Swiss Institute of Bioinformatics

DAY 1, PART 6

Visualisation of structures with Mol*

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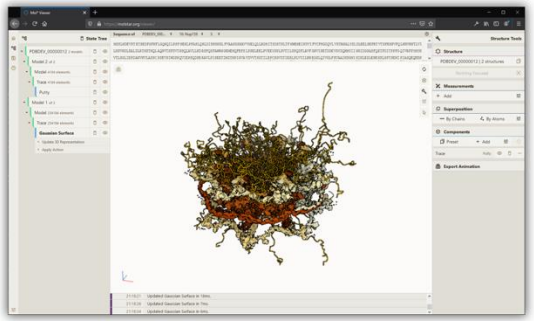
Mol* introduction

Mol* website – molstar.org

Alternatively, use **PyMOL** or **Chimera**

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



Open Mol* Viewer

Viewer Documentation

Issues & Feedback

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

The project is an open collaboration started by

PDBe Protein Data Bank in Europe

RCSB PDB PROTEIN DATA BANK

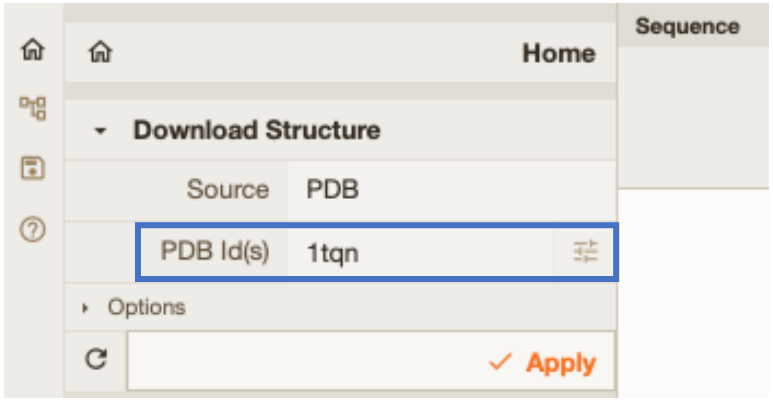
CEITEC central european institute of technology BRNO | CZECH REPUBLIC

elixir CZECH REPUBLIC

Let's get familiar with basic commands in Mol*

Go to Mol* Viewer and upload the suggested structure from the PDB

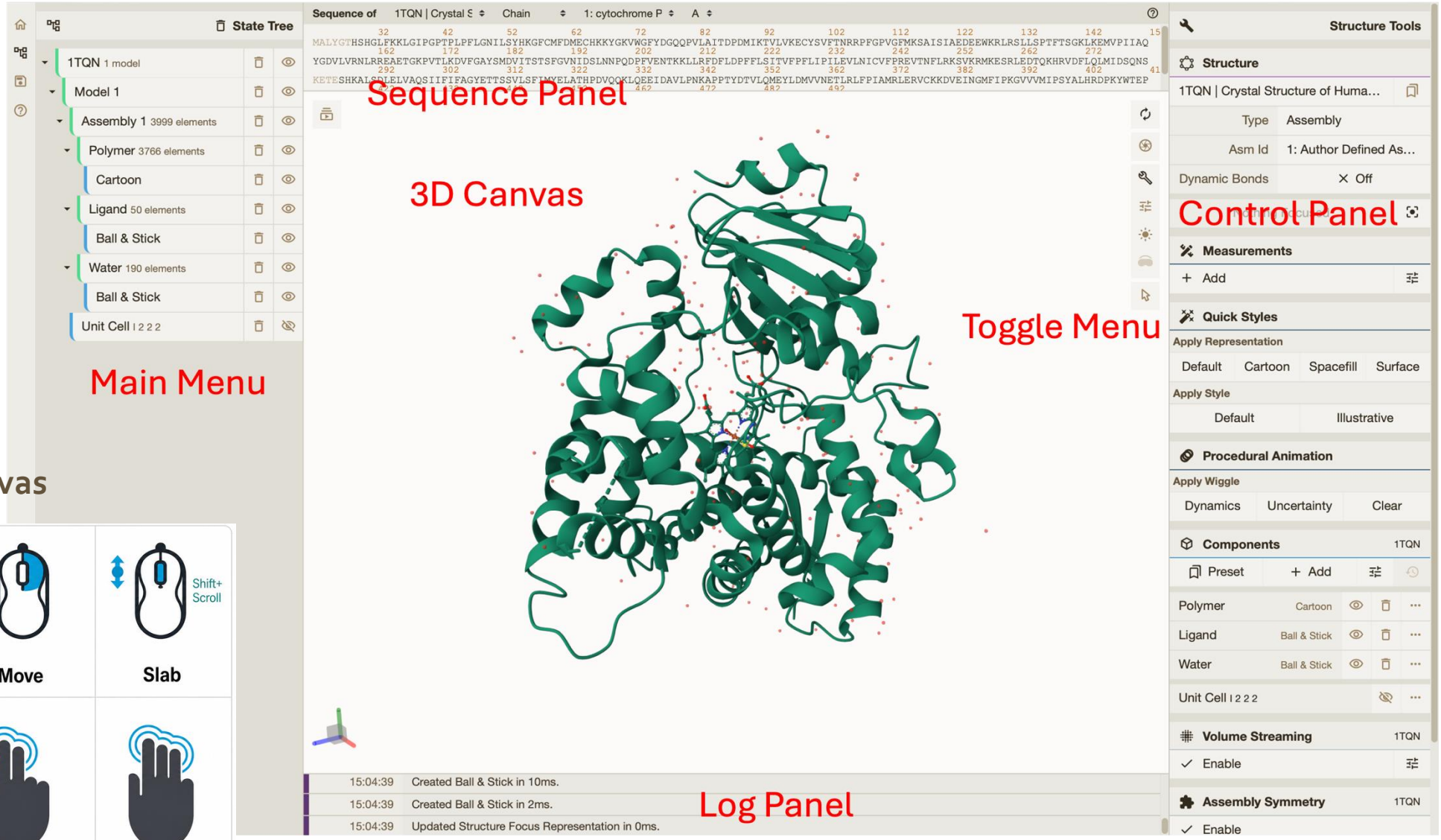
Mol* tutorial with the exercises are on the course website



