Visualização de Macromoléculas

Visualização de Macromoléculas

1. **Seleccionar o modelo que se pretende obter (problema biológico)**

2. **Escolher a base de dados de macromoléculas (geralmente o Protein Data Bank, http://www.rcsb.org)**

3. **Escolher o modelo a analizar, de acordo com as suas características (resolução, número de cadeias, completo, incompleto, condições de cristalização, técnica experimental, ligandos, etc…)**

4. **Descarregar o modelo num dos formatos disponíveis (geralmente formato PDB ou mmCIF)**

5. **Examinar a estrutura num programa de visualização molecular (variados programas de acesso livro, p.exp. PyMOL)**

- O desenvolvimento das técnicas de determinação da estrutura molecular levou à acumulação de um número considerável de estruturas de proteínas (~200000)

- A maior parte das estruturas foram determinadas pelos métodos de difracção (cristalografia) de raios X ou então por ressonância magnética nuclear (RMN)

- A principal base de dados de estruturas de macromoléculas é o Protein Databank (PDB) http://www.rcsb.org

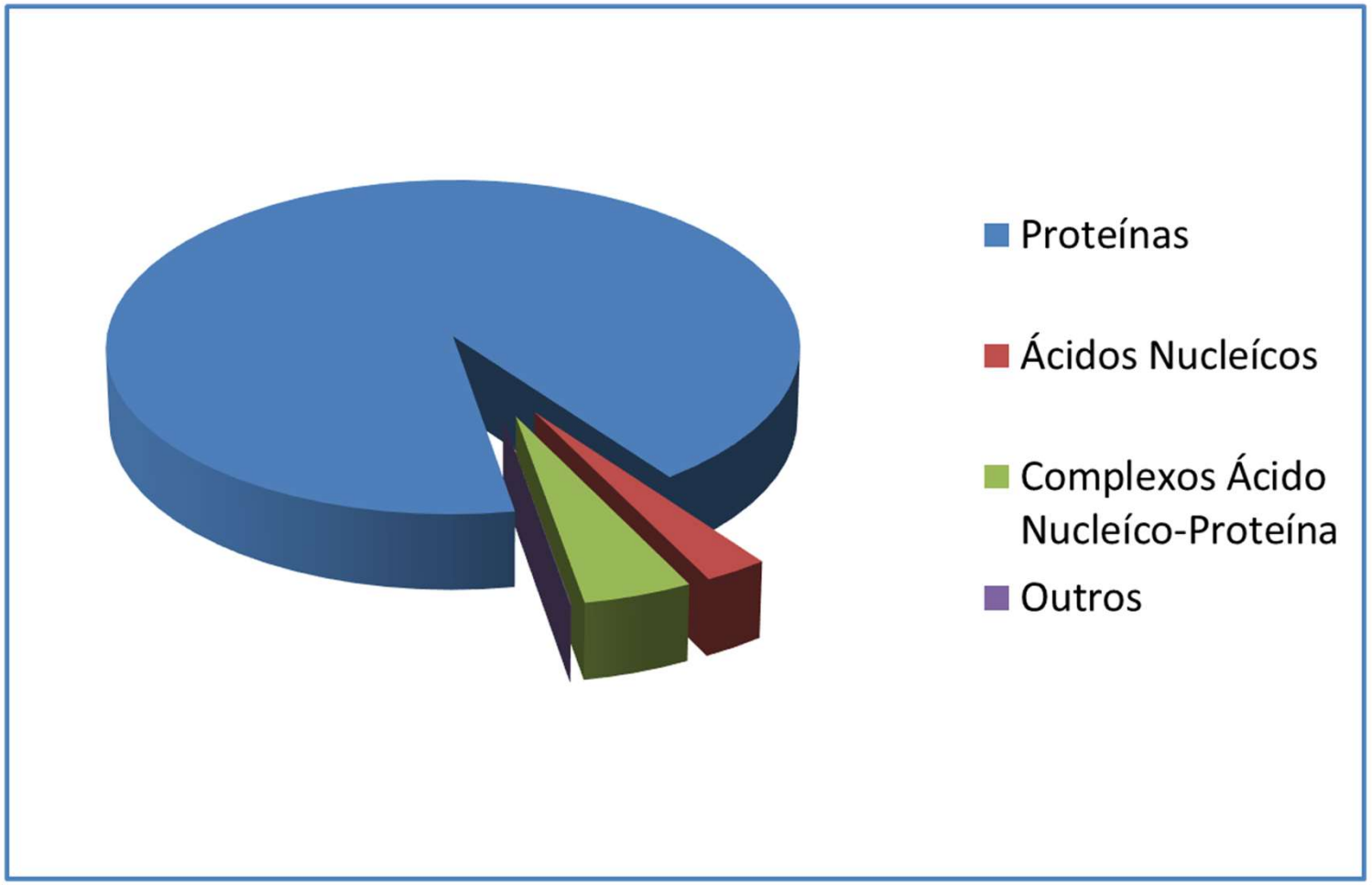
O Protein Data Bank

- 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 RSCB (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 contem hoje em dia outros tipos de moléculas, tais como ácidos nucleicos, lípidos e polissacáridos.
- Número total de estruturas em 2/3/2021: **174994**

Técnica experimental	Proteínas	Ácidos nucleicos	Complexos Ac.Nuc,/Proteína	Outros	Total
Cristalografia de raios X	144855	2164	7208	160	154387
NMR	11636	1347	260	37	13289
Microscopia electrónica	5342	53	1632	3	7030
Outras	270	10	3	5	288
Total	162103	3574	9112	205	**174994**

