

Protein Data Bank and Structure Display with PyMOL

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Bioinformatics Service Support

BioIT, IBMS (生醫所)

Academia Sinica

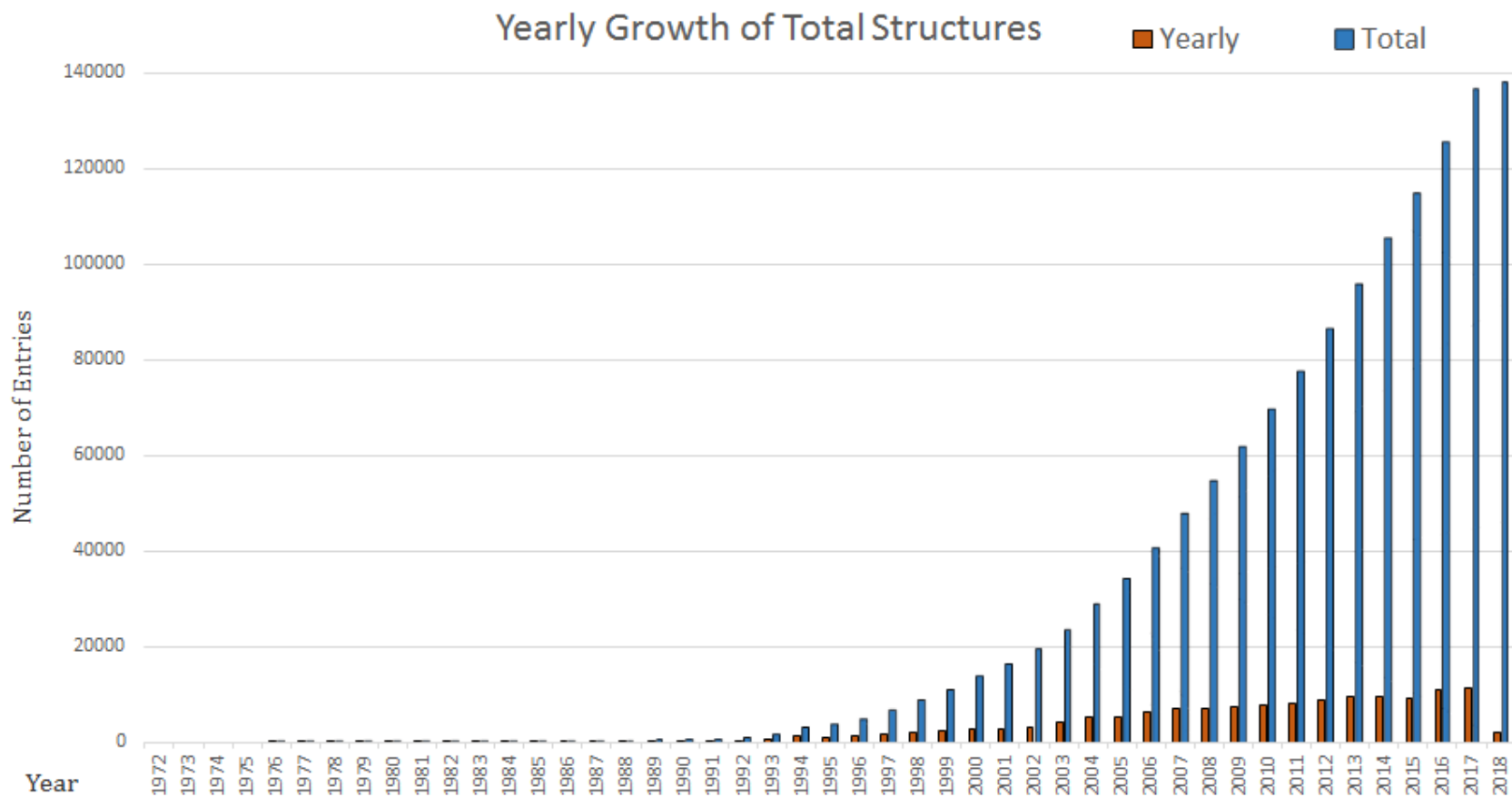
Outline

- About the RCSB PDB and the PDB Archive
- Searching for your structures
- Looking at structures
- Advanced applications in PDB
 - Structure visualization – NGL & JSmol viewers
 - Structure comparison -- jFATCAT-rigid
 - Drug target mapping --DrugBank
 - Protein-ligand interaction -- Ligand Explorer
- PyMOL Basic Applications
- PyMOL Advanced Applications

Worldwide Protein Data Bank (wwPDB)

- **RCSB PDB (USA)** <http://www.rcsb.org/pdb/>
(Nucleic Acids Res. 2017 45:D271-D281)
 - Established in 1971 at Brookhaven National Laboratory (BNL)
 - Taken over in 1998 by Research Collaboratory for Structural Bioinformatics
- **PDBe (Europe)** <http://www.ebi.ac.uk/pdbe/>
(Nucleic Acids Res. 2018 46:D486-D492)
- **PDBj (Japan)** <http://pdbj.org/>
(Nucleic Acids Res. 2017 45:D282-D288)
- **BMRB (USA)** <http://www.bmrwisc.edu/>
 - Biological Magnetic Resonance Bank (BioMagResBank)

RCSB PDB Statistics (1)



RCSB PDB Statistics (2)

- Statistics

Exp. Method	Proteins	Nucleic Acids	Protein / NA complexes	Other	Total
X-ray	116,115	1,916	5,922	10	123,963
NMR	10,660	1,236	249	8	12,153
Electron Microscope	1,459	31	506	0	1,996
Other	210	4	6	13	233
Multi Method	112	4	2	1	119
Total	128,556	3,191	6,685	32	138,464

RCSB PDB (<http://www.rcsb.org/>)

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB

138464 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 PDB EMBL Data Bank UniProt NCBI Protein Data Bank Worldwide Protein Data Bank

Top bar menu

Education PDB-101

Query area
Enter what you want to know ...

Welcome

Deposit

Search

Visualize

Analyze

Download

Learn


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.

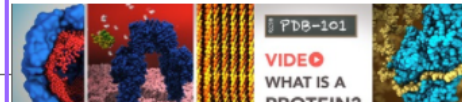
The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

March Molecule of the Month



Vacuolar ATPase

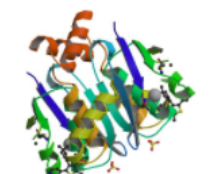
New Video: What is a Protein?



VIDEO WHAT IS A PROTEIN

Latest Entries

As of Tuesday Mar 06 2018



5O18 [PDB Entry](#)

Dissociation of biochemical and antiretroviral activities of Integrase-LEDGF Allosteric Inhibitors revealed by...

Features & Highlights

New Architecture and Services Enable Faster Access to More Information

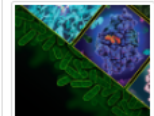
Explore the improved display of PDB Statistics, structure funding information, and 3D views of ligands and electron density.

Implementation of PDB Entry Versioning and Better Revision History to Improve PDB Archive Management

A new FTP repository, <ftp://versioned.wwpdb.org>, now hosts versioned structural model files in PDBx/mmCIF

News

Publications-



Enter the 2017 Video Challenge

High school students are invited to create a story about the *Mechanisms of Bacterial Resistance to Beta-lactam Antibiotics* » 03/06/2018

View Interactions and Maps in 3D » 02/27/2018

wwPDB Biocuration Highlighted in New Publication » 02/20/2018

Meet RCSB PDB at Biophysical Society's Annual Meeting » 02/18/2018

Education portal - PDB-101

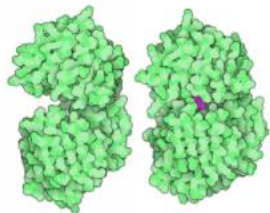
PDB-101 Molecule of the Month - Browse Learn - Global Health - Teach - Geis Archive - Events - More -

RCSB PDB-101 Molecular exploration through biology and chemistry
Educational portal of PDB

Search Molecule of the Month articles and more Go

February 2018

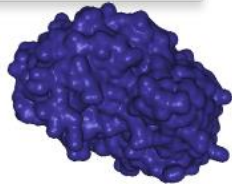
Molecule of the Month



EPSP Synthase and Weedkillers

The weedkiller Roundup attacks a key enzyme involved in the construction of aromatic compounds.

[More](#)



3D View: 2gga

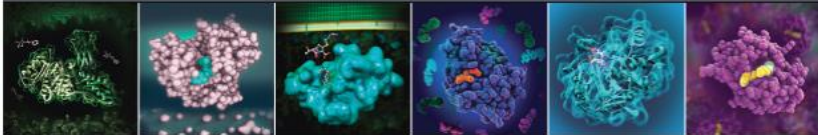
Style	Color	Spin
<input type="radio"/> Cartoon	<input type="radio"/> Rainbow	<input checked="" type="radio"/> On
<input type="radio"/> Spheres	<input checked="" type="radio"/> Chain	<input type="radio"/> Off
<input checked="" type="radio"/> Surface	<input type="radio"/> Structure	

[Browse resources by category](#)

- Health and Disease
- Molecules of Life
- Biotech and Nanotech
- Structures and Structure Determination

All articles: [By Date](#) | [By Category](#) | [By Title](#)

Health Focus: Antimicrobial Resistance



Antibiotics have saved countless lives, but pathogens are quickly finding ways to survive antibiotic treatment. Antibiotic-resistant bacteria are predicted to become the leading cause of death worldwide. They take many approaches: pumping antibiotics out of their cells, altering the molecular machinery that the antibiotics target, and attacking the antibiotics directly. Atomic structures publicly available in the PDB are revealing the details of drug resistance and providing new ways to combat it. Use the PDB-101 resources to learn about protein structures related to antibiotic action and resistance.

