CEITEC

Central European Institute of Technology

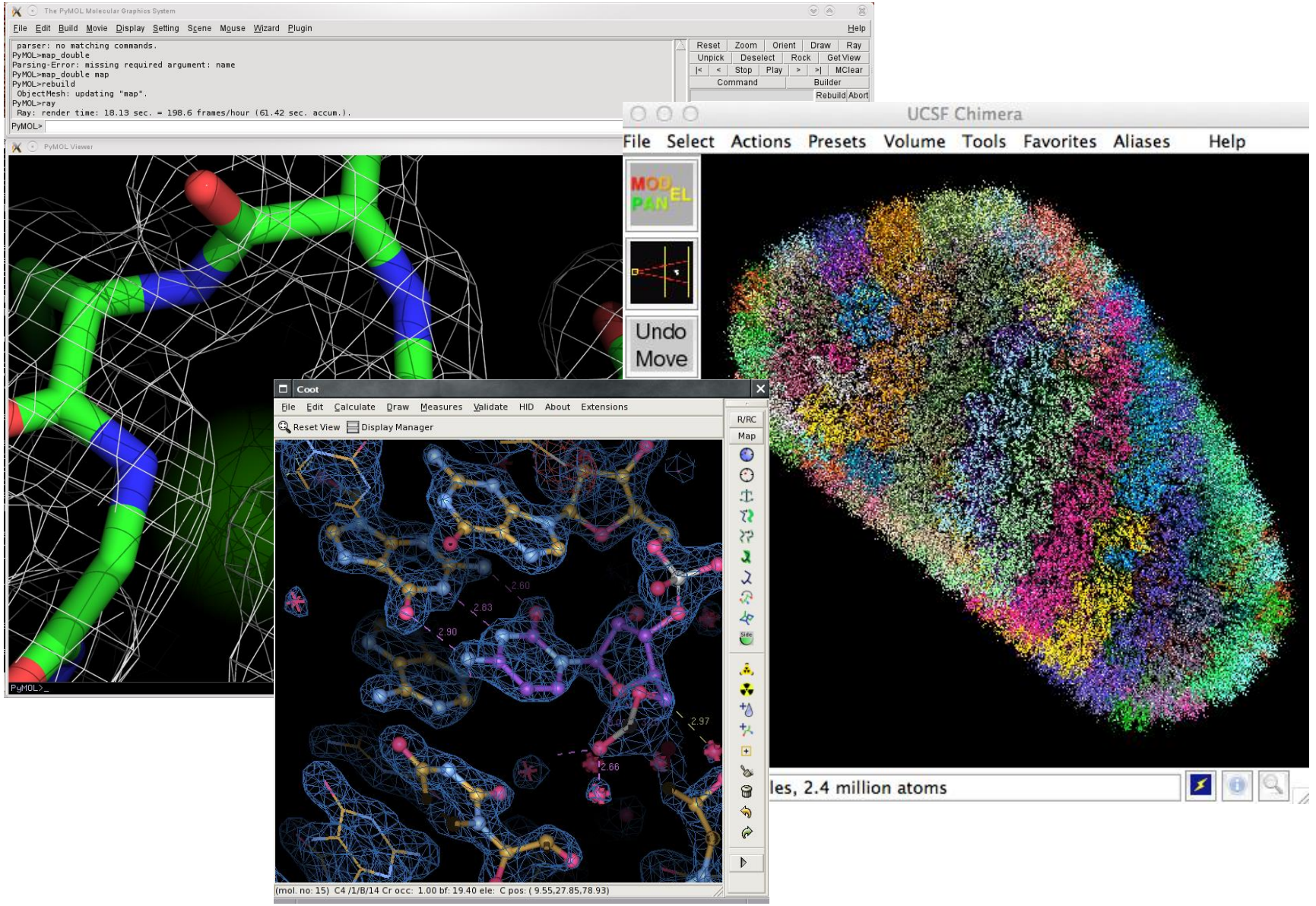
BRNO | CZECH REPUBLIC

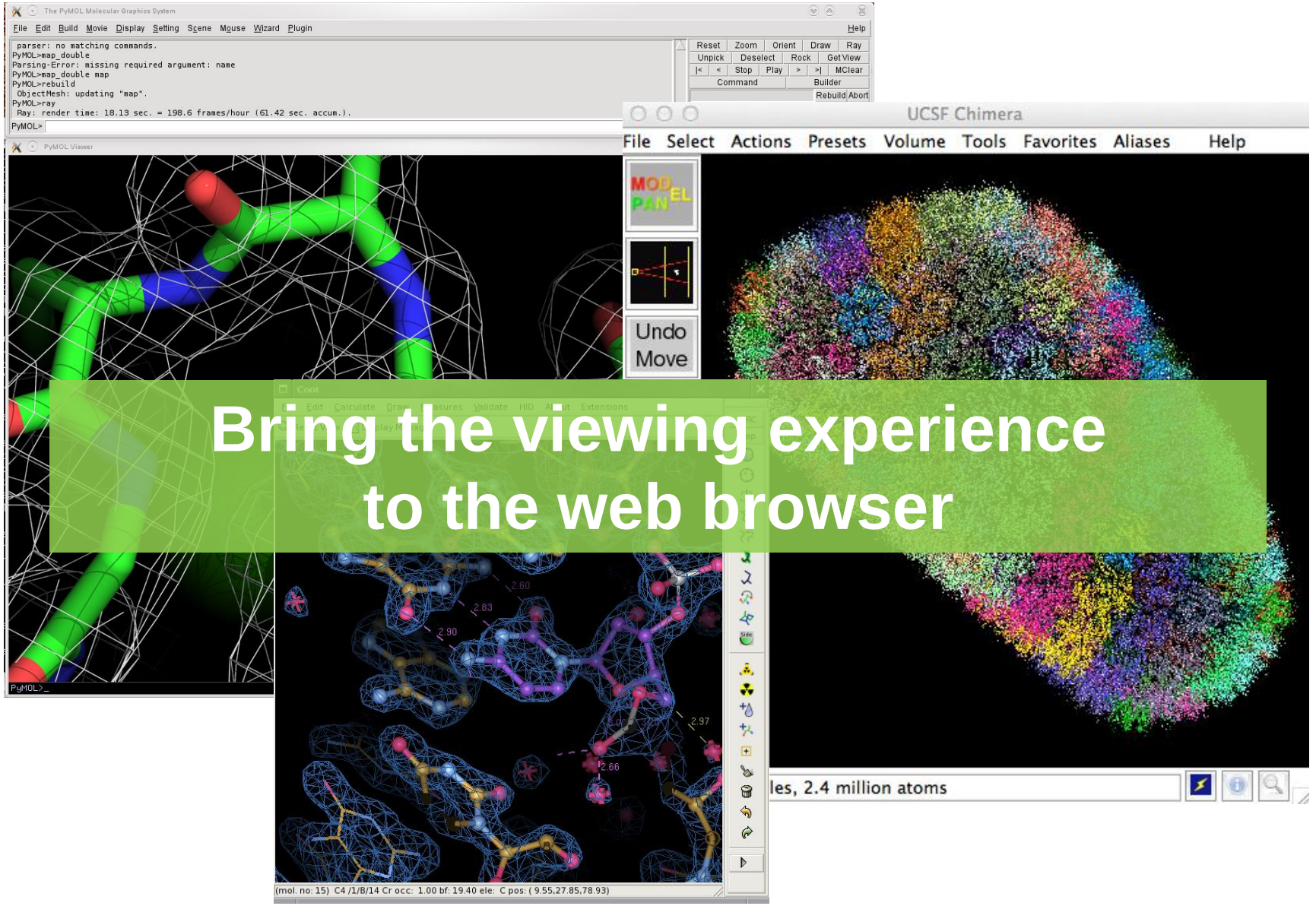
UNIVERSITAS MASARYKIANA BRUNENSIS

LiteMol suite – real-time web-based visualization of large macromolecular structural data

