CEITEC

Central European Institute of Technology
BRNO | CZECH REPUBLIC

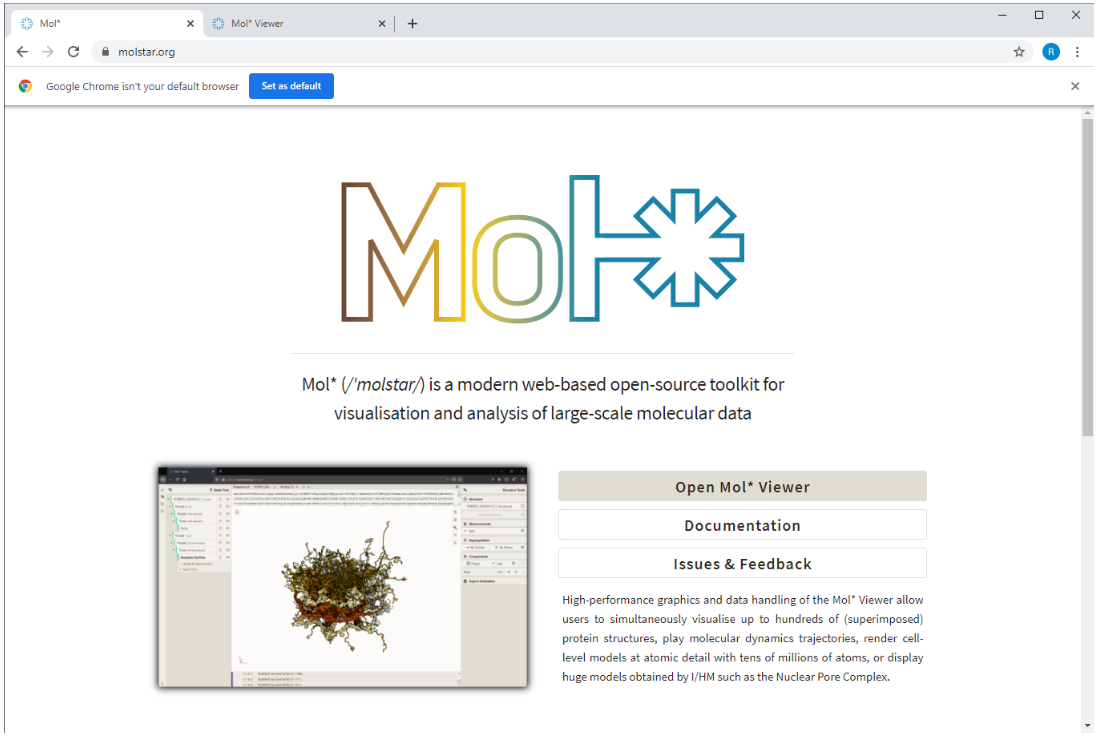
Vizualizace proteinů a ligandů

EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND
INVESTING IN YOUR FUTURE

2007–13
OP Research and
Development for Innovation

MolStar

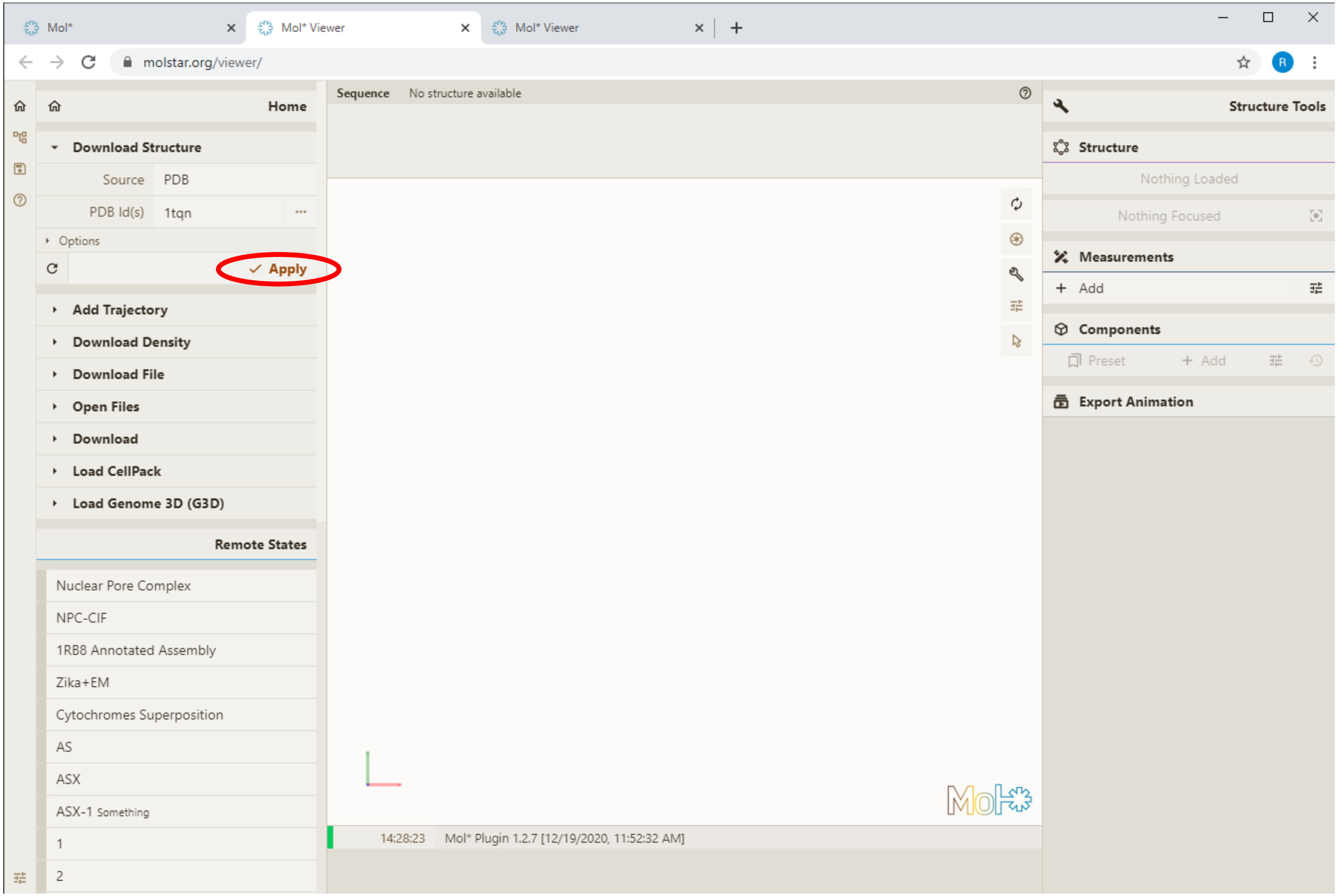
- Webová aplikace pro vizualizaci proteinů a ligandů
- Zvládá i extrémně velké systémy
- Integrovaný v Protein Data Bank
- Vyvíjený u nás v Národním centru pro výzkum biomolekul, ve spolupráci s EMBL EBI a RCSB PDB
- https://molstar.org/



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

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


molstar.org/viewer/

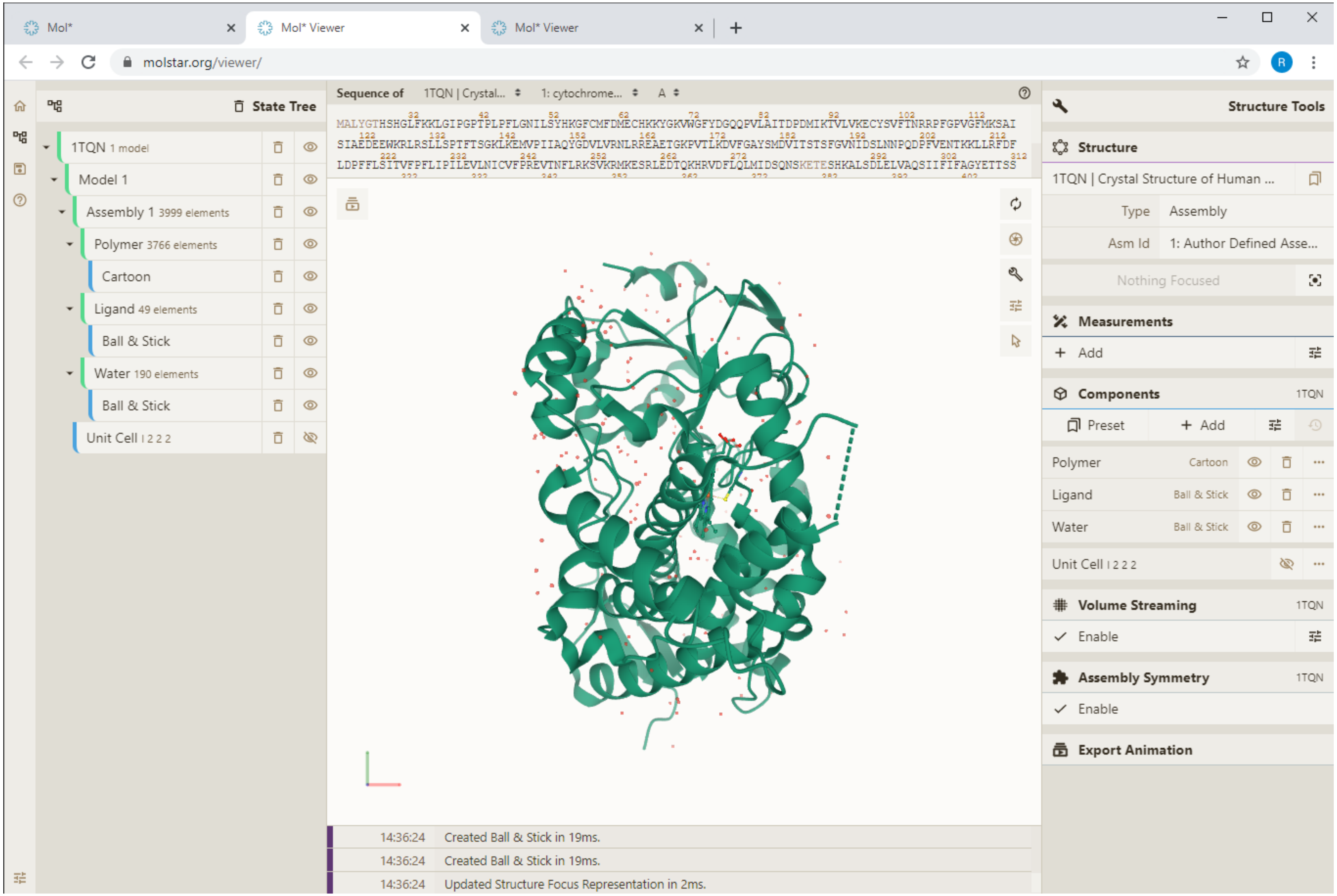
Source: PDB

PDB Id(s): 1tqn

No structure available

14:28:23 Mol* Plugin 1.2.7 [12/19/2020, 11:52:32 AM]

Vizualizace 3D souřadic molekuly
Vizualizační model cartoon



MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI

SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF

LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS

1TQN | Crystal Structure of Human ...

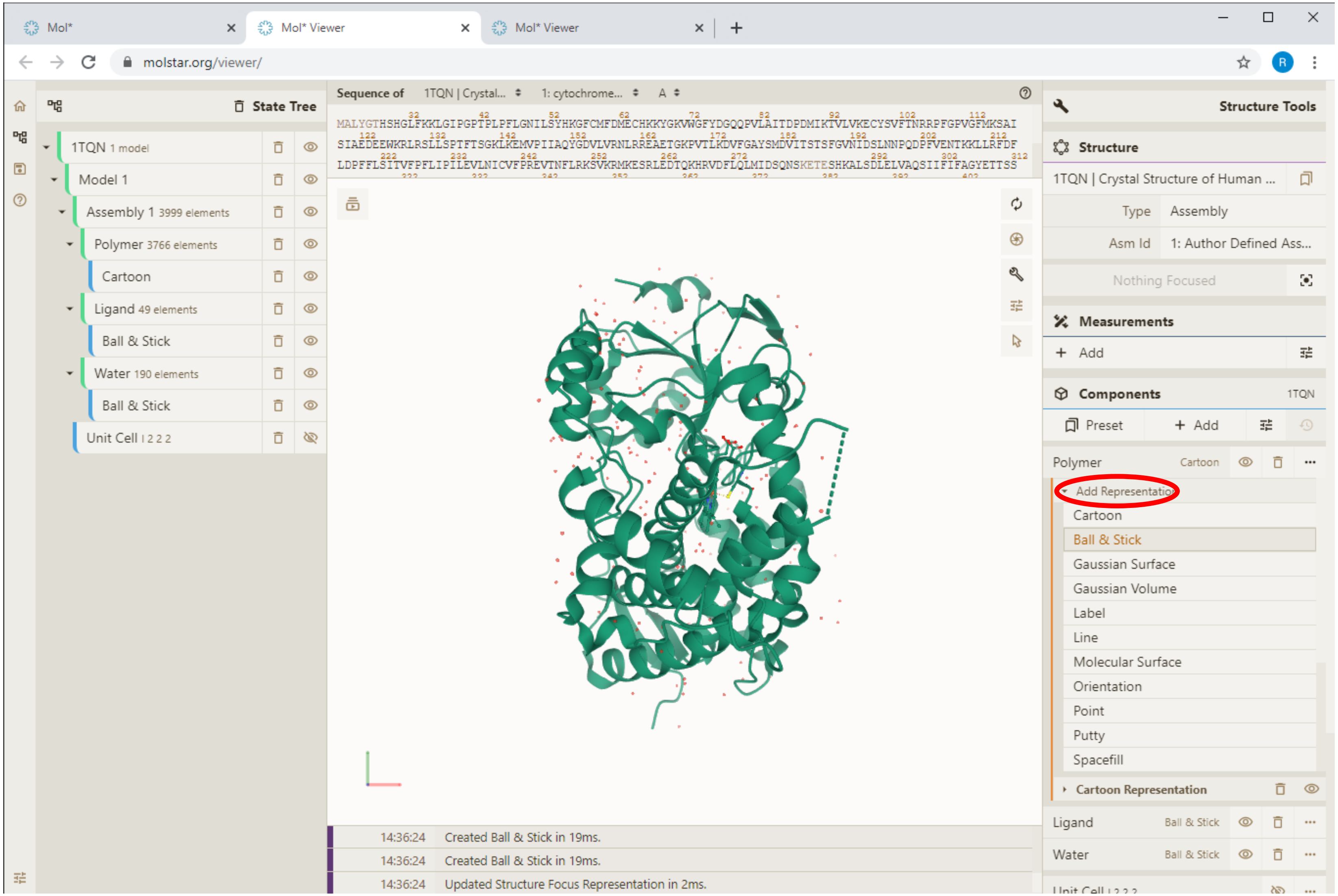
Type: Assembly

Asm Id: 1: Author Defined Asse...

Nothing Focused

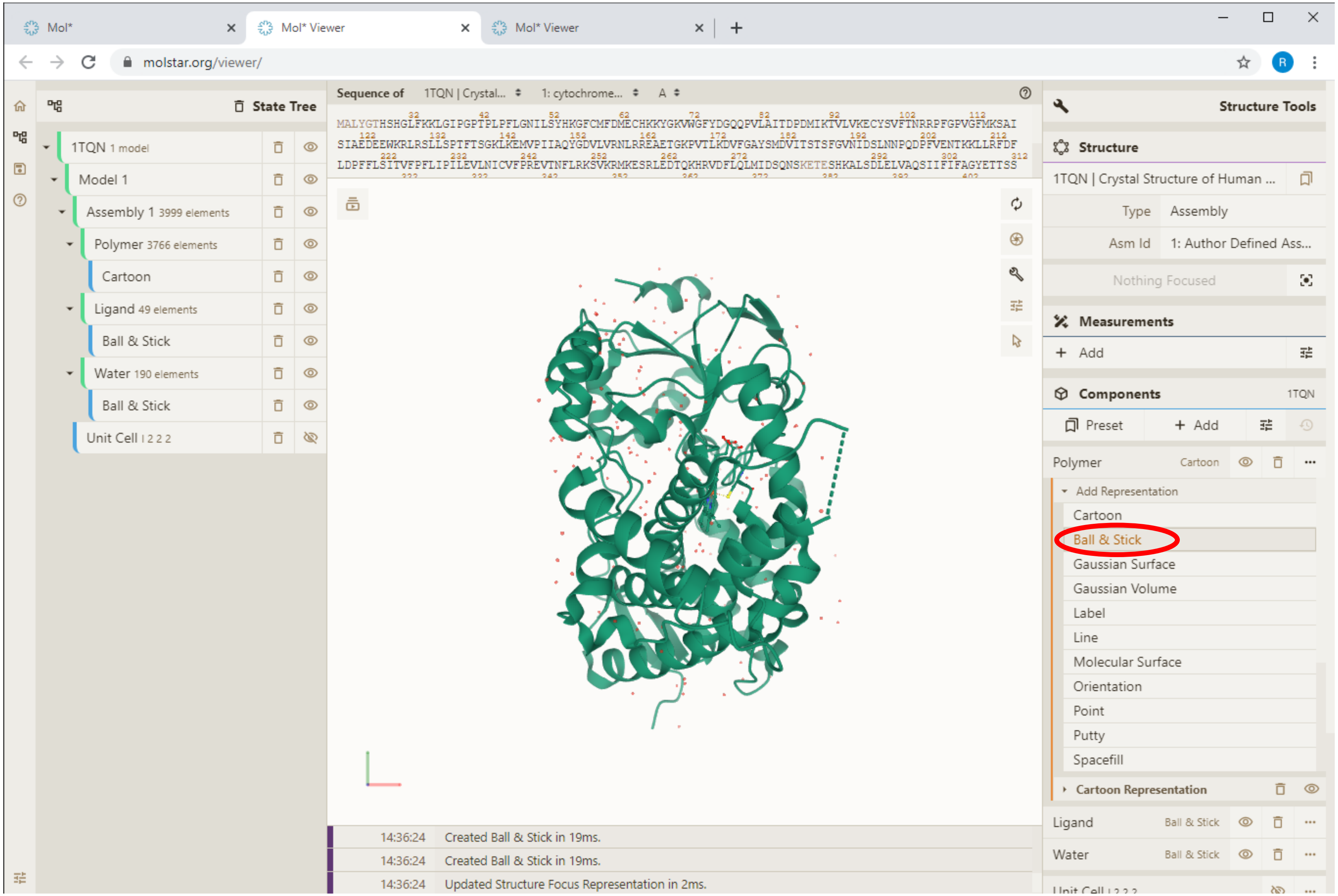
```
14:36:24   Created Ball & Stick in 19ms.
14:36:24   Created Ball & Stick in 19ms.
14:36:24   Updated Structure Focus Representation in 2ms.
```

