

Biomolecular Databases and Formats

Macro vs. Small Molecules

- **Macromolecules:** contain the structure of biological macromolecules. The primary source is the **Protein Data Bank** (<https://www.rcsb.org>).
- **Small molecules:** databanks containing formulas, structures and other information relative to small molecules* . Some of the most important are:
 - PubChem (NCBI) :<https://pubchem.ncbi.nlm.nih.gov/>
 - ZINC (purchasable compounds): <https://zinc.docking.org/>
 - Drugbank (pharma oriented): <https://www.drugbank.ca/>
 - CCDC (crystallographic structures): <https://www.ccdc.cam.ac.uk/>

* The definition of small molecule may vary (~1000-atom limit)

Macromolecules

Macromolecular Databanks

- **Primary databanks:** contain the **raw** information, usually with a set of tools that can be accessed through a portal. Example: **Protein Data Bank** (<https://www.rcsb.org>).
- **Secondary Databanks:** specialized views, collections or filters on the primary databanks. Example: The PDBind database (<http://www.pdbbind.org.cn>)

- The development of molecular structure determination techniques lead to the accumulation of a large body of structures of proteins and nucleic acids (~160000)
- For the most part, those structures were solved using two structure determination methods, X-ray crystallography and nuclear magnetic resonance (NMR)
- The body of structures is stored in the public accessible Protein Databank (PDB) <http://www.rcsb.org>

