

Presentation by Keenan Flynn

# Research Collaboratory for Structural Bioinformatics: a PDB<sup>z</sup>

## <sup>z</sup> RCSB PDB: an Overview

- The Interface: a Day in the RCSB PDB
- “Ins and Outs”
- Methods and Programs
- Review, Critique and Discussion



151079 Biological  
Macromolecular Structures  
Enabling Breakthroughs in  
Research and Education

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

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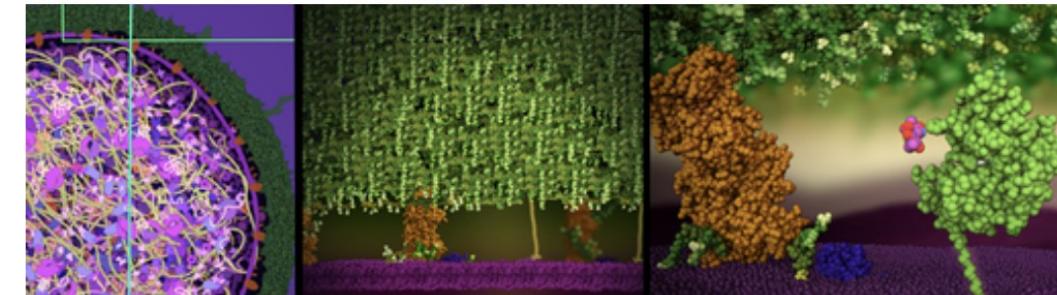
## A Structural View of Biology

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.

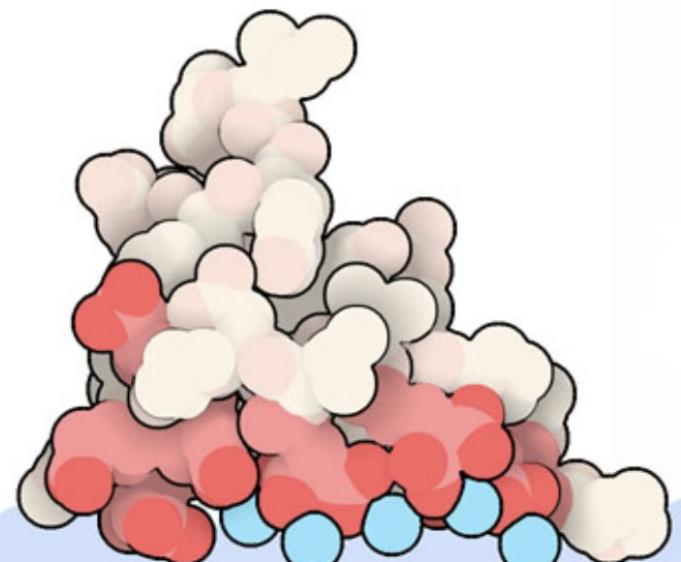
As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.

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.

### New Video: Penicillin and Antibiotic Resistance



## April Molecule of the Month



Proteins and Biominerals



105 Structures

1 Unreleased Structure

51 Citations

37 Ligands

### Search Parameter:

**Text Search for: groel**

[Refine Search](#)

[Save Search to MyPDB](#)

### Refinements



#### ORGANISM

- Escherichia coli (57)
- Homo sapiens (12)
- Methanococcus maripaludis (11)
- Mesorhizobium japonicum (3)
- Mycobacterium tuberculosis (3)
- Thermoplasma acidophilum (3)
- Gallus gallus (2)
- Other (14)

#### UNIPROT MOLECULE NAME

- 60 kDa chaperonin (59)
- 10 kDa chaperonin (17)
- Chaperonin (11)
- 2-oxoisovalerate dehydrog ... (11)
- 2-oxoisovalerate dehydrog ... (11)
- 2-methyl-3-hydroxypyridin ... (3)
- 60 kDa chaperonin 2 (2)
- [Refine Query](#)

#### TAXONOMY

Currently showing 11 - 2525 of 105105 Page: 1 of 55 [← Previous](#) [Next →](#)

Displaying 25 [▼](#) Results

**View:**

Detailed [▼](#)

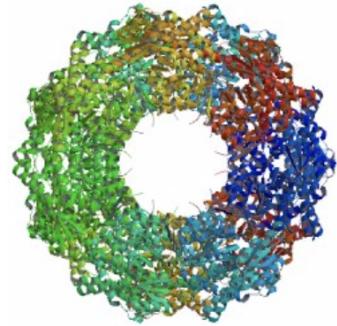
**Reports:**

Select a Report [▼](#)

**Sort:**

↓ Match score: Higher to Lower [▼](#)

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**1SS8**

**GroEL**

[Chaudhry, C.](#), [Horwich, A.L.](#), [Brunger, A.T.](#), [Adams, P.D.](#)

(2004) J Mol Biol **342** 229-245

**Released:** 3/1/2005

**Method:** X-ray Diffraction

**Resolution:** 2.7 Å

**Residue Count:** 3668

**Macromolecule:**

groEL protein (protein)

**Unique Ligands:** --

**Search term match score:** 438.30

[Download File](#) [View File](#)

**Matched fields in 1SS8.cif:**

- **\_citation.title:** Exploring the structural dynamics of the E.coli chaperonin GroEL using translation-libration-screw crystallographic refinement of intermediate states.
- **\_entity.pdbx\_description:** groEL protein
- **\_struct.title:** GroEL

# 1PCQ

Crystal structure of groEL-groES

DOI: [10.2210/pdb1PCQ/pdb](https://doi.org/10.2210/pdb1PCQ/pdb)