Dados de 2/03/2020 em http://www.rcsb.org

O Protein Data Bank contem vários tipos de macromoléculas

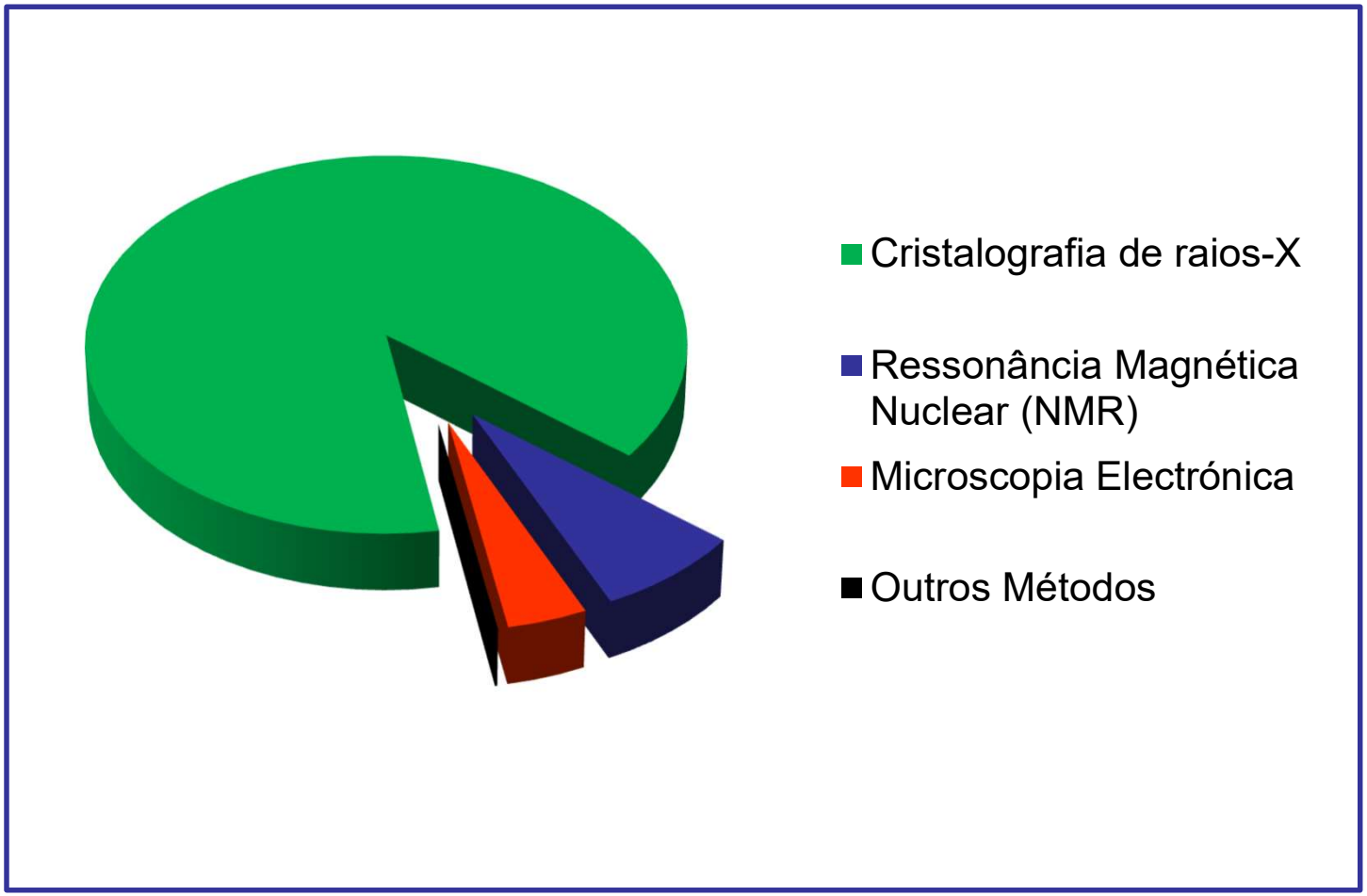


De onde provêm a informação estrutural ?

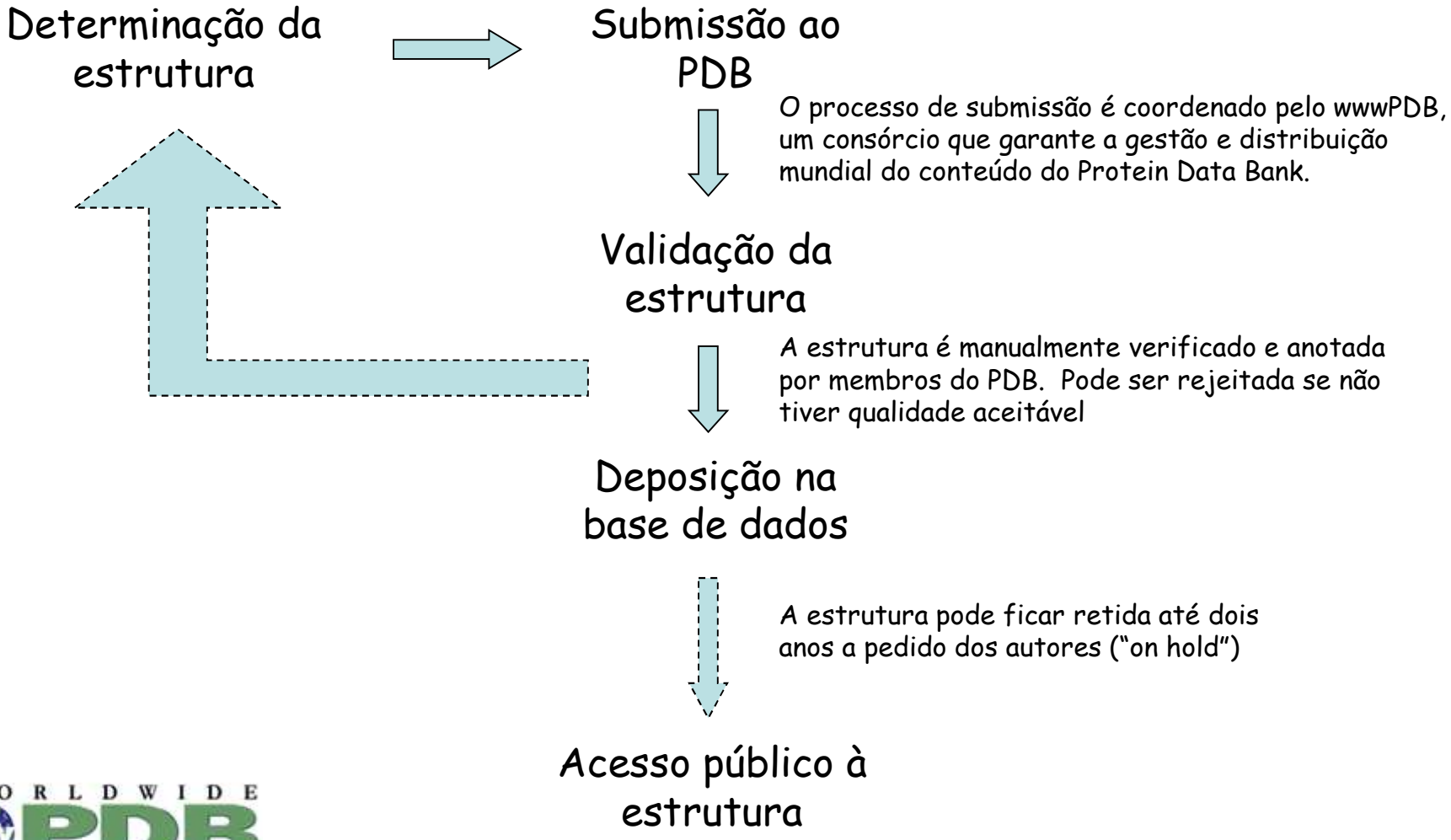
Combinação de vários tipos de conhecimento:

- Teoria da ligação química
- Geometria de moléculas pequenas
- Métodos experimentais para a determinação da estrutura:
  - Cristalografia de raios X
  - Ressonância Magnética Nuclear (NMR)
  - Outros métodos (microscopia, difracção de neutrões, etc…)