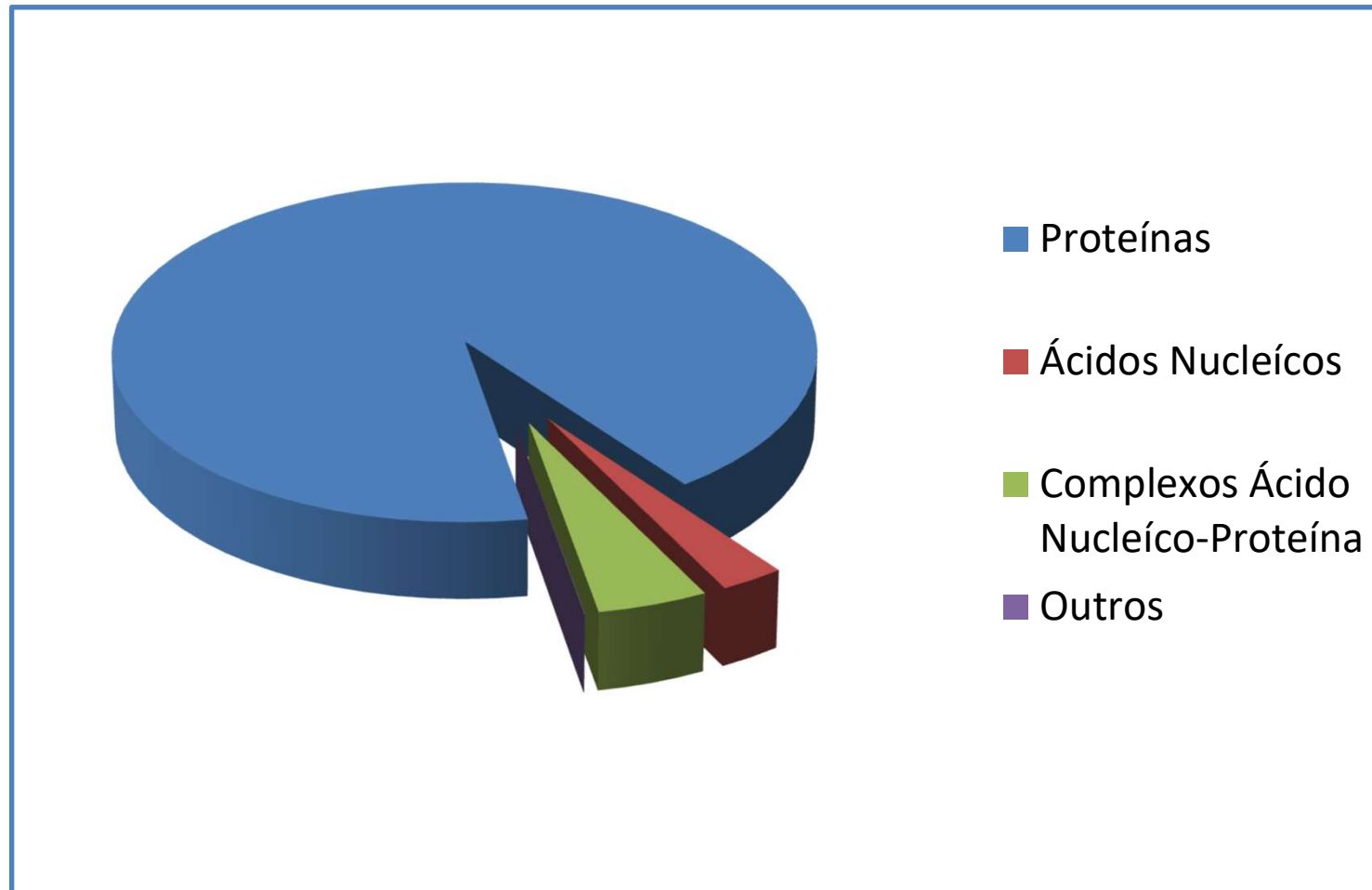
The Protein Data Bank

- O Protein Data Bank (PDB) foi criado em 1971 por E.Meyer e W.Hamilton, do Brookhaven National Laboratory (USA), contendo no início 7 estruturas!
- A gestão do PDB foi transferida em 1998 para os membros do RCSB (Research Collaboratory in Structural Bioinformatics) dos quais a Universidade de Rutgers é o site principal. O PDB (<http://www.rcsb.org>) é um banco de dados de acesso livre.
- Contendo inicialmente estruturas de proteínas, o PDB contém hoje em dia outros tipos de moléculas, tais como ácidos nucleicos, lípidos e polissacáridos.
- Número total de estruturas em 12/12/2019: **158,180**

Técnica experimental	Proteínas	Ácidos nucleicos	Complexos Ac.Nuc./Proteína	Outros	Total
Cristalografia de raios X	132004	2073	6787	8	140872
NMR	11248	1306	262	8	12824
Microscopia electrónica	2974	33	1021	0	4028
Outras	281	4	6	13	304
Combinação	144	5	2	1	152
Total	146651	3421	8078	30	158180

Dados de 12/12/2019 em <http://www.rcsb.org>

The Protein Databank contains different types of biological macromolecules

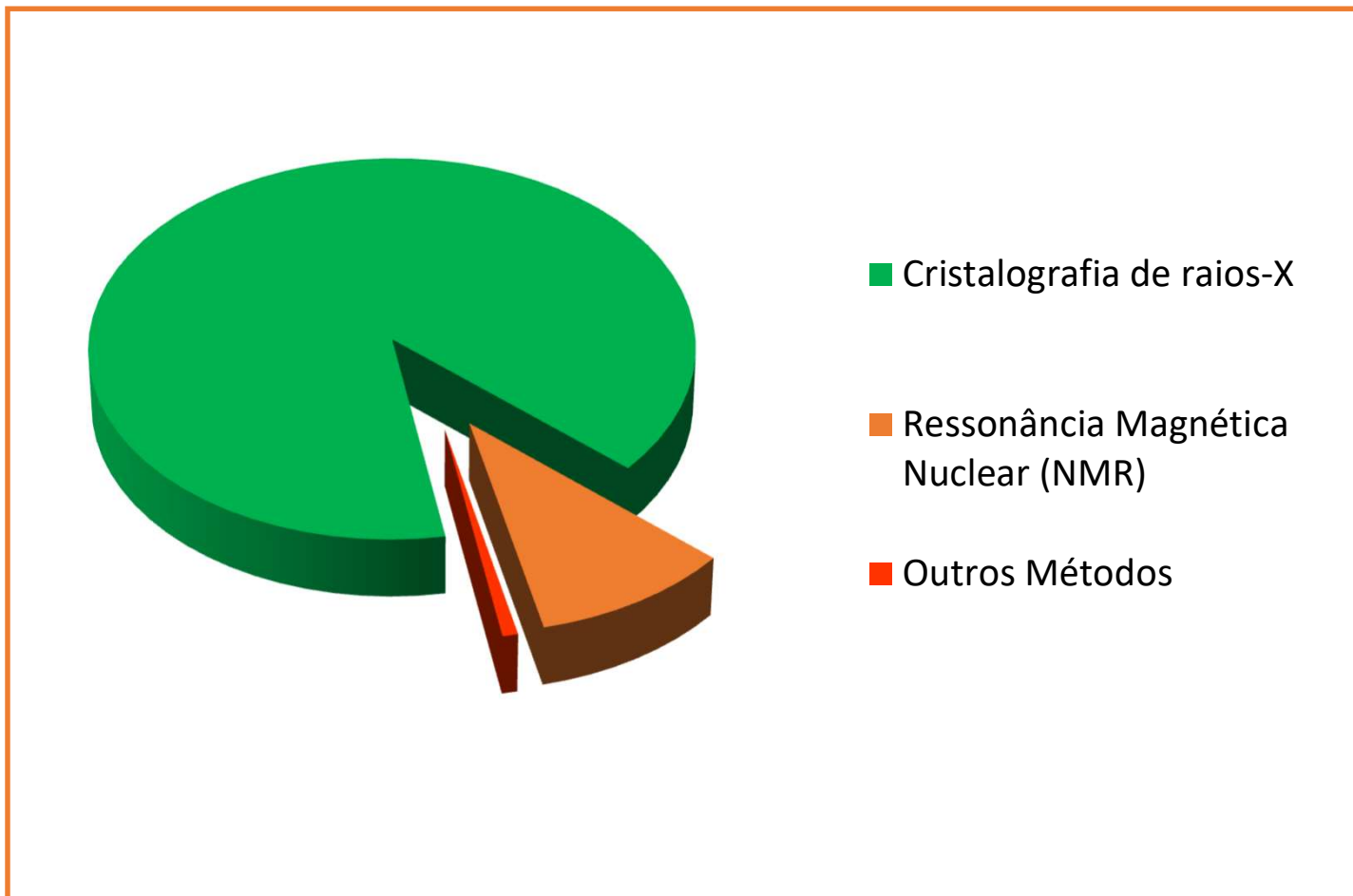


Where does all the structural information come from ?