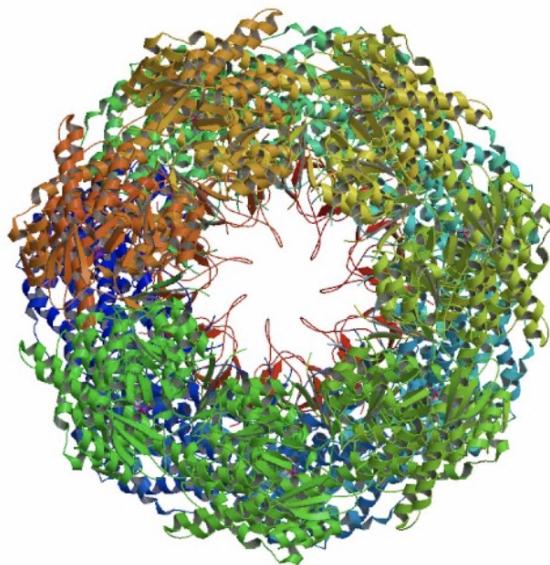
Classification: [CHAPERONE](#)

Organism(s): [Escherichia coli \(strain K12\)](#)

Expression System: [Escherichia coli](#)

Deposited: 2003-05-16 Released: 2003-10-14

Deposition Author(s): [Chaudhry, C.](#), [Farr, G.W.](#), [Todd, M.J.](#), [Rye, H.S.](#), [Brunger, A.T.](#), [Adams, P.D.](#), [Horwich, A.L.](#), [Sigler, P.B.](#)



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

#### Standalone Viewers

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

Global Symmetry: Cyclic - C7 [\(3D View\)](#)

Global Stoichiometry: Hetero 21-mer - A14B7 [\(i\)](#)

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

#### Macromolecule Content

- Total Structure Weight: 849910.13 [\(i\)](#)
- Atom Count: 59304 [\(i\)](#)
- Residue Count: 8015 [\(i\)](#)
- Unique protein chains: 2

#### Experimental Data Snapshot

Method: X-RAY DIFFRACTION

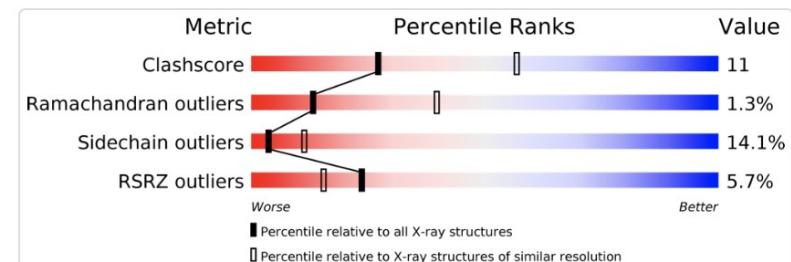
Resolution: 2.808 Å

R-Value Free: 0.278

R-Value Work: 0.262

#### wwPDB Validation

[3D Report](#) [Full Report](#)



This is version 1.2 of the entry. See complete [history](#).

#### Literature

[Download Primary Citation](#) ▾

Role of the gamma-phosphate of ATP in triggering protein folding by GroEL-GroES: function, structure and energetics.

[Chaudhry, C.](#), [Farr, G.W.](#), [Todd, M.J.](#), [Rye, H.S.](#), [Brunger, A.T.](#), [Adams, P.D.](#), [Horwich, A.L.](#), [Sigler, P.B.](#)

(2003) *Embo J.* **22:** 4877-4887

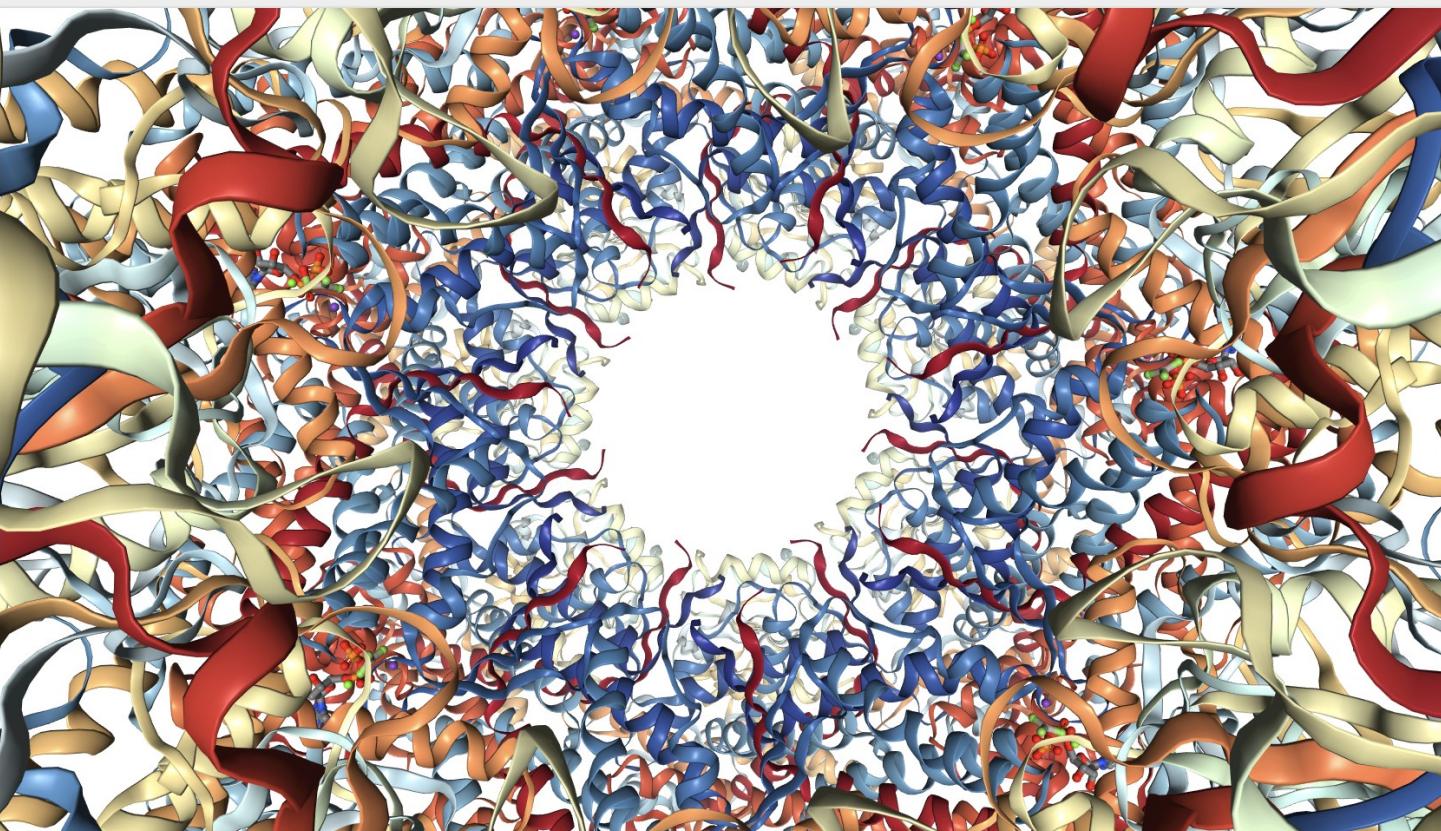
PubMed: [14517228](https://pubmed.ncbi.nlm.nih.gov/14517228/) [Search on PubMed](#) [Search on PubMed Central](#)