PDBe

Protein Data Bank in Europe


The PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help
parser: no matching commands.
PyMOL>map_double
Parsing-Error: missing required argument: name
PyMOL>map_double map
PyMOL>rebuild
ObjectMesh: updating "map".
PyMOL>ray
Ray: render time: 18.13 sec. = 198.6 frames/hour (61.42 sec. accum.).
PyMOL>
Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
Stop Play MClear
Command Builder
Rebuild Abort
PyMOL Viewer
PyMOL>_
UCSF Chimera
File Select Actions Presets Volume Tools Favorites Aliases Help
MODEL PANEL
Undo
Move
les, 2.4 million atoms
Coot
File Edit Calculate Draw Measures Validate HID About Extensions
Reset View
Display Manager
R/RC
Map
2.60
2.83
2.90
2.97
2.66
(mol. no: 15) C4 /1/B/14 Cr occ: 1.00 bf: 19.40 ele: C pos: (9.55,27.85,78.93)



Bring the viewing experience to the web browser

pdbe.org & ncbr.muni.cz/LiteMol

PDBe CEITEC

PDB

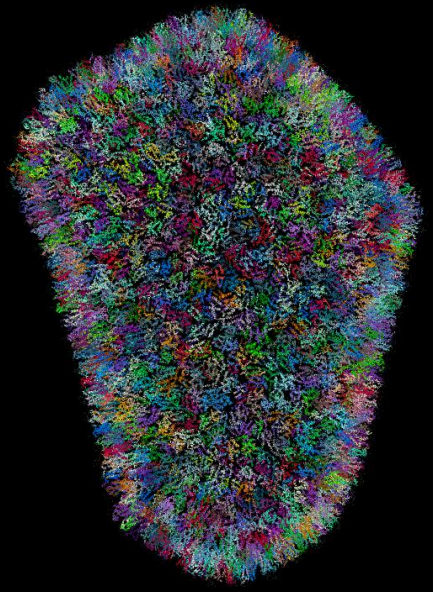
125k entries, +10% per year

Big entries:

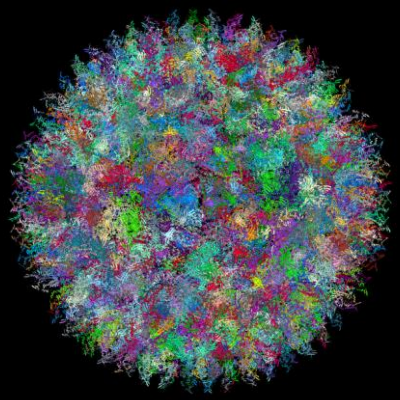
- HIV-1 capsid (3j3q), 2.4M atoms
- Aquareovirus virion (3k1q) assembly, 6M atoms

More large systems will be resolved: ribosomes, viruses, etc.

HIV-1 capsid



Aquareovirus virion



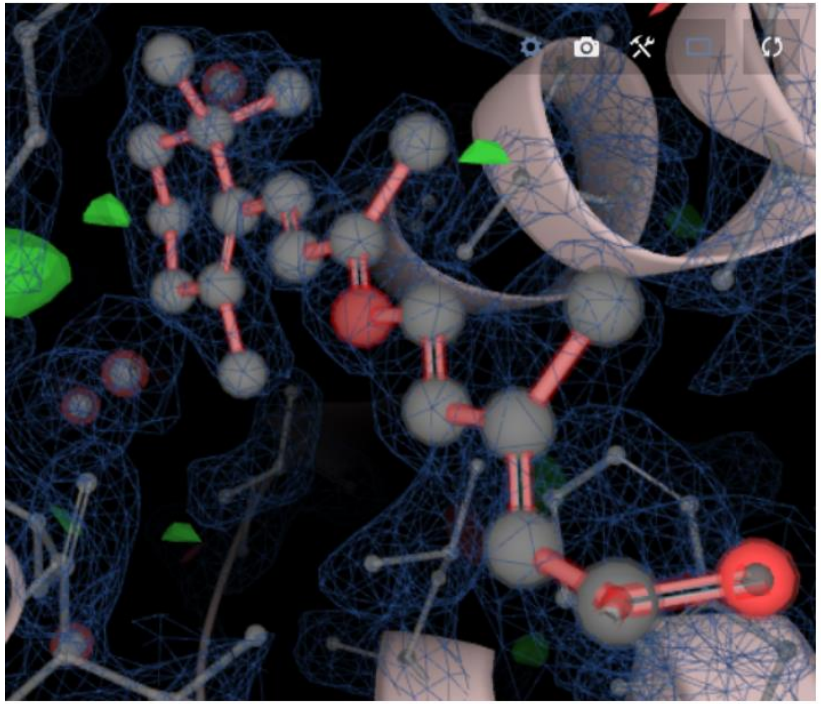
EMBL-EBI

Protein Data Bank in Europe
Bringing Structure to Biology

PDBe home | Deposition | PDBe services | PDBe training | Documentation | About PDBe

About PDBe > News > Exciting visualisation update

Exciting visualisation update



17 August 2016

PDBe is excited to announce some major new updates to our pages at pdbe.org We now have a new, streamlined 3D viewer (LiteMol) that enables visualisation of electron density in the browser with interactive changing of contour levels. For instance, check out retinoic acid in entry 1cbs.

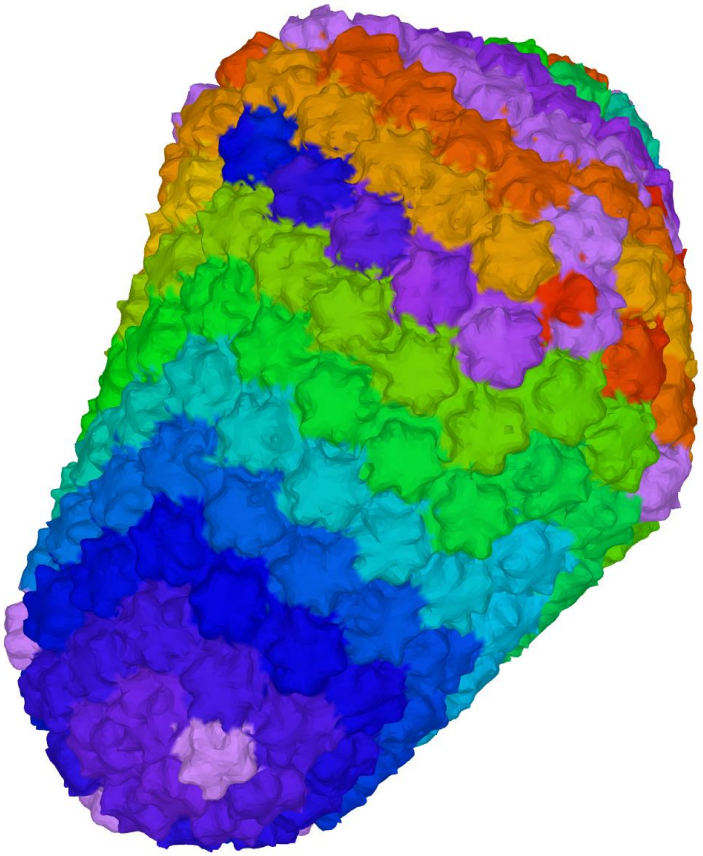
The viewer also has options to view domain annotations (UniProt, CATH SCOP, Pfam, Interpro) and validation information from the wwPDB validation reports - see the annotations for entry 1cbs by clicking the hammer/spanner icon and selecting options in 'Domain Annotation'.

