



Central European Institute of Technology
BRNO | CZECH REPUBLIC

Visualization of proteins and ligands



EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND
INVESTING IN YOUR FUTURE

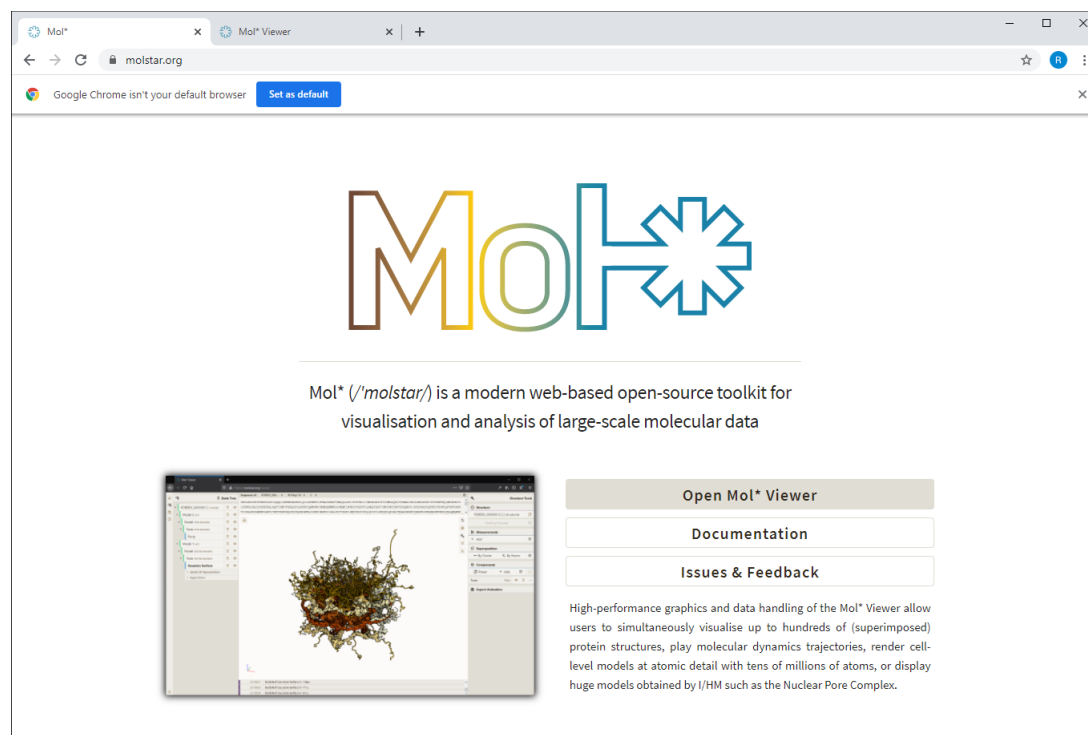


**OP Research and
Development for Innovation**



MolStar

- Web application for visualization of proteins and ligands
- Handles even extremely large systems
- Integrated in Protein Data Bank
- Developed in house at the National Center for Biomolecular Research, in collaboration with EMBL EBI and 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 "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.

Visualization of 3D coordinates of the molecule

Visualization model cartoon

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

Sequence of 1TQN | Crystal...

```
MALYGIHSHGLFKLGI PGPTPLPFLGNILSYHKGF CMFDMECHKKGKWKGFYDGOQFVLAITDPDMIKTVLVKECYSVFNRRPFGVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEMPVPIIAQYGDVLRNLRREAETGKPVTLKDVFGAYSMDVITISFQVNIIDSLNNPQDFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNLCVFPPEVINFLRKSVMKESRLEDTQKHRVDFLQMLIDSONSKETESHKALSDELVAQSIIFIFAGYETTSS
```

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.

Visualization of 3D coordinates of the molecule

Choice of visualization models

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

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

The top panel shows the sequence of 1TQN | Crystal... | 1: cytochrome... | A |. The sequence is: MALYGTSHSHGLFKKLGIPGPTLPLPFLGNILSYHKGFDMCECHKKYGKWNWGFYDGOQVLAITDPPMIKIVLVKECYSVFNRRPFGVGFMKSAI SIAEDEEWKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVLRNLRREARETKGFVTLKDVFGAYSMDVITTSISFGVNIDSLNNFQDPFVENTKLLRFDF LDPFFLSITVFFFLIPFILEVLNICVFFREVINFLRKSVKRMKESRLDITQKHRVDFLQMLMDSQNSKETESHKALSDELVAQSIIFIPAGYETTSS.

