



CEITEC



Central European Institute of Technology  
BRNO | CZECH REPUBLIC

# Vizualizace proteinů a ligandů



EUROPEAN UNION  
EUROPEAN REGIONAL DEVELOPMENT FUND  
INVESTING IN YOUR FUTURE

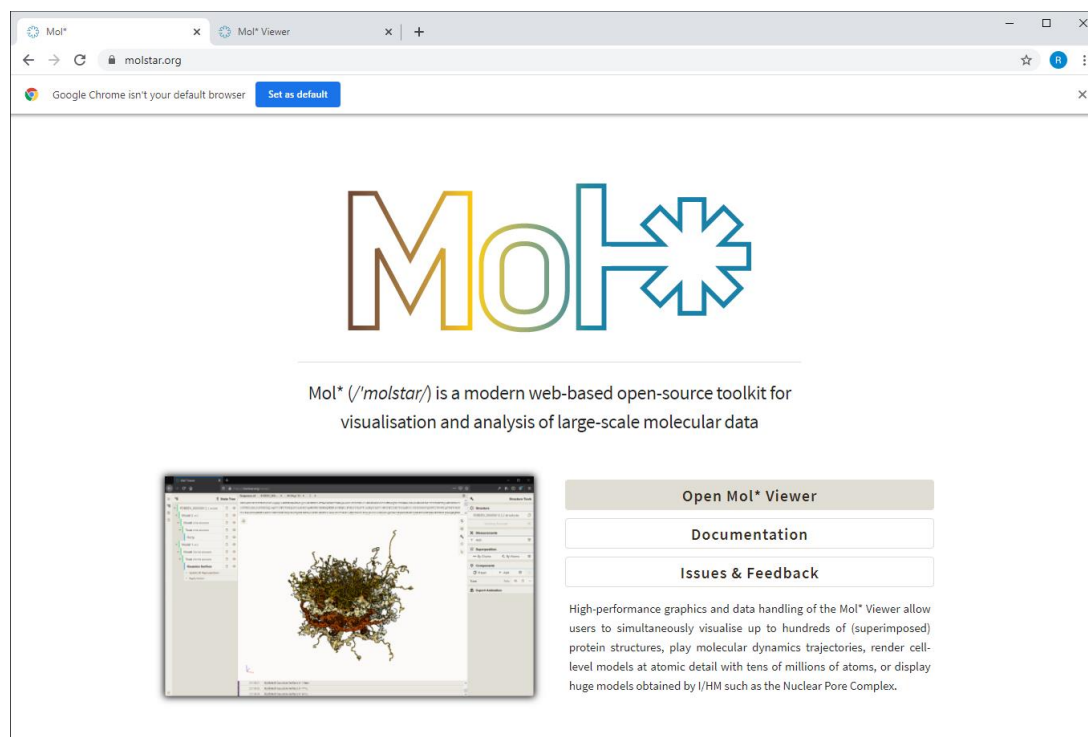


**OP Research and  
Development for Innovation**



# MolStar

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



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

[Open Mol\\* Viewer](#)

[Documentation](#)

[Issues & Feedback](#)

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

The screenshot displays the MolStar web application interface. The browser 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 around 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 souřadic molekuly

## Vizualizační model cartoon

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

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

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

**State Tree**

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

**Structure Tools**

**Structure**

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

**Measurements**

+ Add

**Components** 1TQN

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

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 Created Ball & Stick in 19ms.

