAITDPMIKTVLVKECVSVFTNRRPFGVGFMSAI SIAEDEENKRLRSLSPFTISGKLEMPVPIIAQYGDVLRNLRREAEETGKPEVTLKDVFGAYSMDVITSTSGVNIIDSLNPNQDPPEVENTKKLLRDFD LDPFFLSITVFPFLIPILEVLNICVFPREVTFNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS. 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 'Measurements' with a list of distances, including the selected 2.92 Å. The bottom status bar shows recent actions: 'Created Ball & Stick in 23ms.', 'Created Ball & Stick in 11ms.', and 'Updated Structure Focus Representation in 2ms.'

# Vizualizace anotací

## Obarvení podle vlastností - hydrofobicita

The screenshot displays the Mol\* Viewer interface for the protein structure 1TQN. The central view shows a green ribbon representation of the protein, with a color scale at the bottom indicating hydrophobicity. The scale ranges from 0 (blue) to 1 (red), with a yellow intermediate. The protein structure is surrounded by red dots, likely representing water molecules or other residues.

**Sequence of 1TQN | Crystal...**

```
MALYGTSHSHGLFKLGI PGPTLPFLGNILSYHKGFCMFDMECHKKYGKVGWGFYDQQVLAITDPMIKTVLVKECVSVFTNRRPFGVGFMSAI  
SIAEDEEWKRLRSLLSPTFTSGKLEKMPVILIAQYGDVLRNLRRAEATGKPVILKDFGAYSMQVITSTSFGVNIQSLNPNQDFVENTKLLRDF  
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLRKSVKRMKESRLDITQKRRVDFLQMLIDQNSKETE SHKALSDELEVAQSIIFIFAGYEITTS
```

**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

**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
    - Symmetry
    - Validation
    - Density Fit
    - Geometry Quality
    - Structure Quality Report
    - Modify by Selection
    - Select This
    - Edit Label
    - Cartoon Representation
  - Ligand
    - Ball & Stick
  - Water
    - Ball & Stick
  - Unit Cell 1 2 2 2



# Příkládání struktur

The screenshot displays the Mol\* Viewer web application interface. The browser tabs at the top show 'Mol\*' and 'Mol\* Viewer'. The address bar contains 'molstar.org/viewer/'. The main interface is divided into several sections:

- Home:** A sidebar menu with a 'Download Structure' section. Under this section, the 'PDB Id (s)' field contains '2h7s 2rfc', which is circled in red. Below this field are 'Options' and an 'Apply' button. Other options include 'Add Trajectory', 'Download Density', 'Download File', 'Open Files', 'Download', 'Load CellPack', and 'Load Genome 3D (G3D)'. A 'Remote States' section lists various structures like 'Nuclear Pore Complex', 'NPC-CIF', '1RB8 Annotated Assembly', 'Zika+EM', 'Cytochromes Superposition', 'AS', 'ASX', and 'ASX-1 Something'.
- Sequence:** A central panel with the text 'No structure available'.
- Structure Tools:** A right-hand sidebar with sections for 'Structure' (Nothing Loaded), 'Measurements' (+ Add), 'Components' (Preset, + Add), and 'Export Animation'.

At the bottom of the interface, there is a status bar showing 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.

# Příkládání struktur

The screenshot displays the Mol\* Viewer interface. On the left, the State Tree shows a hierarchical view of the loaded data, including 2H7S 1 model, Model 1, Assembly 1 (3355 elements), Polymer (3201 elements), Cartoon, Ligand (49 elements), Water (111 elements), and Unit Cell P 1 21 1. The main view shows a protein structure in a ribbon representation, colored in green and purple. The right panel contains the Structure Tools menu, which is currently open. The 'Structure' icon is highlighted with a red circle. Below the menu, the 'Components' section shows two structures: Polymer (Cartoon) and Ligand (Ball & Stick). The bottom status bar shows a log of actions: 'Created Ball & Stick in 18ms.', 'Created Ball & Stick in 4ms.', and 'Updated Structure Focus Representation in 2ms.'

