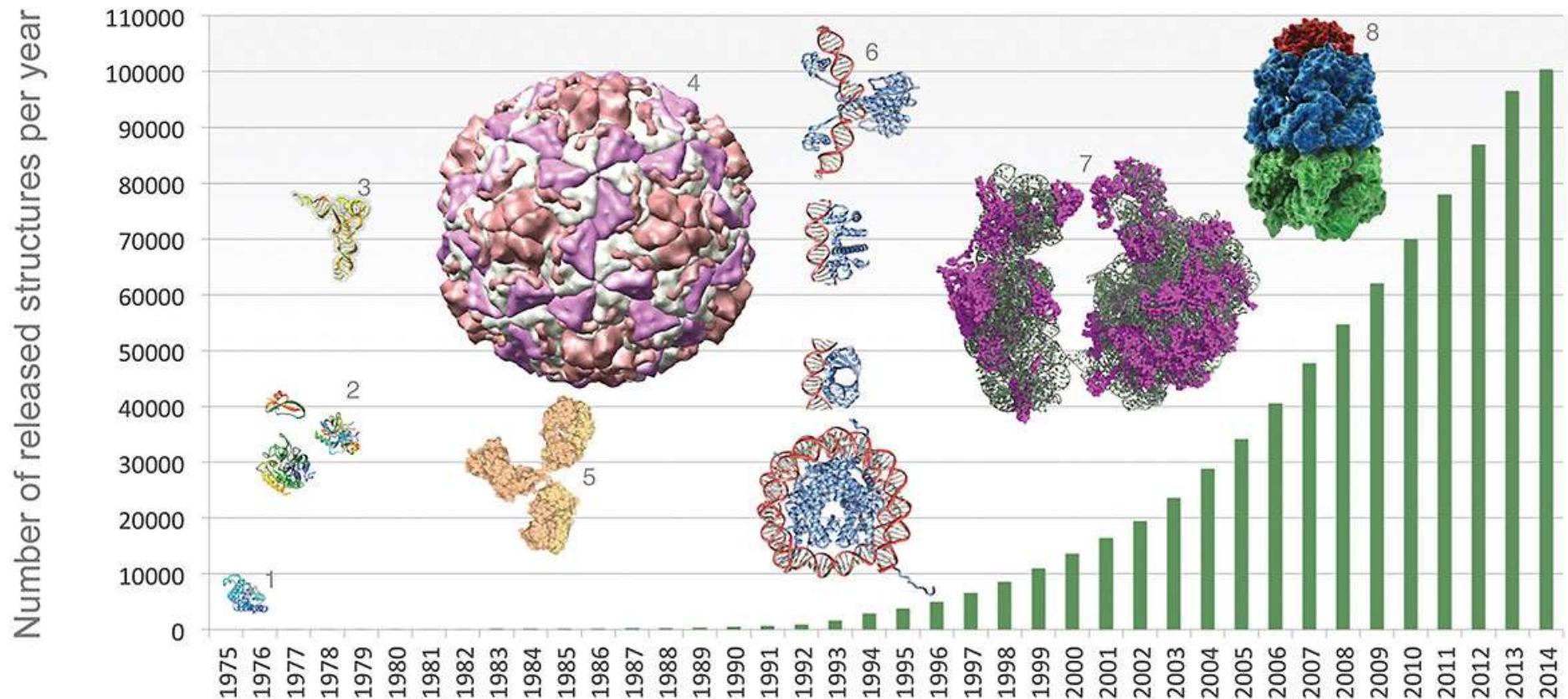


# Introduction:

## Why structural studies?

Corso di Biocristallografia e Microscopia Elettronica

rdezorzi@units.it



# Contents

## Introduction

- Structure function relationships
- Elements of protein structure
- Visualization software and databanks of protein structures

## Protein samples for structural studies

- Recombinant proteins
- Expression and purification
- Evaluation of sample quality and purity
- Analysis of conformational stability

## Practical experiences

- Crystallization of a protein sample
- Sample preparation for data collection
- Data collection at the Elettra Synchrotron
- Data analysis, structure solution and refinement

## Biocrystallography

- Crystallization of proteins
- Symmetry in crystals
- Non-crystallographic symmetries
- Basic concepts of diffraction physics
- Instruments
- Diffraction data collection techniques
- Phase problem in crystallography
- Refinement of the structural model
- Validation

## Transmission electron microscopy

- Basic concepts of optics for TEM
- Instruments
- Single particle techniques
- Image analysis
- 3D reconstruction from images
- Validation
- Electron crystallography

# Objectives of the course

## **Knowledge of:**

- Basic elements of 3D structure of proteins
- Main characteristics of crystals and crystallization techniques
- Physical basis of X-ray diffraction
- X-ray data collection techniques, structural determination and refinement
- Techniques of structural determination by electron microscopy
- Electron microscopy data analysis up to structure validation

## **Apply knowledge to:**

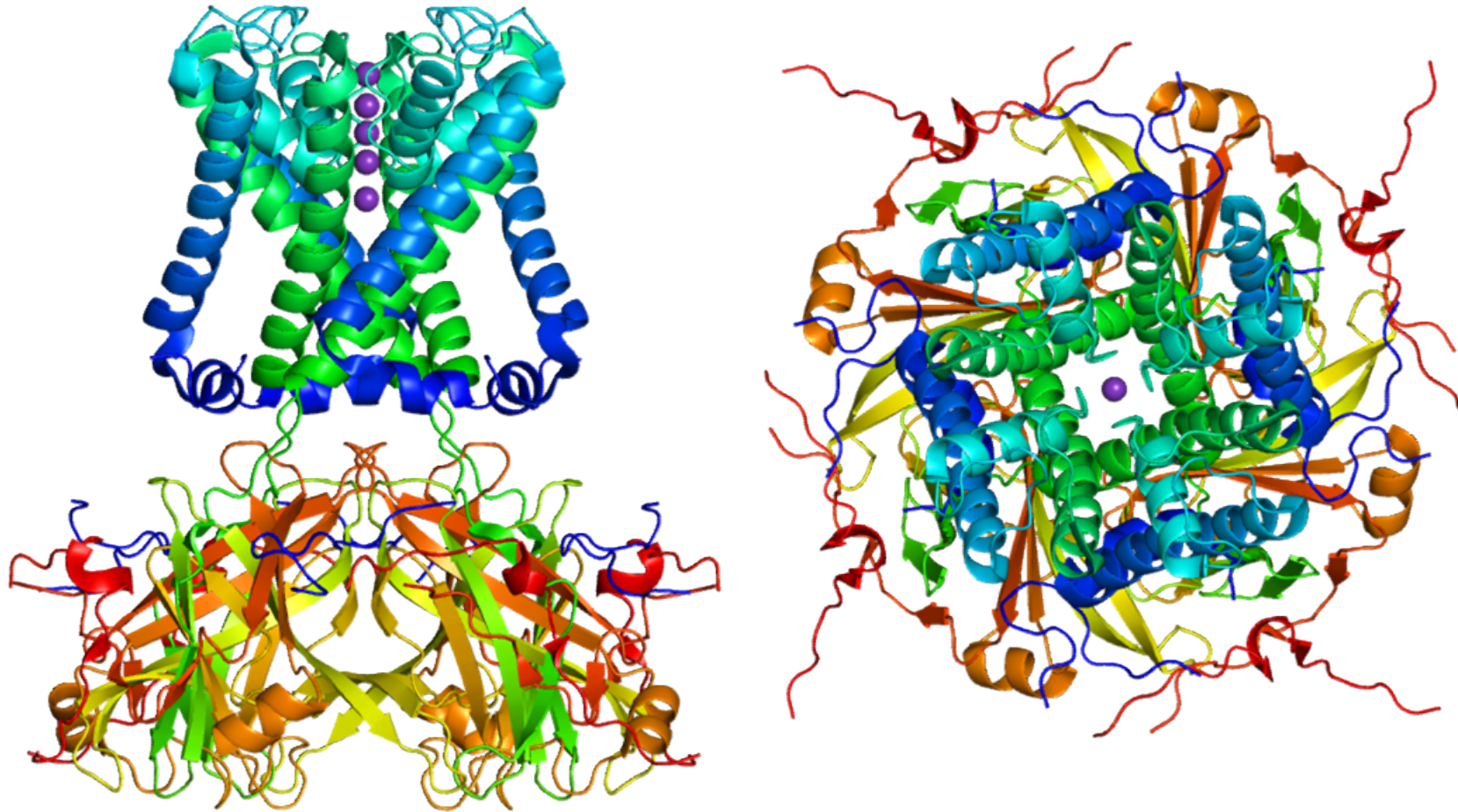
- Describe the 3D structure of a protein
- Plan a X-ray diffraction or electron microscopy experiment, from expression to structure
- Highlight main reasons to chose a structural biology technique over the others
- Recognize crucial factors that can improve/hamper a structural biology experiment
- Identify significant information that can be obtained from a protein structure
- Evaluate quality and reliability of a protein structure obtained through crystallography or EM

## **Communicate:**

- Read and understand a structural biology paper, discussing critical aspects
- Obtain useful information from the available online databases of protein structures
- Present a structural biology study, highlighting useful information obtained from structures
- Obtain images of a protein structure to describe its main features
- Highlight structure-function relationships

# Structure-function relationship

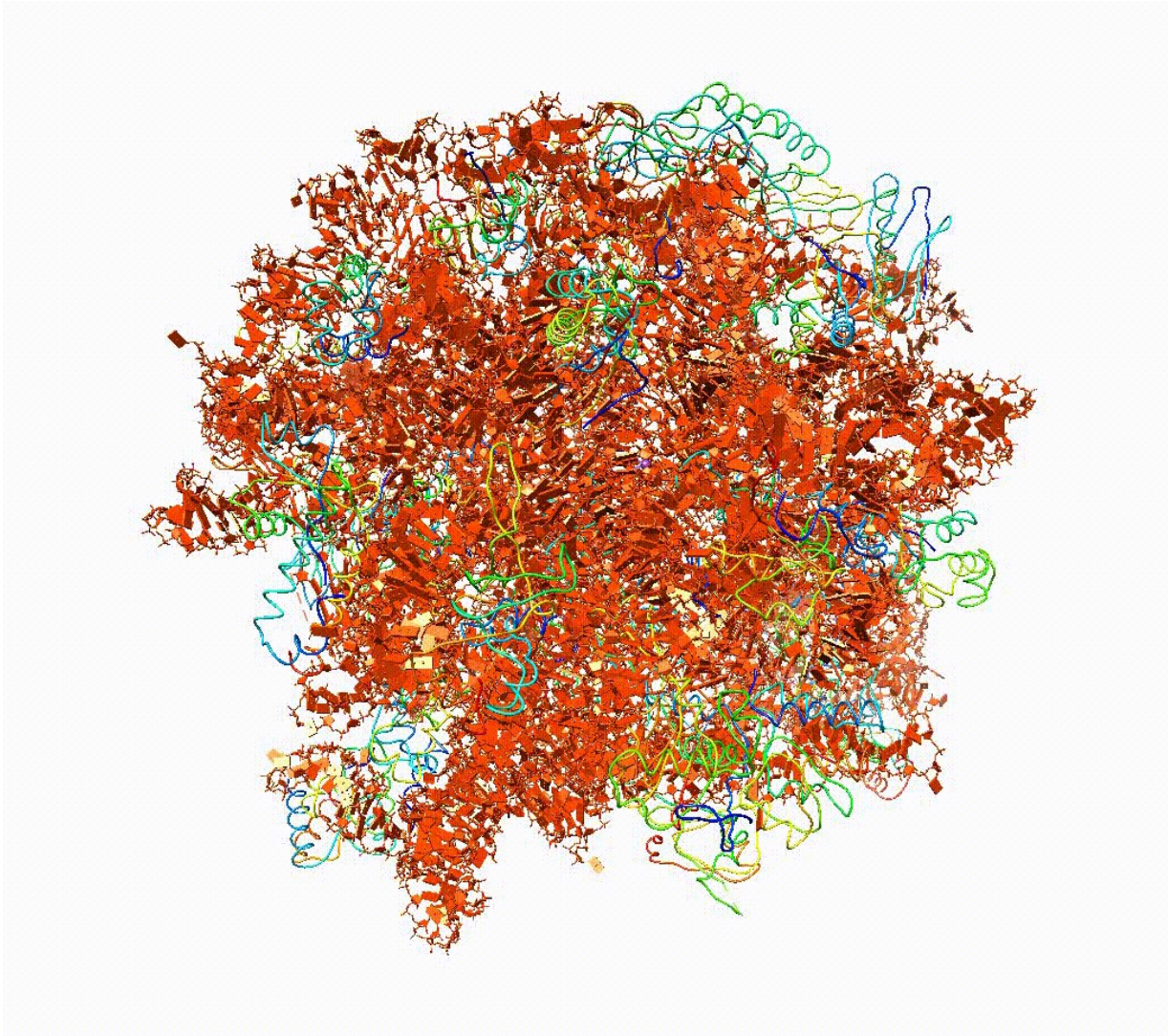
- Mechanisms of biologically relevant proteins and complexes: e.g. Potassium channel



PDB: 3zrs

# Structure-function relationship

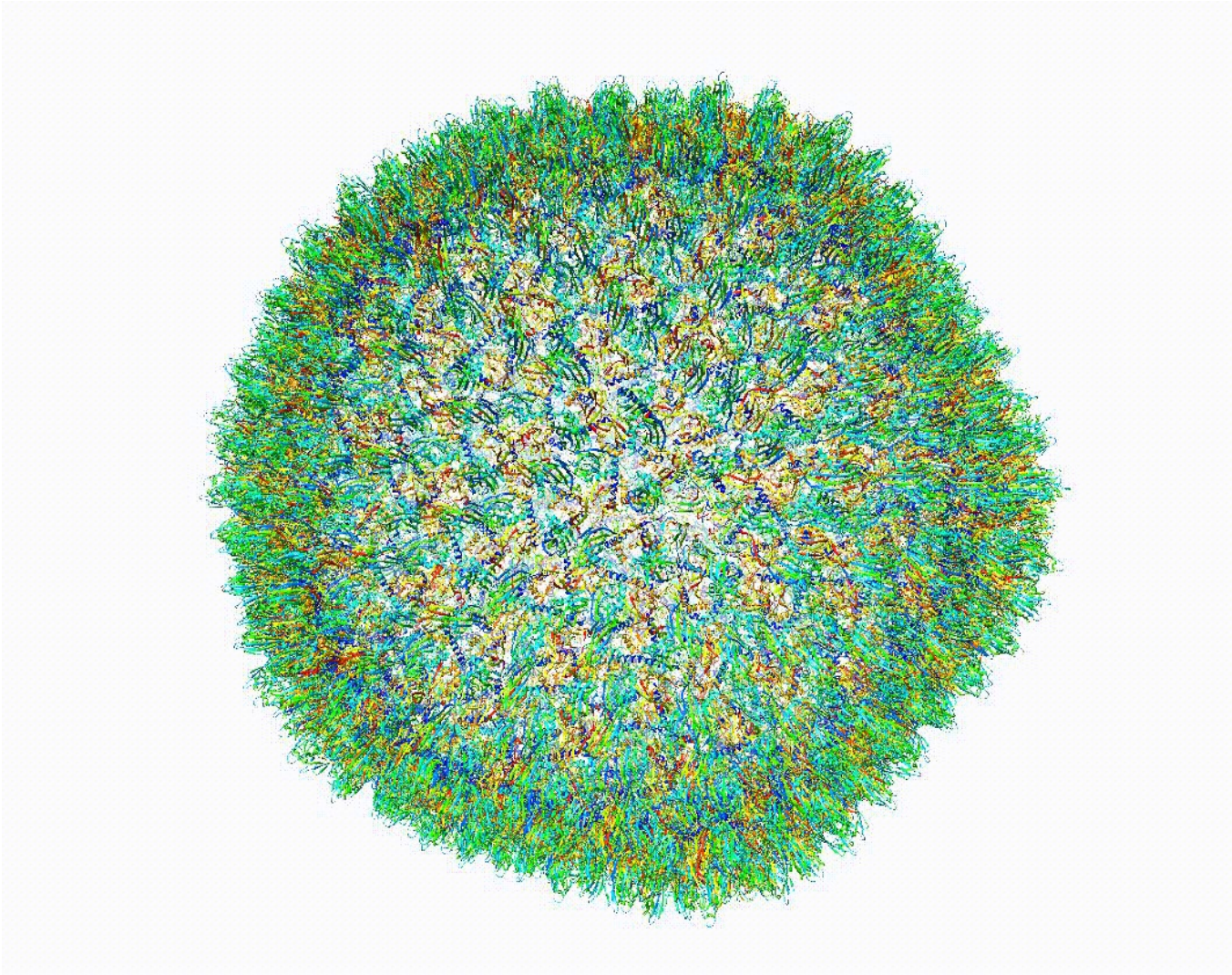
- Mechanisms of biologically relevant proteins and complexes: e.g. ribosome



PDB: 1fft

# Structure-function relationship

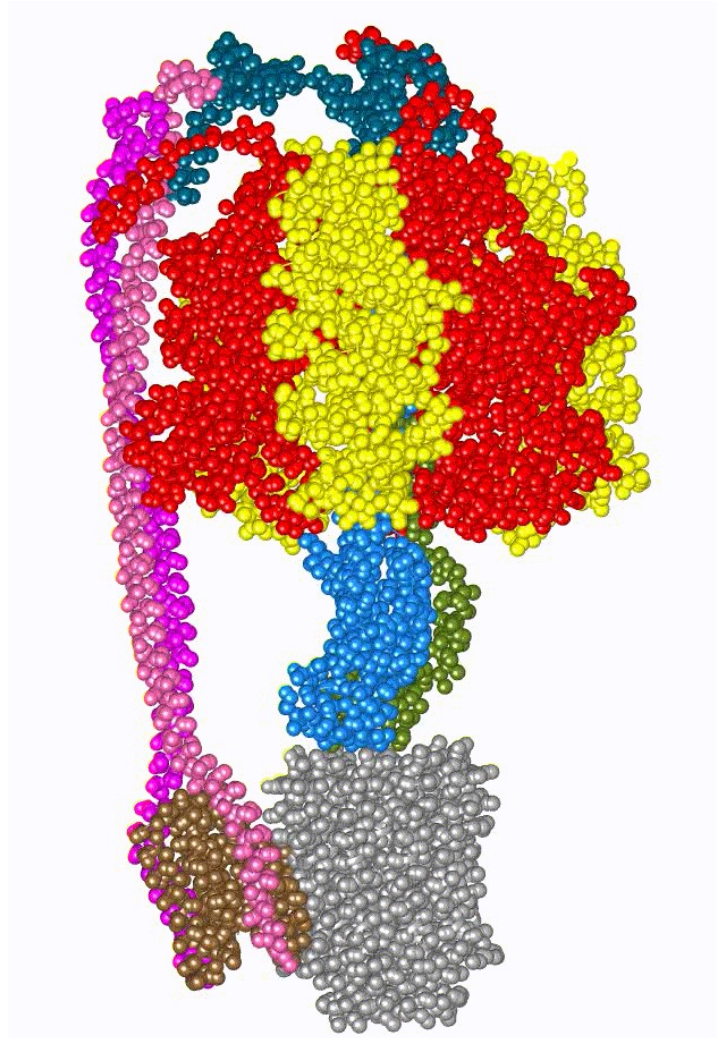
- Mechanisms of biologically relevant proteins and complexes: e.g. virus