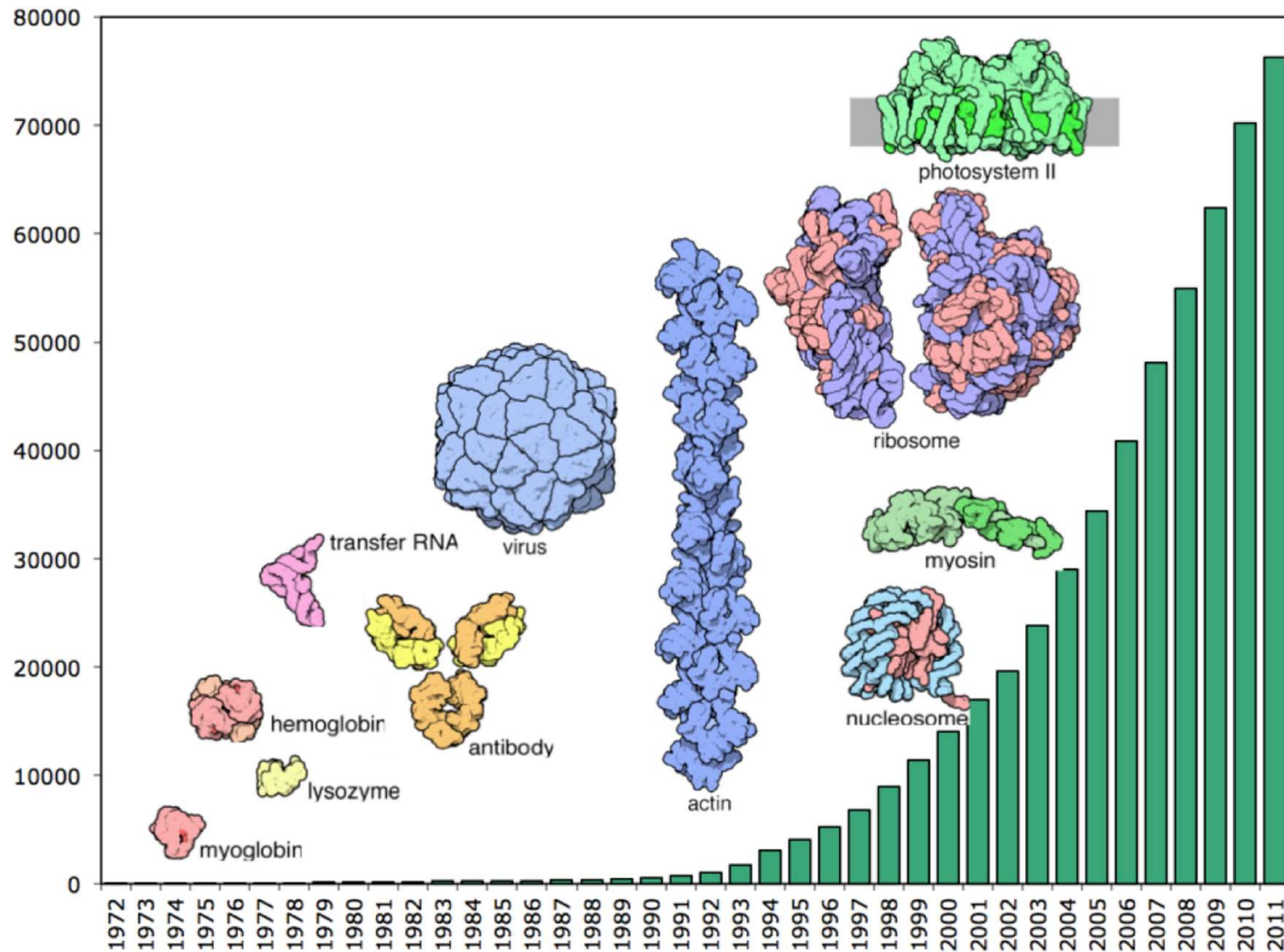
It's a combination of various types of data:

- Molecular geometry and bond theory
- Small molecule geometry
- Experimental Methods of Macromolecular structure determination
 - ❖ X-ray crystallography
 - ❖ Nuclear Magnetic Resonance (NMR)
 - ❖ Other methods (Cryo-EM, neutron diffraction, etc)