News and Events

- Meet RCSB PDB at AAAS
» 02/13/2018
- Special Issue Focused on Tools for Protein Science
» 01/30/2018



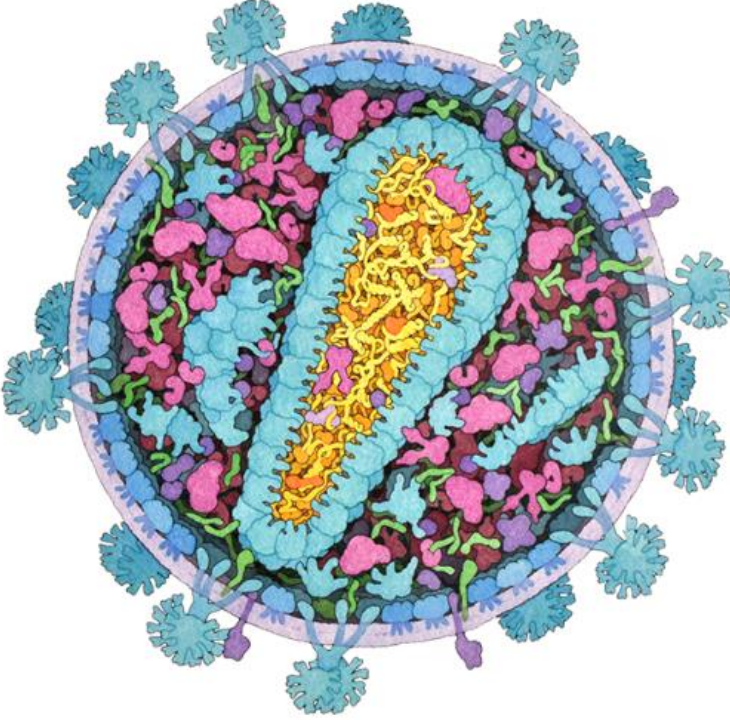
Take an Interactive Tour of the PDB (1)

- Interactive Animations

The Structural Biology of HIV

RCSB PDB-101

Home Viral Proteins: [Structural Proteins](#) [Viral Enzymes](#) [Accessory Proteins](#)



HIV (Human Immunodeficiency Virus) is composed of **two strands of RNA, 15 types of viral proteins, and a few proteins from the last host cell it infected**, all surrounded by a **lipid bilayer membrane**. Together, these molecules allow the virus to infect cells of the immune system and force them to build new copies of the virus. Each molecule in the virus plays a role in this process, from the first steps of viral attachment to the final process of budding.

Since 1986, research on the structural biology of HIV have revealed the atomic details of these proteins. These structures are all publicly available in the Protein Data Bank (PDB) archive. Using these data, researchers have designed new treatments for HIV infection, including effective drug regimens that halt the growth of the virus. The structures also provide new hope for development of a vaccine.

Click anywhere on the virus or choose a protein from the menu to begin exploring.

© RCSB Protein Data Bank

Take an Interactive Tour of the PDB (2)

Molecular Machinery: A Tour of the Protein Data Bank

Scale (nm): 1 5 10 1 nm (nanometer) = 10^{-9} millimeters

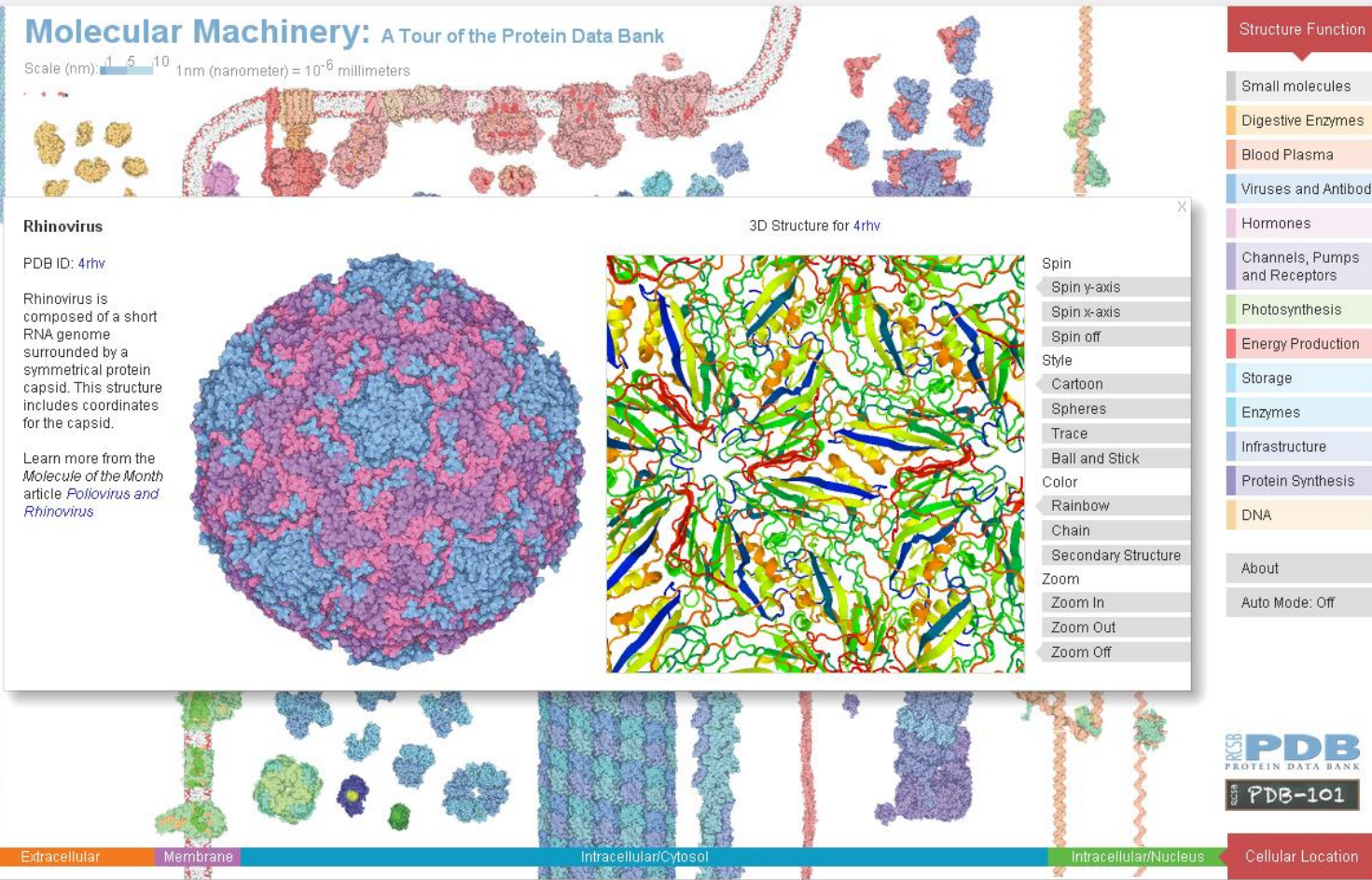
Rhinovirus

PDB ID: 4rhv

Rhinovirus is composed of a short RNA genome surrounded by a symmetrical protein capsid. This structure includes coordinates for the capsid.

Learn more from the *Molecule of the Month* article *Poliovirus and Rhinovirus*

3D Structure for 4rhv



Structure Function

- Small molecules
- Digestive Enzymes
- Blood Plasma
- Viruses and Antibodi
- Hormones
- Channels, Pumps and Receptors
- Photosynthesis
- Energy Production
- Storage
- Enzymes
- Infrastructure
- Protein Synthesis
- DNA

About

Auto Mode: Off

Spin

- Spin y-axis
- Spin x-axis
- Spin off

Style

- Cartoon
- Spheres
- Trace
- Ball and Stick

Color

- Rainbow
- Chain
- Secondary Structure

Zoom

- Zoom In
- Zoom Out
- Zoom Off

Extracellular Membrane Intracellular/Cytosol Intracellular/Nucleus Cellular Location

RCSB PDB PROTEIN DATA BANK

PDB-101

Searching for your structure (1)

The image shows the RCSB PDB website interface. At the top, the navigation bar includes 'RCSB PDB', 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', 'Learn', 'More', and a 'MyPDB' button. The 'Search' dropdown menu is open, listing options: 'Advanced Search', 'Drilldown Search', 'Unreleased & New Entries', 'Sequences' (highlighted with a red arrow), 'Ligands', 'Drugs & Drug Targets', 'Browse by Annotation', and 'PDB Statistics'. Below the navigation bar, there is a search input field with the placeholder text 'Search by PDB ID, author, macromolecule, sequence, or ligal' and a 'Go' button. A secondary search bar contains 'Advanced Search | Browse by Annotations'. The main content area features a 'Welcome' message, a 'Deposit' button, and a 'Search' button. A large section titled 'Explore the PDB Archive' contains a dropdown menu with the following options: 'Organism', 'UniProt Molecule Name', 'Taxonomy', 'Experimental Method', 'X-ray Resolution', 'Release Date', 'Polymer Type', 'Enzyme Classification', 'SCOP Classification', 'Protein Symmetry', 'Protein Stoichiometry', and 'Membrane Proteins'. A pie chart is partially visible below the dropdown menu. On the right side, there is a 'Contact Us' button.

Searching for your structure (2)

Search by Sequences

Choose Option A or B to search for protein and nucleic acid sequences. [Read Tutorial | Advanced Sequence Searching](#)

NOTE Parameters: BLAST method, E-value cutoff: 10.0, Mask Low Complexity: On.

Option A: Use PDB Sequence

Select Associated Chain

B (Seq: 2) ▼

B (Seq: 2)

A (Seq: 1)

Run Sequence Search

or Option B: Paste Sequence

```
GNVDLVFLFDGSMQLPDEFQKILDFMKDVMKKLSNTSYQFAAV
QFSTSYKTEFDYVVKWKDPDALLKHVKHMLLLTN
```

Searching for your structure (3)

Query result browser

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB

Refinements +

Currently showing 1 - 25 of 104 Page: 1 of 5 ← Previous Next →

View: Detailed Reports: Select a Report Displaying 25 Results

Sort: e-value: Best to Worst Download

ORGANISM

- Homo sapiens (88)
- Aquifex aeolicus (4)
- Toxoplasma gondii (3)
- Rattus norvegicus (3)
- Mytilus galloprovincialis (3)
- Mus musculus (3)

UNIPROT MOLECULE NAME

- Integrin alpha-L (32)
- von Willebrand factor (22)
- Integrin alpha-M (13)
- Integrin alpha-1 (10)
- Integrin alpha-X (7)
- Integrin alpha-2 (6)
- Ribonuclease PH (4)
- Refine Query

TAXONOMY

- Eukaryota (100)
- Bacteria (4)

EXPERIMENTAL METHOD

- X-ray (102)
- Solution NMR (2)

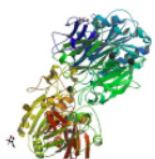
X-RAY RESOLUTION

- less than 1.5 Å (5)
- 1.5 - 2.0 Å (26)
- 2.0 - 2.5 Å (36)
- 2.5 - 3.0 Å (22)
- 3.0 and more Å (13)
- Refine Query

RELEASE DATE

- before 2000 (12)
- 2000 - 2005 (32)
- 2005 - 2010 (20)
- 2010 - 2015 (31)
- 2015 - today (9)
- Refine Query

5E6R: Entity 1 containing Chain A Download File View File



Structures of leukocyte integrin αLβ2: The αI domain, the headpiece, and the pocket for the internal ligand

[Sen, M., Springer, T.A.](#)

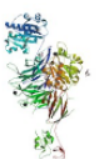
(2016) Proc Natl Acad Sci U S A 113 2940-2945