PDB: 1w8x

# Structure-function relationship

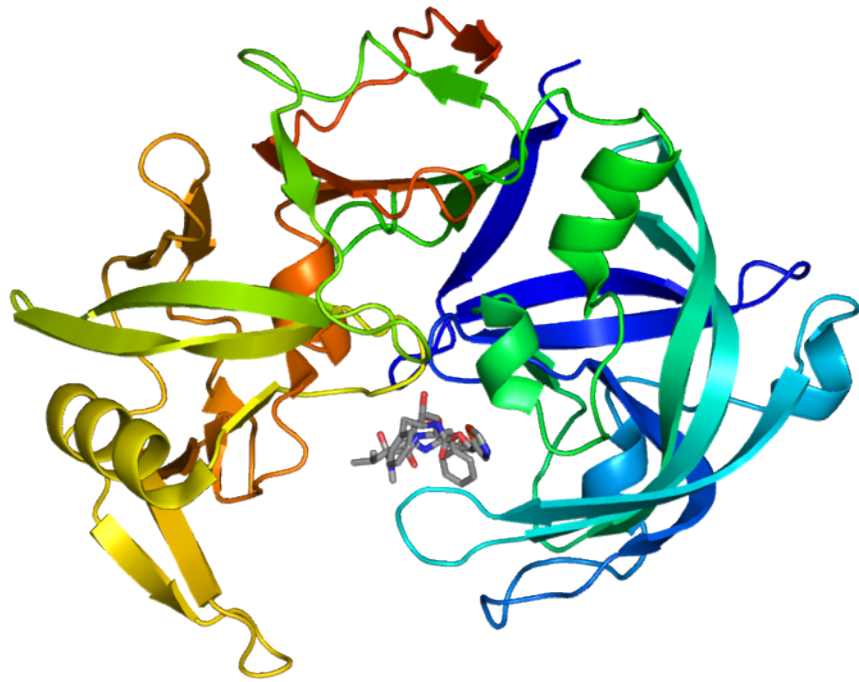
- Mechanisms of biologically relevant proteins and complexes: e.g. ATP-synthase



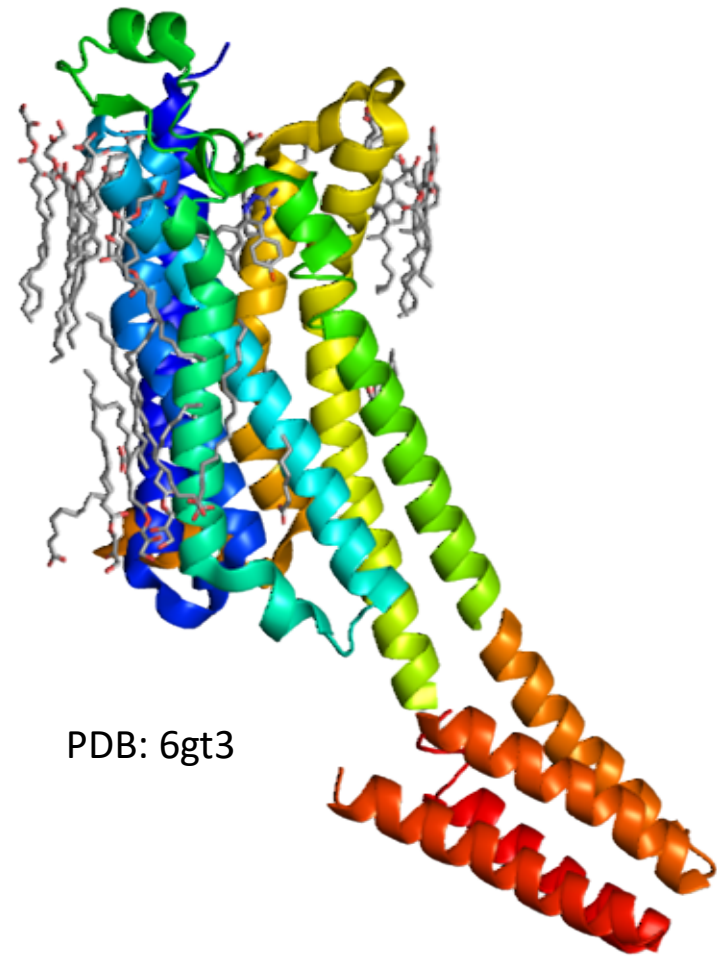
PDB: 5are, 5fil,  
5fij, 5fik, 5ara,  
5ari, 5arh

# Structure-function relationship

- Drug design: e.g. HIV protease inhibitors, GPCR receptors



PDB: 3q70



PDB: 6gt3

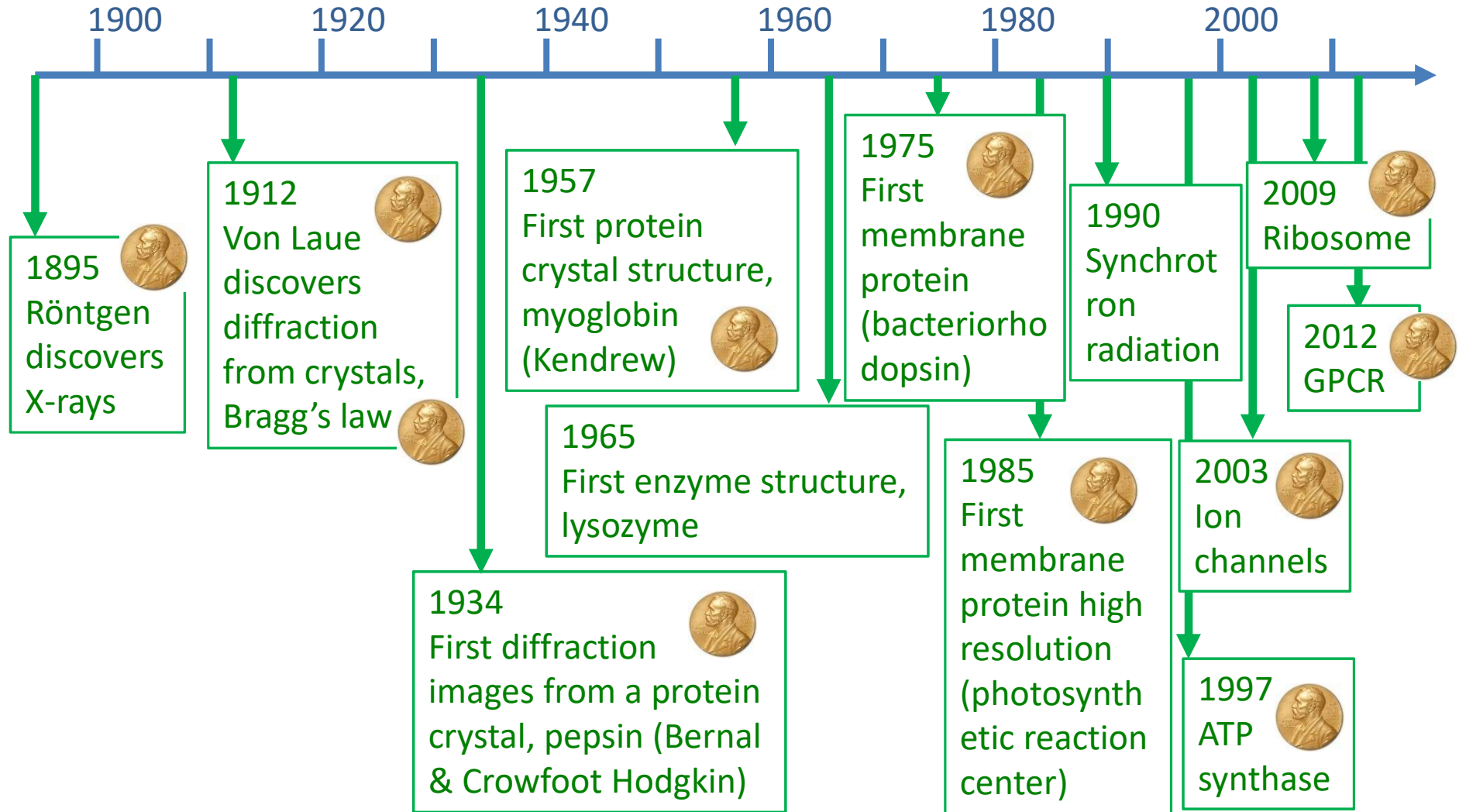


# Structural biology: techniques

	X-ray crystallography	NMR	Electron Microscopy
Protein size	No limitation	< 80 KDa	> 100 kDa
Resolution	Atomic	Atomic	> 2 Å
First structure	1957	1985	Low res: 1975 Medium res: 1990 High res: 2015
Dynamics	No	Yes	(Yes)
Main bottlenecks	Crystallization	Isotope enrichment	Image analysis, model validation

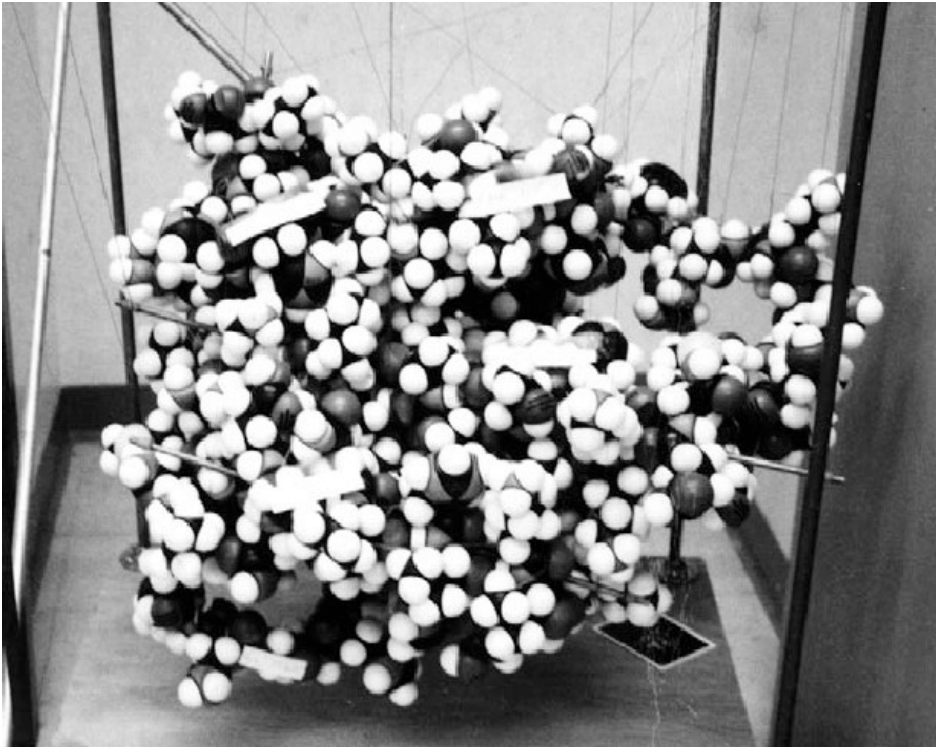
Different structural biology techniques give complementary results!!

# Biocrystallography

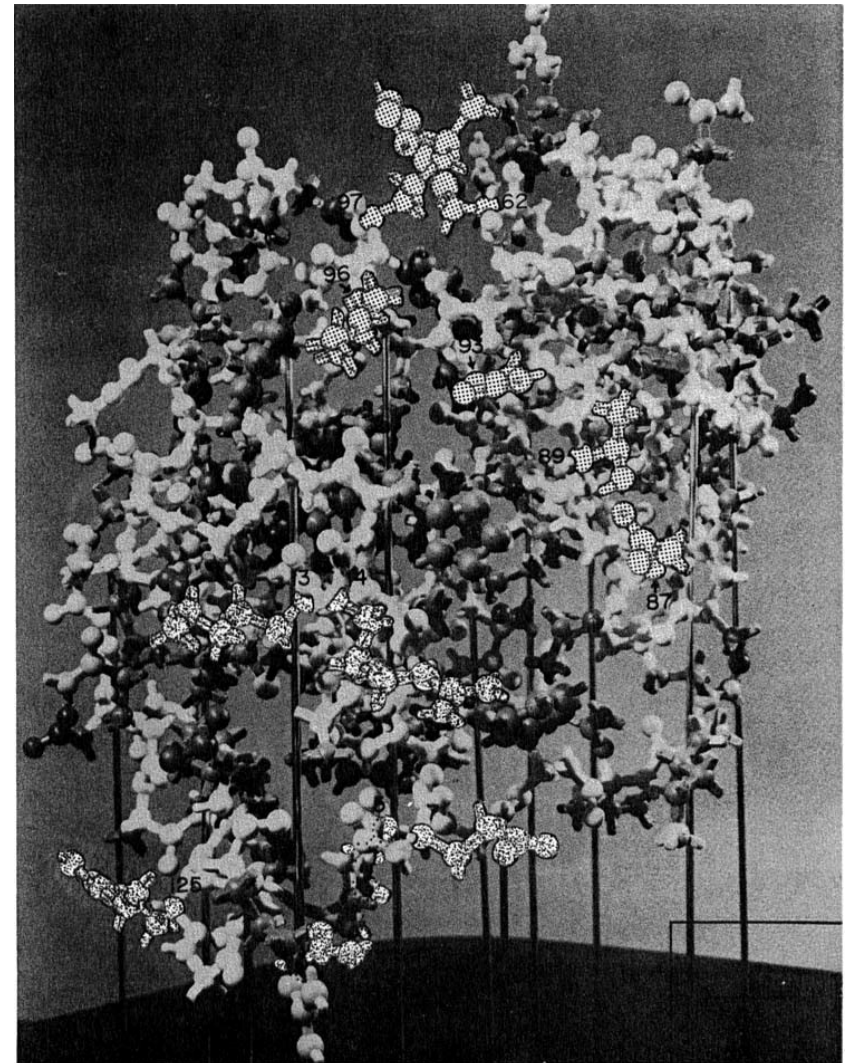


# First protein structures determined by X-ray crystallography

- Myoglobin from sperm whale

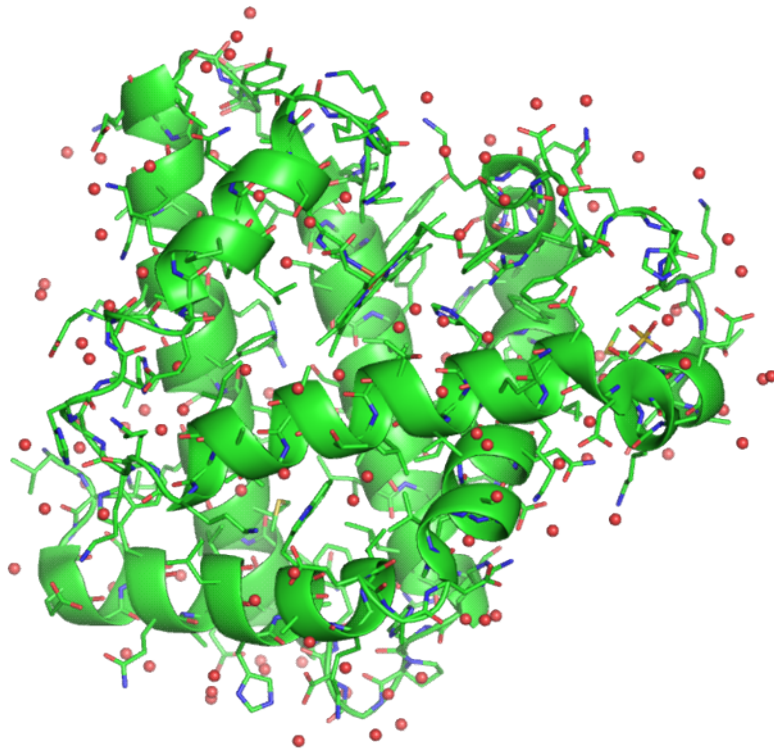


- Lysozyme from chicken egg whites



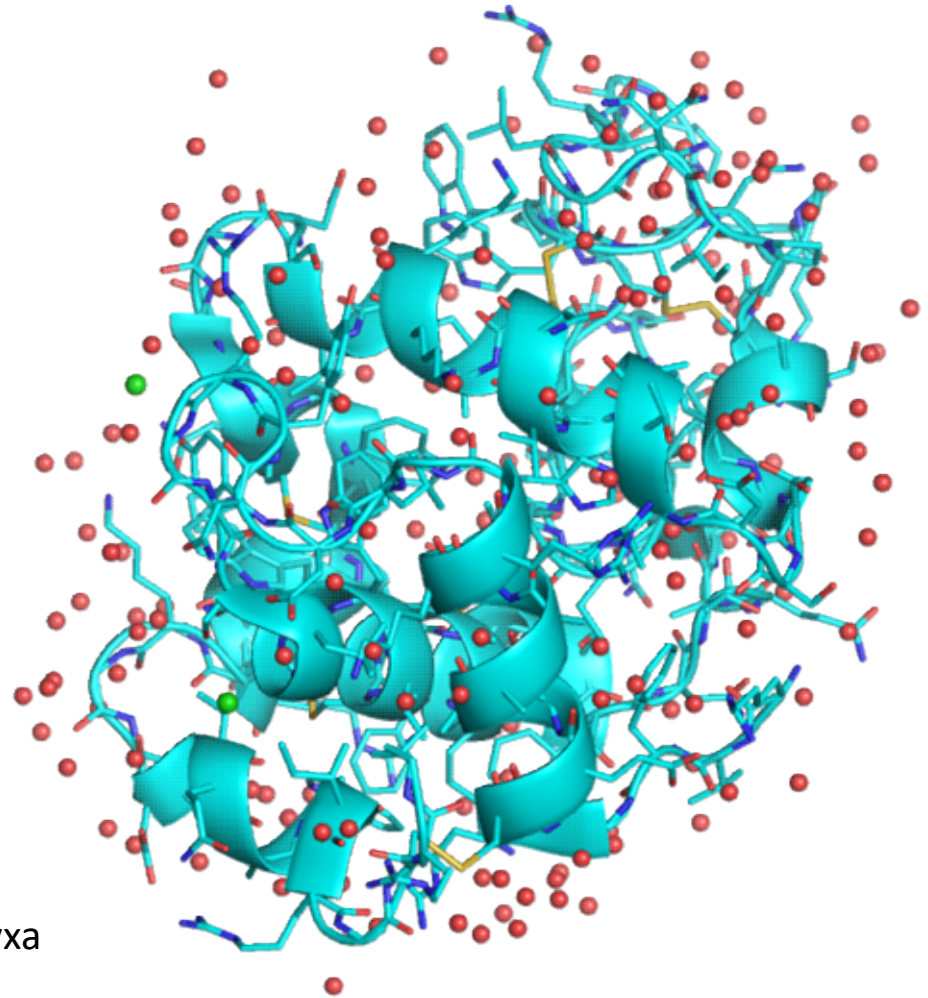
# First protein structures determined by X-ray crystallography