Most structures have been solved by X-ray
cristallography

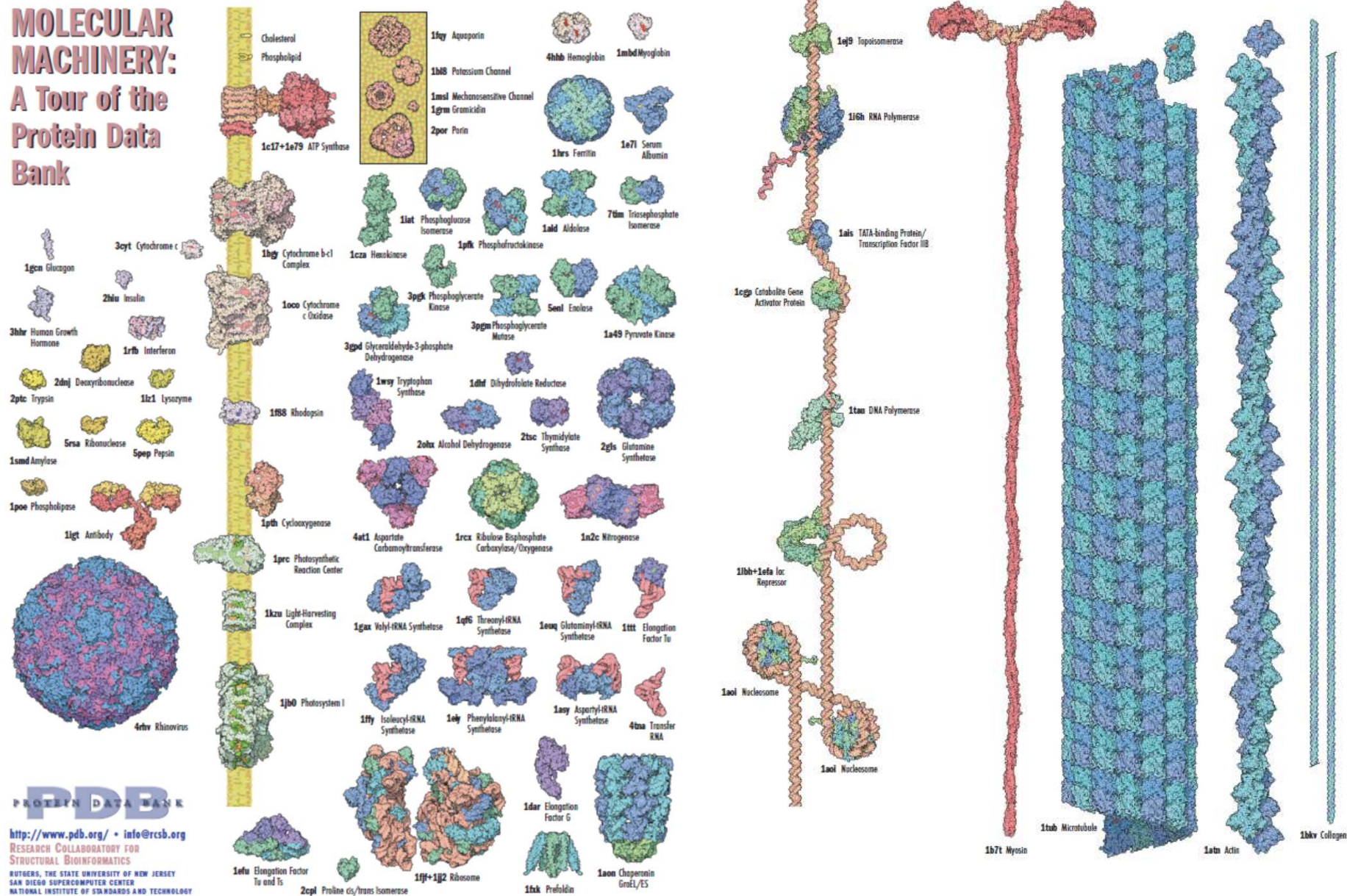


Progress in the determination of macromolecular structures



The PDB contains a very diverse set of structures !

MOLECULAR MACHINERY: A Tour of the Protein Data Bank



PDB Web Portal

RCSB PDB

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RCSB PDB

PROTEIN DATA BANK

158180 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

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

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PDB-101

Worldwide Protein Data Bank

EMDataResource

DOI

Nucleic Acid Database

Worldwide Protein Data Bank Foundation

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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.

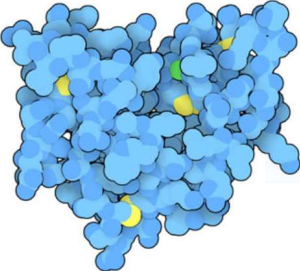
As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.

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.

Video: How Enzymes Work



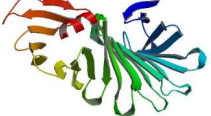
November Molecule of the Month



Phospholipase A2

Latest Entries

As of Tuesday, Nov 26 2019





6J6B


Borrelia burgdorferi OspA via surface entropy reduction (form2)

PDB Entry

Features & Highlights

 New EM map validation in OneDep
Additional validation for electron microscopy maps helps users identify potential discrepancies.

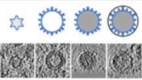
 Improved resolution of DOIs for PDB entries
Access new wwPDB summary pages for released PDB entries with PDB DOIs

 Mandatory PDBx/mmCIF format files submission for MX depositions
Submission of PDBx/mmCIF format files for crystallographic depositions to the PDB will be mandatory from July 1st 2019 onward. PDB format files will no longer be accepted for deposition of structures solved by MX techniques.