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

# Vizualizace 3D souřadnic molekuly

## Volba vizualizačních modelů

The screenshot displays the Mol\* Viewer interface for the protein 1TQN. The central view shows a 3D model of the protein structure in a green cartoon representation. The left sidebar shows the State Tree with the following components:

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

The top of the interface shows the Sequence of 1TQN | Crystal... and the protein sequence: M A L Y G T H S H G L F K K L G I P G P T L P F L G N I L S Y H K G F C M F D M E C H K K Y G K W G F Y D G Q Q P V L A I T D P D M I K T V L V K E C Y S V F I N R R P F G F V G F M K S A I S I A E D E E W K R L R S L L S P T F T S G K L K E M V F I I A Q Y G D V L V R N L R R E A E T G K F V L K D V F G A Y S M D V I T T S T S F G V N I D S L N N F Q D P F V E N T K K L L R F D F L D P F F L S I T V F F L I P I L E V L N I C V F R E V I N F L R K S V K R M K E S R L E D T Q K H R V D F L Q L M I D S Q N S K E T E S H K A L S D L E L V A Q S I I F I P A G Y E T T S S. The right sidebar shows the Structure Tools panel with the following sections:

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

The bottom of the interface shows a log of actions:

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

# Vizualizace 3D souřadnic molekuly

## Vizualizační model Ball & Stick

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

```
MALYGTSHGSLFKLGI PGPTPLPFLGNILSYHKGFDMCHCKYKGVWGFYDQQPVLAITDPDMIKTVLVKCEYSVPTNRRPFVGFVGMKSR I  
SIAEDEEWKRLRSLLSPTFTSGKLEKMFIIAQYGDVLRNLRREAEITGKPVTLKDVFGAYSMDVITSTSFVGNIDSLNPNQDFFVENTKLLRDFD  
LDPFFLSIVFPFLIPILEVNICVFPREVINFLRKSVKRMKESRLEDTQKHRVDFLQMLMIDSONSKETESHKALSDELVAQSIIPFAGYETTSS
```

State Tree

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

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

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

Volume Streaming 1TQN

✓ Enable

Assembly Symmetry 1TQN

✓ Enable

Export Animation

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

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

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

Pozor, ostatní  
módy je nutno  
vypnout

# Vizualizace 3D souřadnic molekuly

## Vizualizační model Line

The screenshot displays the Mol\* Viewer interface for the protein 1TQN (Cytochrome c). The central 3D view shows the protein backbone in a green 'Line' representation. The left sidebar shows a 'State Tree' with the following structure:

- 1TQN 1 model
  - Model 1
    - Assembly 1 3999 elements
      - Polymer 3766 elements
        - Cartoon
        - Ball & Stick
        - Line
      - 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 1TQN | Crystal...' with the following amino acid sequence:

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKWWGFYDQQPVLAITDPDMIKTVLKECYSVFINRRPFGVGFMKSAI  
SIAEDEEWKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVLRNLRREARETGKPVILKDVFGAYSMDVITSTSGVNIIDSLNNPQDFPVENTIKGLLRDFD  
LDPFFLSITVFPFLIPIILEVLNICVFPREVNFRLKSVKRMKESRLDTPKHVDFLQMLIDSONSKETE SHKALSDELVAQSIIIFAGYETTSS
```

The right sidebar contains the 'Structure Tools' panel, which includes sections for 'Structure', 'Measurements', 'Components', 'Volume Streaming', and 'Assembly Symmetry'. The 'Components' section lists the following items:

Component	Representation	Visibility	Actions
Polymer	3 reprs	Visible	Hide, Delete, Refresh
Ligand	Ball & Stick	Visible	Hide, Delete, Refresh
Water	Ball & Stick	Visible	Hide, Delete, Refresh
Unit Cell 1 2 2 2		Visible	Hide, Delete, Refresh

The bottom log shows the following actions:

- 14:36:24 Updated Structure Focus Representation in 2ms.
- 14:41:17 Created Ball & Stick in 255ms.
- 14:53:35 Created Line in 53ms.

# Vizualizace 3D 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 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 recent actions.

**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 | 2 2 2

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