Released: 3/2/2016 Macromolecule: Integrin alpha-L (protein)
Method: X-ray Diffraction Integrin beta-2 (protein)
Resolution: 2.9 Å Unique Ligands: CA, MG, NAG
Residue Count: 1305

Length: 182 E-value: 1.6252E-105 Score: 379.407bits (973) Identities: 182/182 (100%)
Positives: 182/182 (100%) Gaps: 0/182 (0%)

Query: GINVDLVFLFDGSMQLQPDEFQKILDFMKDVMKLSNTSYQFAAVQFSTSYKTEFDFSDYVKWKDPDALLKHVKHMLLLTNTFGAINVY
GINVDLVFLFDGSMQLQPDEFQKILDFMKDVMKLSNTSYQFAAVQFSTSYKTEFDFSDYVKWKDPDALLKHVKHMLLLTNTFGAINVY
Sbjct: GINVDLVFLFDGSMQLQPDEFQKILDFMKDVMKLSNTSYQFAAVQFSTSYKTEFDFSDYVKWKDPDALLKHVKHMLLLTNTFGAINVY

5E6S: Entity 1 containing Chain A, C, E Download File View File



Structures of leukocyte integrin αLB2: The αI domain, the headpiece, and the pocket for the internal ligand

[Sen, M., Springer, T.A.](#)


(2016) Proc Natl Acad Sci U S A 113 2940-2945



Retrieving your structure – 1CQP

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

Biological Assembly 1



1CQP

CRYSTAL STRUCTURE ANALYSIS OF THE COMPLEX LOVASTATIN AT 2.6 Å RESOLUTION

DOI: [10.2210/pdb1CQP/pdb](https://doi.org/10.2210/pdb1CQP/pdb)

Classification: [IMMUNE SYSTEM](#)

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

Deposited: 1999-08-10 Released: 2000-08-07

Deposition Author(s): [Kallen, J.](#), [Welzenbach, K.](#), [Ramage, P.](#), [Geyl, D.](#), [Kriwacki, R.](#), [Legge, G.](#), [Cottens, S.](#), [Weitz-Schmidt, G.](#), [Hommel, U.](#)

Experimental Data Snapshot

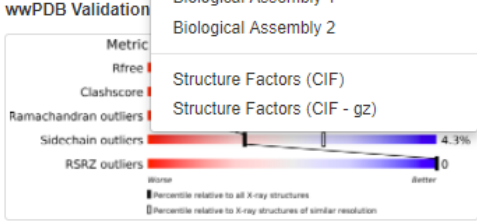
Method: X-RAY DIFFRACTION

Resolution: 2.6 Å

R-Value Free: 0.257

R-Value Work: 0.190

wwPDB Validation



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
- Biological Assembly 2
- Structure Factors (CIF)
- Structure Factors (CIF - gz)

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

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

Global Symmetry: Asymmetric - C1 ⓘ
Global Stoichiometry: Monomer - A ⓘ

Biological assembly 1 assigned by authors.

Macromolecule Content

- Total Structure Weight: 42499.41 ⓘ
- Atom Count: 2998 ⓘ
- Residue Count: 364 ⓘ
- Unique protein chains: 1

This is version 1.3 of the entry. See complete [history](#).

Literature

Download Primary Citation

Structural basis for LFA-1 inhibition upon lovastatin binding to the CD11a I-domain.
[Kallen, J.](#), [Welzenbach, K.](#), [Ramage, P.](#), [Geyl, D.](#), [Kriwacki, R.](#), [Legge, G.](#), [Cottens, S.](#), [Weitz-Schmidt, G.](#), [Hommel, U.](#)
(1999) J.Mol.Biol. 292: 1-9

PubMed: [10493852](#) Search on PubMed
DOI: [10.1006/jmbi.1999.3047](https://doi.org/10.1006/jmbi.1999.3047)

PubMed Abstract:
The lymphocyte function-associated antigen (LFA-1) belongs to the family of beta2-integrins and plays an important role in T-cell activation and leukocyte migration to sites of inflammation. We report here that lovastatin, a drug clinically used for ...

PDB format (2)– 1CQP

Remark records

```
...  
REMARK 2 RESOLUTION. 2.60 ANGSTROMS.  
...  
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY  
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 21  
...  
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS  
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM  
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY  
REMARK 290 RELATED MOLECULES.  
REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000 0.000000  
REMARK 290 SMTRY2 1 0.000000 1.000000 0.000000 0.000000  
REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 0.000000  
REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 36.35000  
REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000 0.000000  
REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 45.90000
```

Heteroatom
records

(non-standard
residues e.g.
ligands, ions
and water)

```
...  
HET MG A 310 1  
HET MG B 310 1  
HET 803 A 311 29  
HET 803 B 311 29  
HETNAM MG MAGNESIUM ION  
HETNAM 803 LOVASTATIN  
HETSYN 803 MK-803; LOVALIP; MEVACOR  
FORMUL 3 MG 2 (MG 2+)  
FORMUL 5 803 2 (C24 H36 O5)  
FORMUL 7 HOH *86 (H2 O)
```



PDB format (3)– 1CQP

Atom records

```
...
ATOM      1  N   GLY A 128      44.810  32.209  24.312  1.00  60.46      N
ATOM      2  CA  GLY A 128      43.318  32.144  24.502  1.00  59.56      C
ATOM      3  C   GLY A 128      42.879  31.077  25.499  1.00  56.37      C
ATOM      4  O   GLY A 128      43.308  31.073  26.654  1.00  57.03      O
...
ATOM    1462  CA  ILE A 309      52.536  35.917  28.130  1.00  58.16      C
ATOM    1463  C   ILE A 309      51.906  37.303  28.426  1.00  65.50      C
ATOM    1464  O   ILE A 309      52.269  38.298  27.740  1.00  70.09      O
ATOM    1465  CB  ILE A 309      51.655  35.083  27.164  1.00  55.20      C
ATOM    1466  CG1 ILE A 309      52.420  33.837  26.734  1.00  50.60      C
ATOM    1467  CG2 ILE A 309      51.255  35.876  25.948  1.00  67.96      C
ATOM    1468  CD1 ILE A 309      53.803  34.136  26.244  1.00  39.29      C
ATOM    1469  OXT ILE A 309      51.061  37.396  29.345  1.00  70.38      O
TER      1470          ILE A 309
ATOM    1471  N   GLY B 128      62.823  33.550  24.044  1.00  67.05      N
ATOM    1472  CA  GLY B 128      64.227  33.694  24.572  1.00  66.00      C
ATOM    1473  C   GLY B 128      64.358  33.241  26.017  1.00  61.57      C
ATOM    1474  O   GLY B 128      63.468  32.572  26.556  1.00  67.10      O
...
ATOM    2931  N   ILE B 309      54.545  27.250  24.474  1.00  43.38      N
ATOM    2932  CA  ILE B 309      54.748  27.915  23.202  1.00  50.44      C
ATOM    2933  C   ILE B 309      55.615  27.111  22.257  1.00  56.16      C
ATOM    2934  O   ILE B 309      56.646  26.621  22.747  1.00  63.24      O
ATOM    2935  CB  ILE B 309      55.413  29.255  23.479  1.00  53.14      C
ATOM    2936  CG1 ILE B 309      54.447  30.132  24.261  1.00  58.81      C
ATOM    2937  CG2 ILE B 309      55.846  29.919  22.204  1.00  63.82      C
ATOM    2938  CD1 ILE B 309      55.101  31.303  24.905  1.00  69.98      C
ATOM    2939  OXT ILE B 309      55.286  27.012  21.049  1.00  62.52      O
TER      2940          ILE B 309
      ●
      ●
      ●
```


PDB format (4)– 1CQP


HETAM
records

```
...
HETATM 2941 MG      MG A 310      48.079  -2.336  22.333  1.00 23.16      MG
HETATM 2942 C1     803 A 311      52.497  19.025  23.052  1.00 43.13      C
HETATM 2943 C2     803 A 311      52.393  17.482  22.971  1.00 36.38      C
HETATM 2944 C3     803 A 311      52.359  16.834  24.377  1.00 33.15      C
HETATM 2945 C21    803 A 311      53.777  16.458  24.857  1.00 27.12      C
...
HETATM 2971 MG      MG B 310      59.074  50.051  55.046  1.00 42.60      MG
HETATM 2972 C1     803 B 311      55.082  39.941  35.863  1.00 39.50      C
HETATM 2973 C2     803 B 311      55.211  40.642  37.236  1.00 34.66      C
HETATM 2974 C3     803 B 311      55.219  39.639  38.406  1.00 26.04      C
HETATM 2975 C21    803 B 311      53.761  39.334  38.807  1.00 28.07      C
...
HETATM 3001 O      HOH A  1      46.704   3.370  17.939  1.00 21.72      O
HETATM 3002 O      HOH A  2      37.676  -1.658  26.021  1.00 24.22      O
HETATM 3003 O      HOH A  3      47.452  -0.486  21.226  1.00 26.23      O
HETATM 3004 O      HOH A  4      46.992  -3.309  17.690  1.00 26.75      O
...
CONNECT   90 2941
CONNECT  104 2941
CONNECT  905 2941
CONNECT 1560 2971
CONNECT 1574 2971
CONNECT 2375 2971
...
MASTER      309      0      4      20      14      0      6      6 3084      2      70      28
END
```

Looking at your structure (1) – 1CQP

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

Biological Assembly 1



1CQP

CRYSTAL STRUCTURE ANALYSIS OF THE COMPLEX LFA-1 (CD11A) I-DOMAIN / LOVASTATIN AT 2.6 Å RESOLUTION

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Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 2.6 Å
R-Value Free: 0.257
R-Value Work: 0.190

wwPDB Validation

Metric	Percentile Ranks	Value
Rfree		0.177
Clashscore		8
Ramachandran outliers		1.1%
Sidechain outliers		4.3%
RSRZ outliers		0

Worse Better
■ Percentile relative to all X-ray structures
□ Percentile relative to X-ray structures of similar resolution

3D View: **Structure** | Electron Density | Ligand Interaction

Standalone Viewers
[Protein Workshop](#) | **Ligand Explorer**

Global Symmetry: Asymmetric - C1
Global Stoichiometry: Monomer - A

Biological assembly 1 assigned by authors.

Macromolecule Content

- Total Structure Weight: 42499.41
- Atom Count: 2998
- Residue Count: 364
- Unique protein chains: 1

This is version 1.3 of the entry. See complete history.