Join Our Team as a Registrar

News

Publications ▾

 Education Corner: Gaming Structural Biology for General Audiences (Part 2)
Learn about Deep Learning, Citizen Science & Puppies from Diamond Light Source's Michele Darrow » 11/26/2019

Introducing Mol* » 11/19/2019

New Papers on Molecular Visualization » 11/12/2019

New EM map validation in OneDep » 11/05/2019

Education Corner: Gaming Structural Biology for General Audiences (Part 1) » 10/29/2019

PDB Turns 48 » 10/20/2019

Happy Birthday, Irving Geis » 10/18/2019

From the Bench to Molecule of the Month » 10/15/2019

PDB at a Glance | 48974 Distinct Protein Sequences | 44467 Structures of Human Sequences | 11504 Nucleic Acid Containing Structures | [More Statistics](#)

<https://www.rcsb.org>

PDB Web Portal

Paulo

RCSB PDB: Homepage x

Secure | <https://www.rcsb.org>

Apps | Acad | AWS | Free | Cell Bits | PDF | Calendario 2017-18 | VTC | NiceHash | LuckPool | Supernova | WTM | WhatToMine | D pmartel | Other bookmarks

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RCSB PDB 137692 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

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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.

New Video: What is a Protein?

February Molecule of the Month

EPSP Synthase and Weedkillers

Latest Entries As of Tuesday Feb 13 2018

Features & Highlights

News Publications

Meet RCSB PDB at AAAS

Learn how RCSB PDB is Sustaining A Living Digital

PDB Web Portal

RCSB PDB - Query Results

www.pdb.org/pdb/results/results.do?tabtoShow=Current&qrid=B13E001B

Gnuplot surprisi... Gnuplot tricks N Old Nabble - G... Music Production Bioinformatics 10.10.20.1/form... + Pocket Other bookmarks

Search | All Categories: lysozyme

Query Parameters: Text Search for: lysozyme

Other search suggestions:

Query Refinements: Select an item or pie chart

Organism Taxonomy Exp. Method X-ray Resolution Release Date Polymer Type

Enzyme Classification SCOP Classification

Refine Query with Advanced Search Remove Similar: Select Percent Similarity

5 Related Molecule of the Month articles

PDB Pioneers Nanobodies Adrenergic Receptors Antibodies Lysozyme

Showing 1 - 25 of 1346 Results Results: 25 Page: 1 of 54

Filter: Check All View: Detailed Reports: Select one.. Sort: Relevance

1JKB HUMAN LYSOZYME MUTANT WITH GLU 35 REPLACED BY ALA

Authors: Muraki, M., Harata, K., Goda, S., Nagahora, H.

Release: 1997-05-15 Classification: Lysozyme

Experiment: X-RAY DIFFRACTION with resolution of 1.66 Å Residue Count: 130

Compound: 1 Polymer [Display Full Polymer Details | Display for All Results]
1 Ligand [Display Full Ligand Details | Display for All Results]

Citation: Importance of van der Waals contact between Glu 35 and Trp 109 to the catalytic action of human lysozyme. (1997) Protein Sci. 6: 473-476 [Display Full Abstract | Display for All Results]

Molecule of the Month: Nanobodies, PDB Pioneers, Antibodies, Lysozyme

Search Hit: Classification: LYSOZYME

1JKC HUMAN LYSOZYME MUTANT WITH TRP 109 REPLACED BY PHE

Authors: Muraki, M., Harata, K., Goda, S., Nagahora, H.

Release: 1997-05-15 Classification: Lysozyme

PDB Web Portal

RCSB Protein Data Bank

www.pdb.org/pdb/explore/explore.do?structureId=1JKB

Gnuplot surprisi... Gnuplot tricks N Old Nabble - G... Music Production Bioinformatics 10.10.20.1/form... + Pocket Other bookmarks

PDB-101 Hide

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Understanding PDB Data
Molecule of the Month
Educational Resources
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Query History (1)

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X-ray | NMR
Validation Server
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Glossary of Terms
RCSB PDB Mobile

Summary Sequence Annotations Seq. Similarity 3D Similarity Literature Biol. & Chem. Methods Geometry Links

HUMAN LYSOZYME MUTANT WITH GLU 35 REPLACED BY ALA

DOI:10.2210/pdb1jkb/pdb

Primary Citation

Importance of van der Waals contact between Glu 35 and Trp 109 to the catalytic action of human lysozyme.

Muraki, M., Goda, S., Nagahora, H., Harata, K.

Journal: (1997) Protein Sci. 6: 473-476

PubMed: 9041653

PubMedCentral: PMC2143631

DOI: 10.1002/pro.5560060227

Search Related Articles in PubMed

PubMed Abstract:

The importance of van der Waals contact between Glu 35 and Trp 109 to the active-site structure and the catalytic properties of human lysozyme (HL) has been investigated by site-directed mutagenesis. The X-ray analysis of mutant HLs revealed that both...

[Read More & Search PubMed Abstracts]

Molecular Description Hide

Classification: Lysozyme

Structure Weight: 14786.71

Molecule: LYSOZYME

Polymer: 1 Type: protein Length: 130

Chains: A

EC#: 3.2.1.17

Mutation: E35A

Organism: Homo sapiens

UniProtKB: Protein Feature View | Search PDB | P61626

P61626 Molec. Processing signal peptide Lysozyme C E.C. 3.2.1.17: Lysozyme

UP Sites

PDB Sites

Secstruc

1JKB.A

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1JKB

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Biological Assembly ?