The right sidebar shows the Structure Tools panel with the following sections:

- Structure: 1TQN | Crystal Structure of Human ...
- Measurements: + Add
- Components: 1TQN
 - Polymer: Cartoon
 - Add Representation
 - Cartoon
 - Ball & Stick** (highlighted)
 - Gaussian Surface
 - Gaussian Volume
 - Label
 - Line
 - Molecular Surface
 - Orientation
 - Point
 - Putty
 - Spacefill
- Ligand: Ball & Stick
- Water: Ball & Stick
- Unit Cell 1 2 2 2

The bottom status bar shows the following 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.

Visualization of 3D coordinates of the molecule

Ball & Stick visualisation model

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

```
MALYGTSHGGLFKLGI PGPTPLPFLGNILSYHKGF CMFDM ECHKYKGVWGFYDQQPVLAITDPDMIKTVLVKECYSVPTNRRPFGVGFMKSR I
SIAEDEEWKRLRSLSPFTTSGKLEKMPV IIAQYGDVLRNLRREAE TGKPVTLKDVFGAYSMDVITSTSGVNI DSNLPQDFFVENTKLLRDFD
LDPFFLSIVVFPFLIPILEVNI CVPPREVINFLRKS VKRMKESRLEDTQKHRVDFLQLMIDSONSKETESHKALSDELVAQSIIPFAGYETTSS
```

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.

Other modes must be switched off

Visualization of 3D coordinates of the molecule

Visualization 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: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMDFMECHKKYGKWWGFYDQQPVLAITDPDMIKTVLVKECYSVFINRRRFGFVGFMKSAI SIAEDEEWKRLRSLSPFTSGKLEKEMVPIIAQYGDVLRNLRREARETGKPVILKDVFGAYSMDVITSTSGVNIIDSLNNPQDFPVENTIKLLRDFD LDFPFLSITVFPFLIPIILEVLNICVFPREVINFLRKSVKRMKESRLÉDTOKHRVDFLQLMIDSONSKETESHKALSDELVAQSIIIFAGYETTSS. The right panel (Structure Tools) shows the structure name '1TQN | Crystal Structure of Human ...', assembly type, and a components table:

Components		1TQN
Preset	+ Add	⌵ ⌵ ⌵
Polymer	3 reprs	⌵ ⌵ ⌵
Ligand	Ball & Stick	⌵ ⌵ ⌵
Water	Ball & Stick	⌵ ⌵ ⌵
Unit Cell	2 2 2	⌵ ⌵ ⌵

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.

Visualization of 3D coordinates of the molecule

Putty visualization model

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central 3D view shows the protein structure rendered as a green putty model, with a small ligand molecule in blue and red sticks. 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.

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

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDECHKKYGKVGWGFYDGOQPVLAITDPMIKIVLVKECYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSPGVNIDSLNPNQDPPFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNLCVFPREVINFLRKSVMKESRLEDYQKHRVDFLQMLIDSONSKETESHKALSDELVQAQSIIFAGYETTSS
```

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

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

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

Visualization of 3D coordinates of the molecule

Spacefil visualization model

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

State Tree

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

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

```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKKYGKRWGFYDGOQPVLAITDPMIKIVLVKCYSVFTNRRPFGVGFMKSAI
SIAEDEEWKRLRSLSPFTFTSGKLEKMPPIAQYGDVLRNLRREAETGKPVTLKQVFGAYSMDVITSTSGVNIIDSLNPNQDPEVENTKGLLRDFD
LDPFFLSITVFFFLIPILEVLNICVFFPREVINFLRKSVMKRESRLEDTQKHRVDFLQMLIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

Structure Tools

- Structure
 - 1TQN | Crystal Structure of Human ...
 - Type Assembly
 - Asm Id 1: Author Defined Asse...
 - Nothing Focused
- Measurements
 - + Add
- Components 1TQN
 - Preset + Add
 - Polymer 5 reprs
 - Ligand Ball & Stick
 - Water Ball & Stick
 - Unit Cell 1 2 2 2
- Volume Streaming 1TQN
 - Enable
- Assembly Symmetry 1TQN
 - Enable
- Export Animation

Log

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

Visualization of the surface of a molecule

Molecular Surface Visualization Model

The screenshot displays the Mol* Viewer interface. The central window shows a 3D molecular surface model of a protein, colored in a teal/green hue. The surface is highly detailed, showing the complex folds and pockets of the protein. A sequence of amino acids is visible at the top, with residue numbers and corresponding letters (e.g., MALYGT...). The left sidebar contains a 'State Tree' with a hierarchical view of the model, including '1TQN 1 model', 'Model 1', 'Assembly 1 3999 elements', 'Polymer 3766 elements', 'Ligand 49 elements', and 'Water 190 elements'. The right sidebar shows 'Structure Tools' and 'Components' panels. The bottom status bar indicates recent actions: 'Created Gaussian Surface in 597ms.', 'Created Gaussian Volume in 64ms.', and 'Created Molecular Surface in 1.749s.'