Vizualizace 3D souřadic molekuly
Volba vizualizačních modelů



```
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 souřadic molekuly
Volba vizualizačních modelů - Ball & Stick



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

1TQN | Crystal Structure of Human ...

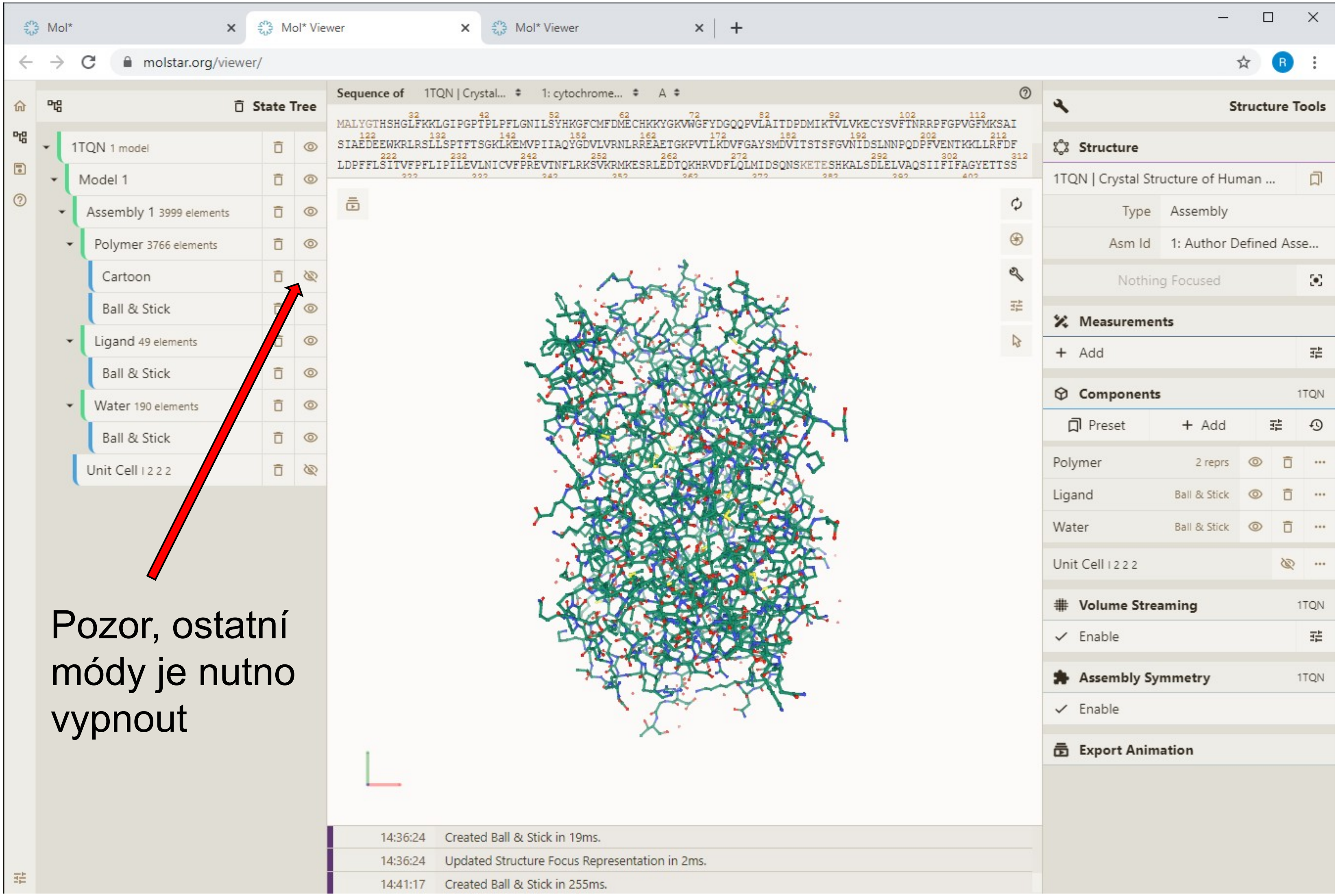
Type: Assembly

Asm Id: 1: Author Defined Ass...

Nothing Focused

```
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.
```

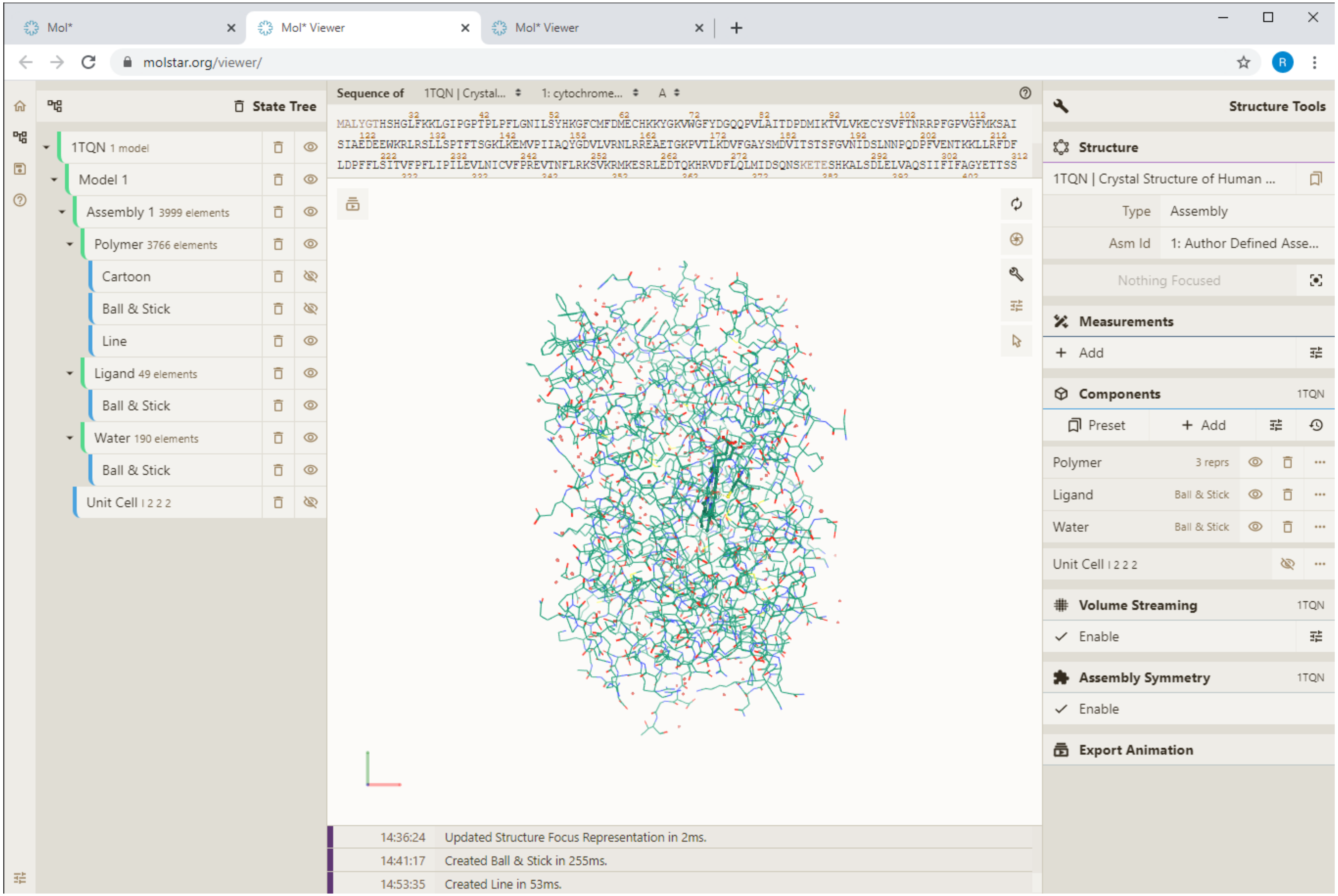
Vizualizace 3D souřadic molekuly
Vizualizační model Ball & Stick



```
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

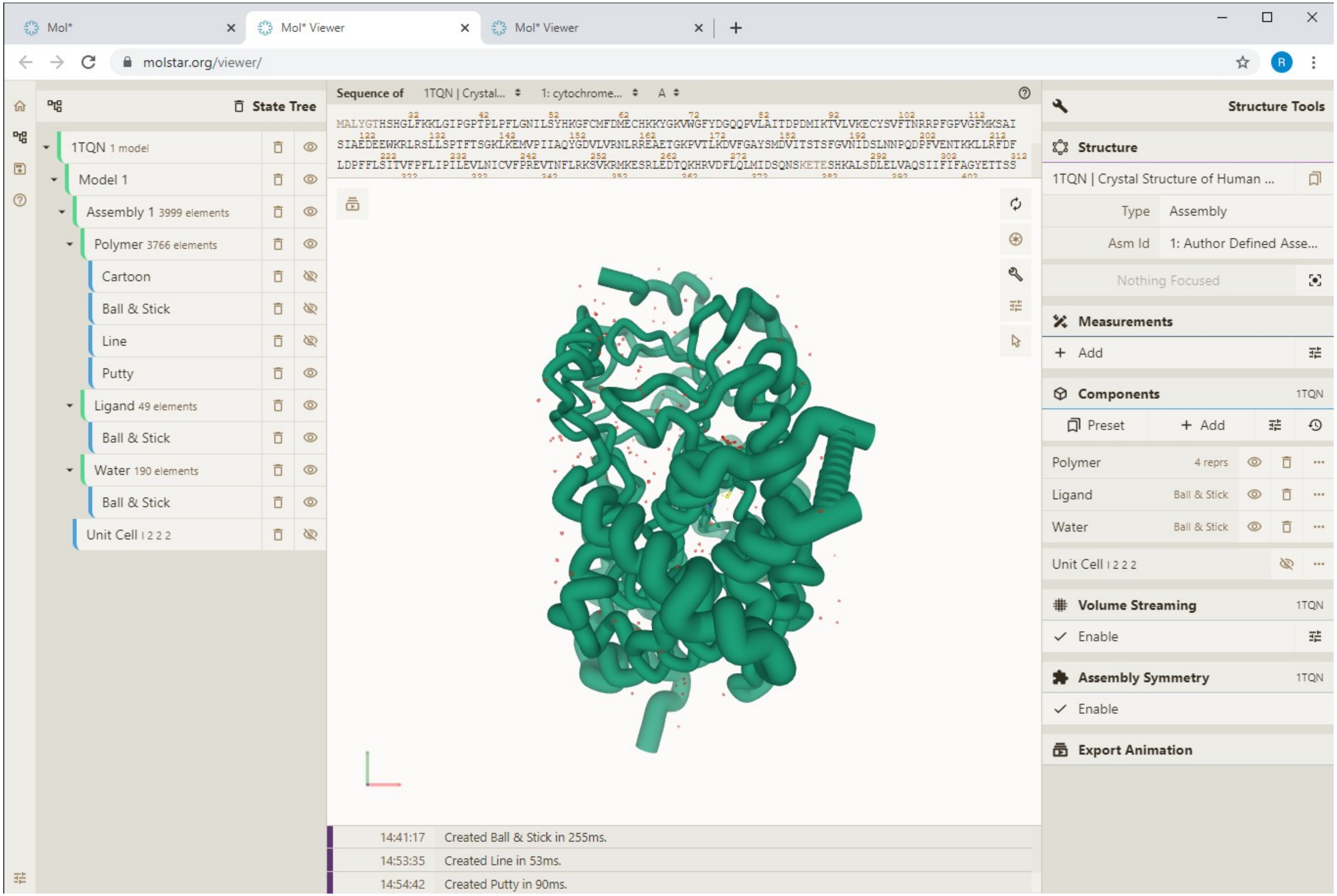
Vizualizace 3D souřadic molekuly
Vizualizační model Line



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

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

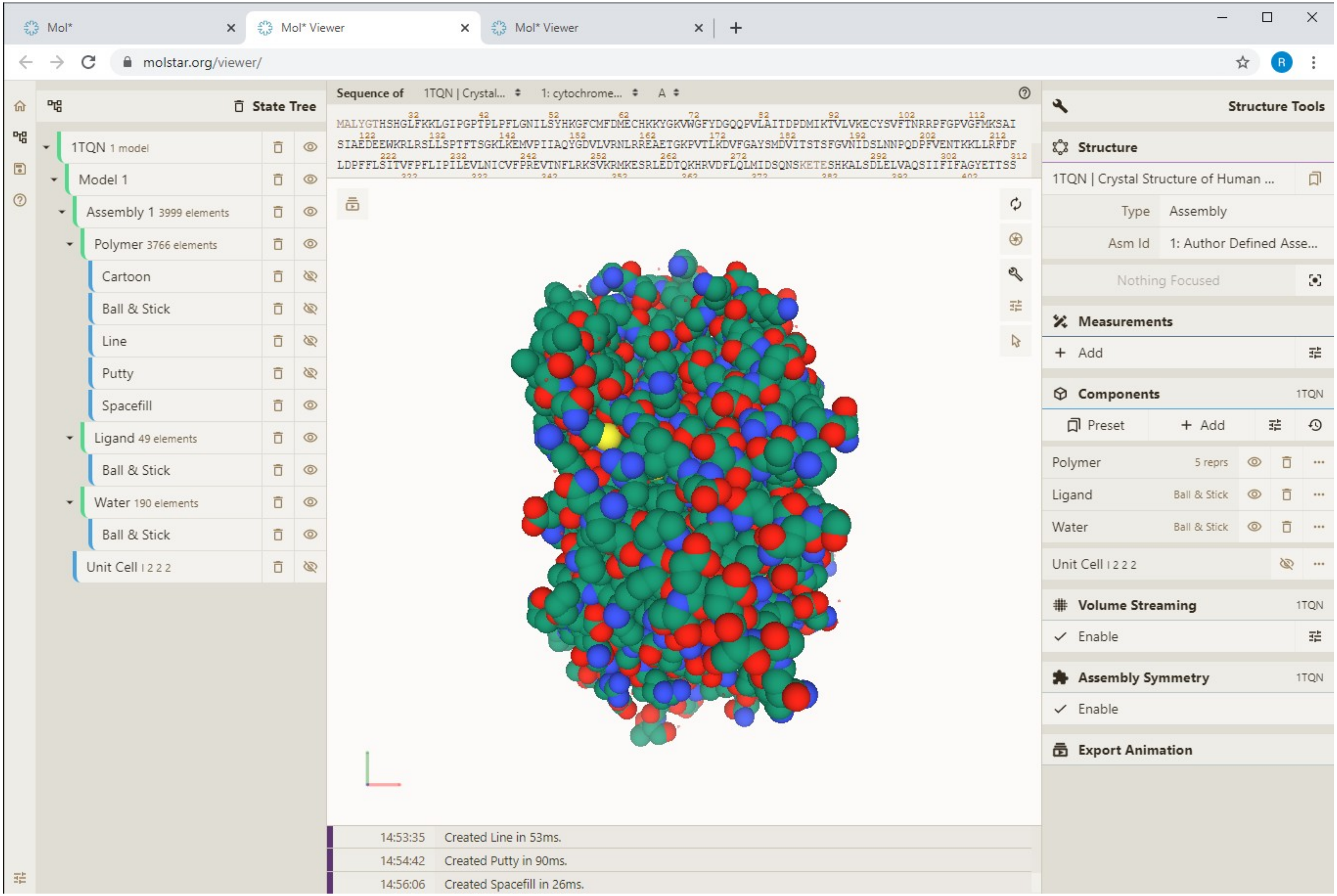
Vizualizace 3D souřadic molekuly
Vizualizační model Putty



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

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

Vizualizace 3D souřadic molekuly
Vizualizační model Spacefil



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SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS

- 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 I 2 2 2

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Polymer 5 reprs

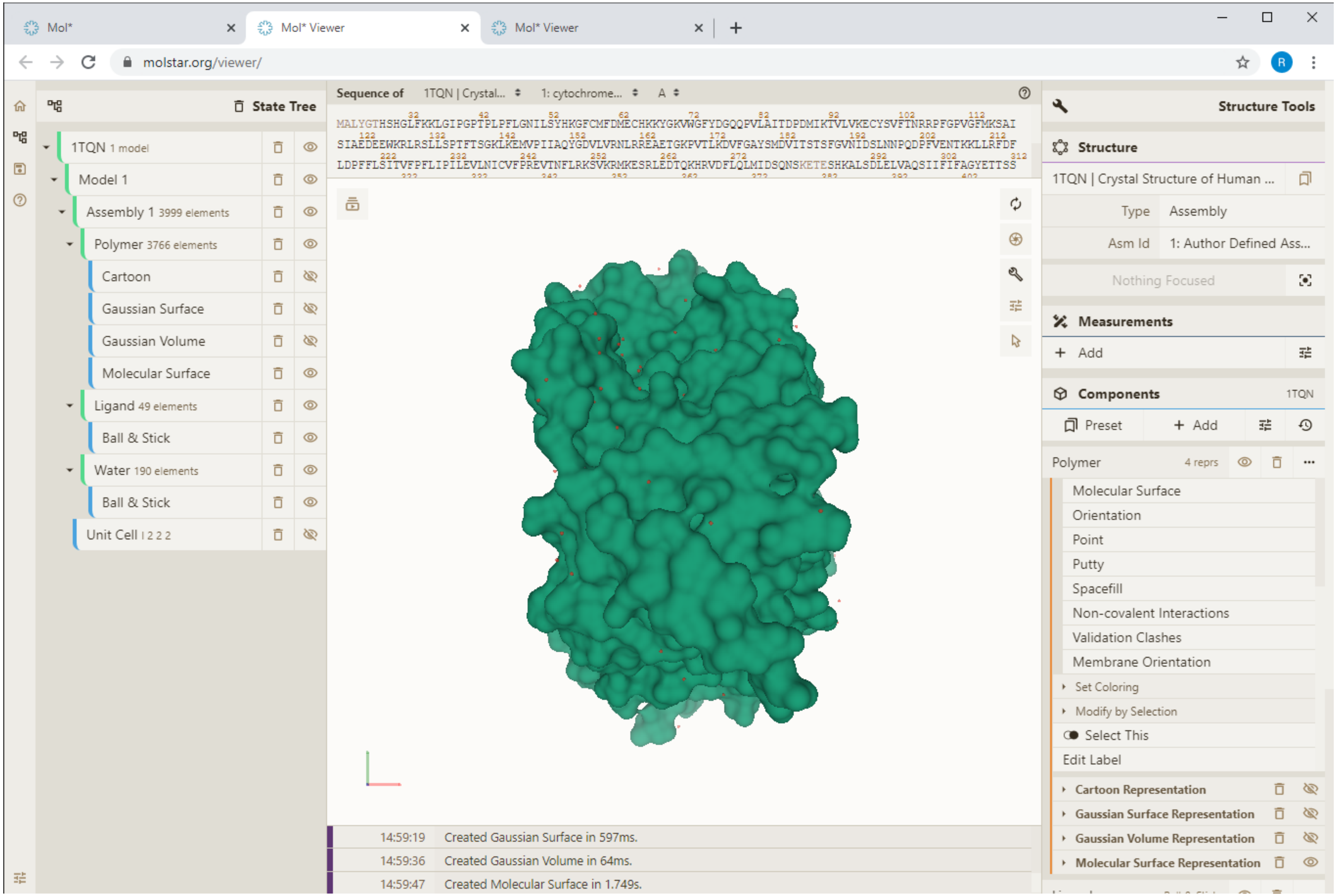
Ligand Ball & Stick

Water Ball & Stick

Unit Cell I 2 2 2

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

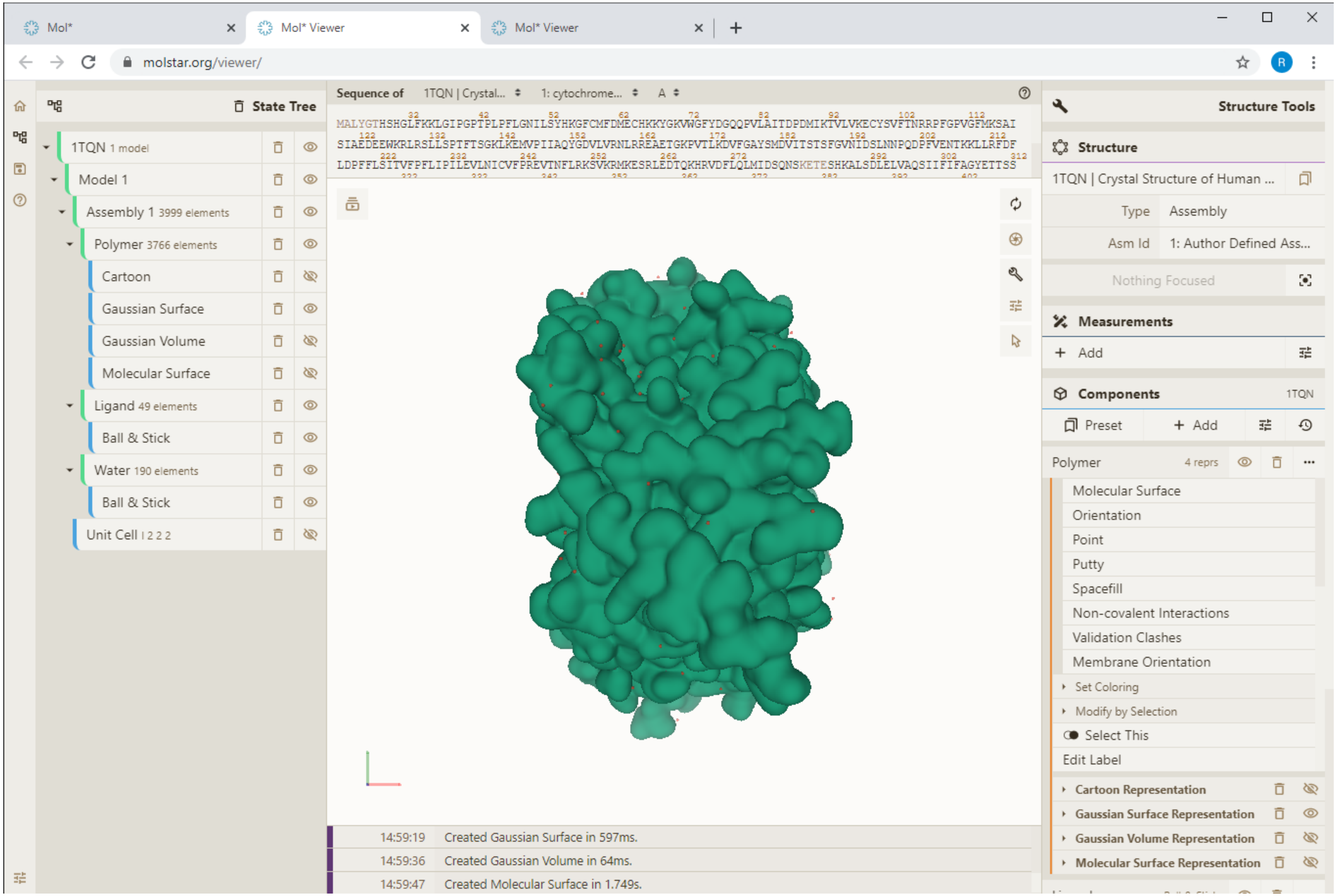
Vizualizace povrchu molekuly
Vizualizační model Molecular Surface



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

```
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.
```

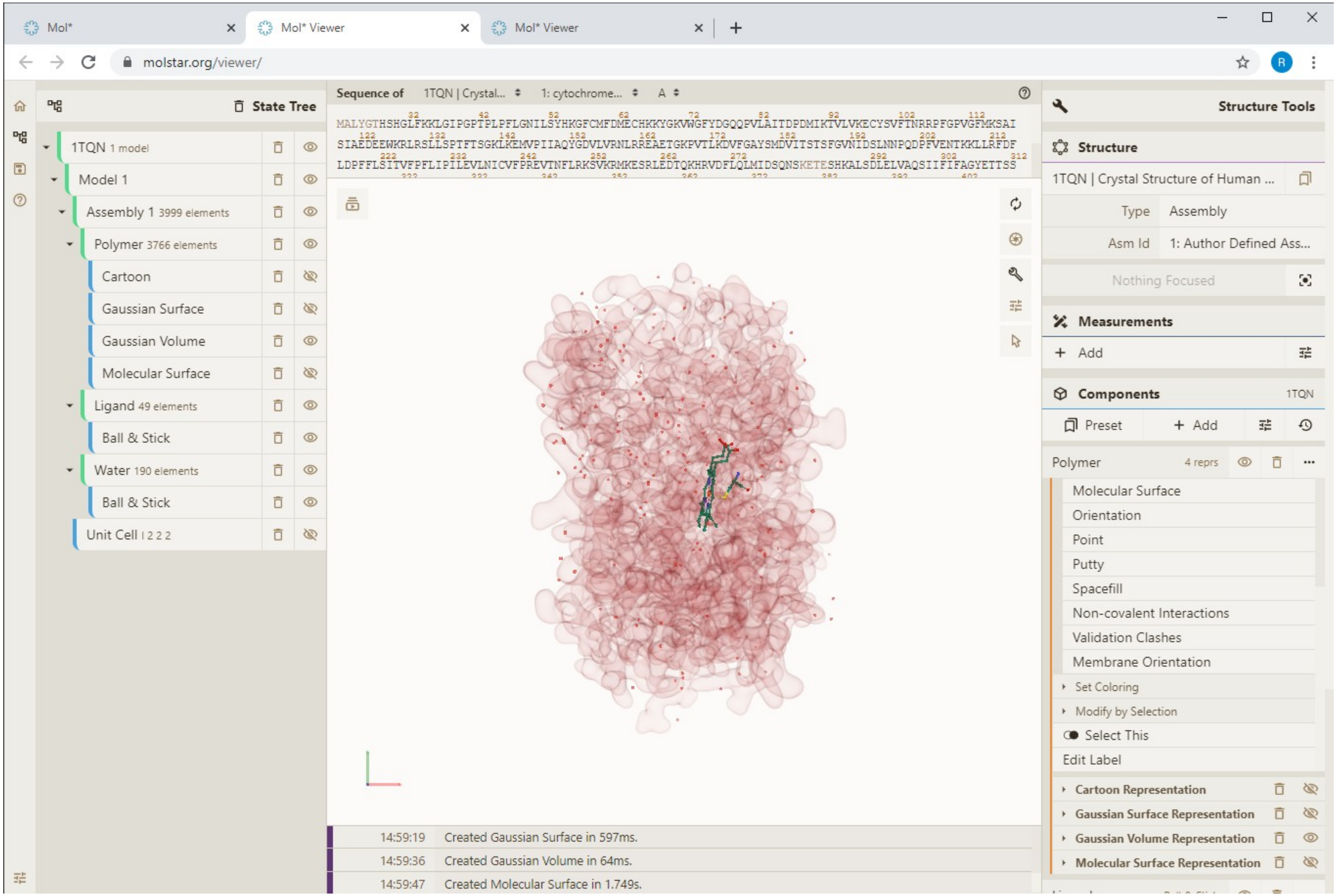
Vizualizace povrchu molekuly
Vizualizační model Gaussian Surface



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

```
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



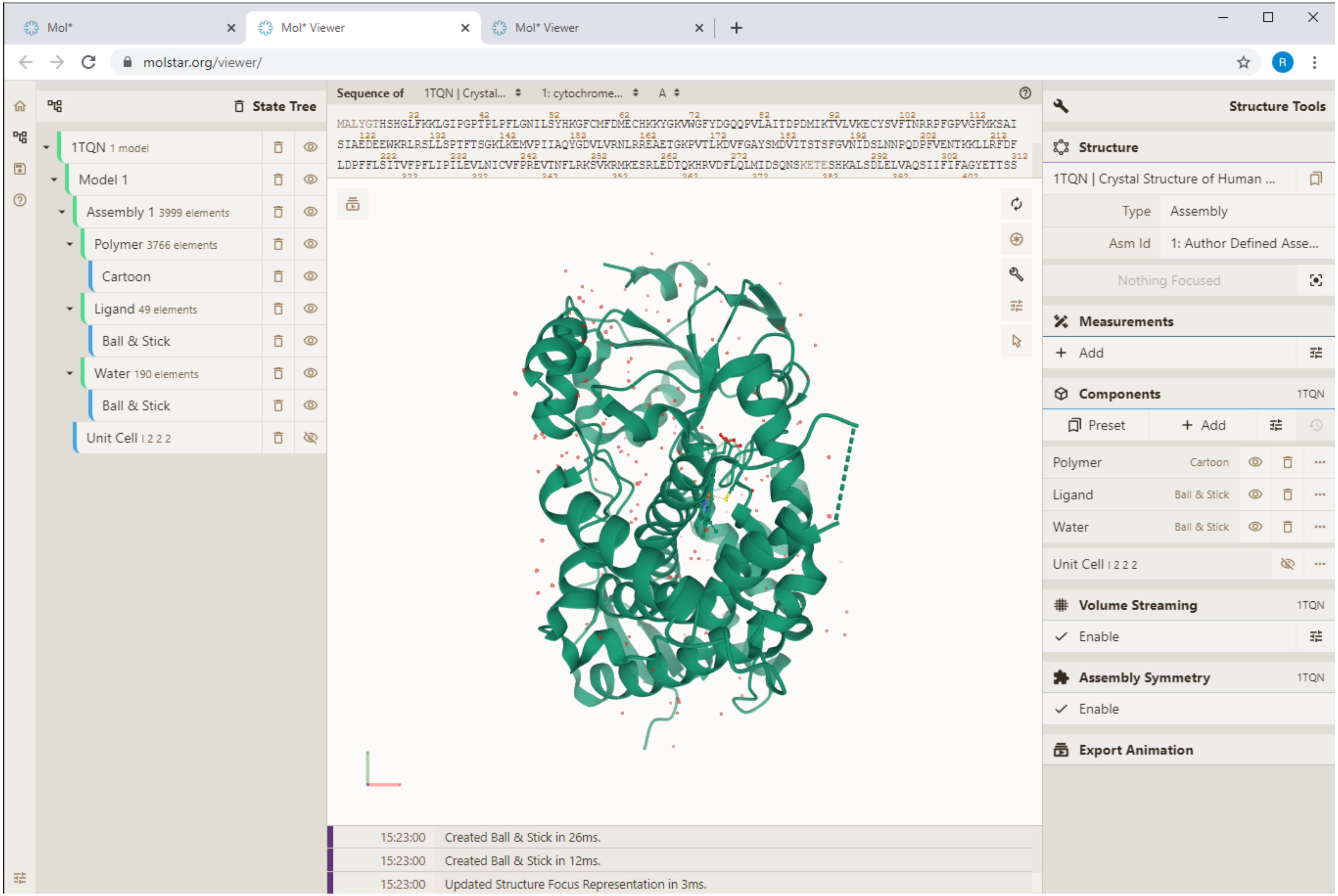
14:59:19 Created Gaussian Surface in 597ms.

14:59:36 Created Gaussian Volume in 64ms.

14:59:47 Created Molecular Surface in 1.749s.

Vizualizace experimentálních dat

Elektronová hustota



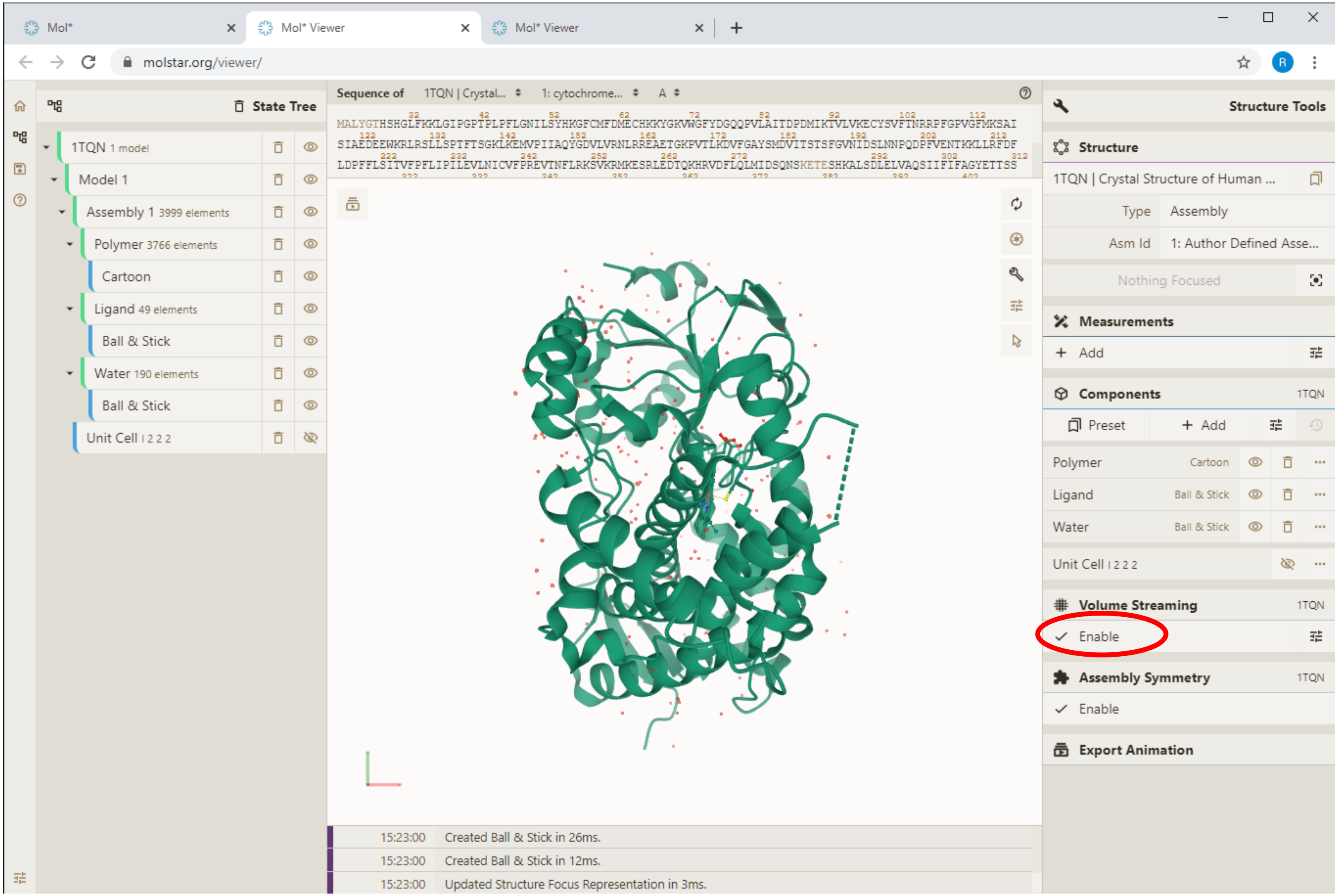
1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Asse...

```
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



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

1TQN | Crystal Structure of Human ...

Type: Assembly

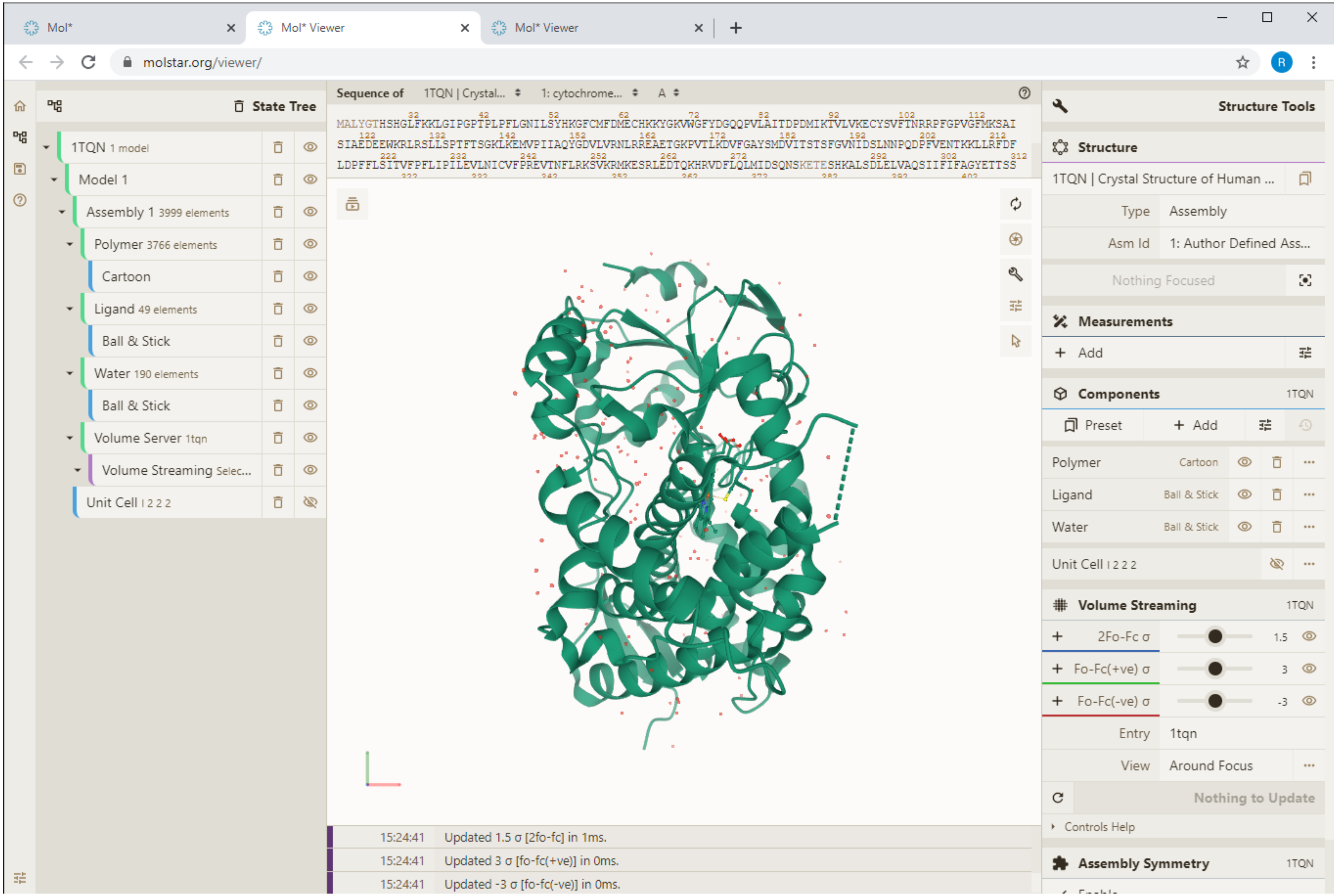
Asm Id: 1: Author Defined Asse...