DOI: [10.1093/emboj/cdg477](https://doi.org/10.1093/emboj/cdg477)

Primary Citation of Related Structures:

## Crystal structure of groEL-groES

Note: Use your mouse to drag, rotate, and zoom in and out of the structure. Mouse-over to identify atoms and bonds. [Mouse controls documentation](#).

[Spin](#)[Center](#)[Fullscreen](#)[Screenshot](#)[Perspective Camera](#)[White background](#)[Focus](#)

0

NGL is a WebGL based 3D viewer powered by [MMTF](#).

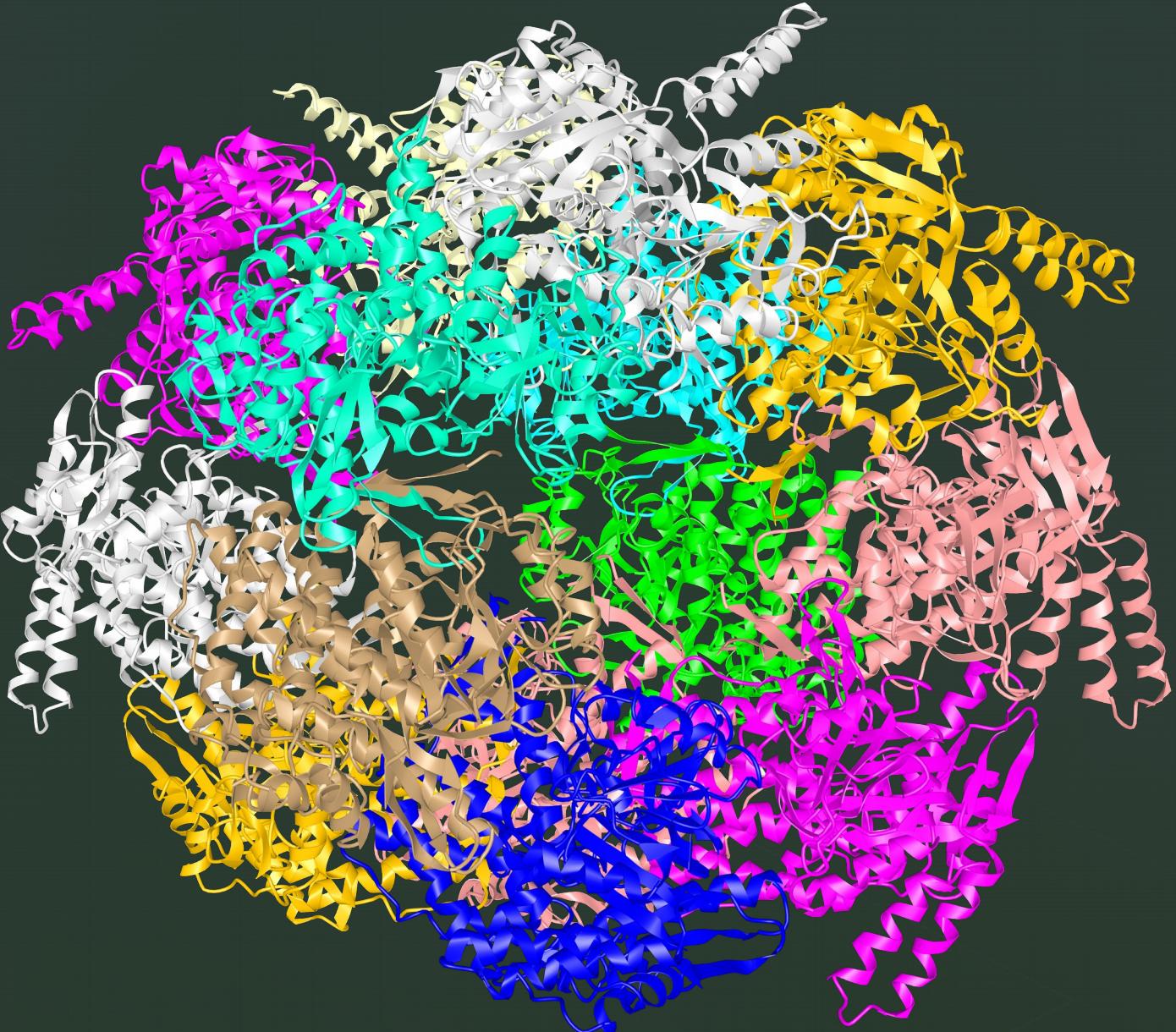
Select a different viewer [NGL \(WebGL\)](#)

**Citation**

Cite images created with the PDB ID and associated publication, NGL Viewer (AS Rose et al. (2018) NGL viewer: web-based molecular graphics for large complexes. Bioinformatics doi:10.1093/bioinformatics/bty419), and RCSB PDB.