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

MALYGT³²HSGLF⁴²PKLGI⁵²PGPT⁶²PLPFL⁷²GNIL⁸²SYHK⁹²GFCM¹⁰²FDM¹¹²CHK¹²²YK¹³²GK¹⁴²W¹⁵²GFY¹⁶²D¹⁷²SQQ¹⁸²VL¹⁹²AI²⁰²IT²¹²DP²²²MI²³²KT²⁴²VL²⁵²V²⁶²KE²⁷²CY²⁸²SV²⁹²FT³⁰²NR³¹²RF³²²GP³³²VG³⁴²FM³⁵²KS³⁶²AI³⁷²
SIA¹²²E¹³²DE¹⁴²EW¹⁵²K¹⁶²R¹⁷²LR¹⁸²SL¹⁹²SP²⁰²FT²¹²SG²²²KL²³²EM²⁴²VP²⁵²II²⁶²AQ²⁷²Y²⁸²GD²⁹²VL³⁰²VR³¹²N³²²LR³³²RE³⁴²AE³⁵²T³⁶²G³⁷²K³⁸²F³⁹²V⁴⁰²IL⁴¹²K⁴²²D⁴³²V⁴⁴²FG⁴⁵²AY⁴⁶²SM⁴⁷²D⁴⁸²V⁴⁹²IT⁵⁰²ST⁵¹²S⁵²²FG⁵³²V⁵⁴²N⁵⁵²ID⁵⁶²SL⁵⁷²NN⁵⁸²P⁵⁹²QD⁶⁰²FF⁶¹²VENT⁶²²KK⁶³²LL⁶⁴²RF⁶⁵²DF⁶⁶²
LD²²²PF²³²FL²⁴²SI²⁵²TV²⁶²FP²⁷²FL²⁸²IP²⁹²ILE³⁰²VL³¹²NI³²²CV³³²FP³⁴²PRE³⁵²V³⁶²IN³⁷²FL³⁸²R³⁹²K⁴⁰²SV⁴¹²K⁴²²RM⁴³²KE⁴⁴²SR⁴⁵²LE⁴⁶²DT⁴⁷²Q⁴⁸²K⁴⁹²HR⁵⁰²VD⁵¹²FL⁵²²QL⁵³²MI⁵⁴²DS⁵⁵²Q⁵⁶²NS⁵⁷²KE⁵⁸²TE⁵⁹²SH⁶⁰²K⁶¹²ALS⁶²²DL⁶³²EL⁶⁴²V⁶⁵²A⁶⁶²Q⁶⁷²SI⁶⁸²IF⁶⁹²F⁷⁰²AG⁷¹²Y⁷²²ET⁷³²TS⁷⁴²S⁷⁵²

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.

Visualisation of the surface of a molecule

Gaussian Surface Visualization Model

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

- 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 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.

Visualisation of the surface of a molecule

Gaussian Volume Visualization Model

The screenshot displays the Mol* web application interface. The browser tabs show 'Mol*' and 'Mol* Viewer'. The address bar is 'molstar.org/viewer/'. The main window shows a protein structure (1TQN) with a Gaussian volume representation (red mesh) and a molecular surface (blue mesh). The left sidebar contains a 'State Tree' with a tree view of the structure, including '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', and 'Unit Cell 1 2 2 2'. The top center shows the 'Sequence of 1TQN | Crystal...' with the amino acid sequence:
MRLYGTHSHGLPKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKYKQWVGFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFPMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLRKEMVPIIAQYGDVLRNLRREAETGKPVILKDFVFGAYSDVITSTSEFVNIIDSLNPDPPFVENTKLLRFD
LDPFFLSITVFFFLIPILEVLNLCVFPREVINFLRKSVKRMKESRLEDITQKHRVDFLQLMIDSQNSKETESHKALSDELVAQSIIIFAGYETTSS
The right sidebar contains 'Structure Tools' and 'Structure' panels. The 'Structure' panel shows '1TQN | Crystal Structure of Human ...' and 'Type Assembly'. The 'Measurements' panel has '+ Add'. The 'Components' panel shows '1TQN' and 'Polymer 4 reprs'. The bottom log shows:
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.