# Příkládání struktur

The screenshot displays the Mol\* web application interface. The browser address bar shows [molstar.org/viewer/](https://molstar.org/viewer/). The main window contains a protein structure visualization of Cytochrome P-450 (2H7S) and 2RFC, shown as a green ribbon structure with a purple ribbon structure overlaid. The structure is surrounded by red spheres representing water molecules. A red circle highlights the 'Residue' button in the top toolbar. The left sidebar shows a 'State Tree' with a hierarchical view of the loaded structures and their components. The right sidebar contains 'Structure Tools' and a 'Structure' panel with various options like 'Measurements', 'Superposition', and 'Components'. The bottom status bar shows recent actions: 'Created Ball & Stick in 18ms.', 'Created Ball & Stick in 4ms.', and 'Updated Structure Focus Representation in 2ms.'

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

TTETIQSNANLAPLPVPHVPEHLVDFDMYNFNSL SAGVQEAMAVLQESNVDFLWTRCNGGHWIATRGQLIREAYEDYRHFSSSECFPIPREAGEAYD  
FIPTSMDFPEQRFALANQVWGMFVVDKLENRIQELACSLIESLRPQGQCNFTEDYAEPPFIRIFMLLAGLPEDIPHLKYLTDQMTRPDGSMTFA  
EAKEALYDYLIPIIEQRQKPGTDAISIVANGQVNGRPI TSDEAKRMC GALLVGGLDIVVNFLSFSMEFLAKSPEHRQELIERPERIPACEELLAR

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 view 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 'Residue', 'Add/Union Selection', 'All', 'Polymer/Carbohydrate Entities', 'Ligand/Non-standard Residue', 'Type', 'Structure Property', '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 assemblies. The right sidebar contains 'Structure Tools' and a 'Structure' panel showing '2 structures'. 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.'

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

```
TTETIQSNANLAPLPPHVEHLVDFDMYNFNSLGSAGVQEAWAVLQESNVFDLWVTRCNGGHWIATRGQLIREAYEDYRHFSSSECFPIPREAGEAYD  
FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRAPOGQCNTEDYAEPPPIRIFMLLAGLPEEDIPHLKYLTDQMTRPDGSMTFA  
EAKEALYDYLIPPIEQRRQKPGTDAISIVANGQVNGRPITSDAQRKMGALLVGGDLTVNVLFSFSEFLAKSPEHRQELIERPERIPACEELLRR
```

# Příkladání struktur

The screenshot displays the Mol\* Viewer interface. The main window shows a protein structure in a ribbon representation, colored in shades of green and purple. A context menu is open over the structure, listing various selection options. The 'Backbone' option is highlighted with a red circle. The left sidebar shows a 'State Tree' with a hierarchy of models and assemblies. The top right panel contains 'Structure Tools' and a list of components. The bottom status bar shows recent actions.

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

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

Residue [Icons]

Add/Union Selection [X]

- All
- Polymer/Carbohydrate Entities
- Ligand/Non-standard Residue
- Type
- Structure Property
- Trace
  - Backbone**
  - Sidechain
  - Sidechain with Trace
  - Helix
  - Beta Strand/Sheet
- Bond Property