A maioria da estruturas do PDB são obtidas por cristalografia de raios X

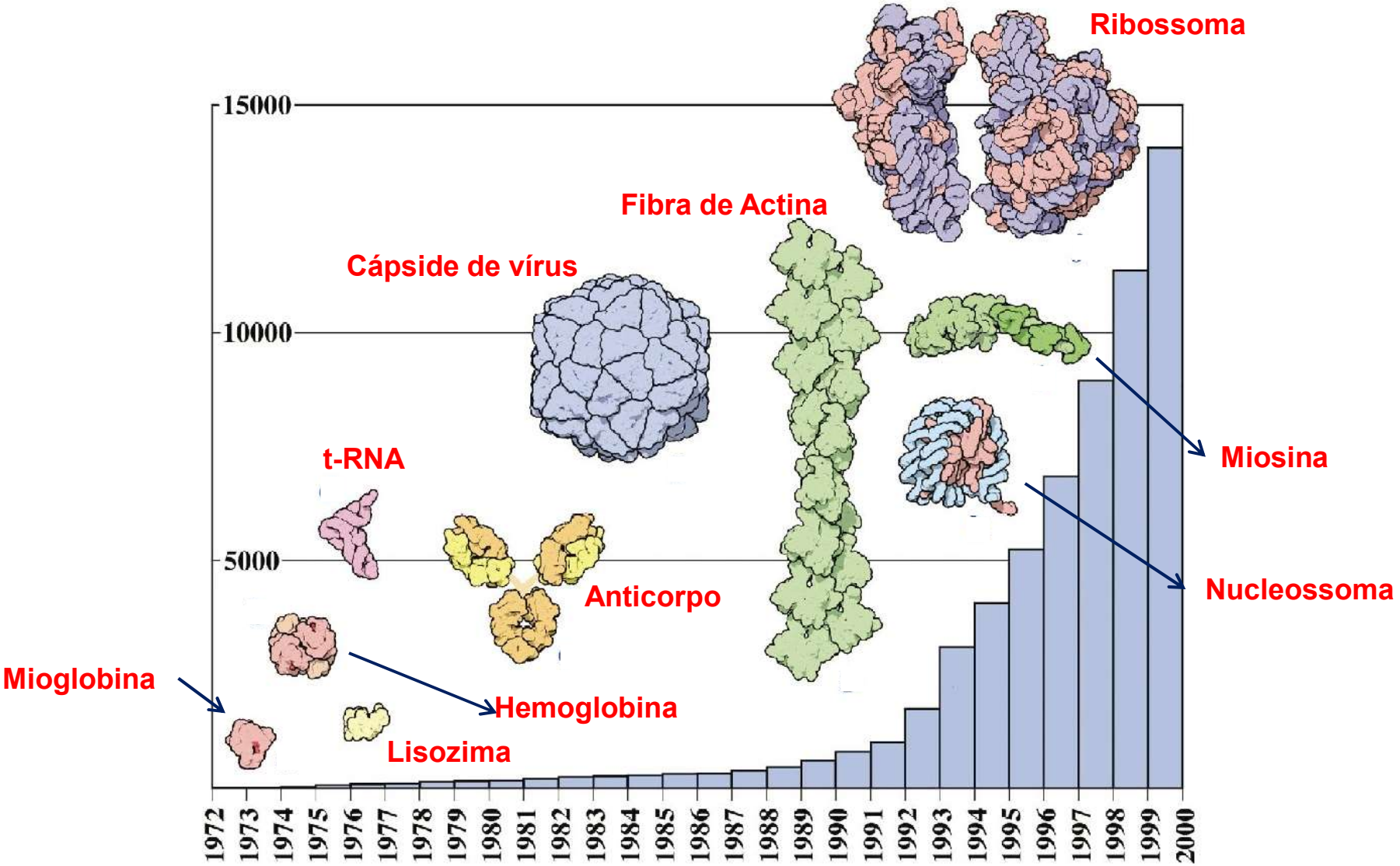


Deposição de estruturas no Protein Data Bank



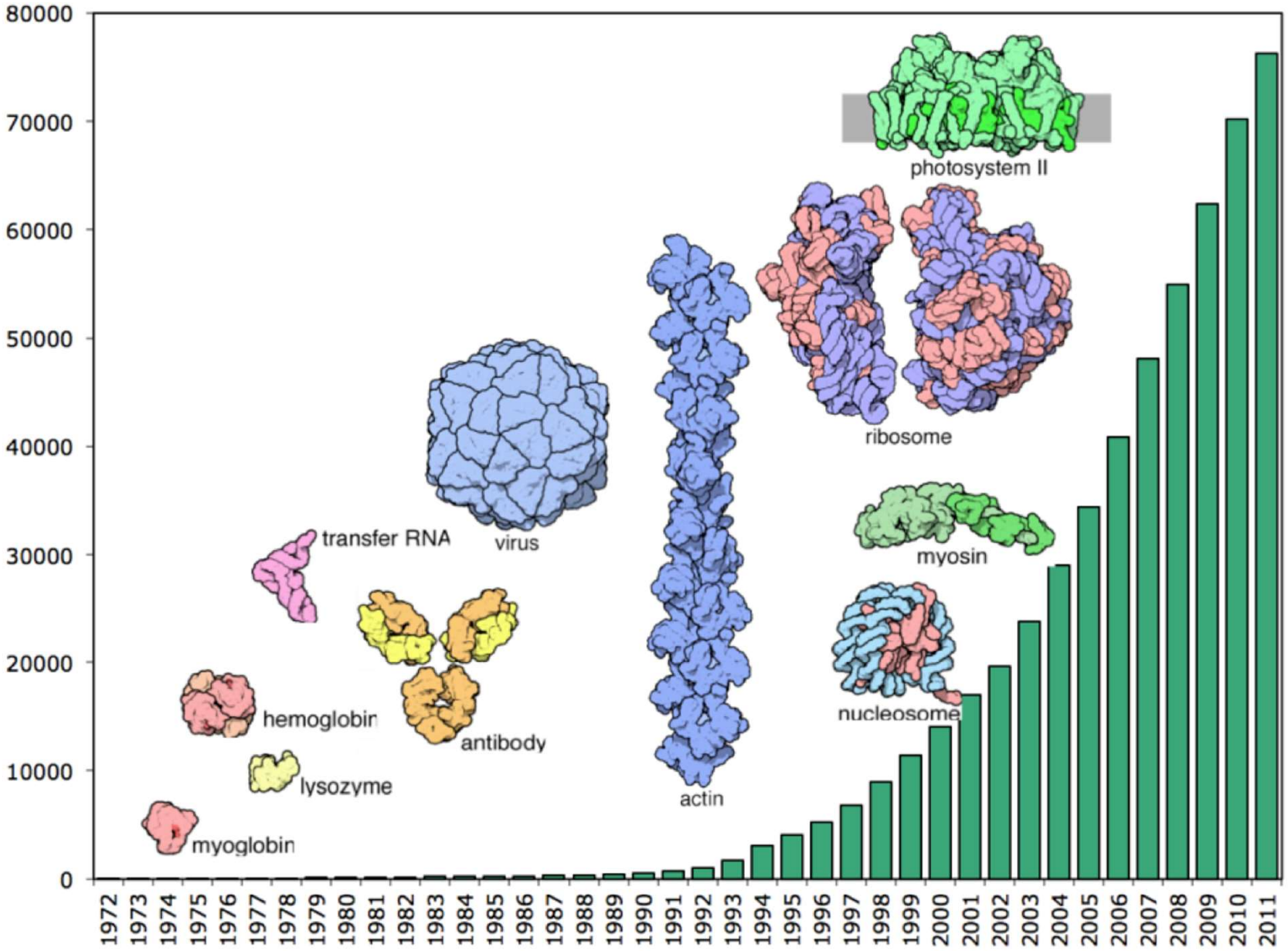
WORLDWIDE PDB