Visualization of experimental data

Electron density

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows a green ribbon representation of the protein structure, with a semi-transparent electron density map overlaid in light green. Red dots are scattered throughout the structure, representing individual atoms or specific residues. The interface includes a 'State Tree' on the left, a 'Sequence of' panel at the top with the amino acid sequence, and a 'Structure Tools' panel on the right. The 'Structure Tools' panel shows the 'Structure' section with '1TQN | Crystal Structure of Human ...' and 'Type: Assembly'. Below this, the 'Measurements' section has a '+ Add' button. The 'Components' section lists '1TQN' with a 'Preset' button and '+ Add' button. The 'Volume Streaming' section is checked and has a '+ Add' button. The 'Assembly Symmetry' section is checked. The 'Export Animation' section has a button. The bottom status bar shows three actions: 'Created Ball & Stick in 26ms.', 'Created Ball & Stick in 12ms.', and 'Updated Structure Focus Representation in 3ms.'

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

```
MALYGTSHSHGLFKKLGIPGFTPLPFLGNILSYHKGFCMPDMECHKKYGKWWGFDGQQPVLAITDPDMIKTVLVEKCYSVFTNRRPFGVGFMSAI  
123 132 142 152 162 172 182 192 202 212  
SIAEDEEWKRLRSLLSPTFTISGKLEKMPVILIAQYGDVLRNLRREAEATGKPVILKDVFGAYSMQVITSTSGVNIIDSLNPNQDPFVENTKLLRDF  
222 232 242 252 262 272 282 292 302 312  
LDPFFLSITIVFFFLIPILEVLMNICVFPREVINFLRKSVMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDELVAQSIIFIFAGYETTSS
```

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.

Visualization of experimental data

Electron density

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows the protein structure in a green cartoon representation, with red dots representing the 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. The 'Volume Streaming' option is checked and circled in red.

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

```
MALYGT32HSHGL42FKKLG52IPGFT62PLPFLGN72ILSY82HKGF92CMFDM102ECHK112YK122GW132WFG142YD152Q162Q172VL182AIT192DP202DM212IK222TV232L242VE252CK262Y272SV282FT292NR302RF312GF322V332GF342M352KS362AI372  
SIAE122DE132EW142K152RL162RS172LL182SPT192FT202IS212GK222L232KEM242VP252II262AQ272Y282GD292V302LV312RN322LR332REA342ET352GK362F372VL382KD392V402FG412AY422S432MD442V452IT462ST472S482FG492V502N512D522SL532NP542QD552PF562V572ENT582K592LL602RF612DF622  
LDP222FF232LS242IT252IV262FP272LI282PI292LEV302LN312IC322VP332PRE342V352IN362FL372RK382SV392K402RM412KE422S432R442LE452DT462Q472K482HR492VD502FL512Q522LM532IS542Q552NS562K572ET582ESH592K602ALS612D622LE632L642V652AQ662SI672IF682F692AG702Y712ET722SS732
```

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset	+ Add	...
Polymer	Cartoon	...
Ligand	Ball & Stick	...
Water	Ball & Stick	...

Unit Cell | 2 2 2

Volume Streaming 1TQN

Enable

Assembly Symmetry 1TQN

Enable

Export Animation

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

Visualization of experimental data

Electron density

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

```
MALYGTSHSHGLFKKLGI PGPTPLPFLGNILSYHKGF CMFDMCHKKYKGVWGFYDQQPVLAITDPDMIKTVLVKECYSVFINRRPFGVGFVGMKSAI
122 132 142 152 162 172 182 192 202 212
SIAEDEENKRLRSLSPFTFTSGKLEKEMVPIIAQYGVLVLRNLRREAEATGKPVILKDFVFGAYSMDEVITSTISFGVNIIDSLNNPQDFEIVENTKLLRDFD
222 232 242 252 262 272 282 292 302 312
LDPFFLSITVFPFLPIPILEVNLICVFPREVINFRLKRSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDELEVAQSIIFIFAGYETTSS
```

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

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	<input type="checkbox"/>	...
Ligand	Ball & Stick	<input type="checkbox"/>	...
Water	Ball & Stick	<input type="checkbox"/>	...
Unit Cell 2 2 2			
Volume Streaming			
1TQN			
+ 2Fo-Fc σ	<input type="range"/>	1.5	<input type="checkbox"/>
+ Fo-Fc(+ve) σ	<input type="range"/>	3	<input type="checkbox"/>
+ Fo-Fc(-ve) σ	<input type="range"/>	-3	<input type="checkbox"/>
Entry	1tqn		
View	Around Focus		
Nothing to Update			
Controls Help			
Assembly Symmetry			
1TQN			