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Biological assembly 1 assigned by authors

Downloadable viewers:

Simple Viewer Protein Workshop Kiosk Viewer

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Deposition Summary Hide

Authors: Muraki, M., Harata, K., Goda, S., Nagahora, H.

Deposition: 1996-11-13

Release: 1997-05-15

Last Modified (REVDAT): 2009-02-24

Revision History ? Hide

Mouse over text for details

Download th structure in PDB format

The screenshot shows the RCSB Protein Data Bank (PDB) website interface. The main content area displays the entry for **HUMAN LYSOZYME MUTANT WITH GLU 35 REPLACED BY ALA** (PDB ID: 1JKB). The left sidebar contains navigation links such as PDB-101, MyPDB, Home, Deposition, Tools, and Help. The right sidebar shows download options and MyPDB personal annotations. A dropdown menu is open, listing various download formats, with **PDB File (Text)** highlighted in a red box.

Summary | Sequence | Annotations | Seq. Similarity | 3D Similarity | Literature | Biol. & Chem. | Methods | Geometry | Links

HUMAN LYSOZYME MUTANT WITH GLU 35 REPLACED BY ALA

DOI:10.2210/pdb1jkb/pdb

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Search Related Articles in PubMed

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Mutation: E35A

Organism: Homo sapiens

UniProtKB: Protein Feature View | Search PDB | P61626

Downloadable viewers:

- Simple Viewer
- Protein Workshop
- Kiosk Viewer

MyPDB Personal Annotations

To save personal annotations, please login to your MyPDB account.

Deposition Summary

Authors: Muraki, M., Harata, K., Goda, S., Nagahora, H.

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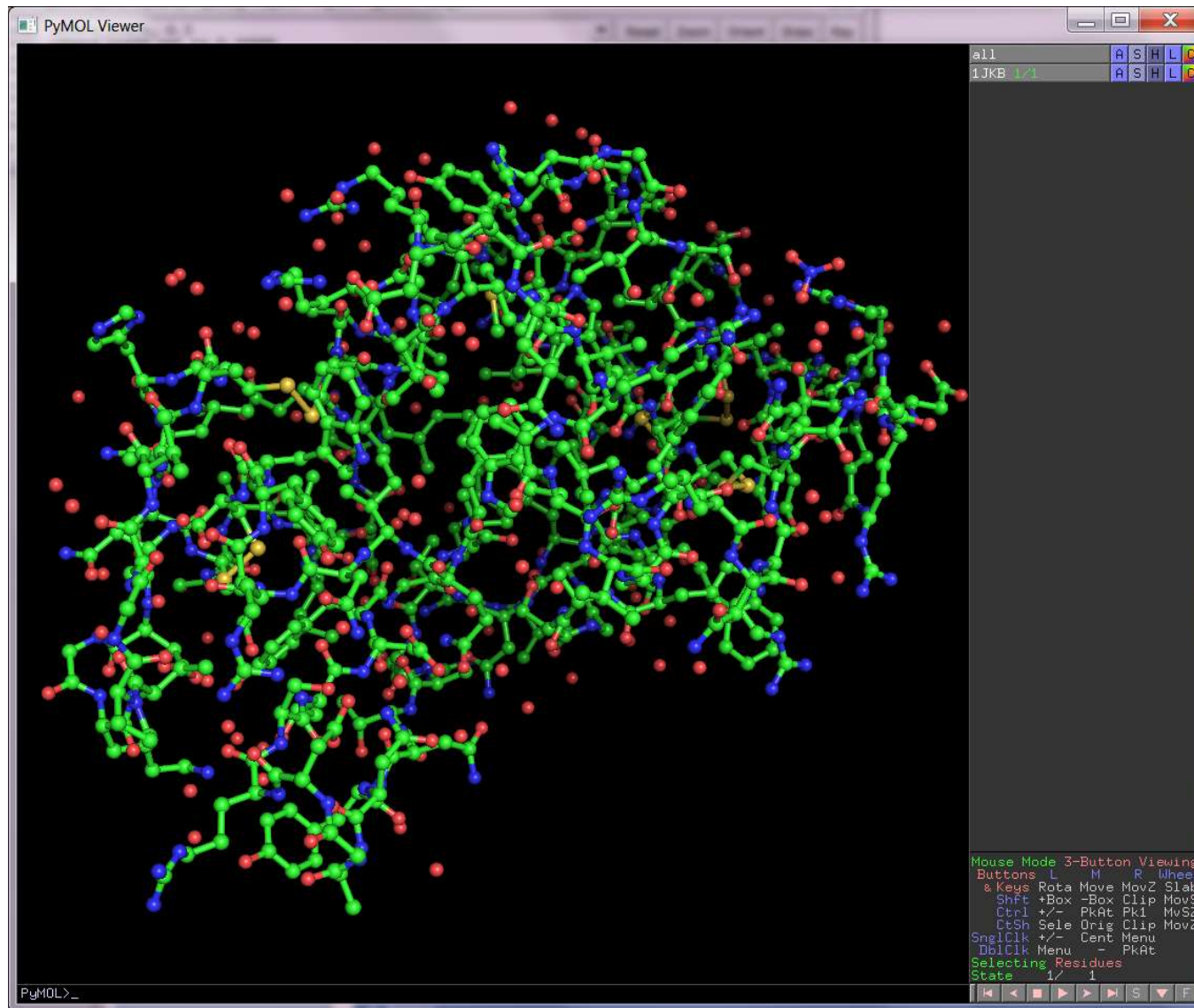
Revision History