Nothing Focused

Component	Representation
Polymer	Cartoon
Ligand	Ball & Stick
Water	Ball & Stick
Unit Cell I 2 2 2	

```
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



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Ass...

Nothing Focused

Polymer: Cartoon

Ligand: Ball & Stick

Water: Ball & Stick

Unit Cell I 2 2 2

2Fo-Fc σ: 1.5

Fo-Fc(+ve) σ: 3

Fo-Fc(-ve) σ: -3

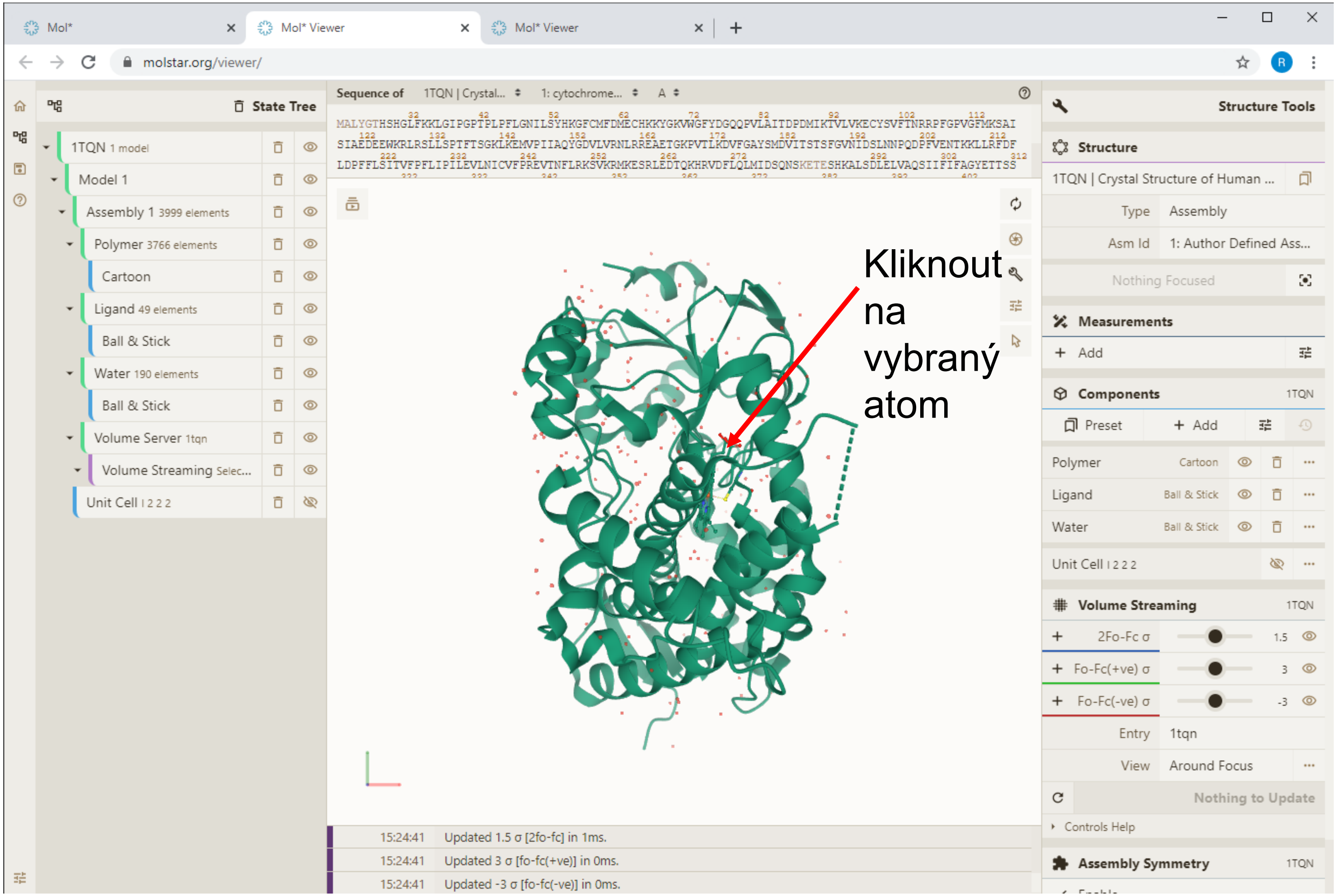
Entry: 1tqn

View: Around Focus

Nothing to Update

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

Vizualizace experimentálních dat
Elektronová hustota



1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Ass...

Nothing Focused

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

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

Entry: 1tqn

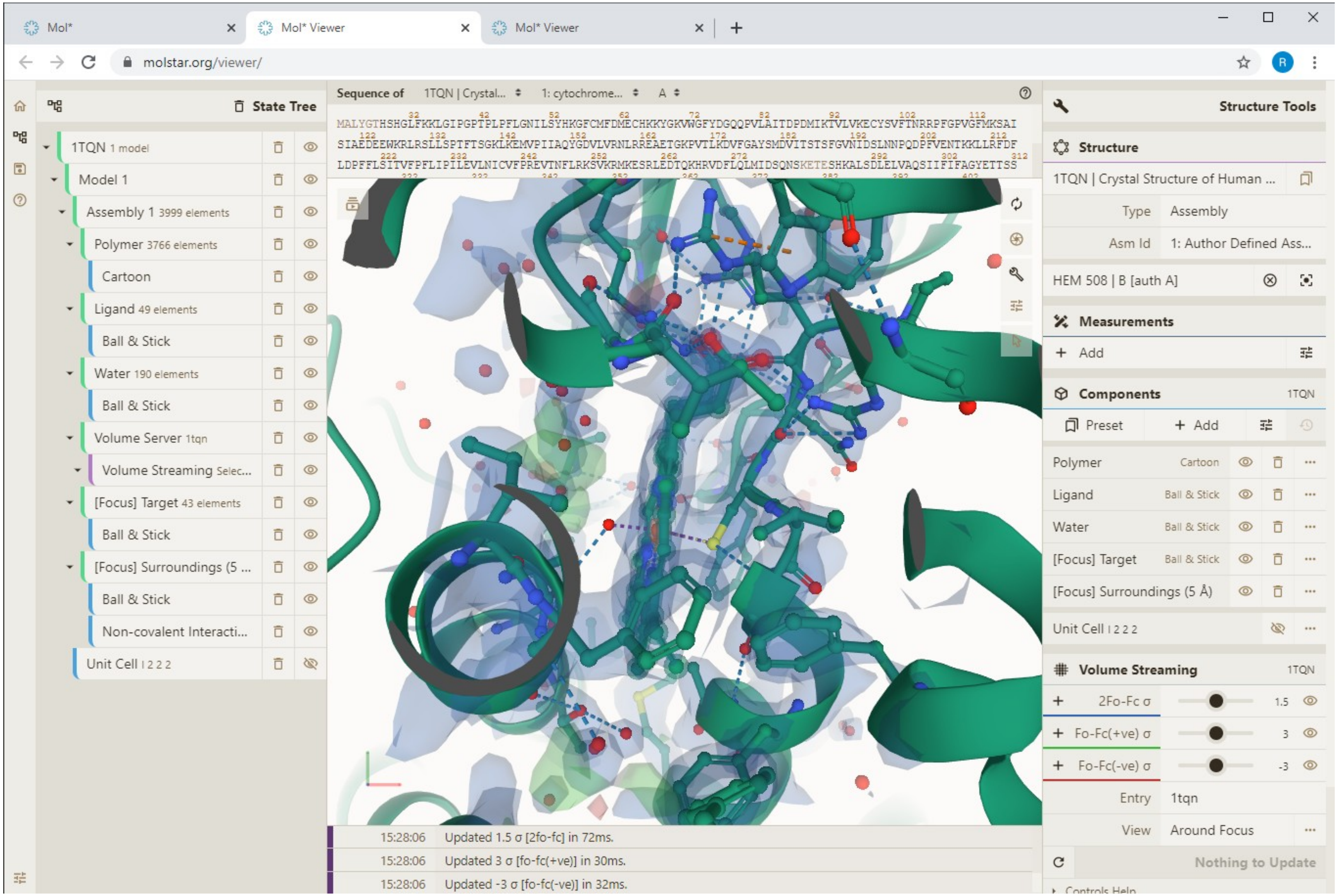
View: Around Focus

Nothing to Update

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

Kliknout na vybraný atom

Vizualizace experimentálních dat
Elektronová hustota



MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS

1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Ass...

HEM 508 | B [auth A]

Polymer	Cartoon	1TQN
Ligand	Ball & Stick	
Water	Ball & Stick	
[Focus] Target	Ball & Stick	
[Focus] Surroundings (5 Å)		
Unit Cell I 2 2 2		

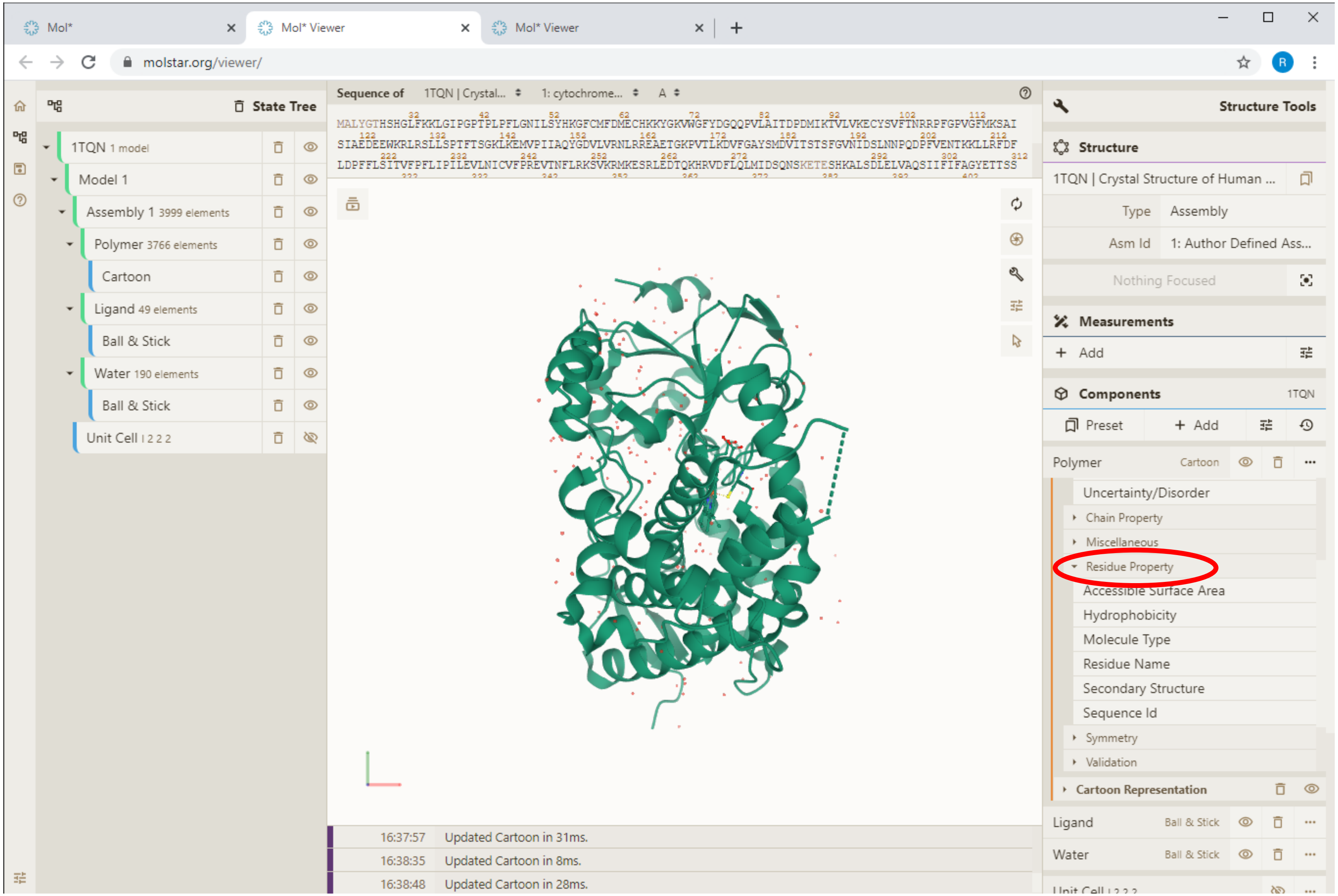
2Fo-Fc σ	1.5
Fo-Fc(+ve) σ	3
Fo-Fc(-ve) σ	-3

Entry: 1tqn

View: Around Focus

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

Vizualizace anotací
Obarvení podle vlastností



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

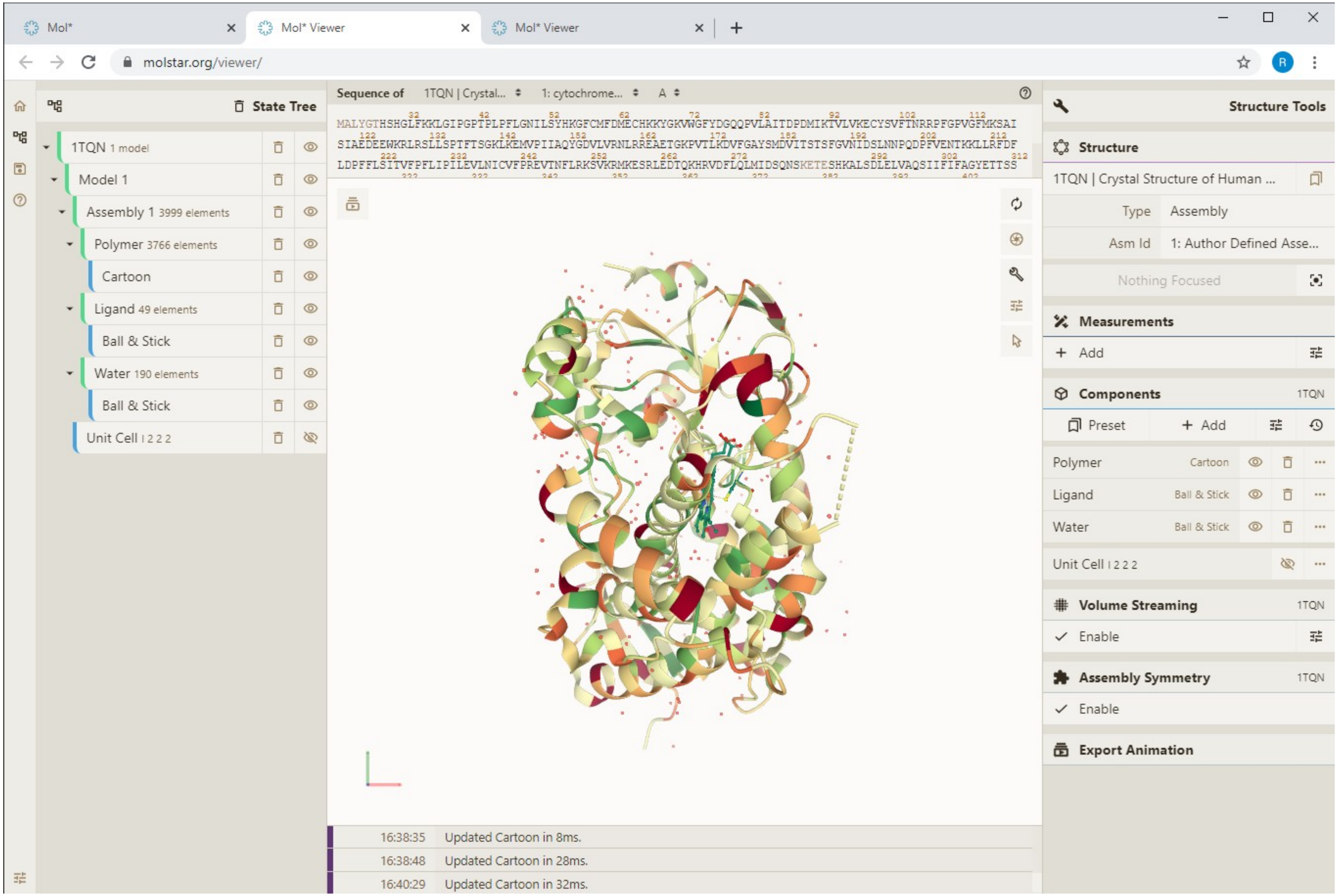
1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Ass...

