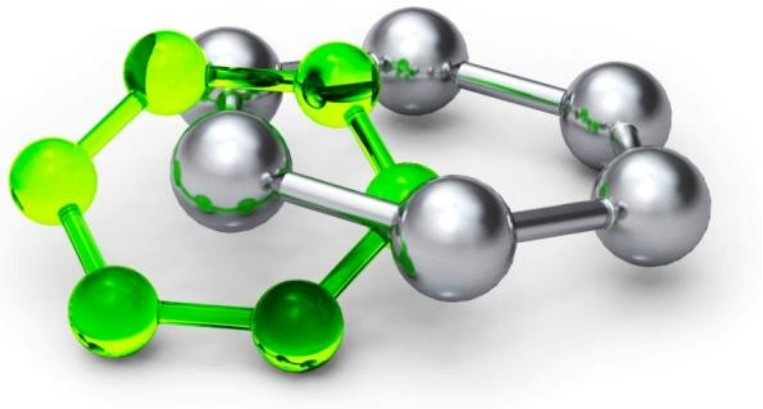
CEITEC

Central European Institute of Technology

BRNO | CZECH REPUBLIC

UNIVERSITAS MASARYKIANA BRUNENSIS

Vizualizace proteinů a ligandů

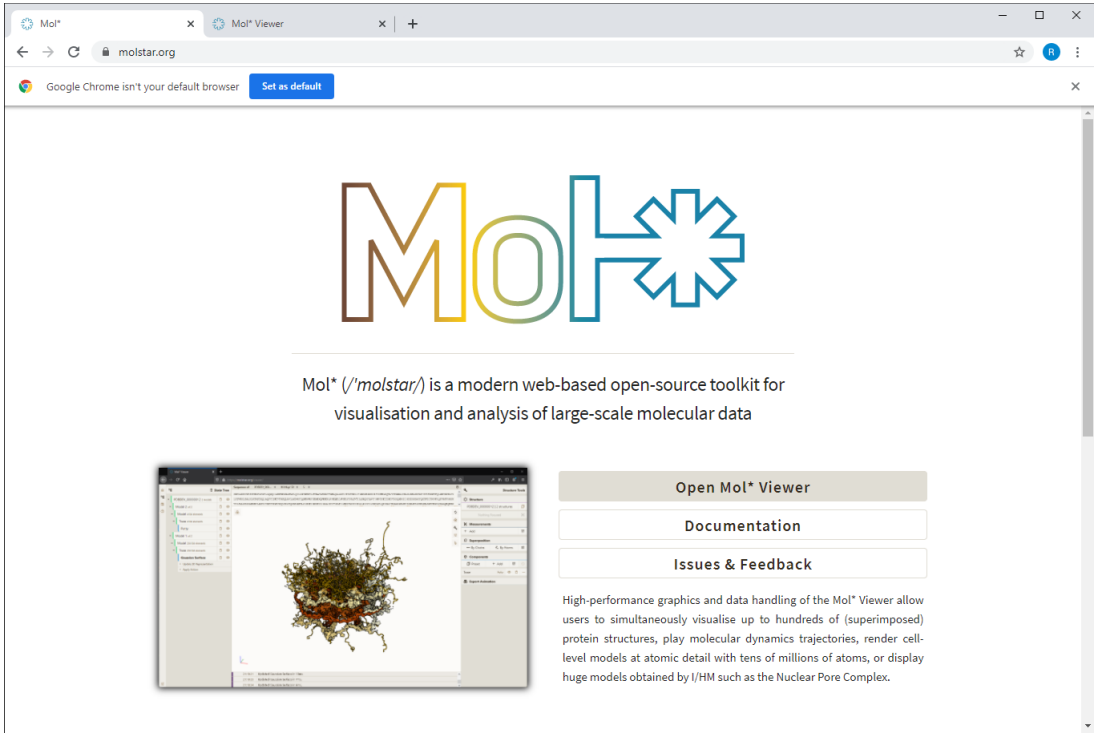


EUROPEAN UNION
EUROPEAN REGIONAL DEVELOPMENT FUND
INVESTING IN YOUR FUTURE

2007–13
OP Research and Development for Innovation

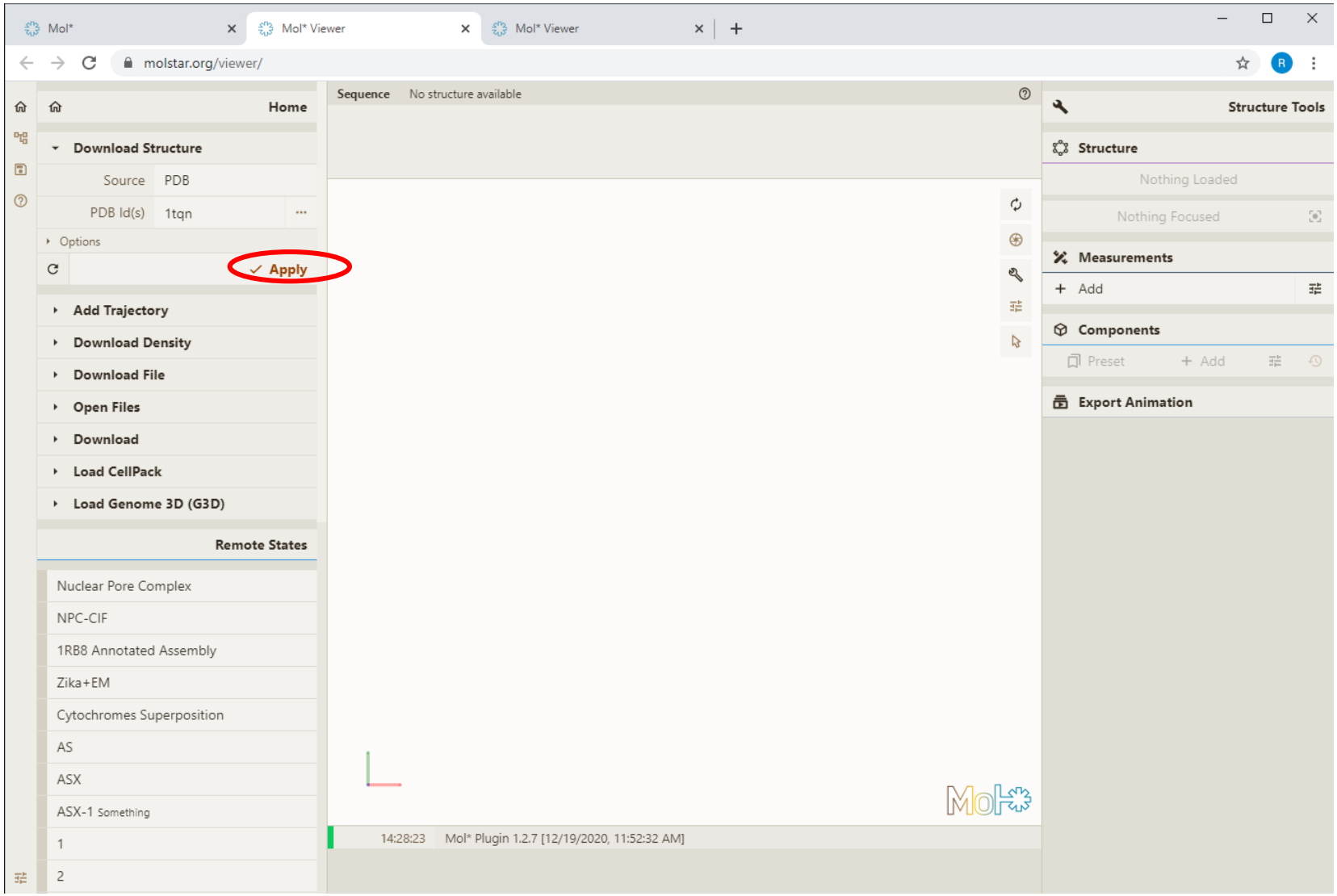
MolStar

- 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/



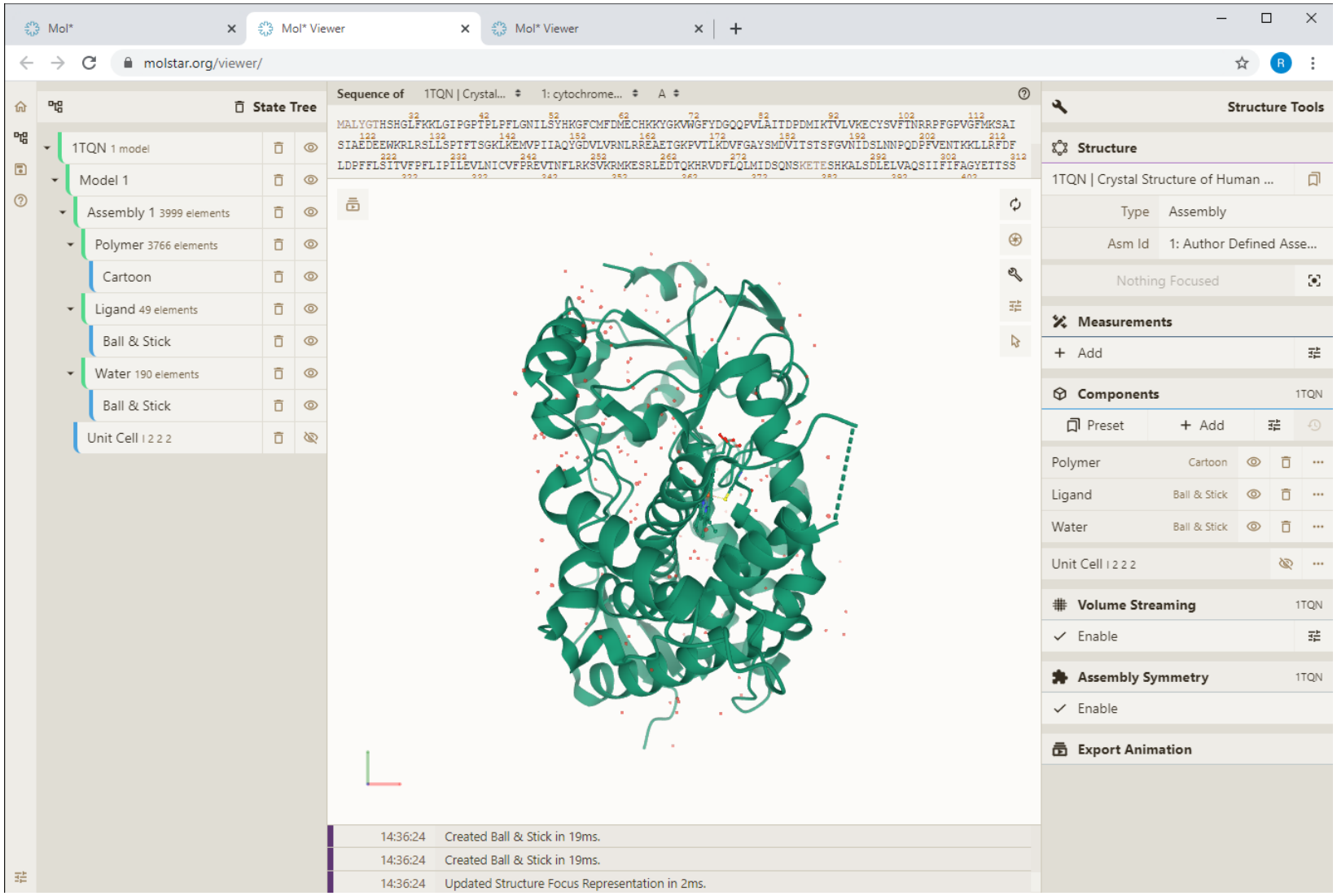