- Myoglobin from sperm whale



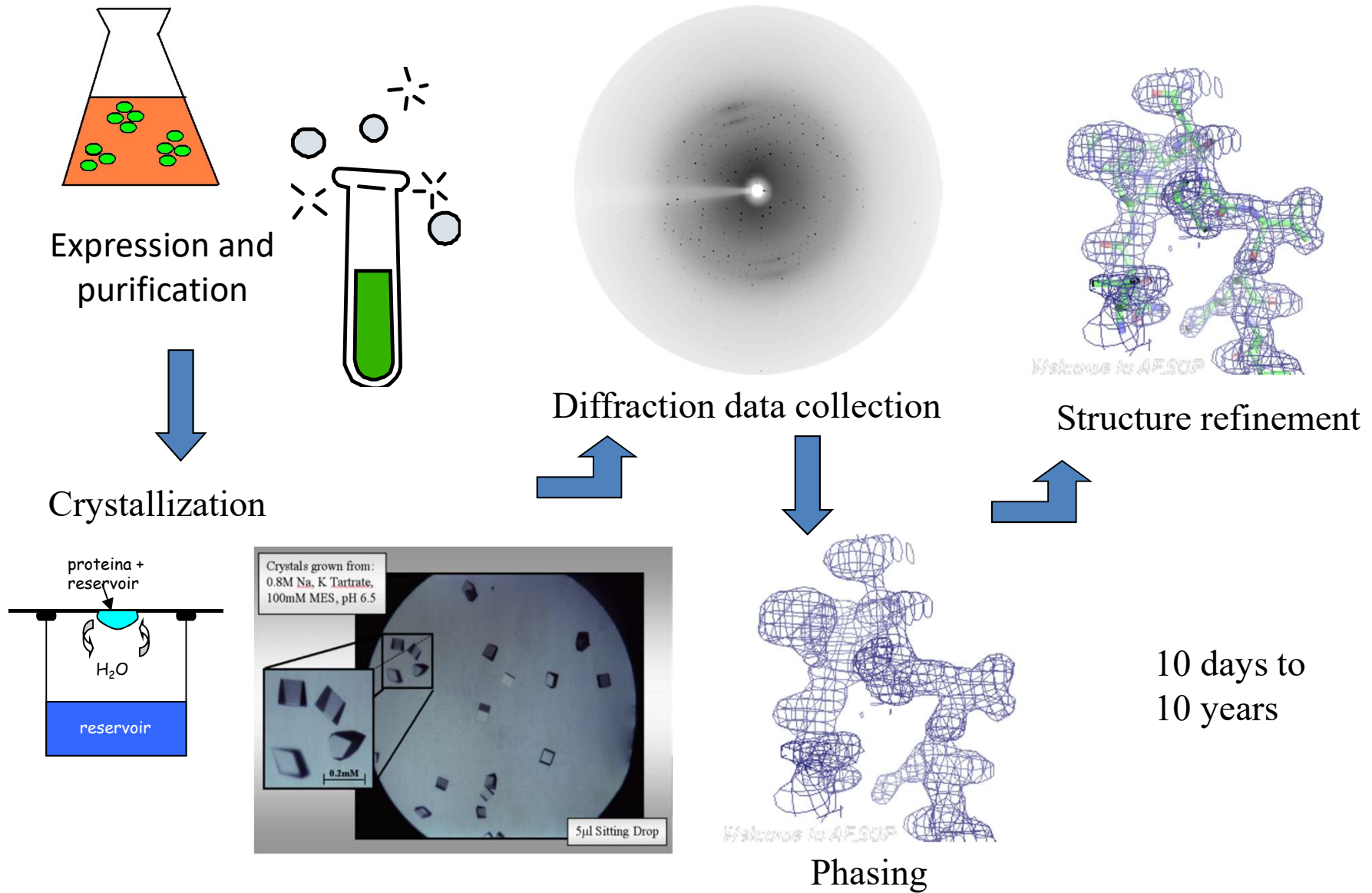
PDB: 1vxa

- Lysozyme from chicken egg whites



PDB: 1vxa

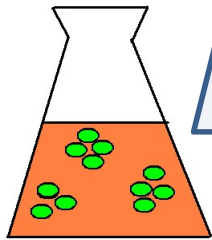
# A biocrystallography experiment



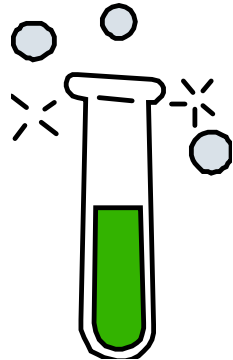
Bioinformatics

# A biocrystallography experiment

Molecular biology

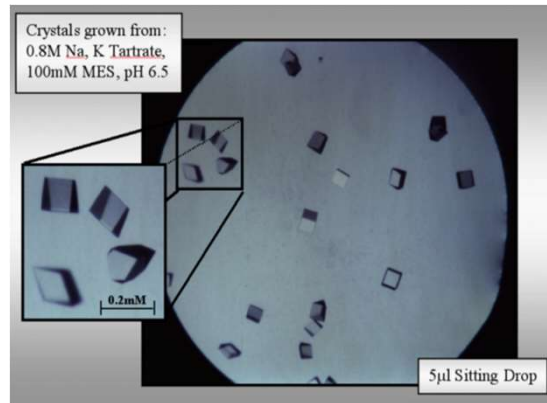
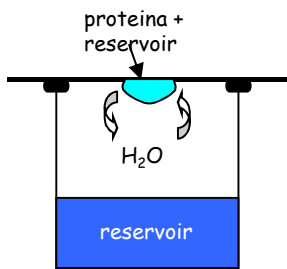


Expression and purification



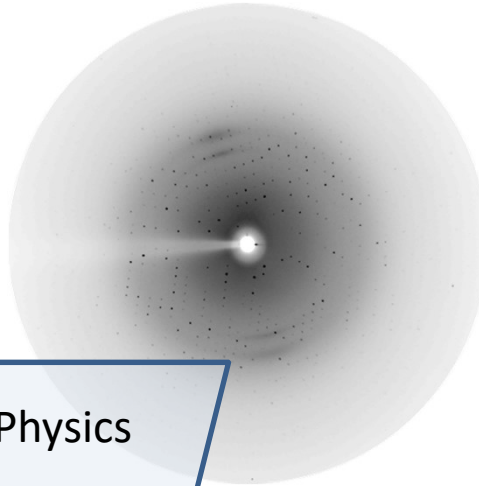
Chemistry

Crystallization

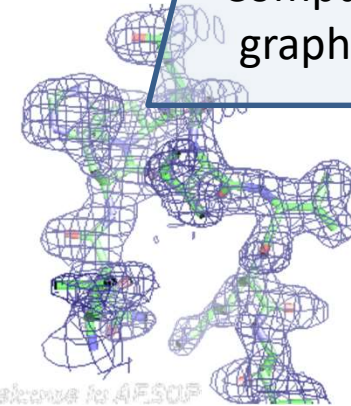


Physics

Diffraction data collection



Computer graphics



Structure refinement

Biology

Biochemistry

10 days to 10 years

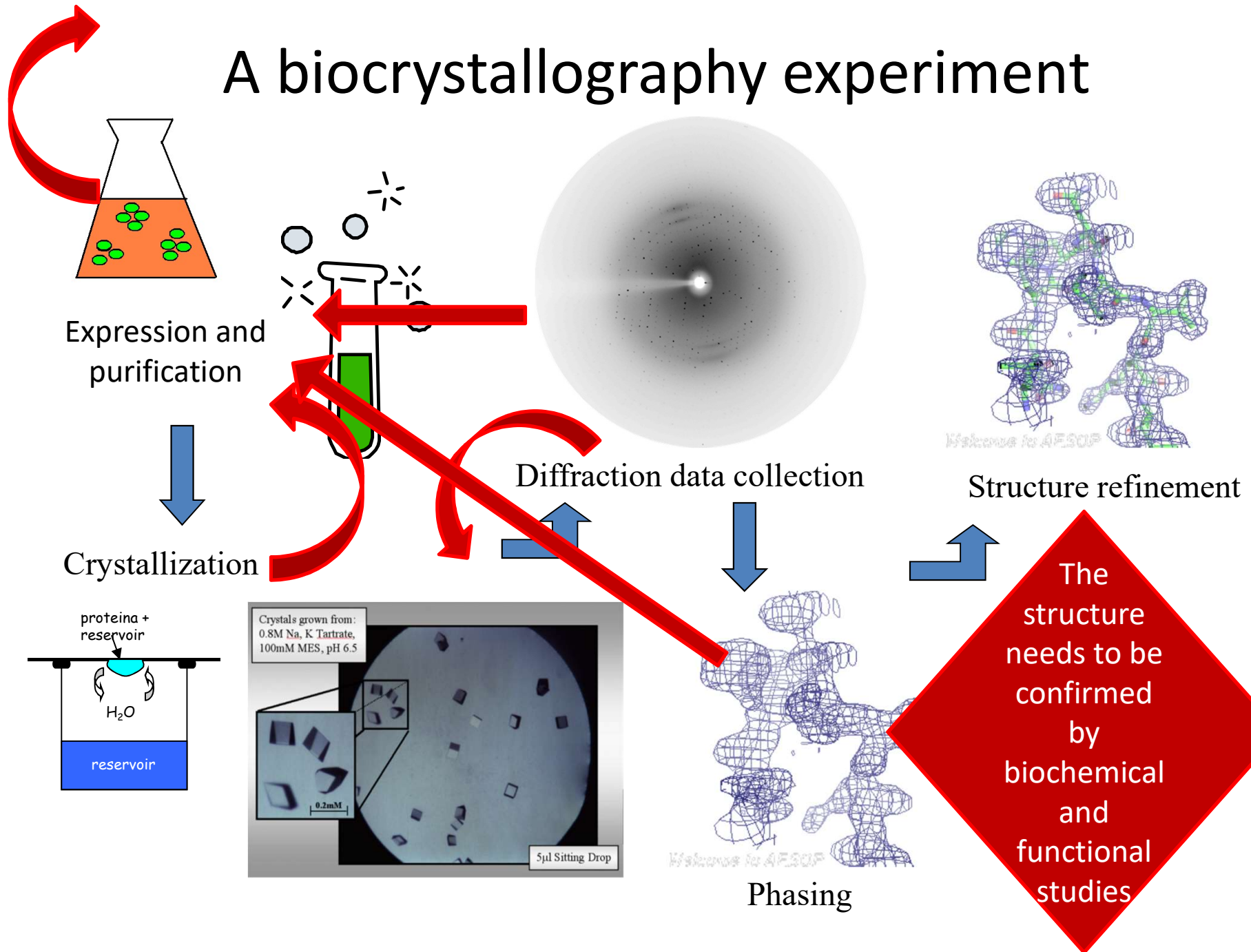
Software development

Mathematics

Statistics

Phasing

# A biocrystallography experiment



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ferritin Go

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## A Structural View of Biology

This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.



## March Molecule of the Month

A 3D molecular structure of a protein complex, primarily colored in blue, with some green and pink components. The structure is complex and multi-domain.

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# Databank resources: PDB (www.rcsb.org)

419 Structures

41 Unreleased Structures

151 Citations

112 Ligands

2 News & PDB-101 Articles

Search Parameter:

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Save Search to MyPDB

Refinements

ORGANISM

- Equus caballus (87)
- Homo sapiens (76)
- Lithobates catesbeianus (47)
- Escherichia coli (24)
- Pseudo-nitzschia multiseriis (16)
- Mycobacterium smegmatis (12)
- Synechococcus sp. CC9311 (11)
- Other (146)

UNIPROT MOLECULE NAME

Ferritin light chain (98)

Currently showing 1 - 25 of 419 Page: 1 of 17 Previous Next Displaying 25 Results

View:

Detailed

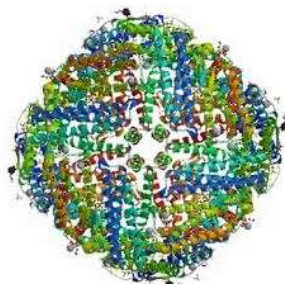
Reports:

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Sort:

Match score: Higher to Lower

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3D View

6A4U

The first crystal structure of crustacean ferritin that is a hybrid type of H and L ferritin

Masuda, T., Zang, J., Zhao, G., Mikami, B.

(2018) Protein Sci 27 1955-1960

Released: 8/22/2018

Method: X-ray Diffraction

Resolution: 1.16 Å

Macromolecule:

Ferritin (protein)

Unique Ligands: CL, EDO, MG, SO4

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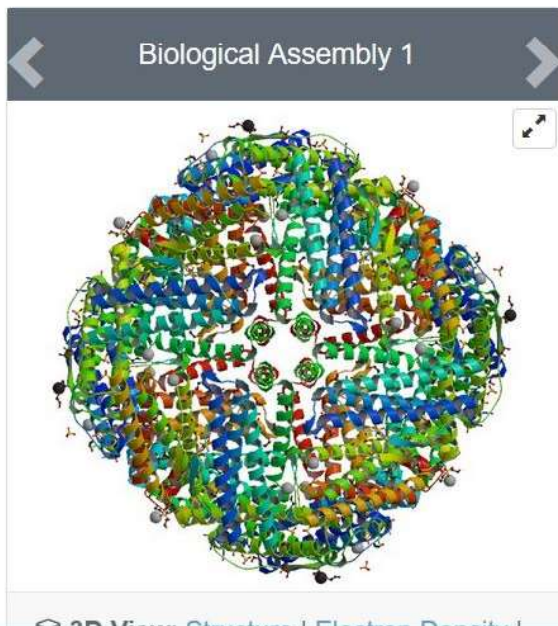
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Structure Summary **3D View** Annotations Sequence Sequence Similarity Structure Similarity Experiment Contact Us



6A4U

The first crystal structure of crustacean ferritin that is a hybrid type of H and L ferritin

DOI: [10.2210/pdb6A4U/pdb](https://doi.org/10.2210/pdb6A4U/pdb)

Classification: [METAL BINDING PROTEIN](#)

Organism(s): [Penaeus japonicus](#)

Expression System: [Escherichia coli BL21\(DE3\)](#)

Mutation(s): 1

Deposited: 2018-06-21 Released: 2018-08-22

Deposition Author(s): [Masuda, T.](#), [Mikami, B.](#), [Zang, J.](#), [Zhao, G.](#)

Funding Organization(s): Japan Society for the Promotion of Science

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**3D View:** [Structure](#) | [Electron Density](#) | [Ligand Interaction](#)

## Standalone Viewers

[Protein Workshop](#) | [Ligand Explorer](#)

**Global Symmetry:** Octahedral - O (3D View)

**Global Stoichiometry:** Homo 24-mer - A24

Biological assembly 1 assigned by authors and generated by PISA (software)

**Biological Assembly Evidence:** gel filtration

## Macromolecule Content

- Total Structure Weight: 120841.39
- Atom Count: 9619
- Residue Count: 1014
- Unique protein chains: 1

**Funding Organization(s):** Japan Society for the Promotion of Science

## Experimental Data Snapshot

**Method:** X-RAY DIFFRACTION

**Resolution:** 1.16 Å

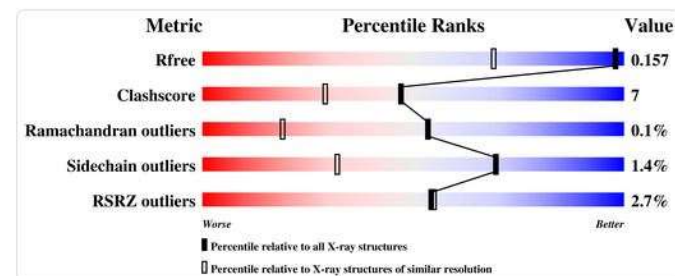
**R-Value Free:** 0.157

**R-Value Work:** 0.138

## wwPDB Validation

[3D Report](#)

[Full Report](#)



This is version 1.1 of the entry. See complete [history](#).

## Literature

[Download Primary Citation](#) ▾

The first crystal structure of crustacean ferritin that is a hybrid type of H and L ferritin

[Masuda, T.](#), [Zang, J.](#), [Zhao, G.](#), [Mikami, B.](#)

(2018) Protein Sci. **27**: 1955-1960

**PubMed:** [30099791](#) [Search on PubMed](#) [Search on PubMed Central](#)

**DOI:** [10.1002/pro.3495](#)

## PubMed Abstract:

Ferritin, a ubiquitous iron storage protein, has a crucial role in innate immunity in arthropods,

# Databank resources: PDB (www.rcsb.org)

## Macromolecules

Find similar proteins by: [Sequence](#) | [Structure](#)

Entity ID: 1

Molecule	Chains	Sequence Length	Organism	Details
Ferritin	A, B, C, D, E, F	169	<a href="#">Panaeus japonicus</a>	Mutation(s): 1 EC: <a href="#">1.16.3.1</a>

Find proteins for [T2B7E1](#) (*Panaeus japonicus*)

Protein Feature View



Full Protein Feature V



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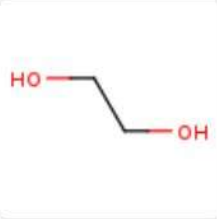

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## Small Molecules

Ligands **4 Unique**

ID	Chains	Name / Formula / InChI Key	2D Diagram & Interactions	3D Interactions
SO4 <a href="#">Query on SO4</a>  <a href="#">Download SDF File</a> ⬇ <a href="#">Download CCD File</a> ⬇	A, B, C, D, E, F	<b>SULFATE ION</b> O <sub>4</sub> S QAOWNCQODCNURD- UHFFFAOYSA-L		<a href="#">Ligand Interaction</a>
CL <a href="#">Query on CL</a>  <a href="#">Download SDF File</a> ⬇ <a href="#">Download CCD File</a> ⬇	B	<b>CHLORIDE ION</b> Cl VEXZGXHMUGYJMC- UHFFFAOYSA-M		<a href="#">Ligand Interaction</a>
EDO <a href="#">Query on EDO</a>  <a href="#">Download SDF File</a> ⬇ <a href="#">Download CCD File</a> ⬇	A, B, C, D, E, F	<b>1,2-ETHANEDIOL</b> <i>ETHYLENE GLYCOL</i> C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> LYCAIKOWRPUZTN- UHFFFAOYSA-N		<a href="#">Ligand Interaction</a>
MG <a href="#">Query on MG</a>	C, D, F	<b>MAGNESIUM ION</b> Mg HVAQYELKONIV		<a href="#">Ligand Interaction</a>

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## Experimental Data & Validation

### Experimental Data

**Method:** X-RAY DIFFRACTION

**Resolution:** 1.16 Å

**R-Value Free:** 0.157

**R-Value Work:** 0.138

**Space Group:** [I 4](#)

**Unit Cell:**

Length (Å)	Angle (°)
a = 124.872	$\alpha$ = 90.00
b = 124.872	$\beta$ = 90.00
c = 175.683	$\gamma$ = 90.00

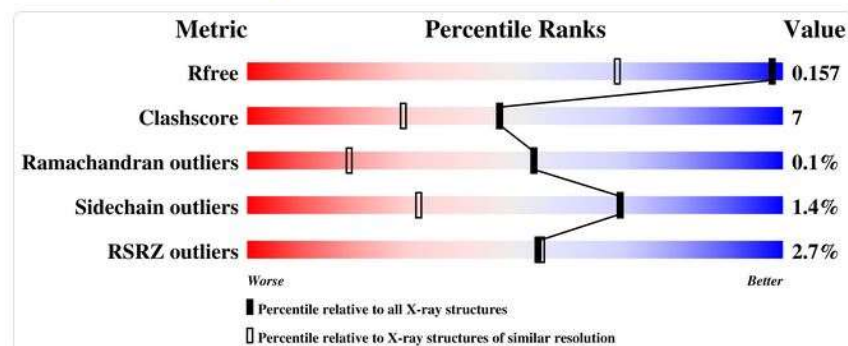
**Software Package:**

Software Name	Purpose
MOLREP	phasing
HKL-2000	data reduction
PHENIX	refinement
HKL-2000	data scaling

[View more in-depth experimental data](#)


### Structure Validation


View [Full Validation Report](#) or [Ramachandran Plots](#)



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# Databank resources: EMDB ([www.ebi.ac.uk/pdbe/emdb/](http://www.ebi.ac.uk/pdbe/emdb/))

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in Europe  
Bringing Structure to Biology

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- EMPIAR
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- 3DEM history

**EMDB**

- Latest maps
- Latest headers
- Latest updates
- Search
- Browse
- FTP archive
- Deposit EM map/model
- EMDB data model
- FAQ
- Policies
- 10,000 entries poster

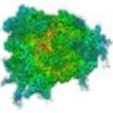
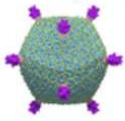

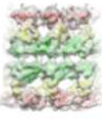


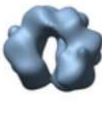

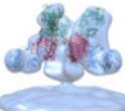
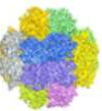


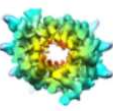
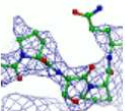
Read about EMPIAR and the EMBL-EBI BioImage Archive in [Nature News, 2 March 2020](#).