```
MALYGIHSHGLFKKLGIPGPTFLPFLGNILSYHMGFCMFDMECHKKYKGVWGFYDQQPVLAITDPMIKIVLVKECYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLSPFTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVTLKQVFGAYSMVDVITSTSPGVNIDSLNPNQDPPFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVNLICVFPREVINFLRKSVMKESRLEDTQKHRVDFLQMLIDSQNSKETESHKALSDELVQAQSIIFAGYETTSS
```

**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		...

Unit Cell | 2 2 2

**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

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

**State Tree:**

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

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

**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

**Log:**

- 14:53:35 Created Line in 53ms.
- 14:54:42 Created Putty in 90ms.
- 14:56:06 Created Spacefill in 26ms.

# Vizualizace povrchu molekuly

## Vizualizační model Molecular Surface

The screenshot displays the Mol\* Viewer interface. The central 3D view shows a protein structure with a green molecular surface representation. The left sidebar contains a 'State Tree' with the following items:

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

The top of the interface shows the sequence of the protein: 1TQN | Crystal... 1: cytochrome... A. The sequence is: MALYGTSHSHGLFKLGI PGPTLPFLGNILSYHKGFCMPDMECHKKYGKWWGFYDQQPVLAITDPDMIKTVLVKECVSVFTNRPRFGVGFMKSAI SIAEDEEWKRLRSLLSPTFTSGKLEKMPV IIAQYGDVLRNLRREAEETGKRVILKDVFGAYSMDEVITSTSGVNIIDSLNPPQDFVENTKLLRDF LDPFFLSITVFPFLIPILEVLNICVFPREVINFLRKSVMKRMKESRLEDTQKHRVDFLQLMIDSDQNSKETE SHKALSDELEVAQSIIFIFAGYETTSS. 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.

The right sidebar contains 'Structure Tools' and 'Structure' information for 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

# 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 | 2 2 2

The top right panel shows the Sequence of 1TQN | Crystal... with the following amino acid sequence:

```
MALYGTSHSHGLFYKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVGFDYDQQQVLAITDPDMIKTVLVKECVSVFTNRRPFGVGFMSAI  
SIAEDDEWKRRLRSLLSPTFTSGKLEMPVILIAQYGDVLRNLRREAEITGKPVILKQVFGAYSMQVITSTSGVNIIDSLNPNQDFFVENTKLLRDF  
LDPFFLSITVFPFLIPILEVNLICVFPREVINFRLKSVKRMKESRLEDITQKHRVDFLQMLMDSQNSKETESHKALSDELEVAQSIIFIFAGYETTSS
```

The right sidebar contains the Structure Tools panel, which includes the following sections:

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

The bottom status bar shows the following log entries:

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

# Vizualizace povrchu molekuly

## Vizualizační model Gaussian Volume

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

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

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

```
MLYGTHTSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKYKWKWGFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFVGVGPKMSAI
122 132 142 152 162 172 182 192 202 212
SIAEDEEWKRLRSLLSPTFTSGKLRKEMVPIIAQYGDVLRNLRREAETGKPVLRKDFGAYSMVITSTSEFVNIIDSLNPDQPFVENTKLLRDF
222 232 242 252 262 272 282 292 302 312
LDPFFLSITVFFFLIPILEVLNLCVFPREVINFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDELVAQSIIIFAGYETSS
```

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

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

The bottom status bar shows the following log entries:

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

# Vizualizace experimentálních dat

## Elektronová hustota

The screenshot displays the Mol\* Viewer interface for the 1TQN protein structure. The central 3D view shows the protein backbone as a green ribbon, with electron density represented by red and yellow 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
        - 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 HSHGLFKLGI PGFTPL PFLGNILSYHKGF C MFDMECHKKYGKWWF YDQQPVLAITDPD MIKTVL VKECYSVFTNRRPFGVGF M KSAI  
123 132 142 152 162 172 182 192 202 212  
SIAE DEEWKRLRSL SPTFTISGK LKEMVPIIAQYGDV LVRNLRREAE T GKPVILKDVFGAYSMDVITSTSFGVNI D SLNPNQD PFVENTK KLLRDF  
222 232 242 252 262 272 282 292 302 312  
LDPFFLSITVFFFLIPILEV LNICVFPREVINFLR KSVKRMKESRLEDI QKRVDFLQLMID SQNSKETESHKALS DLELVAQSIIFIFAGYETTSS  
222 232 242 252 262 272 282 292 302 312
```

