CEITEC

Central European Institute of Technology
BRNO | CZECH REPUBLIC

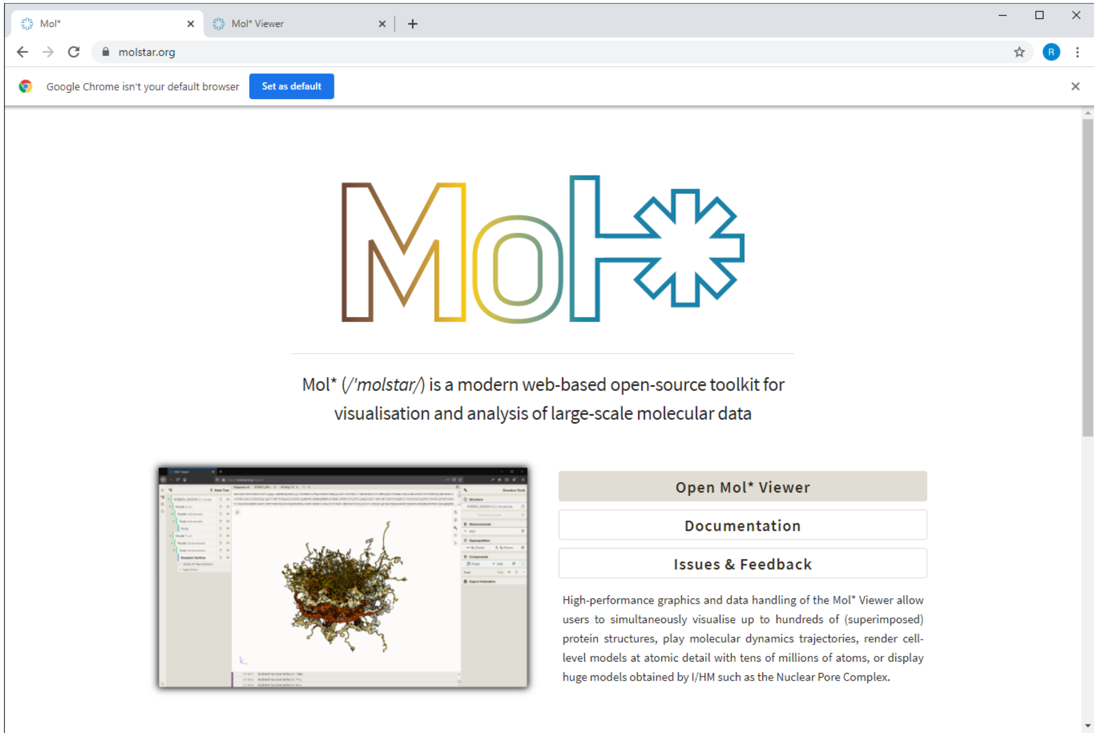
Vizualizace proteinů a ligandů

EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND
INVESTING IN YOUR FUTURE

2007–13
OP Research and
Development for Innovation

MolStar

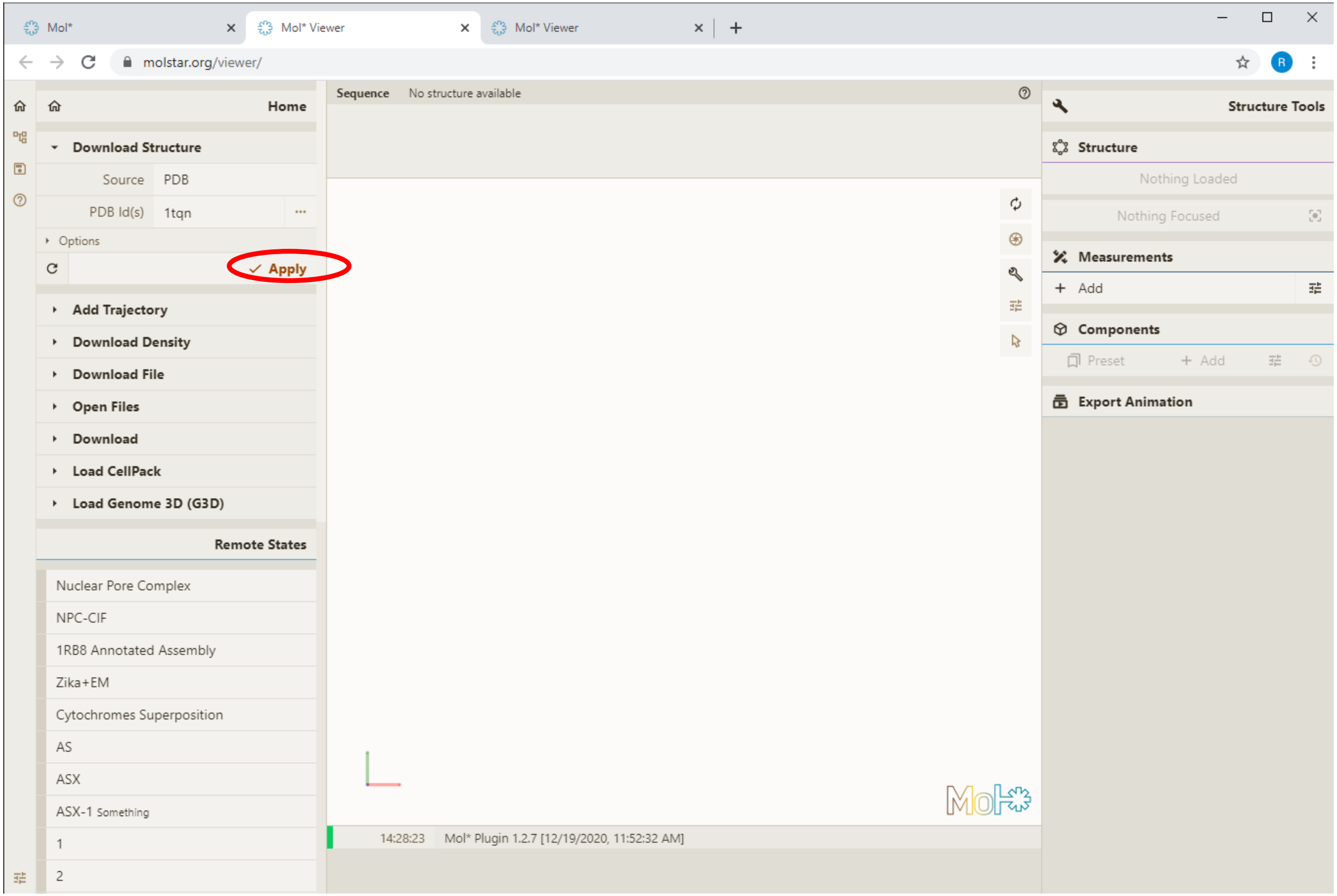
- Webová aplikace pro vizualizaci proteinů a ligandů
- Zvládá i extrémně velké systémy
- Integrovaný v Protein Data Bank
- Vyvíjený u nás v Národním centru pro výzkum biomolekul, ve spolupráci s EMBL EBI a RCSB PDB
- https://molstar.org/



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

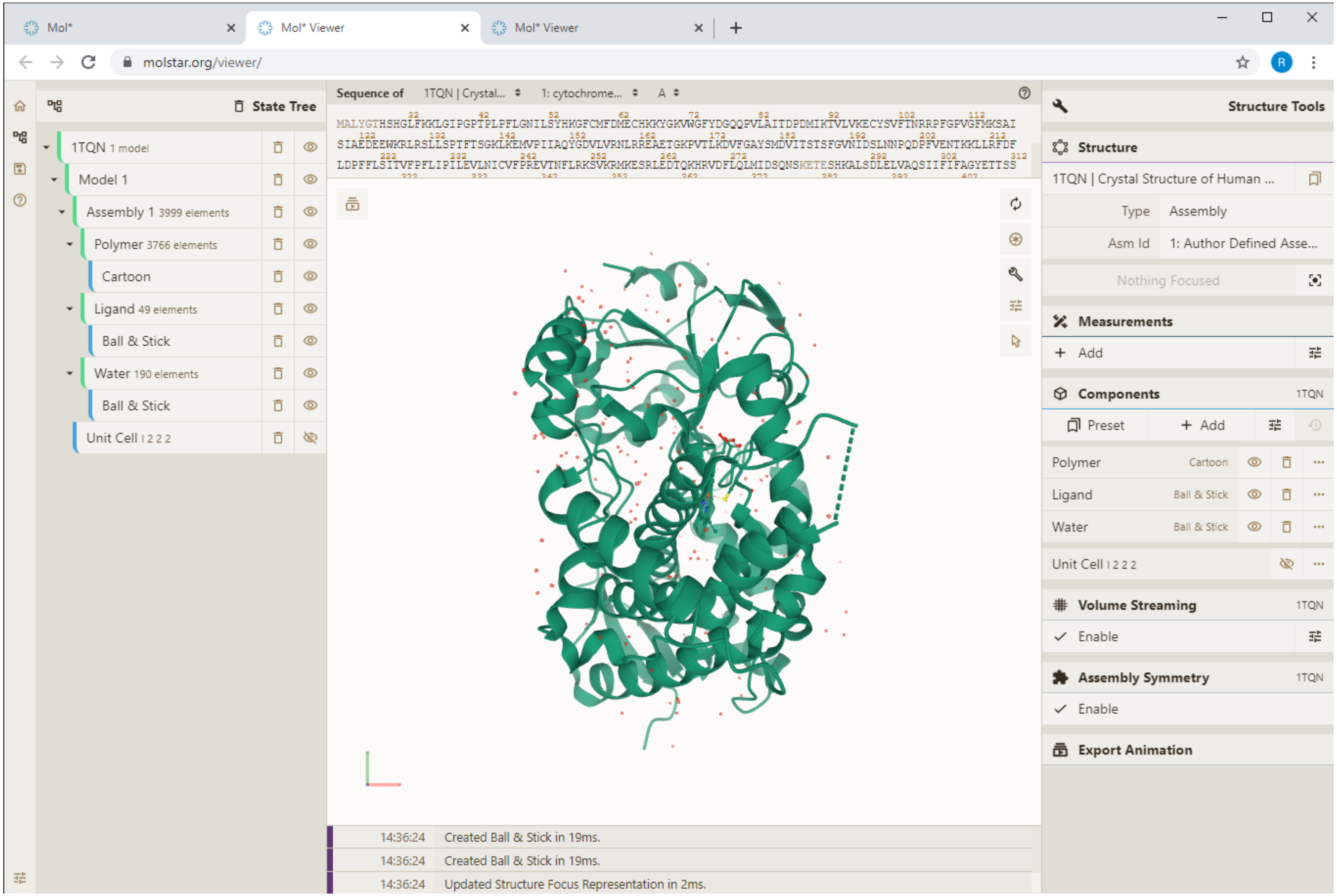
Sequence: No structure available

Nothing Loaded

Nothing Focused

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 ...

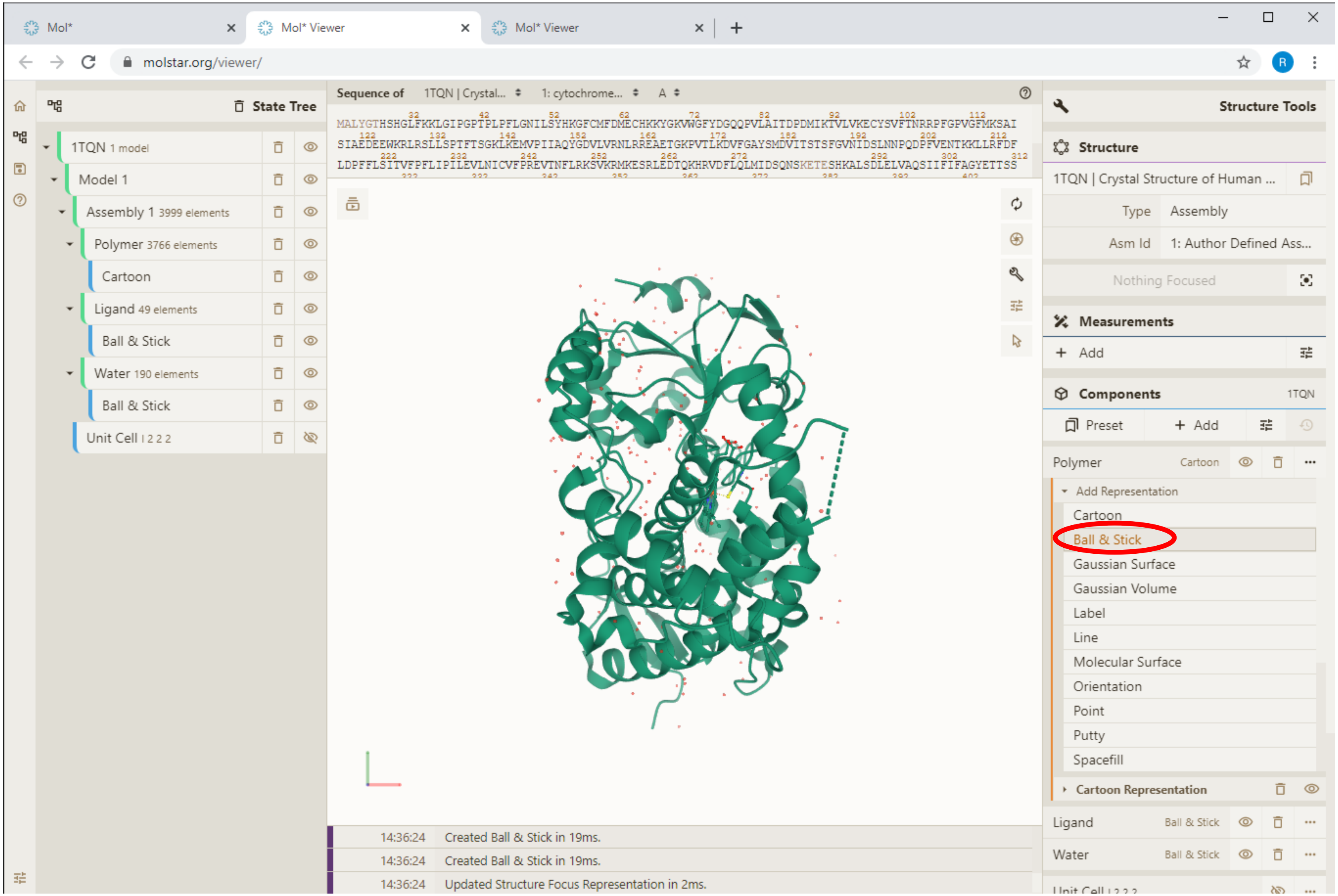
Type: Assembly

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.
```

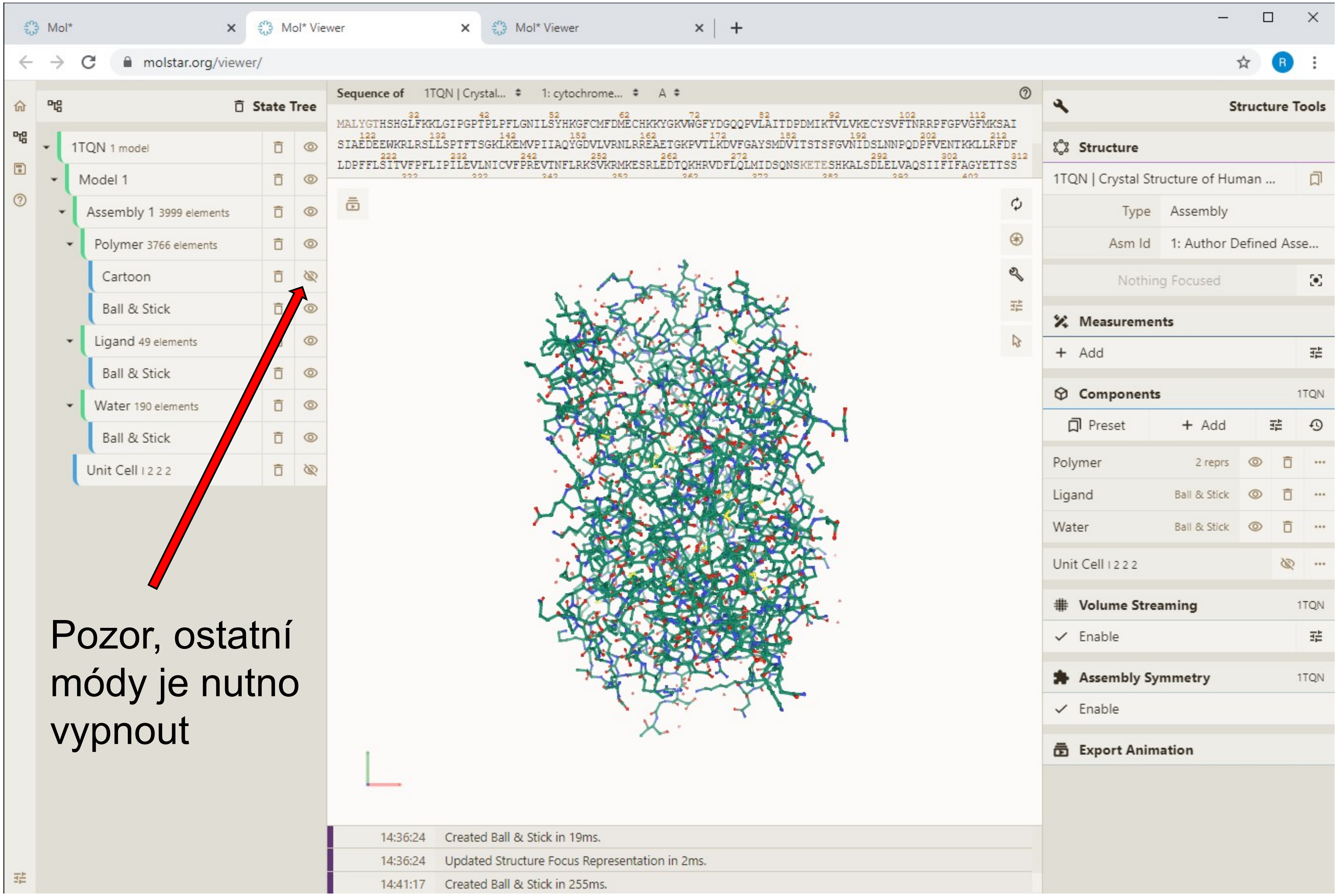
Vizualizace 3D souřadic molekuly
Volba vizualizačních modelů



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

```
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



MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI

SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF

LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS

1TQN | Crystal Structure of Human ...