CEITEC

MolStar

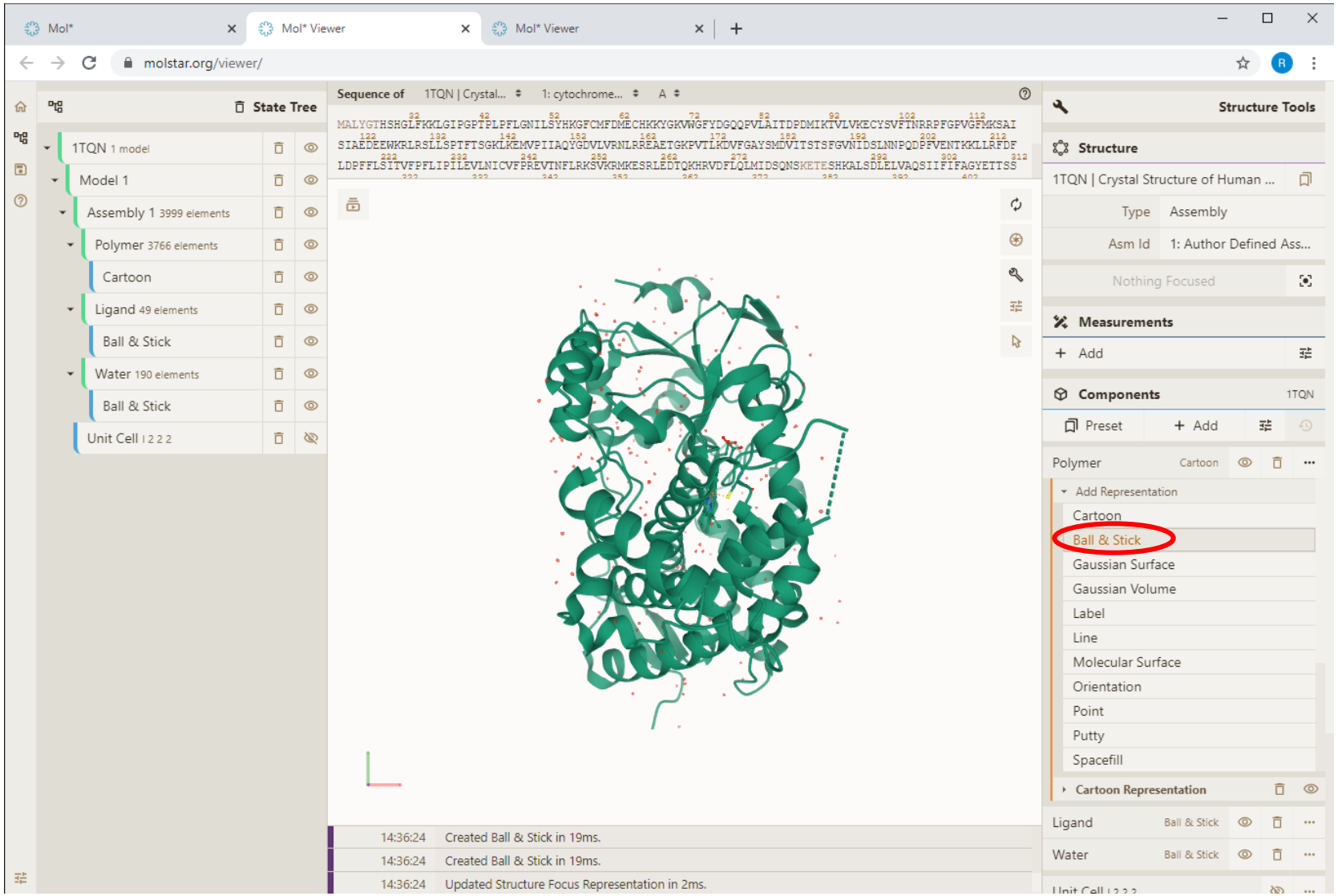


CEITEC

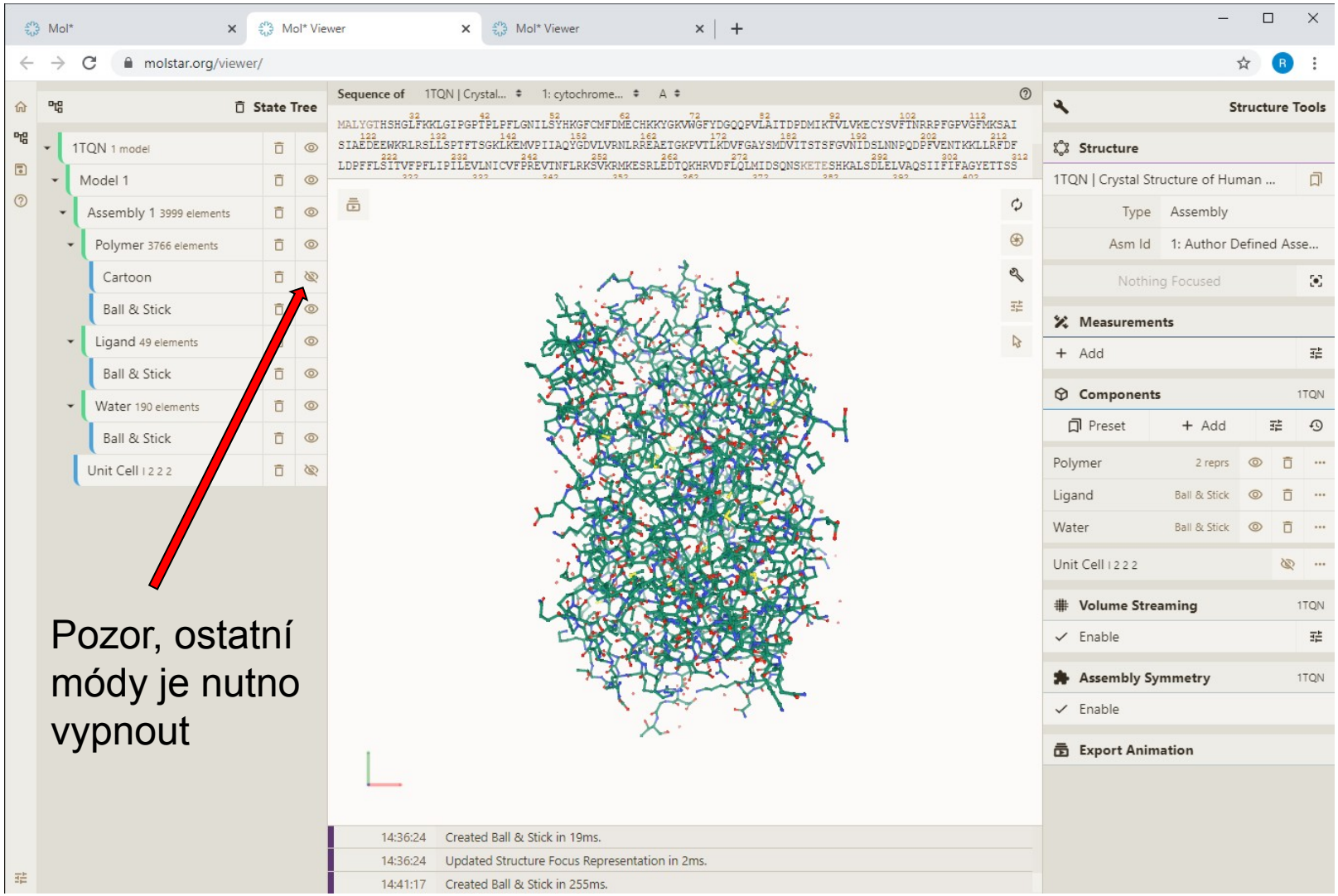
Vizualizace 3D souřadic molekuly
Vizualizační model cartoon



Vizualizace 3D souřadic molekuly
Volba vizualizačních modelů

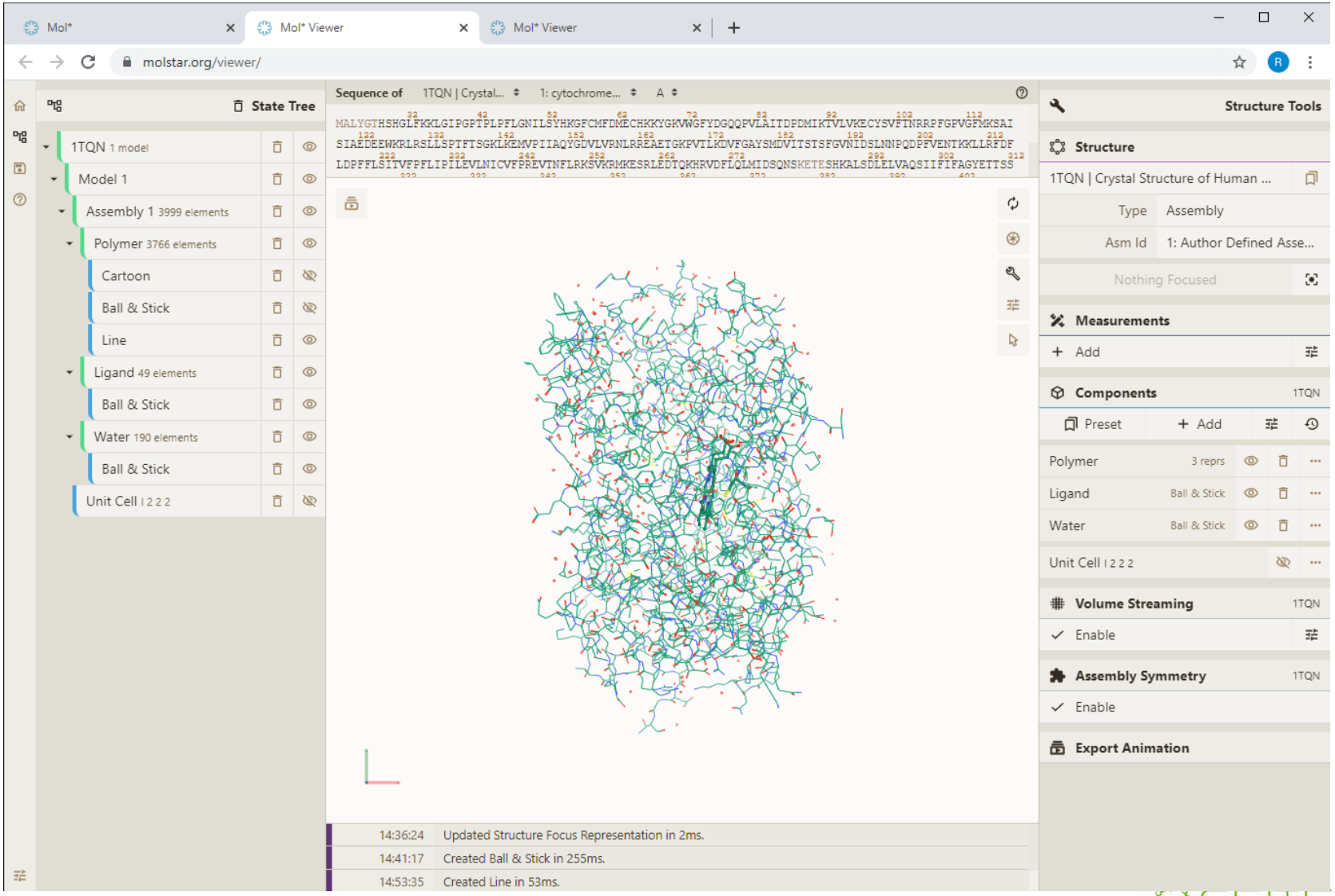


Vizualizace 3D souřadic molekuly
Vizualizační model Ball & Stick

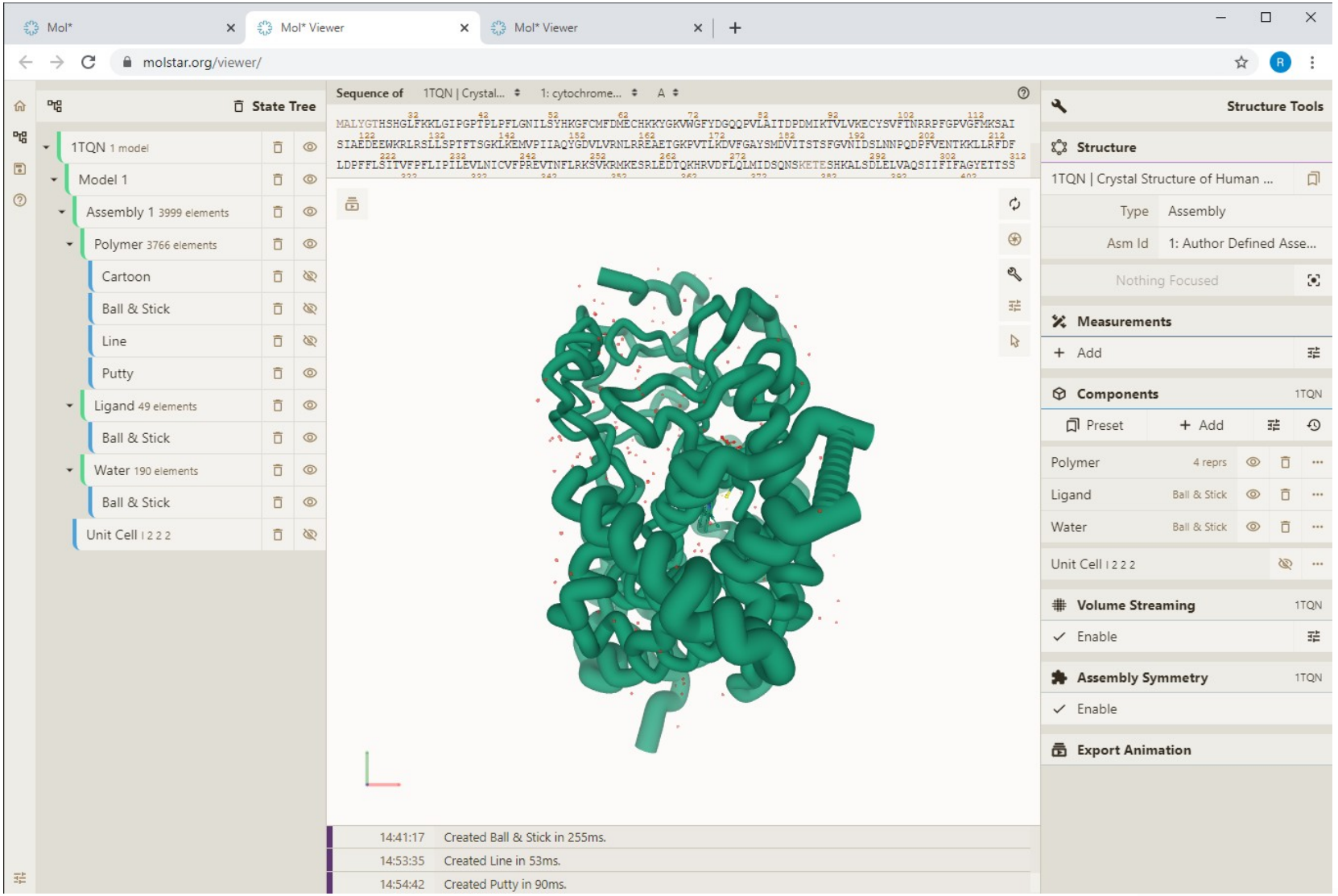


CEITEC

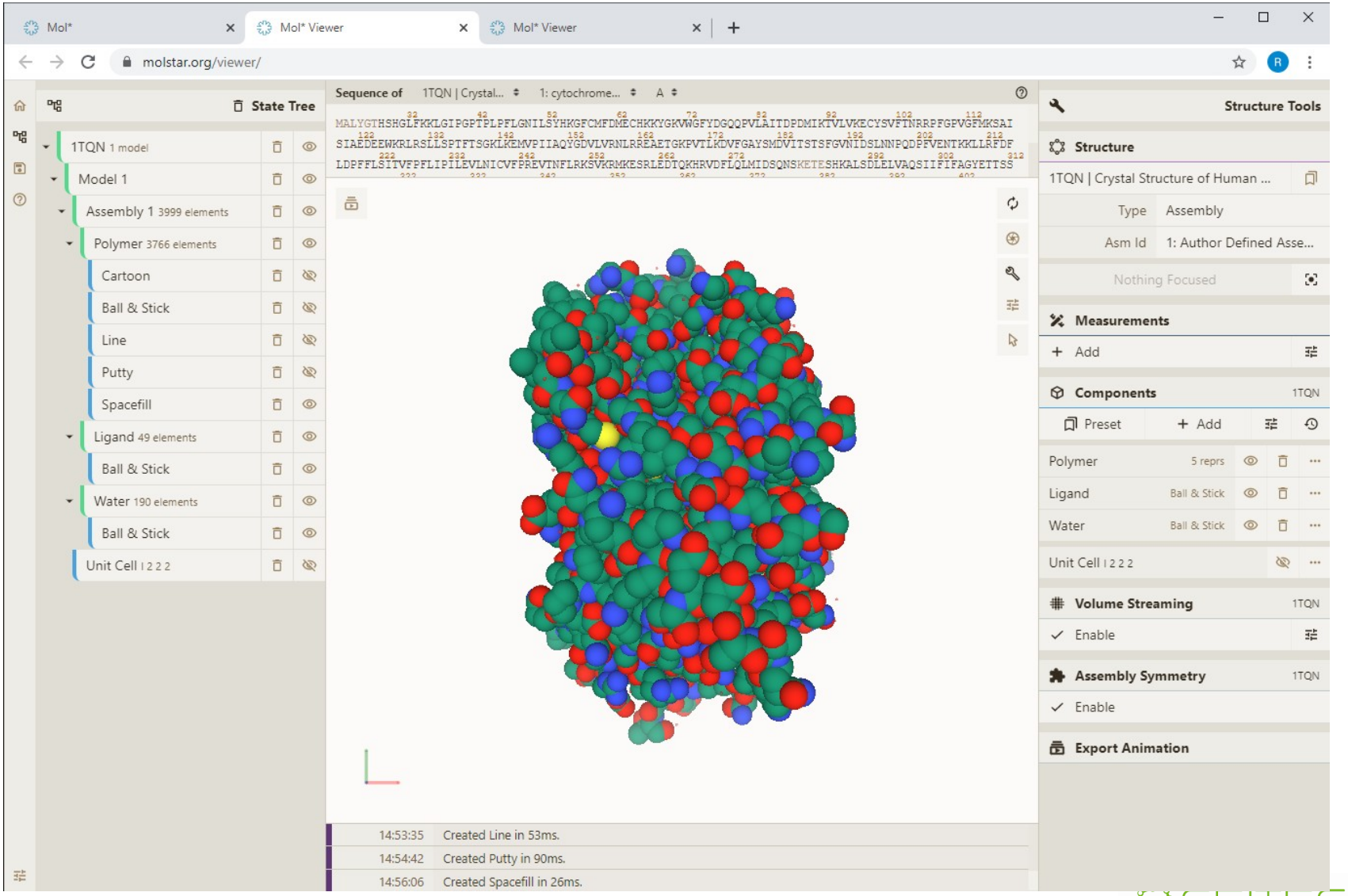
Vizualizace 3D souřadic molekuly
Vizualizační model Line