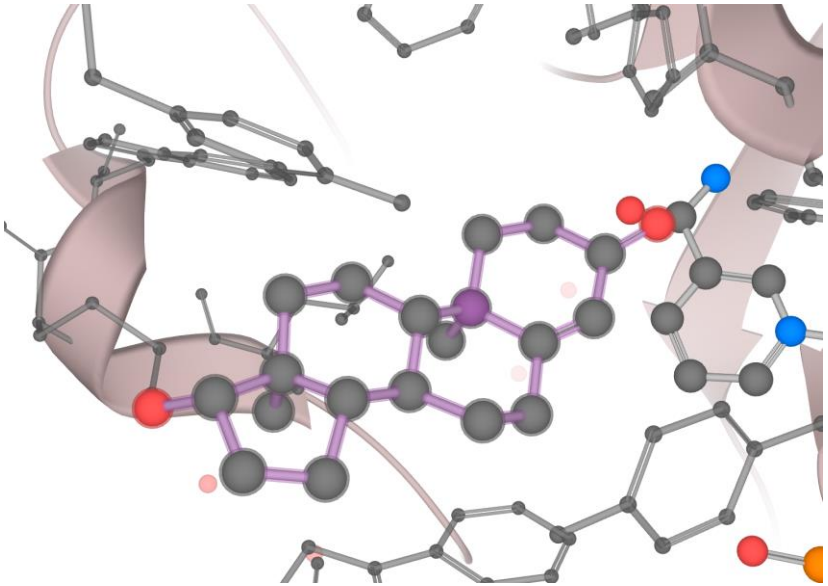
To see all the PDB entries for a given UniProt see "UniProt Coverage Viewer" on the same page.

Initial feedback on the viewer is positive: one user describing it as "Superb 3D performance... you can visualize electron density in the browser as well as or better than molecular graphics programs. It works just as well on my ipad: it is amazing!"

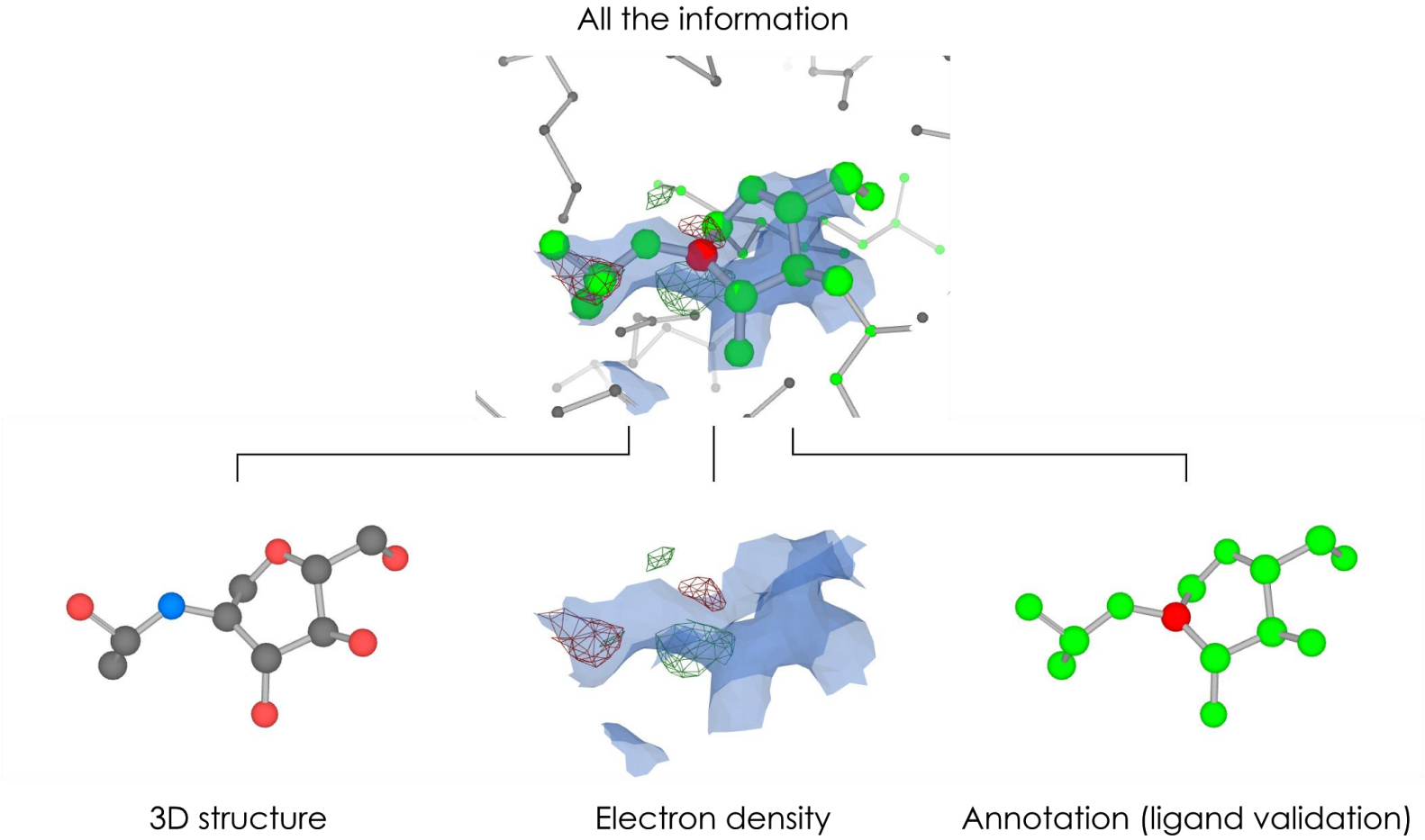
LiteMol is developed by David Sehnal at CEITEC and Mandar Deshpande at PDBe

ENTIRE STRUCTURE or an INTERESTING PART





MODEL, EXPERIMENTAL DATA, and ANNOTATION



Data delivery
takes a long time

Visualization
is computationally demanding

User interaction
must be pleasant

The solution is obvious…

Send only the relevant data

Compress

LiteMol suite

3D coordinate data

Experimental data (density)