Type Assembly

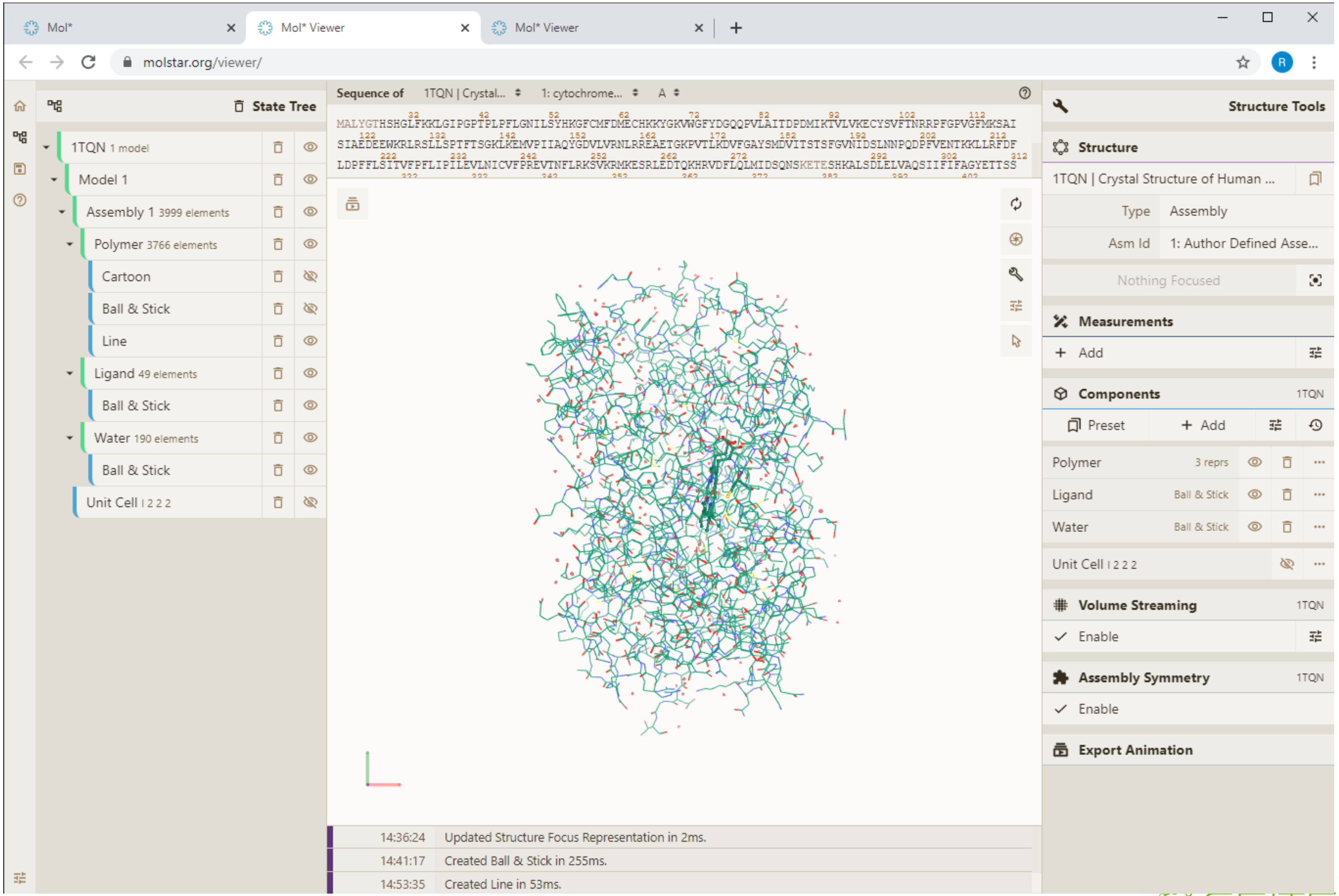
Asm Id 1: Author Defined Asse...

Nothing Focused

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



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SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS

1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Asse...

Nothing Focused

```
14:36:24   Updated Structure Focus Representation in 2ms.
14:41:17   Created Ball & Stick in 255ms.
14:53:35   Created Line in 53ms.
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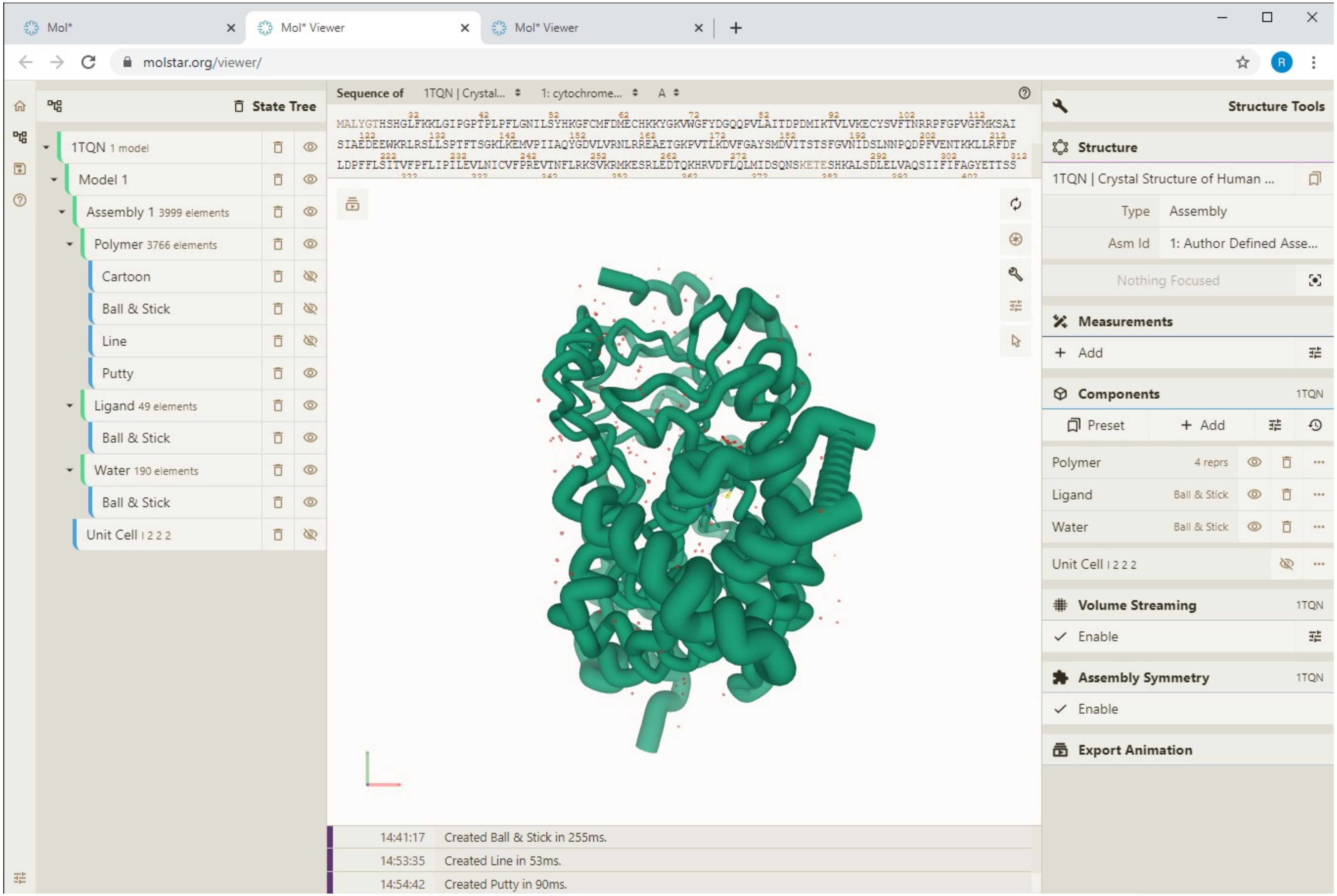
Vizualizace 3D souřadic molekuly
Vizualizační model Putty



```
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SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

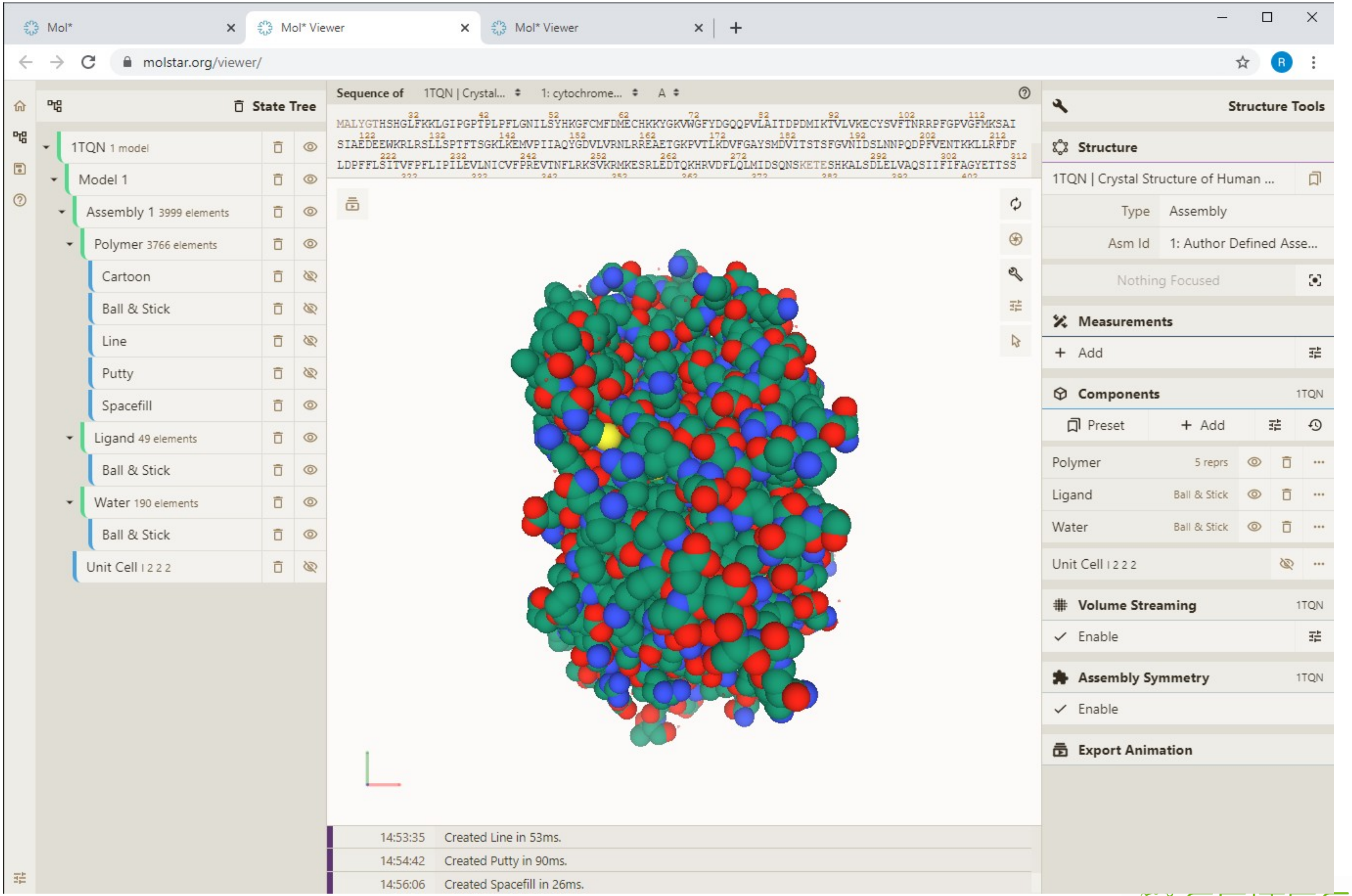
1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

```
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



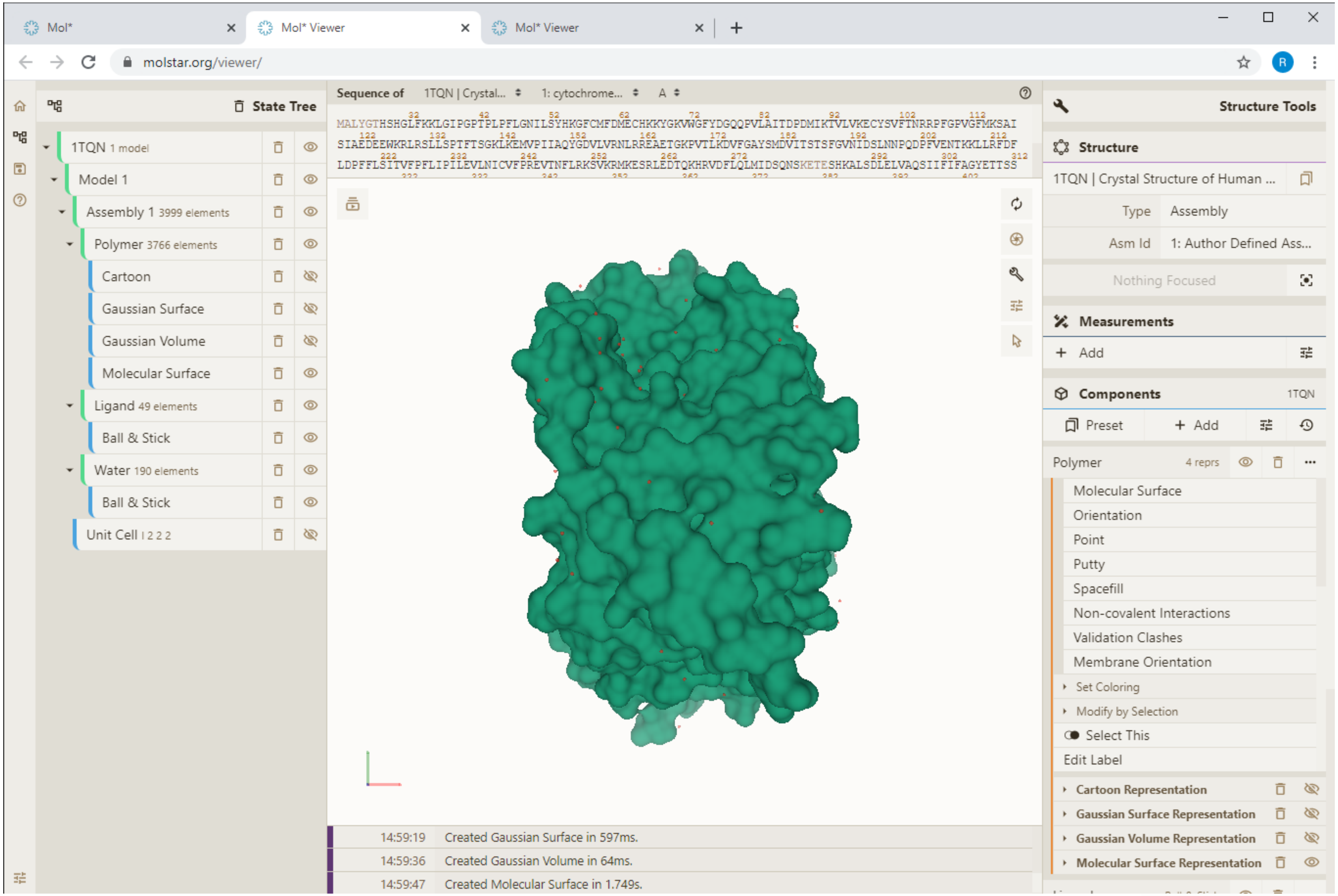
1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Asse...

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

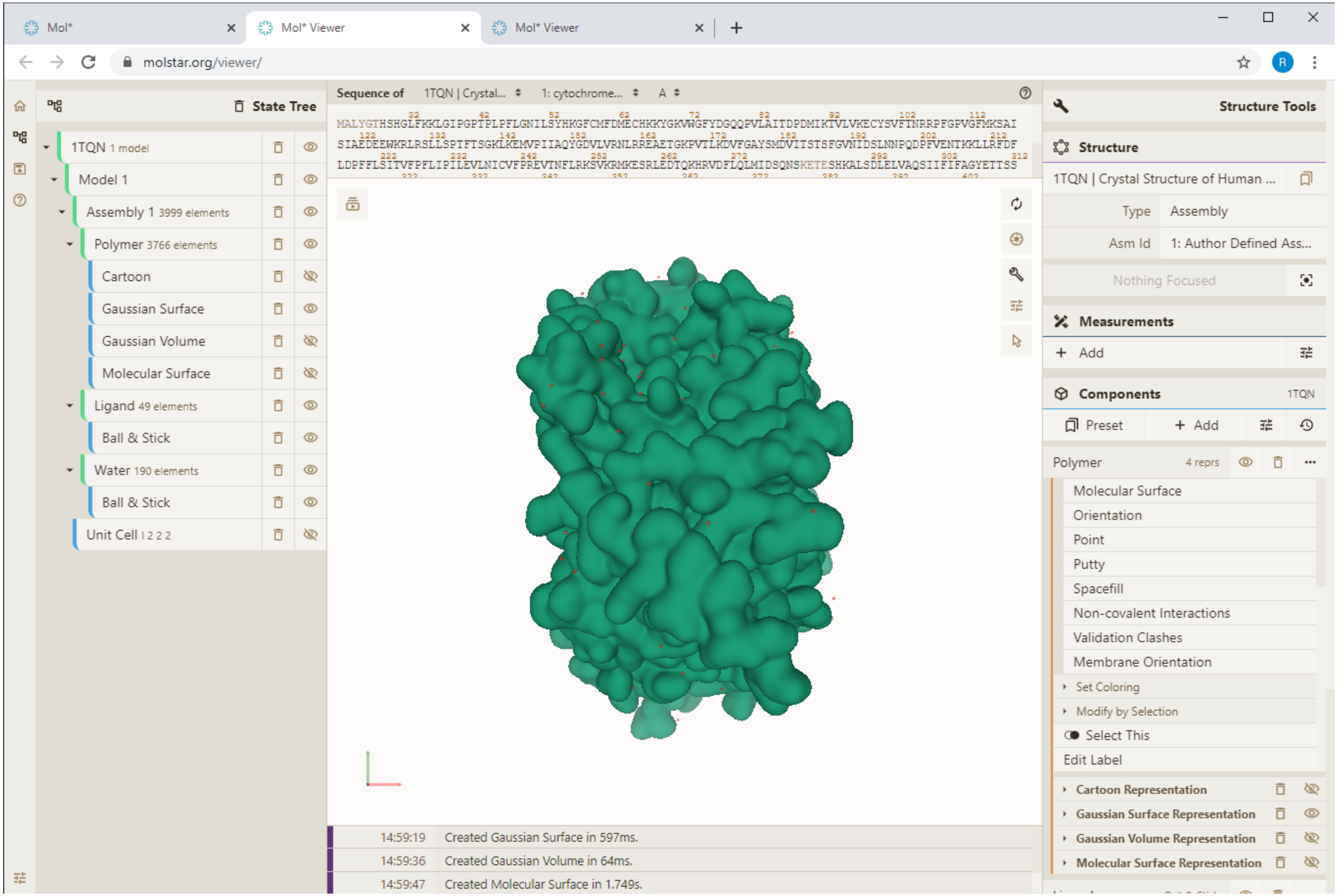
Vizualizace povrchu molekuly
Vizualizační model Molecular Surface