Literature

Download Primary Citation

Structural basis for LFA-1 inhibition upon lovastatin binding to the CD11a I-domain.
[Kallen, J.](#), [Welzenbach, K.](#), [Ramage, P.](#), [Geyl, D.](#), [Kriwacki, R.](#), [Legge, G.](#), [Cottens, S.](#), [Weitz-Schmidt, G.](#), [Hommel, U.](#)
(1999) *J.Mol.Biol.* **292**: 1-9
PubMed: [10493852](#) Search on PubMed
DOI: [10.1006/jmbi.1999.3047](https://doi.org/10.1006/jmbi.1999.3047)

PubMed Abstract:
The lymphocyte function-associated antigen (LFA-1) belongs to the family of beta2-integrins and plays an important role in T-cell activation and leukocyte migration to sites of inflammation. We report here that lovastatin, a drug clinically used for ...

Click it to launch
Ligand Explorer



Looking at your structure (2) – 1CQP

Macromolecules

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

Entity ID: 1

Molecule	Chains	Sequence Length	Organism	Details
ANTIGEN CD11A (P180)	A, B	182	Homo sapiens	Gene Names: ITGAL (CD11A)

Find proteins for [P20701](#) (*Homo sapiens*)

Go to Gene View: [ITGAL](#)

Go to UniProtKB:

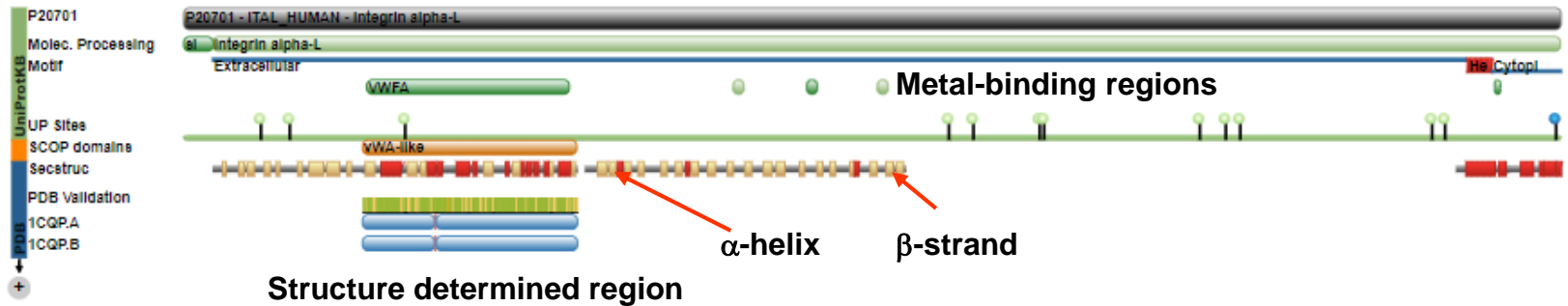
[P20701](#)

Protein Feature View

Full Protein Feature View for [P20701](#)

Actual protein in full-length

Goes to protein feature view



Protein feature view – 1CQP

Viewer: NGL



PDB ID 1CQP.A

Organism: Human Length:1170 UniProt

Isoforms: 3, currently showing only the 'canonical' sequence.

Gene View for ITGAL

Chromosome Location

Other Gene names: CD11A

This protein in other organisms (by gene name):

P20701 - Homo sapiens 34

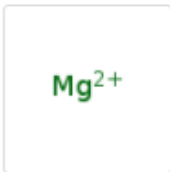

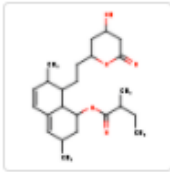
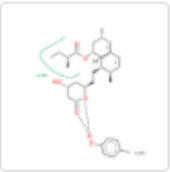
- P24063 - Mus musculus no matching PDB entries
- O43746 - Homo sapiens no matching PDB entries
- Q6TYB8 - Bos taurus no matching PDB entries
- Q9UBC8 - Homo sapiens no matching PDB entries
- Q45H73 - Homo sapiens no matching PDB entries
- Q96HB1 - Homo sapiens no matching PDB entries
- P61625 - Bos taurus no matching PDB entries



Looking at your structure (3) – 1CQP

Small Molecules

Ligands **2 Unique**

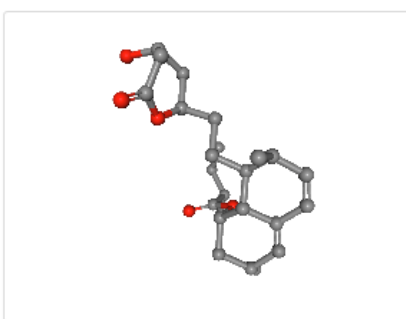
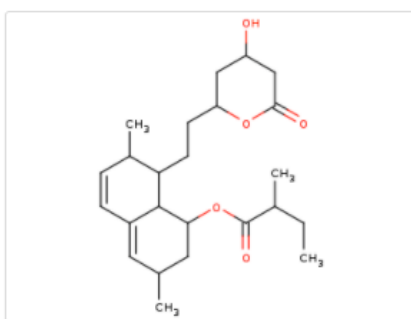
ID	Chains	Name / Formula / InChI Key	2D Diagram & Interactions	3D Interactions
MG Query on MG Download SDF File Download CCD File	A, B	MAGNESIUM ION Mg JLVVSXFLKOJNIY-UHFFFAOYSA-N		Ligand Interaction 
803 Query on 803 Download SDF File Download CCD File	A, B	LOVASTATIN <i>MK-803; LOVALIP; MEVACOR</i> C ₂₄ H ₃₆ O ₅ PCZOHLXUXFIOCF-BXMDZJJMSA-N	 	Ligand Interaction

External Ligand Annotations

ID	Binding Affinity (Sequence Identity %)
803	Kd: 12900 nM (99) BINDINGDB
803	IC50: 2400 nM PDBBIND

•
•
•

Browsing your ligand



Rotate Hydrogens Labels

Chemical Component Summary	
Name	LOVASTATIN
Identifiers	[(1S,3R,7S,8S,8aR)-8-[2-[(2R,4R)-4-hydroxy-6-oxo-oxan-2-yl]ethyl]-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl] (2S)-2-methylbutanoate
Formula	C ₂₄ H ₃₆ O ₅
Molecular Weight	404.54
Type	NON-POLYMER
Isomeric SMILES	CC[C@H](C)C(=O)O[C@H]1C[C@@H](C)C=C2C=C[C@H](C)[C@H](CC[C@@H]3C[C@@H](O)CC(=O)O3)[C@@H]12
InChI	InChI=1S/C24H36O5/c1-5-15(3)24(27)29-21-11-14(2)10-17-7-6-16(4)20(23(17)21)9-8-19-12-18(25)13-22(26)28-19/h6-7,10,14-16,18-21,23,25H,5,8-9,11-13H2,1-4H3/t14-,15-,16-,18+,19+,20-,21-,23-/m0/s1
InChIKey	PCZOHLXUXFIOCF-BXMDZJJMSA-N

Drug Info: DrugBank

DrugBank ID	DB00227 Different stereochemistry
Name	Lovastatin
Groups	<ul style="list-style-type: none">approvedinvestigational

View / Download Files -

803

LOVASTATIN

803 as a free ligand exists in 1 entry. Examples include: 1CQP

Find related ligands: [Stereoisomers](#) [Similar ligands](#)
[Chemical Structure Search](#)

View summary at [Ligand Expo](#)

Related Data Resources for 803
eg. PubChem,
DrugBank,...

Chemical Details	
Formal Charge	0
Atom Count	65
Chiral Atom Count	8
Chiral Atoms	C1, C12, C14, C16, C3, C7, C8, C9
Bond Count	67
Aromatic Bond Count	0
Leaving Atoms	n/a

Chemical information



Looking at your structure (4) – 1CQP

Experimental Data & Validation

Experimental Data

Method: X-RAY DIFFRACTION

Resolution: 2.6 Å

R-Value Free: 0.257

R-Value Work: 0.190

Space Group: [P 2₁ 2₁ 2₁](#)

Unit Cell:

Length (Å)	Angle (°)
a = 72.700	α = 90.00
b = 77.700	β = 90.00
c = 91.800	γ = 90.00

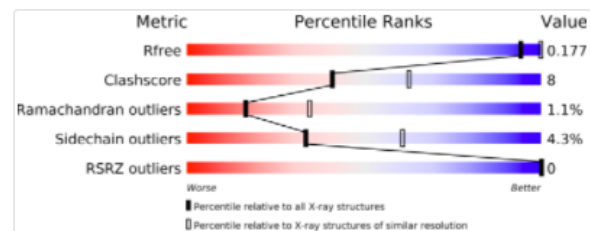
Software Package:

Software Name	Purpose
X-PLOR	phasing
DENZO	data reduction
X-PLOR	refinement
X-PLOR	model building
SCALEPACK	data scaling

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

Structure Validation

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



Entry History

Deposition Data

Deposited Date: 1999-08-10

Released Date: 2000-08-07

Deposition Author(s): [Kallen, J.](#), [Weizenbach, K.](#), [Ramage, P.](#), [Geyl, D.](#), [Kriwacki, R.](#), [Legge, G.](#), [Cottens, S.](#), [Weitz-Schmidt, G.](#), [Hommel, U.](#)

Revision History ⓘ

- **Version 1.0:** 2000-08-07
Type: Initial release
- **Version 1.1:** 2008-04-27
Type: Version format compliance
- **Version 1.2:** 2011-07-13
Type: Version format compliance
- **Version 1.3:** 2014-11-12
Type: Structure summary

Searching for ligand

Breakthroughs in Research and Education

PDB-101 PDB EMBL Data Bank NCBI GenBank World Health Organization

Chemical component search ⓘ
The **Chemical Component Dictionary** gives details of components found in PDB entries including standard solvent molecules.