**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:**

- 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 left sidebar shows the State Tree with the following structure:

- 1TQN 1 model
  - Model 1
    - Assembly 1 3999 elements
      - Polymer 3766 elements
        - Cartoon
      - Ligand 49 elements
        - Ball & Stick
      - Water 190 elements
        - Ball & Stick
      - Volume Server 1tqn
      - Volume Streaming Selec...
      - Unit Cell | 2 2 2

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

```
Sequence of 1TQN | Crystal... 1: cytochrome... A
MALYGTSHSHGLFKKLGIPGPTLPFLGNILSYHKGFCMFDMECHKKYGKVGFDGQQVLAITDIPDMIKTVLVKECYSVFINRRPFGVGFMKSAI
SIAEDEENKRLRSLSPFTFTSGKLEMPVPIIAQYGDVLRNLRREAEATGKPVTLKQVFGAYSMQVITSTISFGVNIIDSLNPNQDPEFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVNLICVFPREVINFLRKSVMKRESRLDTQKRVDFLQLMIDSONSKETE SHKALSDELELVAQSIIFIFAGYETTSS
```

The right sidebar contains the Structure Tools panel, which includes the following sections:

- Structure**
  - 1TQN | Crystal Structure of Human ...
  - Type: Assembly
  - Asm Id: 1: Author Defined Ass...
  - Nothing Focused
- Measurements**
  - + Add
- Components** (1TQN)
  - Preset: + Add
  - Polymer: Cartoon
  - 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

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. A red arrow points to a specific atom, with the text "Kliknout na vybraný atom" (Click on the selected atom) next to it. The interface includes a State Tree on the left, a Sequence of 1TQN | Crystal... at the top, and a Structure Tools panel on the right. The Structure Tools panel shows the Structure section with 1TQN | Crystal Structure of Human ... and the Measurements section with a list of measurements: 2Fo-Fc  $\sigma$  (1.5), Fo-Fc(+ve)  $\sigma$  (3), and Fo-Fc(-ve)  $\sigma$  (-3). The Volume Streaming section is also visible, showing the entry 1tqn and the view Around Focus.

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

MALYGTSHSGLFKGLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYKGVWGFYDGOQFVLAITDIPDMIKTVLVKECYSVFINRRPFGVGVGFMKSAI  
SIAEDEENKRLRSLSPFTFTSGKLEKMPVPIIAQYGVVLRNLRREAEATGKPVTLKDFVFGAYSMDEVITSTISFGVNIIDSLNPNQDFEVNTKLLRDFD  
LDPFFLSITVFPFLIPILEVLNLCVFPREVINFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSONSKETE SHKALSDELELVAQSIIFIFAGYETTSS