```
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



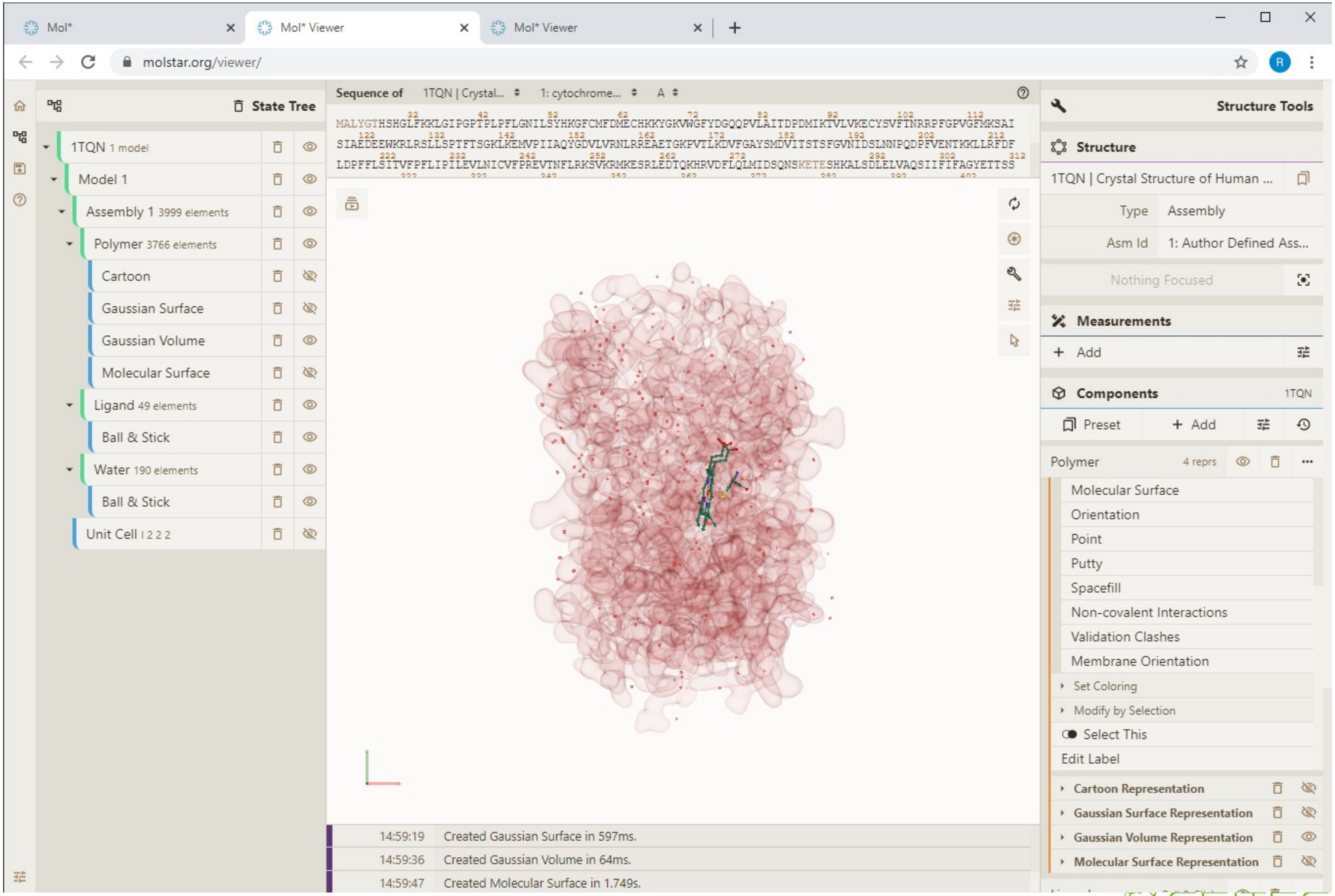
```
                         32        42        52        62        72        82        92       102       112
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
   122       132       142       152       162       172       182       192       202       212
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
      222       232       242       252       262       272                 292       302       312
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.

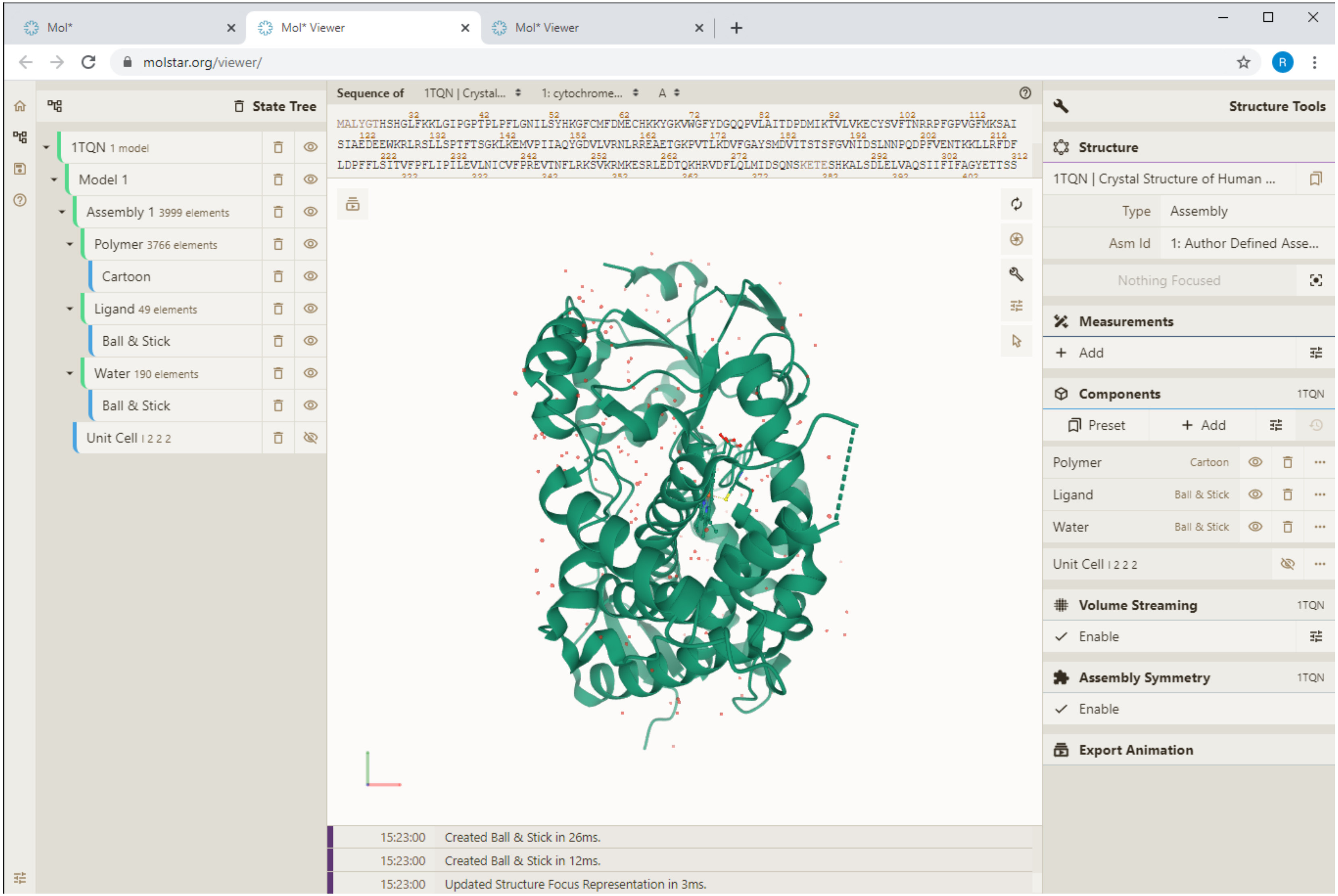
Vizualizace povrchu molekuly
Vizualizační model Gaussian Volume



```
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.
```

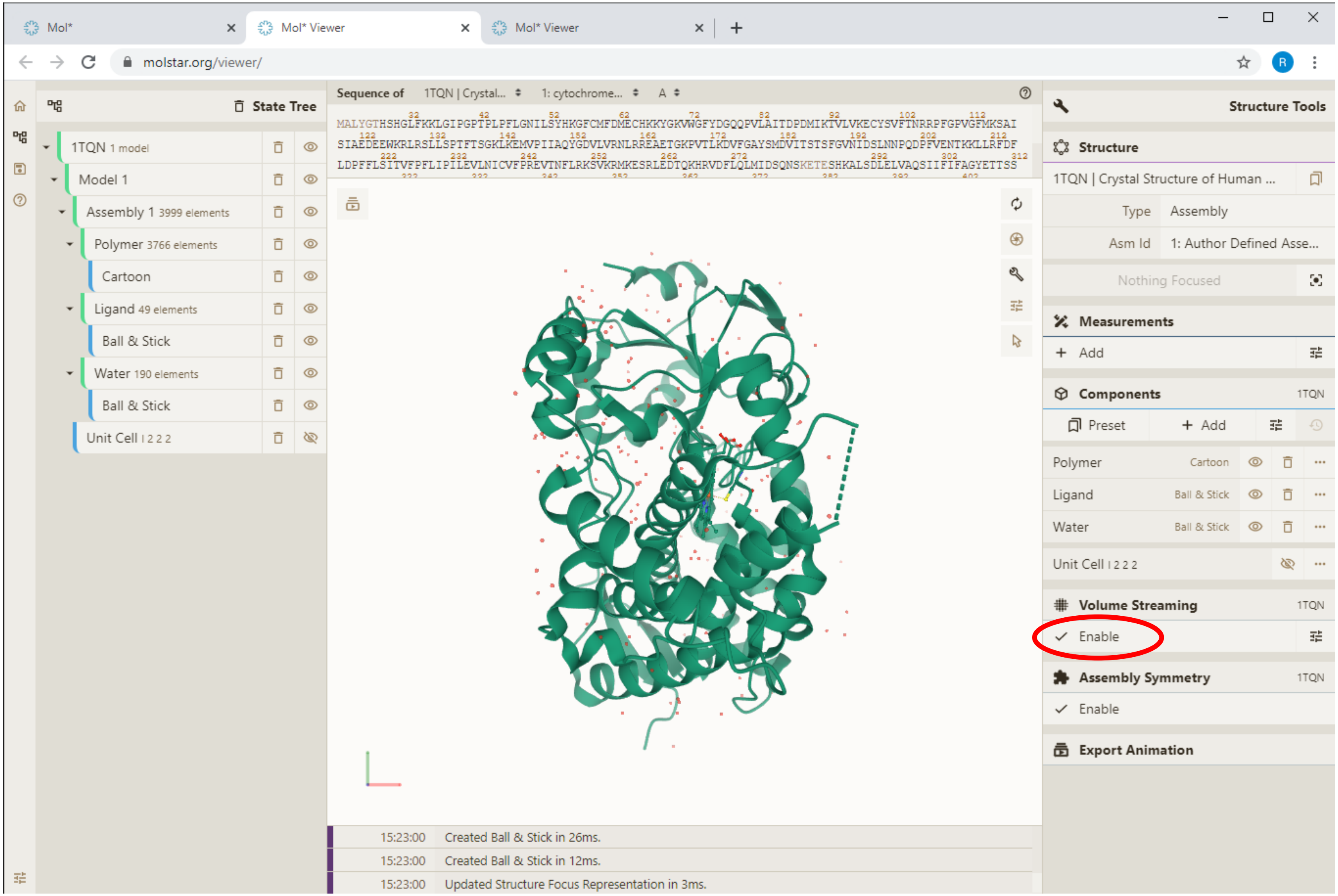
Vizualizace experimentálních dat
Elektronová hustota



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
```

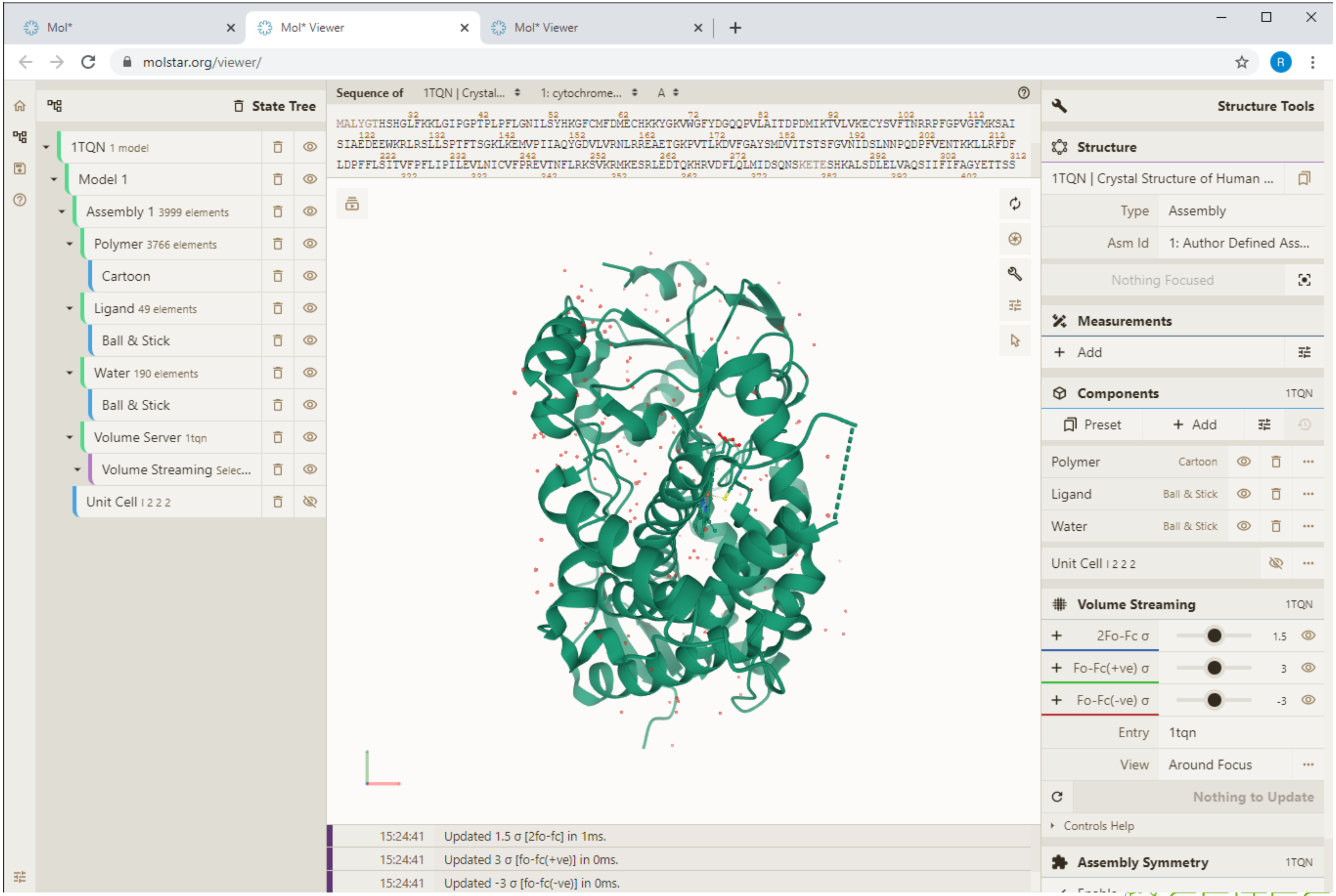
1TQN | Crystal Structure of Human ...