Annotation API

Data compression

Visualization

VISUALIZATION

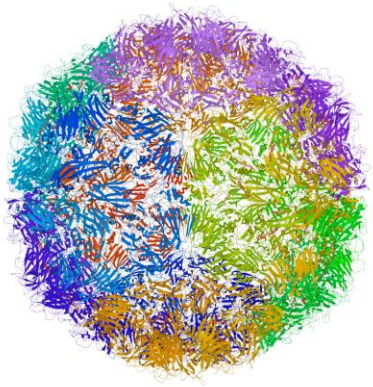
LiteMol Viewer

pdbe.org & ncbr.muni.cz/LiteMol

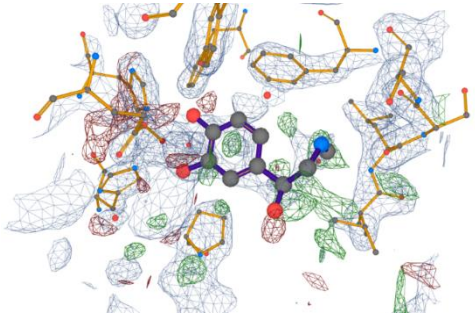
PDBe CEITEC

LiteMol

Web browser based 3D visualization plugin



Common 3D atomic models, assemblies, symmetry

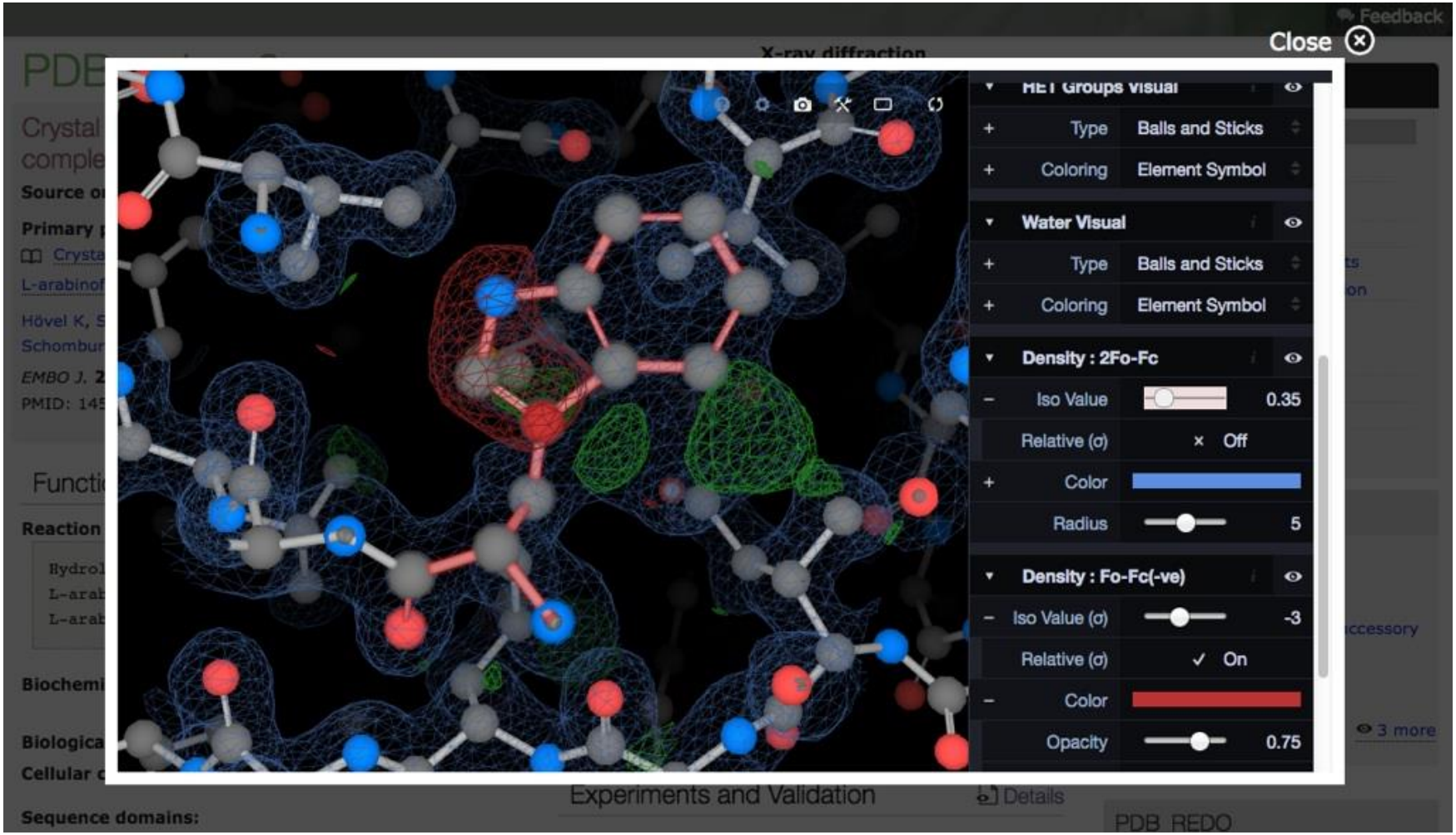


Density maps and Cryo-EM data

Validation data, sequence annotation

…and it's ***fast***

LiteMol in PDBe



pdbe.org/1qrw (3D visualization)

DATA DELIVERY

Coordinate Server

CoordinateServer

On-demand 3D molecular structure

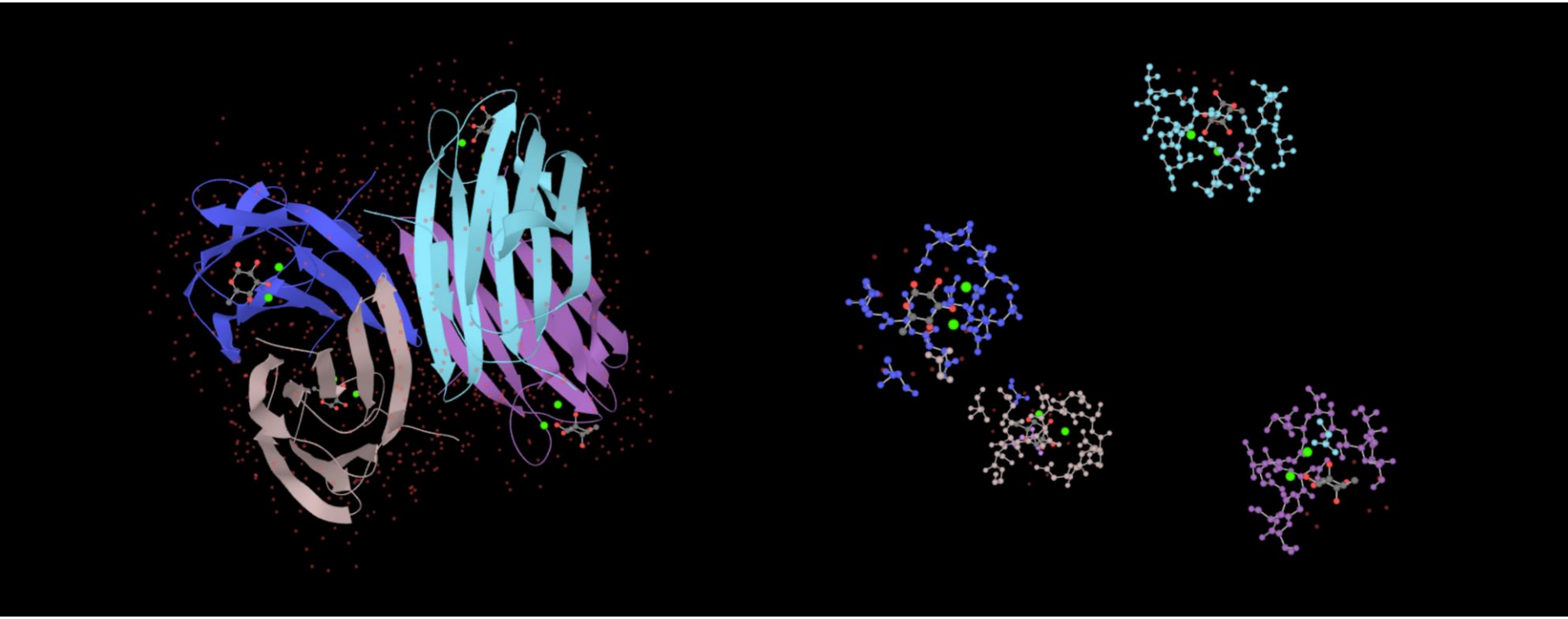
- backbone, individual entities or chains
- ligand interactions
- assemblies, symmetry mates