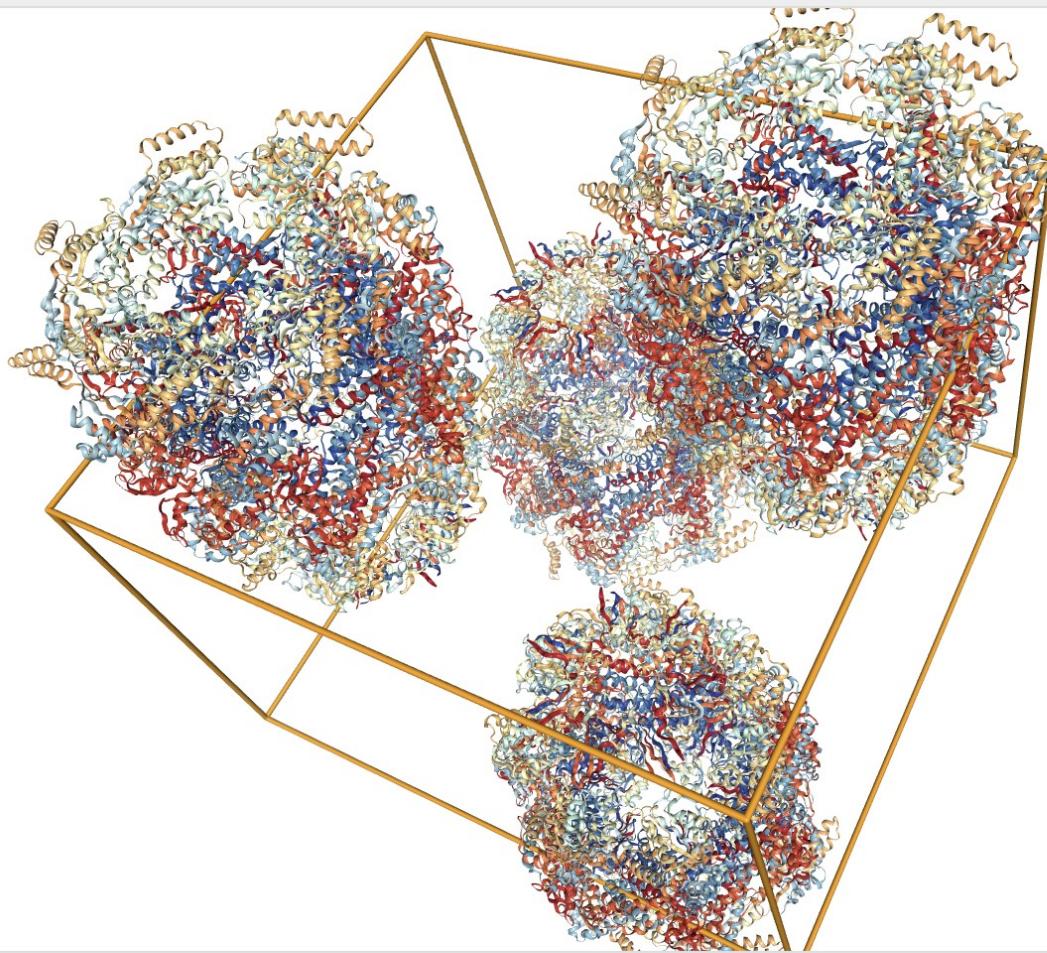
[Structure View](#)[Electron Density Maps](#)[Ligand View](#)[Electron Density Maps Documentation](#)

There are no electron density maps for structure 1PCQ



## Crystal structure of groEL-groES

Note: Use your mouse to drag, rotate, and zoom in and out of the structure. Mouse-over to identify atoms and bonds. [Mouse controls documentation](#).

[Spin ?](#)[Center ?](#)[Fullscreen ?](#)[Screenshot ?](#)[Perspective Camera](#) ▾[White background](#) ▾Focus ? [Structure View](#)[Electron Density Maps](#)[Ligand View](#)[Structure View Documentation](#)

Assembly ?

[Unitcell](#) ▾

Model ?

[Model 1](#) ▾

Symmetry ?

[None](#) ▾

Style ?

[Cartoon](#) ▾

Color ?