```
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



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

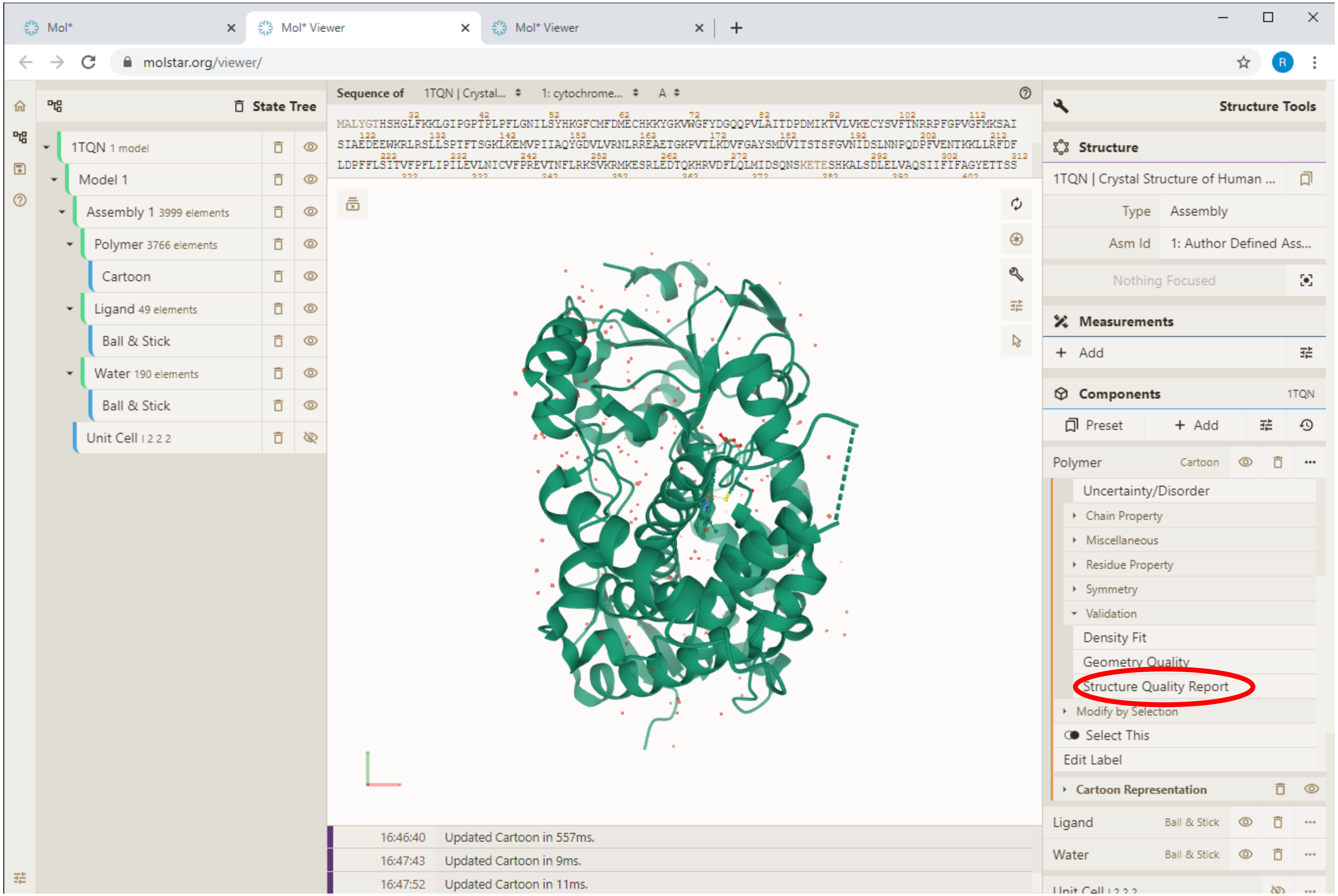
1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Asse...

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

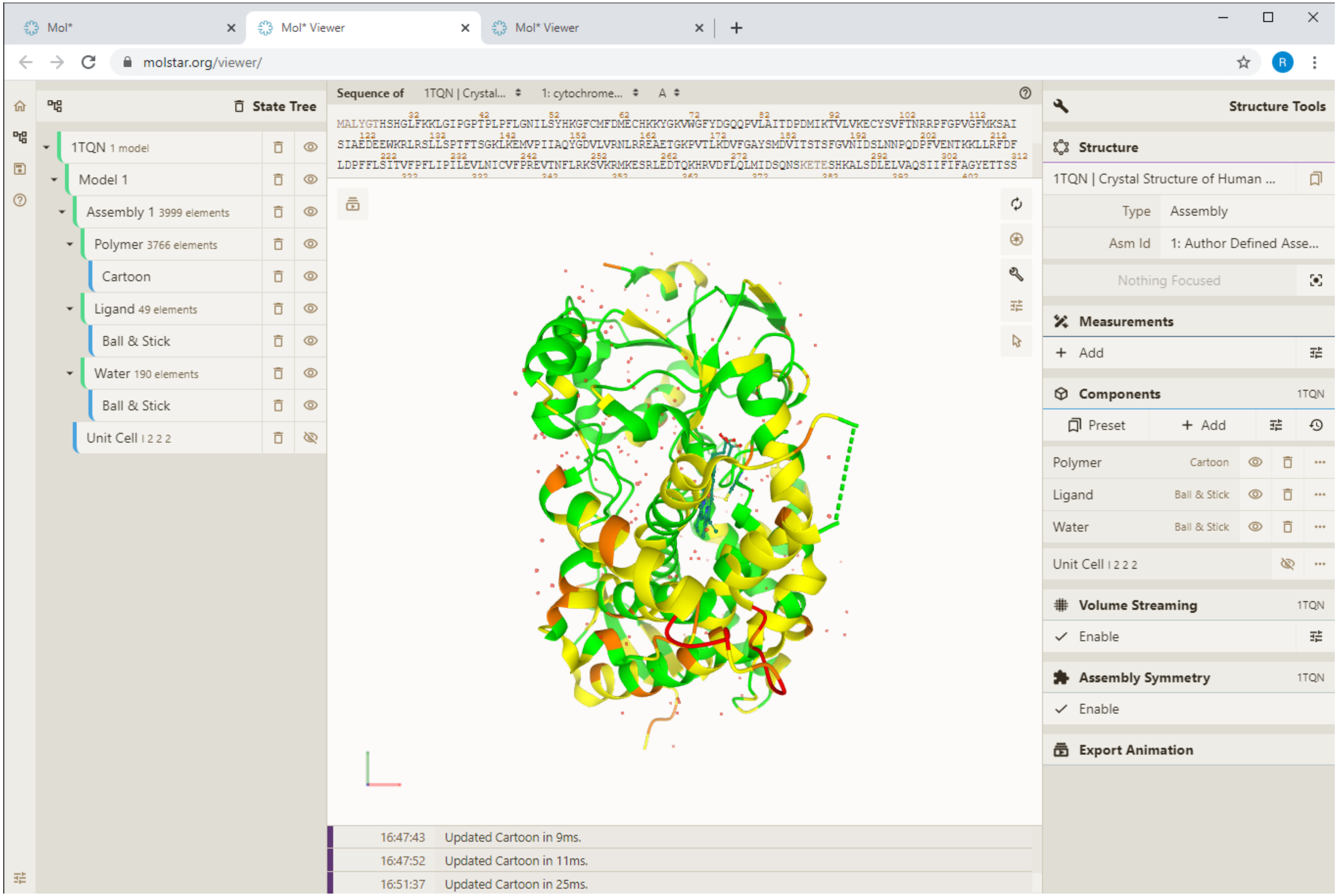
Vizualizace anotací
Obarvení podle vlastností – kvalita



MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS

```
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



MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS

1TQN | Crystal Structure of Human ...

Type: Assembly
Asm Id: 1: Author Defined Asse...
Nothing Focused

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

Měření

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

```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAISIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKP
VTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDFLDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSSVLSFI
MYELATHPDVQQKLQEEIDAVLPNKAPPTYDTVLQMEYLDMVVNETLRLFPIAMRLERVCKKDVEINGMFIPKGVVVMIPSYALHRDPKYWTEPEKFLPERFSKKNKDNIDPYIYTPFGSGPRNCIGMRFALMNMKLALIRVLQNFSF
```

1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Asse...

Dynamic Bonds: ✕ Off

Nothing Focused

Components 1TQN

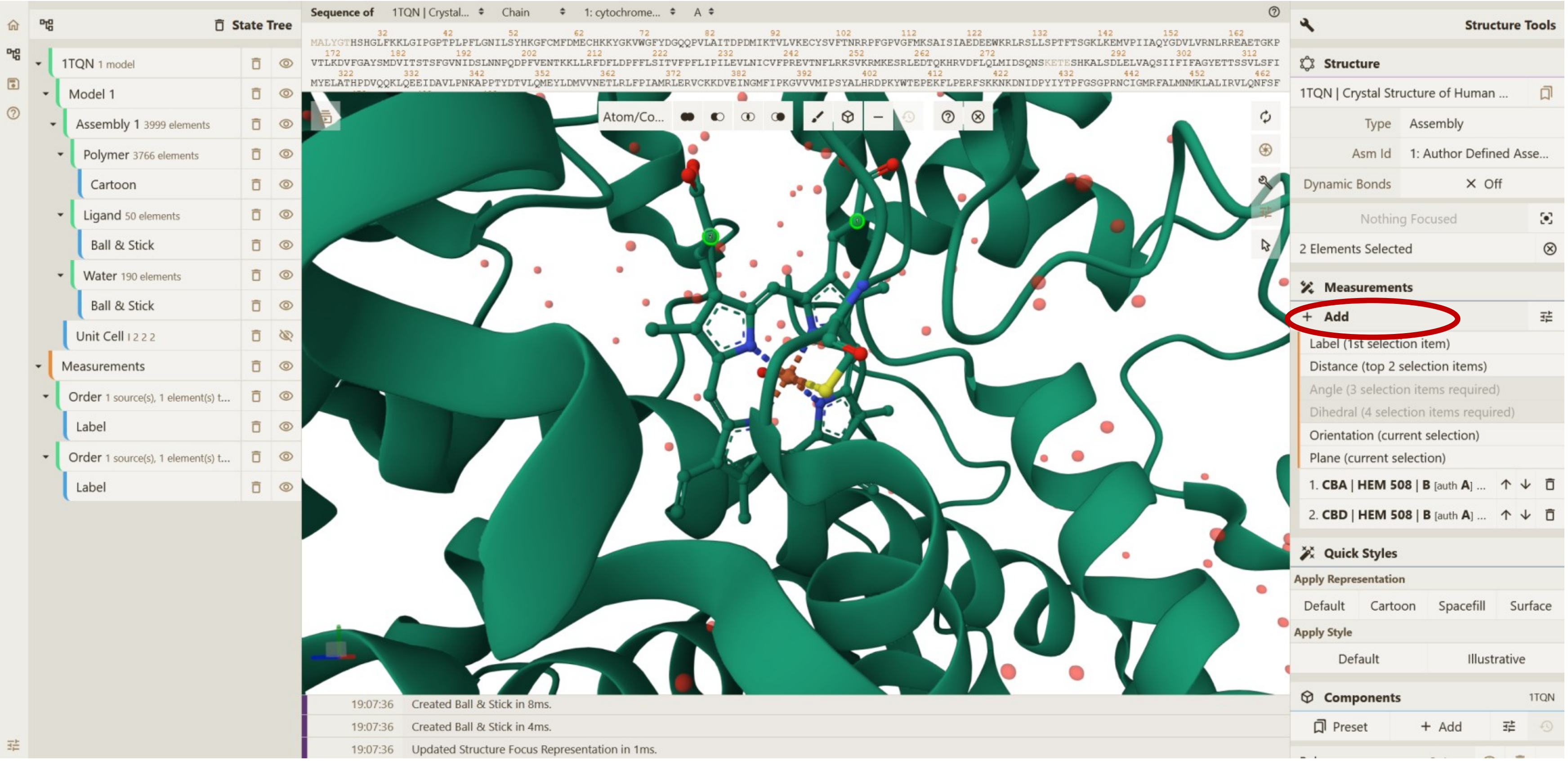
Polymer	Cartoon	
Ligand	Ball & Stick	
Water	Ball & Stick	
Unit Cell 1 2 2 2		

Volume Streaming 1TQN

Assembly Symmetry 1TQN

```
19:07:36   Created Ball & Stick in 8ms.
19:07:36   Created Ball & Stick in 4ms.
19:07:36   Updated Structure Focus Representation in 1ms.
```

Měření



1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

Dynamic Bonds ✕ Off

Nothing Focused

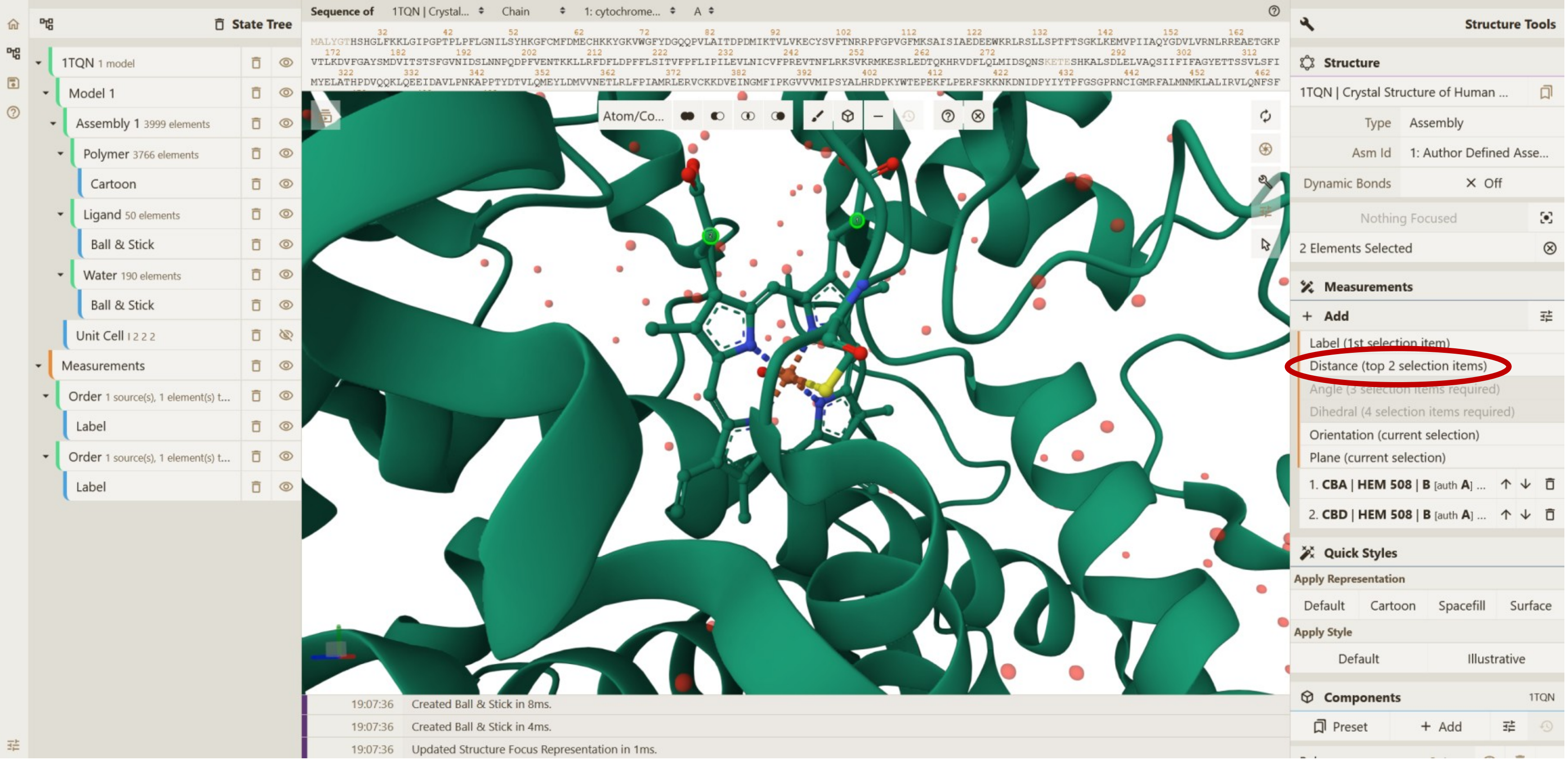
2 Elements Selected

1. **CBA** | **HEM 508** | **B** [auth **A**] ...

2. **CBD** | **HEM 508** | **B** [auth **A**] ...

```
19:07:36   Created Ball & Stick in 8ms.
19:07:36   Created Ball & Stick in 4ms.
19:07:36   Updated Structure Focus Representation in 1ms.
```

Měření



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

```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAISIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKP
VTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDFLDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSSVLSFI
MYELATHPDVQQKLQEEIDAVLPNKAPPTYDTVLQMEYLDMVVNETLRLFPIAMRLERVCKKDVEINGMFIPKGVVVMIPSYALHRDPKYWTEPEKFLPERFSKKNKDNIDPYIYTPFGSGPRNCIGMRFALMNMKLALIRVLQNFSF
```

State Tree

- 1TQN 1 model
  - Model 1
    - Assembly 1 3999 elements
      - Polymer 3766 elements
        - Cartoon
      - Ligand 50 elements
        - Ball & Stick
      - Water 190 elements
        - Ball & Stick
    - Unit Cell 1 2 2 2
- Measurements
  - Order 1 source(s), 1 element(s) t...
    - Label
  - Order 1 source(s), 1 element(s) t...
    - Label

Structure Tools

Structure

1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Asse...

Dynamic Bonds: ✕ Off

Nothing Focused

2 Elements Selected

Measurements

+ Add

- Label (1st selection item)
- Distance (top 2 selection items)
- Angle (3 selection items required)
- Dihedral (4 selection items required)
- Orientation (current selection)
- Plane (current selection)

1. **CBA** | **HEM 508** | **B** [auth **A**] ...
2. **CBD** | **HEM 508** | **B** [auth **A**] ...

Quick Styles

Apply Representation: Default, Cartoon, Spacefill, Surface

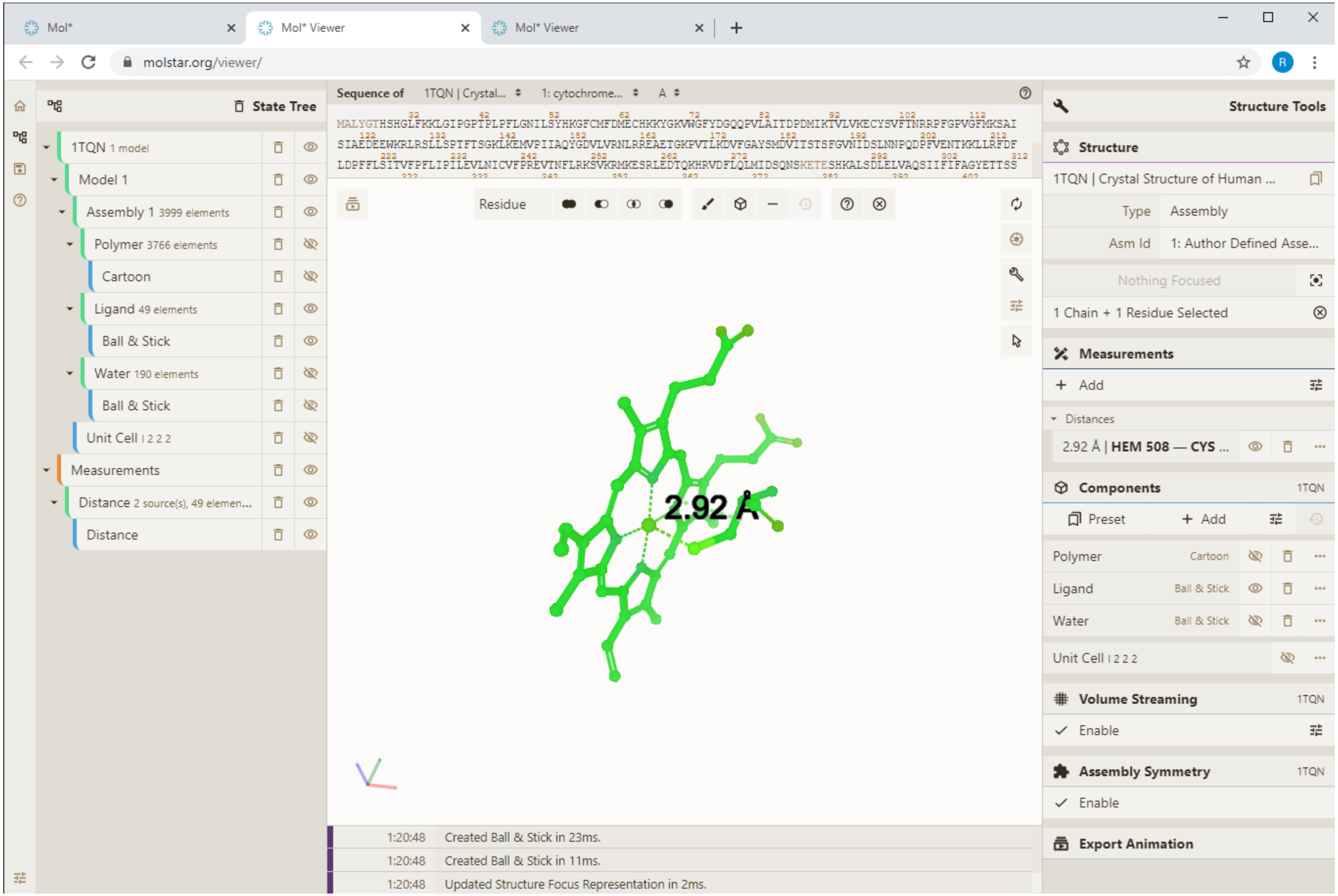
Apply Style: Default, Illustrative

Components 1TQN

Preset + Add