Coordinate Server

CoordinateServer

https://www.ebi.ac.uk/pdbe/coordinates

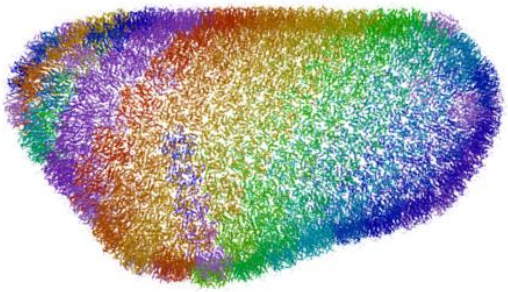
/1gzt/ligandInteraction?name=**FUC**



BinaryCIF

- **An efficient way of storing macromolecules and other data**
- Compatible with the mmCIF standard

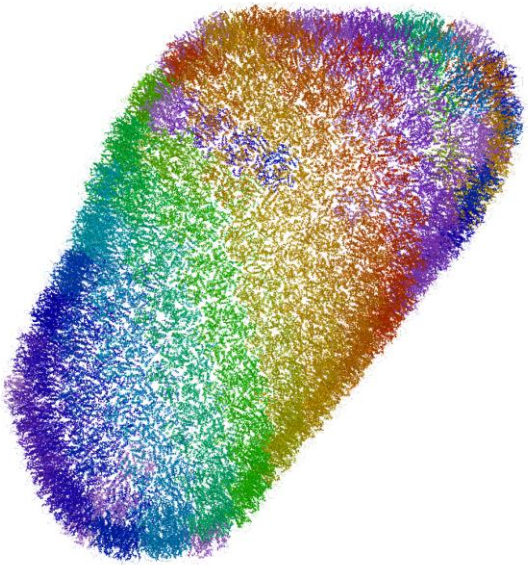
42MB CIF



1.5-12MB

BinaryCIF

Example: Delivery of HIV-1 capsid

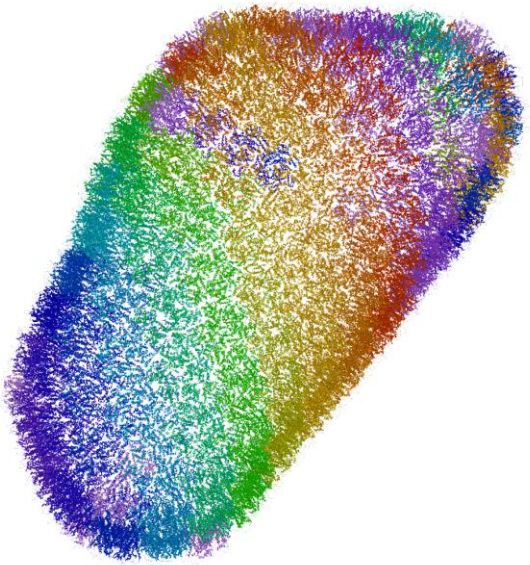


HIV-1 capsid, 2.44M atoms
(PDB ID 3j3q)

Download + Visualization time:

- Full (42 MB):
  - 60s

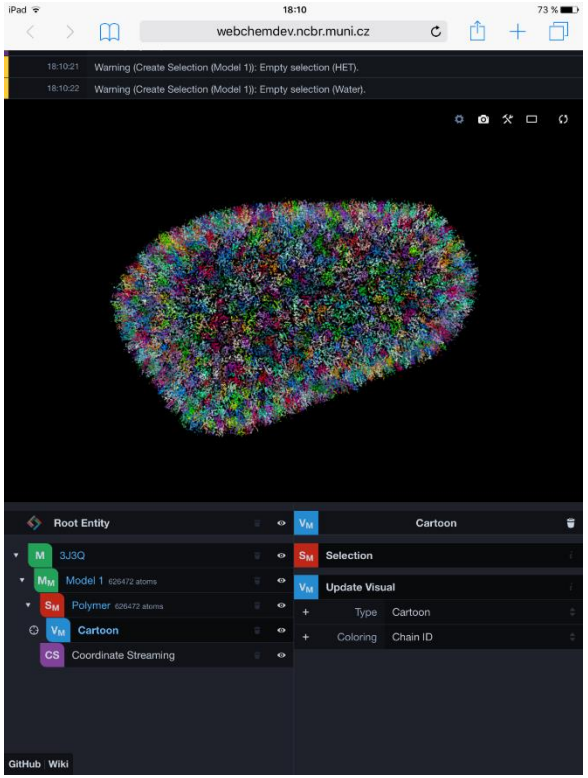
Example: Delivery of HIV-1 capsid

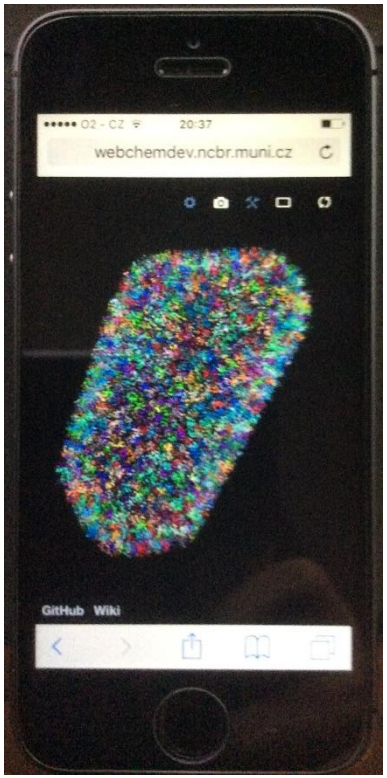


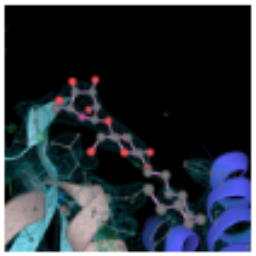
HIV-1 capsid, 2.44M atoms
(PDB ID 3j3q)

Download + Visualization time:

- Full (42 MB):
  - 60s
- **Coordinate Server + BinaryCIF**
  (0.6M atoms, 1.5 MB)**:**
  - **10s**
  - **27x less data**