[Rainbow](#) ▾

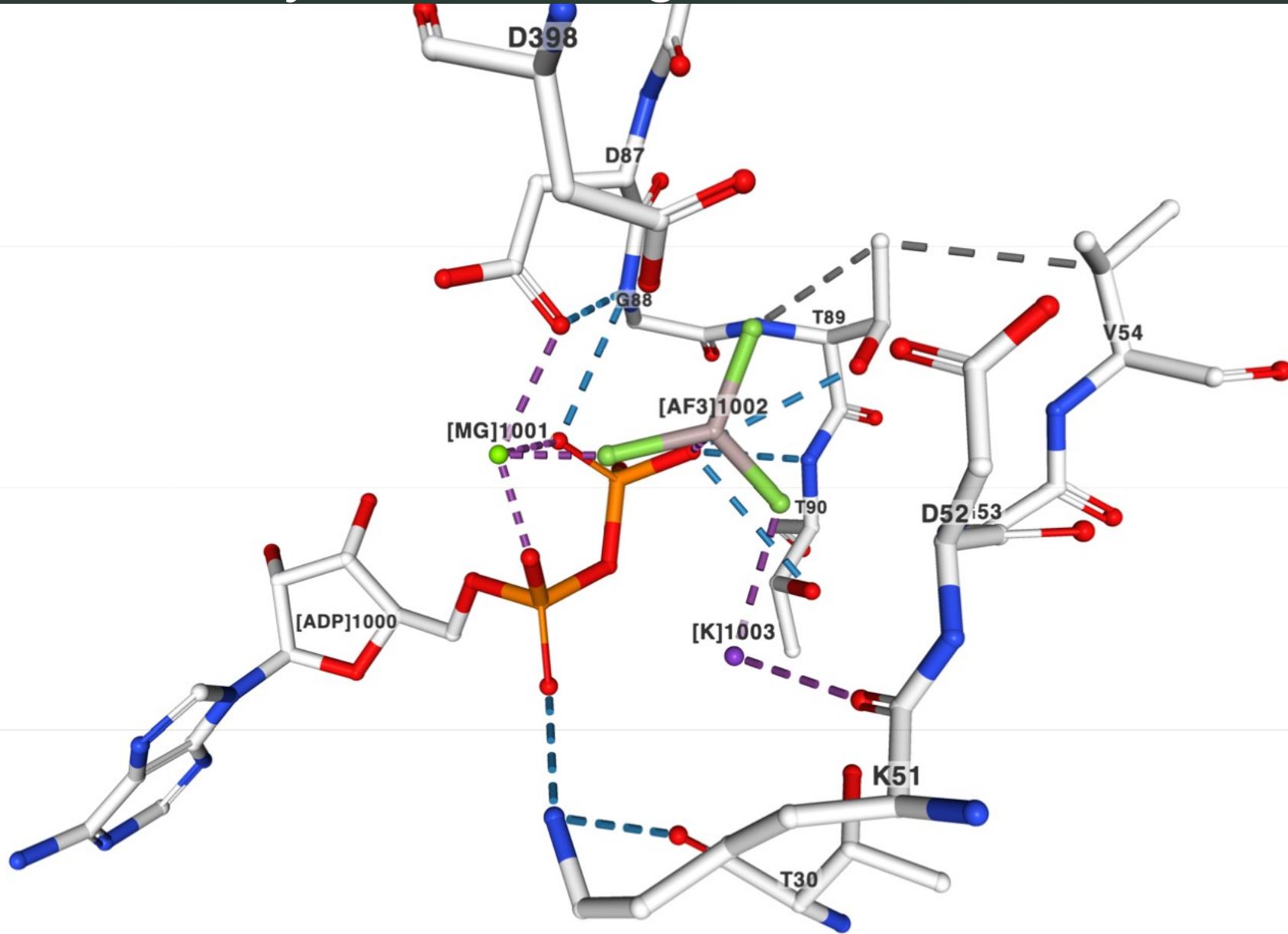
Ligand ?

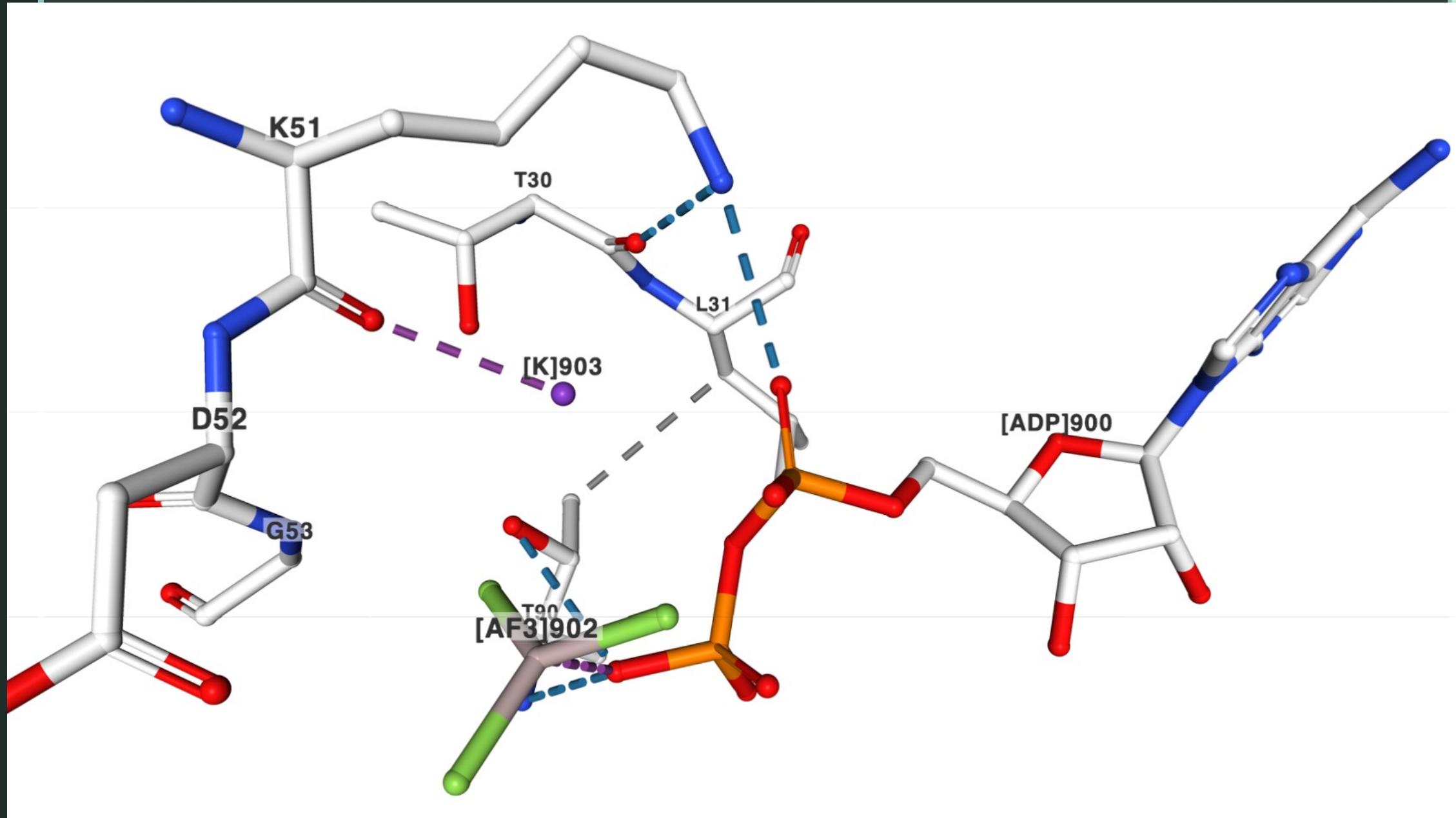
[Ball & Stick](#) ▾

Quality ?