UniProt Molecule Name: Lovastatin hydrolase (9) Find all
Chemical Name: 803: Name...>LOVASTATIN... Find all

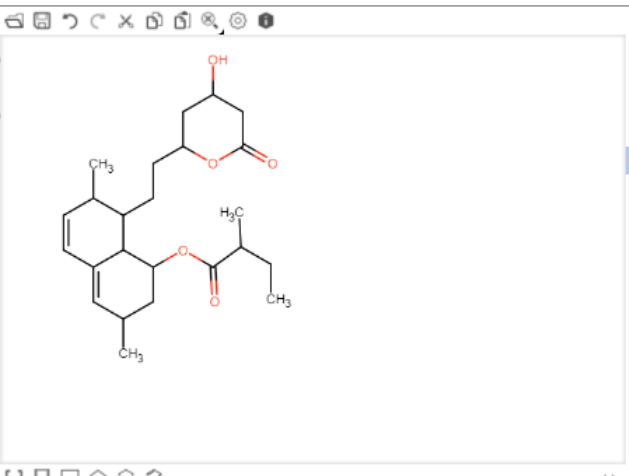
close ✕

Ontology Terms

- D02.455...638.400: Lovast... [... (21)
- D04.615... Lovastatin... (12)

Structure Name/Identifier Formula/Weight

Chemical sketch →
click on the Submit Query



Powered by ChemAxon

Load Chemical ID

SMILES Load SMILES

Search Type: Substru ▾

Molecular weight: From: To:

Submit Query

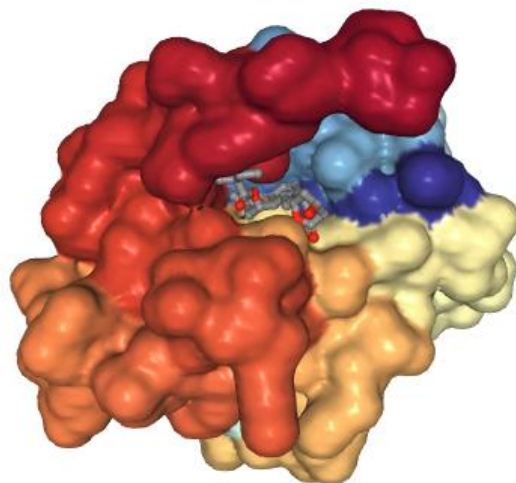
Structure visualization – NGL

1CQP

Display Files Download Files

CRYSTAL STRUCTURE ANALYSIS OF THE COMPLEX LFA-1 (CD11A) I-DOMAIN / LOVASTATIN AT 2.6 Å RESOLUTION

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.



Structure View Electron Density Maps

Ligand Viewer

Structure View Documentation

Assembly Bioassem

Model Model 1

Symmetry None

Style Surface

Color Rainbow

Ligand Ball & Stick

Quality High

Water Ions

Hydrogens Clashes

Default Structure View

Blue to red

Download as PNG image

Spin Fullscreen Center Screenshot Perspective Camera

White background Focus 0

NGL is a WebGL based 3D viewer powered by MMTF.

Select a different viewer

NGL (WebGL)
NGL (WebGL)
JSmol (JavaScript)

Opening JSmol applet

Structure visualization – JSmol (1)

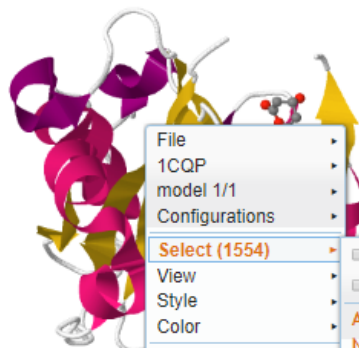
1CQP

CRYSTAL STRUCTURE ANALYSIS OF THE COMPLEX LFA-1 (CD11A) I-DOMAIN / LOVASTATIN AT 2.6 Å RESOLUTION

Display Files

Download Files

NOTE: Use your mouse to drag, rotate, and zoom in and out of the structure. Help



Biological assem

Se

JS

- File
- 1CQP
- model 1/1
- Configurations
- Select (1554)
 - Display Selected Only
 - Selection Halos
 - All
 - None
 - Invert Selection
 - Element
 - Symmetry
 - Protein
 - Nucleic
 - MG - MAGNESIUM ION
 - HOH - WATER
 - 803 - LOVASTATIN
- View
- Style
- Color
- Surfaces
- Symmetry
- Scenes
- Zoom
- Spin
- Vibration
- Spectra
- Animation
- Measurements
- Set picking
- Console
- JavaScript Console
- Show
- Computation
- Language
- About...

Structure Details

Structure

Symmetry Type

Symmetry C1

Stoichiometry A

Select Orientation

Front

Select Display Mode

Secondary Structure

Symmetry

Display Options

By HETATM

- All PDB "HETATM"
- All Solvent
- All Water
- Ligand
 - Nonaqueous HETATM (hetero and not water)
 - Nonaqueous Solvent (solvent and not water)
- Rotation Background
- Polyhedron Axes

Press on the right bottom of mouse to show the drop-down menu

Structure visualization – JSmol (2)

Select → Hetero →
By HETATM → HEM

Style → Scheme →
Ball and Stick

Surface → Dot surface

Select → Hetero →
By HETATM → MG

Color → Atoms →
Cyan

Measurements →
Click for distance
measurement

on the screen:
Click on MG and
[803]311:A C21 #1474
Distance: 19.8Å

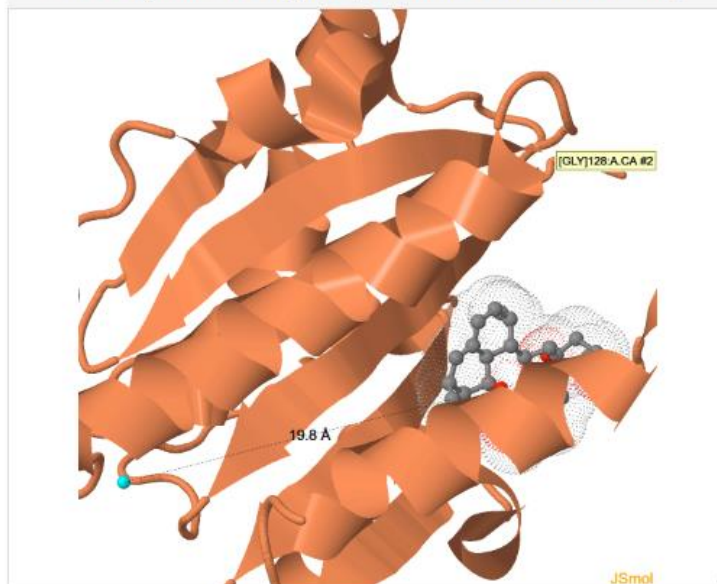
File → Export →
Export PNG image

1CQP

CRYSTAL STRUCTURE ANALYSIS OF THE COMPLEX LFA-1 (CD11A) I-DOMAIN /
LOVASTATIN AT 2.6 Å RESOLUTION

Display Files - Download Files -

NOTE: Use your mouse to drag, rotate, and zoom in and out of the structure. Help



Biological assembly 1 assigned by authors

Select a Viewer

JSmol (Java) ▾

Structure Details

Structure ▾

Symmetry ▾

Type

Symmetry C1

Stoichiometry A

Select Orientation

◀ Front ▶

Select Display Mode

Secondary Structure Subunit ←

Symmetry

Display Options

Style ▾

Color ▾

Surface ▾

H-Bonds SS Bonds
 Rotation Black
 Polyhedron Background
 Axes

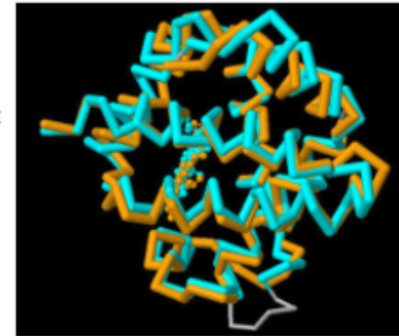
Structure comparison -- jFATCAT-rigid (1)

Analyze Related Features

Sequence & Structure Alignment

RCSB PDB's Comparison Tool calculates pairwise sequence (blast2seq, Needleman-Wunsch, and Smith-Waterman) and structure alignments (FATCAT, CE, Mammoth, TM-Align, TopMatch).

Comparisons can be made for any protein in the PDB archive and for customized or local files not in the PDB. Special features include support for both rigid-body and flexible alignments and detection of circular permutations.



1CQP ↔ 5E6S

Select Associated Chain ID: A (Seq: 1) ↔ A (Seq: YNL D V R G A R S F S P P R A G R H F G Y R V L Q V)

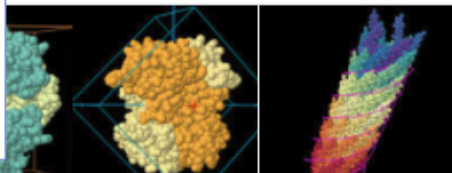
- Select Comparison Method -

- Select Comparison Method -
- Sequence Alignment
 - blast2seq
 - Needleman-Wunsch
 - Smith-Waterman
- Structure Alignment
 - jFATCAT - rigid**
 - jFATCAT - flexible
 - jCE algorithm
 - jCE Circular Permutation
 - External: FatCat
 - External: Mammoth
 - External: TM-Align
 - External: TopMatch

Align More Options

al symmetry among subunits. The view displays the symmetry axes, a polyhedron
asizes the symmetry.

pin Streptavidin Inovirus





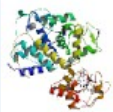
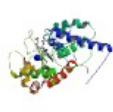
Structure comparison -- jFATCAT-rigid (2)

Structure Alignment View

Pre-calculated jFATCAT_rigid results for 4GED.A vs. 2WD4.A .

This page provides a summary view of the protein structure alignment.

Structure Alignment Results

Alignment Details:	 Query: (orange/dark grey) <i>Ascorbate peroxidase</i>	 Subject: (cyan/light grey) <i>ASCORBATE PEROXIDASE</i>
P-value: 0.00e+00	 PDB ID: 4GED	 PDB ID: 2WD4
Score: 639.52	Chain ID: A	Chain ID: A
RMSD: 1.51	Length: 268	Length: 248
%Id: 38.7%	Similarity: 89%	Similarity: 96%
	EC number: 1.11.1.11	EC number: 1.11.1.11

Comparison Method

Select these two chains for other comparison:
Click [here](#) to align other protein chains. Back to the all vs. all search results for **4GED.A** or **2WD4.A**



Structure comparison -- jFATCAT-rigid (3)

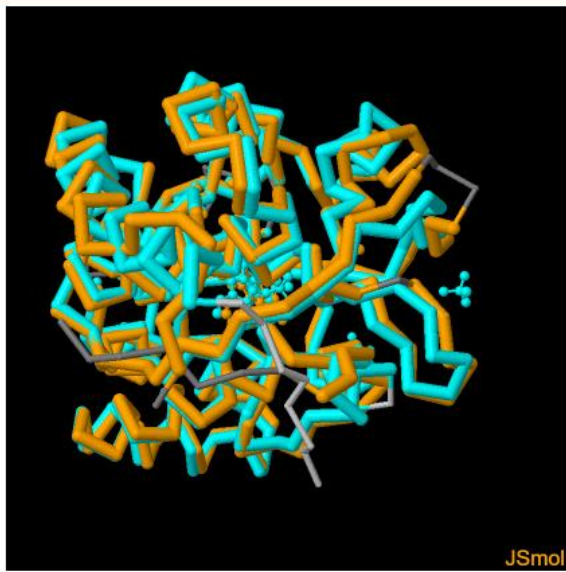
Comparison Method

Select these two chains for other comparison:

--- Select Comparison Method ---

[Click here to align other protein chains.](#) [Back to the all vs. all search results for 4GED.A or 2WD4.A](#)

Jmol



Tip: right-mouse click on Jmol to get access to additional Jmol functionality.