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

# Příkládání struktur

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

- State Tree (Left):** A hierarchical tree showing the loaded structures: 2H7S (1 model), Model 1, Assembly 1 (3355 elements), Polymer (3201 elements), Ligand (49 elements), Water (111 elements), and Unit Cell P 1 21 1. A second structure, 2RFC (1 model), is also listed with its own Model 1, Assembly 1 (2811 elements), Polymer (2752 elements), Ligand (60 elements), Water (5 elements), and Unit Cell P 1 21 1.
- Sequence Viewer (Top):** Shows the amino acid sequence of Cytochrome P-450 2H7S (residues 1-291) with a selection of residues highlighted in green.
- Structure Tools (Right):** A panel with sections for Structure, Measurements, Superposition, and Components. The 'By Chains' option in the Superposition section is highlighted with a red circle.
- 3D View (Center):** A green cartoon representation of the protein structure with a blue and red ligand bound in the active site.
- Log (Bottom):** A log showing 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 structure: 2H7S 1 model, Model 1, Assembly 1 (3355 elements), Polymer (3201 elements), Cartoon, Ligand (49 elements), Water (111 elements), Unit Cell P 1 21 1, 2RFC 1 model, Model 1, Assembly 1 (2811 elements), Polymer (2752 elements), Cartoon, Ligand (60 elements), Water (5 elements), and Unit Cell P 1 21 1.
- Sequence Viewer (Top):** Shows the amino acid sequence of Cytochrome c (2H7S | L244A ...). A segment of the sequence is highlighted in green: `TTETIQSN...NLAPLPPHVP...EHLVDFDMYNF...SNLSAGVQ...EAMAVLQESNV...FDLVMTRCNGGHWIATR...GQLREAYEDVRRHFSSECFPIPREAGEAY...LIF...SMDFPEQRQF...ALANQVVG...FVVDKLENRIQELACSLIESL...FPQQCNFTEDYAE...PFPIRIPMLLAGLPEEDIPHLK...YLTDOMIRPDGSMIF...EAKPEALYDYLPIITEQRORQ...FGTDAISIVANGQVNGR...PITSDEAKRMCGALLVGGLDIVVNF...LFSMEEFLAKSPEHRQELIERPERIPAAACEELLR...`
- Structure Tools (Right):** Contains panels for Structure (2 structures), Measurements, Superposition (By Chains, By Atoms), and Components (2 structures).
- Superposition Panel:** Shows two structures: 2H7S (25 Residues + 1521 Elements) and 2RFC (18 Residues + 1281 Elements). The 'Superpose' button is circled in red.
- Log (Bottom):** 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. The main window shows a protein structure in green cartoon representation with a blue ligand. The interface includes a State Tree on the left, a sequence viewer at the top, and a Structure Tools panel on the right. A log at the bottom shows the superposition of two structures with an RMSD of 4.53.

**State Tree:**

- 2H7S 1 model
  - Model 1
    - Assembly 1 3355 elements
      - Polymer 3201 elements
        - Cartoon
      - Ligand 49 elements
        - Ball & Stick
      - Water 111 elements
        - Ball & Stick
      - Unit Cell P 1 21 1
- 2RFC 1 model
  - Model 1
    - Assembly 1 2811 elements [T...]
      - Polymer 2752 elements
        - Cartoon
      - Ligand 60 elements
        - Ball & Stick
      - Water 5 elements
        - Ball & Stick
      - Unit Cell P 1 21 1

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

```
T T E T I Q S N E 11 N I A L F P P H V P E H I V F D F D N Y N F S N L S A G V Q E A N A V L Q E S N V P D L V W T R C N G S H W I A T R G Q L I R E A Y E D Y A H F S S E C P F I P R L A G E A N Y 81  
101 F I F T S M D P P E Q R Q P A L A N Q V V G M P V V D K L E N R I Q E L A C S L I E S L R P Q S Q C N F T E D Y A E F F I R I F M L L A G L P E E D I P H L K V L I D Q M T R P D G S M T F A 151  
201 E A K E A L Y D V L I P I T E Q R R K P G T D A I S I V A N G Q V N G R P I T S D E A K R M C G A L L V G G L D I V V N F L S F S M E F L A K S P E H S Q E L I E R P E R I P A A C E E L L R R 251
```

**Structure Tools:**

- Structure: 2 structures
- Nothing Focused
- 43 Residues + 2802 Elements Selected
- Measurements: + Add
- Superposition: By Chains, By Atoms
- 25 Residues + 1521 Elements | A | 2H7S
- 18 Residues + 1281 Elements | A | 2RFC
- Superpose
- Components: 2 structures
- Presets: + Add
- Polymer: Cartoon
- Ligand: Ball & Stick
- Water: Ball & Stick
- 2 Unit Cells
- Export Animation

**Log:**

- 21:41:35 Updated Ball & Stick in 2ms.
- 21:41:35 Superposed [25 Residues + 1521 Elements | A | 2H7S] and [18 Residues + 1281 Elements | A | 2RFC] with RMSD 4.53.