```
19:07:36 Created Ball & Stick in 8ms.
19:07:36 Created Ball & Stick in 4ms.
19:07:36 Updated Structure Focus Representation in 1ms.
```

Měření



1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Asse...

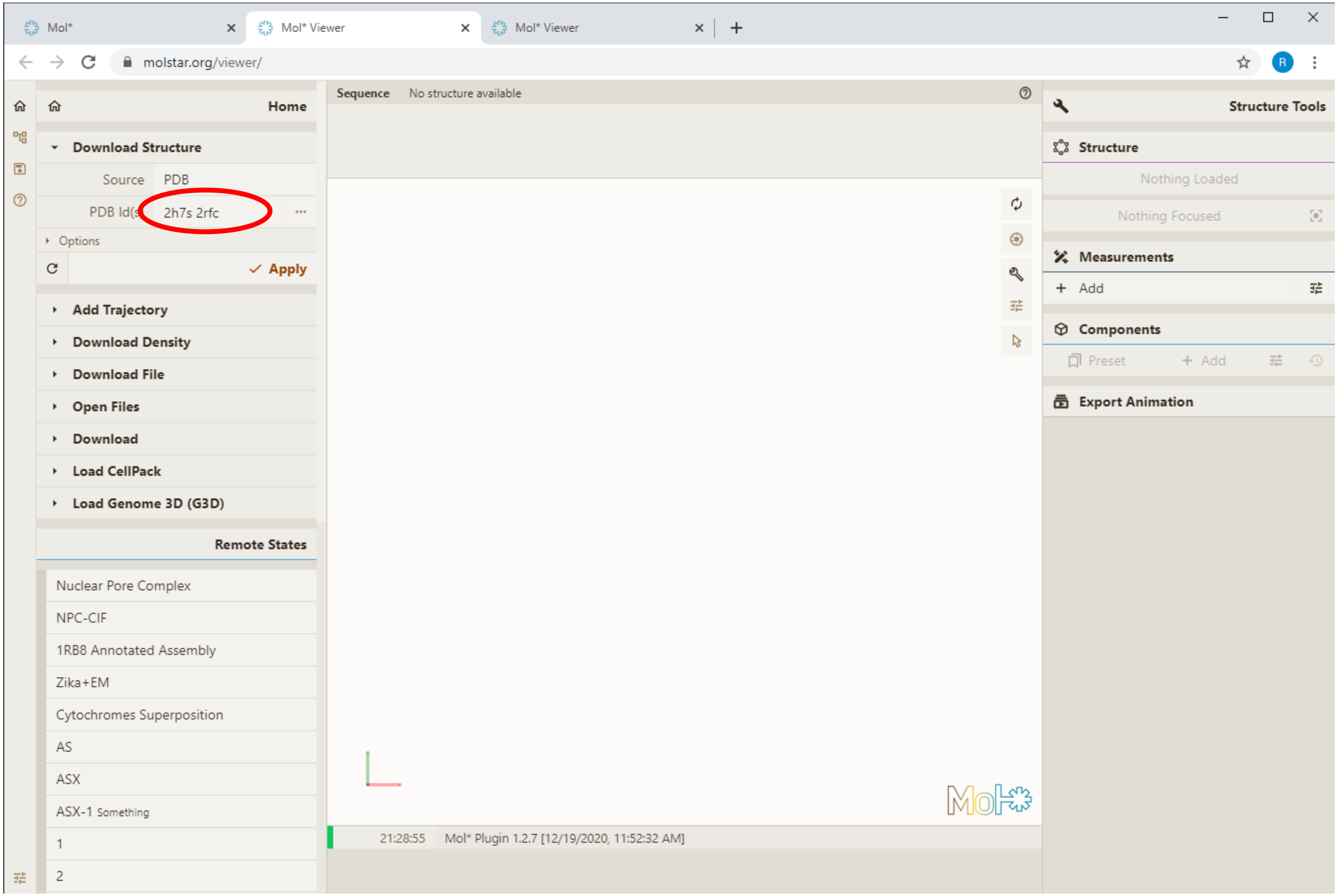
Nothing Focused

1 Chain + 1 Residue Selected

2.92 Å | HEM 508 — CYS ...

```
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.
```

Přikládání struktur



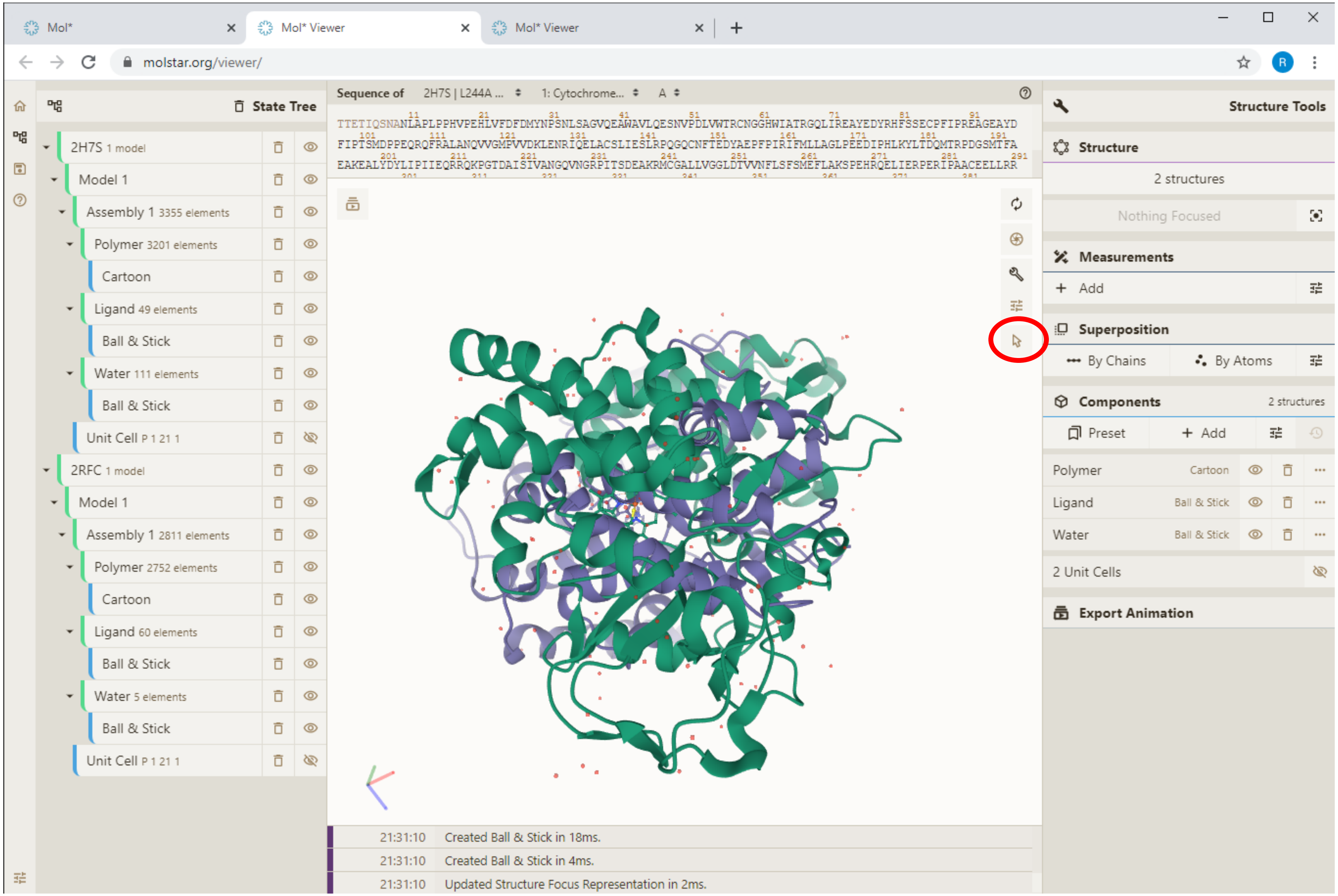
molstar.org/viewer/

Source: PDB

PDB Id(s): 2h7s 2rfc

21:28:55 Mol* Plugin 1.2.7 [12/19/2020, 11:52:32 AM]

Přikládání struktur

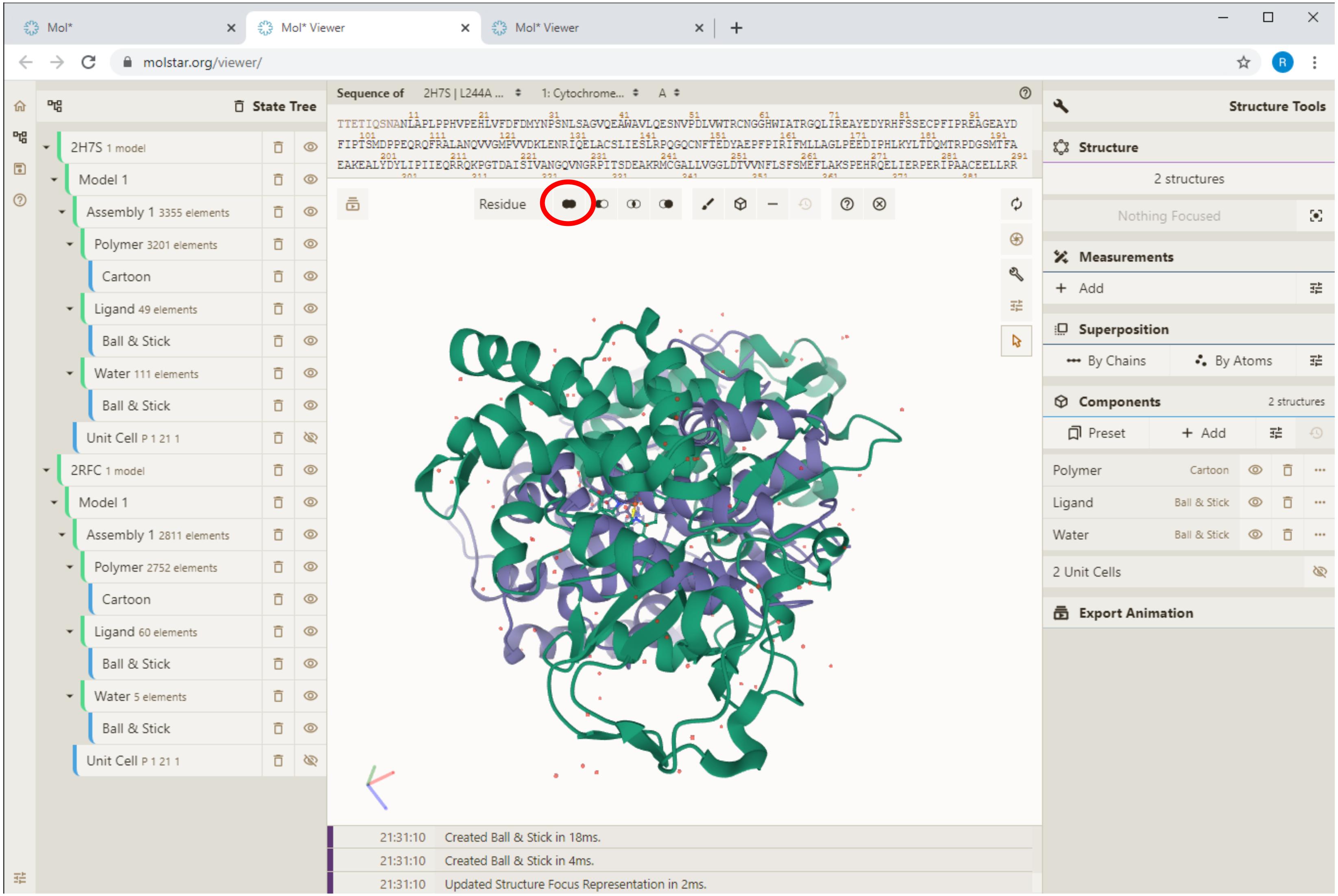


21:31:10 Created Ball & Stick in 18ms.

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

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

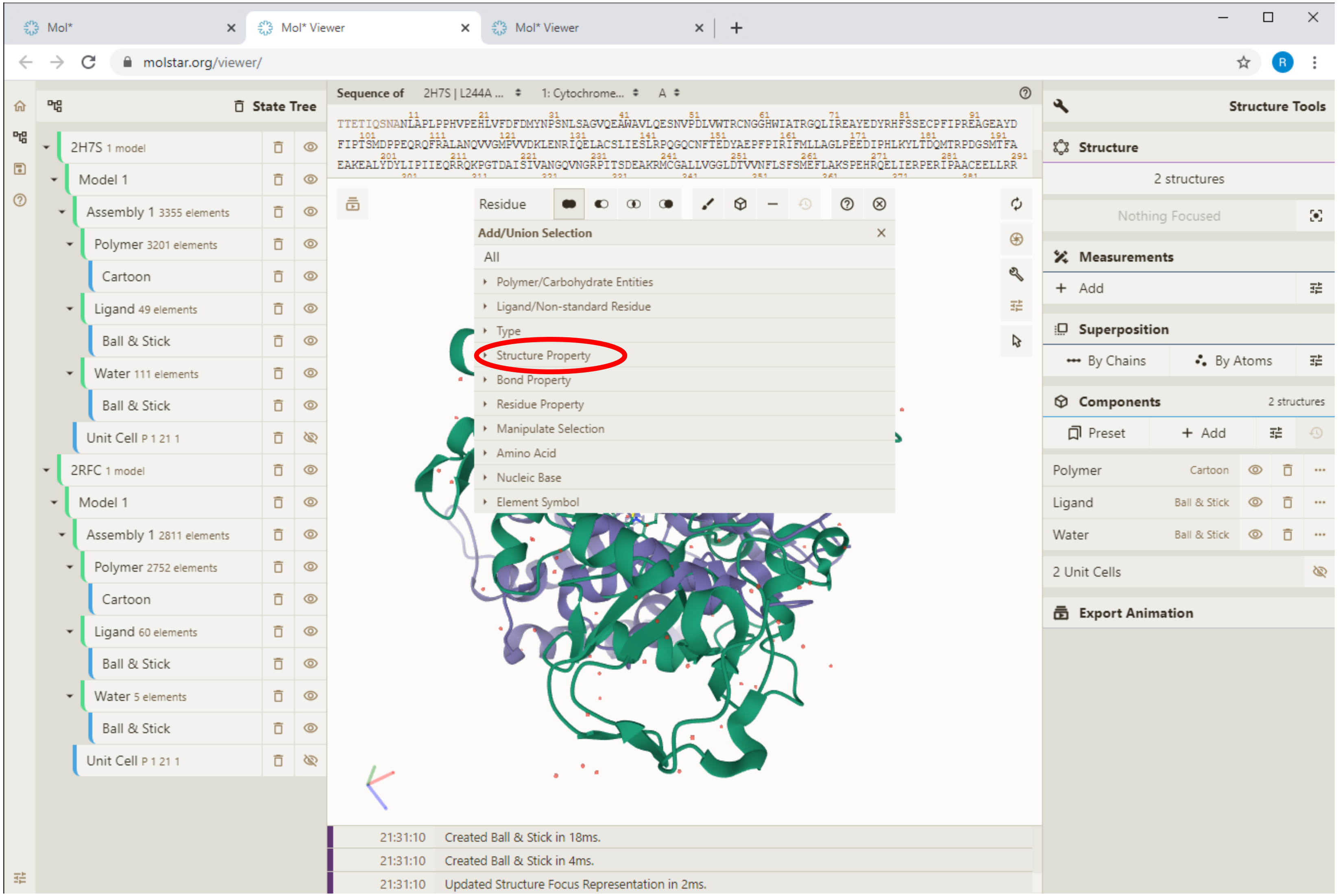
Přikládání struktur



```
TTETIQSNANLAPLPPHVPEHLVFDFDMYNPSNLSAGVQEAWAVLQESNVPDLVWTRCNGGHWIATRGQLIREAYEDYRHFSSECPFIPREAGEAYD
FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRPQGQCNFTEDYAEPFPIRIFMLLAGLPEEDIPHLKYLTDQMTRPDGSMTFA
EAKEALYDYLIPIIEQRRQKPGTDAISIVANGQVNGRPITSDEAKRMCGALLVGGLDTVVNFLSFSMEFLAKSPEHRQELIERPERIPAACEELLRR
```