The EMDB 10,000 entries celebratory poster is now available. Access it by clicking [here](#)


**The Electron Microscopy Data Bank (EMDB) at PDBe**


**Quick access**

Click on one of these categories:

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 <b>Human</b>	 <b>HIV</b>	 <b>Entries with fitted models</b>	 <b>Single particle</b>	 <b>Tomography</b>	 <b>Helical reconstruction</b>	 <b>&lt;5Å resolution</b>

# Databank resources: EMDB ([www.ebi.ac.uk/pdbe/emdb/](http://www.ebi.ac.uk/pdbe/emdb/))

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 **Protein Data Bank in Europe**  
Bringing Structure to Biology

Search  [Search](#)  
Examples: [hemoglobin](#), [BRCA1\\_HUMAN](#) [Advanced search](#)

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## EMDB > EMD-0632

**Rotavirus A-VP3 (RVA-VP3)**

**Source organism:** [Rotavirus A](#) [28875]

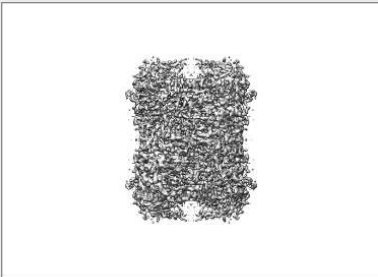
**Fitted atomic model:** [6o6b](#)

**3Dbionotes:** [available for this entry](#)

To be published

**Single particle reconstruction**  
**2.7Å resolution**

**Map released:**  
2020-03-11



**Quick links**

- [EMD-0632 overview](#)
- [Function and Biology](#)
- [Experiments and Validation](#)
- [View](#)
- [Downloads](#)
- [Volume viewer](#)
- [Volume slicer](#)
- [Visual analysis](#)

**Function and Biology** [Details](#) | **Experimental Information** [Details](#)

<b>Sample name:</b>	VP3	<b>Resolution:</b>	2.7Å
<b>Ligand:</b>	GUANOSINE-5'-MONOPHOSPHATE	<b>Resolution method:</b>	FSC 0.143 CUT-OFF
<b>Proteins:</b>	VP3, Protein VP3	<b>Applied symmetry:</b>	D2
		<b>Reconstruction software:</b>	RELION
		<b>Microscope:</b>	JEOL 3200FSC
		<b>Detector:</b>	GATAN K2 SUMMIT (4k x 4k)

**Related entries**

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- [By sample](#)
- [By organism](#)



# Structure atomic coordinates: pdb file

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RCSB PDB PROTEIN DATA BANK 161470 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

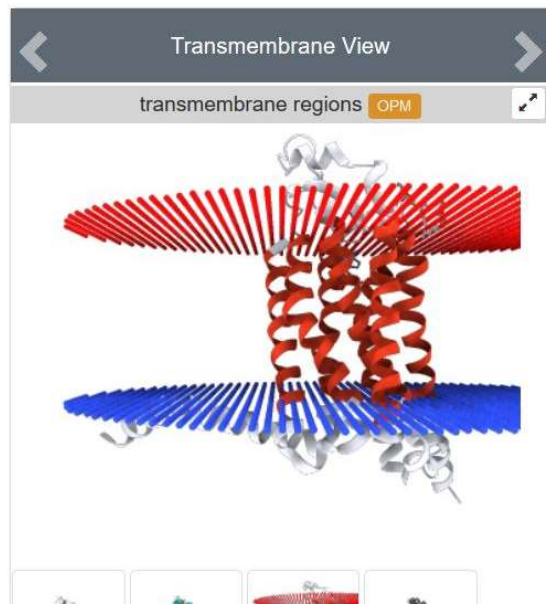
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RCSB PDB-101 WORLDWIDE PDB PROTEIN DATA BANK EMDatabank Unified Data Resource for 3DEM NDB NUCLEIC ACID DATABASE Worldwide Protein Data Bank Foundation

f t y d

- Structure Summary
- 3D View
- Annotations
- Sequence
- Sequence Similarity
- Structure Similarity
- Experiment



## 2YDO

Thermostabilised HUMAN A2a Receptor with adenosine bound

DOI: 10.2210/pdb2YDO/pdb

Classification: [RECEPTOR](#)

Organism(s): [Homo sapiens](#)

Expression System: [Trichoplusia ni](#)

Mutation(s): 5

Deposited: 2011-03-23 Released: 2011-05-18

Deposition Author(s): [Lebon, G.](#), [Warne, T.](#), [Edwards, P.C.](#), [Bennett, K.](#), [Langmead, C.J.](#), [Leslie, A.G.W.](#), [Tate, C.G.](#)

### Experimental Data Snapshot

Method: X-RAY DIFFRACTION  
Resolution: 3 Å  
R-Value Free: 0.269  
R-Value Work: 0.244

### wwPDB Validation



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# Structure atomic coordinates: pdb file

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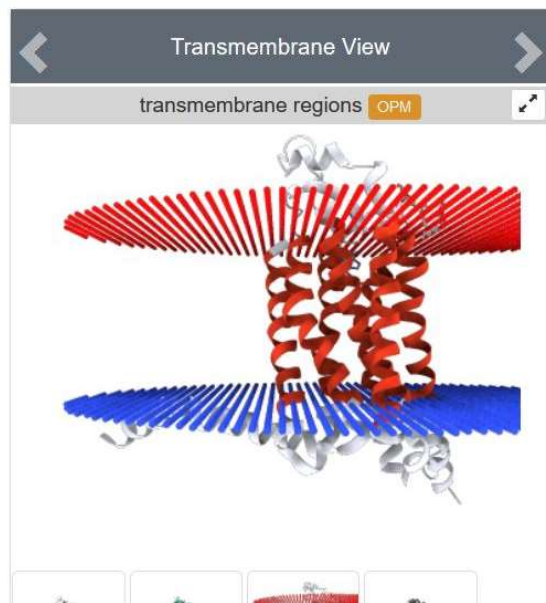
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Advanced Search | Browse by Annotations

PDB-101 WORLDWIDE PDB PROTEIN DATA BANK EMDatabank Unified Data Resource for ISEM NDB NUCLEIC ACID DATABASE Worldwide Protein Data Bank Foundation

f t v y

- Structure Summary
- 3D View
- Annotations
- Sequence
- Sequence Similarity
- Structure Similarity
- Experiment



## 2YDO

Thermostabilised HUMAN A2a Receptor with adenosine

DOI: [10.2210/pdb2YDO/pdb](https://doi.org/10.2210/pdb2YDO/pdb)

Classification: [RECEPTOR](#)

Organism(s): [Homo sapiens](#)

Expression System: [Trichoplusia ni](#)

Mutation(s): 5

Deposited: 2011-03-23 Released: 2011-05-18

Deposition Author(s): [Lebon, G.](#), [Warne, T.](#), [Edwards, P.C.](#), [Bennett, K.](#), [L...](#)

### Experimental Data Snapshot

Method: X-RAY DIFFRACTION

Resolution: 3 Å

R-Value Free: 0.269

R-Value Work: 0.244

### wwPDB Validation

Metric	Value
Clashscore	1.8
Ramachandran outliers	0.0%
Rotamer outliers	0.0%

Display Files Download Files

- FASTA Sequence
- PDB Format**
- PDB Format (gz)**
- PDBx/mmCIF Format
- PDBx/mmCIF Format (gz)
- PDBML/XML Format (gz)
- Biological Assembly 1
- Structure Factors (CIF)
- Structure Factors (CIF - gz)
- 2fo-fc Map (DMSO)

# Structure atomic coordinates: pdb file

```
2ydo.pdb - Blocco note di Windows
File Modifica Formato Visualizza ?
HEADER RECEPTOR 23-MAR-11 2YDO
TITLE THERMOSTABILISED HUMAN A2A RECEPTOR WITH ADENOSINE BOUND
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: ADENOSINE RECEPTOR A2A;
COMPND 3 CHAIN: A;
COMPND 4 FRAGMENT: RESIDUES 1-317;
COMPND 5 SYNONYM: THERMOSTABILISED HUMAN A2A RECEPTOR;
COMPND 6 ENGINEERED: YES;
COMPND 7 MUTATION: YES
SOURCE MOL_ID: 1;
SOURCE 2 ORGANISM_SCIENTIFIC: HOMO SAPIENS;
SOURCE 3 ORGANISM_COMMON: HUMAN;
SOURCE 4 ORGANISM_TAXID: 9606;
SOURCE 5 TISSUE: BRAIN;
SOURCE 6 EXPRESSION_SYSTEM: TRICHOPLUSIA NI;
SOURCE 7 EXPRESSION_SYSTEM_COMMON: CABBAGE LOOPER;
SOURCE 8 EXPRESSION_SYSTEM_TAXID: 7111;
SOURCE 9 EXPRESSION_SYSTEM_CELL_LINE: HIGH FIVE;
SOURCE 10 EXPRESSION_SYSTEM_VECTOR_TYPE: BACULOVIRUS;
SOURCE 11 EXPRESSION_SYSTEM_PLASMID: PBACPAK8
KEYWDS RECEPTOR, G PROTEIN COUPLED RECEPTOR, SEVEN-HELIX RECEPTOR, AGONIST
KEYWDS 2 BOUND FORM, THERMOSTABILISING POINT MUTATIONS, GPCR, 7TM RECEPTOR
EXPDTA X-RAY DIFFRACTION
AUTHOR G. LEBON, T. WARNE, P. C. EDWARDS, K. BENNETT, C. J. LANGMEAD, A. G. W. LESLIE,
AUTHOR 2 C. G. TATE
REVDAT 4 03-APR-19 2YDO 1 SOURCE
REVDAT 3 22-JUN-11 2YDO 1 JRNL
REVDAT 2 01-JUN-11 2YDO 1 REMARK MASTER
REVDAT 1 18-MAY-11 2YDO 0
JRNL AUTH G. LEBON, T. WARNE, P. C. EDWARDS, K. BENNETT, C. J. LANGMEAD,
JRNL AUTH 2 A. G. W. LESLIE, C. G. TATE
JRNL TITL AGONIST-BOUND ADENOSINE A(2A) RECEPTOR STRUCTURES REVEAL
JRNL TITL 2 COMMON FEATURES OF GPCR ACTIVATION.
JRNL REF NATURE V 474 521 2011
```

Information  
about the  
protein

Information  
about the  
publication

# Structure atomic coordinates: pdb file

```
2ydo.pdb - Blocco note di Windows
File Modifica Formato Visualizza ?
REMARK 3
REMARK 3 DATA USED IN REFINEMENT.
REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 3.00
REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 60.42
REMARK 3 DATA CUTOFF (SIGMA(F)) : NULL
REMARK 3 COMPLETENESS FOR RANGE (%) : 93.5
REMARK 3 NUMBER OF REFLECTIONS : 10556
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING + TEST SET) : 0.246
REMARK 3 R VALUE (WORKING SET) : 0.244
REMARK 3 FREE R VALUE : 0.269
REMARK 3 FREE R VALUE TEST SET SIZE (%) : 5.200
REMARK 3 FREE R VALUE TEST SET COUNT : 575
REMARK 3
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK 3 TOTAL NUMBER OF BINS USED : 20
REMARK 3 BIN RESOLUTION RANGE HIGH (A) : 3.00
REMARK 3 BIN RESOLUTION RANGE LOW (A) : 3.08
REMARK 3 REFLECTION IN BIN (WORKING SET) : 745
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 91.87
REMARK 3 BIN R VALUE (WORKING SET) : 0.3360
REMARK 3 BIN FREE R VALUE SET COUNT : 35
REMARK 3 BIN FREE R VALUE : 0.2600
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 2410
REMARK 3 NUCLEIC ACID ATOMS : 0
REMARK 3 HETEROGEN ATOMS : 59
REMARK 3 SOLVENT ATOMS : 18
REMARK 3
```

Information  
about  
crystal  
structure  
and  
refinement

# Structure atomic coordinates: pdb file

```
2ydo.pdb - Blocco note di Windows
File Modifica Formato Visualizza ?
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : 09-DEC-10
REMARK 200 TEMPERATURE (KELVIN) : 100
REMARK 200 PH : 7.6
REMARK 200 NUMBER OF CRYSTALS USED : 2
REMARK 200
REMARK 200 SYNCHROTRON (Y/N) : Y
REMARK 200 RADIATION SOURCE : DIAMOND
REMARK 200 BEAMLINE : I24
REMARK 200 X-RAY GENERATOR MODEL : NULL
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A) : 0.9778
REMARK 200 MONOCHROMATOR : NULL
REMARK 200 OPTICS : NULL
REMARK 200
REMARK 200 DETECTOR TYPE : PIXEL
REMARK 200 DETECTOR MANUFACTURER : DECTRIS PILATUS 6M
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : MOSFLM
REMARK 200 DATA SCALING SOFTWARE : SCALA
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 10556
REMARK 200 RESOLUTION RANGE HIGH (A) : 3.000
REMARK 200 RESOLUTION RANGE LOW (A) : 79.340
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : 0.000
REMARK 200
REMARK 200 OVERALL.
REMARK 200 COMPLETENESS FOR RANGE (%) : 93.9
REMARK 200 DATA REDUNDANCY : 2.600
REMARK 200 R MERGE (I) : 0.10000
REMARK 200 R SYM (I) : NULL
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 7.1000
```

Information  
about the  
crystallographic  
experiment

# Structure atomic coordinates: pdb file

```
File Modifica Formato Visualizza ?
SITE      3 AC1 11 HOH A2016 HOH A2017 HOH A2018
SITE      1 AC2  1 TYR A 179
SITE      1 AC3  5 GLY A 142 TRP A 143 ASN A 144 ASN A 145
SITE      1 AC3  5 GLN A 148
CRYST1    76.465  98.869  79.516  90.00  93.49  90.00 C 1 2 1 4
ORIGX1    1.000000  0.000000  0.000000  0.000000
ORIGX2    0.000000  1.000000  0.000000  0.000000
ORIGX3    0.000000  0.000000  1.000000  0.000000
SCALE1    0.013078  0.000000  0.000798  0.000000
SCALE2    0.000000  0.010114  0.000000  0.000000
SCALE3    0.000000  0.000000  0.012500  0.000000
ATOM      1  N  SER  A  6  -28.148  4.590 -7.800  1.00 113.33  N
ATOM      2  CA SER  A  6  -26.785  4.701 -7.207  1.00 115.91  C
ATOM      3  C  SER  A  6  -26.419  6.159 -6.970  1.00 114.54  C
ATOM      4  O  SER  A  6  -26.103  6.886 -7.915  1.00 110.10  O
ATOM      5  CB SER  A  6  -25.744  4.037 -8.113  1.00 116.34  C
ATOM      6  OG SER  A  6  -26.087  2.689 -8.379  1.00 121.40  O
ATOM      7  N  SER  A  7  -26.458  6.572 -5.703  1.00 116.37  N
ATOM      8  CA SER  A  7  -26.153  7.952 -5.306  1.00 112.95  C
ATOM      9  C  SER  A  7  -24.758  8.391 -5.751  1.00 109.79  C
ATOM     10  O  SER  A  7  -24.497  9.586 -5.902  1.00 104.20  O
ATOM     11  CB SER  A  7  -26.313  8.125 -3.794  1.00 113.79  C
ATOM     12  OG SER  A  7  -25.474  7.228 -3.088  1.00 117.64  O
ATOM     13  N  VAL  A  8  -23.879  7.409 -5.959  1.00 108.84  N
ATOM     14  CA VAL  A  8  -22.535  7.626 -6.501  1.00 108.75  C
ATOM     15  C  VAL  A  8  -22.622  8.258 -7.895  1.00 110.01  C
ATOM     16  O  VAL  A  8  -21.895  9.207 -8.205  1.00 105.91  O
ATOM     17  CB VAL  A  8  -21.739  6.295 -6.599  1.00 108.46  C
ATOM     18  CG1 VAL  A  8  -20.240  6.568 -6.638  1.00 107.74  C
ATOM     19  CG2 VAL  A  8  -22.087  5.355 -5.443  1.00 105.56  C
ATOM     20  N  TYR  A  9  -23.521  7.717 -8.719  1.00 108.80  N
ATOM     21  CA TYR  A  9  -23.812  8.252 -10.048 1.00 102.10  C
ATOM     22  C  TYR  A  9  -24.618  9.551 -9.966  1.00  98.51  C
ATOM     23  O  TYR  A  9  -24.331 10.506 -10.688 1.00  94.86  O
```

Unit cell  
and  
symmetry

List of atoms  
with:

1. Atom name
2. Residue type and number
3. Chain
4. Cartesian coordinates
5. Occupancy
6. Thermal factor
7. Atom type

# Structure atomic coordinates: mmCIF file

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB

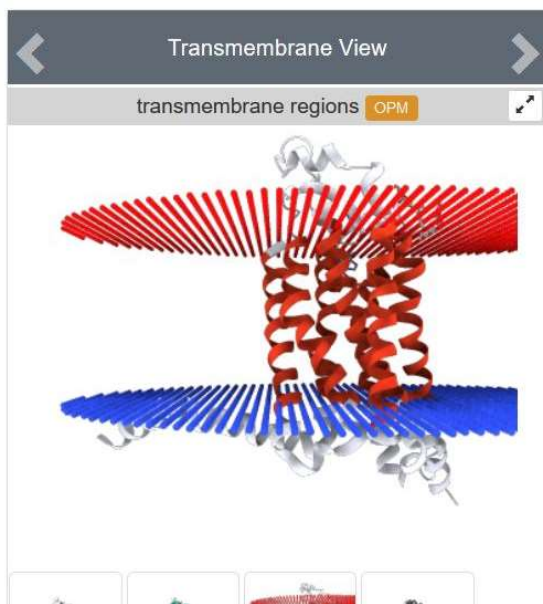
RCSB PDB PROTEIN DATA BANK 161470 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

Search by PDB ID, author, macromolecule, sequence, or ligands Go

Advanced Search | Browse by Annotations

PDB-101 WORLDWIDE PDB PROTEIN DATA BANK EMDatabank Unified Data Resource for SDEM NDB NUCLEIC ACID DATABASE Worldwide Protein Data Bank Foundation

- Structure Summary
- 3D View
- Annotations
- Sequence
- Sequence Similarity
- Structure Similarity
- Experiment



## 2YDO

Thermostabilised HUMAN A2a Receptor with adenosine bou

DOI: 10.2210/pdb2YDO/pdb

Classification: [RECEPTOR](#)

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Expression System: [Trichoplusia ni](#)