PROTEIN DATA BANK

Progresso na determinação das estruturas

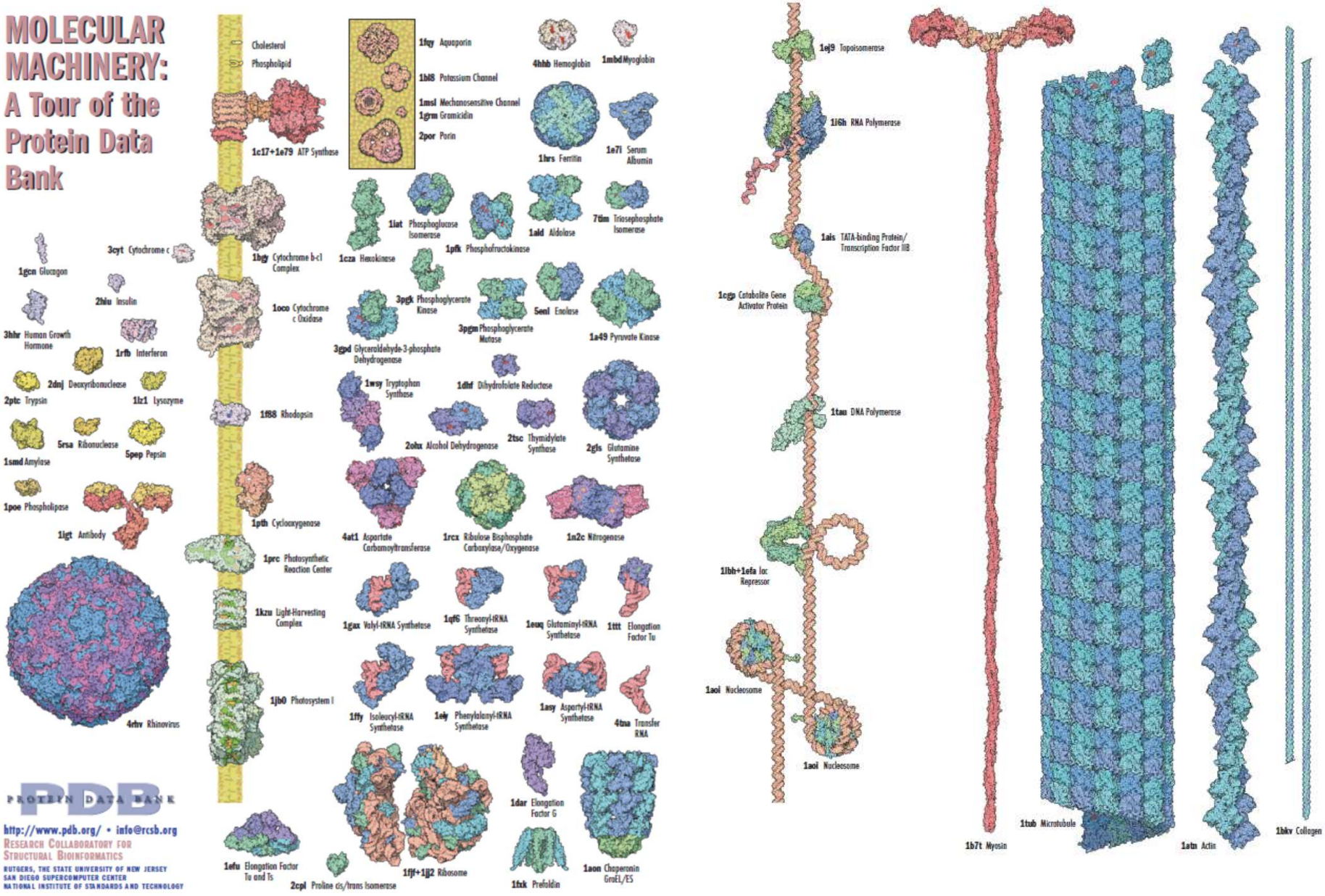


http://www.pdb.org

Progresso na determinação das estruturas



O PDB contém uma enorme diversidade estrutural!