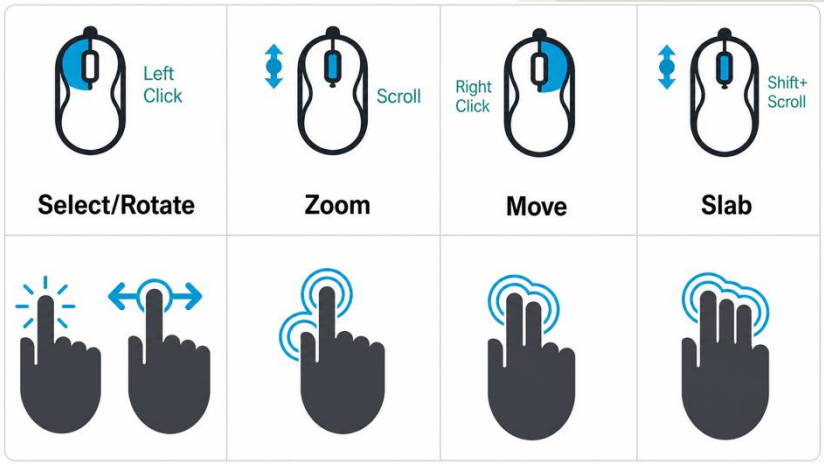
Mol* introduction

Reset View
Press *t*

Spin Animation
Press i
(to disable press i again)



To Navigate the 3D Canvas



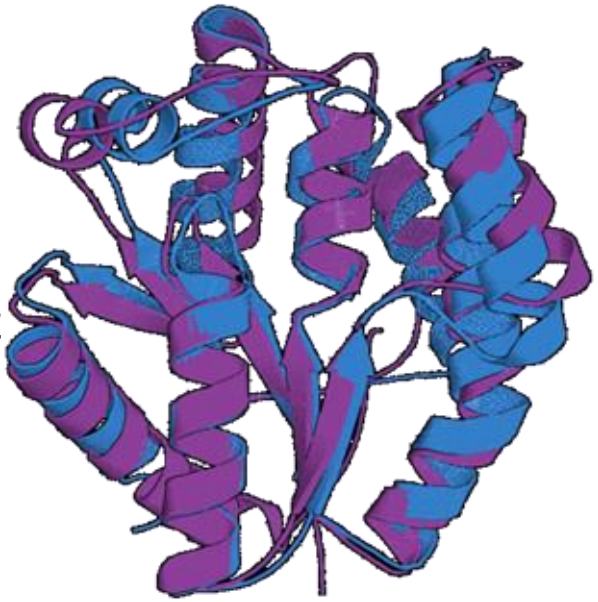
Structure Alignment

What is Structural Alignment?

Structure alignment establishes residue-residue correspondences between macromolecular structures based on optimal superposition of their 3D conformation

When is Structure Alignment useful?

- Structure is more conserved than sequence → alignment helps detect evolutionary relationships where sequence-based methods struggle due to low sequence identity
- Pairwise comparison reveals conformational changes upon ligand binding
- Analysis of structural variation within evolutionary families and identification of common structural domains
- Determining prediction quality



High structural similarity

PDB ids: 4S35,1NMY
TM-score: 0.82
Sequence identity: 28%

Structure Alignment

In Mol* there two options for structural alignment:

RMSD-based Superposition – rigidly rotates and translates one structure onto another to minimize the RMSD of paired atoms, sequence-guided

RMSD-score: good value ~2 Å or less, protein length dependent

TM-align Superposition – sequence-independent alignment algorithm

TM-score: protein length independent, only aligned residues included

Scores < 0.2 usually indicate that the proteins are unrelated while those >0.5 generally have the same protein fold

Mol* Exercises

Exercise 1 (together)

Superpose human myoglobin (PDB ID: **1MBO**) to one of the chains of hemoglobin (PDB ID: **4HHB**).

Exercise 2

Superpose the best model for PIGU protein to PIGU protein in the glycosylphosphatidylinositol (GPI) transamidase complex (PDB ID: **7W72**)