# Přikládání struktur

The screenshot displays the Mol\* web interface for a protein structure. The main view shows a ribbon representation of the protein structure, colored in green and purple, with a sequence viewer at the top. The sequence viewer shows the amino acid sequence: TTETIQSNANLAPLPPHVPHEHLVDFDMYNFNSLSAGVQEAQAVLQESNVDFLWVTRCNGGHWIATRGQLIREAYEDYRHFSSSECFPIPREAGEAYD... The interface includes a state tree on the left, a structure tools panel on the right, and a log at the bottom.

**State Tree**

- 2H7S 1 model
  - Model 1
    - Assembly 1 3355 elements
      - Polymer 3201 elements
        - Cartoon
        - Ligand 49 elements
          - Ball & Stick
        - Water 111 elements
          - Ball & Stick
      - Unit Cell P 1 21 1
- 2RFC 1 model
  - Model 1
    - Assembly 1 2811 elements [T...]
      - Polymer 2752 elements
        - Cartoon
        - Ligand 60 elements
          - Ball & Stick
        - Water 5 elements
          - Ball & Stick
      - Unit Cell P 1 21 1

**Structure Tools**

- Structure
  - 2 structures
  - Nothing Focused
- Measurements
  - + Add
- Superposition
  - By Chains
  - By Atoms
  - Add 2 or more selections (toggle mode) from separate structures. Selections must be limited to single polymer chains or residues therein.
- Components
  - 2 structures
  - Preset + Add
  - Polymer: Cartoon
  - Ligand: Ball & Stick
  - Water: Ball & Stick
  - 2 Unit Cells
- Export Animation

**Log**

- 21:41:35 Updated Ball & Stick in 2ms.
- 21:41:35 Superposed [25 Residues + 1521 Elements | A | 2H7S] and [18 Residues + 1281 Elements | A | 2RFC] with RMSD 4.53.

**Cytochrome P450-cam**  
2H7S | Model 1 | Instance ASM\_1 | A | ARG 290

# 2DProts: Integration of AlphaFoldDB

AlphaFold Protein Structure Database

Home About FAQs Downloads

# AlphaFold Protein Structure Database

Developed by DeepMind and EMBL-EBI

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

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

Feedback on structure: Contact DeepMind

# 2DProts: Integration of AlphaFoldDB

AlphaFold Protein Structure Database

Home About FAQs Downloads

AlphaFold DB provides open access to over 200 million protein structure predictions to accelerate scientific research.

Developed by DeepMind and EMBL-EBI

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

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

Feedback on structure: Contact DeepMind

# Přikládání struktur – PDB a AlphaFold

## Pairwise Structure Alignment

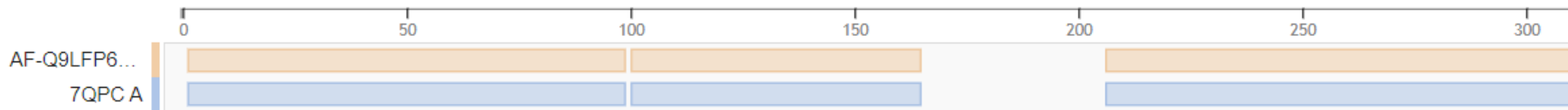
[Help](#)

▸ Compare Protein Structures

Entry ID	Chain ID	Description	Organism	Sequence Length	Modeled Residues
AF-Q9LFP6-F1	A	N/A	N/A	367	367
7QPC	A	Auxin efflux carrier component 8	Arabidopsis thaliana	376	327

**SEQUENCE ALIGNMENT**

SCORES



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

# Přikládání struktur – PDB a AlphaFold