Type: Assembly

Asm Id: 1: Author Defined Asse...

```
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



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MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```
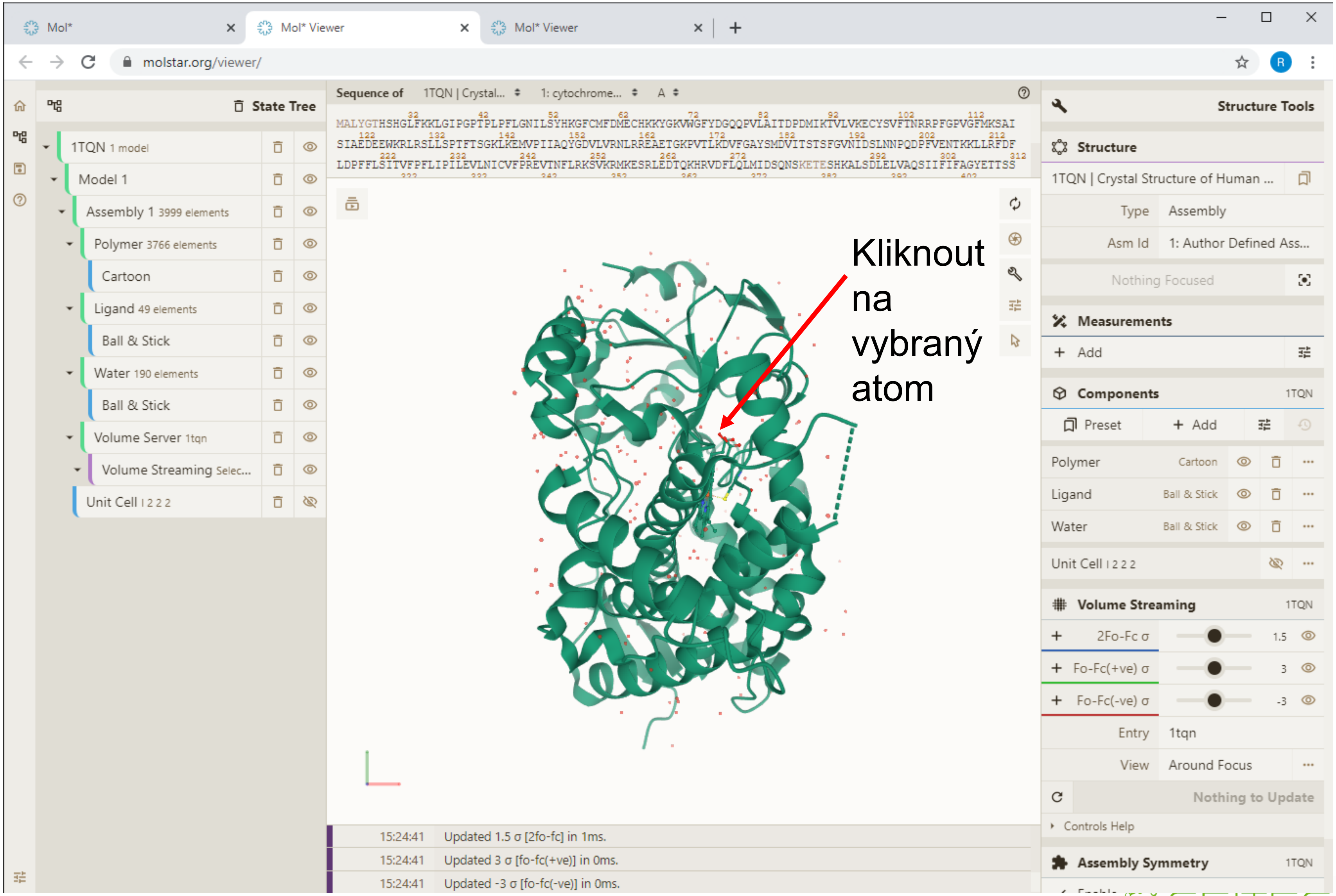

Type: Assembly
Asm Id: 1: Author Defined Ass...

2Fo-Fc σ: 1.5
Fo-Fc(+ve) σ: 3
Fo-Fc(-ve) σ: -3
Entry: 1tqn
View: Around Focus

```
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



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

Type Assembly

Asm Id 1: Author Defined Ass...

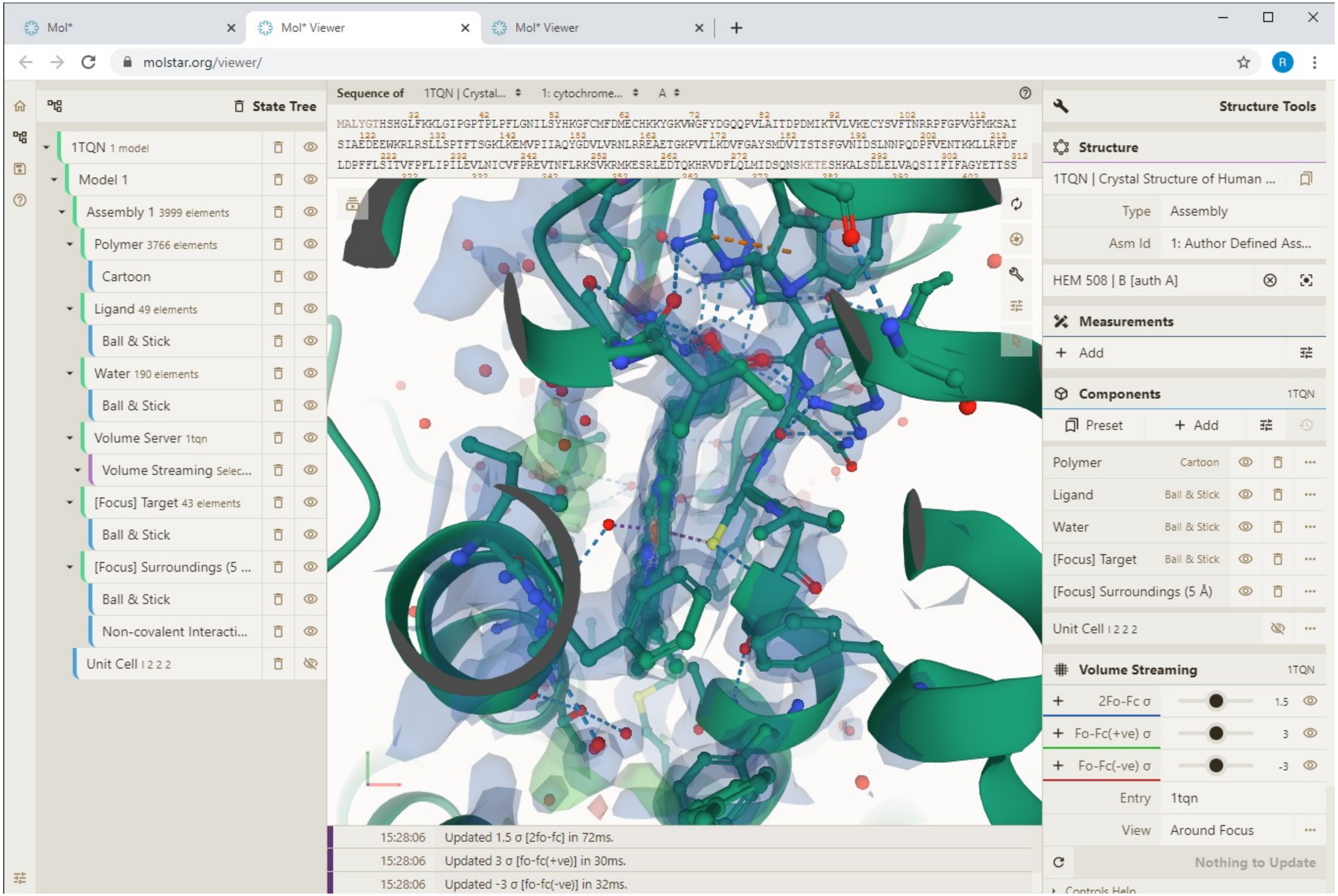
Entry 1tqn

View Around Focus

```
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



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LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

Type: Assembly

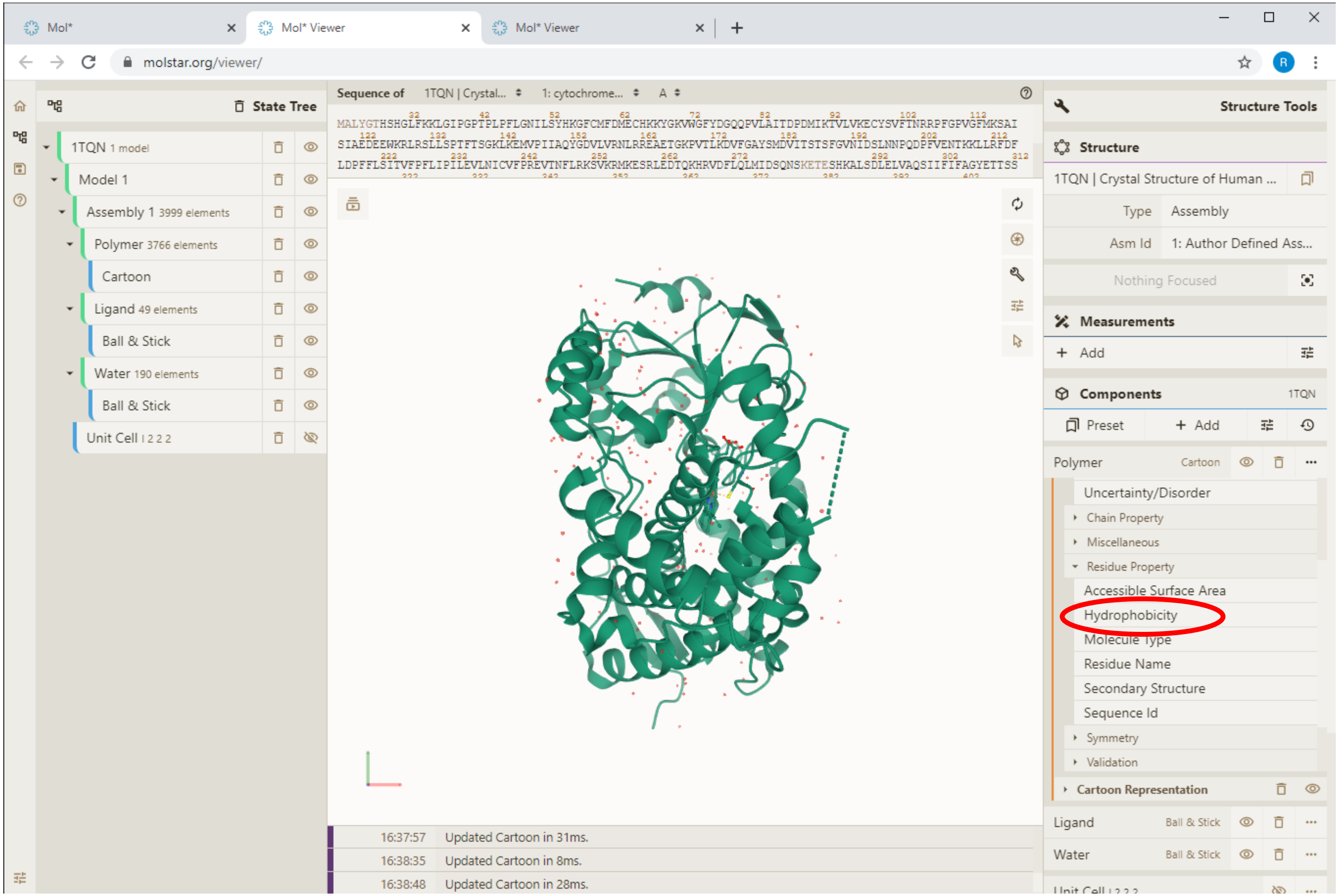
Asm Id: 1: Author Defined Ass...

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 ...

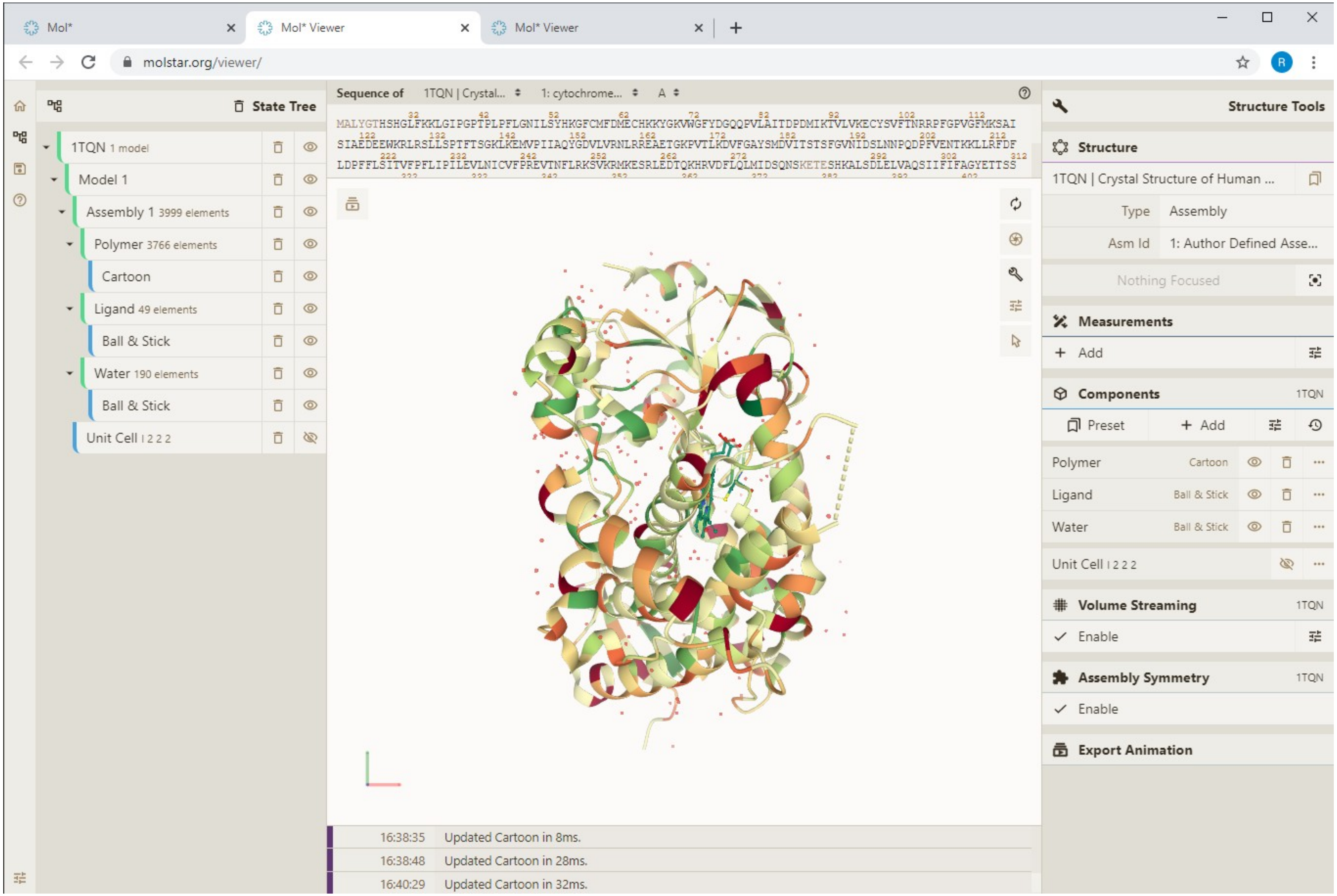
Type: Assembly

Asm Id: 1: Author Defined Ass...

Nothing Focused

```
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 ...