Visualization of experimental data

Electron density

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central view shows a green ribbon representation of the protein structure, overlaid with semi-transparent electron density maps. A red arrow points to a specific atom in the structure, with the text "Click on the selected atom" next to it. The interface includes a "State Tree" on the left, a "Sequence" panel 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 "Type Assembly". Below this, the "Measurements" section has a "+ Add" button. The "Components" section lists "1TQN" with "Preset" and "+ Add" buttons. The "Volume Streaming" section shows "1TQN" with three entries: "2Fo-Fc σ " (1.5), "Fo-Fc(+ve) σ " (3), and "Fo-Fc(-ve) σ " (-3). The "Assembly Symmetry" section shows "1TQN". The bottom status bar shows update times and actions: "15:24:41 Updated 1.5 σ [2fo-fc] in 1ms.", "15:24:41 Updated 3 σ [fo-fc(+ve)] in 0ms.", and "15:24:41 Updated -3 σ [fo-fc(-ve)] in 0ms."

Visualization of experimental data

Electron density

The image shows a screenshot of the Mol* Viewer web application. The central view displays a 3D molecular model of the protein 1TQN (Cytochrome P450) in green, with electron density maps overlaid in semi-transparent blue and green. The density maps are shown as mesh surfaces around the atoms. 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...

```
MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFDMFMECHKYKQWGFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGVGFPMKSAI
SIAEDEWKRRLRSLSPTFTSGKLELVPIIAQYGVVLVRNLRREARETGKQVTLKQVFGAYSMDEVITSTSFQWVNSLNNPQDPFVENTKLLRDF
LDPFFLSITVFPFLIPILEVLNLCVFFREVINFLRKSVKRMKESRLDQTQKRVDFLQMLIDSONSKETE SHKALSDELVAQSIIIFIFAGYETISS
```

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.

Visualisation of annotations

Colouring by properties

The screenshot displays the Mol* web viewer interface. The central view shows a protein structure (1TQN) rendered in a green cartoon representation, with red dots indicating specific annotations. The right-hand panel, titled 'Structure Tools', contains a list of properties for the selected polymer. The 'Hydrophobicity' property is highlighted with a red circle. The left-hand panel, titled 'State Tree', shows a hierarchical view of the model, including '1TQN 1 model', 'Model 1', 'Assembly 1' (3999 elements), 'Polymer' (3766 elements), 'Ligand' (49 elements), and 'Water' (190 elements). The top panel shows the protein sequence with residue numbers: MALYGTSHSHGLFKLGI... SIAEDEENKRLRSLLS... LDPFFLSITVFPFLIP... The bottom panel shows a log of recent updates: '16:37:57 Updated Cartoon in 31ms.', '16:38:35 Updated Cartoon in 8ms.', and '16:38:48 Updated Cartoon in 28ms.'

Visualisation of annotations

Colouring by properties - hydrophobicity

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central visualization shows the protein structure colored by hydrophobicity, with a color scale from green (low) to red (high). 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

```
MALYGIHSHGLFKKLGIPGPTLPFLGNILSYHKGFCEMDECHKYKGVWGFYDQQPVLAITDPDMIKITVLVKECYSVETNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLEMPVPIIAQYGDVLRNLRREAETGKPFVTLKQVFGAYSMDVITSTISFGVNI DLSLNNPQDPFVENTKLLRFD
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLLRKSVMKESRLEDYQKHRVDFLQLMIDSQNSKETE SHKALSDLELVAQSIITFPAGYETTS
```

Structure Tools:

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

Log:

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

Visualisation of annotations

Colouring by properties - quality

The screenshot displays the Mol* web interface for the protein 1TQN. The central view shows a green ribbon representation of the protein structure, with numerous red dots scattered across it, representing quality annotations. 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 list of properties for the polymer, including 'Structure Quality Report' which is circled in red. The bottom status bar shows a log of updates.

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

```
MALYGTSHSHGLFKKLGIPGPTLPFLGNILSYHKGFCMFDMECHKRYGKMGWGYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGVGVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLRKEMVPIIAQYGDVLRNLRREAEITGKQVTLKDVFGAYSMDVITSTISFGVNIIDSLNPNQDPPFVENTKLLRDFD
LDPFFLSITVFPFLIPLEVLNICVFPREVINFLRKSVKRMKESRLEDTQKHRVDFLQMLMIDSQNSKETESHKALSDELVAQSIIIFAGYETTSS
```

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

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

Visualisation of annotations

Colouring by properties - quality

The screenshot displays the Mol* Viewer interface for the protein 1TQN. The central visualization shows a ribbon representation of the protein structure, colored by quality. The color gradient ranges from green (high quality) to red (low quality). The interface includes a state tree on the left, a sequence viewer at the top, and a control panel on the right.