Mutation(s): 5

Deposited: 2011-03-23 Released: 2011-05-18

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Method: X-RAY DIFFRACTION

Resolution: 3 Å

R-Value Free: 0.269

R-Value Work: 0.244

### wwPDB Validation

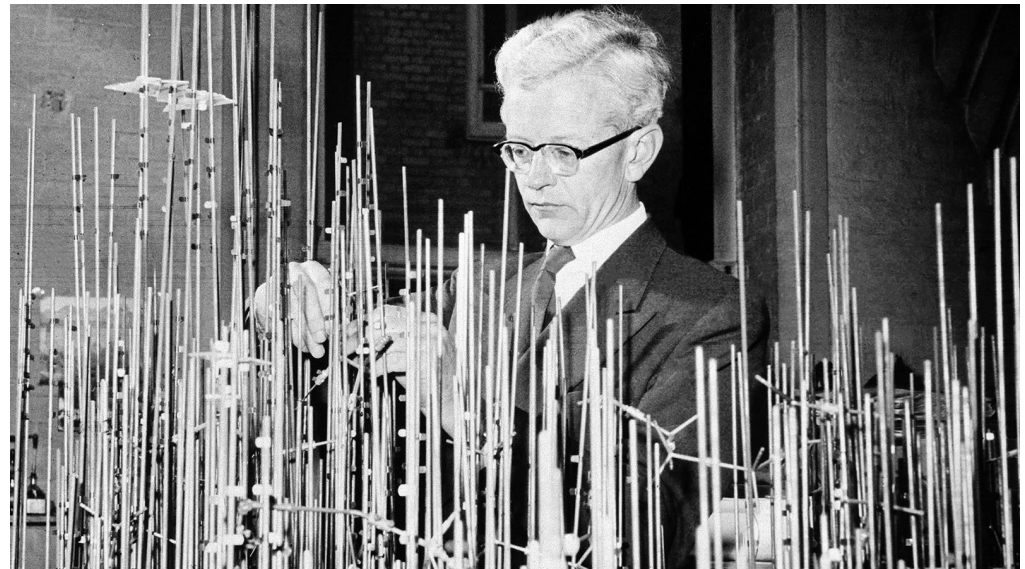
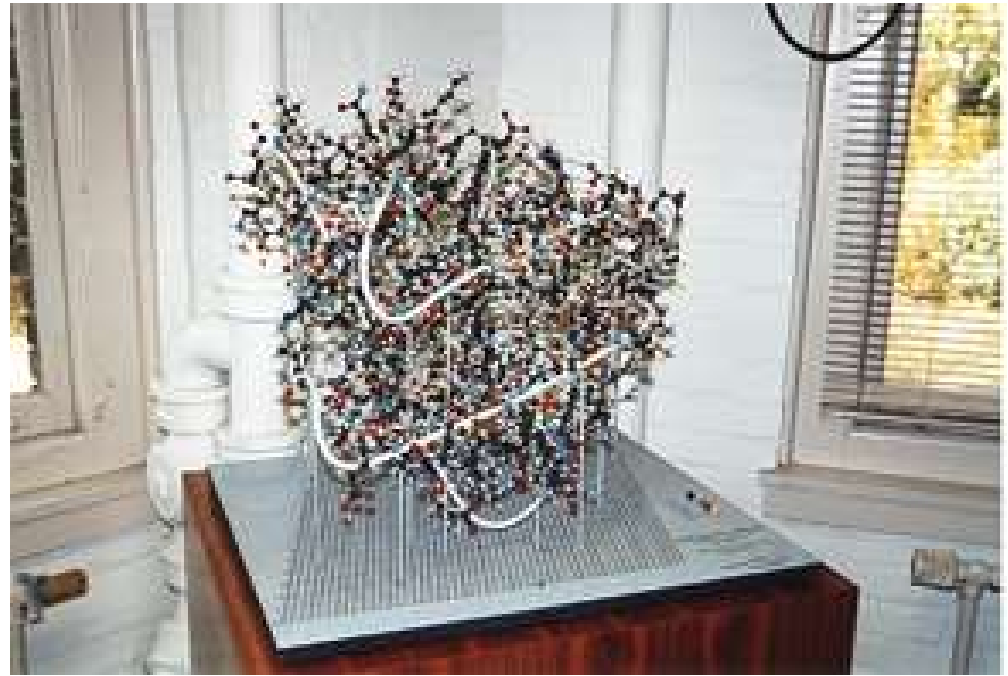
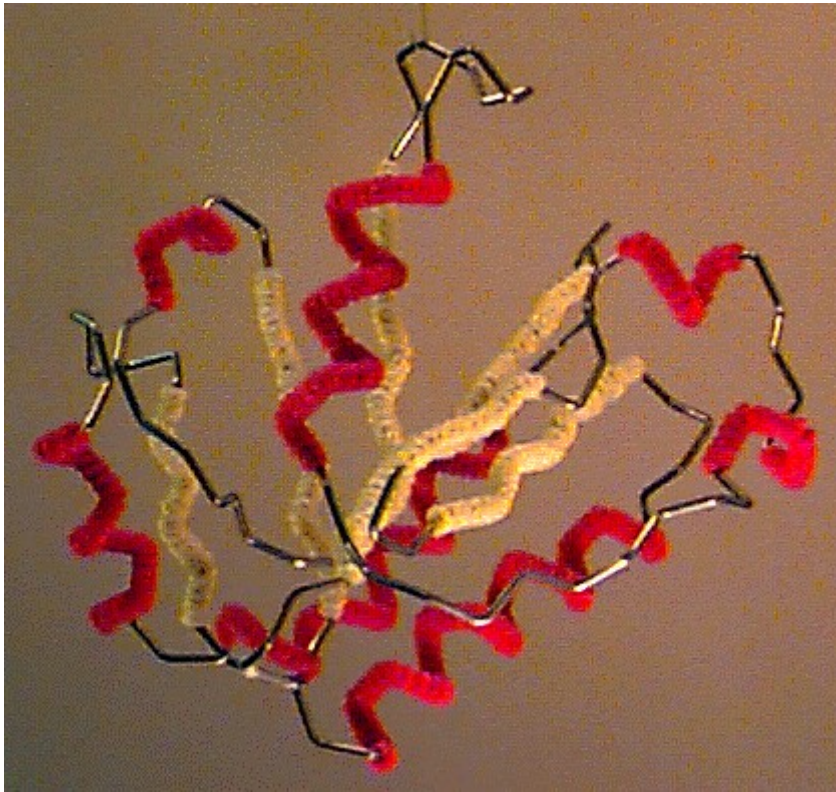
Metric	Value
Clashscore	1.8
Ramachandran outliers	0.0%
Rotamer outliers	0.0%

Display Files Download Files

- FASTA Sequence
- PDB Format
- PDB Format (gz)
- PDBx/mmCIF Format**
- PDBx/mmCIF Format (gz)
- PDBML/XML Format (gz)
- Biological Assembly 1
- Structure Factors (CIF)**
- Structure Factors (CIF - gz)
- 2fo-fc Map (DMNA)

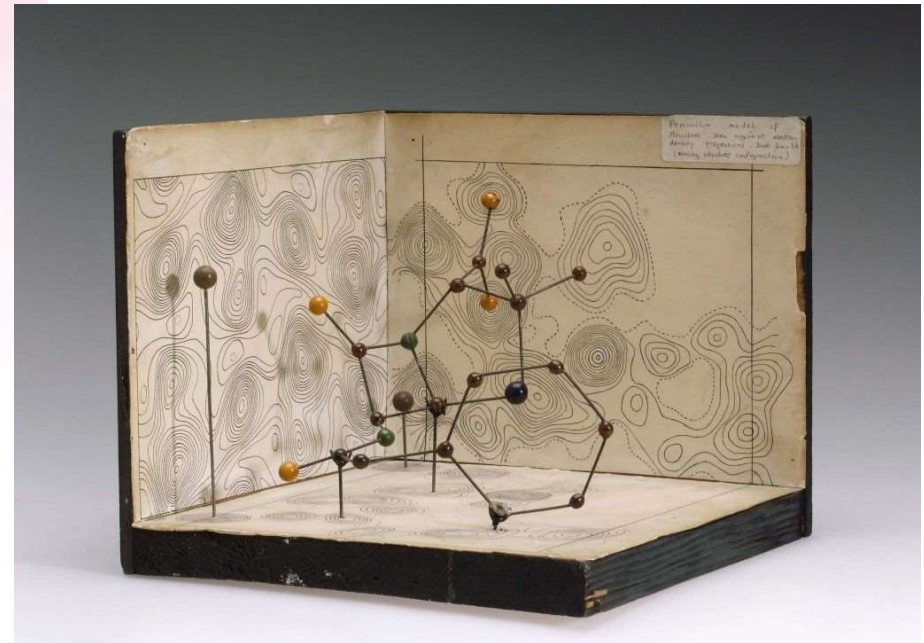
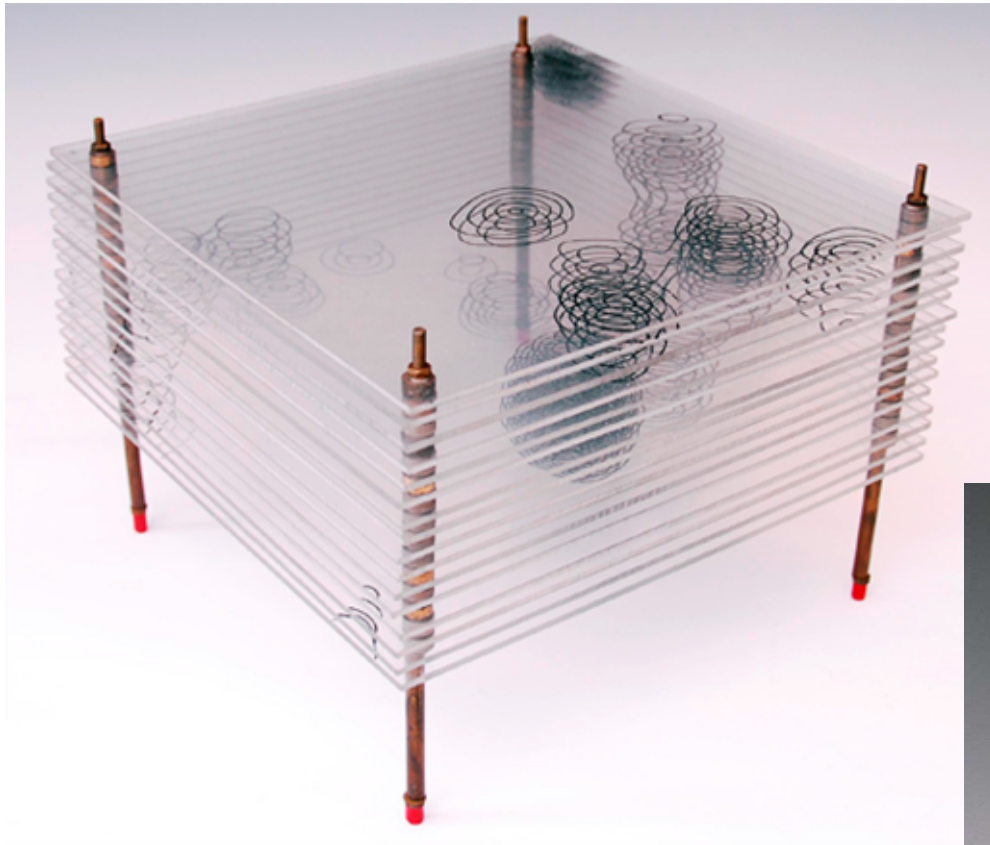
for the electron density!!!

# Graphical software: in the old days...





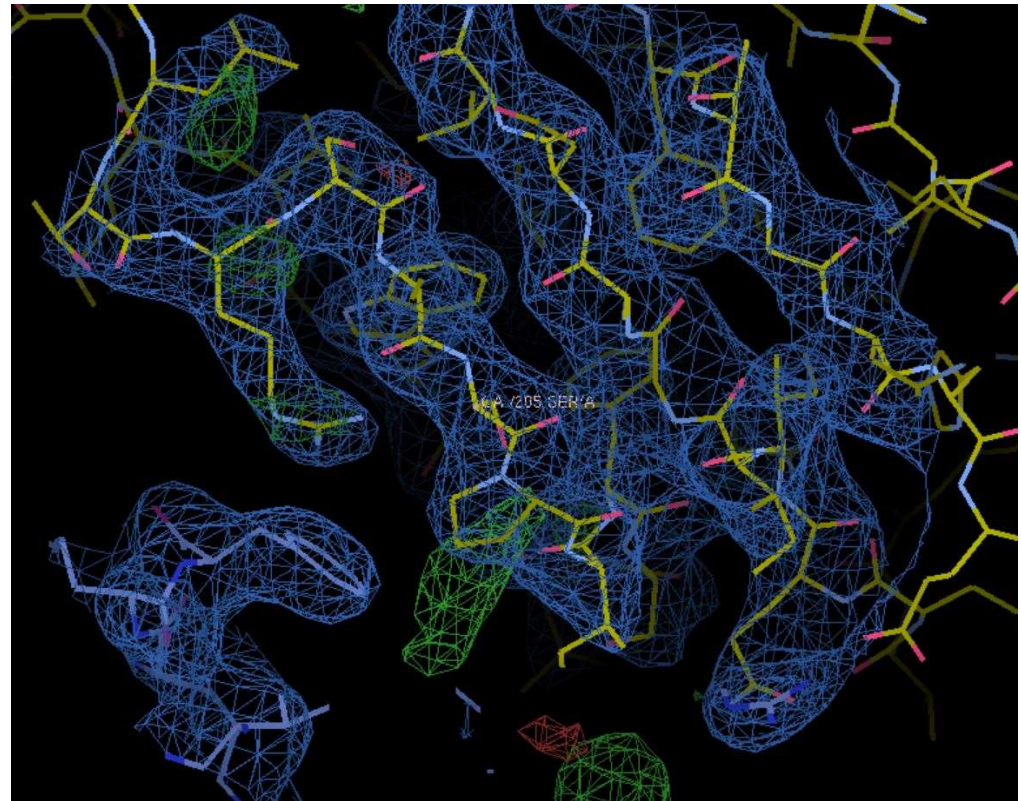
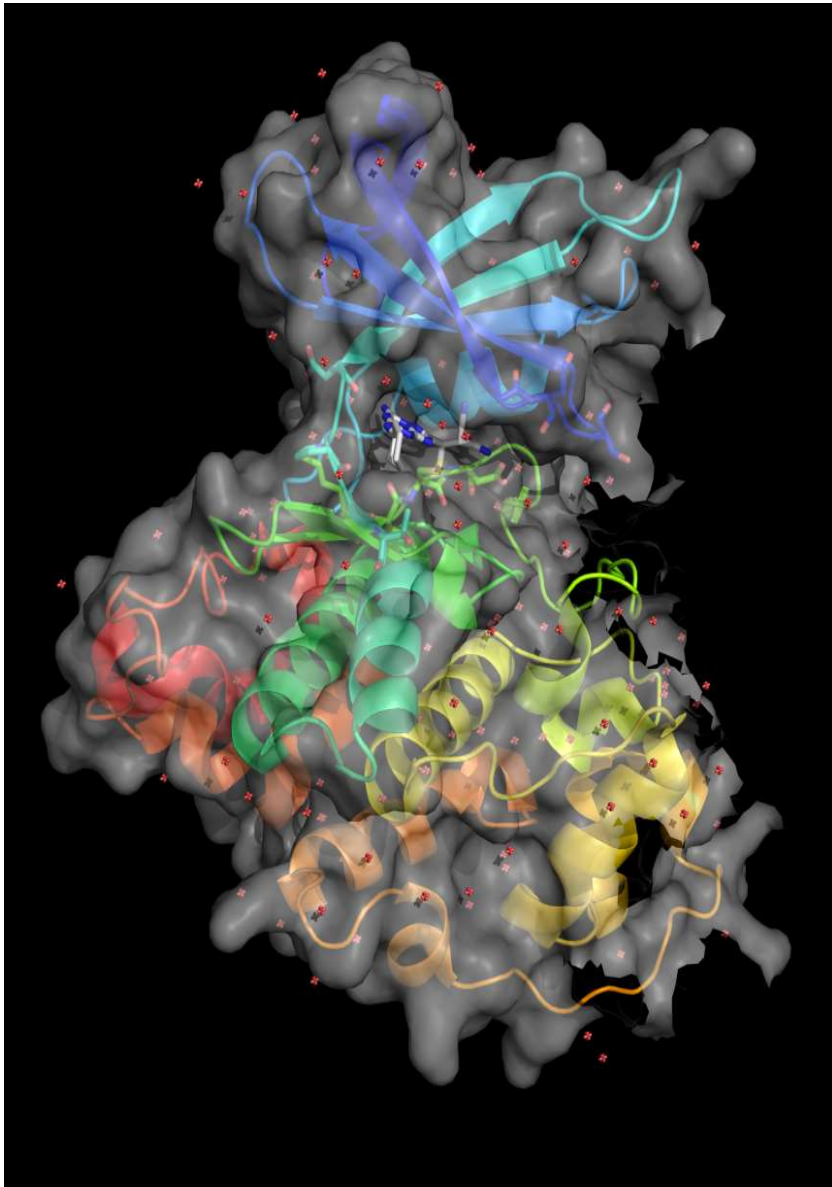
# Graphical software: in the old days...



# Graphical software: in the old days...



# Graphical software:... today

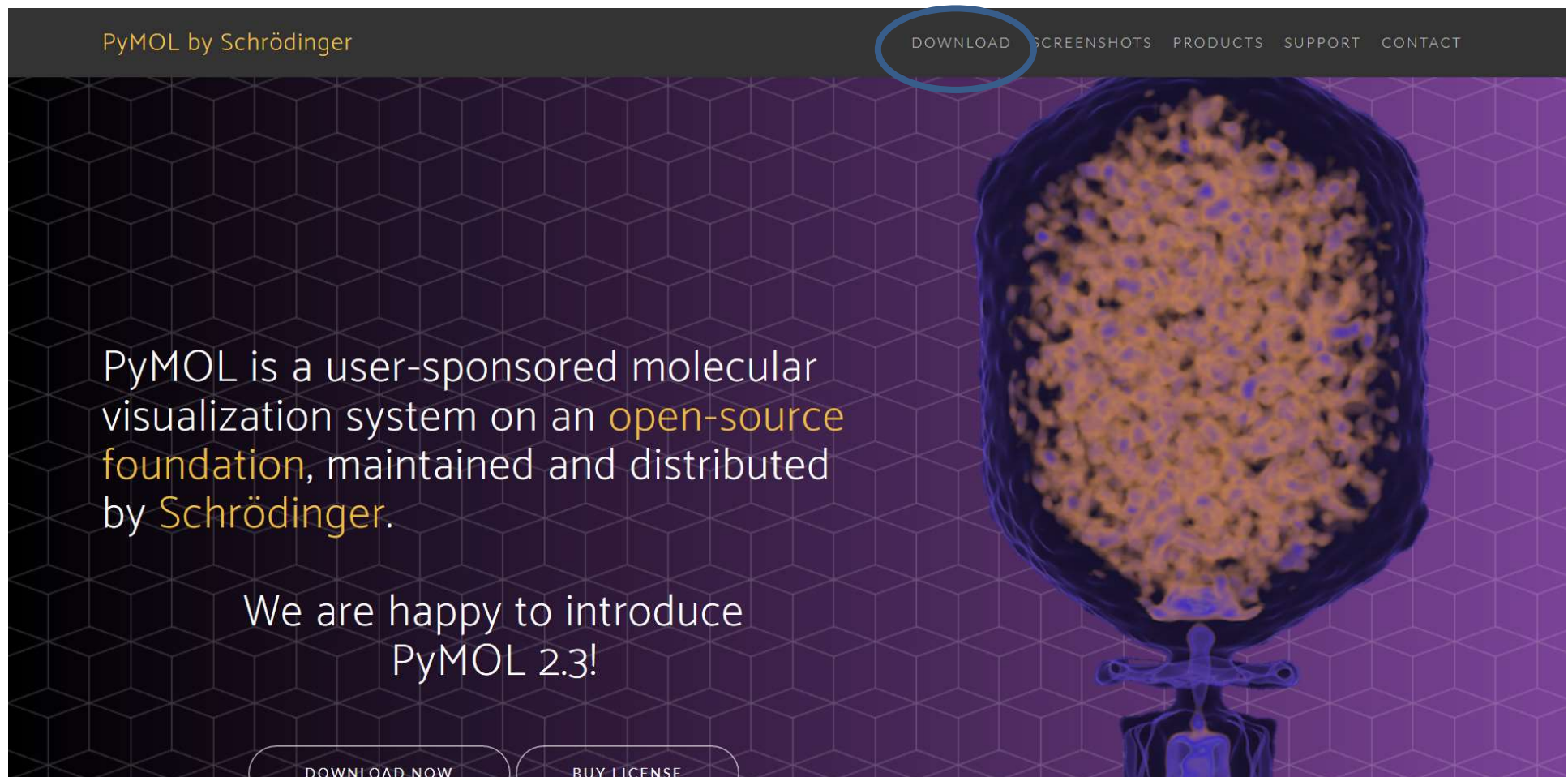


# Graphical software:... today



# Graphical software: Pymol

1. Download: <https://pymol.org/2/>



The image shows a screenshot of the PyMOL website homepage. The background is a dark purple with a subtle geometric pattern. On the right side, there is a large, glowing 3D molecular model of a protein structure, rendered in shades of orange and blue. The text on the page is white and yellow. At the top left, it says "PyMOL by Schrödinger". At the top right, there is a navigation menu with the word "DOWNLOAD" circled in blue. Below the navigation menu, the main text reads: "PyMOL is a user-sponsored molecular visualization system on an open-source foundation, maintained and distributed by Schrödinger." Below this, it says "We are happy to introduce PyMOL 2.3!". At the bottom, there are two buttons: "DOWNLOAD NOW" and "BUY LICENSE".