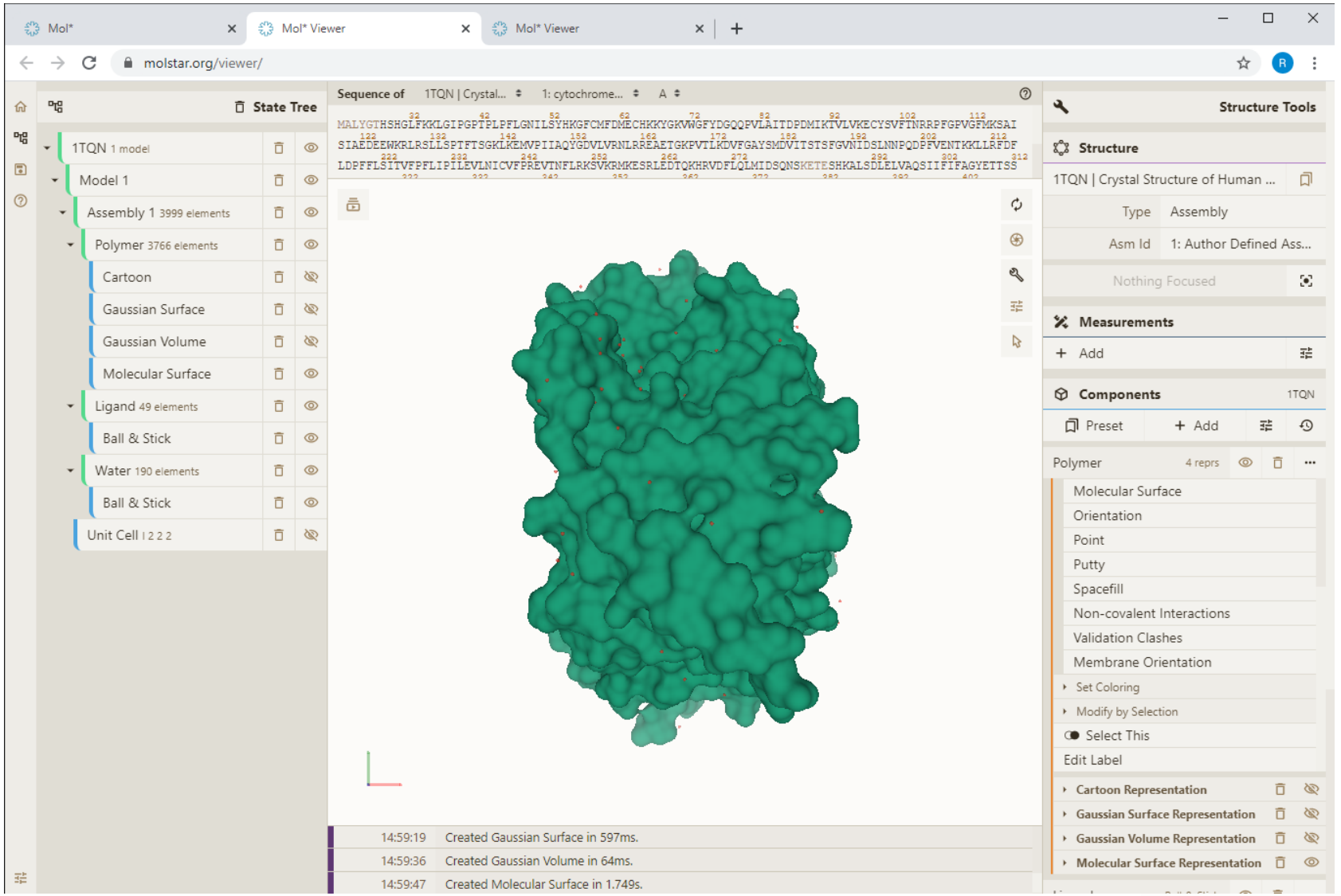
Vizualizace 3D souřadic molekuly
Vizualizační model Putty



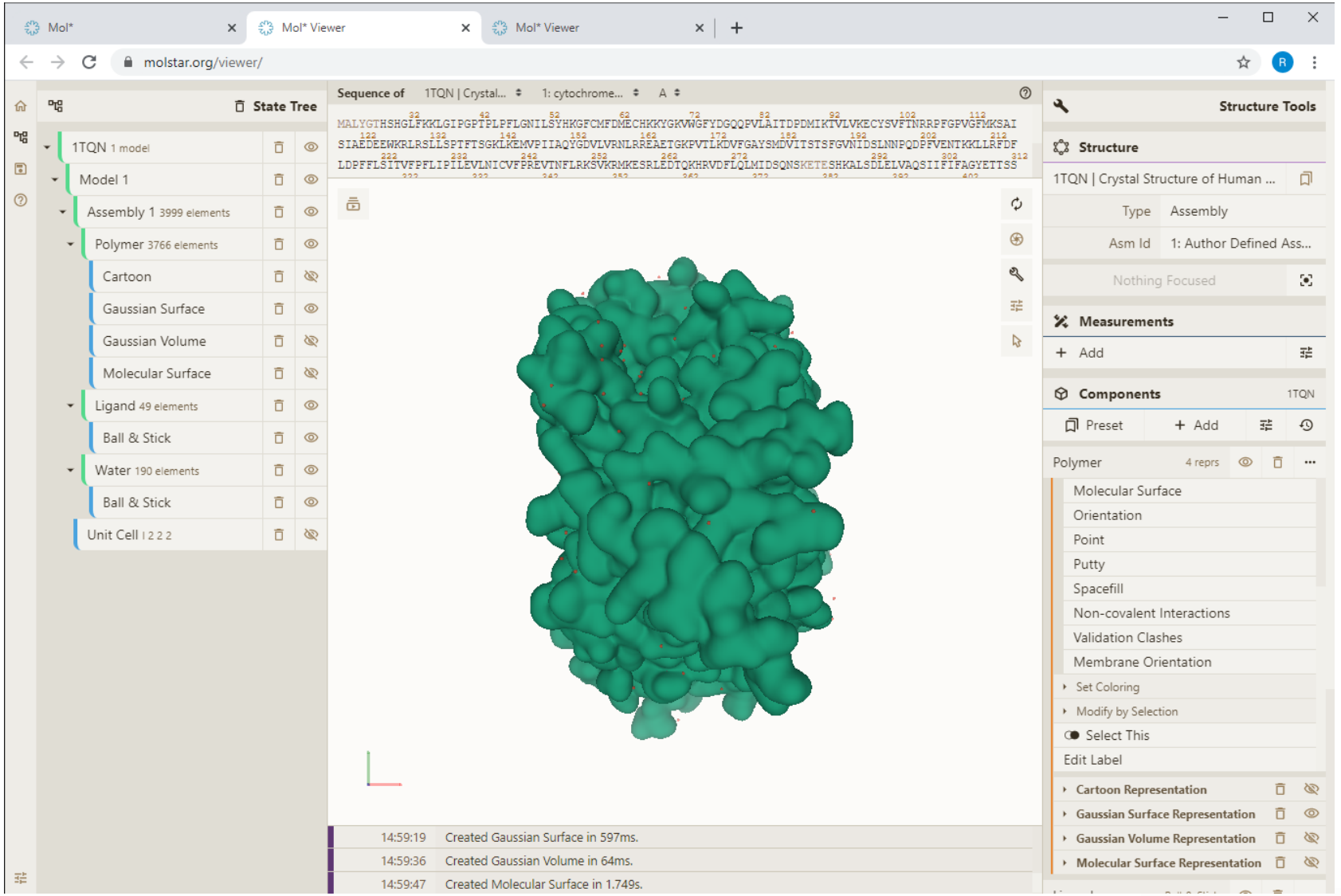
Vizualizace 3D souřadic molekuly
Vizualizační model Spacefil



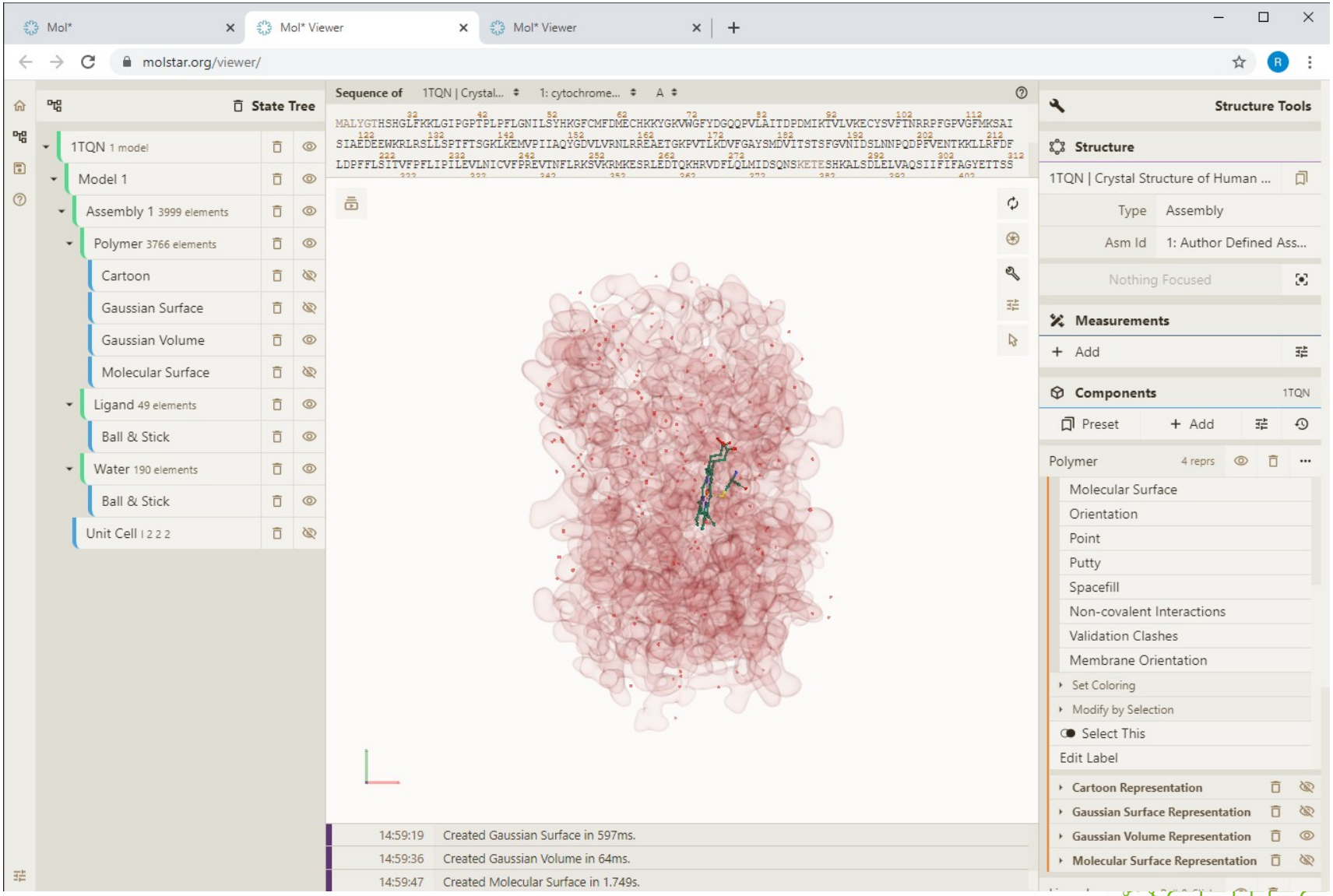
Vizualizace povrchu molekuly
Vizualizační model Molecular Surface



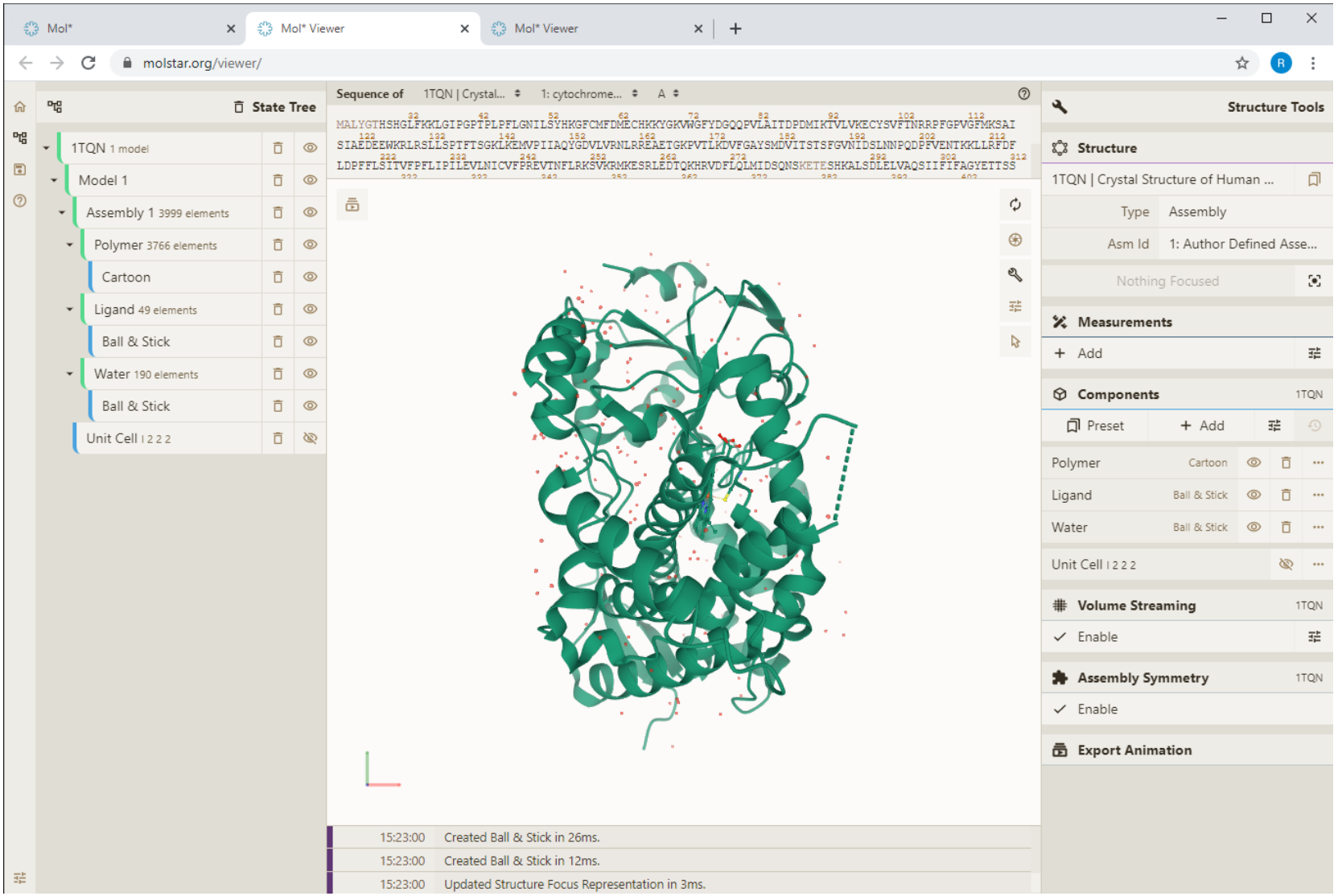
Vizualizace povrchu molekuly
Vizualizační model Gaussian Surface