Reset Display

Jmol Script

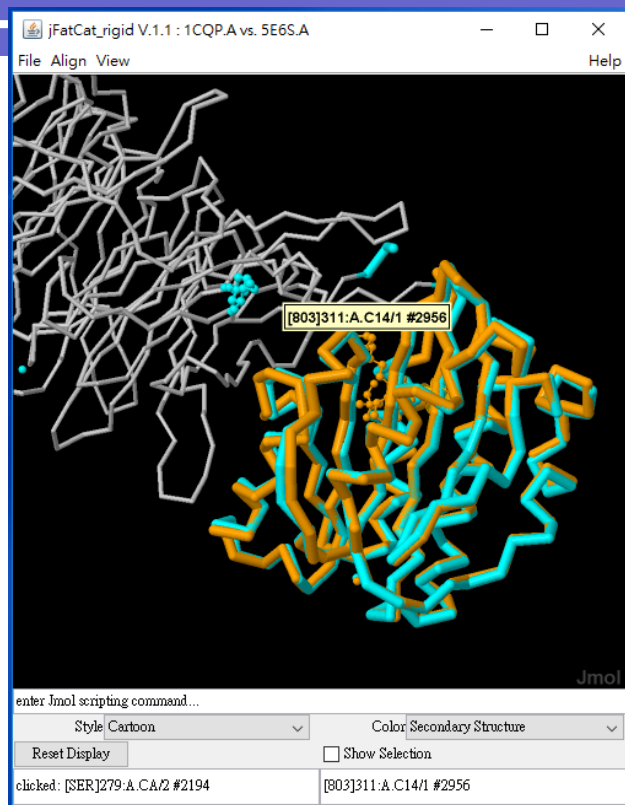
Display Query & Target Show Both Style Backbone Color Secondary Structure
Toggle Selection H-Bonds SS Bonds Rotation Antialias Display (nicer) Black Background
Color Legend ■ 4GED.A ■ 2WD4.A

It is also possible to view this alignment using the stand-alone Java Web Start application.

 Launch Web Start



Structure comparison -- jFATCAT-rigid (5)

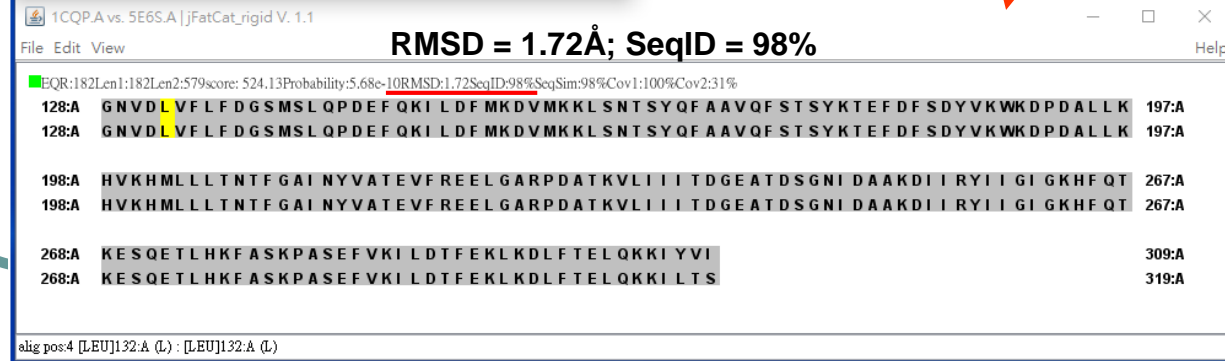


This structure alignment also can be viewed using the stand-alone Java Web Start application.

Click on [Launch Web Start](#)

← Structure alignment

Sequence alignment



RMSD = 1.72Å; SeqID = 98%

EQR:182Len1:182Len2:579score: 524.13Probability:5.68e-10RMSD:1.72SeqID:98%SeqSim:98%Cov1:100%Cov2:31%

128:A	G N V D L V F L F D G S M S L Q P D E F Q K I L D F M K D V M K K L S N T S Y Q F A A V Q F S T S Y K T E F D F S D Y V K W K D P D A L L K	197:A
128:A	G N V D L V F L F D G S M S L Q P D E F Q K I L D F M K D V M K K L S N T S Y Q F A A V Q F S T S Y K T E F D F S D Y V K W K D P D A L L K	197:A
198:A	H V K H M L L L T N T F G A I N Y V A T E V F R E E L G A R P D A T K V L I I T D G E A T D S G N I D A A K D I R Y I I G I G K H F Q T	267:A
198:A	H V K H M L L L T N T F G A I N Y V A T E V F R E E L G A R P D A T K V L I I T D G E A T D S G N I D A A K D I R Y I I G I G K H F Q T	267:A
268:A	K E S Q E T L H K F A S K P A S E F V K I L D T F E K L K D L F T E L Q K K I Y V I	309:A
268:A	K E S Q E T L H K F A S K P A S E F V K I L D T F E K L K D L F T E L Q K K I L T S	319:A

align pos:4 [LEU]132:A (L) : [LEU]132:A (L)

Drug and Drug Target Mapping

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB

PDB-101 PDB

Advanced Search
Drilldown Search
Unreleased & New Entries
Sequences
Ligands
Drugs & Drug Targets
Browse by Annotation
PDB Statistics

Drug and Drug

Two tables provide access to drug target information from DrugBank that are mapped to PDB entries with each weekly update.

- **Drugs Bound to Primary Targets:** Lists drugs bound to primary target(s), or a homolog of primary target(s), i.e., co-crystal structures of drugs.
- **Primary Drug Targets:** Lists primary drug targets in the PDB, regardless if the drug molecule is part of the PDB entry (e.g., apo forms of drug targets, drug target with different bound ligands). Biotherapeutics, such as complexes with monoclonal antibodies, are included.

See description of column names

Search by Generic or Brand Names
(separate multiple drugs by commas)

Drugs Bound to Primary Targets Primary Drug Targets

The top 3 PDB IDs for each drug based on the **drug target sequence similarity search**. If the sequence identities are same, the PDB ID with better resolution will take precedence.

Click on column headers to sort up/down. Click again to reverse order. [CSV](#)

Page 1 of 179 View 1 - 20 of 3,580

	Generic Name	Brand Name	DrugBa ID	ATC Codes	Target Name	UniProt ID	PDB ID 1	Seq. Identit	PDB ID 2	Seq. Identit	PDB ID 3	Seq. Identit	All PDB
1	3,4-Methylene		DB01454		Synaptic vesicular amine transporter	Q05940							
2	3,4-Methylene		DB01454		Sodium-dependent noradrenaline transporter	P23975	4XP6	59%	4XP6	59%	4XP5	59%	Find
3	3,4-Methylene		DB01454		Sodium-dependent serotonin transporter	P31645	5I6X	99%	5I71	99%	5I73	99%	Find

Protein-ligand interaction (1)

Save the image

RCSB PDB Ligand Explorer 4.2.0 (powered by the MBT): 1CQP

File Analysis Help

Full Sequences Contact Map

Chain G N V D L V F L F D G S M S L O P D E F O K I L D F M K D V M K K L S N T S Y O F A A V O F S T S Y K T E F D F S D V V K W K D P D A

A: L L K H V K H M L L L I N T F G A I N V V A T E V F R E E L G A R P D A T K V L I I T D G E A T D S G N I D A A K D I I R V I I G I

128 140 150 160 170 180 190

195 200 210 220 230 240 250 Y257 260

G K H F O T K E S O E T L H K F A S K P A S E F V K I L D T F E K L K D L F I E L O K K I V V I

Choose a ligand to analyze...

- A
 - MG (A 310)
 - 803 (A 311)
- B
 - MG (B 310)
 - 803 (B 311)

Choose interactions & thresholds...

- Hydrogen Bond 3.3
- Hydrophobic 3.9
- Bridged H-Bond 3.3
- Metal Interaction 3.5
- Neighbor Residues 4.0

Label interactions by distance

Surfaces

Off Transparent Opaque

Color by Hydrophobicity

Distance 6.5 Type Solid

Status: Atom: CA Residue TYR 257 Chain A

Protein-ligand interaction (2)

1CQP

Display Files - Download Files -

CRYSTAL STRUCTURE ANALYSIS OF THE COMPLEX LFA-1 (CD11A) I-DOMAIN / LOVASTATIN AT 2.6 Å RESOLUTION

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](#).

Structure View Electron Density Maps

Ligand Viewer

Structure View Documentation

Assembly 1 Bioassem

Model 1

Symmetry None

Style None

Color Rainbow

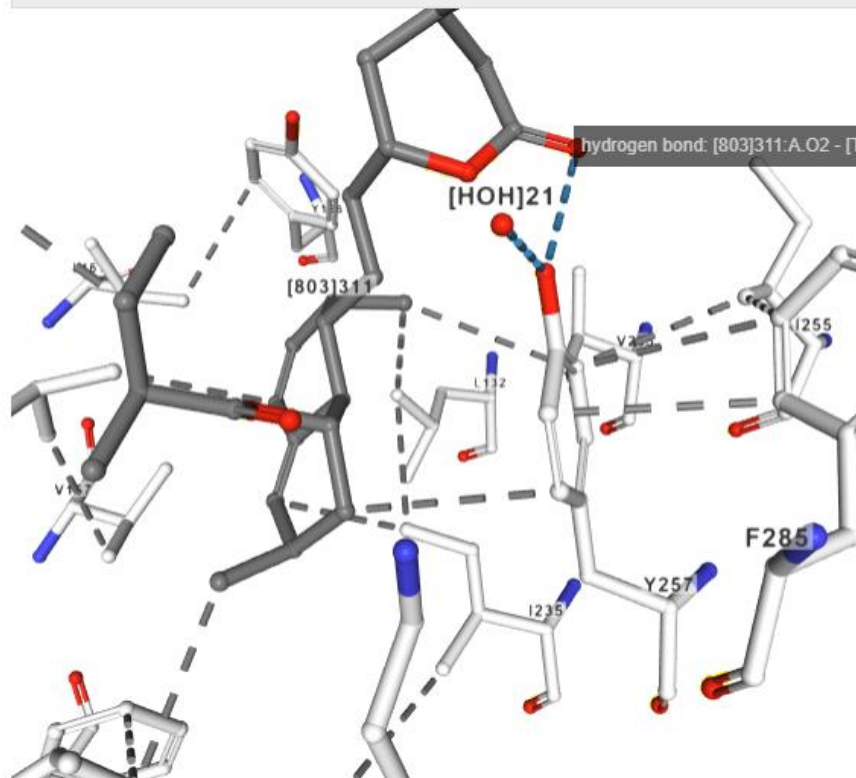
Ligand None

Quality High

Water Ions

Hydrogens Clashes

Default Structure View



Spin Fullscreen Center Screenshot Perspective Camera

White background Focus 0

NGL is a WebGL based 3D viewer powered by MMTF.