PyMOL by Schrödinger

DOWNLOAD SCREENSHOTS PRODUCTS SUPPORT CONTACT

PyMOL is a user-sponsored molecular visualization system on an **open-source foundation**, maintained and distributed by **Schrödinger**.

We are happy to introduce  
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# Graphical software: Pymol

1. Download: <https://pymol.org/2/>

PyMOL by Schrödinger

[DOWNLOAD](#) [SCREENSHOTS](#) [PRODUCTS](#) [SUPPORT](#) [CONTACT](#)

## Download PyMOL 2.3

Version 2.3.5 - Updated March 3rd 2020 ([installation instructions](#))

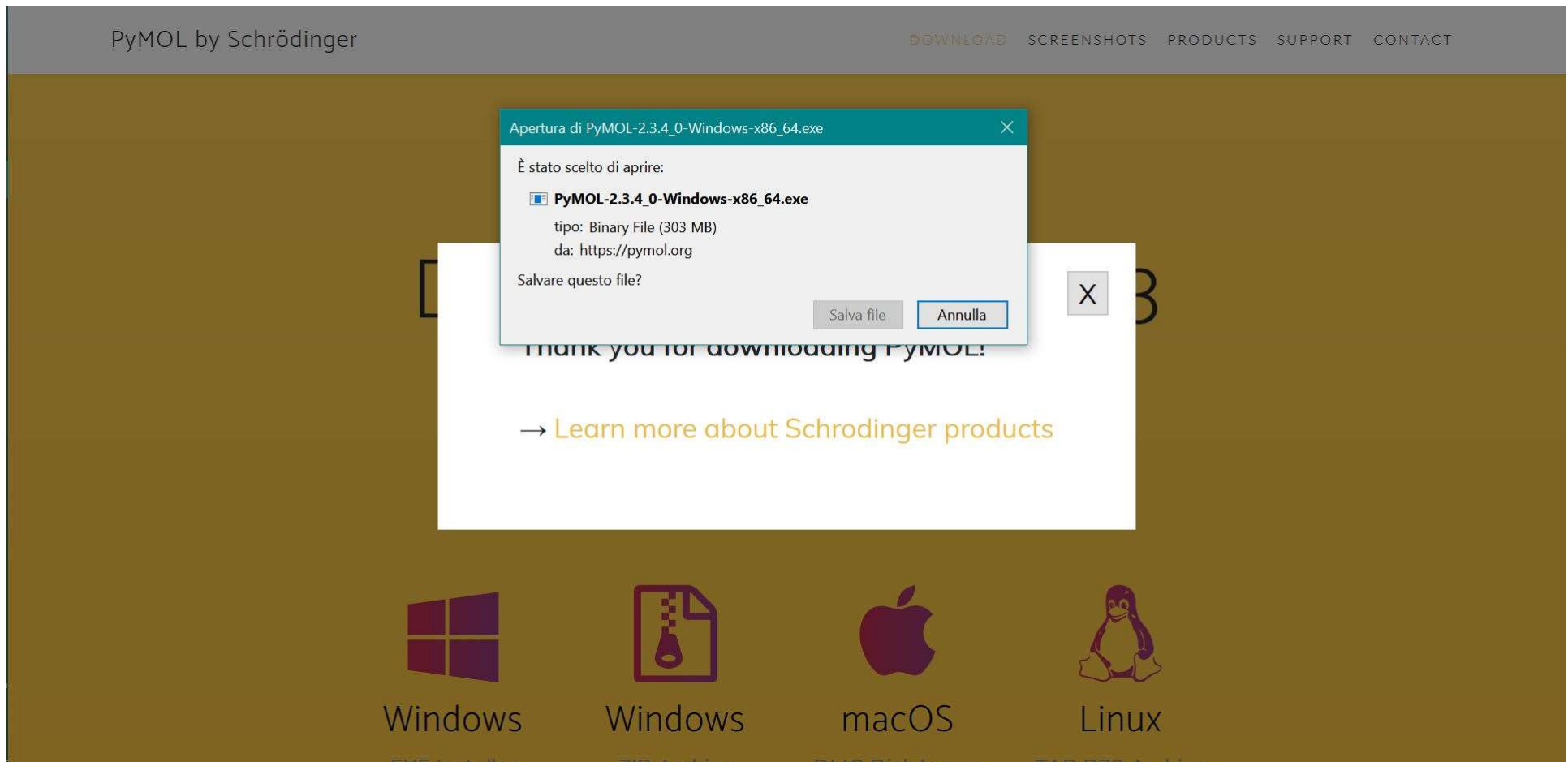
For previous versions and Python 2.7 bundles, [see here](#).

**These bundles include Python 3.7**



# Graphical software: Pymol

1. Download: <https://pymol.org/2/>



## 2. Open and load pdb file

The image shows two overlapping windows from the PyMOL software. The top window is the 'PyMOL Tcl/Tk GUI' and the bottom window is the 'PyMOL Viewer'.

**PyMOL Tcl/Tk GUI**

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help Tutorial

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This PyMOL Executable Build incorporates Open-Source PyMOL 0.99rc6.

Reset Zoom Draw Ray Rock  
Unpick Deselect Get View  
< < Stop Play > >| MClear  
Command Builder

**PyMOL Viewer**

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**Warren L. DeLano, Ph.D.** Principal Scientist  
**Joni W. Lam,** Operations Manager

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**DeLano Scientific LLC**  
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South San Francisco, CA 94080  
United States of America  
650-872-0942 Fax: 650-872-0273  
[www.delanoscientific.com](http://www.delanoscientific.com)

all A S H L C

Mouse Mode 3-Button Viewing  
Buttons L M R Wheel  
& Keys Rota Move MovZ Slab  
Shift +Box -Box Clip MovS  
Ctrl +/- PkAt Pk1 MvSZ  
CtSh Sele Orig Clip MovZ  
SnglClk +/- Cent Menu  
DblClk Menu - PkAt  
Selecting Residues  
Frame [ 1 / 11 0/sec



## 2. Open and load pdb file

The screenshot shows the PyMOL Tk GUI interface. The 'File' menu is open, displaying options such as 'Open...', 'Save Session', 'Save Session As...', 'Save Molecule...', 'Save Image...', 'Save Movie...', 'Log...', 'Resume...', 'Append...', 'Close Log', 'Run...', 'Quit', and 'Reinitialize'. The main window displays a 'Terms of Usage' dialog box for the PyMOL Executable Build. The dialog text includes copyright information for DeLano Scientific LLC (2006) and outlines the terms for use, including requirements for sponsorship and acknowledgment. A logo for DeLano Scientific LLC is visible, featuring a molecular structure with blue spheres and black arrows. The dialog also provides contact information for Warren L. DeLano, Ph.D. and Joni W. Lam, and a link to the funding page. A terminal window in the bottom right corner shows the command 'all' and a list of mouse controls for 3-button viewing, including buttons for rotation, translation, and zooming.

PyMOL Tk GUI

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help Tutorial

Open...  
Save Session  
Save Session As...  
Save Molecule...  
Save Image...  
Save Movie...  
Log...  
Resume...  
Append...  
Close Log  
Run...  
Quit  
Reinitialize

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Maintenance and/or Support Subscription may be required  
this Build beyond a finite honor-system evaluation period.  
//www.pymol.org/funding.html for more information.  
able Build incorporates Open-Source PyMOL 0.99rc6.

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All non-sponsors who use this Build to prepare a publication, presentation, animation, or web site must therein acknowledge PyMOL by name. Failure to do so creates a sponsorship obligation in the form of a liability for payment of current-year PyMOL subscription fees to DeLano Scientific LLC.

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<http://www.pymol.org/funding.html> or email: [sales@delsci.com](mailto:sales@delsci.com)

Thank you for your cooperation, support, and participation.

**Warren L. DeLano, Ph.D.** Principal Scientist  
**Joni W. Lam,** Operations Manager

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Please purchase a subscription so that we can continue to develop PyMOL as open-source software for research, drug discovery, and education!

**DeLano Scientific LLC**  
400 Oyster Point Blvd. Ste 213  
South San Francisco, CA 94080  
United States of America  
650-872-0942 Fax: 650-872-0273  
[www.delanoscientific.com](http://www.delanoscientific.com)

all A S H L C

Mouse Mode 3-Button Viewing  
Buttons L M R Wheel  
& Keys Rota Move MovZ Slab  
Shft +Box -Box Clip MovS  
Ctrl +/- PkAt Pk1 MvSZ  
CtSh Sele Orig Clip MovZ  
SnglClk +/- Cent Menu  
Db1Clk Menu - PkAt  
Selecting Residues  
Frame [ 1 / 1 ] 0/sec

## 2. Open and load pdb file

The screenshot displays the PyMOL software interface. The top window, titled "PyMOL Tcl/Tk GUI", contains a menu bar (File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Plugin, Help, Tutorial) and a command console. The console shows the following text:

```
COMPND  MOL_ID: 1;  
COMPND  2 MOLECULE: INSULIN;  
COMPND  3 CHAIN: A, C;  
COMPND  4 MOL_ID: 2;  
COMPND  5 MOLECULE: INSULIN;  
COMPND  6 CHAIN: B, D  
ObjectMolecule: Read secondary structure assignments.  
ObjectMolecule: Read crystal symmetry information.  
Symmetry: Found 9 symmetry operators.  
CmdLoad: "C:/Users/Rita/Downloads/1zni.pdb" loaded as "1zni".
```

Below the command console is a toolbar with buttons for Reset, Zoom, Draw, Ray, Rock, Unpick, Deselect, Get View, navigation arrows, Stop, Play, MClear, Command, and Builder.

The bottom window, titled "PyMOL Viewer", shows a 3D molecular model of insulin. The protein backbone is rendered in green sticks, with side chains in blue and red. The model is set against a black background. To the right of the viewer is a legend table:

all	A	S	H	L	C
1zni	A	S	H	L	C

At the bottom right of the viewer window, there is a mouse control panel with the following text:

```
Mouse Mode 3-Button Viewing  
Buttons L M R Wheel  
& Keys Rota Move MovZ Slab  
Shft +Box -Box Clip MovS  
Ctrl +/- PKAt Pk1 MvSZ  
CtSh Sele Orig Clip MovZ  
SnglClk +/- Cent Menu  
DblClk Menu - PKAt  
Selecting Residues  
Frame [ 1 / 1 ] 28/sec
```

# 3. Menu options

The screenshot displays the PyMOL software interface. At the top, the title bar reads "PyMOL Td/Tk GUI". Below it is a menu bar with options: File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Plugin, Help, and Tutorial. A command console on the left shows the following text:

```
COMPND  MOL_ID: 1;  
COMPND  2 MOLECULE: INSULIN;  
COMPND  3 CHAIN: A, C;  
COMPND  4 MOL_ID: 2;  
COMPND  5 MOLECULE: INSULIN;  
COMPND  6 CHAIN: B, D  
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Symmetry: Found 9 symmetry operators.  
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```

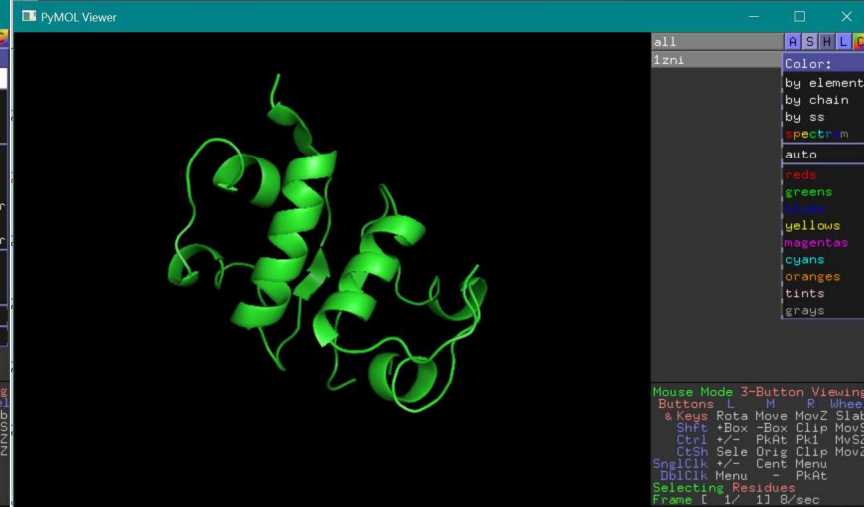
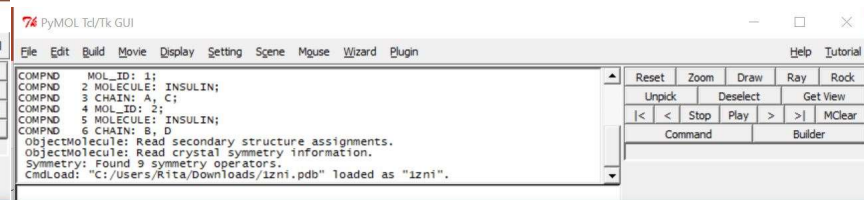
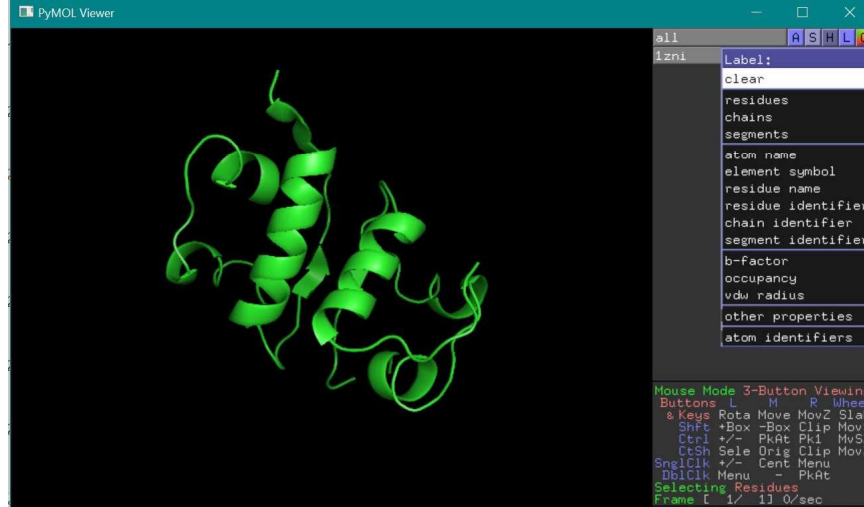
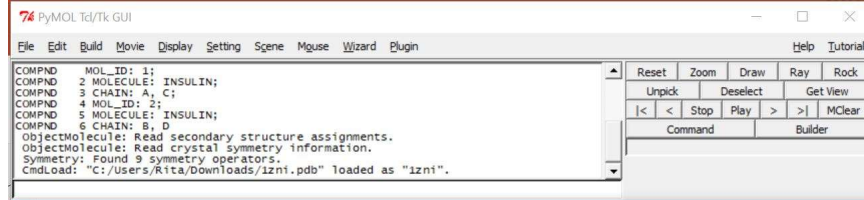
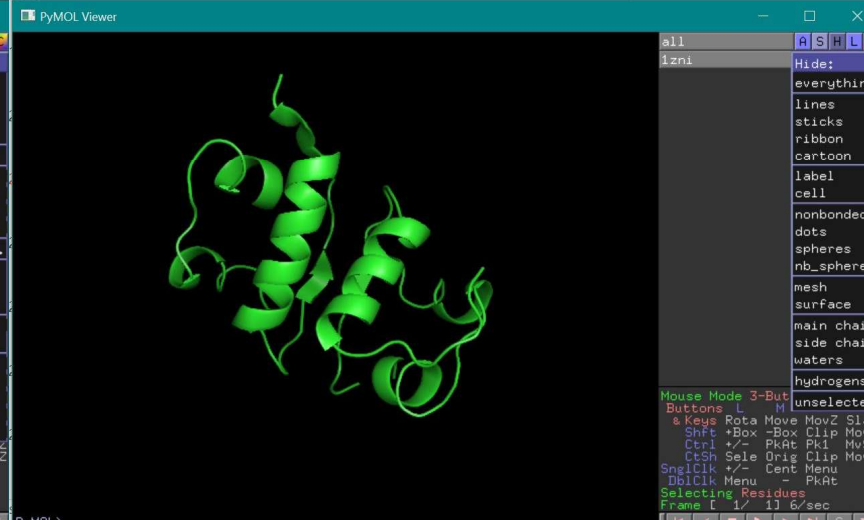
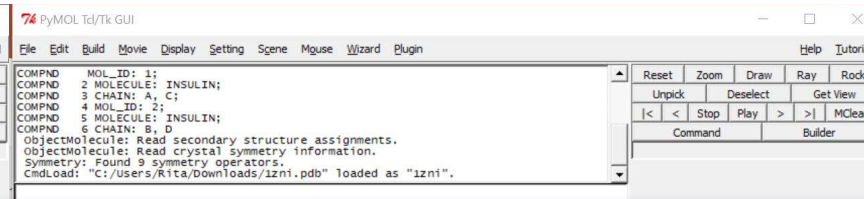
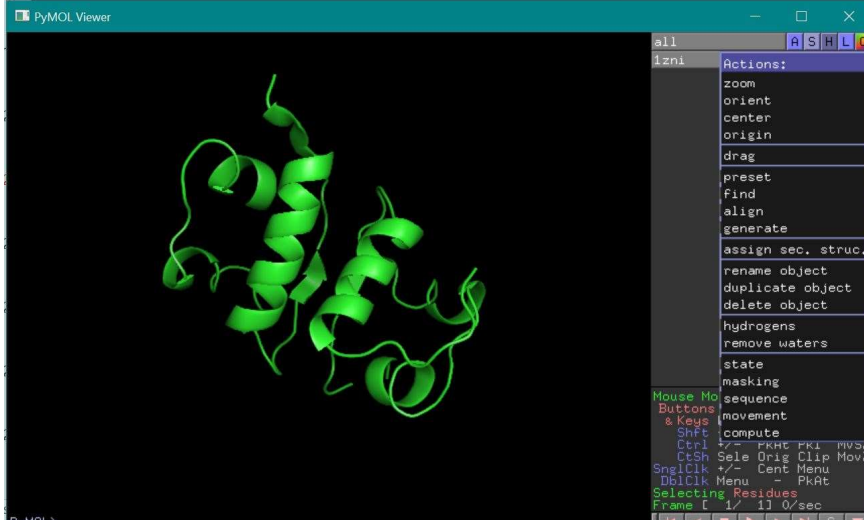
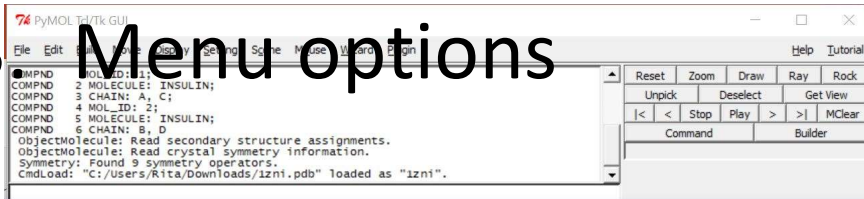
To the right of the console is a toolbar with buttons: Reset, Zoom, Draw, Ray, Rock, Unpick, Deselect, Get View, navigation arrows, Command, and Builder. The main window, titled "PyMOL Viewer", shows a 3D molecular model of insulin. A context menu is open over the model, listing various display options:

As:	Show:
lines	as
sticks	lines
ribbon	sticks
cartoon	ribbon
label	cartoon
cell	label
nonbonded	cell
dots	nonbonded
spheres	dots
nb_spheres	spheres
mesh	nb_spheres
surface	mesh
	surface
	organic
	main chain
	side chain
	disulfides

Below the menu, the status bar displays mouse controls and frame information:

```
Mouse Mode 3-Button Viewing  
Buttons L M R Wheel  
& Keys Rota Move MovZ Slab  
Shft +Box -Box Clip MovS  
Ctrl +/- PkAt Pk1 MvSZ  
CtSh Sele Orig Clip MovZ  
SnglClk +/- Cent Menu  
DblClk Menu - PkAt  
Selecting Residues  
Frame [ 1/ 1] 11/sec
```

# 3 Menu options





# Graphical software: UCSF Chimera

1. Download: [www.cgl.ucsf.edu/chimera/](http://www.cgl.ucsf.edu/chimera/)

**UCSF CHIMERA**  
an Extensible Molecular Modeling System

UCSF Chimera is a highly extensible program for interactive visualization and analysis of molecular structures and related data, including density maps, supramolecular assemblies, sequence alignments, docking results, trajectories, and conformational ensembles. High-quality images and animations can be generated. Chimera includes complete documentation and several tutorials, and can be downloaded free of charge for academic, government, nonprofit, and personal use. Chimera is developed by the [Resource for Biocomputing, Visualization, and Informatics \(RBVI\)](#), supported in part by the [National Institutes of Health \(P41-GM103311\)](#).

UCSF ChimeraX (or simply ChimeraX) is the next-generation molecular visualization program from the RBVI, following UCSF Chimera.

**Feature Highlight**

**B-Factor Coloring**

A structure can be colored to show values of an attribute such as atomic B-factor. The image includes a molecular surface that has been clipped and capped, 2D labels, and a color key. Color Zone was used to color the planar cross-section of the surface (see [image how-to](#)).

(More features...)

Galactose/Glucose-Binding Protein (2gbp)

B-factor ( $\text{\AA}^2$ )

2 30 50

**Chimera Search**

Go

Google™ Search

**News**

**November 13, 2019**

Chimera production release 1.14 is now available. See the [release notes](#) for what's new.

**September 21, 2019**

A production release candidate (version 1.14) is available; please try it and report any problems. See the [release notes](#) for what's new.

**November 17, 2018**

Chimera production release 1.13.1 is now available; see the [release notes](#) for what's new. The Mac version requires OS 10.10 or later.

(Previous news...)

**Upcoming Events**

**Recent Citations**


Measurement of atom resolvability in cryo-EM maps with Q-scores, Pintilie C, Zhou K, et al. *Nat Methods*. 2020

**Gallery Sample**

**Thermosome**

# Graphical software: UCSF Chimera

1. Download: [www.cgl.ucsf.edu/chimera/](http://www.cgl.ucsf.edu/chimera/)



**UCSF CHIMERA**  
an Extensible Molecular Modeling System

**Download Chimera**

- [Daily Builds](#)
- [Snapshot Releases](#)
- [Unsupported Releases](#)
- [Old Releases](#)
- [Bug Tracking System](#)
- [Licensing Information](#)
- [Experimental Chimera Features](#)
- [Plug-ins on the Web](#)
- [Graphics Driver Bugs](#)
- [Benchmark Results](#)
- [Chimera Source Code](#)
- [Cygwin Source Code](#)

**Current Production Releases**

- See the [release notes](#) for a list of new features and other information.
- For [more recent changes](#), use the [snapshot](#) and [daily](#) builds; they are less tested but usually reliable.

**64-bit Releases:**

Platform	Installer, Size, and Checksum	Date	Notes
Microsoft Windows 64-bit	<a href="#">chimera-1.14-win64.exe</a> Size: 152229635 bytes MD5: a3eddc25f84e55c4c49ff6f6f7643b	Nov 13, 2019	<a href="#">Instructions</a> <a href="#">Documentation</a> Runs on Windows 7 or later.
Mac OS X 64-bit	<a href="#">chimera-1.14-mac64.dmg</a> Size: 135741903 bytes MD5: c763aa87af928ae6dc7d39a8f6bf92d5	Nov 13, 2019	<a href="#">Instructions</a> <a href="#">Documentation</a> Runs on Mac OS X 10.10 or later.

**Quick Links**

**Documentation**

- [Getting Started](#)
- [User's Guide](#)
- [Command Index](#)
- [Tutorials and Videos](#)
- [Guide to Volume Data](#)
- [Release Notes](#)

**Download**

- [What's New in Daily Builds](#)
- [Map of Download Locations](#)