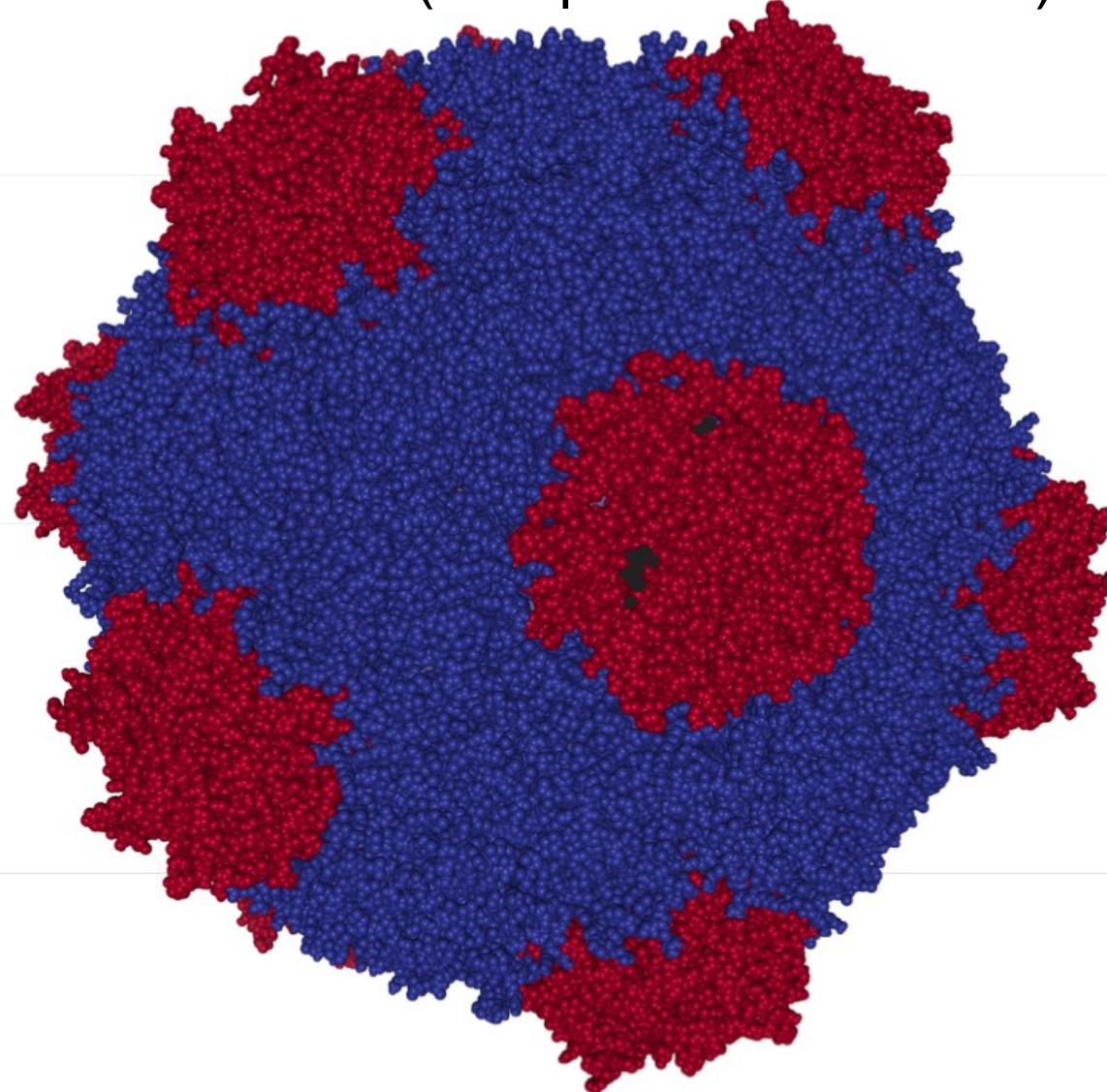
[Automatic](#) ▾Water ? Ions ? Hydrogens ? Clashes ? [Default Structure View ?](#)

# Key Feature: Ligand View





Key Feature: Macromolecular structures  
Below: CPMV (Cowpea Mosaic Virus)



## “Ins and Outs”

Input File type	Results	Output file
Atomic coordinate file	Visual image with toggle features	PDB, mmCIF, XML

Display Files ▾ Download Files ▾

FASTA Sequence

PDB Format

PDB Format (Header)

mmCIF Format

mmCIF Format (Header)