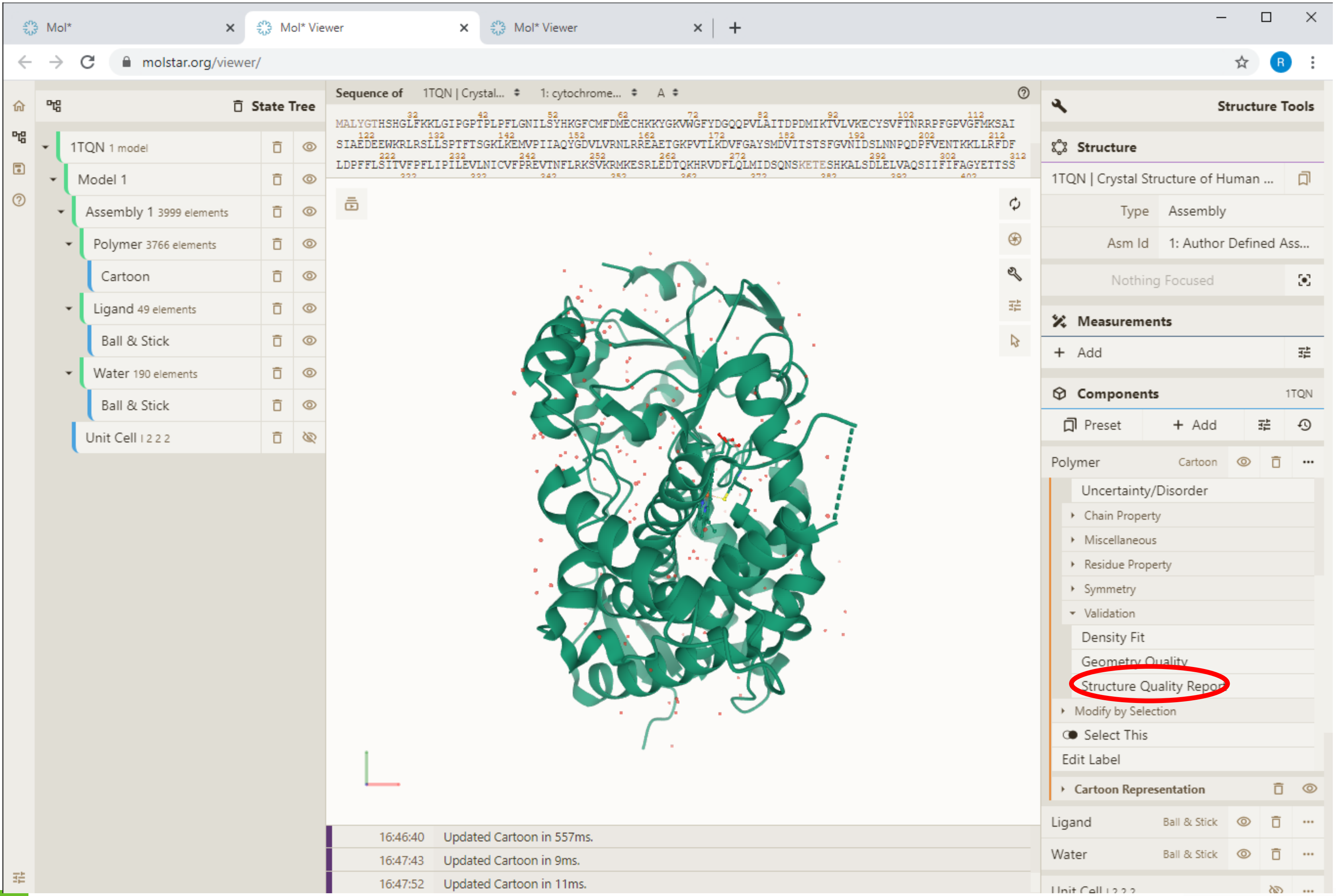
Type: Assembly

Asm Id: 1: Author Defined Asse...

Nothing Focused

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

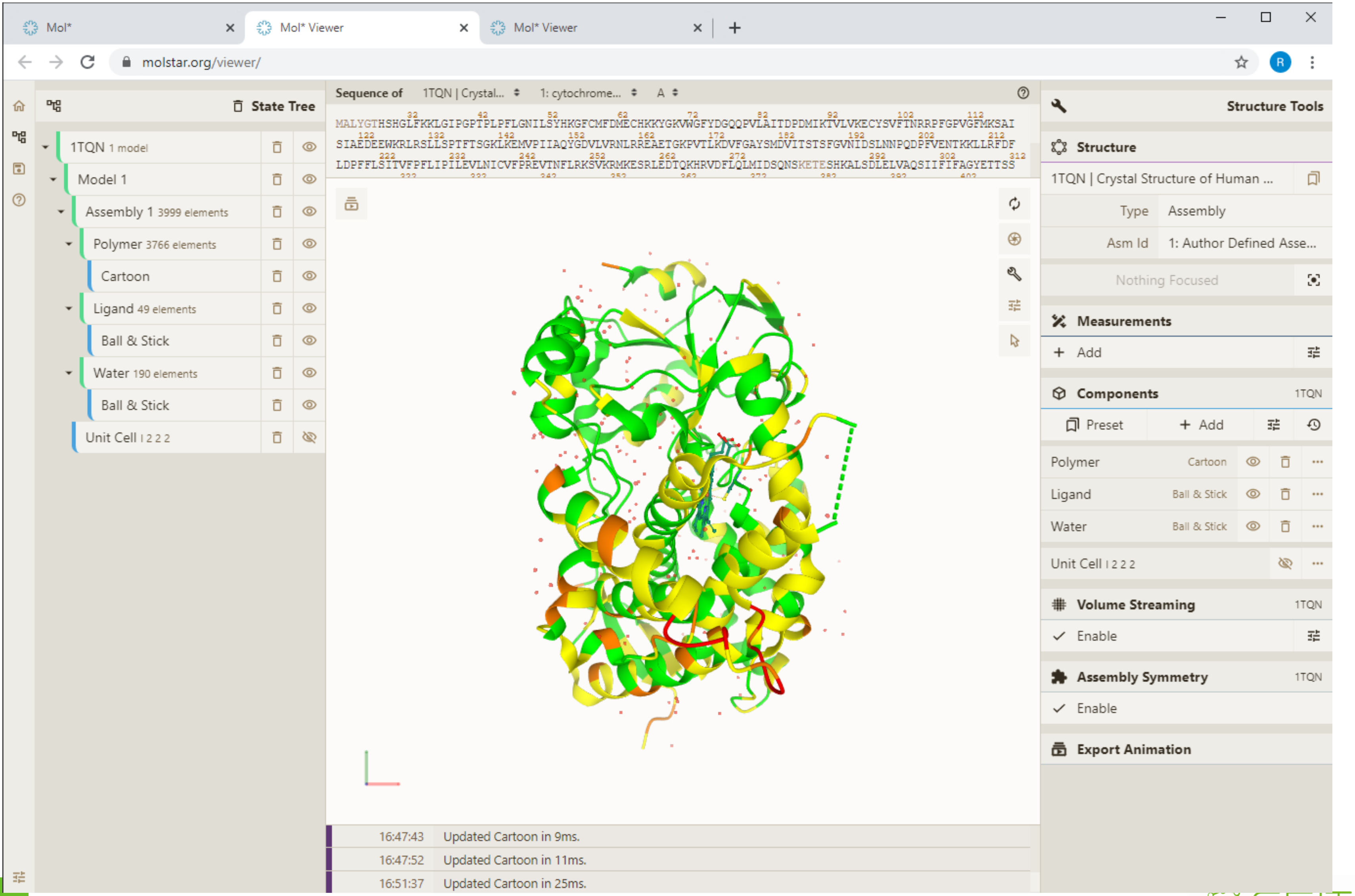
Vizualizace anotací
Obarvení podle vlastností – kvalita



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

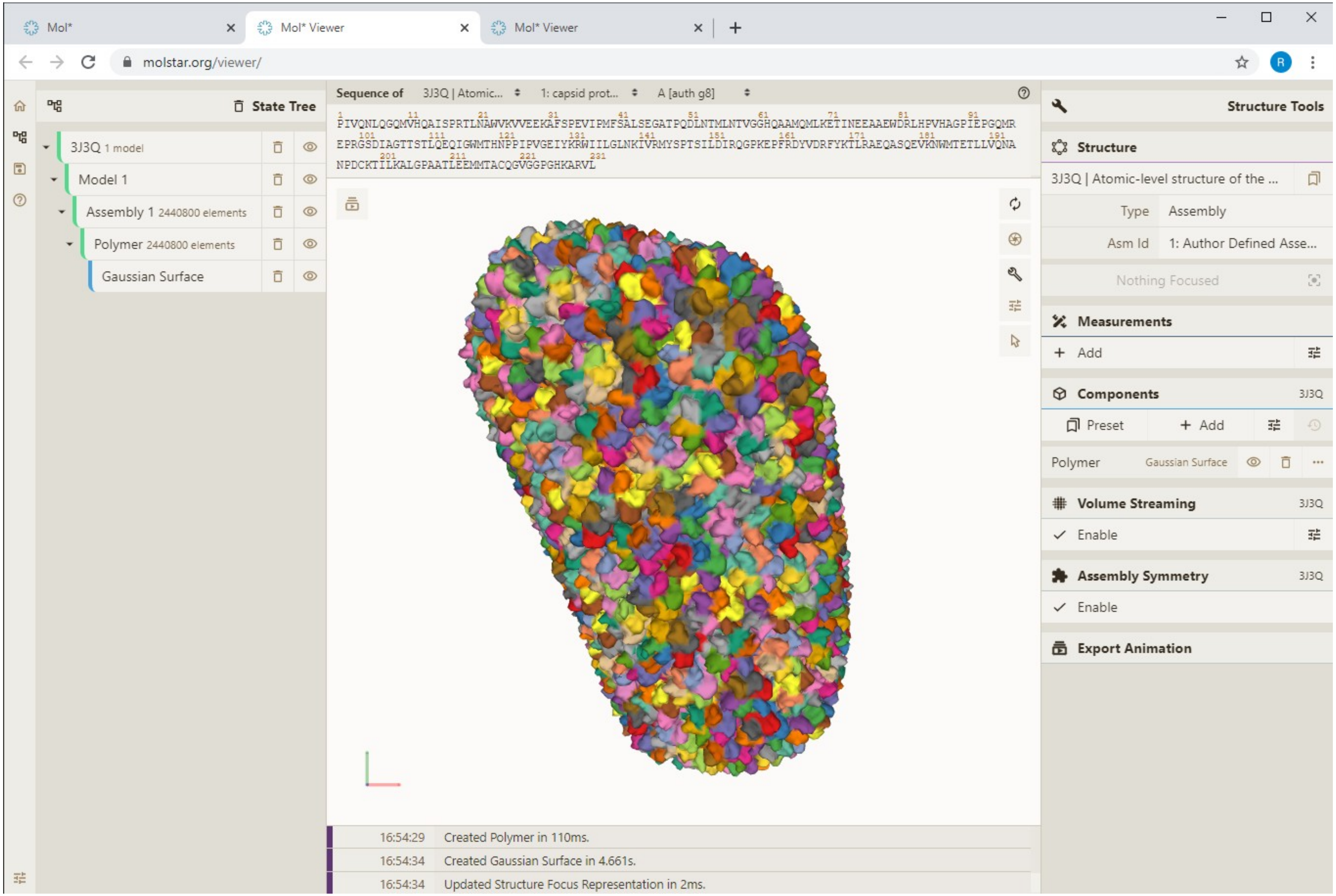
```
16:46:40   Updated Cartoon in 557ms.
16:47:43   Updated Cartoon in 9ms.
16:47:52   Updated Cartoon in 11ms.
```

Vizualizace anotací
Obarvení podle vlastností - kvalita



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

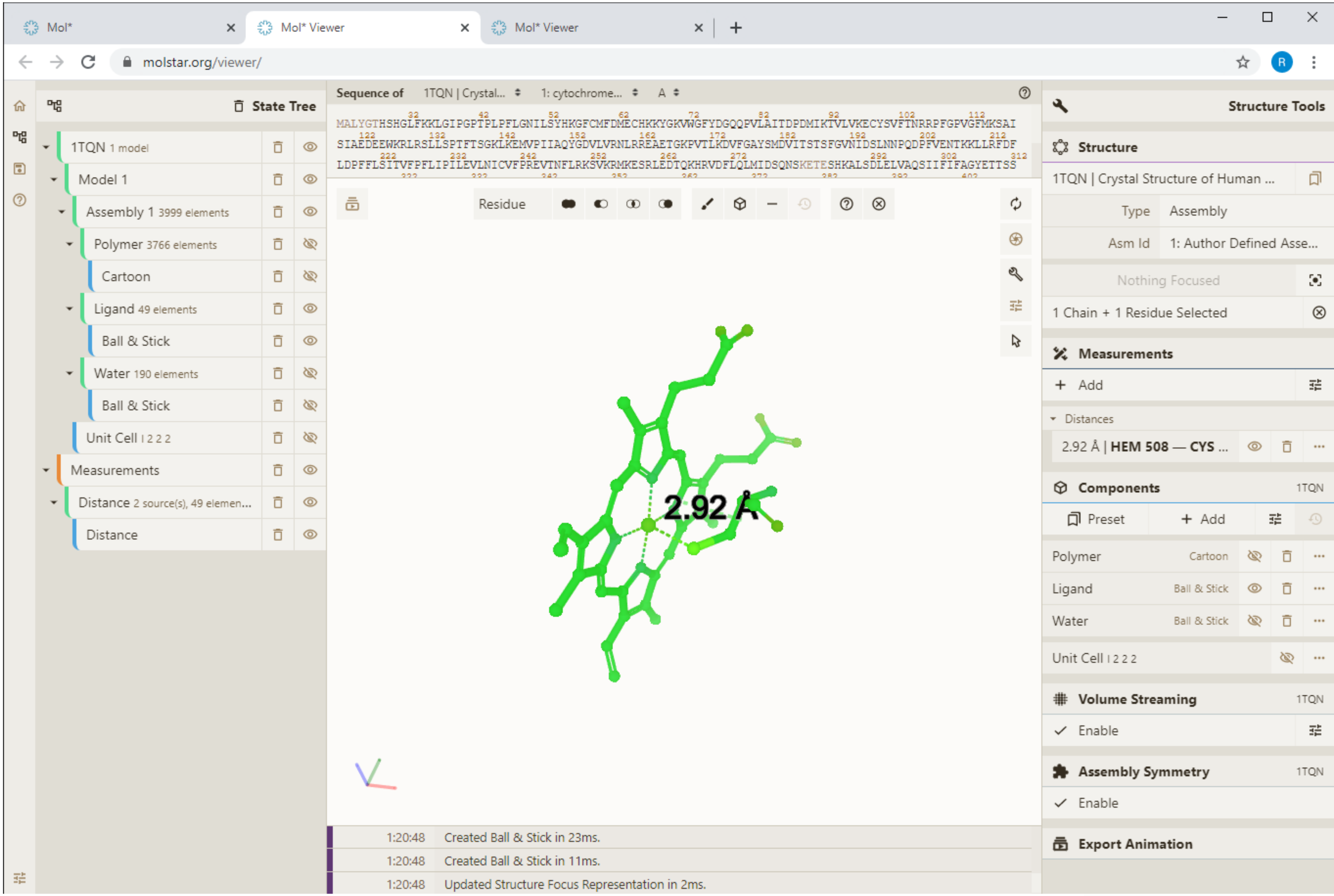
Vizualizace proteinových assemblies



```
PIVQNLQGQMVHQAISPRTLNAWVKVVEEKAFSPEVIPMFSALSEGATPQDLNTMLNTVGGHQAAMQMLKETINEEAAEWDRLHPVHAGPIEPGQMR
EPRGSDIAGTTSTLQEQIGWMTHNPPIPVGEIYKRWIILGLNKIVRMYSPTSILDIRQGPKEPFRDYVDRFYKTLRAEQASQEVKNWMTETLLVQNA
NPDCKTILKALGPAATLEEMMTACQGVGGPGHKARVL
```

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

Měření



MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS

1TQN | Crystal Structure of Human ...

Type Assembly

Asm Id 1: Author Defined Asse...