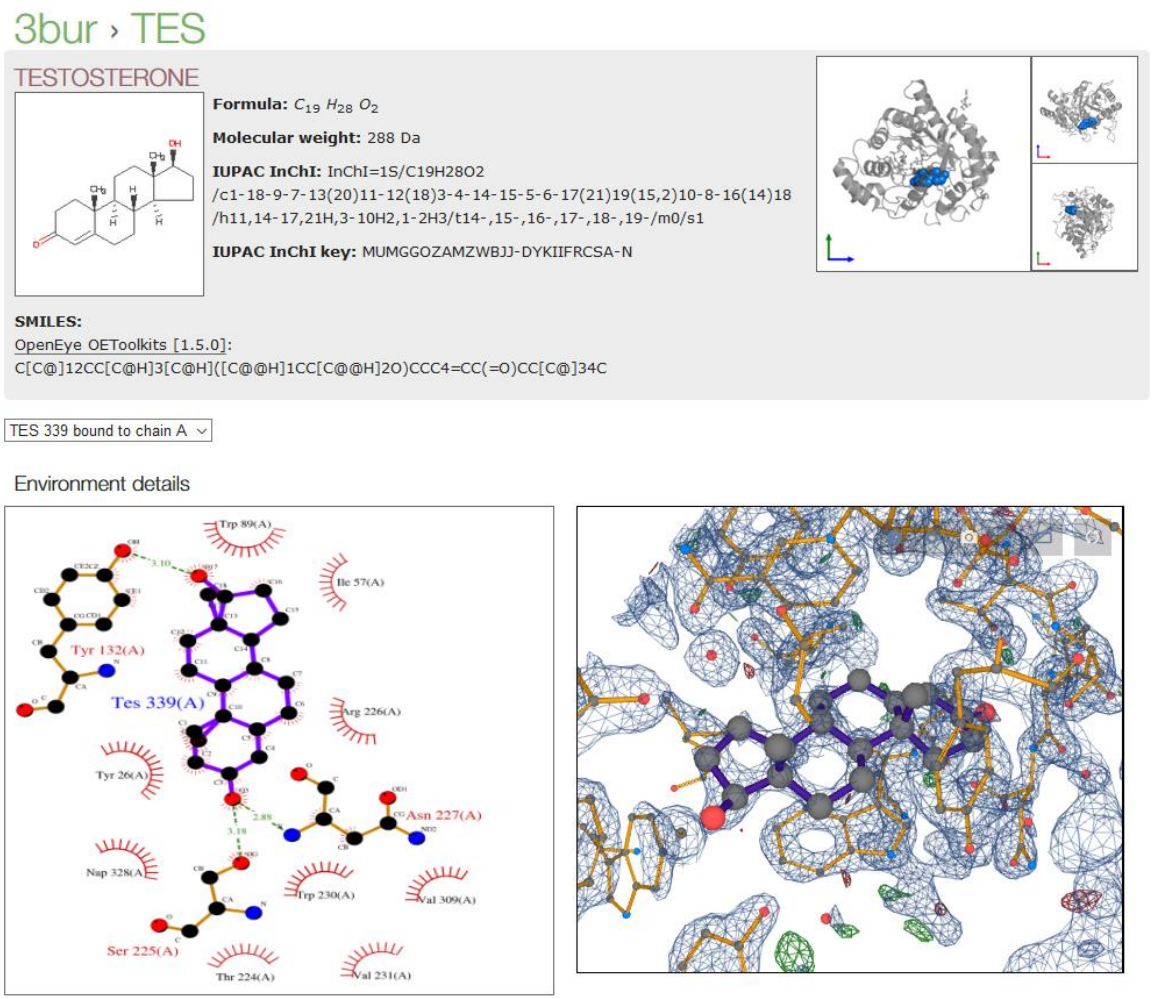




Hari Jay @harijay

@PDBeurope I finally believe tablets can be used for structure browsing. Amazed at how well the Lite Molecular viewer works on Ipad

PDBe Ligand Pages



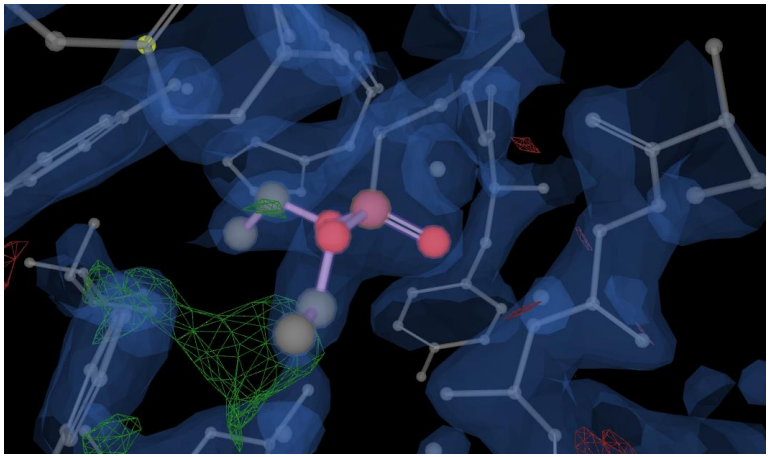
www.ebi.ac.uk/pdbe/entry/pdb/3bur/bound/TES

EXPERIMENTAL DATA

DensityServer

DensityServer

- **On-demand experimental data**
  - *Instantly* access any slice of available density
- **Uses the BinaryCIF format**
- **Works in a way similar to the CoordinateServer**

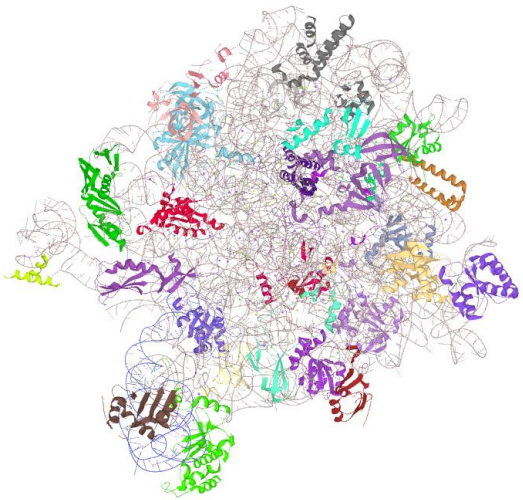


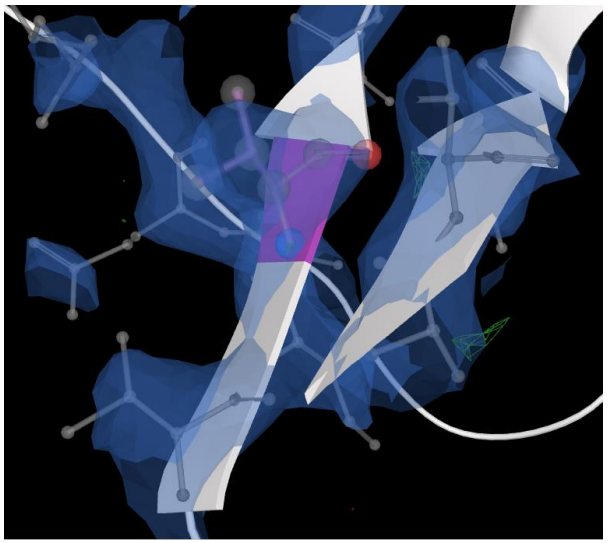
DensityServer Example

DensityServer

Fully Refined Crystal Structure of the Haloarcula marismortui Large Ribosomal Subunit at 2.4 Å Resolution (X-ray, PDB id 1JJ2)

- **145MB** of CCP4 density data, **10+s latency**
- 5Å around any residue: **10-30KB, 150ms latency**