Vizualizace povrchu molekuly
Vizualizační model Gaussian Volume

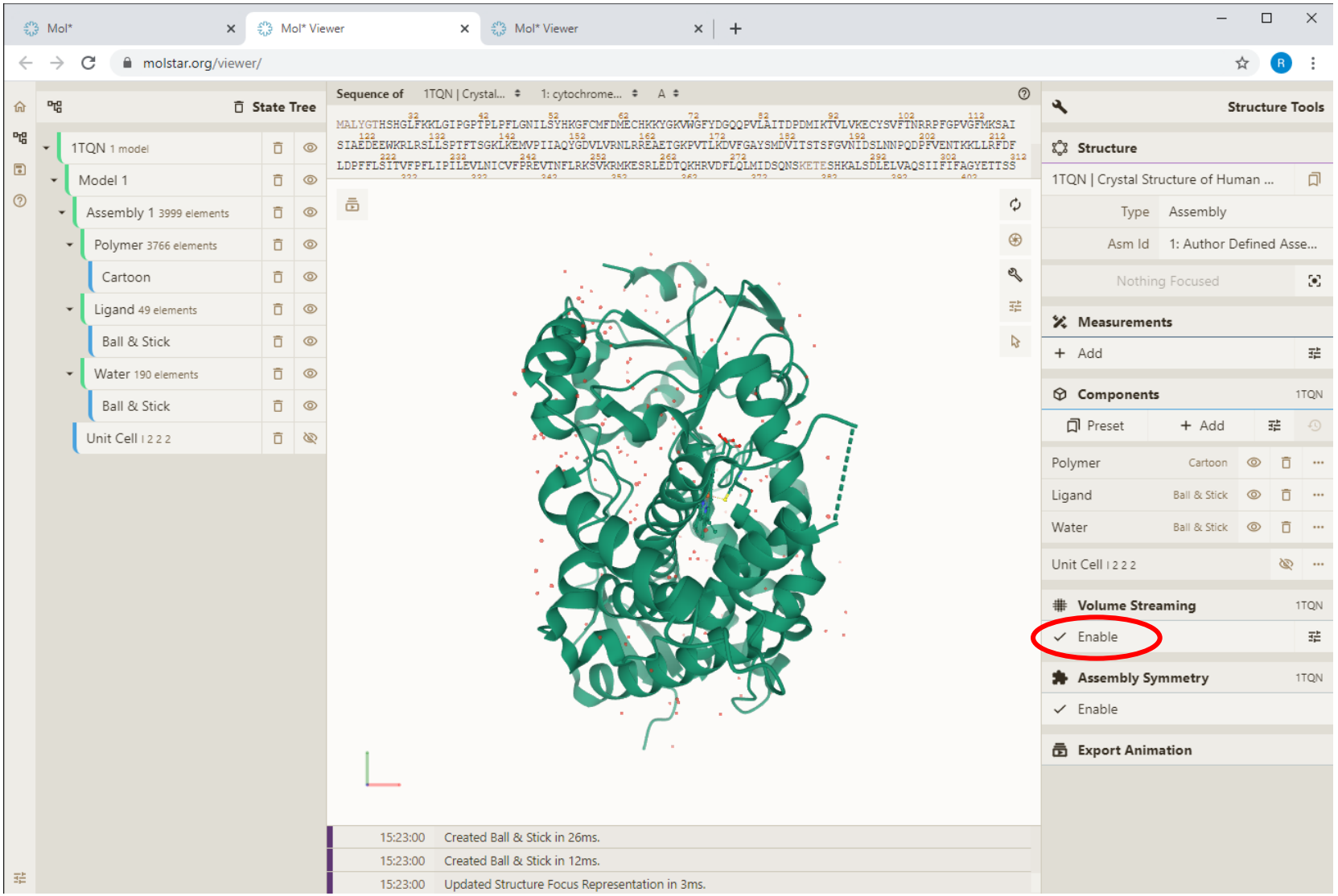


Vizualizace experimentálních dat
Elektronová hustota



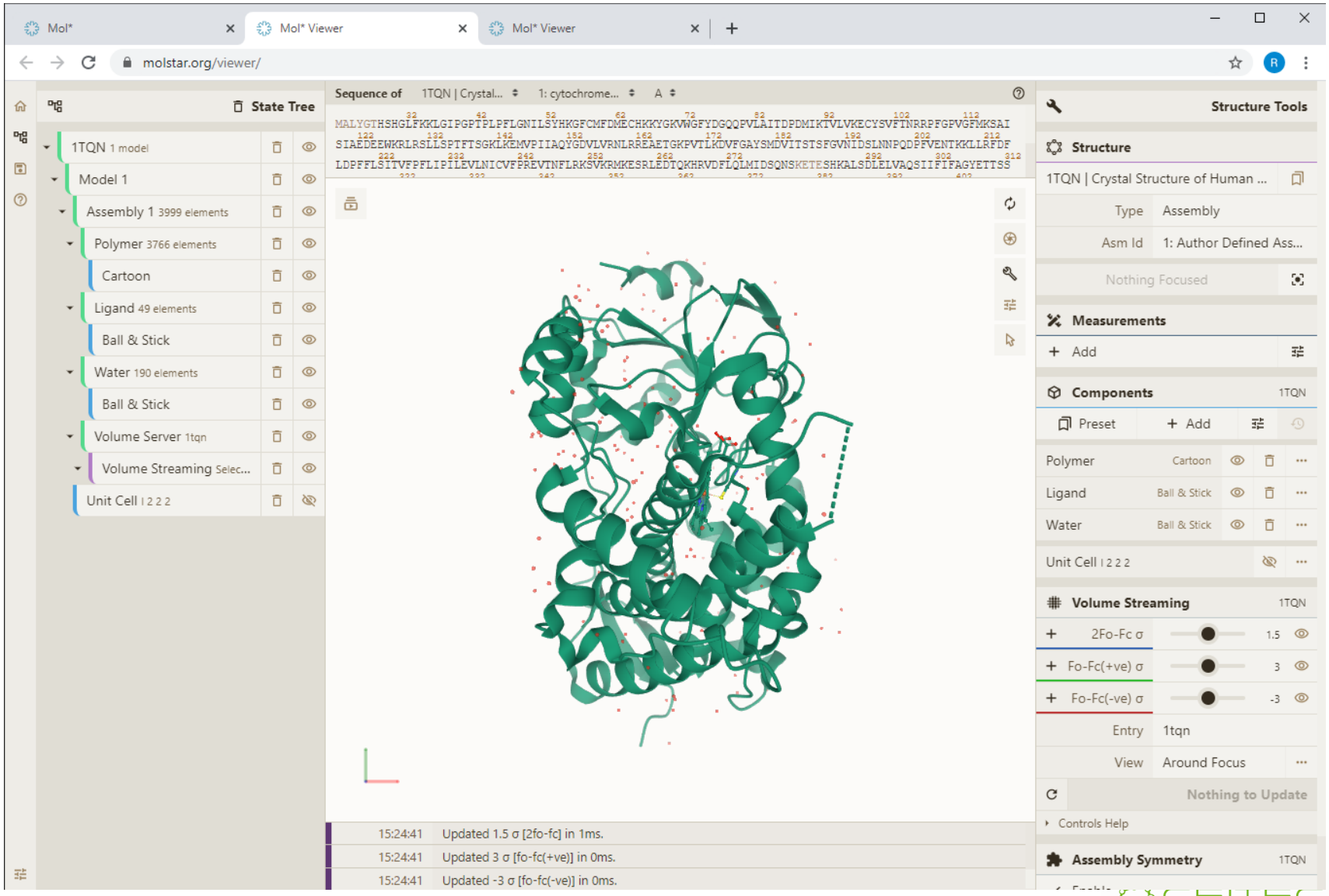
CEITEC

Vizualizace experimentálních dat
Elektronová hustota

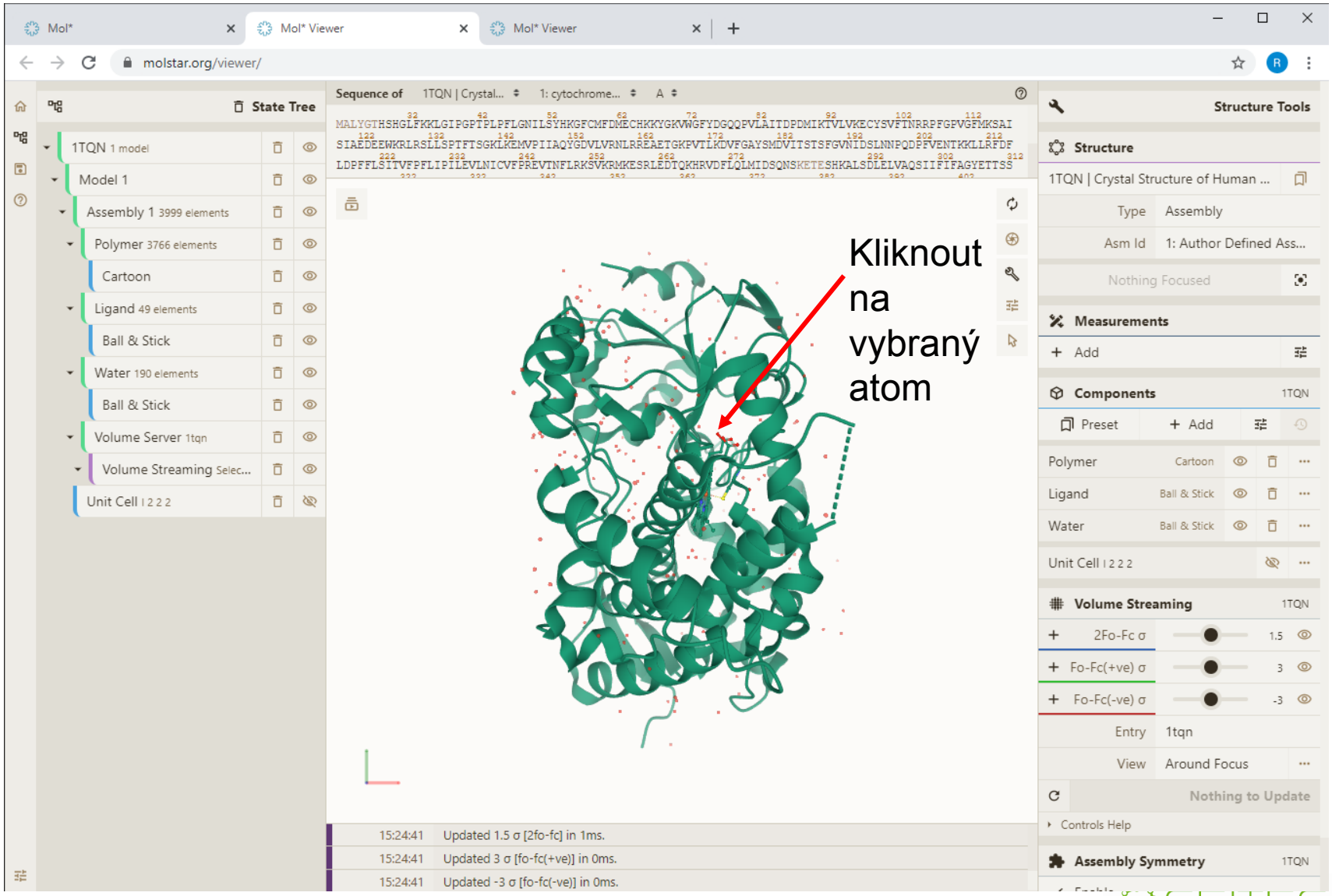


CEITEC

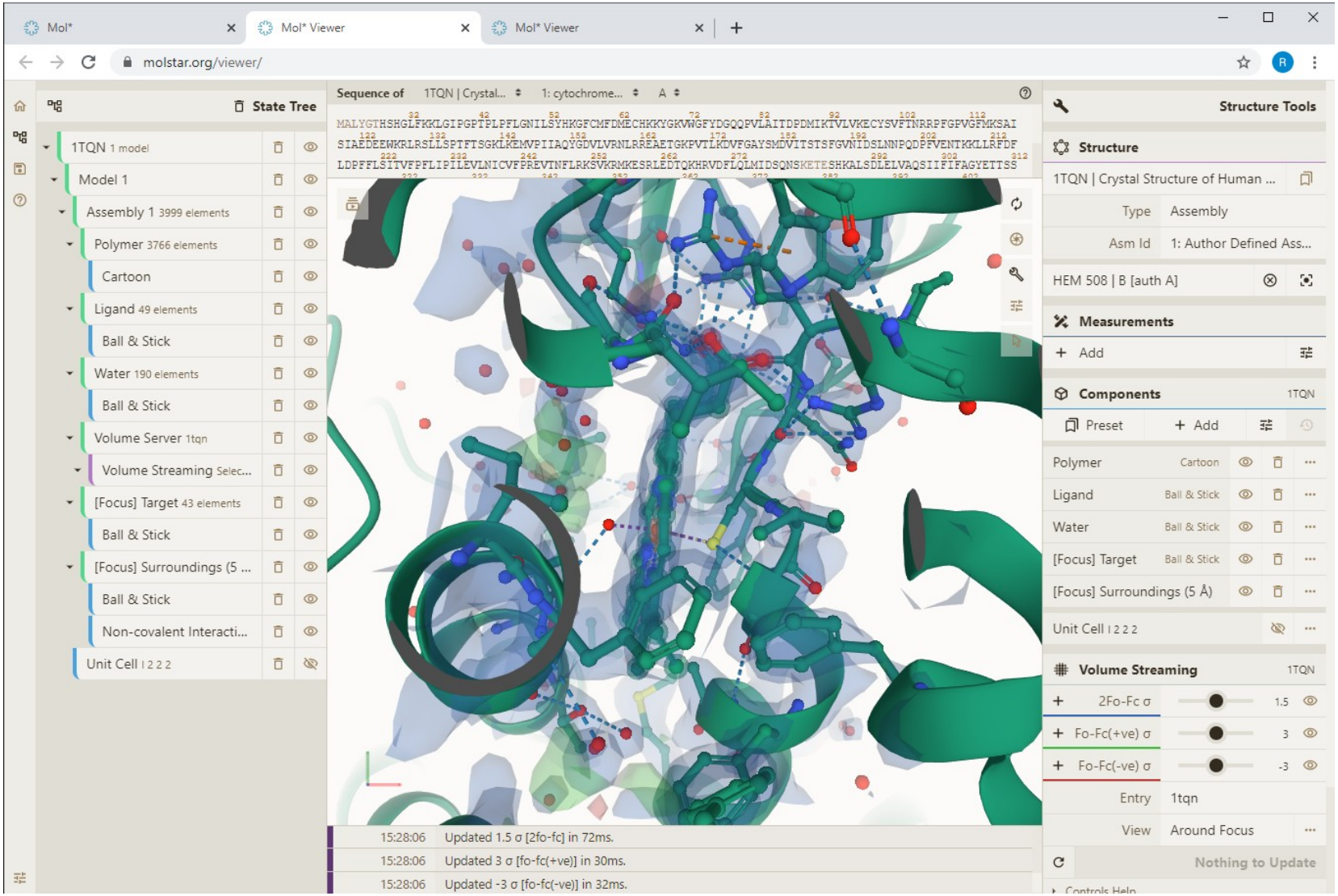
Vizualizace experimentálních dat
Elektronová hustota



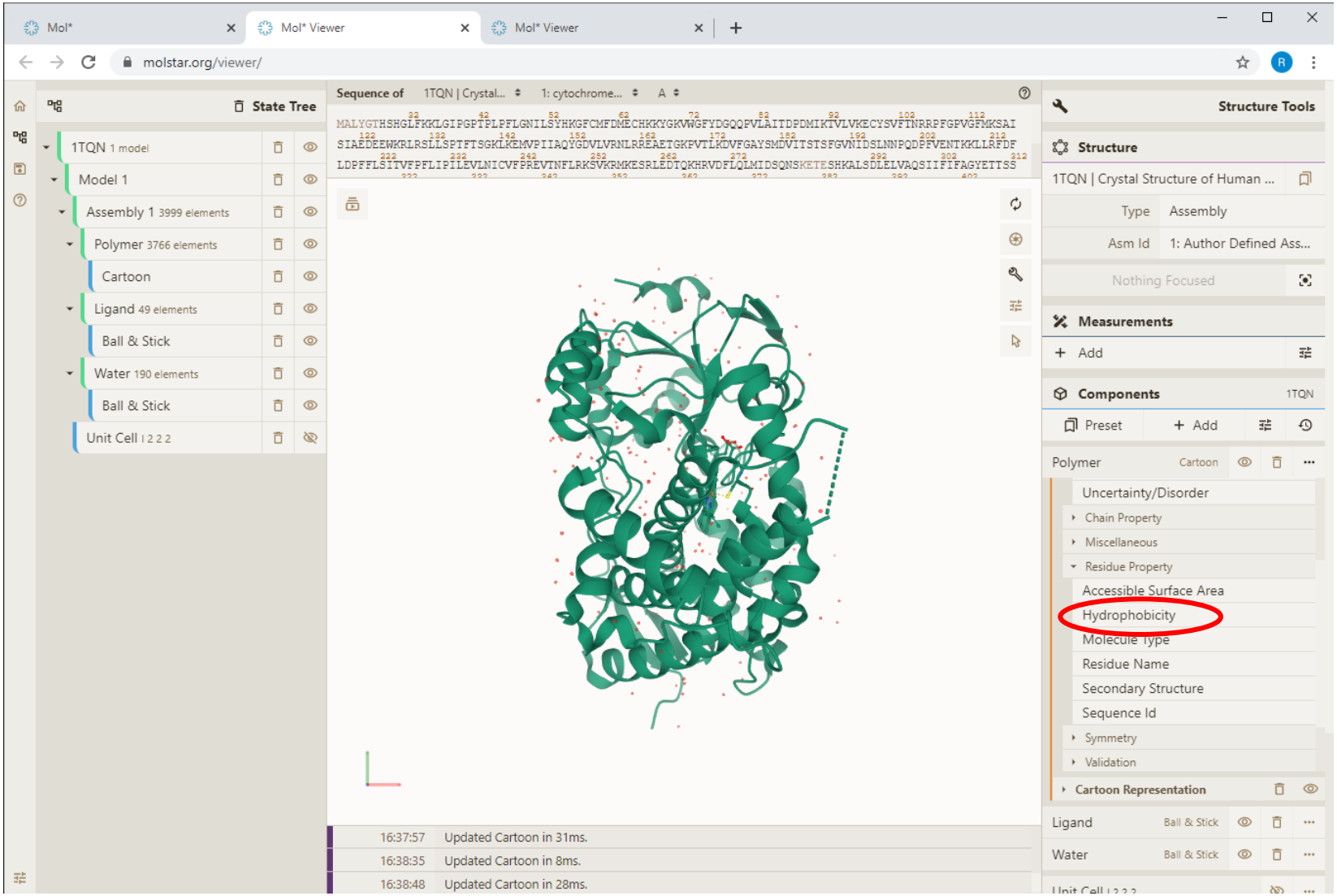
Vizualizace experimentálních dat
Elektronová hustota