Sequence of 1TQN | Crystal...

```
MALYGTSHSHGLFKLGI PGPTLPFLGNILSYHKGFDMFMECHKYKQWGFYDQQPVLAITDPDMIKTVLVKECYSVFTNRRPFPGVGFMKSAI
SIAEDEWKRRLRSLLSPTFTSGKLEKMPVIAAQYGDVLRNLRREAETGKPVILKDFGAYSMQVITSTSGVNIIDSLNPNQDFFVENTKLLRDFD
LDPFFLSITVFPFLIPILEVLNICVFPREVINFLAKSVKRMKRESRLDITQKRHVDVFLQMLMIDSQNSKETESHKALSDELVAQSIIIFAGYETTSS
```

State Tree

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

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Asse...

Nothing Focused

Measurements

+ Add

Components 1TQN

Preset	+ Add	☰	🔄
Polymer	Cartoon	👁	🗑
Ligand	Ball & Stick	👁	🗑
Water	Ball & Stick	👁	🗑
Unit Cell 2 2 2		👁	🗑

Volume Streaming 1TQN

✓ Enable

Assembly Symmetry 1TQN

✓ Enable

Export Animation

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

Visualization of protein assemblies

The screenshot displays the Mol* web interface for visualizing a protein assembly. The central view shows a large, multi-colored protein assembly. The left sidebar shows a state tree with the following items:

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

The top right shows the protein sequence for 3J3Q:

```
Sequence of 3J3Q | Atomic... 1: capsid prot... A [auth g8]  
1 BIVNLOGQMVHQAI SPRTLNANVVKVVEEKAFSPVEIPMFSALSSEGATPODLNTMLNTVGGHQAAOMQLKETINEEAAEWDRLHPVHAGPIEPGQMR  
EPRGSDIAGTTSTLQEIQIGWMTNHPPIPVGGEIYKRWII LGLNKIVRMYSPTSIDIRQGPKEPRFRDYDRFYKTLRAEQASQEVKQWMMTETLLVQNA  
NPDCKTILKALGPAATLEEMMTACQGVGGPGHKARVL
```

The right sidebar contains 'Structure Tools' with the following sections:

- 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**

The bottom status bar shows the following log entries:

- 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.

Measurements

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 distance measurement of 2.92 Å is highlighted between two atoms, with dashed lines indicating the path. The top of the interface shows the sequence of the protein: MALYGTSHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKWWGFYDGOQVLAITDPMIKTVLVKECVSVFTNRRPFGVGFMSAI SIAEDEENKRLRSLLSPTFTSGKLEKEMVPIIAQYGDVLRNLRREARETGKPEVTLKDVFGAYSMDVITSTSGVNIIDSLNPNQDPPEVENTKKLLRDFD LDPFFLSITVFPFLIPILEVLNICVFPREVTFNLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS. The left sidebar contains a State Tree with categories like 1TQN 1 model, Model 1, Assembly 1, Polymer, Ligand, Water, and Measurements. The right sidebar shows Structure Tools, Structure information (1TQN | Crystal Structure of Human ...), and a Measurements panel with a table of distances.

Measurements	
+ Add	
Distances	
2.92 Å	HEM 508 — CYS ...

Components	
Polymer	Cartoon
Ligand	Ball & Stick
Water	Ball & Stick
Unit Cell 2 2 2	

Volume Streaming	
✓ Enable	

Assembly Symmetry	
✓ Enable	

Export Animation	

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.

Superimposition of structures

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

The left sidebar contains a "Home" section with a "Download Structure" menu. Under this menu, the "Source" is set to "PDB". A search input field contains the text "PDB Id (s) 2h7s 2rfc", which is circled in red. Below the search field, there is an "Options" section with an "Apply" button. Further down, there are several expandable menu items: "Add Trajectory", "Download Density", "Download File", "Open Files", "Download", "Load CellPack", and "Load Genome 3D (G3D)".

Below the "Download Structure" section is a "Remote States" section, which lists several pre-defined states: "Nuclear Pore Complex", "NPC-CIF", "1RB8 Annotated Assembly", "Zika+EM", "Cytochromes Superposition", "AS", "ASX", and "ASX-1 Something". At the bottom of this list, there are two numbered entries: "1" and "2".

The right sidebar is titled "Structure Tools" and contains several sections: "Structure" (with "Nothing Loaded" and "Nothing Focused" indicators), "Measurements" (with a "+ Add" button), "Components" (with a "Preset" button, a "+ Add" button, and a refresh icon), and "Export Animation".