```
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.
```

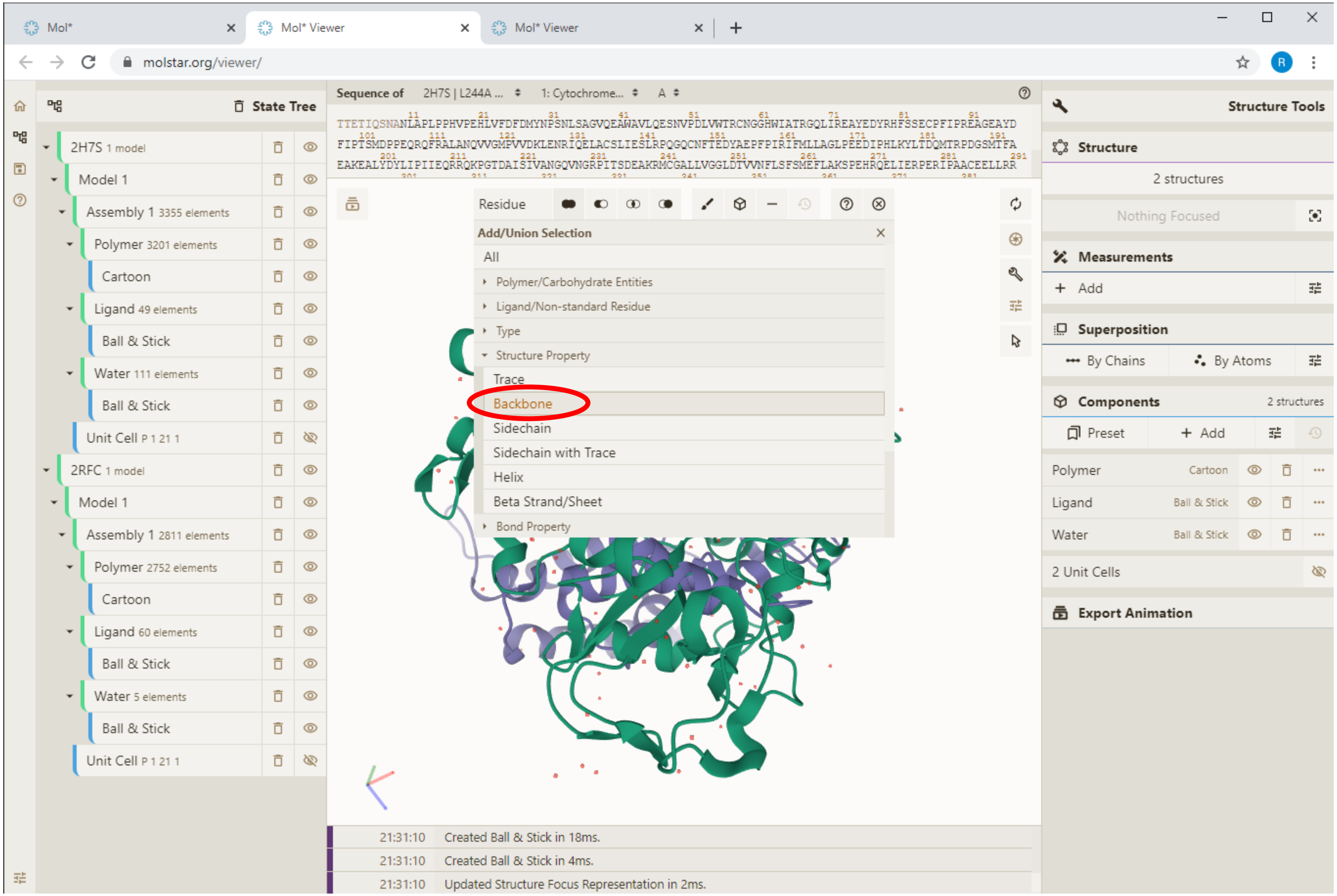
Přikládání struktur



TTETIQSNANLAPLPPHVPEHLVFDFDMYNPSNLSAGVQEAWAVLQESNVPDLVWTRCNGGHWIATRGQLIREAYEDYRHFSSECPFIPREAGEAYD
FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRPQGQCNFTEDYAEPFPIRIFMLLAGLPEEDIPHLKYLTDQMTRPDGSMTFA
EAKEALYDYLIPIIEQRRQKPGTDAISIVANGQVNGRPITSDEAKRMCGALLVGGLDTVVNFLSFSMEFLAKSPEHRQELIERPERIPAACEELLRR

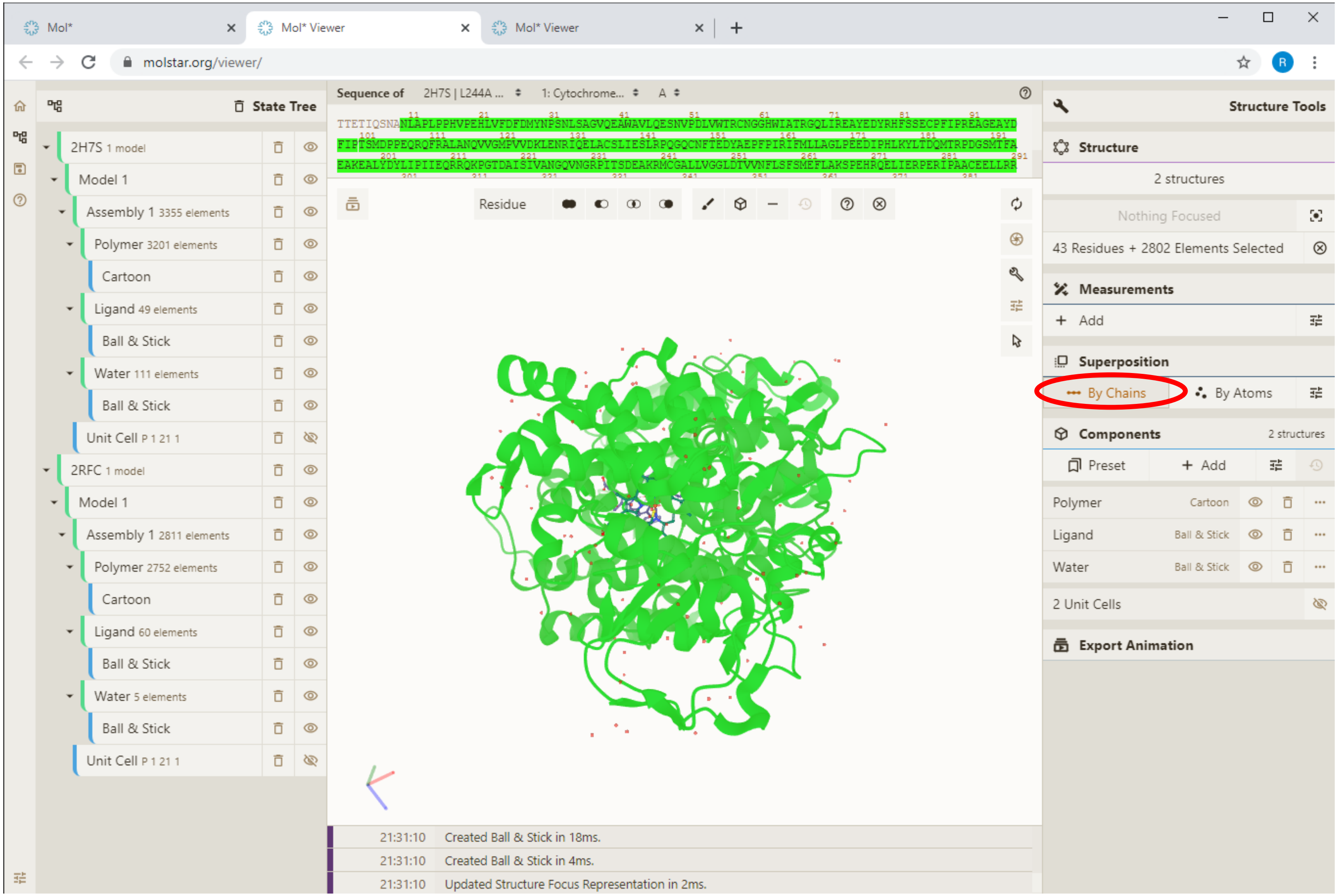
```
21:31:10   Created Ball & Stick in 18ms.
21:31:10   Created Ball & Stick in 4ms.
21:31:10   Updated Structure Focus Representation in 2ms.
```

Přikládání struktur



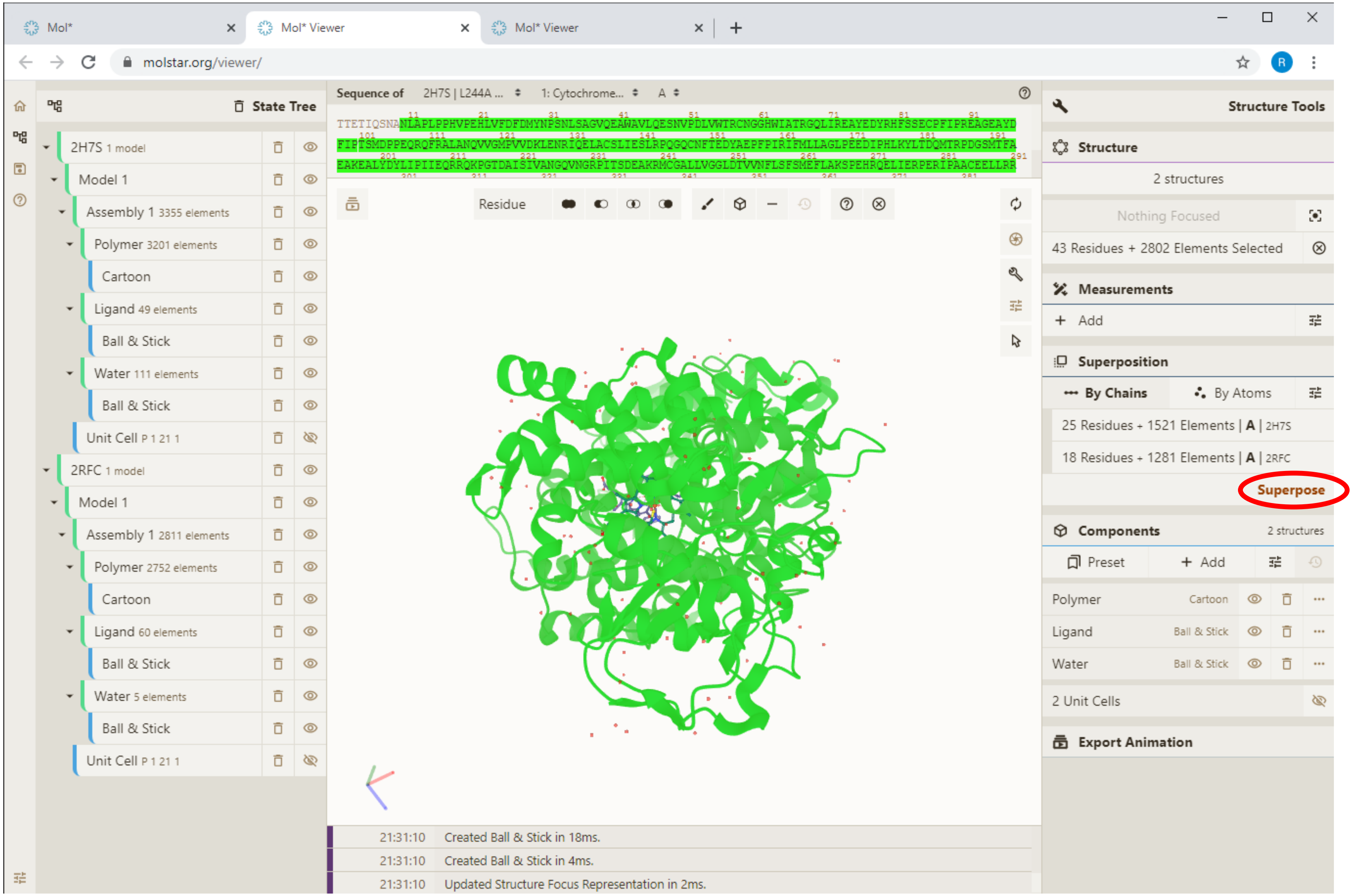
```
21:31:10   Created Ball & Stick in 18ms.
21:31:10   Created Ball & Stick in 4ms.
21:31:10   Updated Structure Focus Representation in 2ms.
```

Přikládání struktur



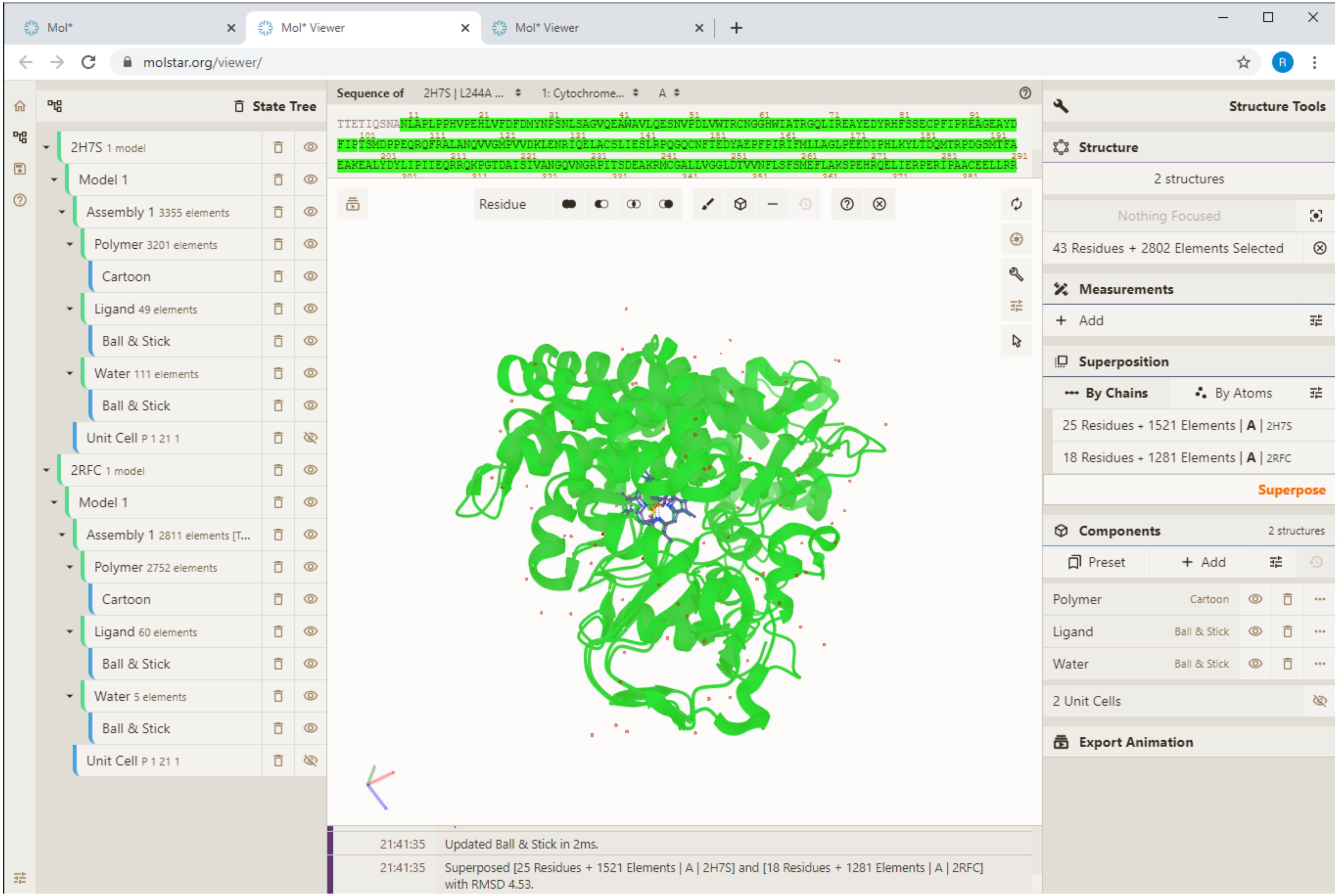
```
21:31:10   Created Ball & Stick in 18ms.
21:31:10   Created Ball & Stick in 4ms.
21:31:10   Updated Structure Focus Representation in 2ms.
```

Přikládání struktur



```
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.
```

Přikládání struktur

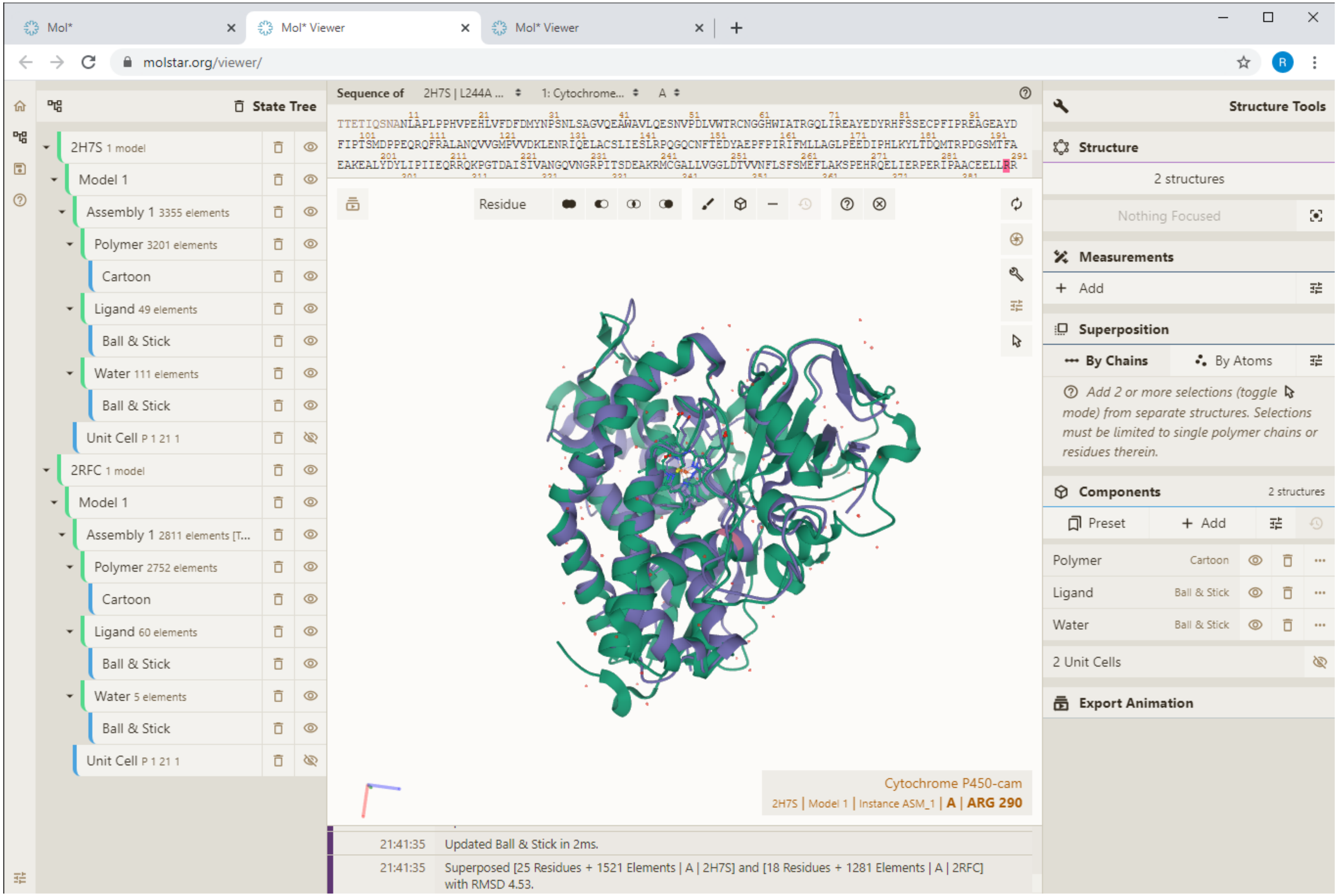