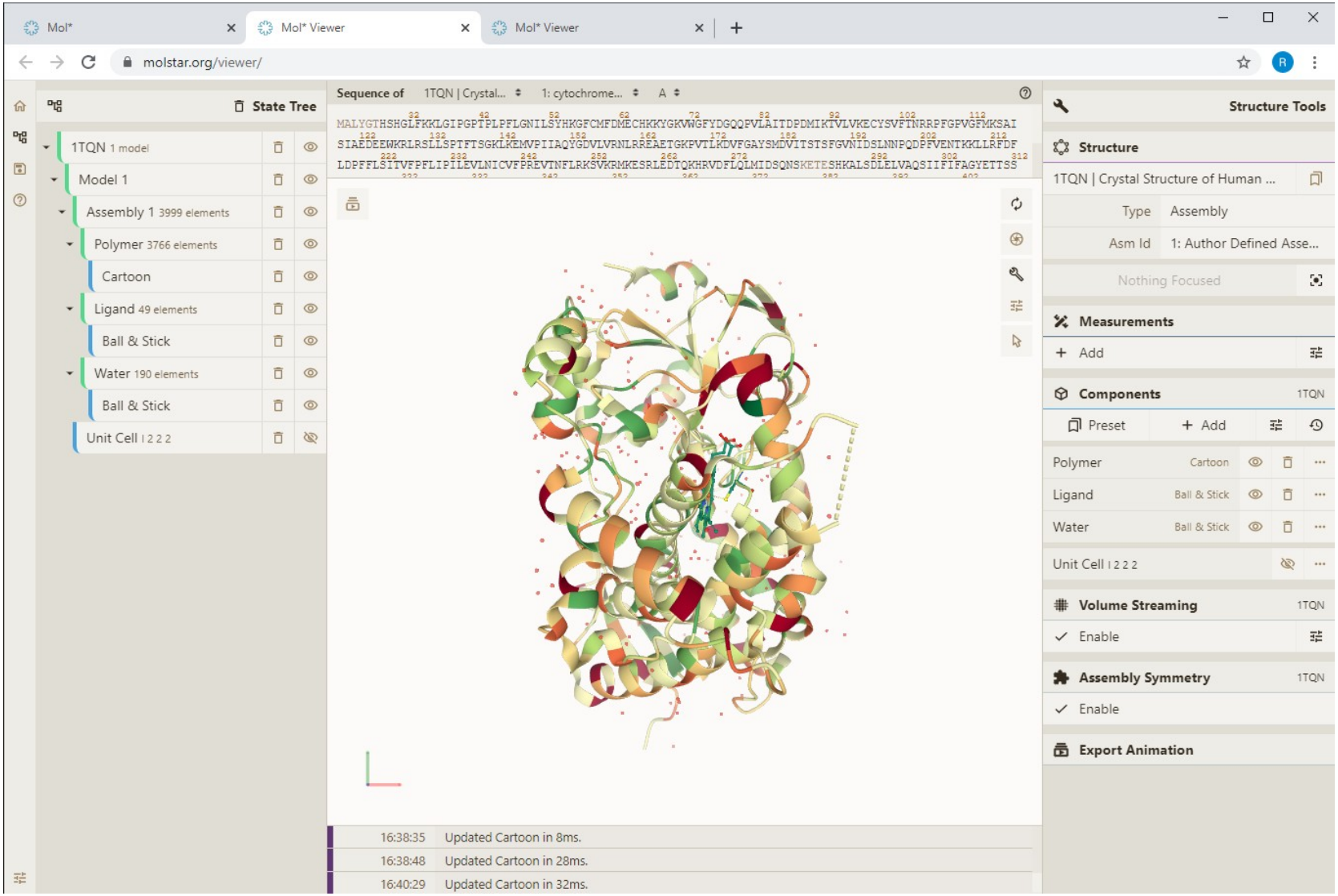
Vizualizace experimentálních dat
Elektronová hustota



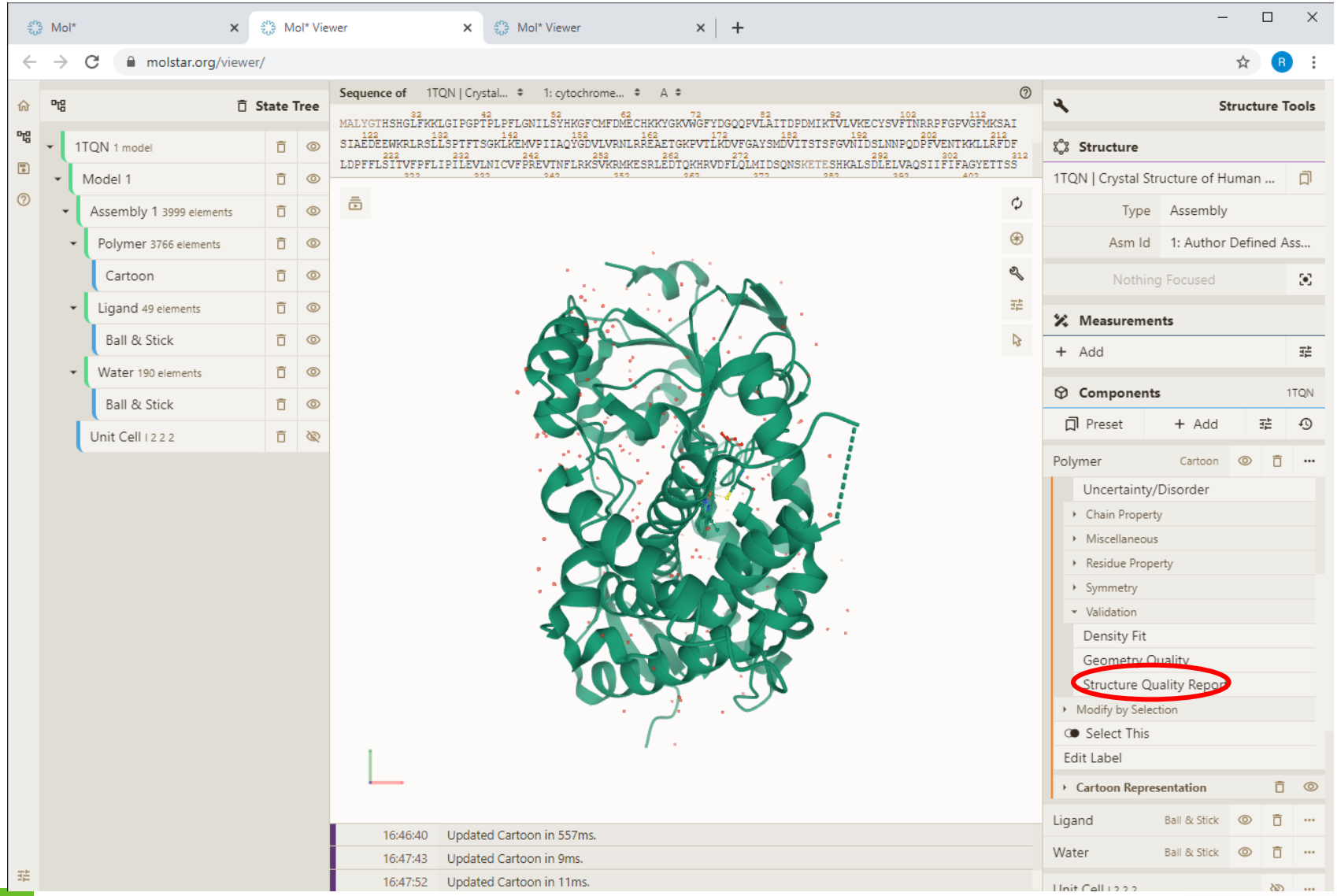
Vizualizace anotací
Obarvení podle vlastností



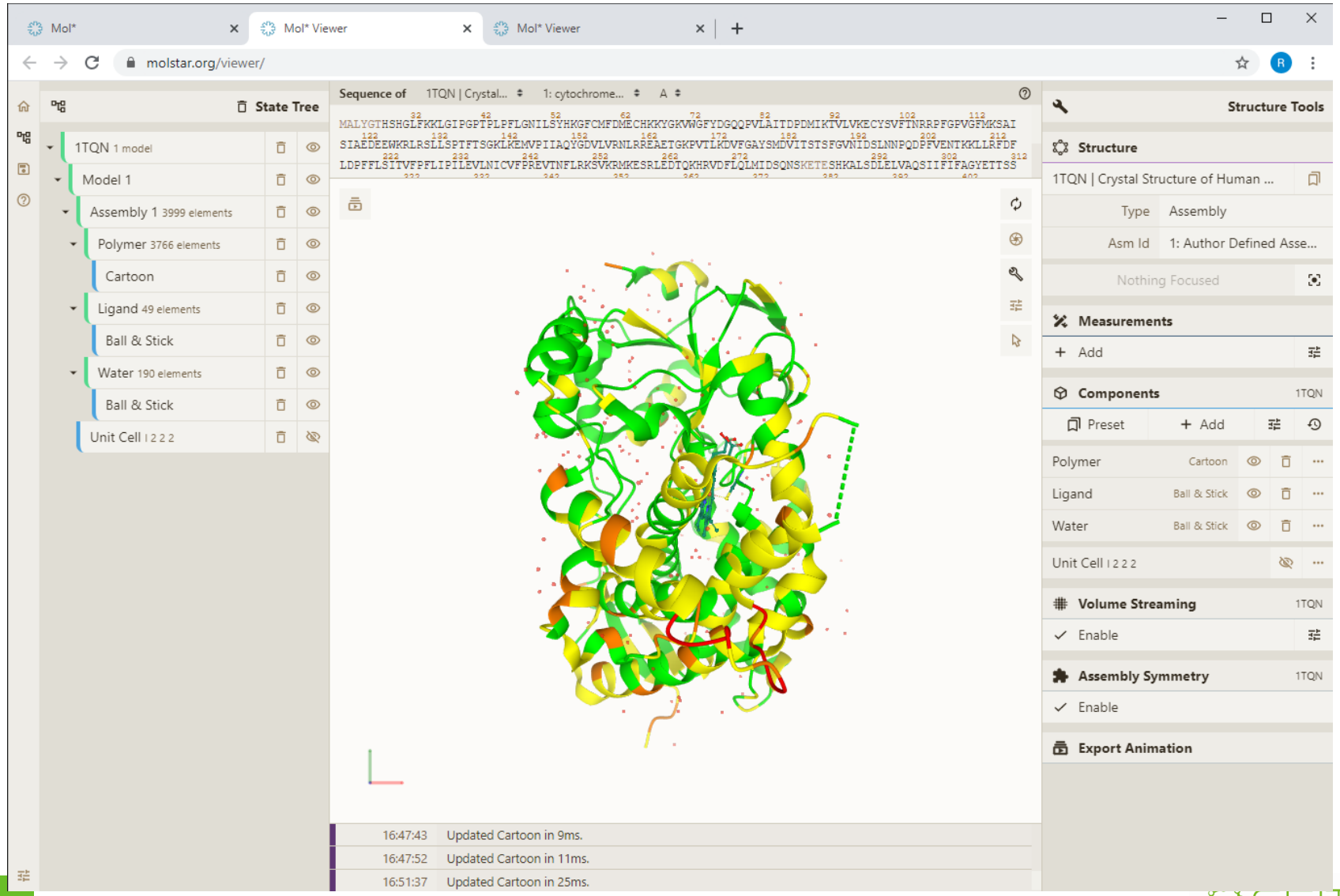
Vizualizace anotací
Obarvení podle vlastností - hydrofobicita



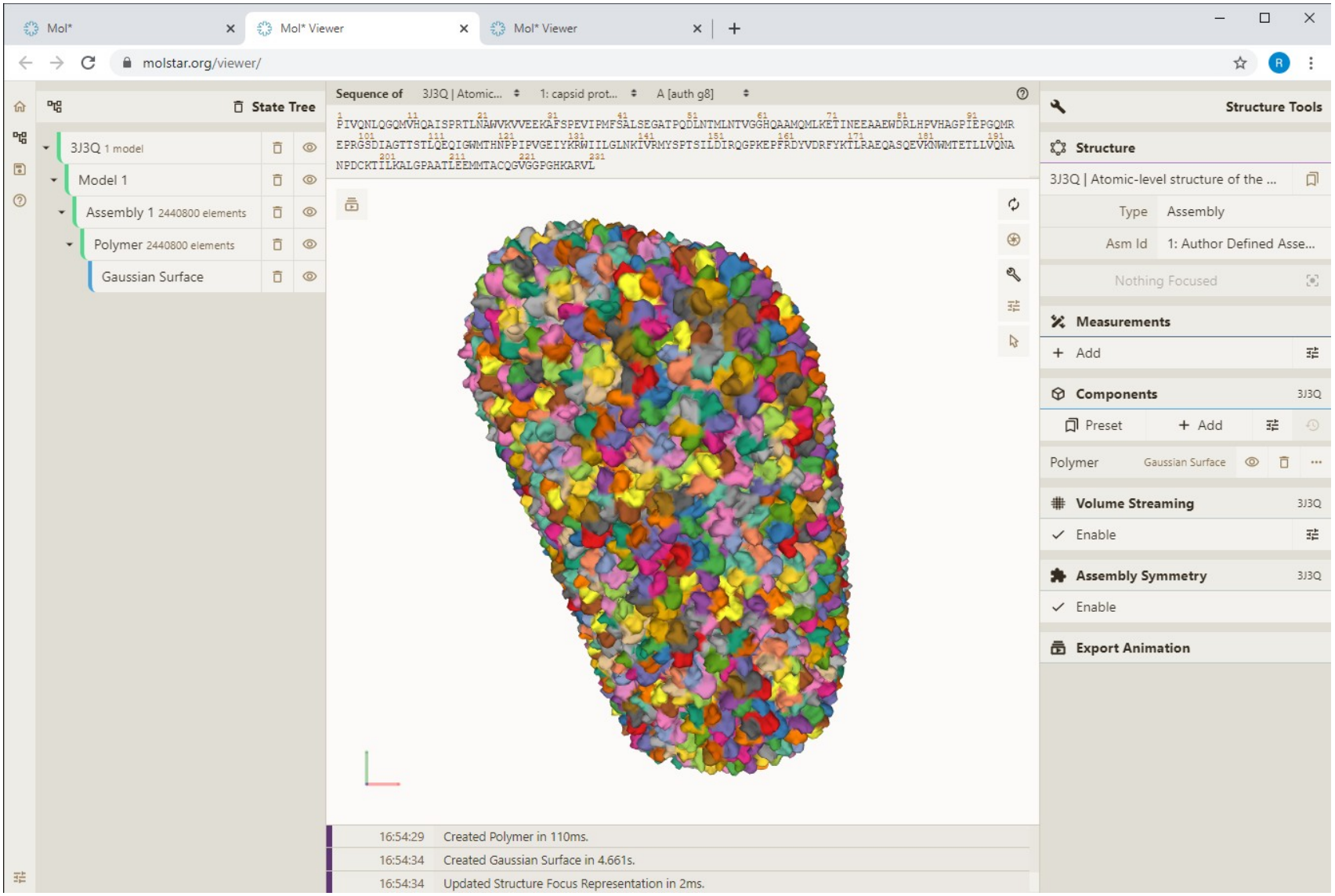
Vizualizace anotací
Obarvení podle vlastností – kvalita