Kliknout na vybraný atom

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

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

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKYKWKWGFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRFPFGVGFMSAI
SIAEDEEWKRLRSLSPTFTSGKLEAVPIIAQYGVVLRNLRREAEITGKEVTLKQVFGAYSMDVITSTSFQVNISSLNPPQDFVENTKLLRDF
LDPFFLSITVFFFLIPILEVNI CVFPRVFNFLRKSVKRMKESRLÉDTQKHRVDFLQMLIDSONSKETE SHKALSDELVAQSII FIFAGYETISS
```

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

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 $\sigma$	<input type="checkbox"/>	1.5	<input type="checkbox"/>
+ Fo-Fc(+ve) $\sigma$	<input type="checkbox"/>	3	<input type="checkbox"/>
+ Fo-Fc(-ve) $\sigma$	<input type="checkbox"/>	-3	<input type="checkbox"/>

Entry 1tqn

View Around Focus

Nothing to Update

# Vizualizace anotací

## Obarvení podle vlastností

The screenshot displays the Mol\* web application interface. The central view shows a protein structure (1TQN) rendered as a green cartoon ribbon. The interface is divided into several panels:

- State Tree (Left):** A hierarchical list of the model's components, including '1TQN 1 model', 'Model 1', 'Assembly 1 3999 elements', 'Polymer 3766 elements', 'Cartoon', 'Ligand 49 elements', 'Ball & Stick', 'Water 190 elements', and 'Unit Cell 1 2.2.2'.
- Sequence Viewer (Top):** Shows the amino acid sequence of the protein: `MALYGTSHSHGLFKLGI PGPTLP LFLGNILSYHKGFCMFDMECHKKYGKWWFYDQQQVLAITDPDMIKTVLVKECYSVFTNRRFPVGFVGMKSAI SIAEDEENKRLRSLLSPTFTSGKLRKEMWPIIAQYGDVLRNLRREAETGKPVILKQVFGAYSMQVITSTISFGVNISSLNPNQDFFVENTKLLRDF LDPFFLSITVFPFLIPILVNLNICVFPREVINFLLRSVKRMKESRLEDTQKHRVDFLQMLIDSQNSKETESHKALSDELVAQSIIIFAGVETISS`. Residue numbers are indicated below the sequence.
- Structure Tools (Right):** A panel for interacting with the structure. It includes sections for 'Structure' (showing '1TQN | Crystal Structure of Human ...'), 'Measurements' (with an 'Add' button), and 'Components' (showing '1TQN'). Under 'Components', the 'Hydrophobicity' property is highlighted with a red circle.

At the bottom of the interface, a log shows recent updates: '16:37:57 Updated Cartoon in 31ms.', '16:38:35 Updated Cartoon in 8ms.', and '16:38:48 Updated Cartoon in 28ms.'

# Vizualizace anotací

## Obarvení podle vlastností - hydrofobicita

The screenshot displays the Mol\* Viewer interface for the protein structure 1TQN (Crystal Structure of Human Cytochrome c). The protein is visualized as a ribbon structure with a color gradient from green (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.

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

```
MALYGIHSHGLFKLGIPTLPFLGNILSYHKGFDMCKKYGKVGFDGQQPVLAITDPDMIKTVLVKECYSVETNRRPFGPVGFMKSAI  
SIAEDEEWKRLRSLSPFTSGKLEKEMVPIIAQYGDVIVNLRREAETGKPVTLKQVFGAYSMVDVITSTSGVNI DLSLNNPQDPFVENTKLLRDFD  
LDPFFLSITVFPFLIPILEVLNICVFPREVTFNFLRRSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETE 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

**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

**Log**

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

# Vizualizace anotací

## Obarvení podle vlastností – kvalita

The screenshot displays the Mol\* Viewer interface for the protein structure 1TQN. The central view shows the protein as a green cartoon ribbon. The left sidebar (State Tree) lists the hierarchy: 1TQN 1 model, Model 1, Assembly 1 (3999 elements), Polymer (3766 elements), and Water (190 elements). The top panel shows the protein sequence: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMCHKKYKWKWGFYDQQPVLAITDPDMIKTVLVKECYSVFINRRPFGVGFMKSAI... The right sidebar (Structure Tools) shows the 'Structure' section with '1TQN | Crystal Structure of Human ...' and 'Structure Quality Report' highlighted in red. The bottom log shows: 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 representation of the protein, colored by quality. The ribbon is primarily green and yellow, with some orange and red segments, indicating different quality levels. The protein is surrounded by water molecules shown as small red and white spheres.