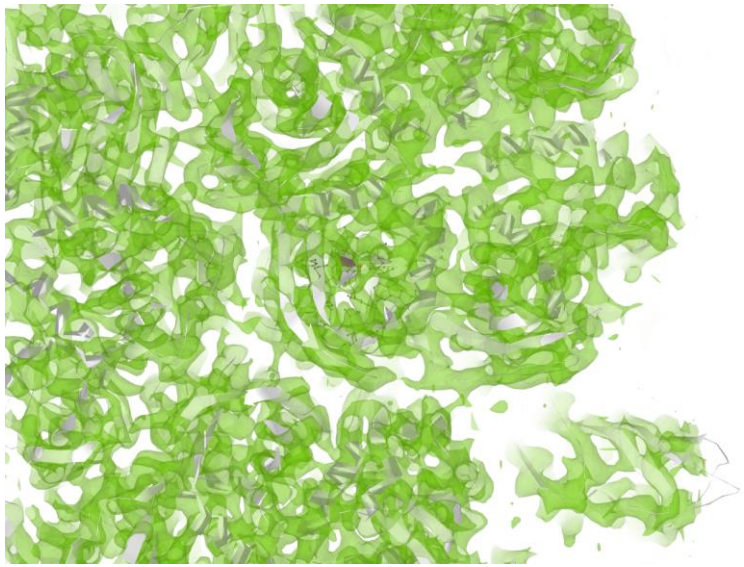


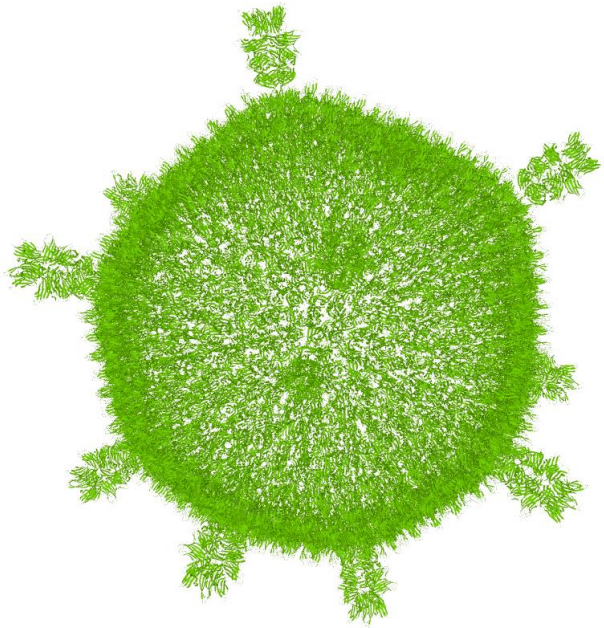
DensityServer Example

DensityServer

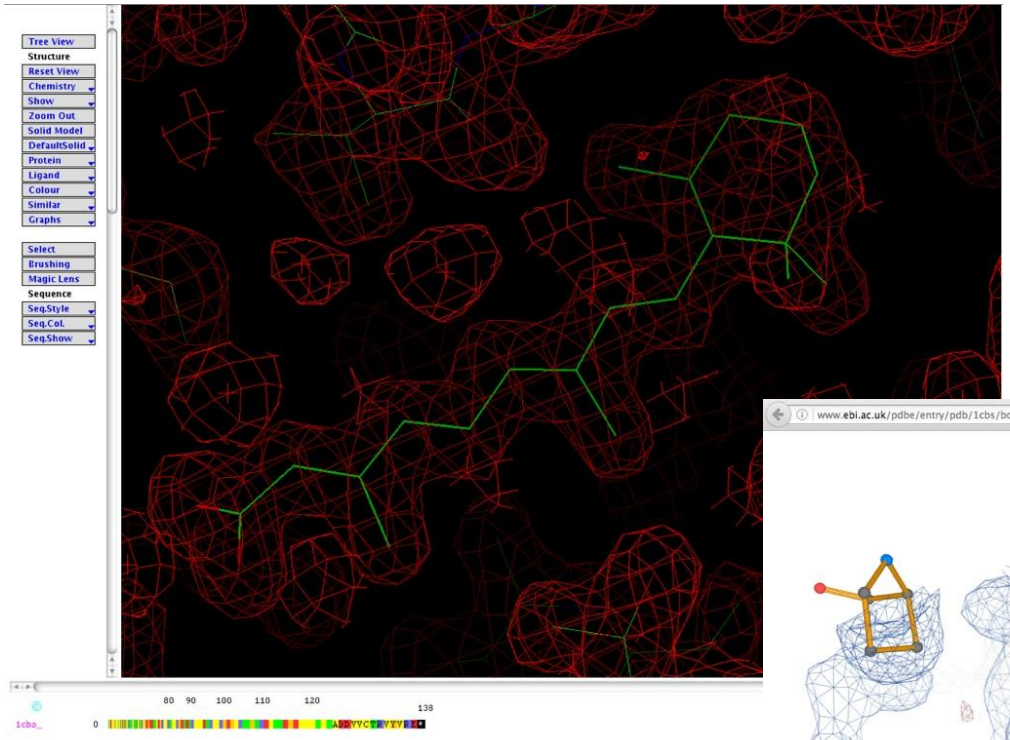
Life in the extremes: atomic structure of Sulfolobus Turreted Icosahedral Virus (2.7M atoms, Cryo-EM, PDB id 3j31)

- **4GB** of CCP4 density data
- 50Å sphere anywhere: **400KB in <0.5s**

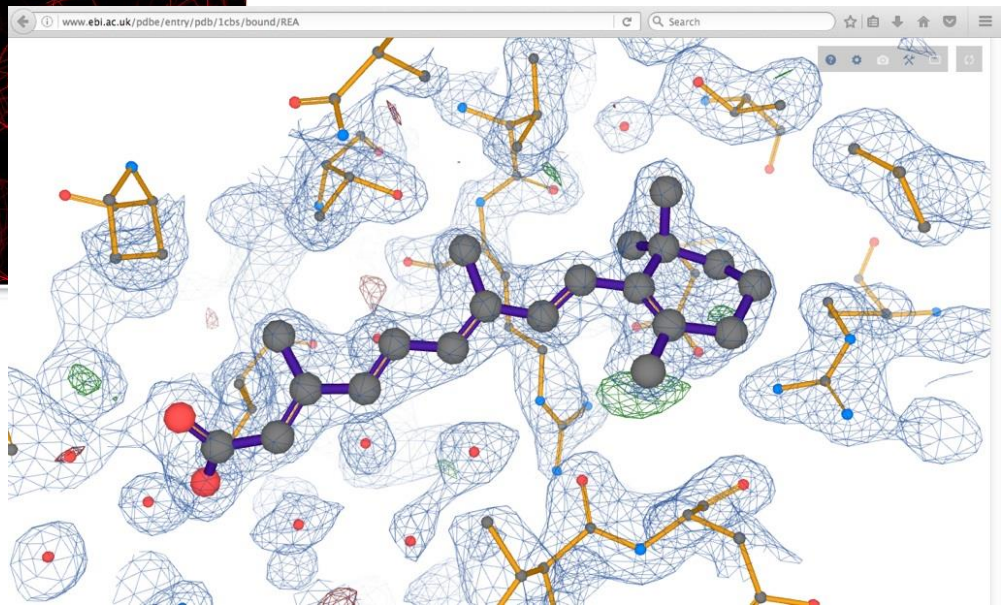




Uppsala Electron Density Server retired



AstexViewer (Java)