Formatos de representação da estrutura

- A representação da estrutura molecular em bancos de dados passa pela descrição das **coordenadas atómicas**, 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 interna 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           N
ATOM      2  CA  PRO A  13       9.718  29.013  43.919  1.00 37.33           C
ATOM      3  C   PRO A  13       9.566  29.662  42.541  1.00 37.52           C
ATOM      4  O   PRO A  13       9.275  30.855  42.444  1.00 38.00           O
ATOM      5  CB  PRO A  13       8.383  28.488  44.434  1.00 37.68           C
ATOM      6  CG  PRO A  13       7.919  29.624  45.336  1.00 36.60           C
ATOM      7  CD  PRO A  13       9.196  30.126  45.995  1.00 36.47           C
ATOM      8  N   ASP A  14       9.777  28.879  41.483  1.00 36.83           N
ATOM      9  CA  ASP A  14       9.671  29.384  40.116  1.00 36.13           C
                    ..........
MASTER      299    0    6    3    0    0    0    6  378    1   38    4
END
```

Cabeçalho

Coordenadas

Portal de acesso ao Protein Data Bank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LYSOZYME
Immune system, Lysozyme
in UniProt Molecule Name
Lysozyme
Lysozyme 1
Lysozyme C
Lysozyme C I
Lysozyme C II
Lysozyme C, milk isozyme
Lysozyme C-1
Lysozyme C-2
Lysozyme M1
Lysozyme g
in Additional Structure Keywords
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from protein synthesis to health and dise
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The RCSB PDB builds upon the data by
research and education in molecular bio
biology, and beyond.
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ecule of the Month
Cisplatin and DNA
Latest Entries
As of Tue Feb 23 2021
6LZU
F411A mutant of chitin-specific solute binding protein from Vibrio harveyi co-crystalized with chitobiose.
Features & Highlights
Search for Structural Motifs
Explore residue patterns that recur throughout the PDB
IQB and ERN: Electron Microscopy Community Voice of the Customer
Register for the online February 11 workshop that will solicit feedback from microscopists and facility managers about IT challenges
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PDB50: Submit Posters by March 15
Join the wwPDB May 4-5 for a symposium of speakers from around
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174994 Structures
51529 Structures of Human Sequences
12764 Nucleic Acid Containing Structures
More Statistics

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Celebrating 50 YEARS OF Protein Data Bank

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QUERY: Full Text = "Lysozyme" Open In Query Builder JSON MyPDB Login

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Refinements Clear All

SCIENTIFIC NAME OF SOURCE ORGANISM Clear

- Homo sapiens (966)
- Gallus gallus (922)
- Escherichia virus T4 (741)
- Mus musculus (164)
- Escherichia coli (134)
- synthetic construct (127)
- Escherichia coli K-12 (109)
- Bos taurus (83)
- Saccharomyces cerevisiae S288C (62)
- Camelus dromedarius (61)

More...

TAXONOMY Clear

- Eukaryota (2725)
- Bacteria (1448)
- Duplodnaviria (810)
- other sequences (127)
- Riboviria (95)
- Archaea (94)
- Varidnaviria (6)
- Monodnaviria (5)
- unclassified sequences (3)
- unclassified bacterial viruses (2)

More...

EXPERIMENTAL METHOD Clear

- X-RAY DIFFRACTION (4937)
- SOLUTION NMR (33)
- ELECTRON MICROSCOPY (21)
- POWDER DIFFRACTION (14)
- ELECTRON CRYSTALLOGRAPHY (13)
- NEUTRON DIFFRACTION (10)
- EPR (4)
- SOLID-STATE NMR (1)

POLYMER ENTITY TYPE Clear

- Protein (5001)
- DNA (56)
- RNA (25)

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Displaying 1 to 25 of 5023 **Structures** Page 1 of 201 ← Previous Next → Display 25 per page

3D View

6LZM

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COMPARISON OF THE CRYSTAL STRUCTURE OF BACTERIOPHAGE T4 LYSOZYME AT LOW, MEDIUM, AND HIGH IONIC STRENGTHS

Bell, J.A., Wilson, K., Zhang, X.-J., Faber, H.R., Nicholson, H., Matthews, B.W.

(1991) Proteins **10**: 10-21

Released	1992-07-15
Method	X-RAY DIFFRACTION 1.8 Å
Organisms	Escherichia virus T4
Macromolecule	T4 LYSOZYME (protein)
Unique Ligands	BME, CL

3D View

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Method	X-RAY DIFFRACTION 1.8 Å
Organisms	Escherichia virus T4
Macromolecule	T4 LYSOZYME (protein)
Unique Ligands	BME, CL

3D View

4LZM

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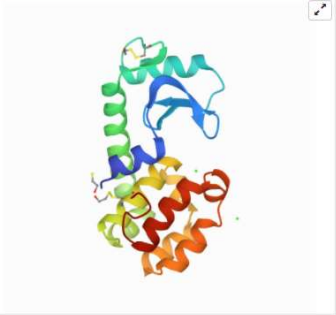
(1991) Proteins **10**: 10-21

Released	1992-07-15
Method	X-RAY DIFFRACTION 1.7 Å
Organisms	Escherichia virus T4
Macromolecule	T4 LYSOZYME (protein)
Unique Ligands	BME, CL

Biological Assembly 1



3D View: Structure | Electron Density | Ligand Interaction

Global Symmetry: Asymmetric - C1
Global Stoichiometry: Monomer - A1

Find Similar Assemblies

Biological assembly 1 assigned by authors.

Macromolecule Content

- Total Structure Weight: 18.97 kDa
- Atom Count: 1400
- Residue Count: 162
- Unique protein chains: 1

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COMPARISON OF THE CRYSTAL STRUCTURE OF BACTERIOPHAGE T4 LYSOZYME AT LOW, MEDIUM, AND HIGH IONIC STRENGTHS

DOI: 10.2210/pdb6LZM/pdb

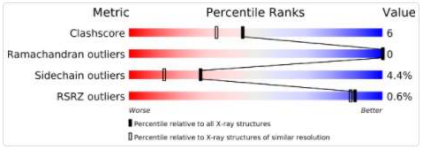
Classification: HYDROLASE (O-GLYCOSYL)
Organism(s): Escherichia virus T4
Mutation(s): No

Deposited: 1991-01-25 **Released:** 1992-07-15
Deposition Author(s): Bell, J.A., Wilson, K., Zhang, X.-J., Faber, H.R., Nicholson, H., Matthews, B.W.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 1.80 Å
R-Value Observed: 0.160

wwPDB Validation 3D Report Full Report



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Literature

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Bell, J.A., Wilson, K.P., Zhang, X.J., Faber, H.R., Nicholson, H., Matthews, B.W.
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PubMed: 2062826 Search on PubMed
DOI: 10.1002/prot.340100103
Primary Citation of Related Structures:
7LZM, 6LZM, 5LZM, 4LZM

PubMed Abstract:
Crystals of bacteriophage T4 lysozyme used for structural studies are routinely grown from concentrated phosphate solutions. It has been found that crystals in the same space group can also be grown from solutions containing 0.05 M imidazole chloride, 0. ...

Macromolecules

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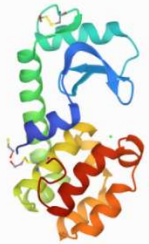

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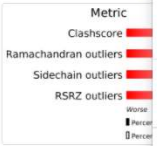

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- FASTA Sequence
- PDB Format
- PDB Format (gz)
- PDBx/mmCIF Format
- PDBx/mmCIF Format (gz)
- PDBML/XML Format (gz)
- Biological Assembly 1
- Structure Factors (CIF)
- Structure Factors (CIF - gz)
- Validation Full PDF
- Validation XML
- fo-fc Map (DSN6)
- 2fo-fc Map (DSN6)
- Map Coefficients (MTZ format)

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Macromolecules

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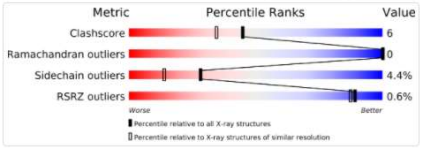

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Macromolecules

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COMPARISON OF THE CRYSTAL STRUCTURE OF BACTERIOPHAGE T4 LYSOZYME AT LOW, MEDIUM, AND HIGH IONIC STRENGTHS

Help

Sequence of 6LZM | COMP... Chain 1: T4 LYSOZYME A

```
1          11         21         31         41         51         61         71         81         91         101        111
MNIFEMLRIDEGLRLKIYKDTEGYYTIGIGHLLTKSPSLNAAKSELDKAIGRNCNGVITKDEAEKLFNQDVDAAVRGILRNAKLKPVYDSLDAVRRCALINMVFQMGETGVAGF
          121        131        141        151        161
TNSLRMLQQKRWDEAAVNLAKSRWYNQTPNRAKRVITTFRTGTWDAYKNL
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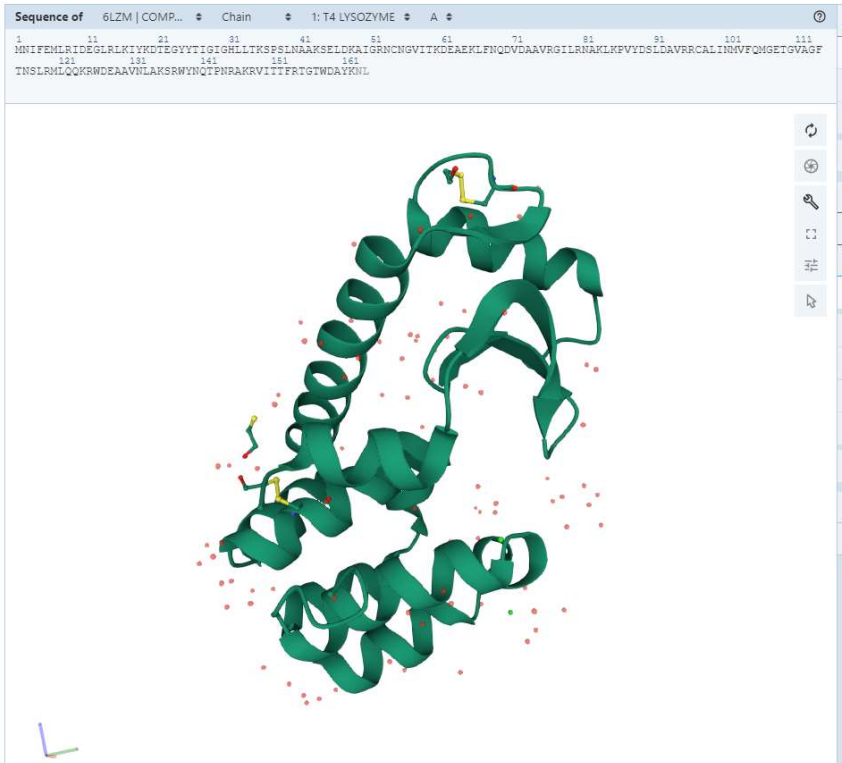
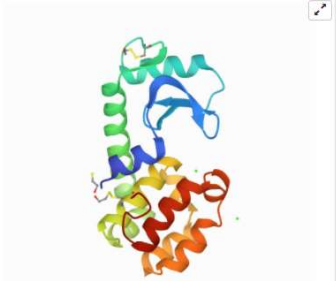