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

Superimposition of structures

The screenshot displays the Mol* Viewer interface for superimposing two protein structures. The main window shows a 3D ribbon representation of a protein structure, with two different conformations overlaid in green and purple. The interface is divided into several panels:

- State Tree (Left):** A hierarchical tree showing the loaded components, 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. A second structure, 2RFC (1 model), is also listed below.
- Sequence Viewer (Top):** Displays the amino acid sequence for 2H7S | L244A... and 1: Cytochrome... with residue numbers 11, 21, 31, 41, 51, 61, 71, 81, 91, 101, 111, 121, 131, 141, 151, 161, 171, 181, 191, 201, 211, 221, 231, 241, 251, 261, 271, 281, 291.
- Structure Tools (Right):** A panel with various tools. The 'Superposition' tool is highlighted with a red circle. It includes options for 'By Chains' and 'By Atoms'. Below it, the 'Components' section shows a table of loaded elements:

Component	Representation	Visible	Deleted	More
Polymer	Cartoon	<input checked="" type="checkbox"/>	<input type="checkbox"/>	...
Ligand	Ball & Stick	<input type="checkbox"/>	<input type="checkbox"/>	...
Water	Ball & Stick	<input type="checkbox"/>	<input type="checkbox"/>	...

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.

Superimposition of structures

The screenshot displays the Mol* Viewer interface for superimposing two protein structures. The central 3D view shows two protein chains: one in green and one in purple, both rendered as ribbons. 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 (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
 - Polymer 2752 elements
 - Cartoon
 - Ligand 60 elements
 - Ball & Stick
 - Water 5 elements
 - Ball & Stick
 - Unit Cell P 1 21 1

Sequence Viewer (Top):

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

TTETIQSNANLAPLPPHVPHELVDFDMYNFNSL SAGVQEA WVLQESNVDFLWTRCNGGHWIATRGQLIREAYEDYRHFSSSECFPIPREAGEAYD
FIPTSMDFPEQRFALANQVGMFVVDKLENRIQELACSLIESLSPQGCNFTEDYAEFPPIRIFMLLAGLPEDIPHLKYLTDQMTRPDGSMTFA
EAKEALYDYLPIIIEQRQKPGTDAISIVANGQVNGRPITSDEAKRMC GALLVGGLDIVWNFLSFSMEFLAKSPEHRQELIERPERIPACEELLAR

Structure Tools Panel (Right):

- Structure: 2 structures
- Measurements: + Add
- Superposition: By Chains, By Atoms
- Components: 2 structures
 - Polymer: Cartoon
 - Ligand: Ball & Stick
 - Water: Ball & Stick
- Export Animation

Bottom 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.

Superimposition of structures

The screenshot displays the Mol* Viewer interface with two protein structures superimposed. The left structure is shown in green, and the right structure is in purple. A context menu is open over the green structure, with 'Structure Property' highlighted in red. The interface includes a 'State Tree' on the left, a 'Sequence of' window at the top, and a 'Structure Tools' panel on the right. The 'Structure Tools' panel shows '2 structures' and 'Nothing Focused' under the 'Structure' section. The 'Superposition' section has 'By Chains' and 'By Atoms' options. The 'Components' section lists 'Polymer', 'Ligand', and 'Water' with their respective representations. The 'Export Animation' section is also visible.

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

```
TTETIQSNANLAPLPPHVEHLVDFDMYNFSNLSAGVQEAWAVLQESNVFDLWVTRCNGGHWIATRGQLIREAYEDYRHFSSSECFIPREAGEAYD
FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRPOGQCNTEDYAEPPPIRIFMLLAGLPEEDIPHLKYLTDQMRPDGSMIFA
EAKEALYDYLIPPIEQRRQKPGTDAISIVANGVNGRPIITSEAKRMCGALLVGGGLDIVNVLFSFSEFLAKSPEHRQELIERPERIPACELLLR
```

Residue [Icons]

Add/Union Selection X

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

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

Superimposition of structures

The screenshot displays the Mol* Viewer interface with two protein structures superimposed. The left sidebar shows a 'State Tree' with the following structure:

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

The main view shows the protein backbone in green and purple. A context menu is open over the structure, with the 'Backbone' option highlighted in red. The menu items are:

 - 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
 - Bond Property

The right sidebar contains the following sections:

- 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

The bottom status bar shows the following 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.

Superimposition of structures

The screenshot displays the Mol* Viewer interface for superimposing two protein structures. The left sidebar shows a state tree with two models: 2H7S (1 model) and 2RFC (1 model). The central view shows a green protein structure with a blue ligand. The right sidebar shows the 'Structure Tools' panel with 'By Chains' selected under 'Superposition'.