Mouse over text for details

Source

www.pdb.org/pdb/download/downloadFile.do?fileFormat=pdb&compression=NO&structureId=1JKB

Viewing the structure with a molecular visualizer (PyMOL)



Formatos de representação da estrutura

- A representação da estrutura molecular em bancos de dados passa pela descrição das **coordenadas atômicas**, do **tipo de átomo**, e das **ligações químicas** presentes.
- A descrição do tipo de átomos e ligações que os unem designa-se como **topologia** da molécula.
- No caso das proteínas, a topologia dos 20 aminoácidos standard pode ser assumida *a priori*, pois a estrutura dos aminoácidos é conhecida
- A topologia de outras moléculas, tais como grupos prostéticos , deverá ser especificada
- O formato "tradicional" de representação de estrutura no Protein Data Bank é o formato **PDB**.

Formato da informação no Protein Data Bank

- A informação contida no Protein Databank inclui coordenadas atómicas, topologias de ligação (descrição das ligações químicas), nomes dos átomos e grupos químicos, dados associados ao processo de determinação experimental da estruturas e outras informações sobre a função, ligandos, propriedades, etc...
- Presentemente a informação no PDB está disponível nos seguintes formatos:
 - **pdb file**: O formato "flat file", um tipo de ficheiro chamado "ficheiro PDB". Estes ficheiros são os mais utilizados pelos softwares de manipulação e visualização de estruturas e têm geralmente a extensão ".pdb"
 - **mmCIF**: - um formato mais poderoso e estruturado que o ficheiro PDB, ainda não tendo sido largamente adoptado
 - **XML**: - extended mark-up language, um formato muito geral de representação de informação, compatível com um vasto número de aplicações de software.

Formato do ficheiro PDB

```
HEADER      METAL BINDING PROTEIN                      21-AUG-03   1Q8H
TITLE       CRYSTAL STRUCTURE OF PORCINE OSTEOCALCIN
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: OSTEOCALCIN;
COMPND      3 CHAIN: A
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: SUS SCROFA;
SOURCE      3 ORGANISM_COMMON: PIG
KEYWDS      HELIX-TURN-HELIX-TURN-HELIX, PAPER-CLIP, HYDROXYAPATITE
KEYWDS      2 CRYSTAL SURFACE BINDING PROTEIN, CALCIUM BINDING PROTEIN,
KEYWDS      3 BONE GLA PROTEIN
EXPDTA      X-RAY DIFFRACTION
AUTHOR      Q.Q.HOANG,F.SICHERI,A.J.HOWARD,D.S.YANG
REVDAT      1 11-NOV-03 1Q8H 0
JRNL        AUTH  Q.Q.HOANG,F.SICHERI,A.J.HOWARD,D.S.YANG
JRNL        TITL   BONE RECOGNITION MECHANISM OF PORCINE OSTEOCALCIN
JRNL        TITL 2 FROM CRYSTAL STRUCTURE.
JRNL        REF    NATURE                      V. 425   977 2003
JRNL        REFN   ASTM NATUAS   UK ISSN 0028-0836
REMARK      1
REMARK      2
REMARK      2 RESOLUTION. 2.00 ANGSTROMS.
REMARK      3
REMARK      3 REFINEMENT.
REMARK      3   PROGRAM      : CNS 1.1
REMARK      3   AUTHORS      : BRUNGER, ADAMS, CLORE, DELANO, GROS, GROSSE-
.....
ATOM        1  N   PRO A  13      10.210  29.966  44.935  1.00 38.06
ATOM        2  CA  PRO A  13       9.718  29.013  43.919  1.00 37.33
ATOM        3  C   PRO A  13       9.566  29.662  42.541  1.00 37.52
ATOM        4  O   PRO A  13       9.275  30.855  42.444  1.00 38.00
ATOM        5  CB  PRO A  13       8.383  28.488  44.434  1.00 37.68
ATOM        6  CG  PRO A  13       7.919  29.624  45.336  1.00 36.60
ATOM        7  CD  PRO A  13       9.196  30.126  45.995  1.00 36.47
ATOM        8  N   ASP A  14       9.777  28.879  41.483  1.00 36.83
ATOM        9  CA  ASP A  14       9.671  29.384  40.116  1.00 36.13
.....
MASTER      299    0    6    3    0    0    0    6  378    1  38    4
END
```

Cabeçalho

Coordenadas

Interligação entre Uniprot e PDB

The screenshot shows the UniProtKB entry for P00760 (TRY1_BOVIN). The 'Cross-refs' tab is highlighted in red. The entry is a reviewed protein from Bos taurus (Bovine) with the recommended name 'Cationic trypsin' (EC=3.4.21.4). It is cleaved into two chains: Alpha-trypsin chain 1 and Alpha-trypsin chain 2. The taxonomic lineage is Eukaryota > Metazoa > Chordata > Craniata > Vertebrata > Euteleostomi > Mammalia > Eutheria > Laurasiatheria > Cetartiodactyla > Ruminantia > Pecora > Bovidae > Bovinae > Bos.