**State Tree (Left Panel):**

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

**Sequence (Top):**

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

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

**Structure Tools (Right Panel):**

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

**Log (Bottom):**

- 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. At the top, the browser address bar shows `molstar.org/viewer/`. The main window is divided into several sections:

- State Tree (Left):** A hierarchical list of loaded models and components, including "3J3Q 1 model", "Model 1", "Assembly 1 2440800 elements", "Polymer 2440800 elements", and "Gaussian Surface".
- Sequence Viewer (Top):** Displays the amino acid sequence for protein 3J3Q, with residue numbers 1 through 231 indicated above the sequence. The sequence is: `1 BIVONLQGMVHQAI SPRTLNANVVKVVEEKAFSPVEVIMFSA LSEGATPODLNTMLNTVGGHQAA MQMLKETINEEA EWDR LHPVHAGPIEPGQMR  
101 EPRGSDIAGTTSTLQE QIGWMTNHPPIPVGGEIYKRWII LGLNKIVMYSPTSILDIRQGPKEPFRDYDRFYKTLRAEQASQEVKQWMMTETLLVQNA  
201 NPDKCTILKALGPARTLEEMMTACQGVGGPGHKARVL`
- 3D Visualization (Center):** A large, colorful 3D representation of the protein assembly, showing a dense, roughly spherical structure composed of many individual protein subunits.
- Structure Tools (Right):** A panel with various controls for the visualization, including "Structure" (3J3Q | Atomic-level structure of the ...), "Measurements", "Components" (3J3Q), "Volume Streaming" (3J3Q), and "Assembly Symmetry" (3J3Q).
- Log (Bottom):** A list of recent actions:
  - 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.



# 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 options like 'Download Structure', 'Add Trajectory', 'Download Density', 'Download File', 'Open Files', 'Download', 'Load CellPack', and 'Load Genome 3D (G3D)'. The 'Download Structure' section is expanded, showing a 'Source' dropdown set to 'PDB' and a search input field containing '2h7s 2rfc', which is circled in red. Below this is an 'Apply' button and a 'Remote States' list with items like 'Nuclear Pore Complex', 'NPC-CIF', '1RB8 Annotated Assembly', 'Zika+EM', 'Cytochromes Superposition', 'AS', 'ASX', and 'ASX-1 Something'.
- Sequence:** A header area with the text 'No structure available'.
- Structure Tools:** A sidebar on the right with sections for 'Structure' (Nothing Loaded), 'Measurements' (+ Add), 'Components' (Preset, + Add), and 'Export Animation'.

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





# Příkládání struktur

The screenshot displays the Mol\* Viewer interface for a protein structure. The main view shows a ribbon representation of the protein, colored in shades of green and purple. The interface is divided into several panels:

- 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):** Displays the amino acid sequence of the protein, with residue numbers and a red circle highlighting the 'Residue' button in the Structure Tools panel.
- Structure Tools (Right):** A panel with various tools for interacting with the structure, including buttons for 'Structure', 'Measurements', 'Superposition', 'Components', and 'Export Animation'. The 'Residue' button is highlighted with a red circle.

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\* Viewer interface. On the left is a 'State Tree' panel listing various components like '2H7S 1 model', 'Model 1', 'Assembly 1', 'Polymer', 'Ligand', and 'Water'. The central area shows a protein structure in a ribbon representation. A context menu is open over the structure, with the 'Backbone' option highlighted in red. The menu includes options like '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'. At the top, a sequence of amino acids is visible: 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 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 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 V V N F L S F S M E F L A K S F E H R Q E L I E R P E R I P A C E L L R R. The right sidebar contains 'Structure Tools', 'Structure' (2 structures), 'Measurements', 'Superposition', 'Components' (2 structures), and 'Export Animation'. A log at the bottom shows recent actions: 'Created Ball & Stick in 18ms.', 'Created Ball & Stick in 4ms.', and 'Updated Structure Focus Representation in 2ms.'