Structure
6LZM | COMPARISON OF THE CRYST...
Type Assembly
Asm Id 1: Author Defined Asse...
Nothing Focused
Measurements
Structural Motif Search
Components 6LZM
Preset + Add
Polymer Cartoon
Ligand Ball & Stick
Water Ball & Stick
Ion Ball & Stick
Unit Cell P 32 2 1
Density
Assembly Symmetry

Select a different viewer Mol* (Javascript)

Citation

Biological Assembly 1



3D View: Structure | Electron Density | Ligand Interaction

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- Residue Count: 162
- Unique protein chains: 1

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COMPARISON OF THE CRYSTAL STRUCTURE OF BACTERIOPHAGE T4 LYSOZYME AT LOW, MEDIUM, AND HIGH IONIC STRENGTHS

DOI: 10.2210/pdb6LZM/pdb

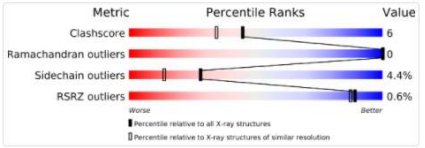
Classification: HYDROLASE (O-GLYCOSYL)
Organism(s): Escherichia virus T4
Mutation(s): No

Deposited: 1991-01-25 **Released:** 1992-07-15
Deposition Author(s): Bell, J.A., Wilson, K., Zhang, X.-J., Faber, H.R., Nicholson, H., Matthews, B.W.

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 1.80 Å
R-Value Observed: 0.160

wwPDB Validation 3D Report Full Report



This is version 1.4 of the entry. See complete history.

Literature

Download Primary Citation

Comparison of the crystal structure of bacteriophage T4 lysozyme at low, medium, and high ionic strengths.

Bell, J.A., Wilson, K.P., Zhang, X.J., Faber, H.R., Nicholson, H., Matthews, B.W.
(1991) Proteins **10**: 10-21

PubMed: 2062826 Search on PubMed
DOI: 10.1002/prot.340100103
Primary Citation of Related Structures:
7LZM, 6LZM, 5LZM, 4LZM

PubMed Abstract:
Crystals of bacteriophage T4 lysozyme used for structural studies are routinely grown from concentrated phosphate solutions. It has been found that crystals in the same space group can also be grown from solutions containing 0.05 M imidazole chloride, 0. ...

Macromolecules

6LZM

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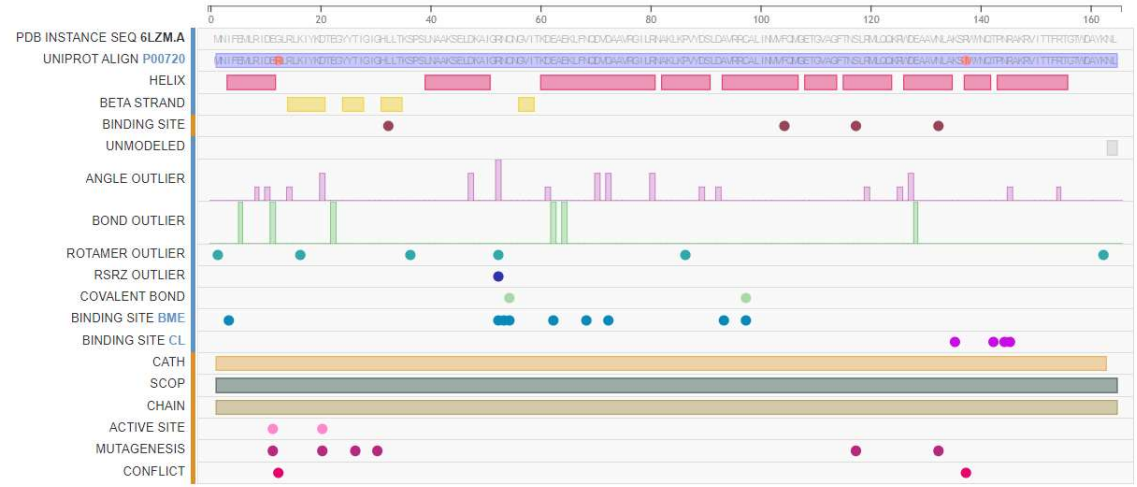
COMPARISON OF THE CRYSTAL STRUCTURE OF BACTERIOPHAGE T4 LYSOZYME AT LOW, MEDIUM, AND HIGH IONIC STRENGTHS