1 Chain + 1 Residue Selected

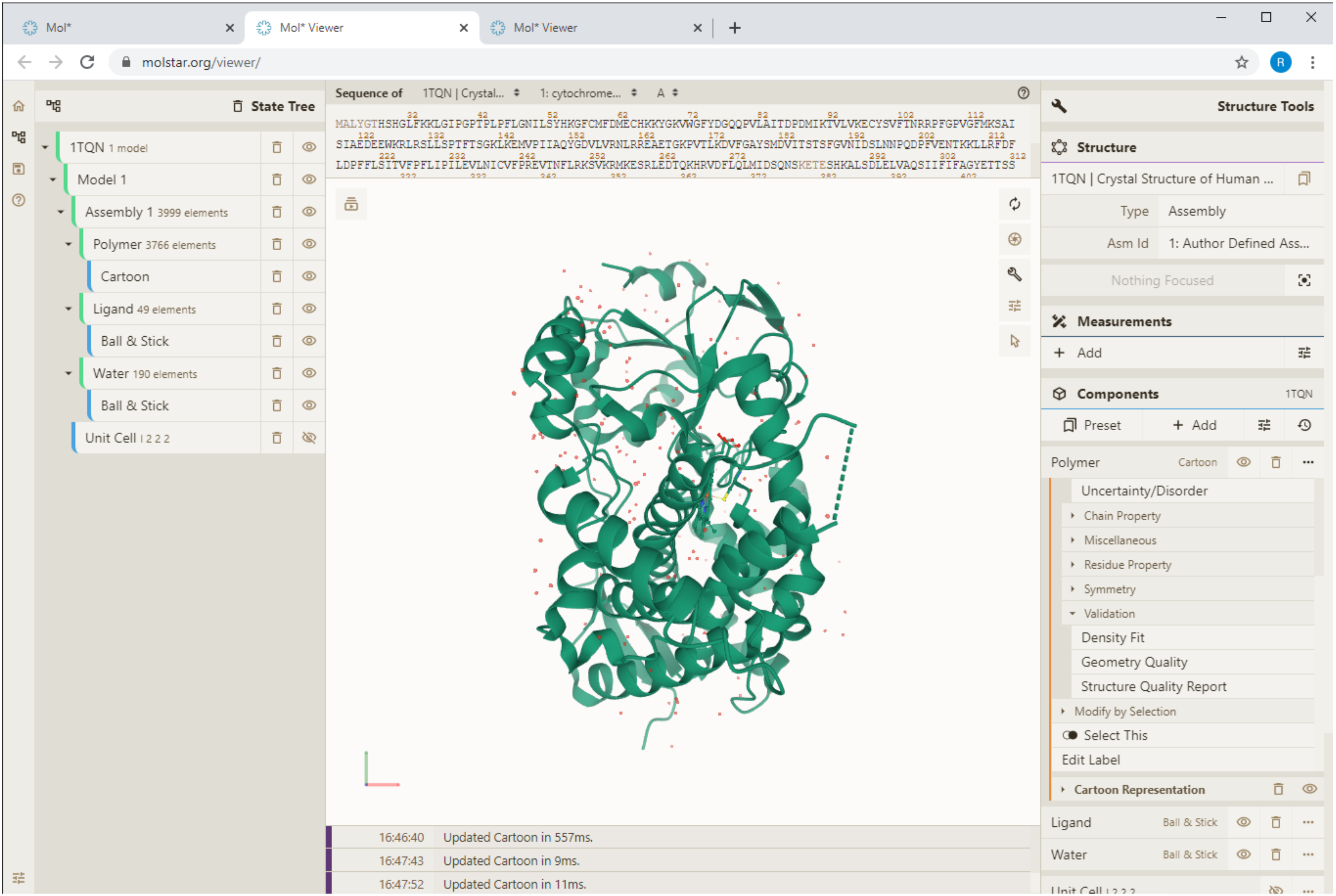
2.92 Å | **HEM 508 — CYS ...**

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.

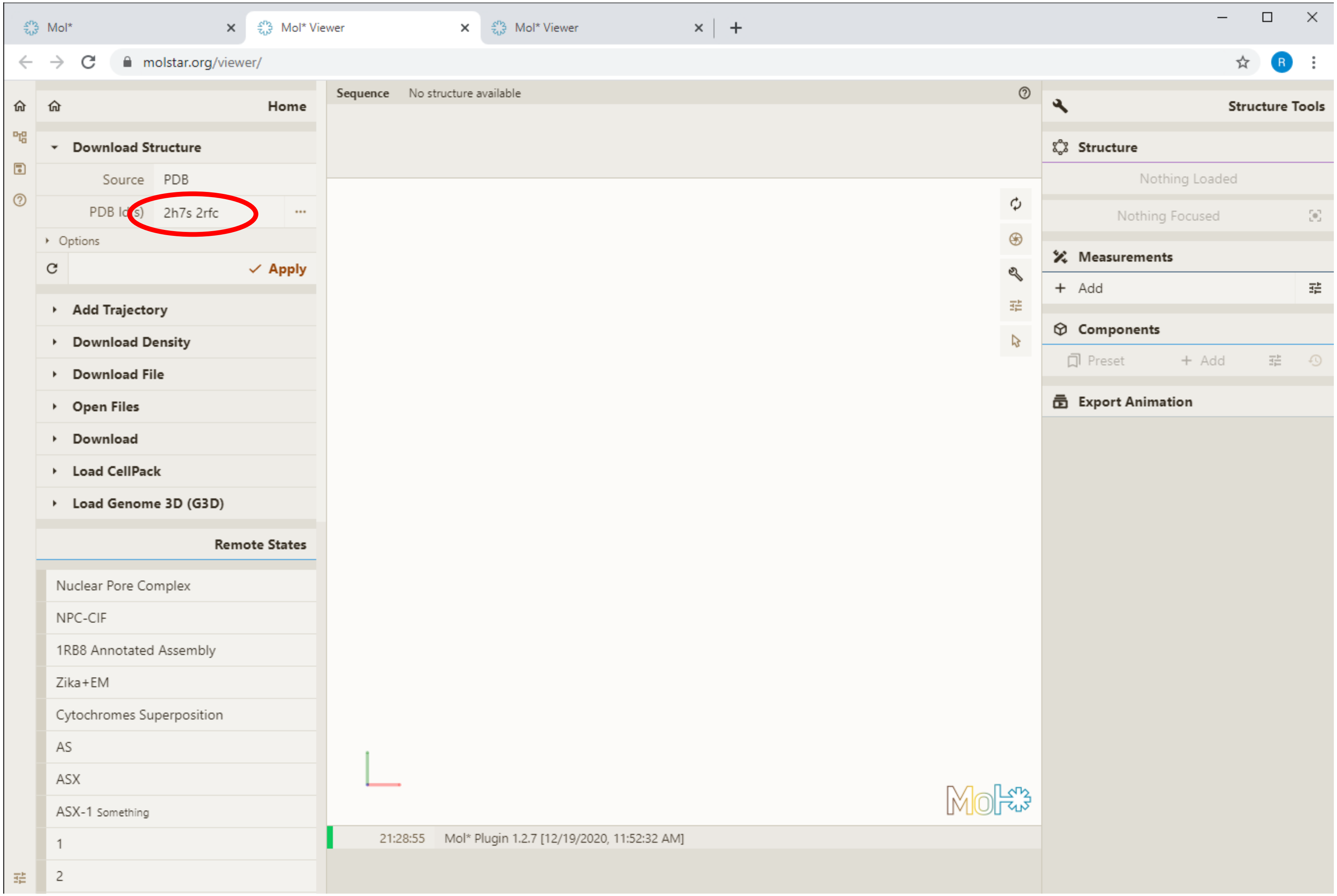
Vizualizace anotací
Obarvení podle vlastností - hydrofobicita



```
MALYGTHSHGLFKKLGIPGPTPLPFLGNILSYHKGFCMFDMECHKKYGKVWGFYDGQQPVLAITDPDMIKTVLVKECYSVFTNRRPFGPVGFMKSAI
SIAEDEEWKRLRSLLSPTFTSGKLKEMVPIIAQYGDVLVRNLRREAETGKPVTLKDVFGAYSMDVITSTSFGVNIDSLNNPQDPFVENTKKLLRFDF
LDPFFLSITVFPFLIPILEVLNICVFPREVTNFLRKSVKRMKESRLEDTQKHRVDFLQLMIDSQNSKETESHKALSDLELVAQSIIFIFAGYETTSS
```

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

Přikládání struktur



Download Structure

Source PDB

PDB Id(s) 2h7s 2rfc

No structure available

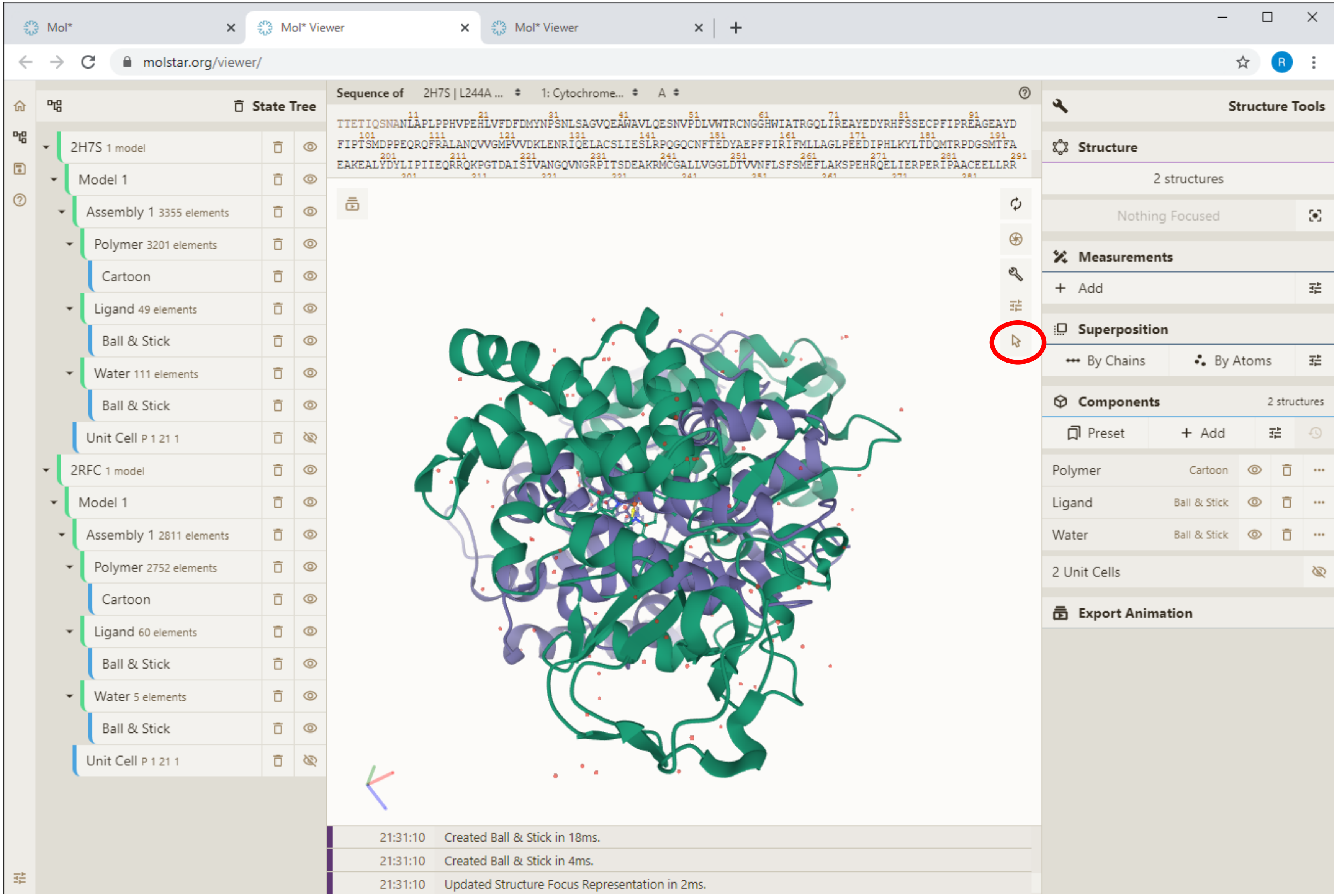
Nothing Loaded

Nothing Focused

Nuclear Pore Complex
NPC-CIF
1RB8 Annotated Assembly
Zika+EM
Cytochromes Superposition
AS
ASX
ASX-1 Something
1
2

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

Přikládání struktur



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FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRPQGQCNFTEDYAEPFPIRIFMLLAGLPEEDIPHLKYLTDQMTRPDGSMTFA
EAKEALYDYLIPIIEQRRQKPGTDAISIVANGQVNGRPITSDEAKRMCGALLVGGLDTVVNFLSFSMEFLAKSPEHRQELIERPERIPAACEELLRR
```
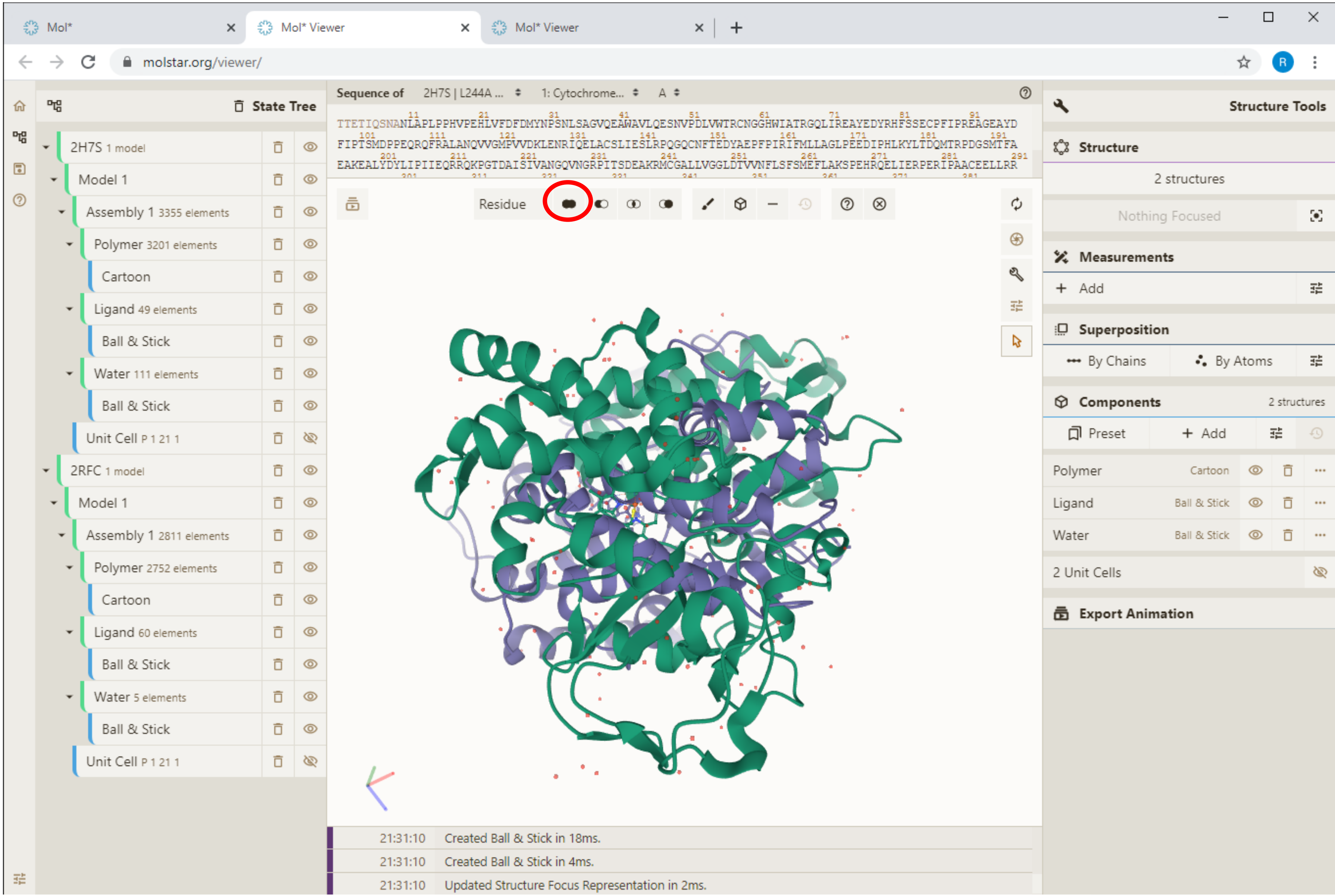
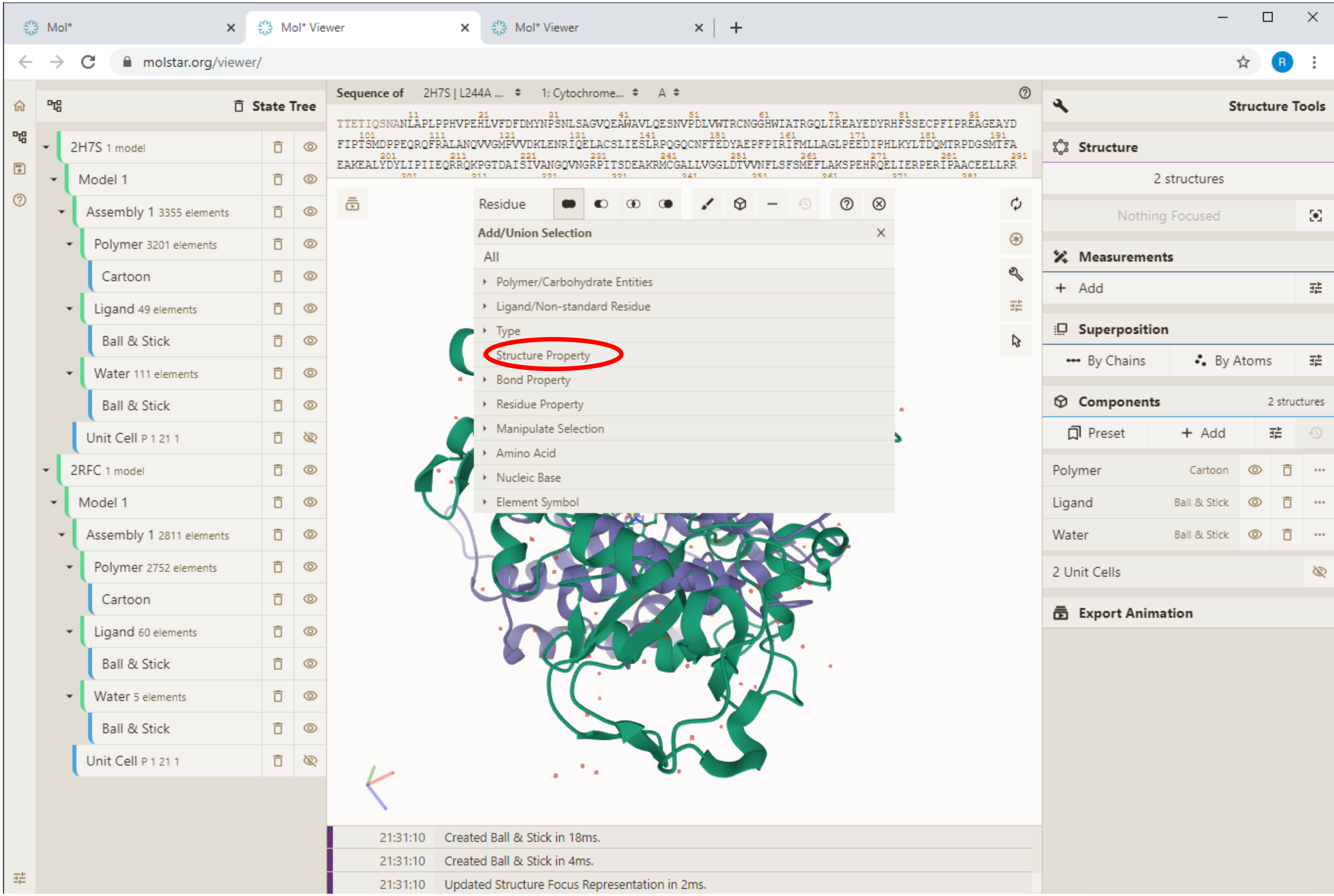