# 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...DMYNF...NSAGV...EAWLQ...ESNV...PDLVW...TRCNG...GHWI...ATRG...LI...REAY...EDY...RHF...S...E...C...P...F...I...P...R...E...A...G...E...A...Y...D...I...P...I...T...S...M...D...P...P...E...Q...R...Q...P...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...I...E...S...L...A...P...Q...G...Q...C...N...F...T...E...D...Y...A...E...P...P...F...I...R...I...E...M...L...I...A...G...L...P...E...E...D...I...S...H...L...K...Y...L...D...Q...M...I...R...P...D...G...S...M...I...E...A...K...E...A...L...Y...D...Y...I...L...I...E...I...E...Q...R...R...K...P...G...I...D...A...I...S...I...V...A...N...G...Q...V...N...G...R...P...I...T...S...D...E...A...K...R...M...G...A...I...V...G...G...L...D...I...V...N...F...L...S...F...S...M...E...F...L...A...K...S...P...E...H...R...Q...E...L...I...E...R...P...E...R...I...P...A...C...E...E...L...L...R...`. The central 3D view shows a protein structure in green cartoon representation. The right panel contains the Structure Tools, with the 'Superposition' section having 'By Chains' selected and circled in red. The bottom log 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\* web application interface. The central panel shows a protein structure rendered in green cartoon representation. Above the structure, a sequence alignment is visible, with the sequence: TTETIQSN...NLAPLPPHVP...EHLVDFDMYNF...SNLSAGVQ...EAMAVLQ...ESNV...DLVWTR...CNGSHW...IATRG...QLREAY...EDYR...HFSSECF...FIPREAGEAY...  
FIFTSMDP...PPEQR...FRALANQ...VVGMP...VVDKLEN...RIQ...ELAG...SLIES...LRP...QG...CNFT...EDYAE...PFI...R...P...M...L...AG...LP...E...D...I...P...H...K...Y...L...T...D...Q...M...I...R...P...D...G...S...M...T...F...  
EANEAL...Y...D...Y...L...I...P...I...E...O...R...R...O...K...P...G...I...D...A...I...S...I...V...A...N...G...Q...V...N...G...R...P...I...T...S...D...E...A...K...R...M...O...G...A...L...L...V...G...G...L...D...I...V...N...F...L...S...F...S...M...E...F...L...A...K...S...P...E...H...R...O...E...L...I...E...R...P...E...I...P...A...C...E...L...L...E...R...  
The left sidebar contains a 'State Tree' with a hierarchical view of the structure, including models, assemblies, polymers, ligands, and water molecules. The right sidebar contains 'Structure Tools' and a 'Structure' panel with various options like 'Measurements', 'Superposition', and 'Components'. The 'Superposition' panel is highlighted with a red circle, and the 'Superpose' button is also circled in red. 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.'

# Přikládání struktur

The screenshot displays the Mol\* web application interface. The main window shows a 3D visualization of a protein structure (2H7S) in green cartoon representation, with a blue ligand molecule bound in the center. The protein is surrounded by red dots representing water molecules. The interface includes a left sidebar with a 'State Tree' showing the hierarchy of the loaded structure (2H7S 1 model, Model 1, Assembly 1, Polymer, Cartoon, Ligand, Water, Unit Cell). The top center shows the 'Sequence of' section with the amino acid sequence of the protein, with a segment highlighted in green. The right sidebar contains 'Structure Tools' and a 'Structure' panel showing two structures: 2H7S (25 Residues + 1521 Elements) and 2RFC (18 Residues + 1281 Elements). The 'Superposition' panel shows the structures are superposed by chains, with an RMSD of 4.53. The 'Components' panel lists the loaded components: Polymer (Cartoon), Ligand (Ball & Stick), Water (Ball & Stick), and 2 Unit Cells. The bottom status bar shows the time and actions performed: 'Updated Ball & Stick in 2ms.' and 'Superposed [25 Residues + 1521 Elements | A | 2H7S] and [18 Residues + 1281 Elements | A | 2RFC] with RMSD 4.53.'

# Příkládání struktur

The screenshot displays the Mol\* web application interface. The main window shows a 3D protein structure of Cytochrome P450-cam, rendered in a cartoon style with green and purple ribbons. The structure is superposed with another model, as indicated by the log at the bottom.

**State Tree (Left Panel):**

- 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 (Right Panel):**

- 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
- Export Animation

**Log (Bottom):**

- 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.