Vizualizace anotací
Obarvení podle vlastností - kvalita

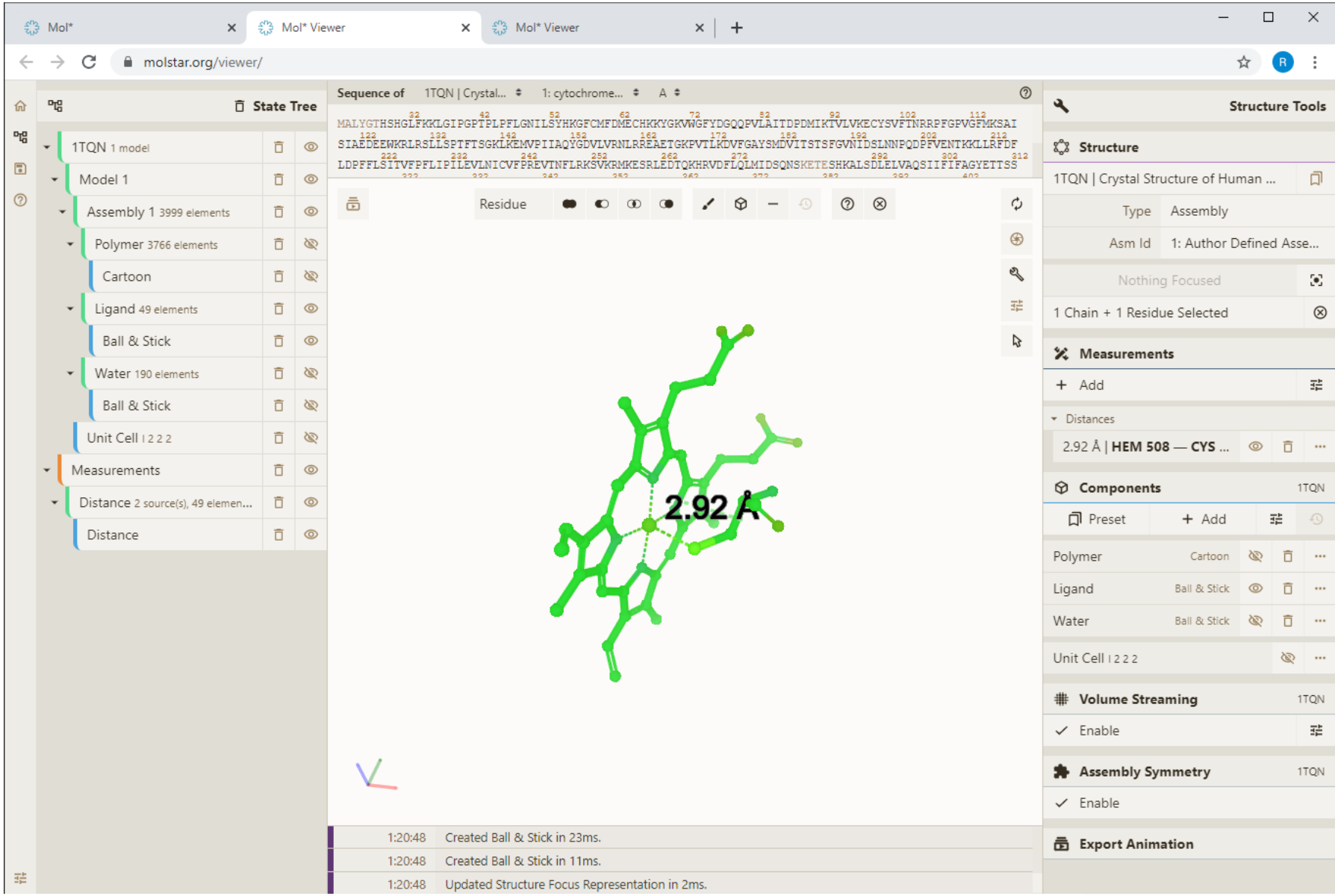


Vizualizace proteinových assemblies



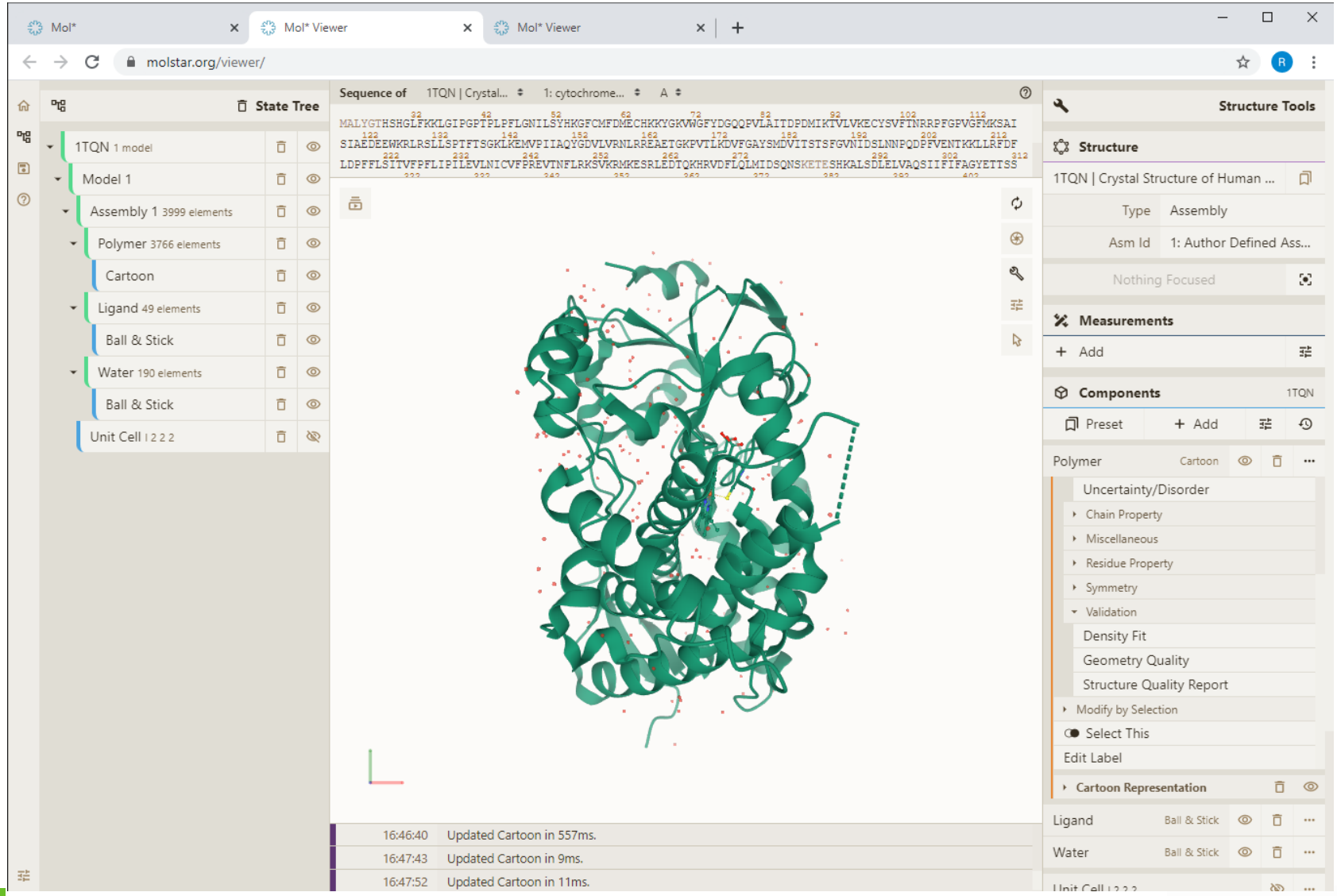
CEITEC

Měření

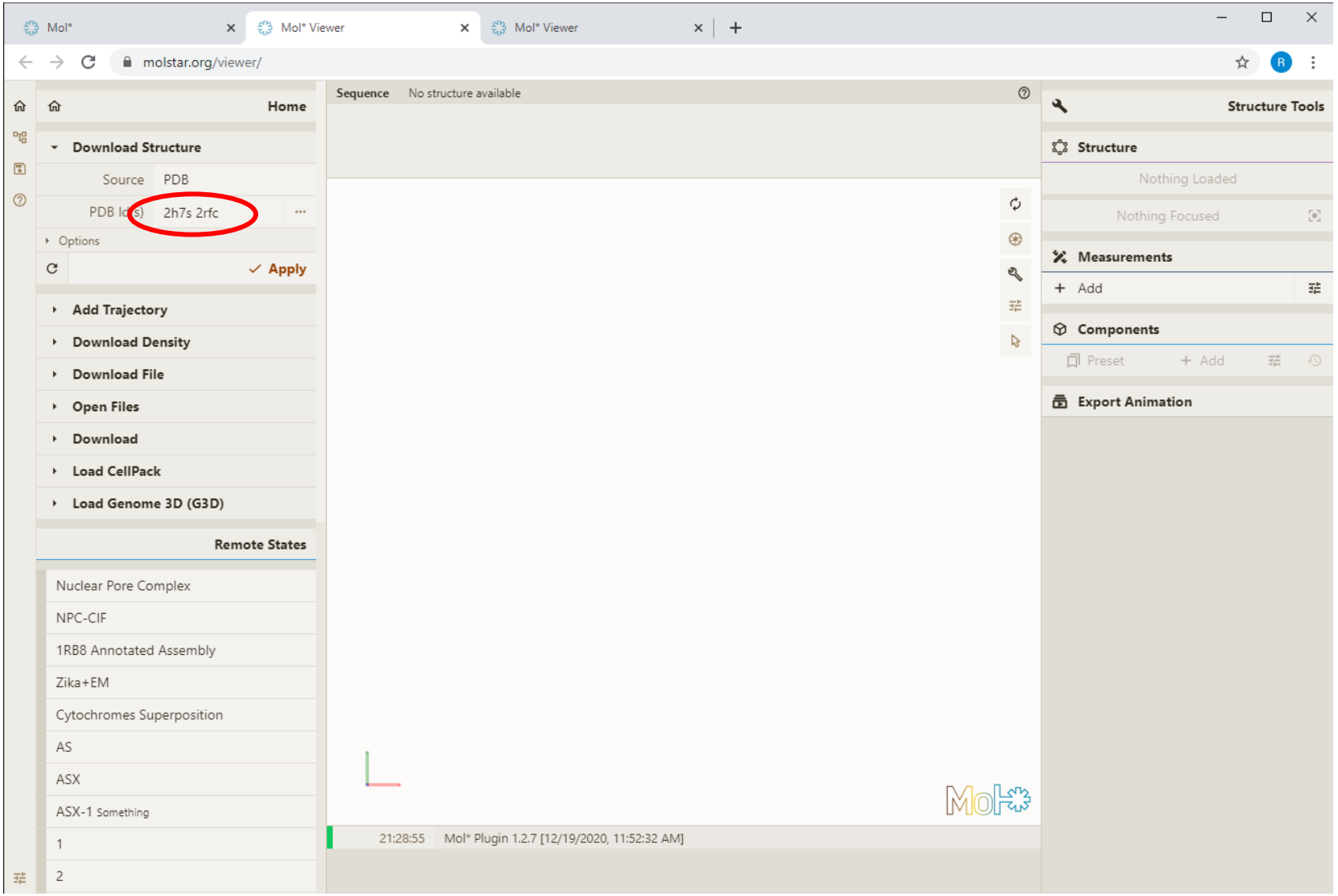


CEITEC

Vizualizace anotací
Obarvení podle vlastností - hydrofobicita

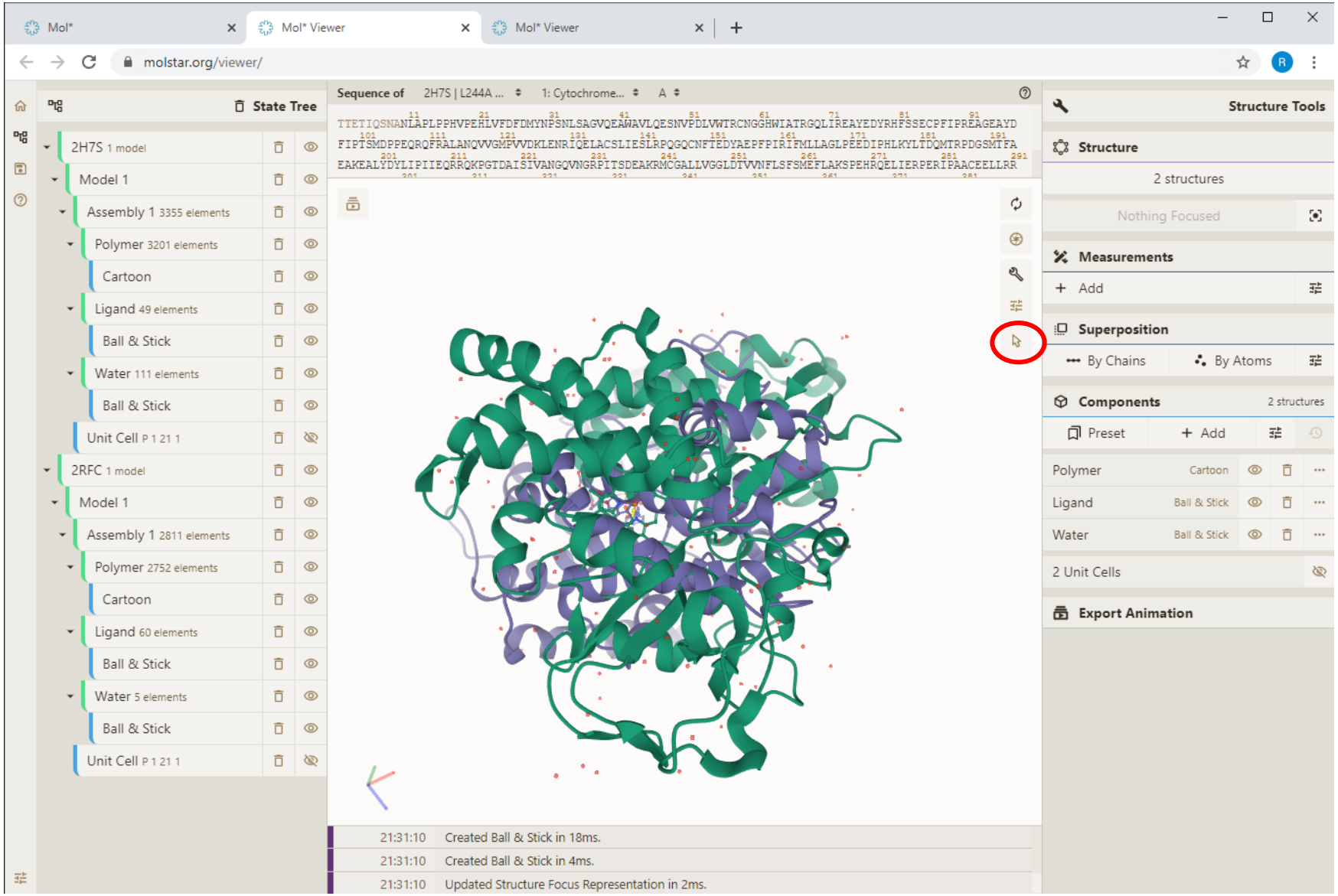


Přikládání struktur

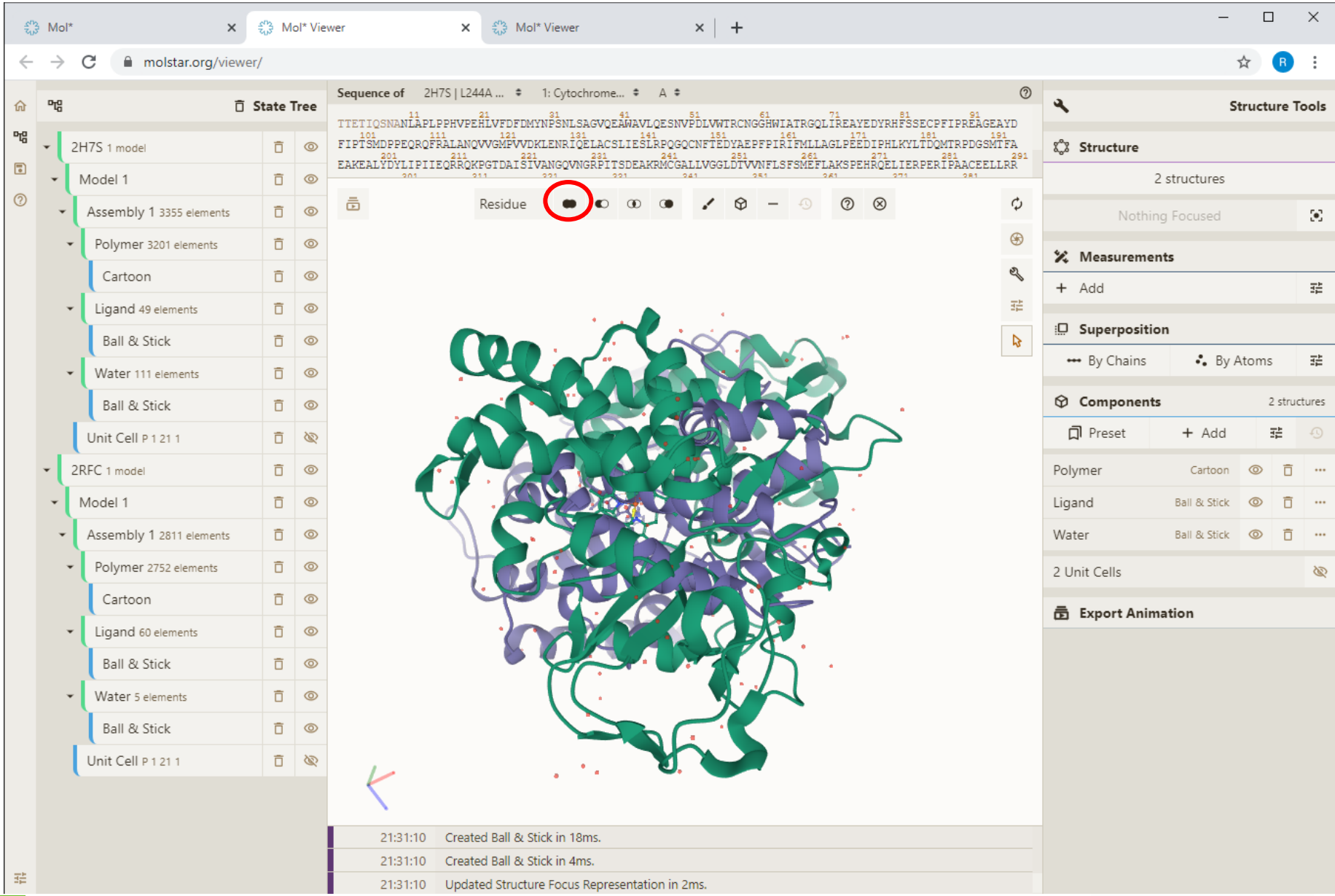


CEITEC

Přikládání struktur