```
21:31:10   Created Ball & Stick in 18ms.
21:31:10   Created Ball & Stick in 4ms.
21:31:10   Updated Structure Focus Representation in 2ms.
```

Přikládání struktur



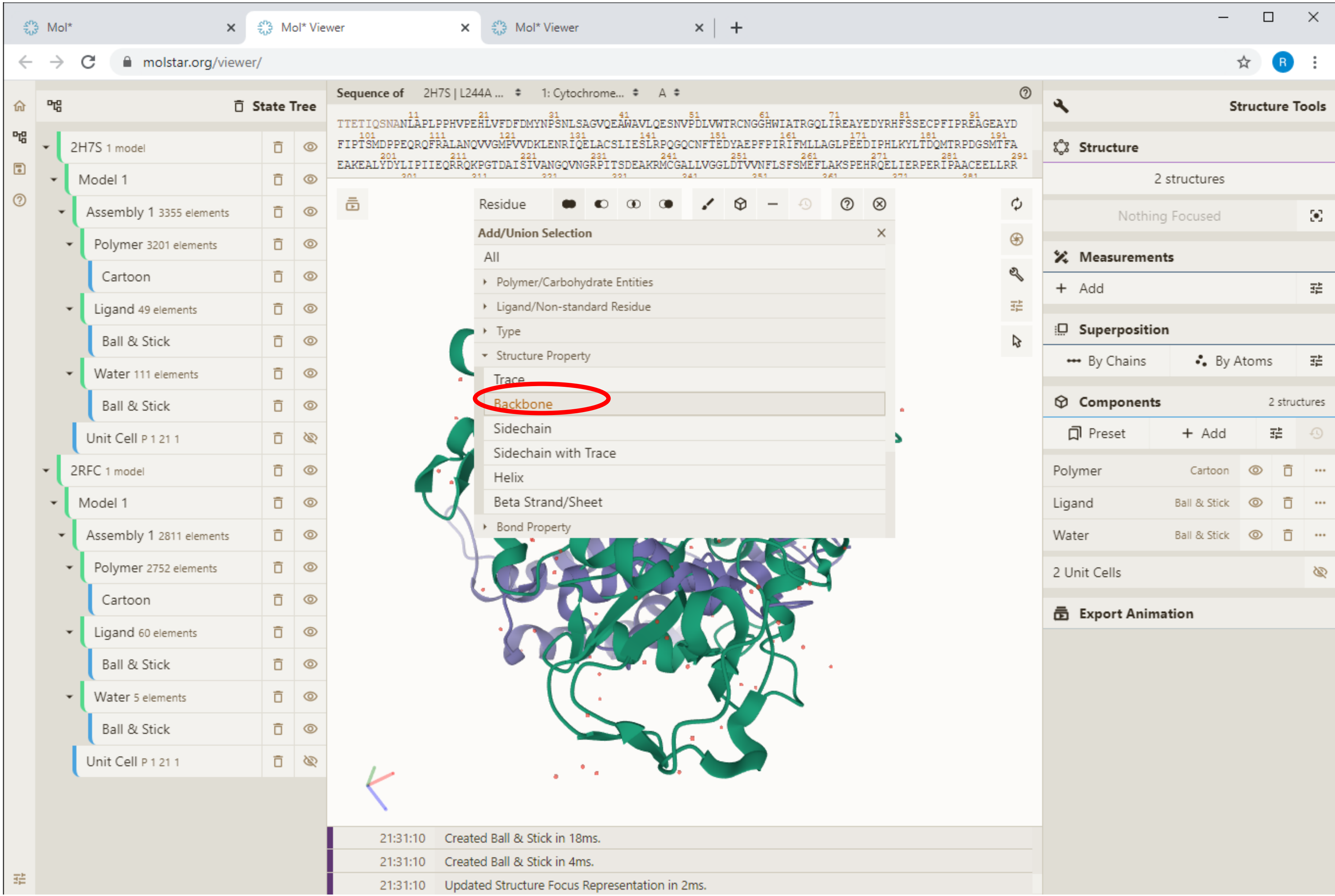
```
21:31:10   Created Ball & Stick in 18ms.
21:31:10   Created Ball & Stick in 4ms.
21:31:10   Updated Structure Focus Representation in 2ms.
```

Přikládání struktur



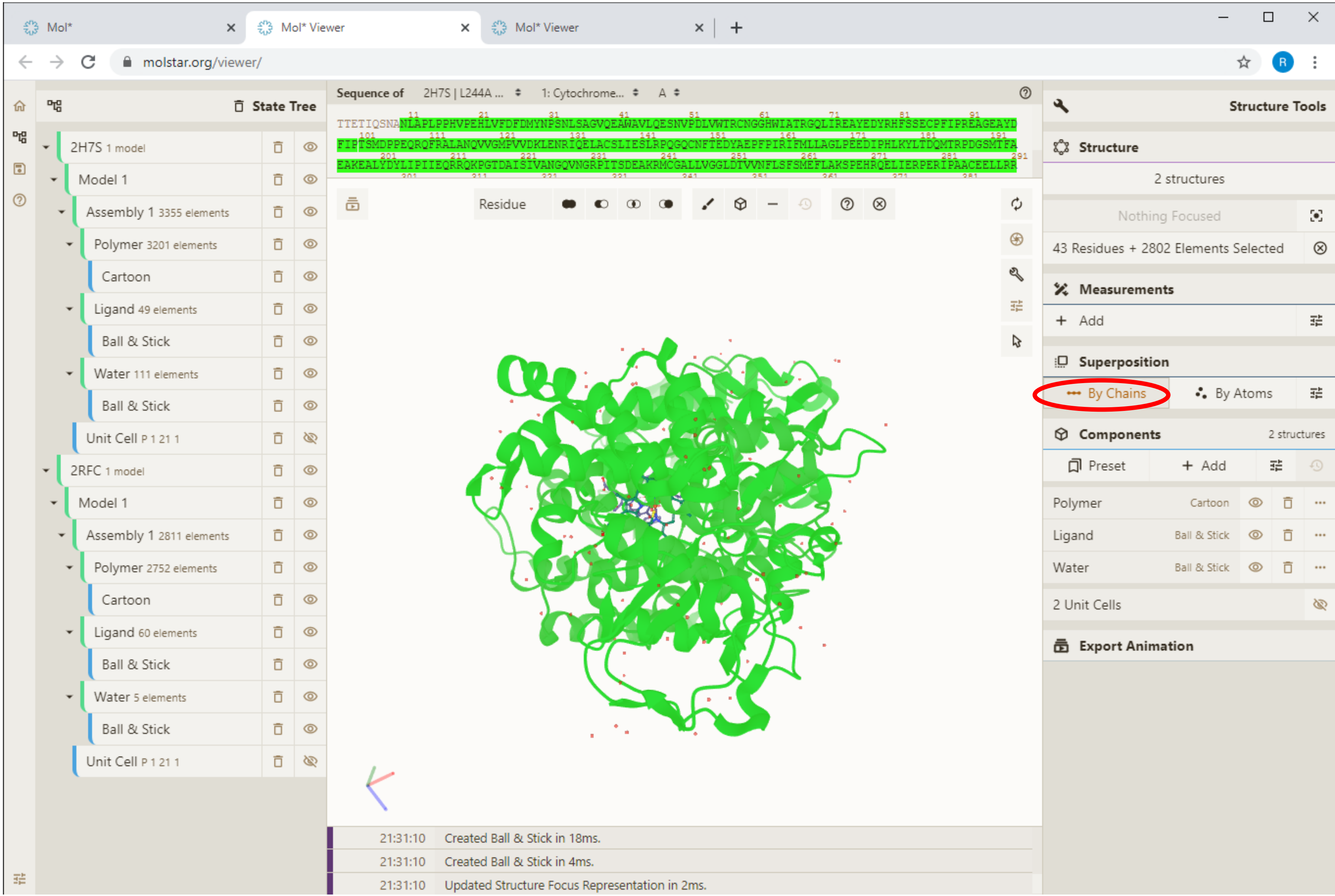
```
21:31:10   Created Ball & Stick in 18ms.
21:31:10   Created Ball & Stick in 4ms.
21:31:10   Updated Structure Focus Representation in 2ms.
```

Přikládání struktur



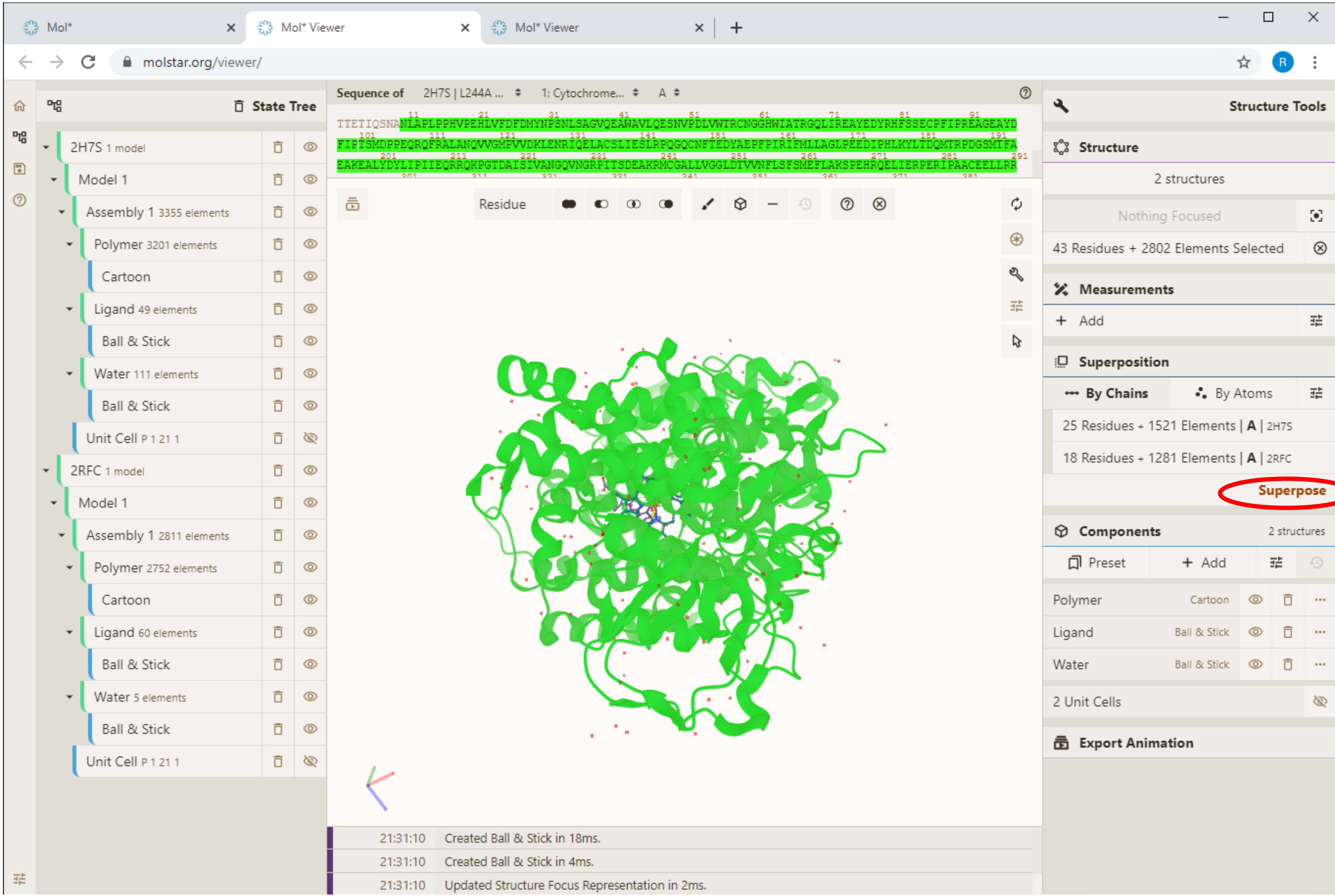
```
21:31:10   Created Ball & Stick in 18ms.
21:31:10   Created Ball & Stick in 4ms.
21:31:10   Updated Structure Focus Representation in 2ms.
```

Přikládání struktur



```
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



```
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FIPTSMDPPEQRQFRALANQVVGMPVVDKLENRIQELACSLIESLRPQGQCNFTEDYAEPFPIRIFMLLAGLPEEDIPHLKYLTDQMTRPDGSMTFA
EAKEALYDYLIPIIEQRRQKPGTDAISIVANGQVNGRPITSDEAKRMCGALLVGGLDTVVNFLSFSMEFLAKSPEHRQELIERPERIPAACEELLRR
```
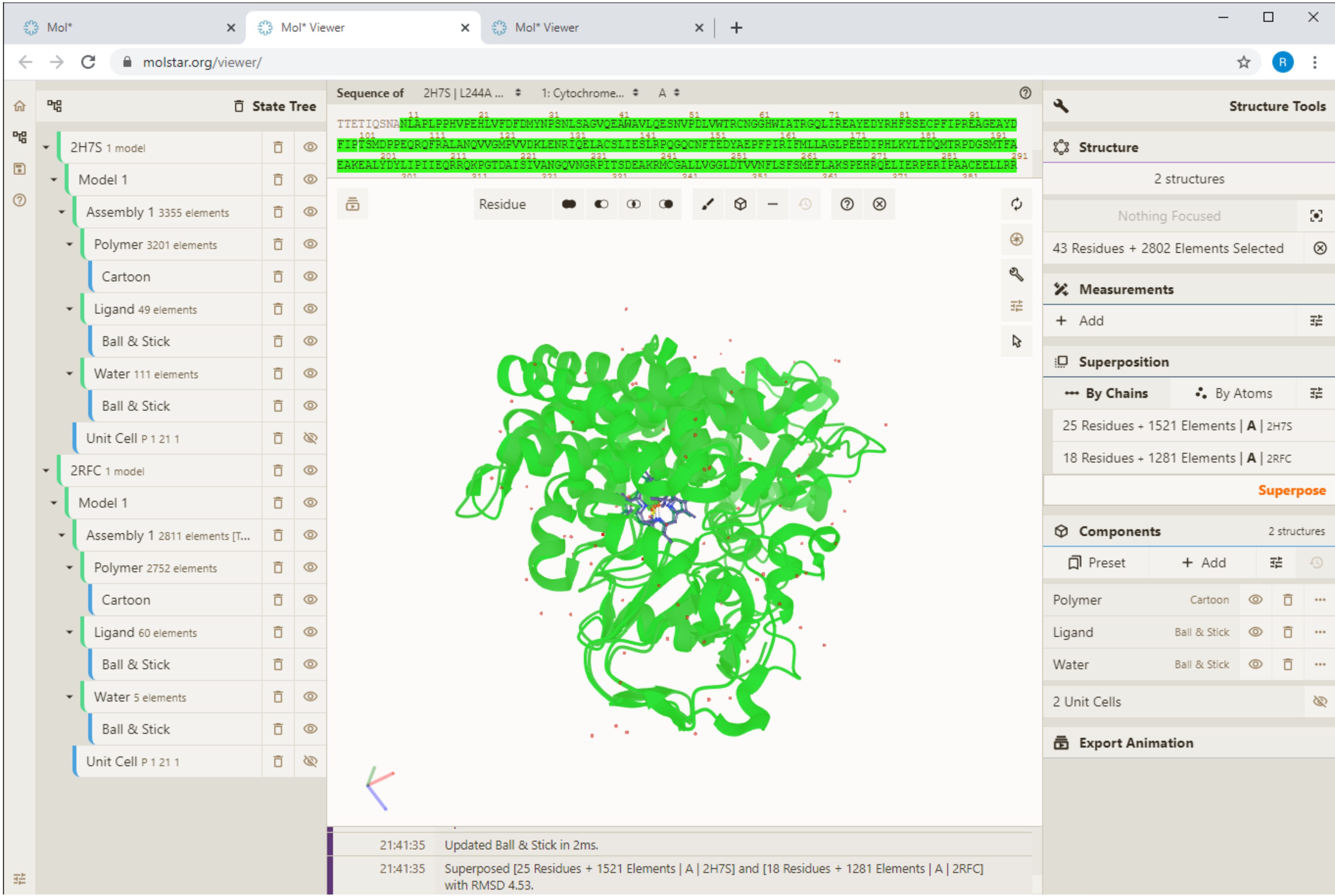

```
21:31:10   Created Ball & Stick in 18ms.
21:31:10   Created Ball & Stick in 4ms.
21:31:10   Updated Structure Focus Representation in 2ms.
```