Blues Drums Bund x thelooploft's stre x Gravidade - Cinec x Mino Cinelu - Wiki x RCSB Protein Data x Configurar - Appl x Over To You: Mac x Cationic trypsin pr x

www.uniprot.org/uniprot/P00760#section_x-ref

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Search in Protein Knowledgebase (UniProtKB) Query Search Advanced Search » Clear

P00760 (TRY1_BOVIN) ★ Reviewed, UniProtKB/Swiss-Prot
Last modified October 16, 2013. Version 149. History...

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Clusters with 100%, 90%, 50% identity | Documents (3) | Third-party data text xml rdf/xml gff fasta

Names · Attributes · General annotation · Ontologies · Interactions · Sequence annotation · Sequences · References · Web links **Cross-refs**

Entry info · Documents Customize order

Names and origin

Protein names	<i>Recommended name:</i> Cationic trypsin EC=3.4.21.4 <i>Alternative name(s):</i> Beta-trypsin <i>Cleaved into the following 2 chains:</i> 1. Alpha-trypsin chain 1 2. Alpha-trypsin chain 2
Organism	Bos taurus (Bovine) [Reference proteome]
Taxonomic identifier	9913 [NCBI]
Taxonomic lineage	Eukaryota > Metazoa > Chordata > Craniata > Vertebrata > Euteleostomi > Mammalia > Eutheria > Laurasiatheria > Cetartiodactyla > Ruminantia > Pecora > Bovidae > Bovinae > Bos

Interligação entre Uniprot e PDB

Blues Drums Bundle x thelooploft's stream x W Mino Cinelu - Wikip x RCSB Protein Data B x Configurar - Apple S x Over To You: MacBoi x Cationic trypsin prec x

www.uniprot.org/uniprot/P00760#section_x-ref

Names · Attributes · General annotation · Ontologies · Interactions · Sequence annotation · Sequences · References · Web links · Cross-refs · Entry info · Documents Customize order

Cross-references

Sequence databases

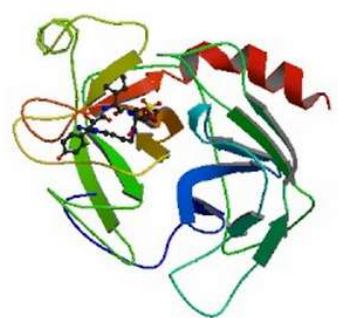
<input checked="" type="radio"/> EMBL	BC134797 mRNA. Translation: AAI34798.1 .
<input type="radio"/> GenBank	BC146041 mRNA. Translation: AAI46042.1 .
<input type="radio"/> DDBJ	D38507 mRNA. Translation: BAA07516.1 .
IPI	IPI00706427 .
PIR	TRBOTR . A90164.
RefSeq	NP_001107199.1 . NM_001113727.1 .
UniGene	Bt.91423 .

3D structure databases

<input checked="" type="radio"/> PDBe	Entry	Method	Resolution (Å)	Chain	Positions	PDBsum
<input type="radio"/> RCSB PDB	1AQ7	X-ray	2.20	A	24-246	[>]
<input type="radio"/> PDBj	1AUJ	X-ray	2.10	A	24-246	[>]
	1AZ8	X-ray	1.80	A	24-246	[>]
	1BJU	X-ray	1.80	A	24-246	[>]
	1BJV	X-ray	1.80	A	24-246	[>]
	1BTP	X-ray	2.20	A	18-246	[>]
	1BTW	X-ray	1.70	A	18-246	[>]
	1BTX	X-ray	1.70	A	18-246	[>]
	1BTY	X-ray	1.50	A	18-246	[>]
	1BTZ	X-ray	2.00	A	18-246	[>]

Blues Drums Bundle x thelooploft's stream x Mino Cinelu - Wikip x RCSB Protein Data B x Configurar - Apple S x Over To You: MacBoi x RCSB Protein Data B x



www.pdb.org/pdb/explore/explore.do?structureId=1AQ7

RCSB PDB PROTEIN DATA BANK  A MEMBER OF THE **PDB** | **EMDataBank**

An Information Portal to Biological Macromolecular Structures
As of Tuesday Oct 29, 2013 at 5 PM PDT there are 95113 Structures | [PDB Statistics](#) | [Email](#) | [RSS](#) | [Help](#)

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Everything Author Macromolecule Sequence Ligand ?

 e.g., PDB ID, molecule name, author 

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TRYPSIN WITH INHIBITOR AERUGINOSIN 98-B

1AQ7  Display Files ▾
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DOI:10.2210/pdb1aq7/pdb

Primary Citation


Atomic Structure of the Trypsin-Aeruginosin 98-B Complex


Sandler, B., Murakami, M., Clardy, J.


Journal: (1998) J.Am.Chem.Soc. **120**: 595-596

PubMed ID is not available

↑ Molecular Description **Hide**

Classification: Hydrolase/hydrolase Inhibitor 

Structure Weight: 23979.18 

Molecule:	TRYPSIN	Type:	protein	Length:	223
Polymer:	1				
Chains:	A				
EC#:	3.4.21.4 				

Biological Assembly ?