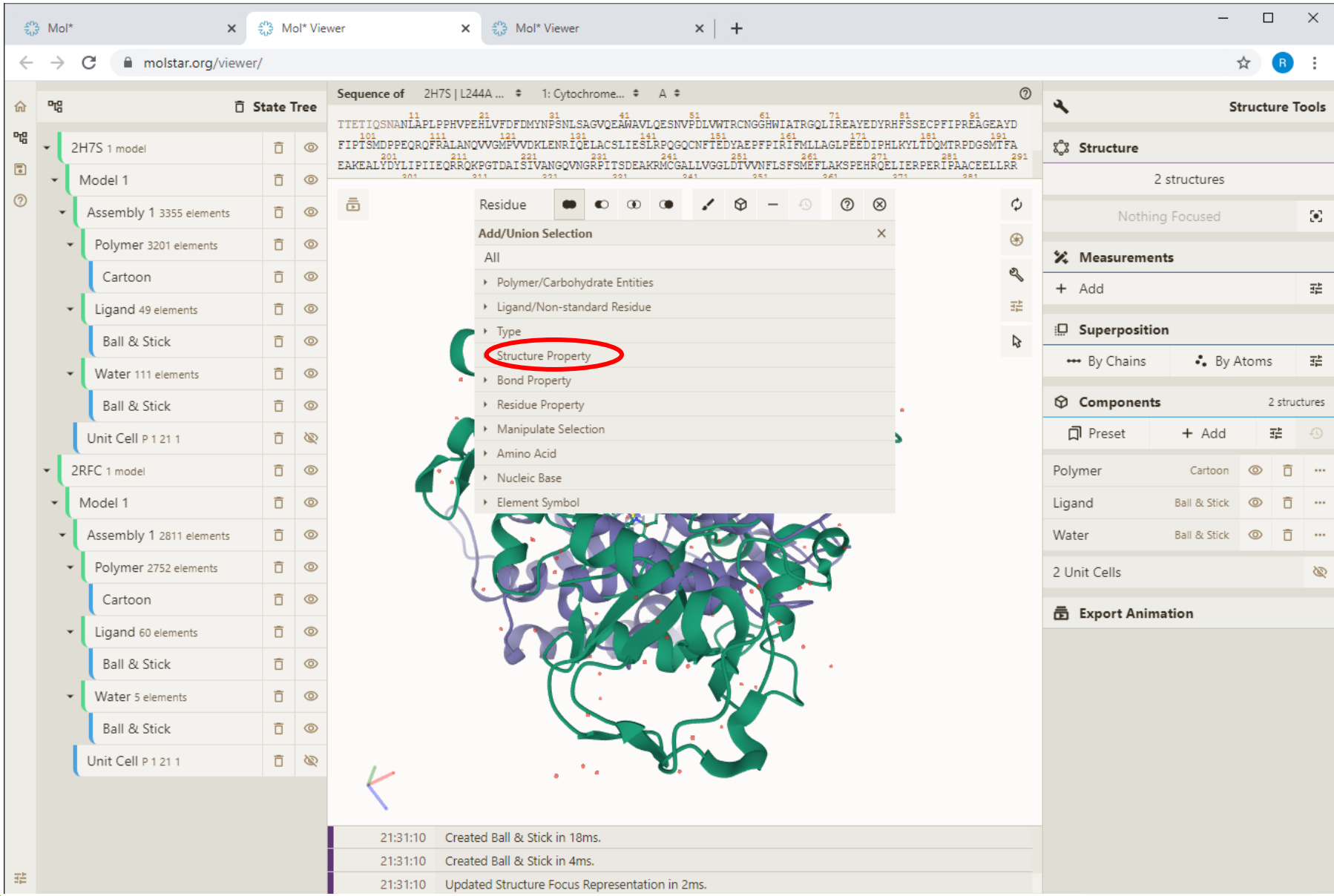


Přikládání struktur

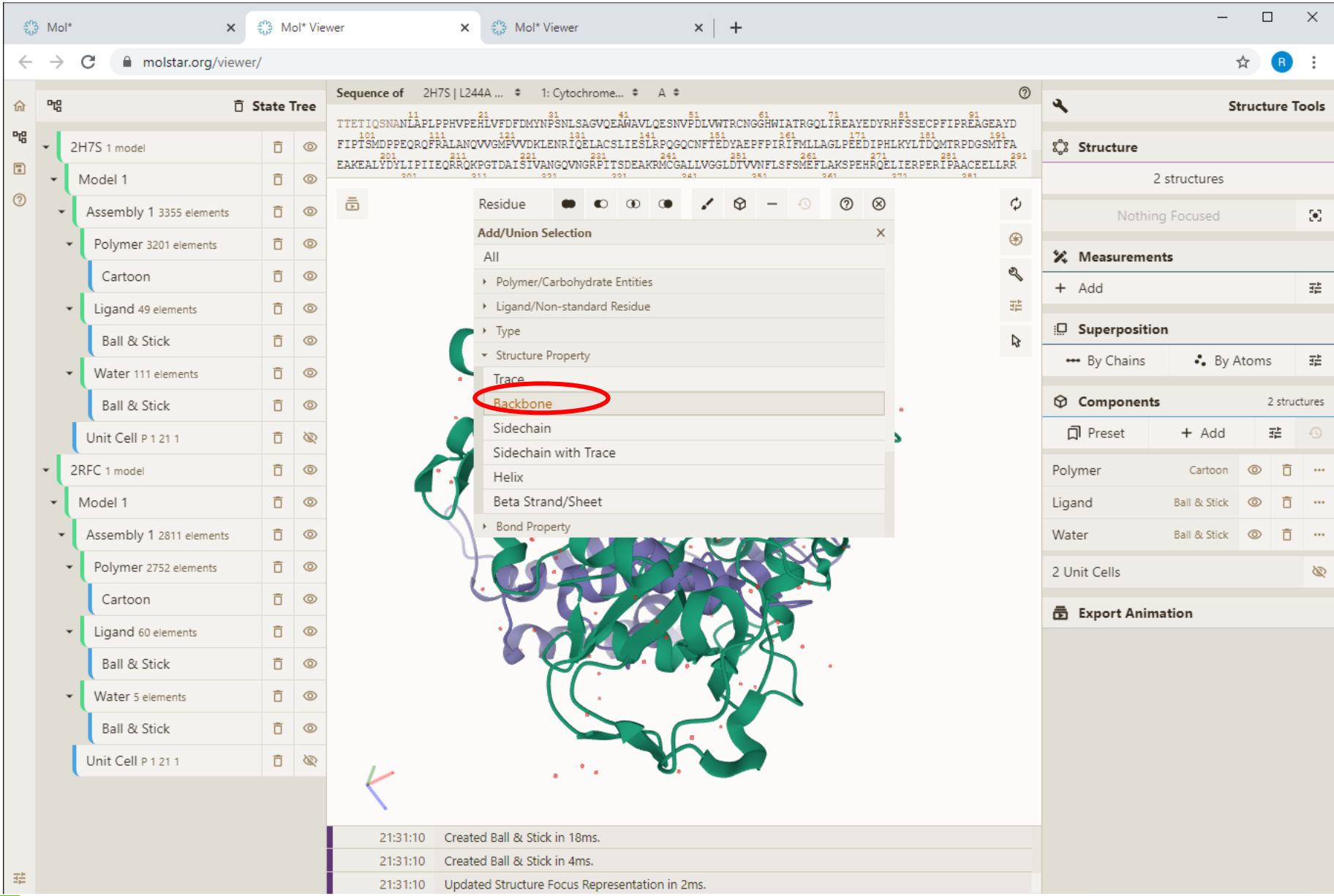


CEITEC

Přikládání struktur

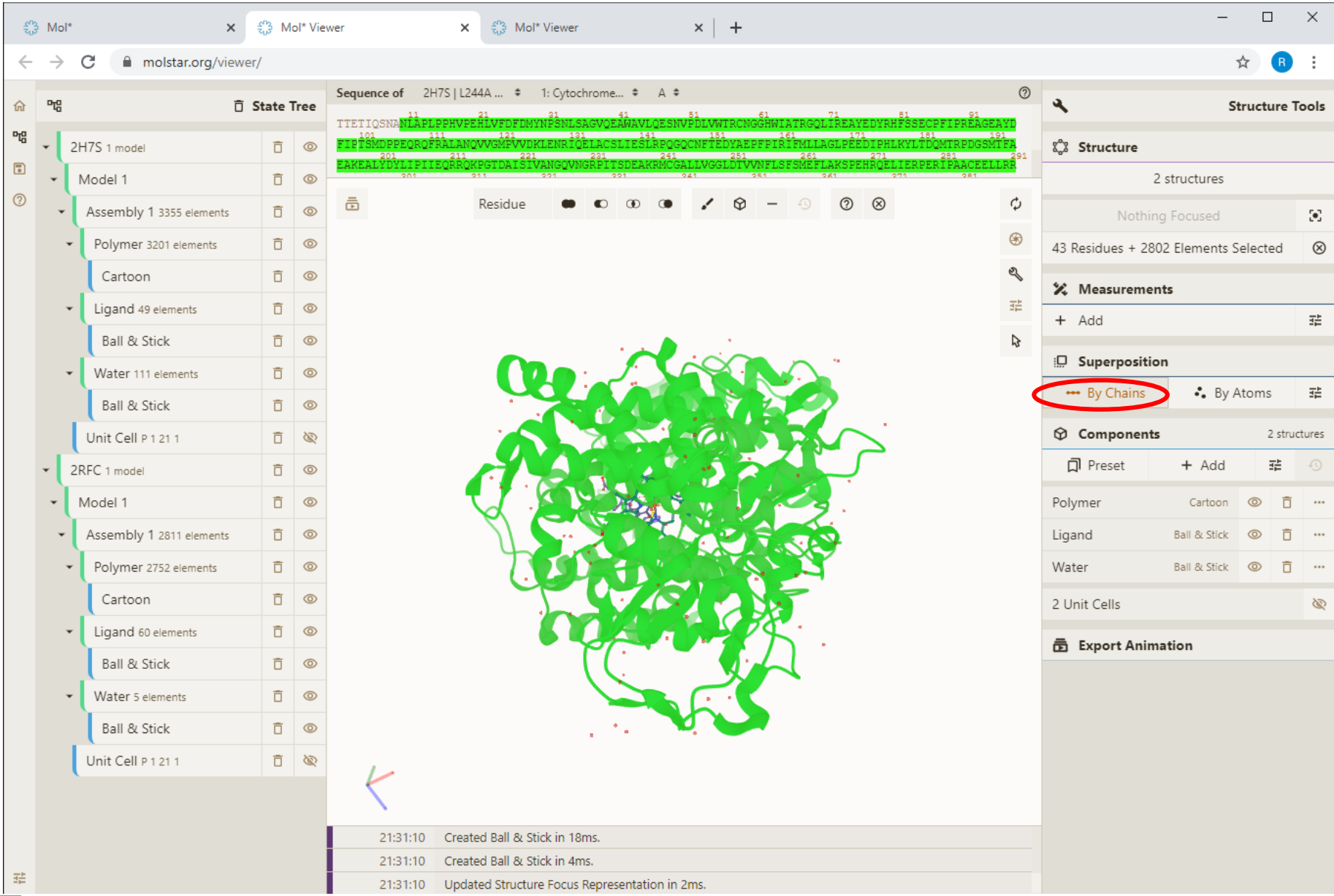


Přikládání struktur



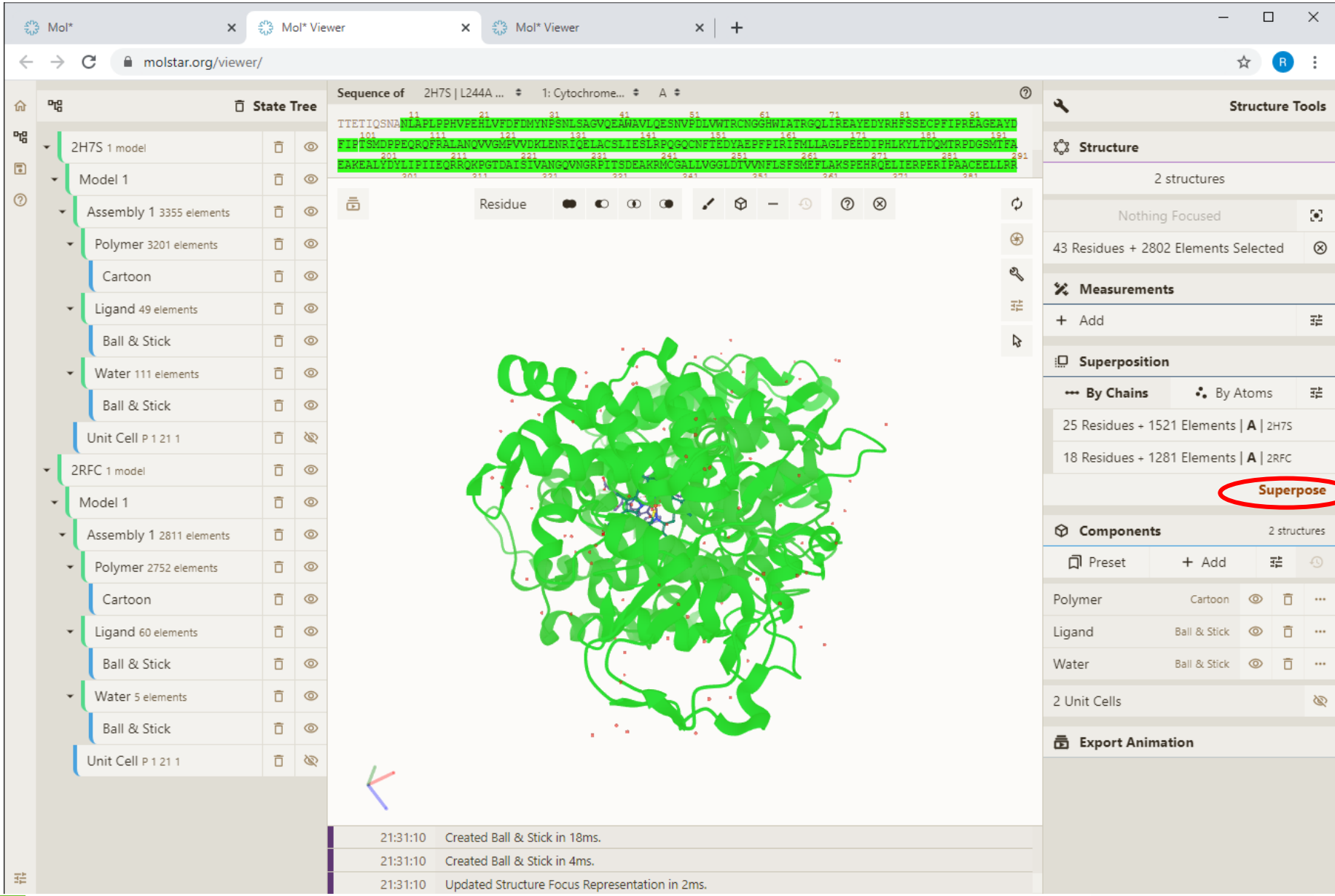
CEITEC

Přikládání struktur



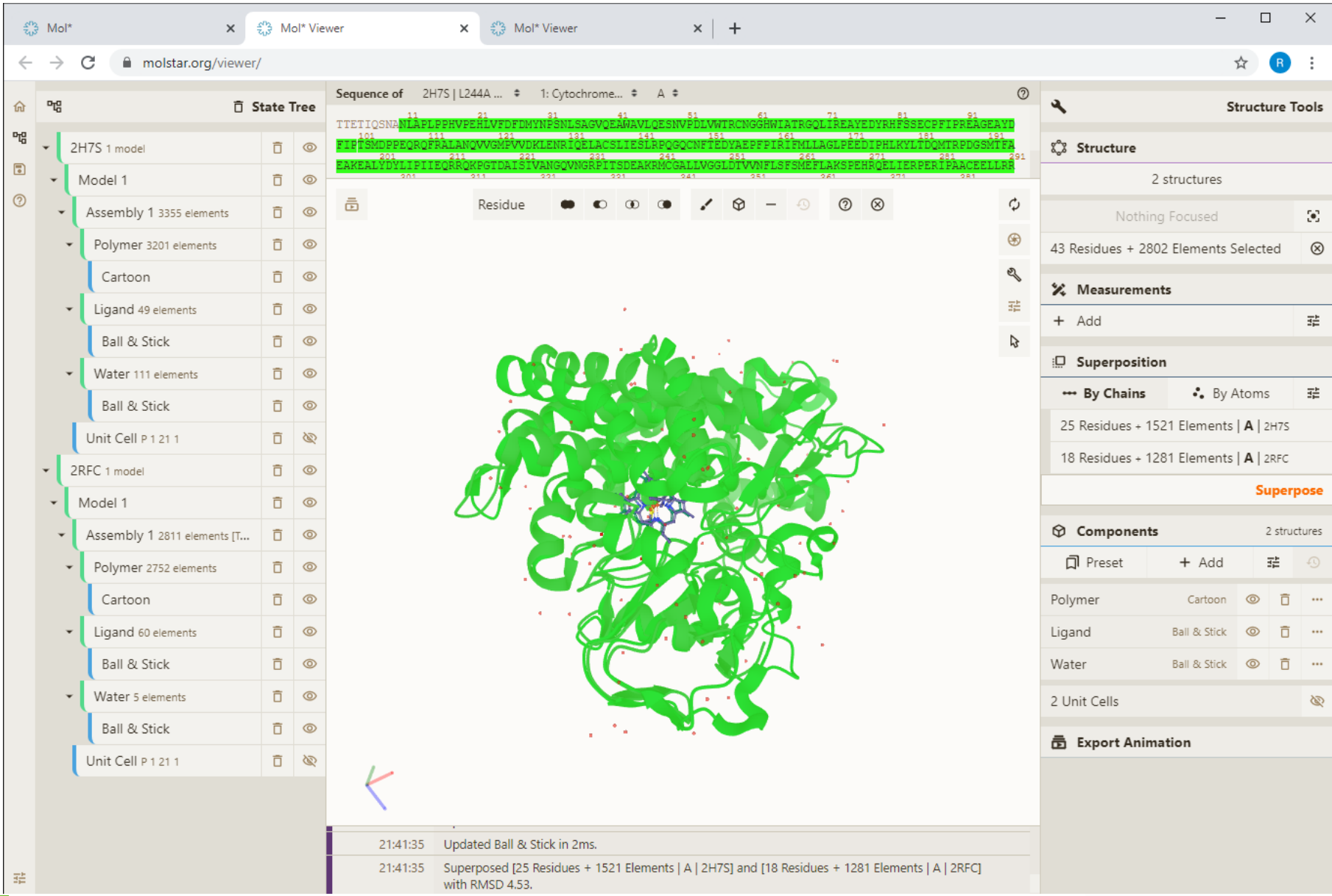
CEITEC

Přikládání struktur



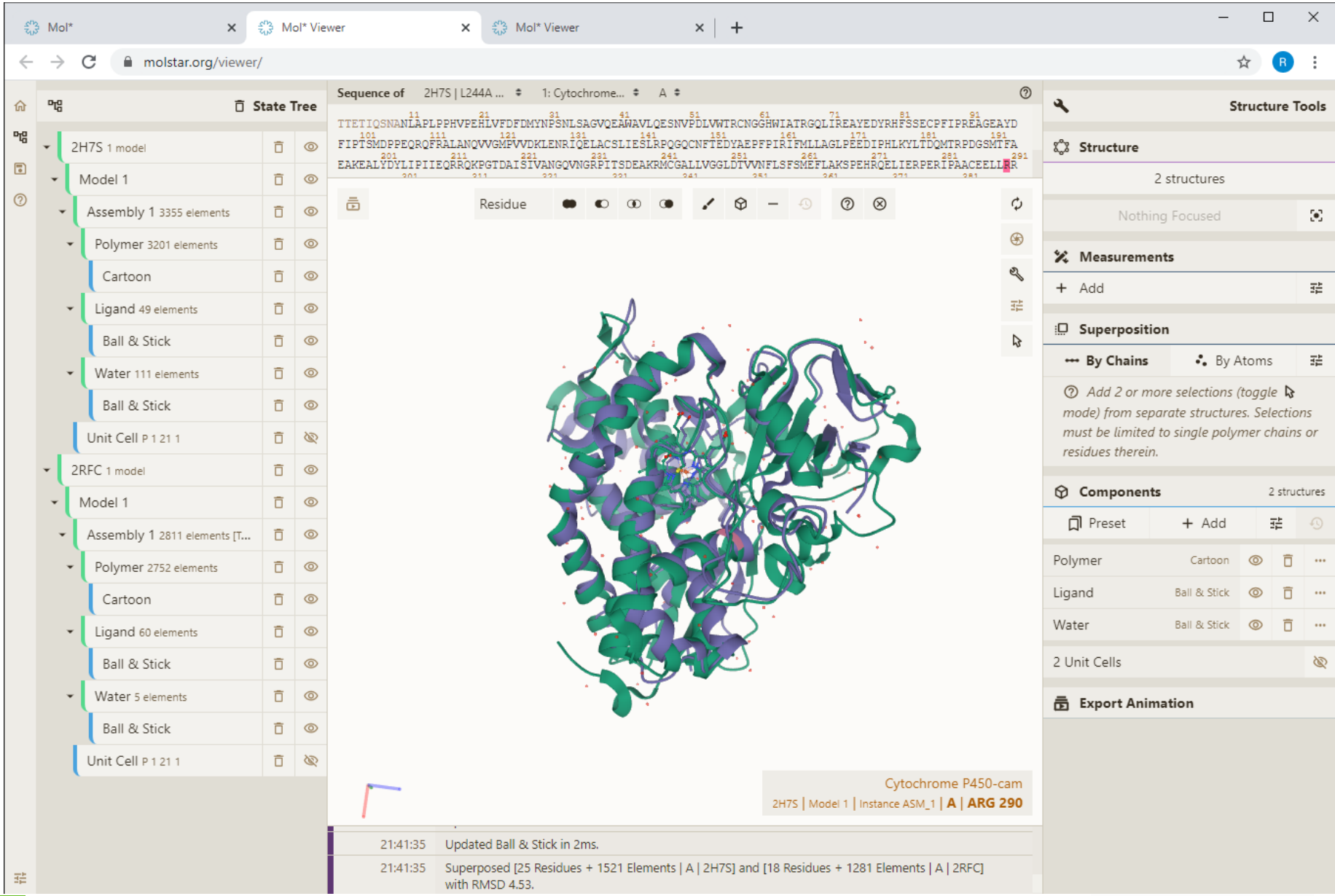
CEITEC

Přikládání struktur



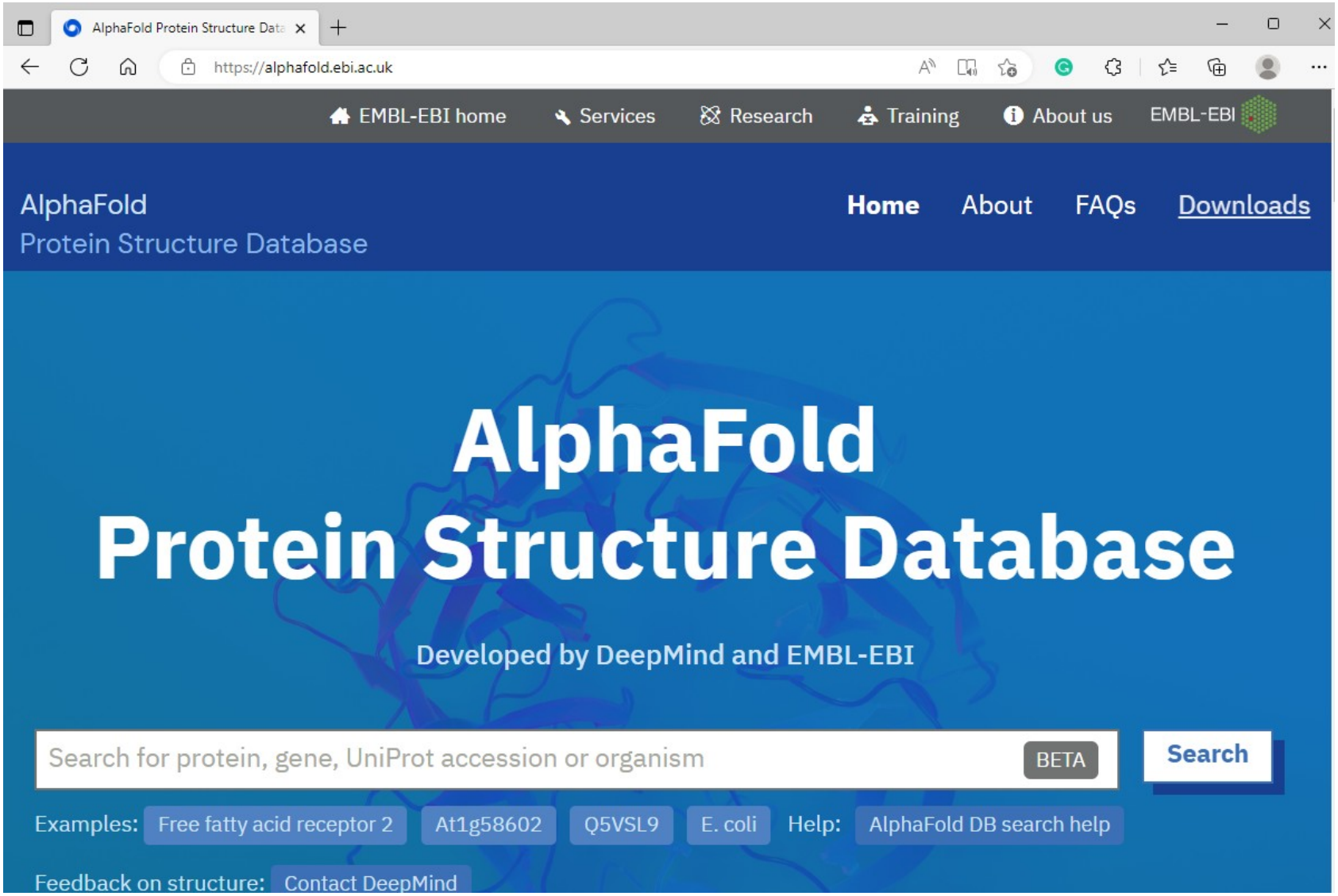
CEITEC

Přikládání struktur