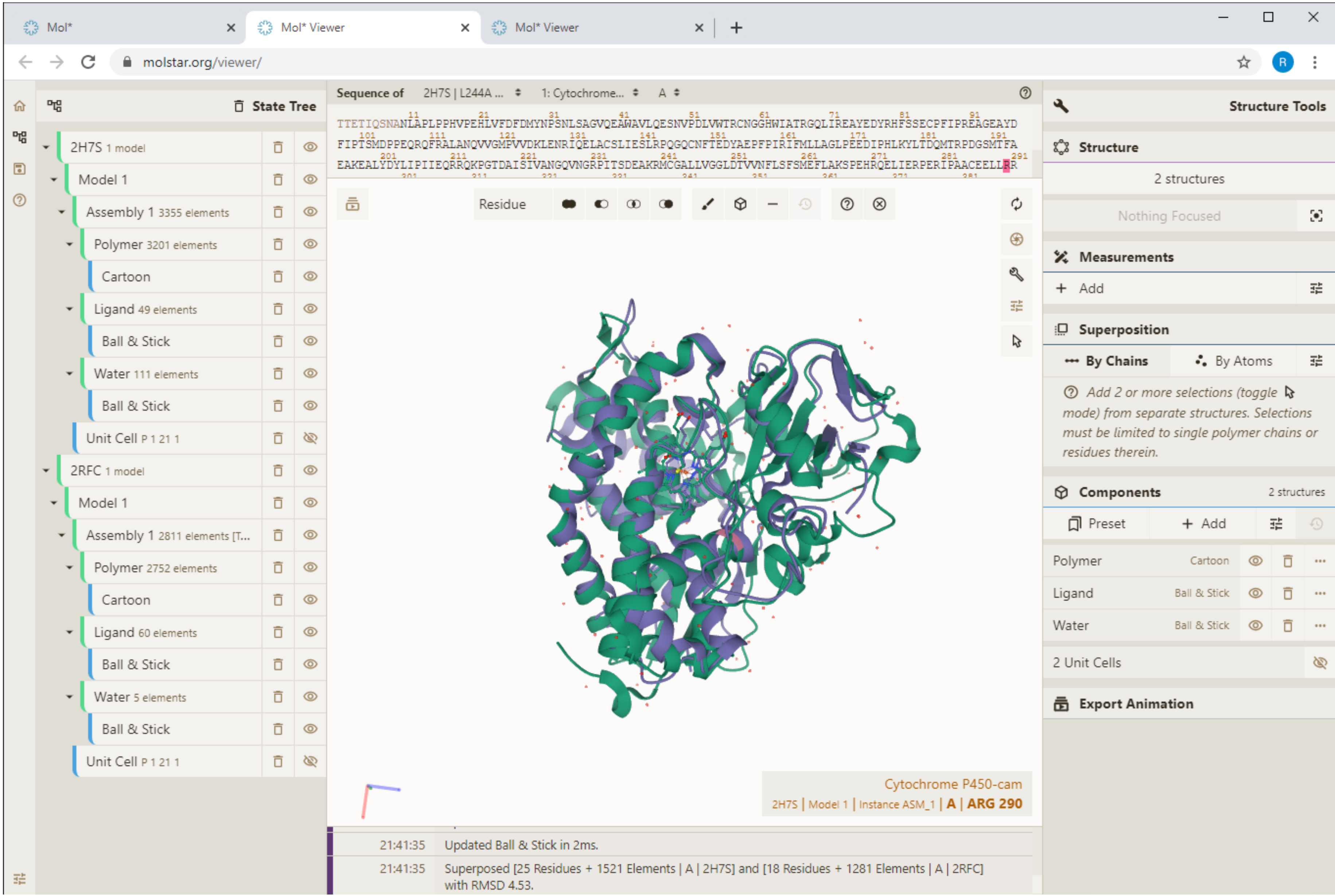
Přikládání struktur



21:41:35 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.

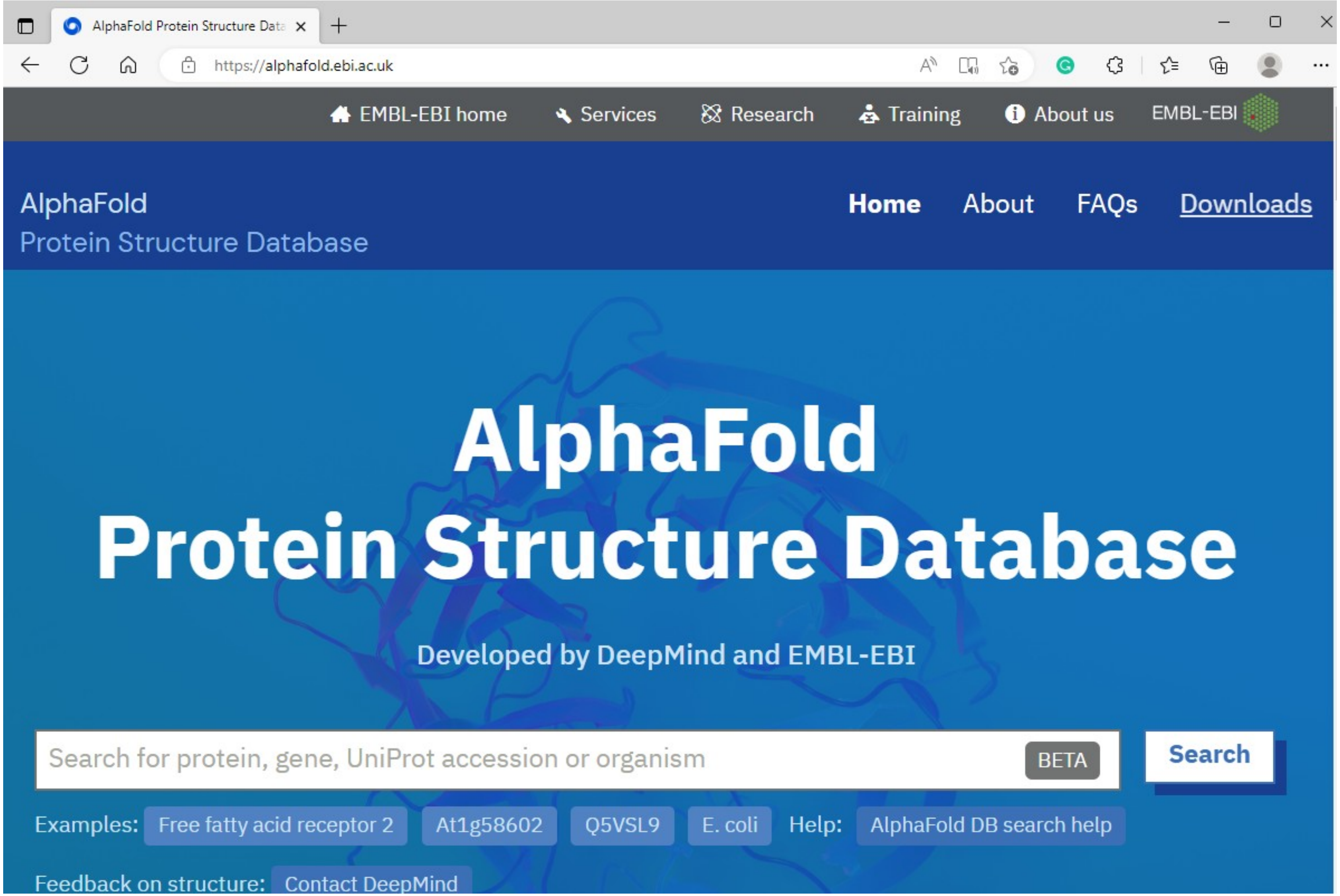
Přikládání struktur



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.
```

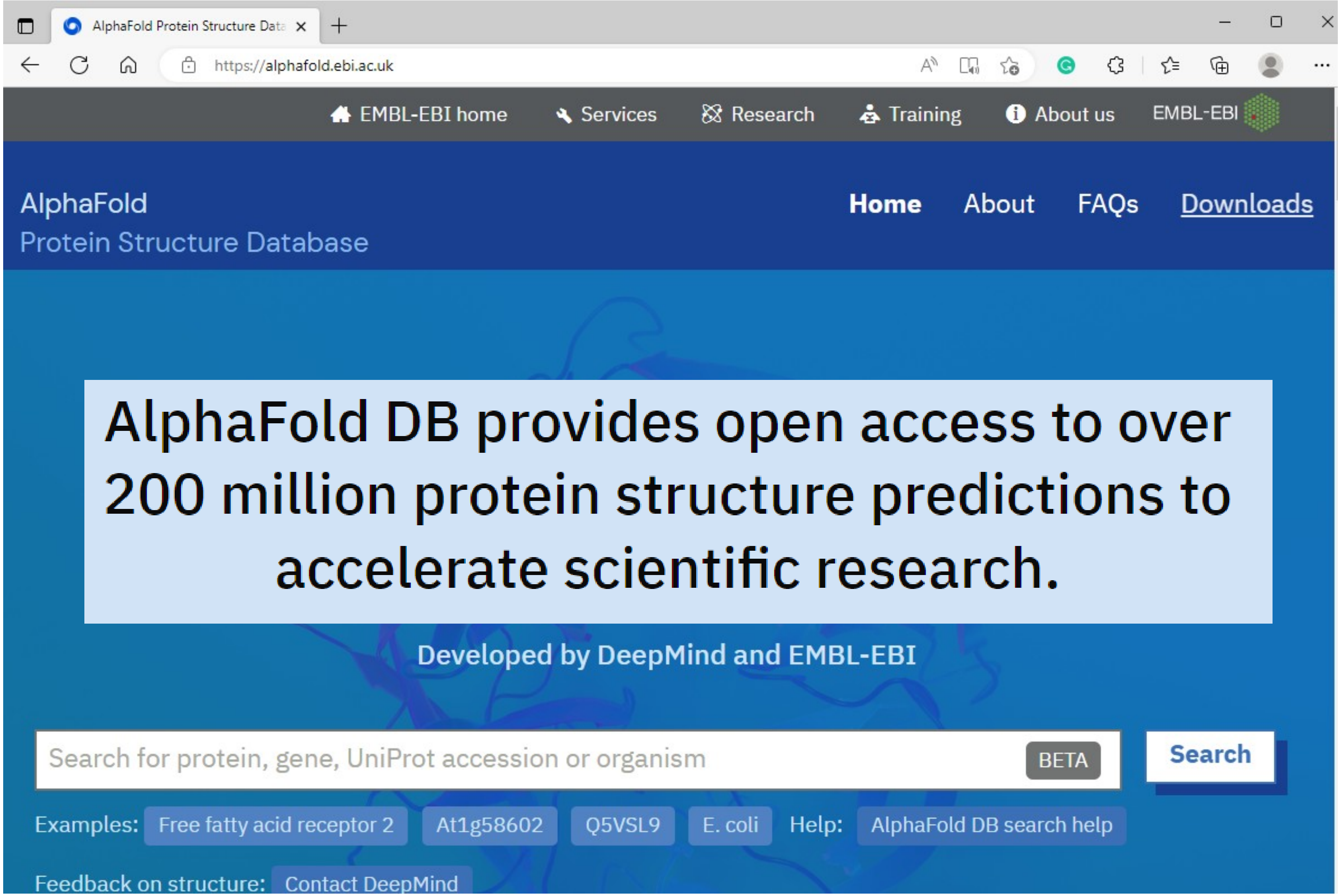
2DProts: Integration of AlphaFoldDB



AlphaFold
Protein Structure Database

Developed by DeepMind and EMBL-EBI

2DProts: Integration of AlphaFoldDB



AlphaFold
Protein Structure Database

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

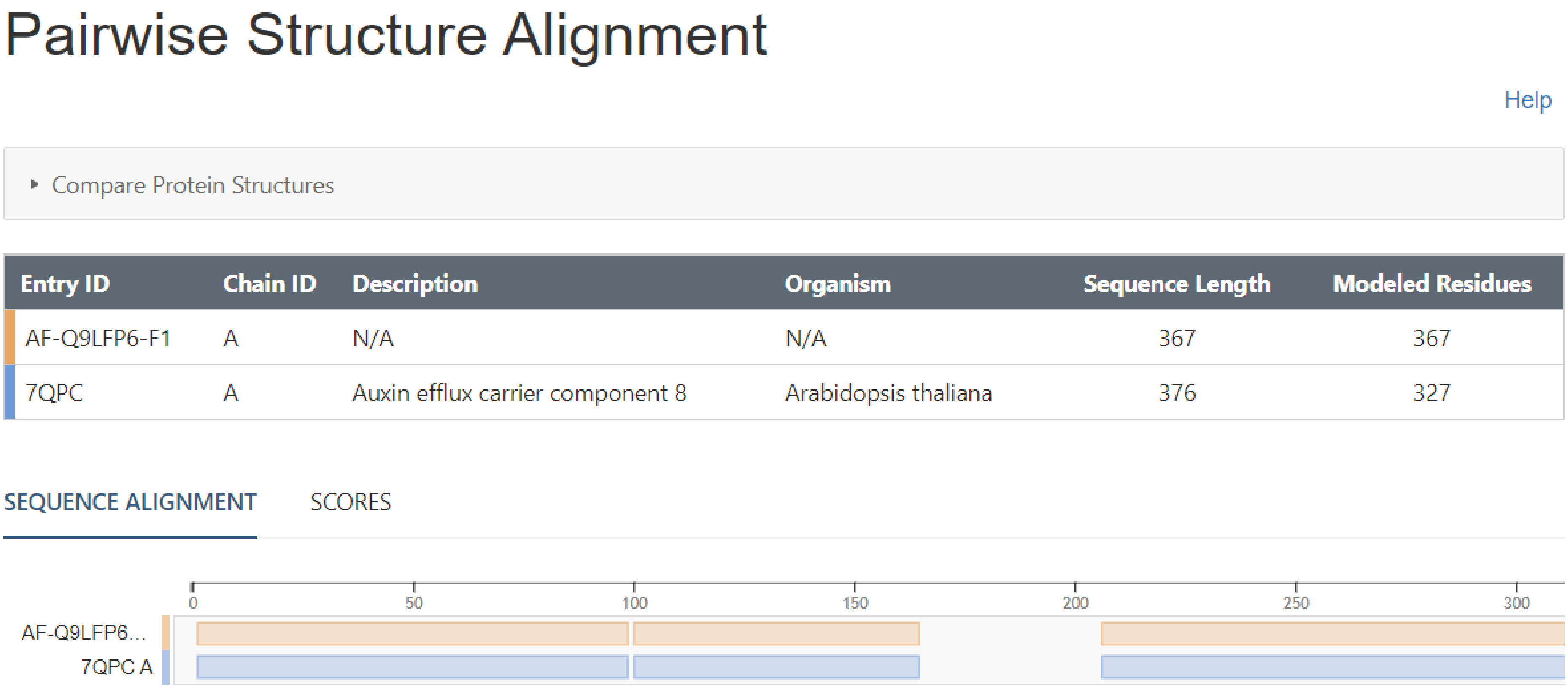
Developed by DeepMind and EMBL-EBI

Search for protein, gene, UniProt accession or organism

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

Feedback on structure: Contact DeepMind

Přikládání struktur – PDB a AlphaFold



Pairwise Structure Alignment

Help

▸ Compare Protein Structures

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

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

Přikládání struktur – PDB a AlphaFold