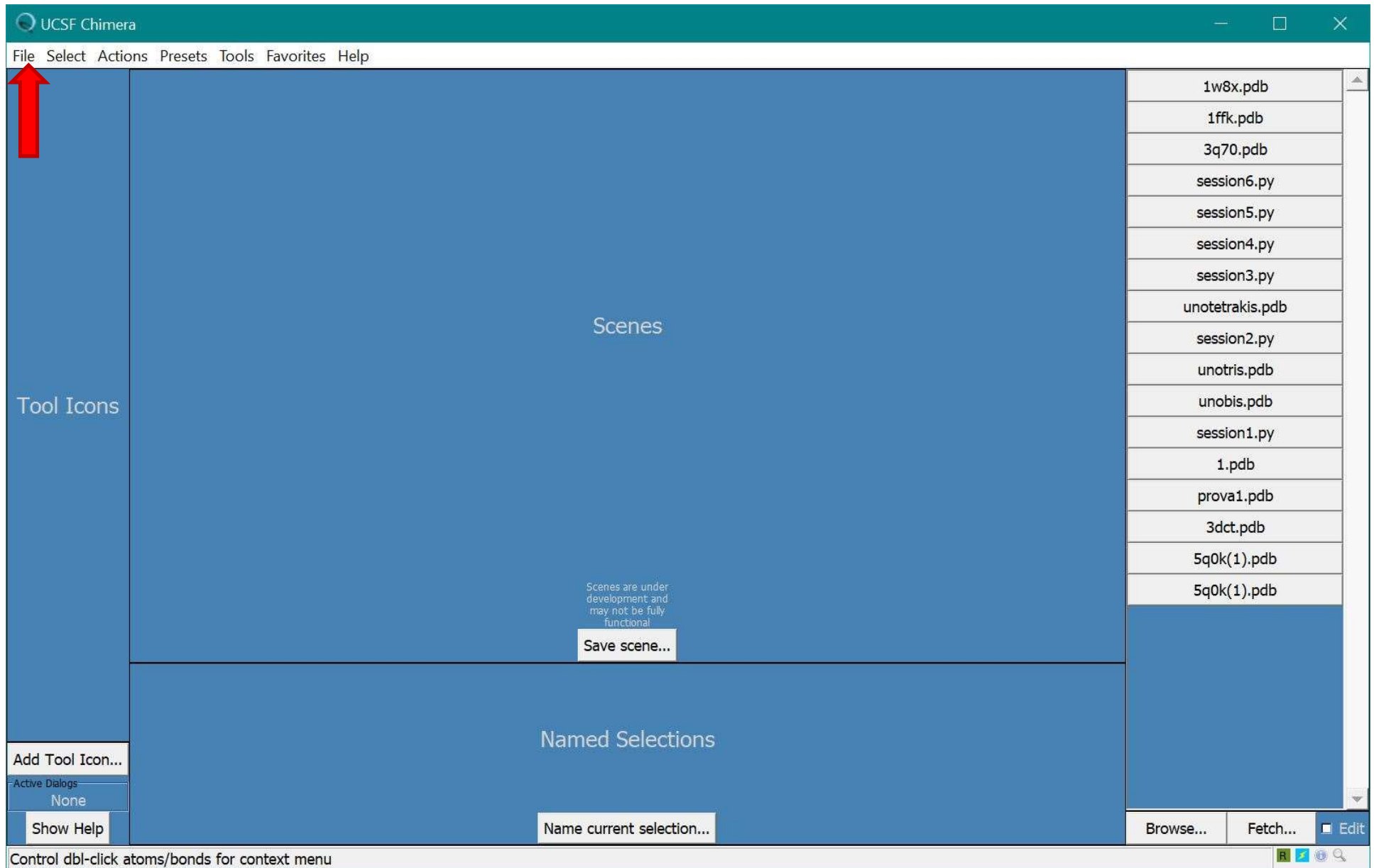
**Galleries**

- [Image Gallery](#)
- [Animation Gallery](#)

**Publications**

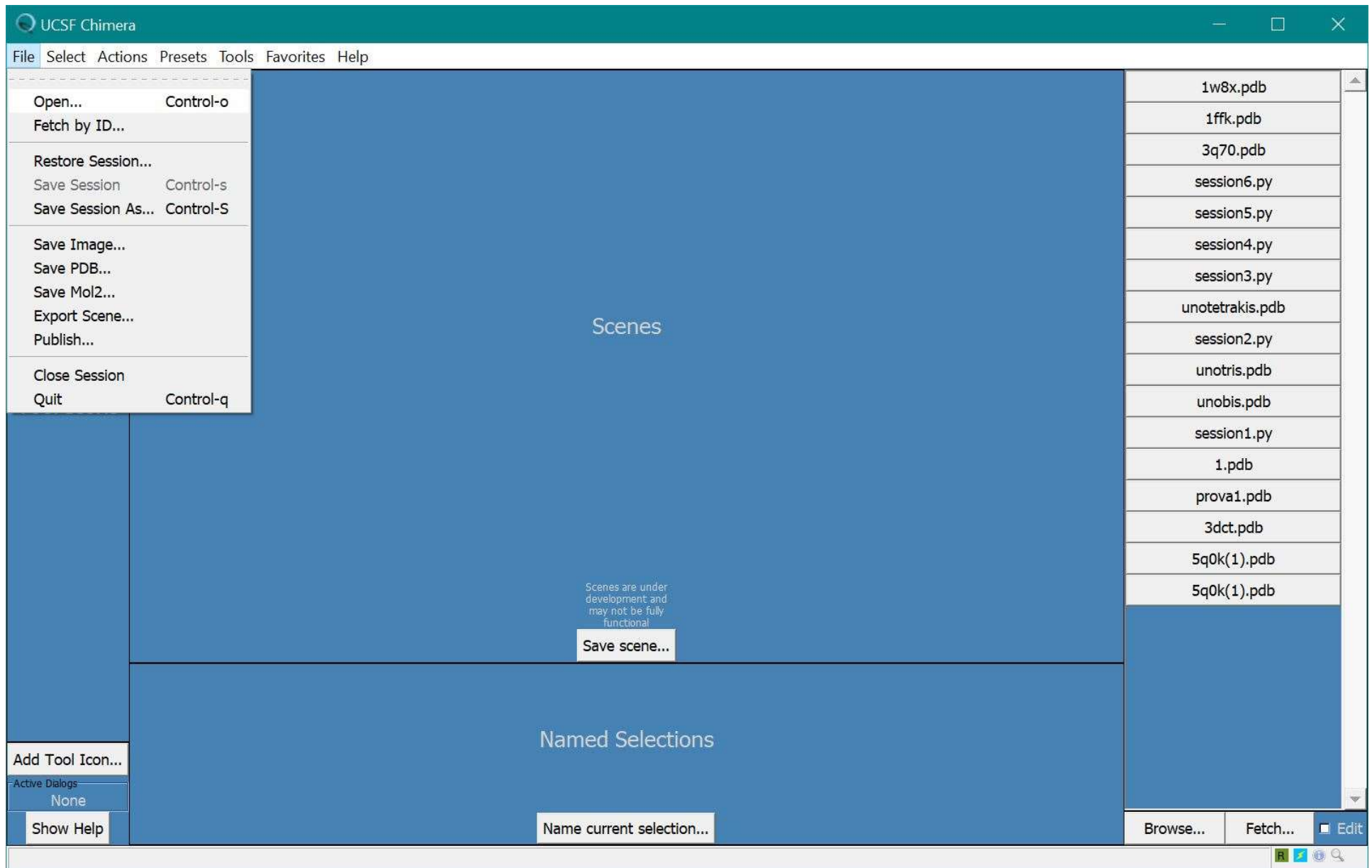
- [Related Databases and Software](#)
- [Citing Chimera](#)
- [Contact Us](#)

## 2. Open and load pdb file

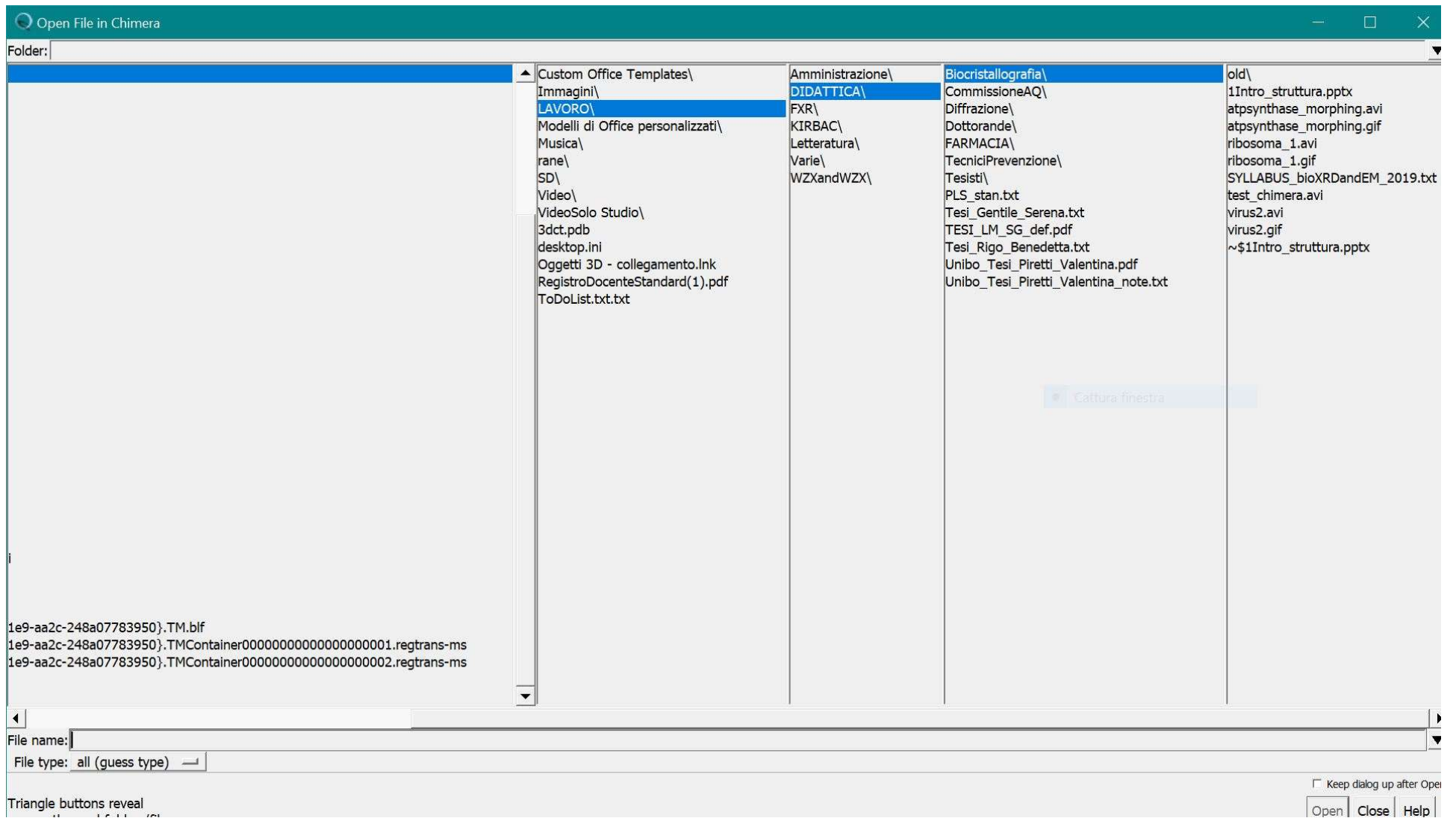




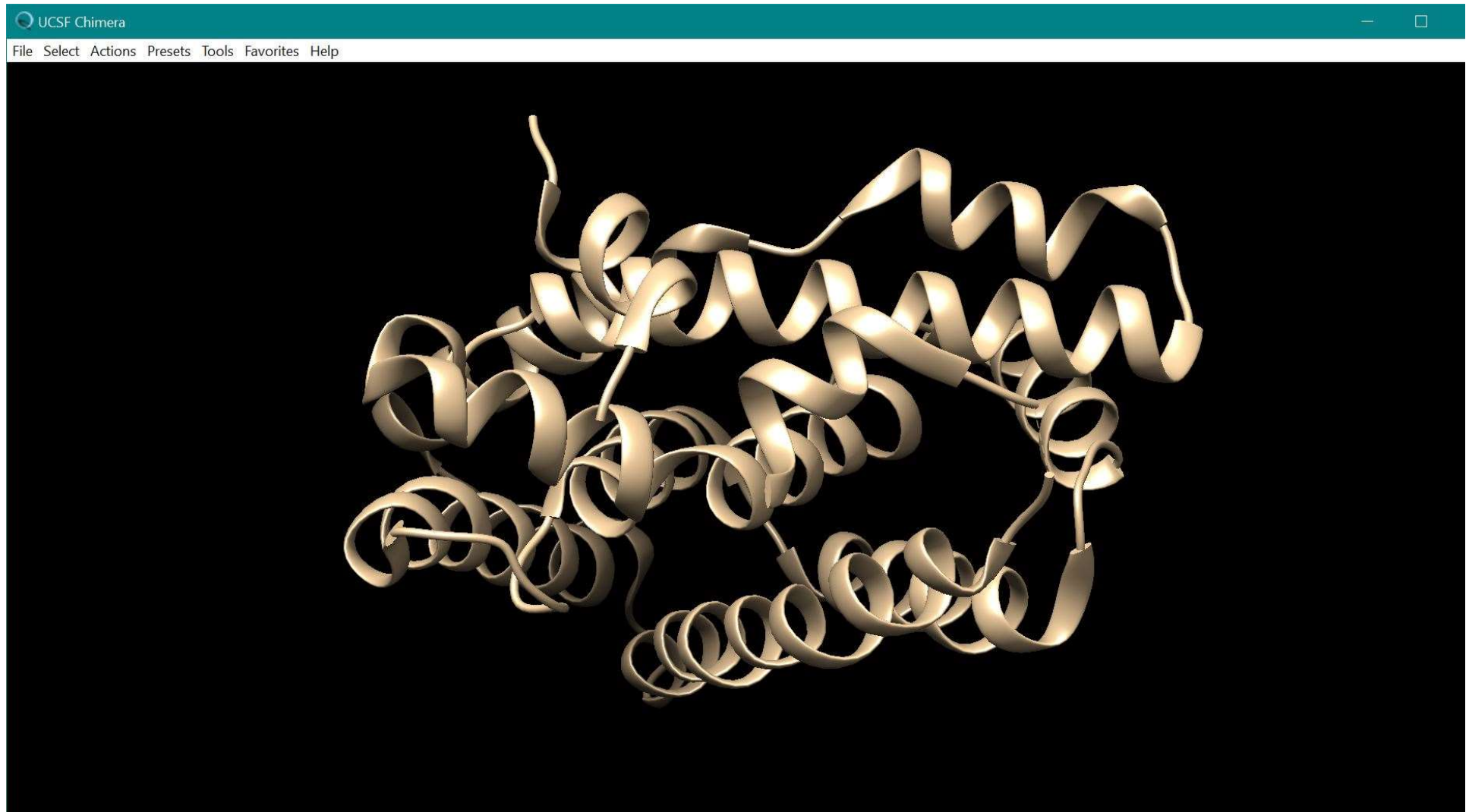
## 2. Open and load pdb file



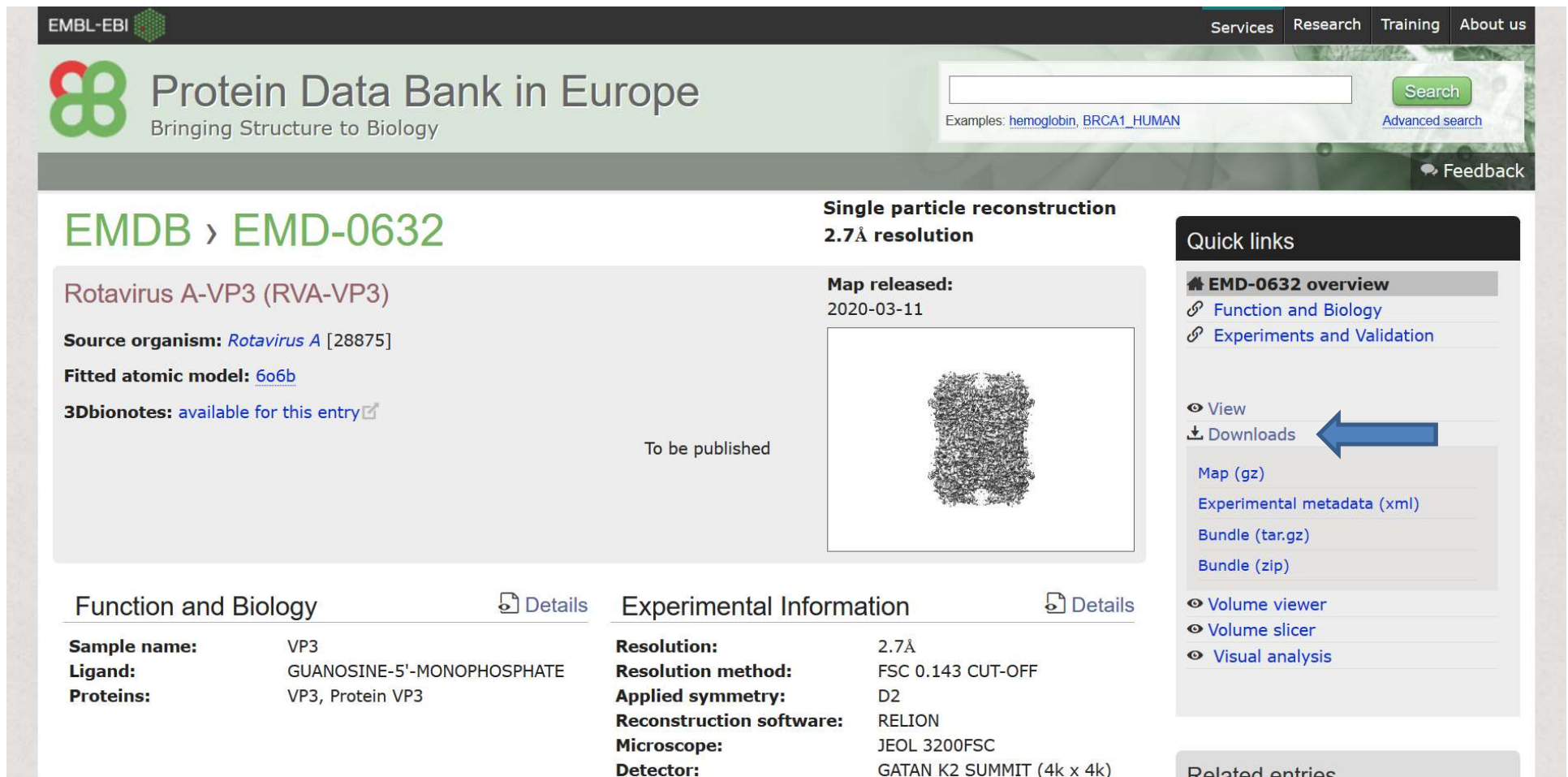
## 2. Open and load pdb file



## 2. Open and load pdb file



### 3. Load a map file (electron density!) (www.ebi.ac.uk/pdbe/emdb/)



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**Protein Data Bank in Europe**  
Bringing Structure to Biology

Search [Advanced search](#)

Examples: [hemoglobin](#), [BRCA1\\_HUMAN](#)

Feedback

## EMDB > EMD-0632

**Rotavirus A-VP3 (RVA-VP3)**

Source organism: [Rotavirus A](#) [28875]

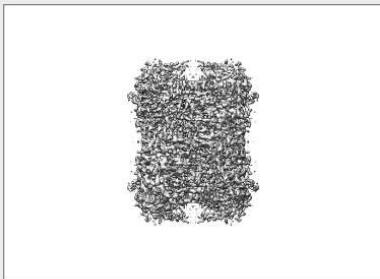
Fitted atomic model: [6o6b](#)

3Dbionotes: [available for this entry](#)

To be published

**Single particle reconstruction**  
**2.7 Å resolution**

Map released:  
2020-03-11



**Function and Biology** [Details](#) | **Experimental Information** [Details](#)

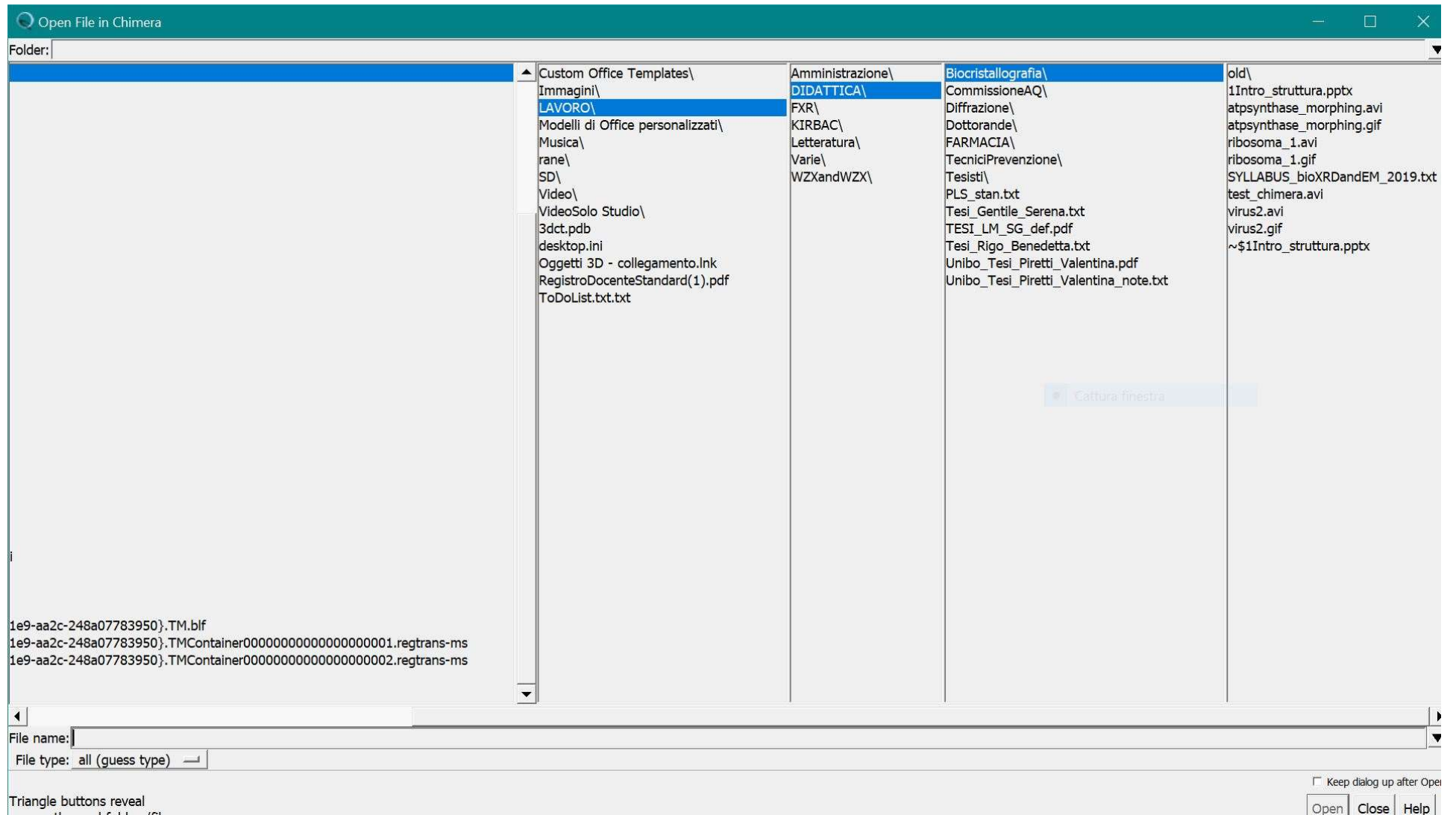
<b>Sample name:</b>	VP3	<b>Resolution:</b>	2.7 Å
<b>Ligand:</b>	GUANOSINE-5'-MONOPHOSPHATE	<b>Resolution method:</b>	FSC 0.143 CUT-OFF
<b>Proteins:</b>	VP3, Protein VP3	<b>Applied symmetry:</b>	D2
		<b>Reconstruction software:</b>	RELION
		<b>Microscope:</b>	JEOL 3200FSC
		<b>Detector:</b>	GATAN K2 SUMMIT (4k x 4k)

**Quick links**

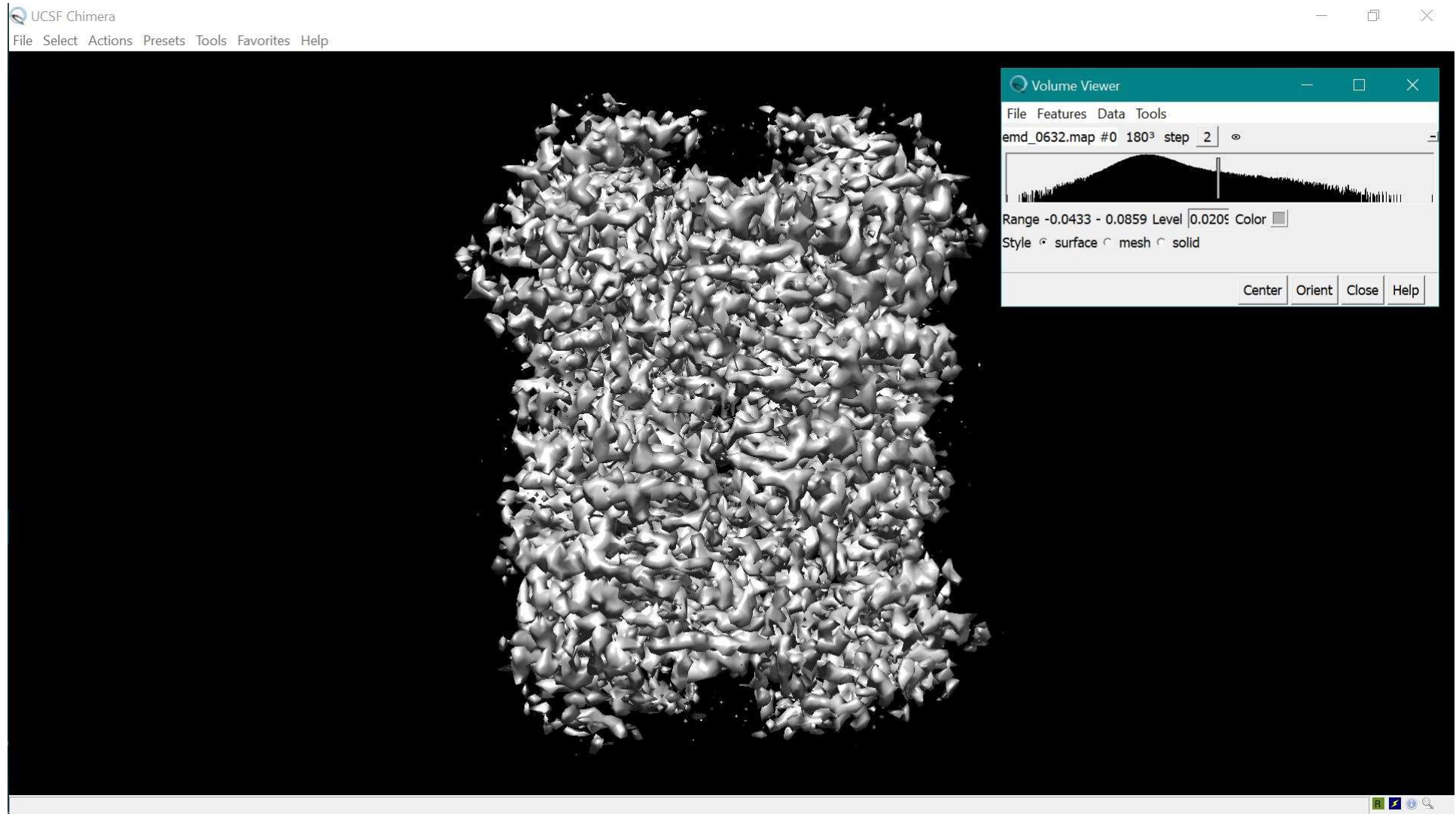
- EMD-0632 overview**
- [Function and Biology](#)
- [Experiments and Validation](#)
- [View](#)
- Downloads** ←
- [Map \(gz\)](#)
- [Experimental metadata \(xml\)](#)
- [Bundle \(tar.gz\)](#)
- [Bundle \(zip\)](#)
- [Volume viewer](#)
- [Volume slicer](#)
- [Visual analysis](#)

**Related entries**

### 3. Load a map file (electron density!)



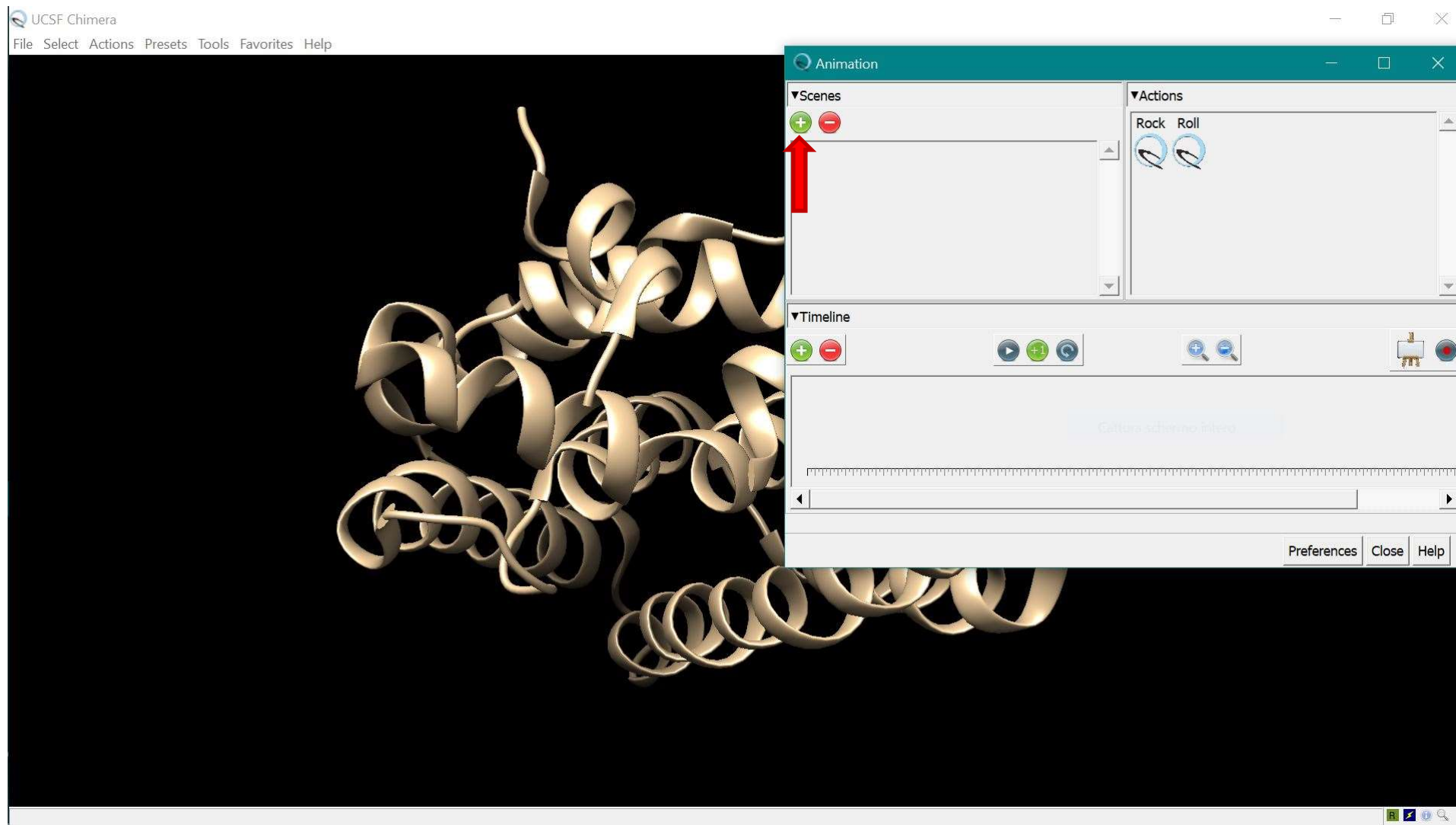
### 3. Load a map file (electron density!)



# 99.Animation!



# 99.Animation!





# 99.Animation!

The image shows a screenshot of the UCSF Chimera software interface. The main window displays a 3D ribbon representation of a protein structure, colored in a light tan or beige hue, set against a black background. The protein is a complex, multi-domain structure with several loops and helices. In the top-left corner, the UCSF Chimera logo and menu items (File, Select, Actions, Presets, Tools, Favorites, Help) are visible. On the right side, the 'Animation' panel is open, showing a 'Scenes' section with four numbered slots (1, 2, 3, 4) and an 'Actions' section with two actions labeled 'Rock' and 'Roll'. Below these is a 'Timeline' section with a play button, a plus sign, a minus sign, and a search icon. A red curved arrow points from the 'Scenes' section down to the 'Timeline' section, indicating the relationship between the two. At the bottom right of the Animation panel, there are buttons for 'Preferences', 'Close', and 'Help'. The overall interface is clean and professional, typical of scientific software.

# 99.Animation!

The image shows the UCSF Chimera software interface. The main window displays a protein structure as a yellow ribbon on a black background. The 'Animation' panel is open on the right, showing a timeline with four scenes labeled '1: 4', '2: 2', '3: 1', and '4: 1'. A red arrow points to the play button in the timeline controls, and another red arrow points to the stop button. The 'Actions' panel shows 'Rock' and 'Roll' actions. The status bar at the bottom indicates 'Movie saved to \C:Users\...\Bicristallografia\test\_chimera.avi'.

UCSF Chimera  
File Select Actions Presets Tools Favorites Help

Animation

Scenes

1 2 3 4

Actions

Rock Roll

Timeline

1: 4 2: 2 3: 1 4: 1

Timeline: 1 (4 of 4)

Movie saved to \C:Users\...\Bicristallografia\test\_chimera.avi

# 99.Animation!