```
TTETIQSNANLAPLPPHVPEHLVFDFDMYNPSNLSAGVQEAWAVLQESNVPDLVWTRCNGGHWIATRGQLIREAYEDYRHFSSECPFIPREAGEAYD
FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRPQGQCNFTEDYAEPFPIRIFMLLAGLPEEDIPHLKYLTDQMTRPDGSMTFA
EAKEALYDYLIPIIEQRRQKPGTDAISIVANGQVNGRPITSDEAKRMCGALLVGGLDTVVNFLSFSMEFLAKSPEHRQELIERPERIPAACEELLRR
```

- 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

```
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

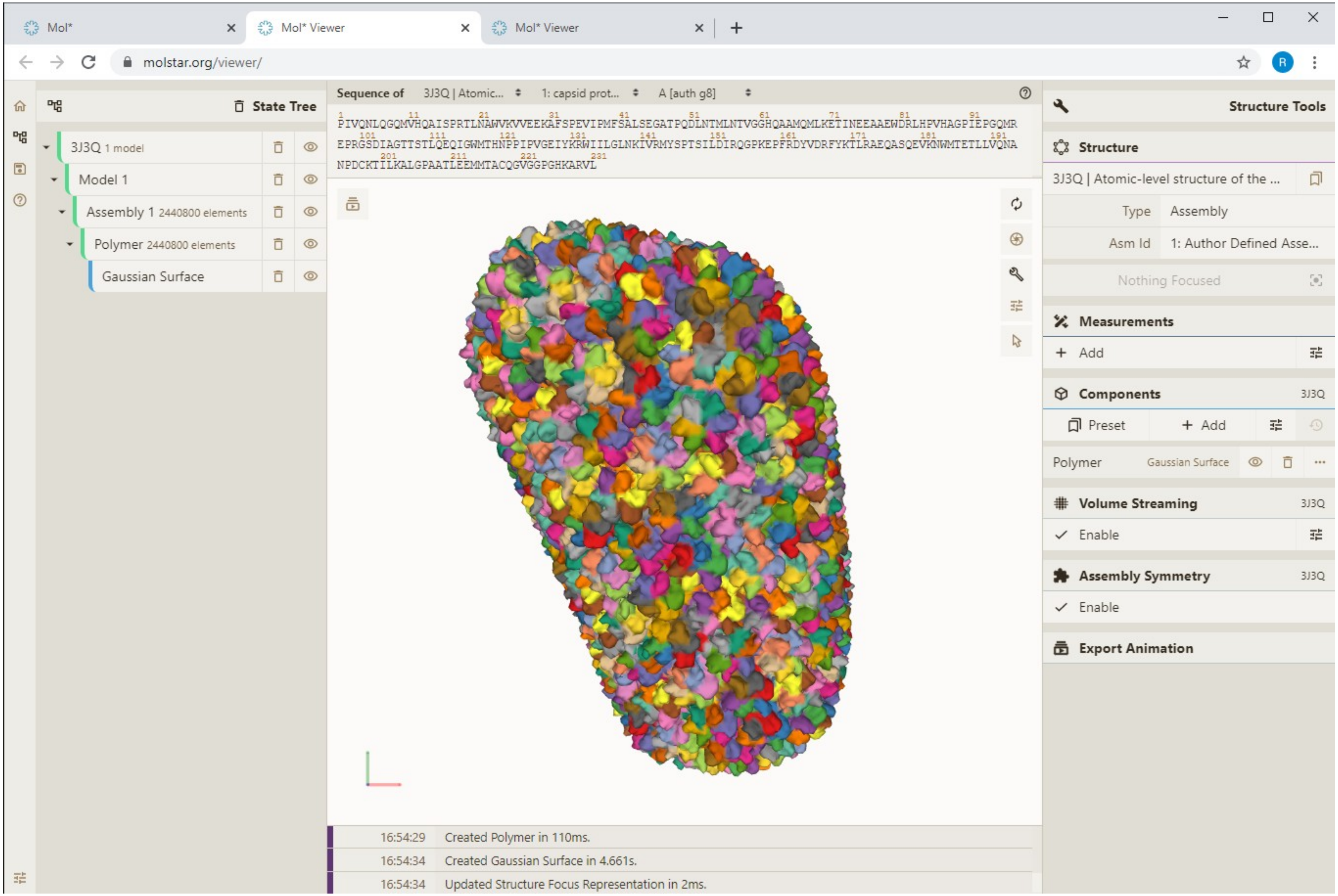


```
TTETIQSNANLAPLPPHVPEHLVFDFDMYNPSNLSAGVQEAWAVLQESNVPDLVWTRCNGGHWIATRGQLIREAYEDYRHFSSECPFIPREAGEAYD
FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRPQGQCNFTEDYAEPFPIRIFMLLAGLPEEDIPHLKYLTDQMTRPDGSMTFA
EAKEALYDYLIPIIEQRRQKPGTDAISIVANGQVNGRPITSDEAKRMCGALLVGGLDTVVNFLSFSMEFLAKSPEHRQELIERPERIPAACEELLRR
```

Add 2 or more selections (toggle mode) from separate structures. Selections must be limited to single polymer chains or residues therein.

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

Vizualizace proteinových assemblies



Sequence of 3J3Q | Atomic... 1: capsid prot... A [auth g8]

```
1         11        21        31        41        51        61        71        81        91
PIVQNLQGQMVHQAISPRTLNAWVKVVEEKAFSPEVIPMFSALSEGATPQDLNTMLNTVGGHQAAMQMLKETINEEAAEWDRLHPVHAGPIEPGQMR
  101       111       121       131       141       151       161       171       181       191
EPRGSDIAGTTSTLQEQIGWMTHNPPIPVGEIYKRWIILGLNKIVRMYSPTSILDIRQGPKEPFRDYVDRFYKTLRAEQASQEVKNWMTETLLVQNA
     201       211       221       231
NPDCKTILKALGPAATLEEMMTACQGVGGPGHKARVL
```

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

Type: Assembly

Asm Id: 1: Author Defined Asse...

Nothing Focused

Polymer: Gaussian Surface

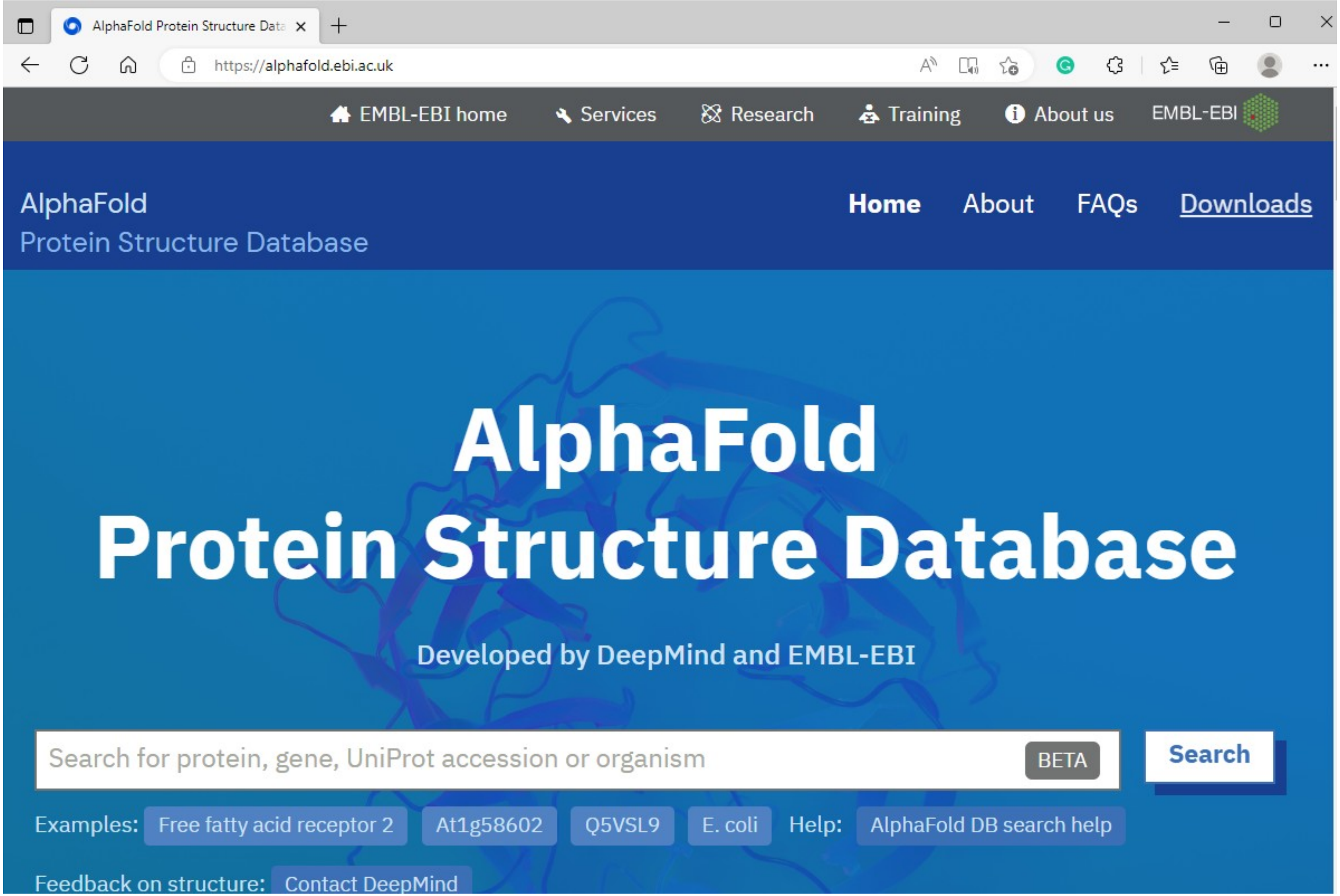
```
16:54:29   Created Polymer in 110ms.
16:54:34   Created Gaussian Surface in 4.661s.
16:54:34   Updated Structure Focus Representation in 2ms.
```

CEITEC

Molstar Integrace

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

AlphaFoldDB

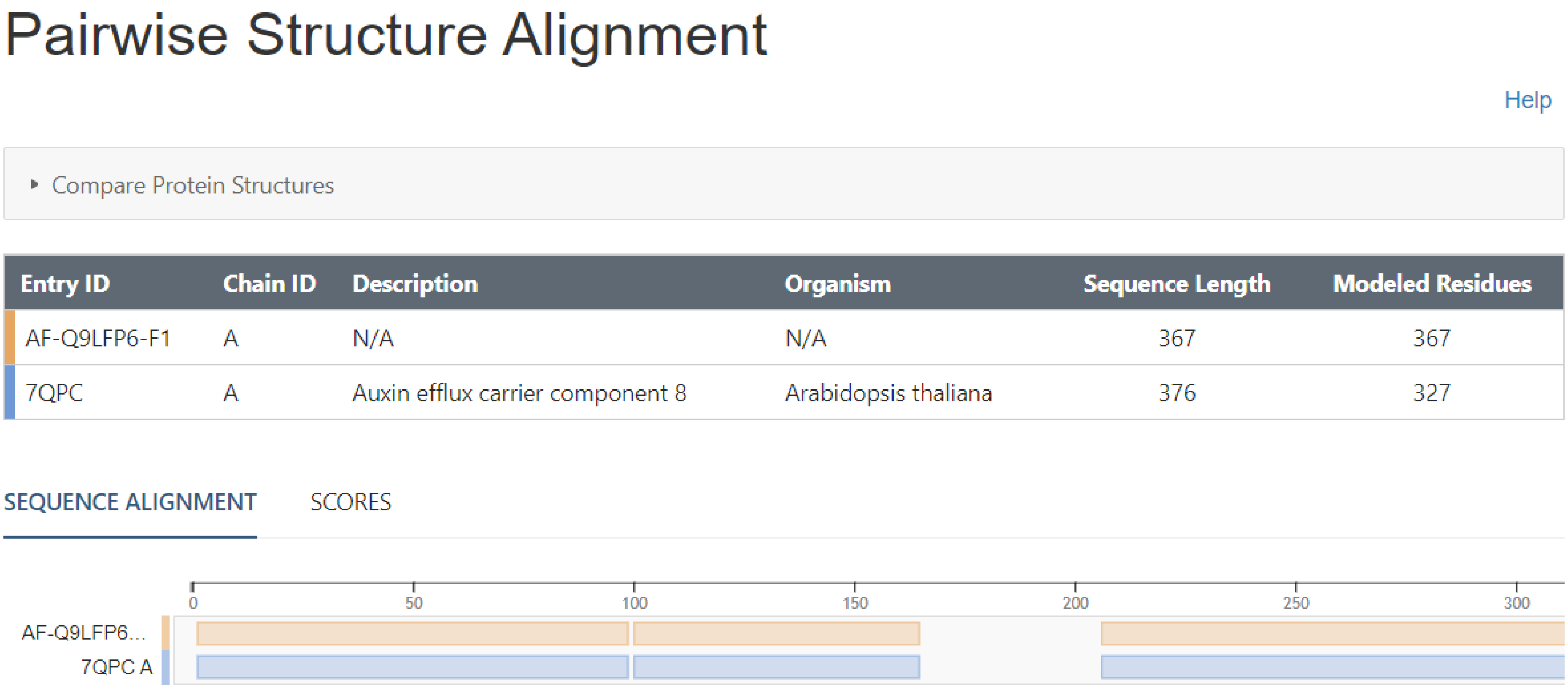


AlphaFold

Protein Structure Database

Developed by DeepMind and EMBL-EBI

Přikládání struktur – PDB a AlphaFold

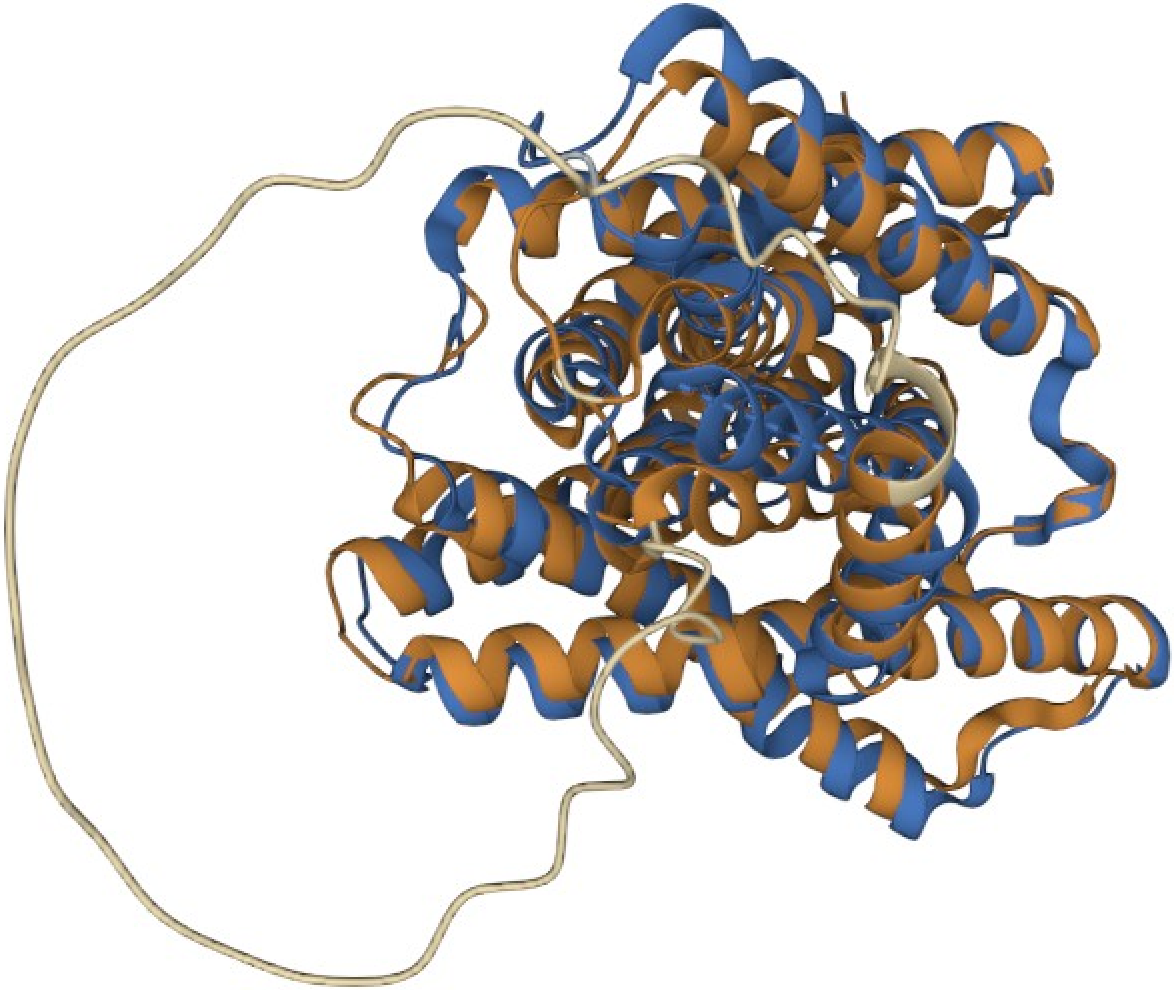


Pairwise Structure Alignment

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

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

Přikládání struktur – PDB a AlphaFold



Molstar Rozšíření

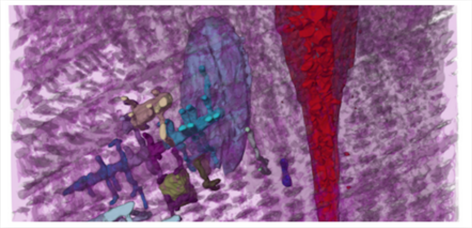
Extensions

MolViewSpec

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

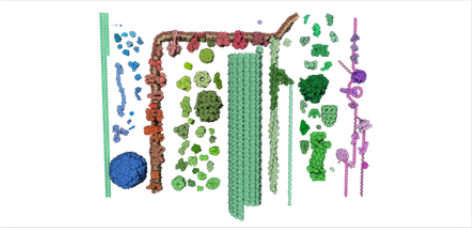
MolViewSpec provides a generic mechanism for describing visual scenes or views that are used in molecular visualizations. It adopts declarative data-driven approach to describe, load, render, and visually deliver molecular structures, along with 3D representations, coloring schemes, and associated structural,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

Volumes and Segmentations



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

Mesoscale Explorer



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