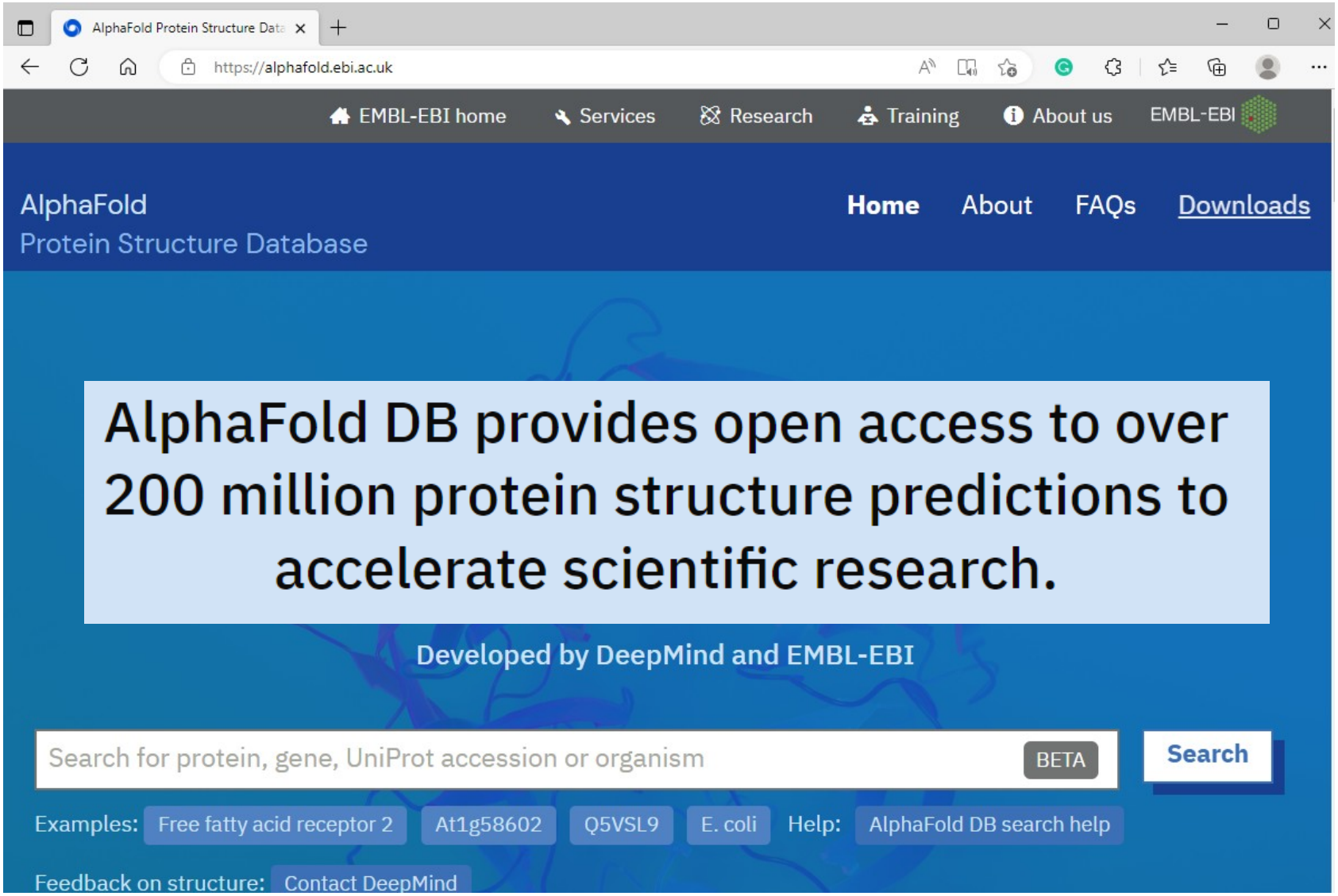


CEITEC

2DProts: Integration of AlphaFoldDB



2DProts: Integration of AlphaFoldDB



Přikládání struktur – PDB a AlphaFold

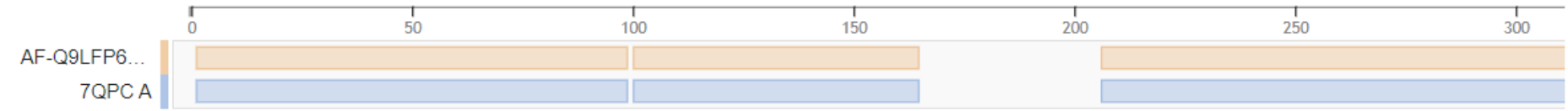
Pairwise Structure Alignment

Help

▸ Compare Protein Structures

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

SEQUENCE ALIGNMENT SCORES



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

CEITEC

Přikládání struktur – PDB a AlphaFold