Select a different viewer NGL (WebGL)

Other features

- Human Gene View
- Pathway View
- Transmembrane Proteins

Genome Assembly GRCh37 - ?

Full Screen

14,20,923,289..20,925,666

Genome: 20,923,500 20,924,000 20,924,500 20,925,000 20,925,500

4QHE A
1CGGB

Genes

- ENST0000055414.1
- ENST00000216714.3
- ENST00000553881.1
- ENST00000554813.1
- ENST00000558296.1
- ENST00000557344.1
- ENST0000055306.1
- ENST00000553555.1
- ENST00000388030.4

4QHE_A APEX1: 4QHEA

Method P27695

Location 14:20925150-20925664

Links APEX1

Note Crystal structure of Mg²⁺ bound human APE1

P27695 Map genomic region to protein sequence P27695

RCSB 4QHE

Structure

Summary

Image

About: The PDB track gives a graphical summary of the region of a gene for which an experimentally obtained protein structure is available from the Protein Data Bank.

This feature requires an up-to-date web browser.

Legend

The genome browser is based on [Biodalliance browser](#)

The tracks display the following information:

Track	Info
Genome	A ruler that provides location information. If the zoom level is high enough, it can show the nucleotides at the corresponding location, or a graphical encoding for each nucleotide (A: green, T: red, G: yellow, C: blue).
PDB	The blue boxes on this track indicate regions for which coordinates have been observed in PDB. Clicking on this track shows

GRCh37 assembly

RCSB PDB

Pathway View: Map PDB Data onto Metabolic Pathways

Select an organism and a metabolic pathway from the pull-down menus to view a map.

Organism

Please select ...

- Please select ...
- Escherichia coli
- Homo sapiens

Map

Please select ...

- Please select ...
- Amino acid metabolism (partial)
- Carbohydrate metabolism
- Glycolysis TCA PPP
- Inositol retinol metabolism
- Tryptophan metabolism

- In a reaction pathway map, each arrow represents a reaction and each node represents a metabolite.
- The size and color of each reaction arrow indicates the number of PDB entries or homology models that are associated with it.
 - If there is no PDB entry associated with a reaction, its arrow will be gray.
 - If there are only homology models associated with a reaction, its arrow will be yellow.
 - If there are PDB entries associated with a reaction, the color of its arrow will vary from light blue to dark blue depending on the number of associated entries in that map.
- The color of a metabolite node indicates the presence (blue) or absence (gray) of the compound in the [wvPDB Chemical Component Dictionary \(CCD\)](#).
- Clicking on a node or arrow will reveal the associated ligand ID or a list of the associated PDB entries, respectively.
- The last character of a metabolite may indicate its compartment: `_c` -> cytosolic, `_m` -> mitochondrial, `_e` -> extracellular space
- The lighter numbers displays the stoichiometry of the metabolite in the reaction. When it is 1, we hide the number.

The PDB to Reaction mapping is based on the data provided by [GEM-PRO](#) project. In brief, genes are linked to proteins and proteins interact with metabolites. Therefore genes and proteins can be associated with reactions and metabolites in the provided genome-scale models. In order to associate a PDB id with a reaction, we use the relation from Gene to UniProt to PDB. (Gene -> UniProt -> PDB). The UniProt to PDB mapping is available from the [SIFTS](#) initiative.

Transmembrane View

transmembrane regions OPM

see also Brunk et al. BMC Systems Biology (2016).

Multiple file downloading

The screenshot displays the PDB Batch Download interface. On the left is a dark blue sidebar with navigation links: Welcome, Deposit, Search, Visualize, Analyze, Download, and Learn. The main content area is titled "Batch Download" and "Coordinates & Experimental Data". It features a text input field containing the PDB IDs "4D2I,4CS4,4CIW,4Q4W". Below the input field are three sections of radio button options: "Coordinates" (PDB, PDBx/mmCIF, PDBML/XML, Biological Assemblies), "Experimental Data" (Structure Factors, NMR Restraints), and "Compression Type" (uncompressed, gzipped). A "Launch Download Application" button is located at the bottom right of the interface.

Batch Download

Coordinates & Experimental Data

Sequences

Ligands

FTP Archive & Services

HTTPS Services

Web Services

RESTful Web Services

Download: Coordinates & Experimental Data

Enter PDB IDs separated by comma or white space. Note: The Download Tool is launched as a stand-alone application using the Java Web Start protocol. [More Download Help](#) ?

4D2I,4CS4,4CIW,4Q4W

Coordinates: PDB PDBx/mmCIF PDBML/XML Biological Assemblies

Experimental Data: Structure Factors NMR Restraints

Compression Type: uncompressed gzipped

Launch Download Application



PyMOL

What PyMOL Can Do ...

- Open source
 - Support multiple file formats including pdb, mol2, sdf,...
 - Manipulate multiple molecules
 - High quality rendering
 - Read in density maps in CCP4 or X-PLOR format
 - Van der Waals surface rendering
 - Extensive animation generation
 - Written in C and Python languages
-
- Get the free source code or purchase licenses
(<https://pymol.org/> and <https://sourceforge.net/projects/pymol/>)

Visualize 1CQP using PyMOL

The screenshot displays the PyMOL graphical user interface. At the top, a menu bar includes File, Edit, Build, Movie, Display, Setting, Scene, Mouse, Wizard, Plugin, and Help. Below the menu bar is a command line area with a list of files being deleted (e.g., PyMOL.pdb, PyMOL.pml, etc.) and a prompt 'PyMOL>'. The main viewer window shows a protein structure in green ribbon representation. A context menu is open over the structure, listing various display options under 'Ligand Sites' and 'Preset'. A mouse mode menu is also visible at the bottom right, showing '3-Button Viewing' and '3-Button Editing' options. A frame indicator at the bottom shows 'State 1/ 1'.

External
GUI window

Name panel

A: Active S: Show
H: Hide L: Label
C: Colour

Viewer window

Mouse Mode

3-Button Viewing
3-Button Editing

Frame indicator

Command lines

The command language

- The majority of simple functions, such as open, save..., are available via the external GUI menu. Commands can also be used to interact with PyMOL.
- Commonly-used commands:
 - load <\$PYMOL_PATH/filename>
 - select </object_name/segment_identifier/chain_identifier/residue_identifier/name_identifier>
 - color <color>
 - show <representation type>
 - hide < representation type >
 - set <parameter>
 - zoom <select or object>
 - distance <two atoms>
 -
 -
 -
- Arguments are separated by one or more commas.
 - show cartoon, chain A

PyMOL Basic Application (1)

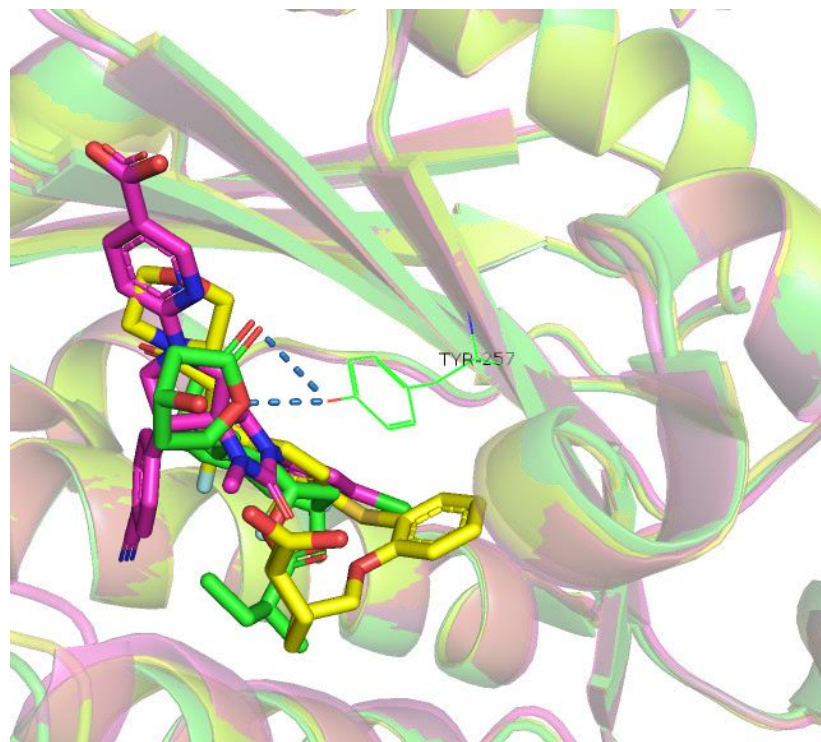
- File → Open 1cqp.pdb
- Display → Sequence
- PyMOL>select /1cqp//A
- (sele) A → rename selection → chain_a
- 1cqp H → everything
- (chain_a) S → cartoon
- (chain_a) C → by ss
- click on 803
- (sele) S → sticks
- (sele) C → by element
- File → Export Image As → PNG
- [or] Draw/Ray → Save Image to File



Exercise: PyMOL>select /1cqp//B
(sele) A → remove atoms
Display → Sequence
click on 803 and Y257
(sele) S → sticks
PyMOL>distance 257/OH, 311/O1

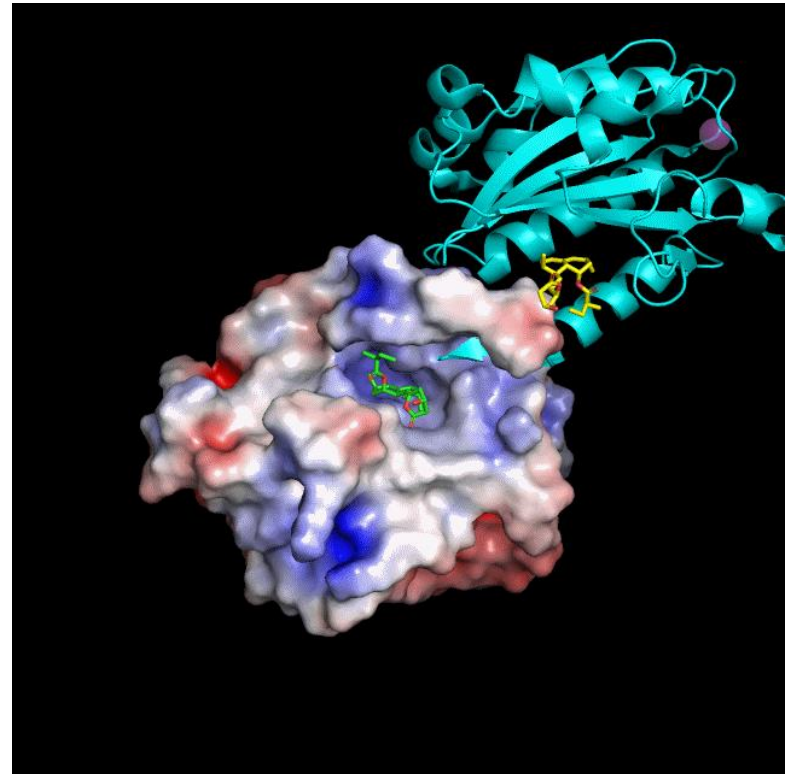
PyMOL Basic Application (2)