Model ? Model 1

Ligand View Documentation Unitcell

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

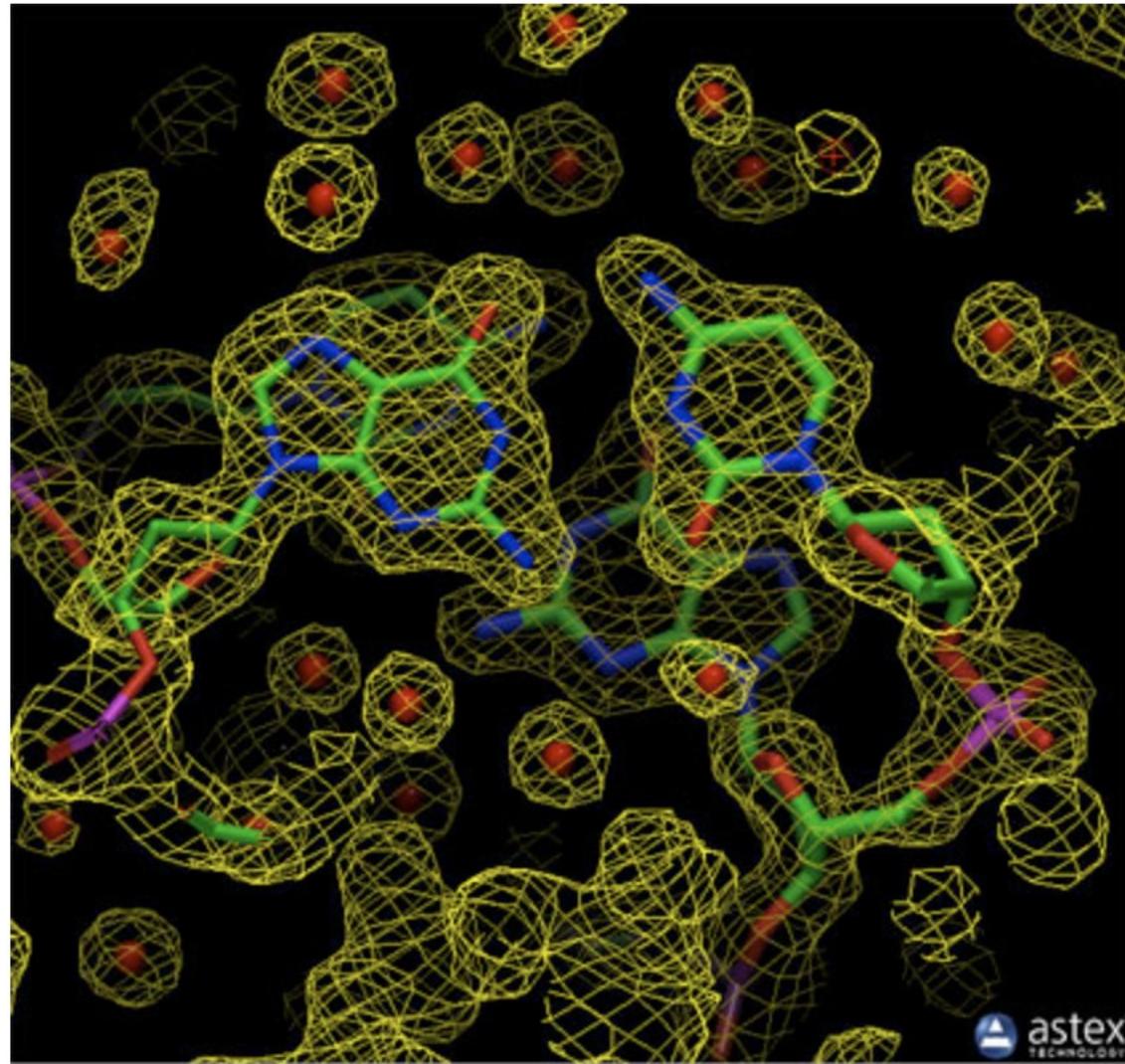
Structure Factors (CIF)

Structure Factors (CIF - gz)

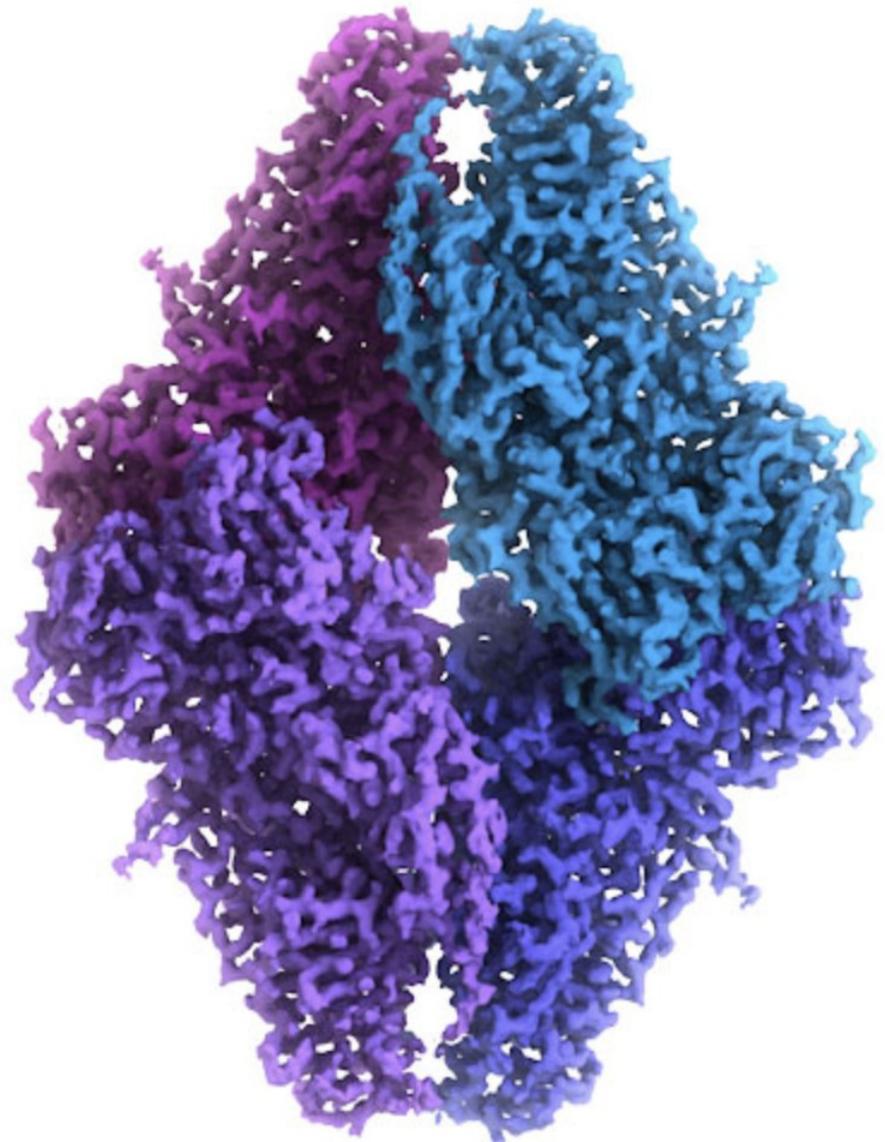
Ligand ? Ball & Stick

<sup>z</sup> How was this data obtained?