LiteMol

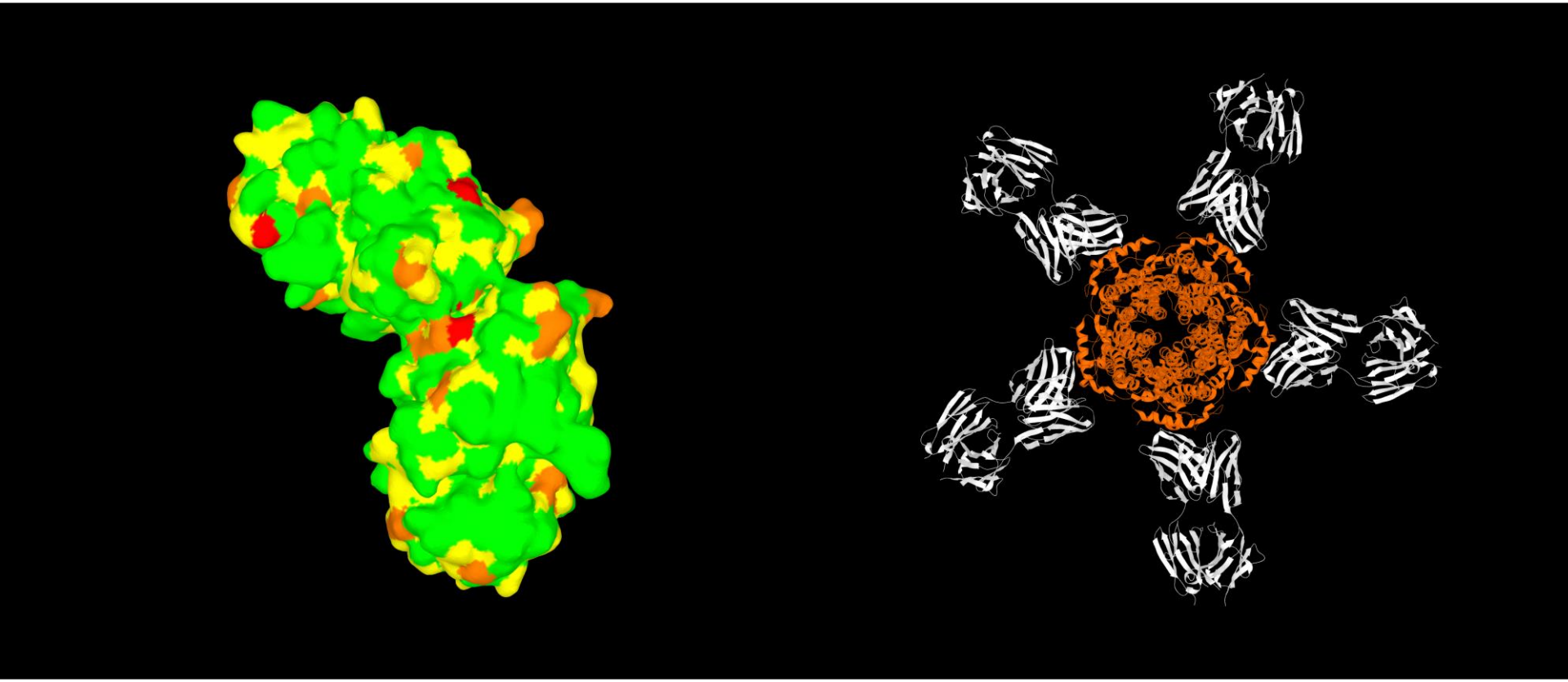
pdbe.org/eds

ANNOTATION

Validation and Sequence Annotation

Nipah Virus G Attachment Glycoprotein
3D12

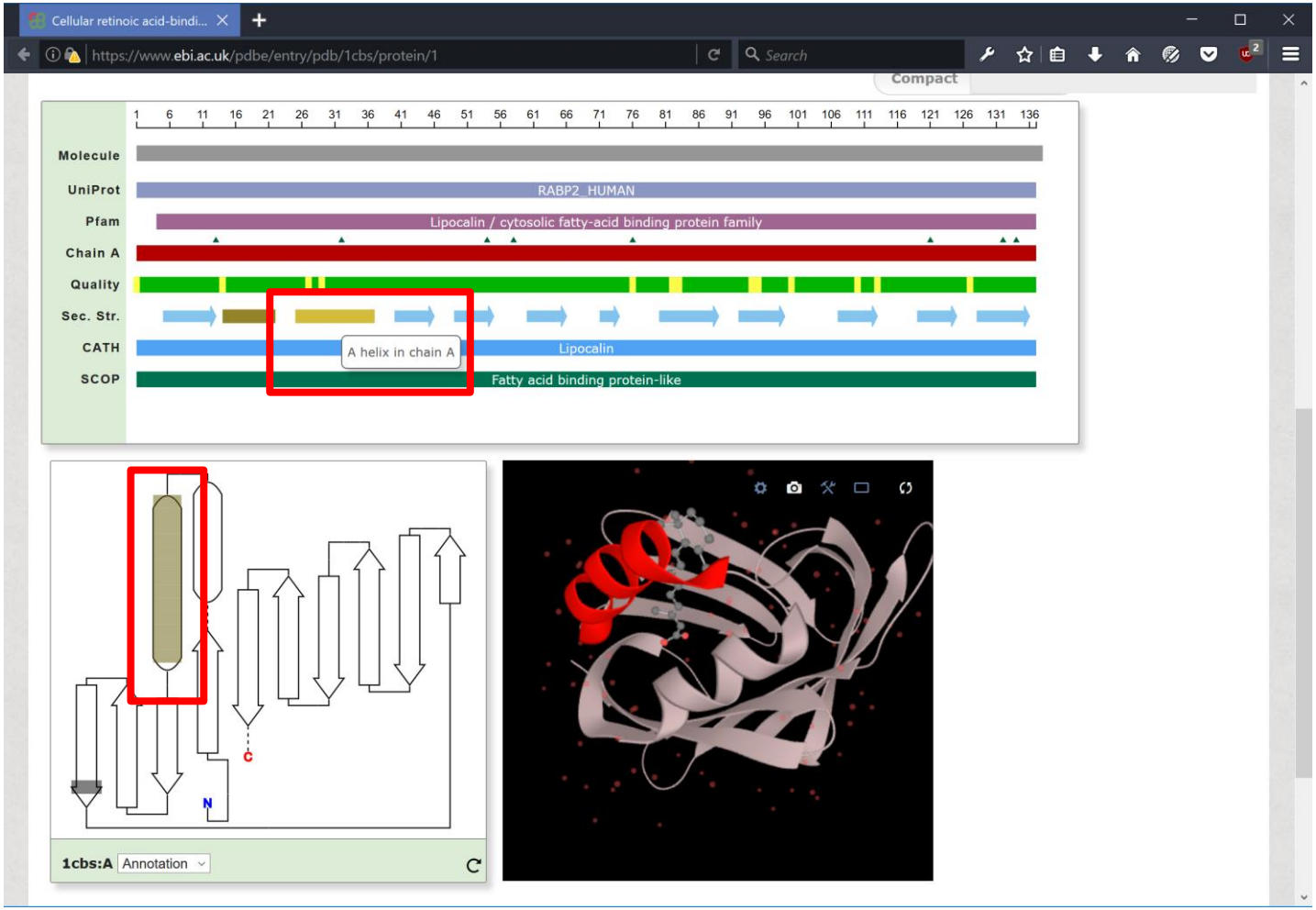
Chloride Channel Complex
5T5N



PDBe validation score

UNIPROT annotation

Interactive 1D, 2D and 3D structure



www.ebi.ac.uk/pdbe/entry/pdb/1cbs/protein/1

IT’S FOR EVERYONE

It’s for everyone

- Accessible from *PDBe* and *LiteMol Viewer*
- Services can be consumed by 3rd parties
- *LiteMol* in your applications

Summary

- Rich visualization available in the web browser
- Integrated into PDBe
- Available for everyone