- Display → Background → white
- File → Open 1cqp.pdb (3e2m.pdb & 3m6f.pdb)
- PyMOL>select /1cqp//A (select /3e2m//A)
- (sele) A → rename selection → 1cqp_a (3e2m_a)
- (3e2m_a) C → yellows; A → align → to selection → 1cqp_a (RMS = 0.317Å)
- 3m6f A → align → to selection → 1cqp_a (RMS = 0.37Å)
- all H → everything
- 3m6f (1cqp_a & 3e2m_a) S → cartoon
- Click on 803 (E2M & BJZ) S → sticks; C → by element
- Click on 1cqp_a Y257 (sele) S → lines; C → by element; S → label
- Setting → Transparency → Cartoon → 50%
- Wizard → Measurement Distances; click on oxygen atoms of Y257 & 803
- measure01 C → skyblue; H → labels
- measure02 C → skyblue; H → labels
- File → Export Image As → PNG
- File → Save Session As → *.pse



PyMOL Advanced Applications

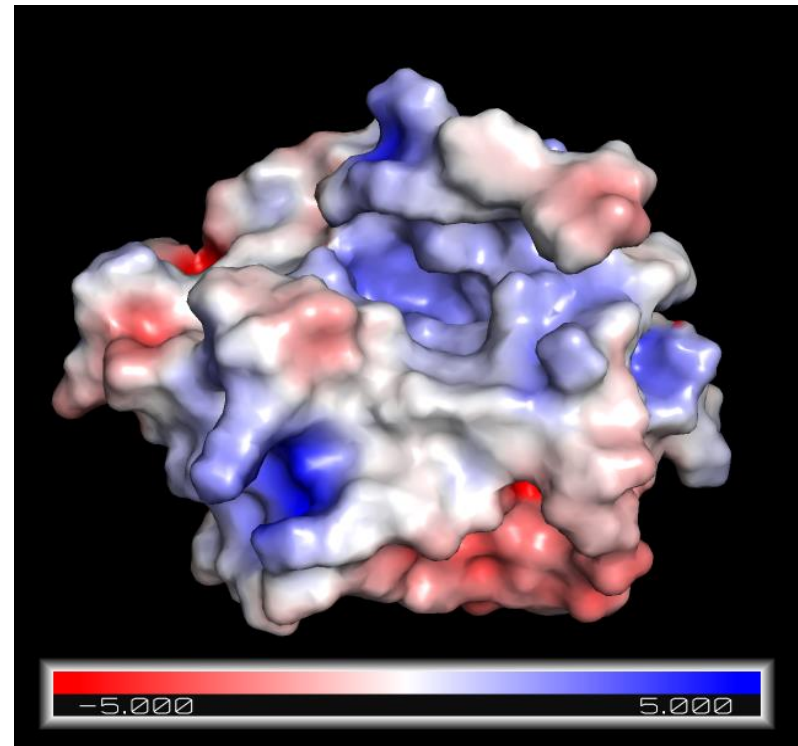
- Electrostatic surface
- Plugin
- Molecular movement
- Animation
- Script



Electrostatic surface and plugin

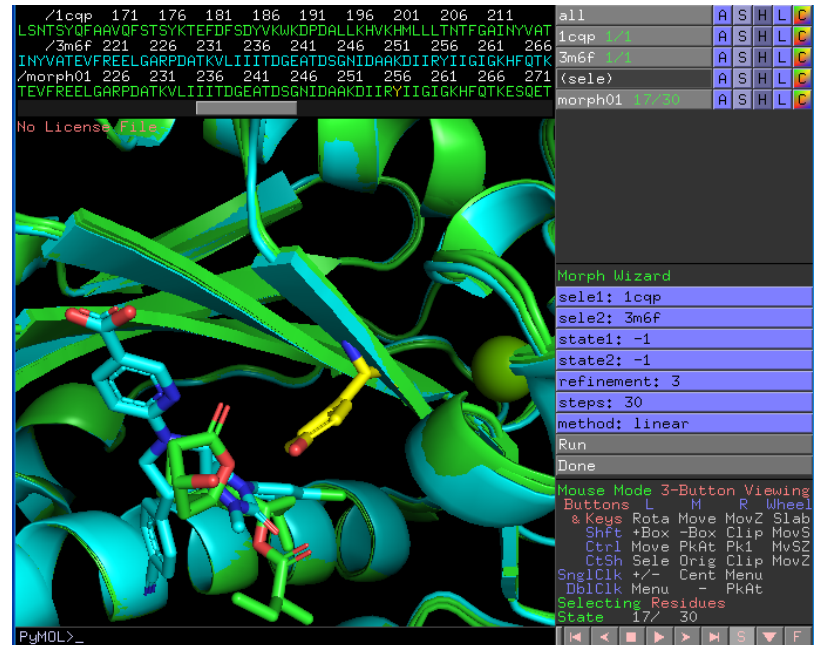
- An input file of APBS (Adaptive Poisson-Boltzmann Solver) is required to generate the electrostatic surface for the structure. This file can be obtained from PDB2PQR web server. (http://nbc-222.ucsd.edu/pdb2pqr_2.0.0/)
- File → Open 1cqp.pdb
- File → Open 15209457729-pot-PE0.dx
- Plugin → Initialize Plugin System
- Plugin → APBS Electrostatics → run

Exercise: File → Open 1cqp.pdb
1cqp C → by chain; H → waters
Mouse Mode → Residues
click on 803 of chain B
(sele) C → by element →
carbon atoms in yellow
click on MG C → magentas →
purple
Setting → Transparency →
Sphere → 50%



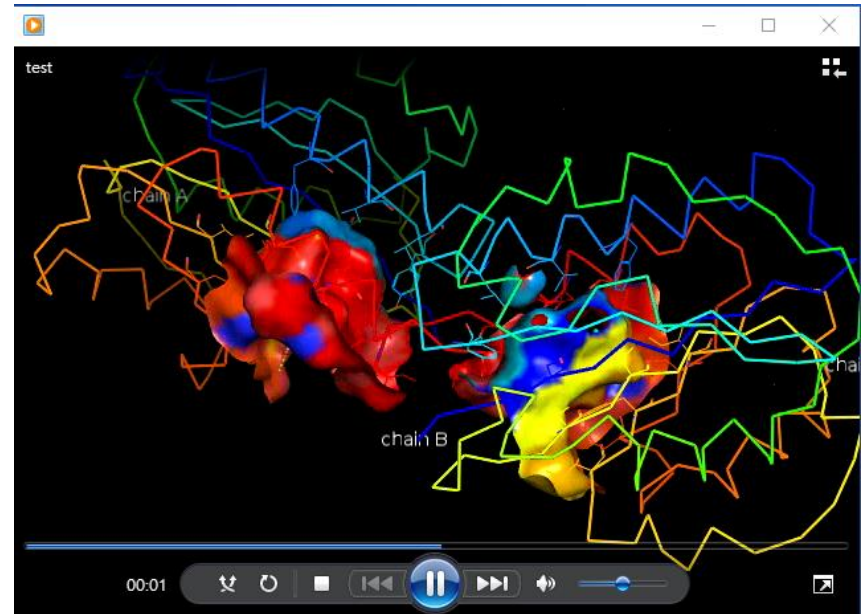
Molecular movement

- File → Open 1cqp.pdb
- select /1cqp//B
- (sele) A → remove atoms
- File → Open 3m6f.pdb
- Plugin → Alignment/Superposition → one by one
- 1cqp A → center
- 1cqp A → generate → wizard...
- Morph Wizard → sele2: **3m6f**;
method: **linear** → run
- Display → Sequence
- click on Y257 of morph01
- (sele) S → sticks; C → by element → carbon atoms in yellow
- Morph Wizard → run



Movie and animation

- File → Open 1cqp.pdb
 - 1cqp A → present → ligand sites → solid surface
 - 1cqp L → chains
 - Movie → 30 FPS; Program → Camera Loop → X-Roll → 4 seconds
 - File → Export Movie As → Save Movie as
 - File → Export Movie As → PNG Images
-
- At this step, 120 PNG images are saved. An external software is used to convert these images into a movie or an animation.



A Simple PyMOL Script

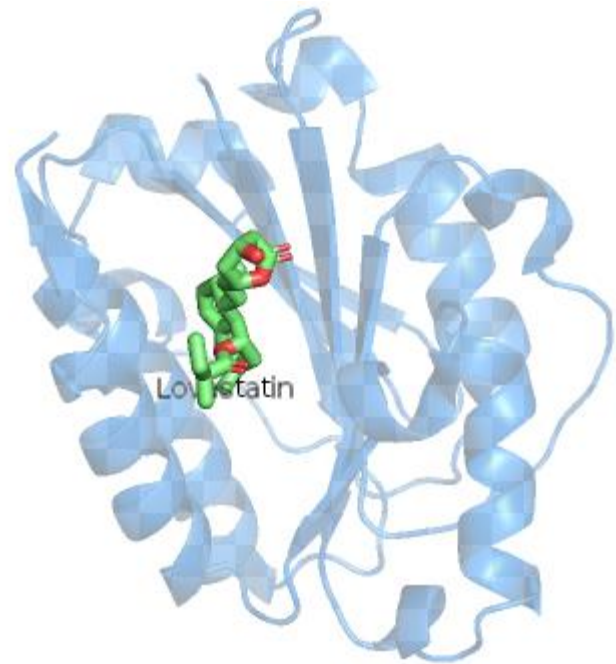
- Make a text file of commands:

- BasicScript.pml

```
load C:\Users\USERX\Desktop\1cqp.pdb
bg_color white
select chB, chain B
remove chB
hide everything
show cartoon
set cartoon_color, marine
set cartoon_transparency, 0.5
select ligand, /1cqp//A/311
show sticks,ligand
set_bond stick_radius, 0.5
label (311/C21),"%s" % "Lovastatin"
alter 190-192/,ss="L"
alter 267-268/,ss="L"
rebuild
center all
draw
```

- Run this script file by typing in:

- run FILEPATH\BasicScript.pml
[or] @FILEPATH\BasicScript.pml



Practice Makes Perfect!

Thank You