- X-Ray Diffraction
- X-Ray Crystallography
- X-Ray Free Electron Lasers (XFEL)
- NMR Spectroscopy
- 3D Electron Microscopy



The experimental electron density from a structure of DNA is shown here (PDB entry [196d](#)), along with the atomic model that was generated based on the data. The contours surround regions with high densities of electrons, which correspond to the atoms in the molecule.



This cryo-EM map of beta-galactosidase was built from over 90,000 images of the molecule frozen in ice, which was detailed enough to provide an atomic model. The cryoEM map is at EMDataBank entry [EMD-2984](#), and the atomic coordinates are in PDB entry [5a1a](#). Image courtesy of Veronica Falconieri and Siriam Subramaniam, National Cancer Institute.

# The Program: MBT Protein Workshop

## Molecular Graphics Software Links

- [BioBlender](#)  
Open Source viewer that includes features for morphing proteins and visualization of lipophilic and electrostatic potentials.
- [BRAGI](#)  
A protein visualization and modeling program
- [CCP4mg](#)  
Create beautiful publication quality images and movies. Users can superpose and analyse structures as well. The program runs 'out of the box' on Linux, Mac OSX and Windows platforms.
- [Chimera](#)  
Interactive molecular modeling system, free to academic/non-profit; displays multiple sequence alignments and associated structures, atom-type and H-bond identification, molecular dynamics trajectories (AMBER format), and offers ligand-screening interface (DOCK), filter by number/position of H-bonds, and extensibility to create custom modules - for Windows, Linux, Mac OS X, IRIX, and Tru64 Unix
- [Cn3D](#)  
Simultaneously displays structure, sequence, and alignment, with annotation and alignment editing features, for use with 3-D structures from NCBI's Entrez; available for Windows, Macintosh, and Unix
- [CrystalMaker](#)  
A program for building, displaying and manipulating all kinds of crystal and molecular structures.
- [ePMV](#)  
Embedded Python Molecular Viewer (ePMV) is an open-source plug-in that runs molecular modeling software directly inside of professional 3D animation applications
- [EzMol](#)  
A simple-to-use web-based molecular visualisation tool particularly designed for the occasional user which works with most common browsers so there is no need for any installation or a licence. The final visualisation model can be downloaded for publication or saved for subsequent use.
- [Foldit](#)  
Foldit is a crowdsourcing computer game based on protein modeling.
- [ICM-Browser](#)  
Software (free download) for browsing molecules and making fully-interactive 3D molecule documents for embedding in PowerPoint and the Web using ActiveICM.
- [MVM](#)  
Molecular Visualization Program and GUI of ZMM. MVM is a free molecular viewer that can be used to display protein, nucleic acids, oligosaccharides, small and macromolecules. It has an intuitive interface. In addition to being a molecular viewer, it is the user interface of a very powerful molecular mechanics engine (ZMM).
- [Nanome](#)  
A Virtual Reality interface for immersive molecular design, visualization and collaboration. Import molecular structures from your database and export them to PDB/MMCIF format. Manipulate molecular structures by grabbing, rotating, or enlarging with your hands. Share a virtual lab in real time with colleagues across the globe. Or spectate VR sessions via a 2D interface.
- [PMV \(Python Molecular Viewer\)](#)  
An interactive molecular visualization and modeling environment for manipulation and viewing of multiple molecules.
- [PocketMol](#)  
Program to view and manipulate PDB files on a PocketPC
- [POLYVIEW](#)
  - [POLYVIEW-2D](#)  
Protein structure annotation using sequence profiles
  - [POLYVIEW-3D](#)  
Versatile annotation and high quality visualization of macromolecular structures
  - [POLYVIEW-MM](#)  
Analysis and visualization of macromolecular motions
- [Prosat](#)  
Mapping protein sequence annotations onto a protein structure and visualizing them simultaneously with the structure.
- [PyMOL](#)  
A free and open-source molecular graphics system for visualization, animation, editing, and publication-quality imagery. PyMOL is scriptable and can be extended using the Python language. Supports Windows, Mac OSX, Unix, and Linux
- [QuteMol](#)  
An open source (GPL), interactive, high quality molecular visualization system. QuteMol exploits the current GPU capabilities through OpenGL shaders to offer an array of innovative visual effects.
- [RasMol](#)

z Discussion and Review

- Redundancy
- Usefulness
- Robustness

Z

# Any Questions?

BIOLOGY IS LARGELY SOLVED.  
DNA IS THE SOURCE CODE  
FOR OUR BODIES. NOW THAT  
GENE SEQUENCING IS EASY,  
WE JUST HAVE TO READ IT.

IT'S NOT JUST "SOURCE  
CODE". THERE'S A TON  
OF FEEDBACK AND  
EXTERNAL PROCESSING.



BUT EVEN IF IT WERE, DNA IS THE  
RESULT OF THE MOST AGGRESSIVE  
OPTIMIZATION PROCESS IN THE  
UNIVERSE, RUNNING IN PARALLEL  
AT EVERY LEVEL, IN EVERY LIVING  
THING, FOR FOUR BILLION YEARS.

IT'S STILL JUST CODE.



OK, TRY OPENING GOOGLE.COM  
AND CLICKING "VIEW SOURCE."

| OK, I-... OH MY GOD.

THAT'S JUST A FEW YEARS OF  
OPTIMIZATION BY GOOGLE DEVs.  
DNA IS THOUSANDS OF TIMES  
LONGER AND WAY, WAY WORSE.

| WOW, BIOLOGY  
IS IMPOSSIBLE.