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

```
TTETIQSN11NL21AP31PP41PH51VE61RL71VD81FD91MY101N111FS121NL131S141AG151VE161AV171LQ181ES191NP201DL211VR221CG231NG241GH251WI261AT271RG281QL291IR301E311AY321ED331YR341HF351SE361CP371IF381RE391AGE401AY411  
F101I111F121SM131DP141PE151Q161R171FR181AL191AN201Q211V221GM231F241V251VD261K271LEN281RI291Q301EL311AG321SL331IE341SL351NP361Q371QC381N391F401TE411D421Y431AE441PP451PI461RI471FM481LL491AG501LP511ED521IP531HL541K551YL561TD571QM581IR591PD601GS611MT621  
E201A211KE221AL231Y241D251YL261IL271PI281IE291QR301R311CK321PG331IDA341LS351IV361ANG371Q381V391NG401R411PI421TS431DE441AK451K461MC471G481ALL491V501GG511LD521IV531VN541FL551S561FM571E581FL591AK601S611PE621HR631Q641EL651EA661PER671I681PA691ACE701ELL711ER
```

Structure Tools

Structure

2 structures

Nothing Focused

43 Residues + 2802 Elements Selected

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.

Superimposition of structures

The screenshot displays the Mol* Viewer interface with two protein structures superimposed. The left sidebar shows a 'State Tree' with two main models: '2H7S 1 model' and '2RFC 1 model'. The central panel shows the protein structure in green cartoon representation, with a blue stick model of a ligand. The right sidebar contains 'Structure Tools' and a 'Superposition' panel. The 'Superposition' panel shows two structures: '25 Residues + 1521 Elements | A | 2H7S' and '18 Residues + 1281 Elements | A | 2RFC'. The 'Superpose' button is highlighted with a red circle. The bottom status bar shows a log of actions: 'Created Ball & Stick in 18ms.', 'Created Ball & Stick in 4ms.', and 'Updated Structure Focus Representation in 2ms.'

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

```
TTETIQSN11...21...31...41...51...61...71...81...91...101...111...121...131...141...151...161...171...181...191...201...211...221...231...241...251...261...271...281...291
```

Residue [Icons]

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

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

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

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

Superimposition of structures

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 L 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 E L G E A N Y 81  
101 I 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 I 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 S Q E L I E R P E R I P A A C E E L L R R 251  
261 271 281 291
```

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.

Superimposition of structures

The screenshot displays the Mol* Viewer interface for superimposing two protein structures. The central 3D view shows two protein chains, one in green and one in purple, overlaid to compare their conformations. The left sidebar contains a 'State Tree' with a hierarchical view of the loaded structures: 2H7S (1 model) and 2RFC (1 model). The right sidebar, 'Structure Tools', shows the current view is '2 structures' and provides options for 'Measurements' and 'Superposition'. The 'Superposition' section is active, showing 'By Chains' mode and a description: 'Add 2 or more selections (toggle mode) from separate structures. Selections must be limited to single polymer chains or residues therein.' The 'Components' section lists '2 structures' with a 'Preset' button and an 'Add' button. The 'Export Animation' section is also visible.

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

TTETIQSNANLAPLPPHVPEHLVDFDMYNFNSLSAGVQEAHVLQESNVDFLWVTRCNGGHWIATRGQLIREAYEDYRHFSSSECFPIPREAGEAYD
FIPTSMDFPEQRFALANQVWGMFVVDKLENRIQELACSLIESLSRPGQCNTEDYAEFPPIRIFMLLAGLPEDIPHLKYLTDQMTRPDGSMTFA
EAKEALYDYLPIIEQRQKPGIDAISSIVANGQVNGRPITSDEAKRMCGALLVGGLDIVVNFSLFSMEFLAKSPEHRQELIERPERIPAAACEELLR

Residue [tools]

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.

Superimposition of structures – PDB and AlphaFold

Pairwise Structure Alignment

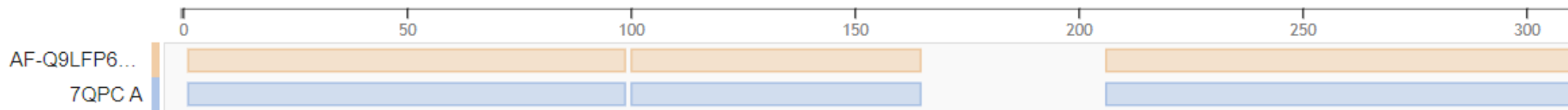
[Help](#)

▸ 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/>

Superimposition of structures – PDB and AlphaFold