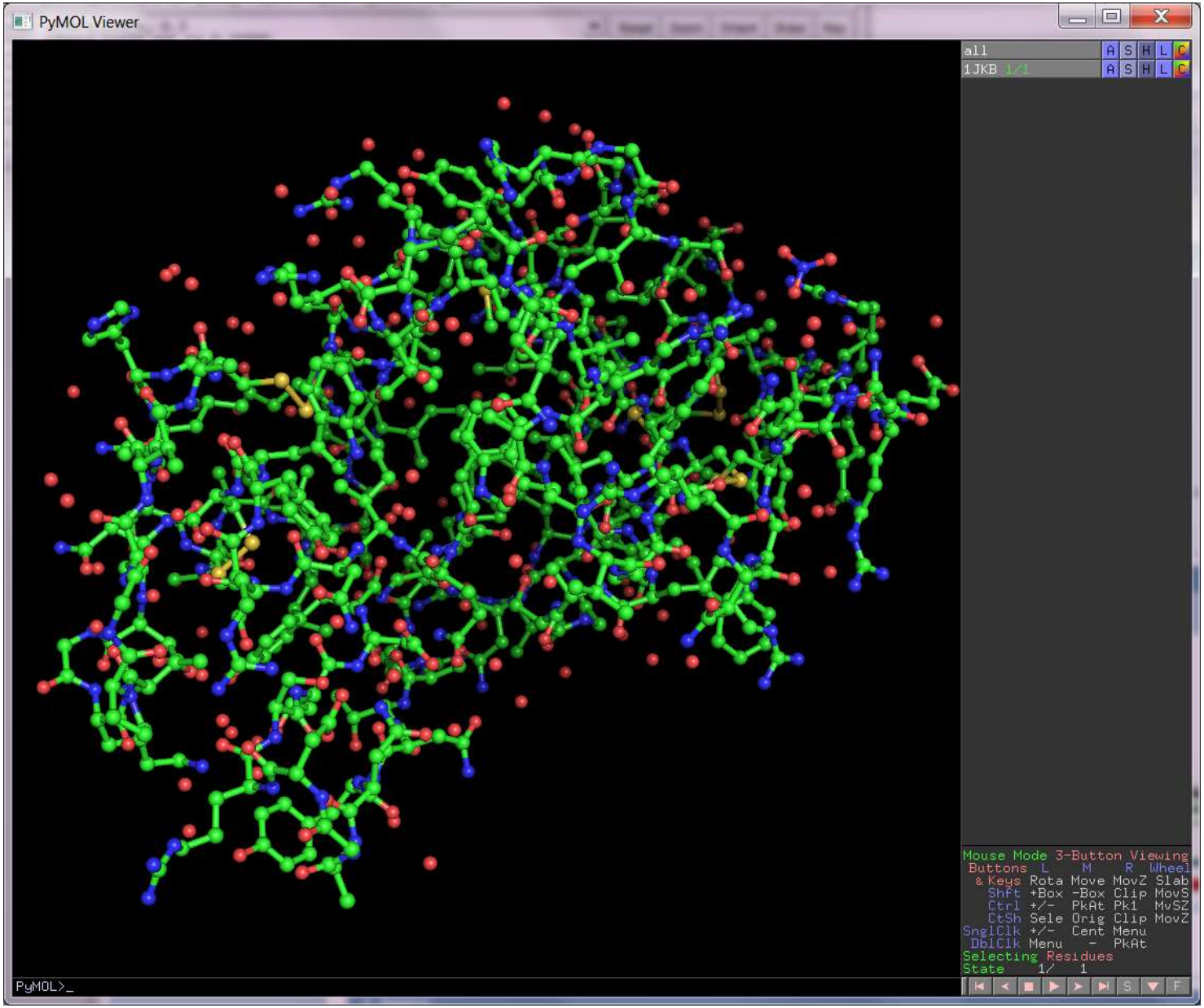
Help

6LZM.A T4 LYSOZYME - Escherichia virus T4

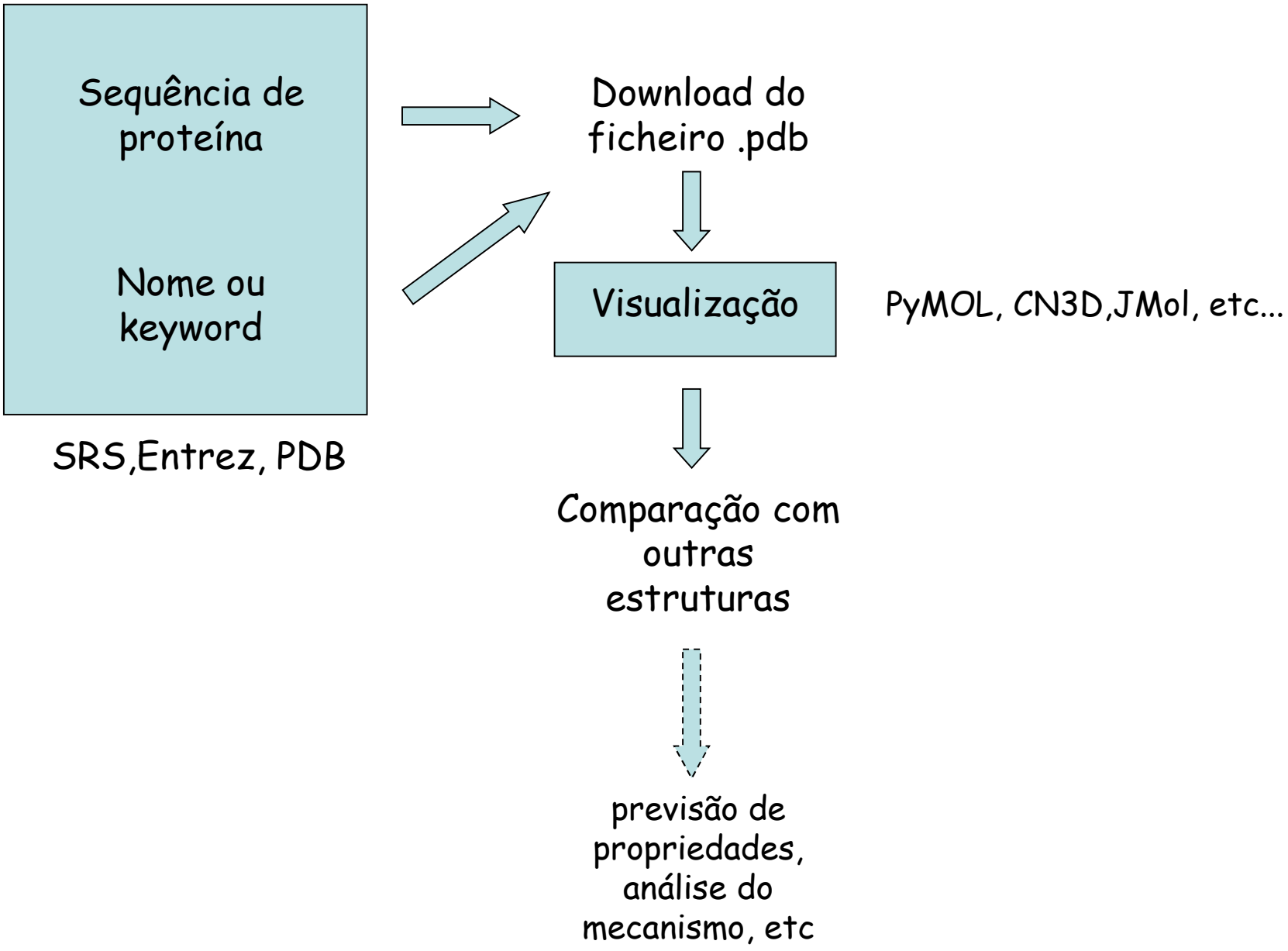


RCSB PDB is funded by the National Science Foundation (DBI-1832184), the US Department of Energy (DE-SC0019749), and the National Cancer Institute, National Institute of Allergy and Infectious Diseases, and National Institute of General Medical Sciences of the National Institutes of Health under grant R01GM133198.

Visualizar o ficheiro de estrutura no programa PyMOL



Visualização de estruturas moleculares



Software para visualização molecular

Aplicações de software que permitem a visualização de ficheiros de estrutura molecular (ficheiros PDB e outros formatos), permitindo a análise e cálculo de propriedades moleculares e a comparação de diferentes estruturas

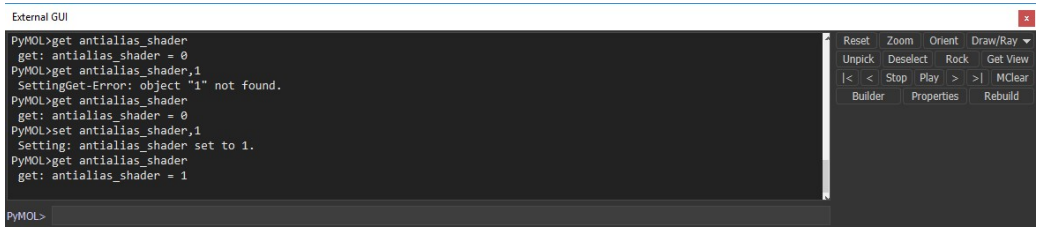
Instaláveis:

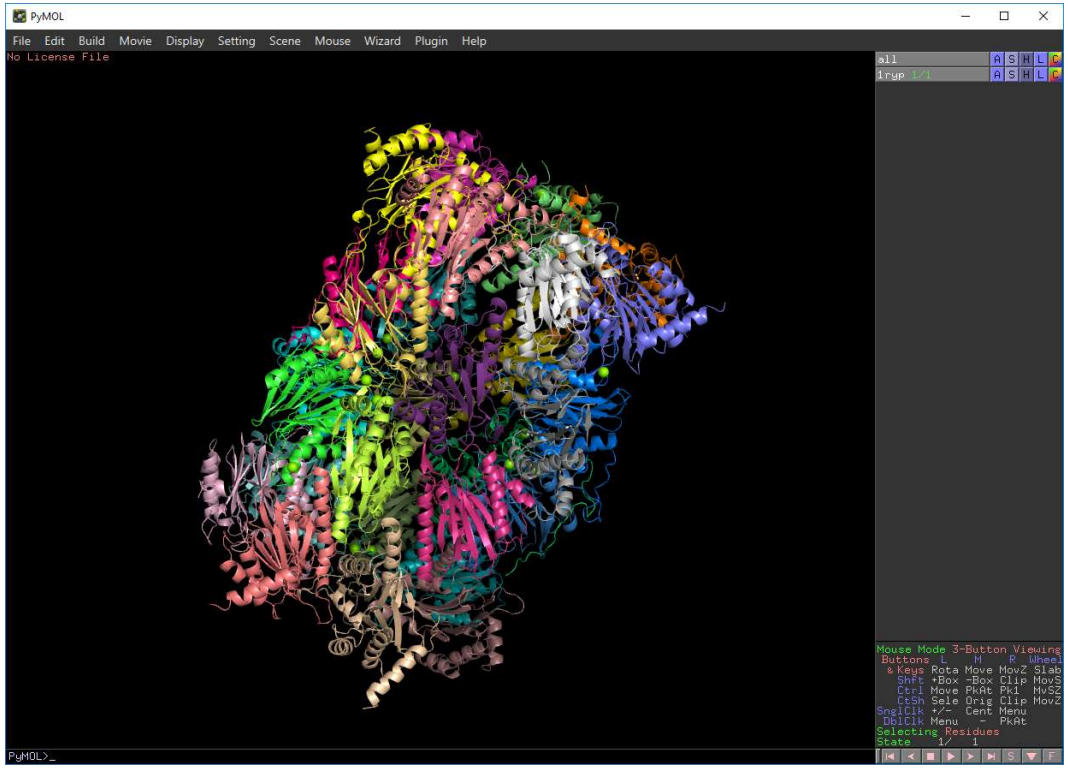
- **PyMOL:** http://www.pymol.org
- **ICM :** http://www.ncbi.nlm.nih.gov/Structure/CN3D/cn3d.shtml
- **QuteMol:** http://qutemol.sourceforge.net/
- **SwissPDB viewer:** http://www.expasy.org/spdbv/

On-line:

- **nglviewr:** http://nglviewer.org/
- **ICMJS:** http://www.molsoft.com
- **Jmol/JSMol:** http://jmol.sourceforge.net/

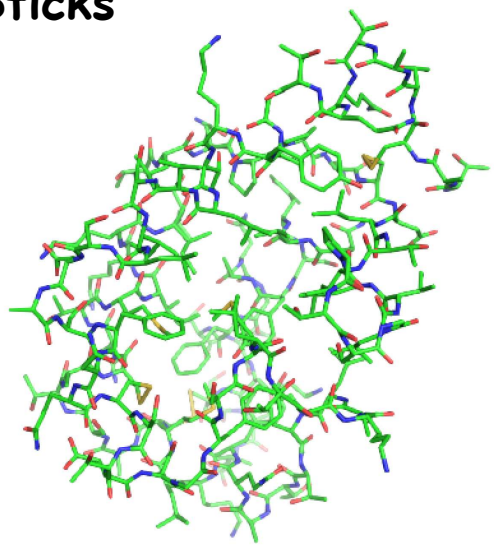
PyMOL (www.pymol.org)



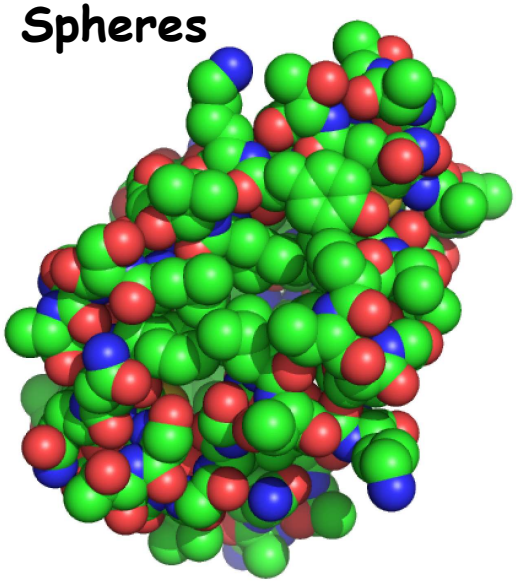


- Open Source
- Acesso livre
- Python / C
- Visualização de macromoléculas
- Animações moleculares
- Comparação de estruturas
- Medições
- Scripting
- Windows / Mac / Linux

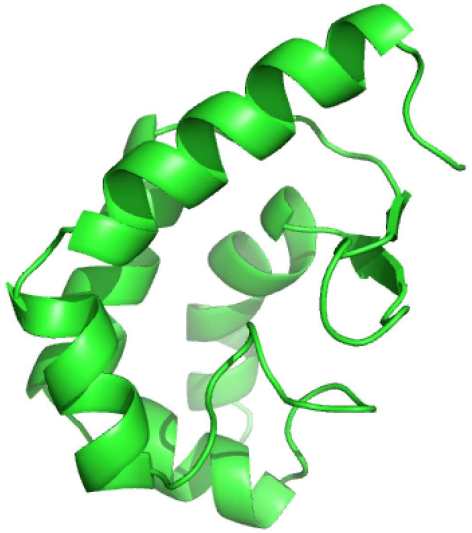
Sticks



Spheres

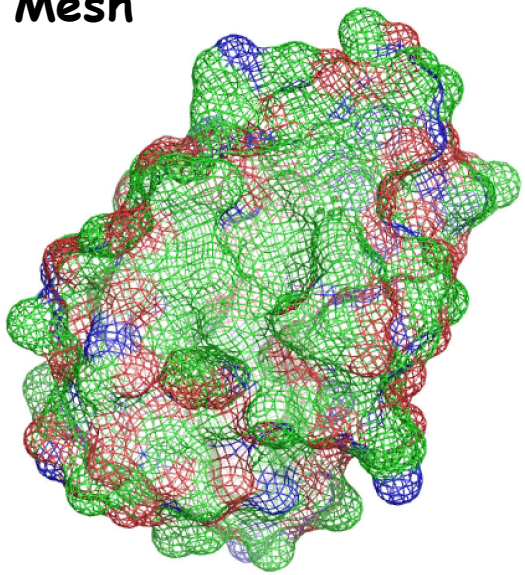


Cartoon

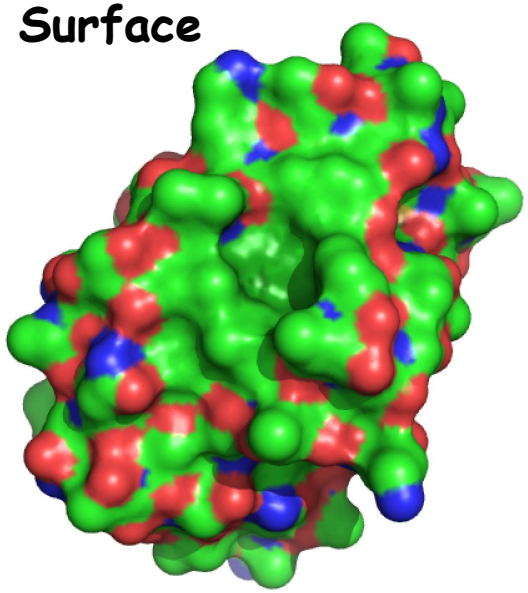


Ribbon

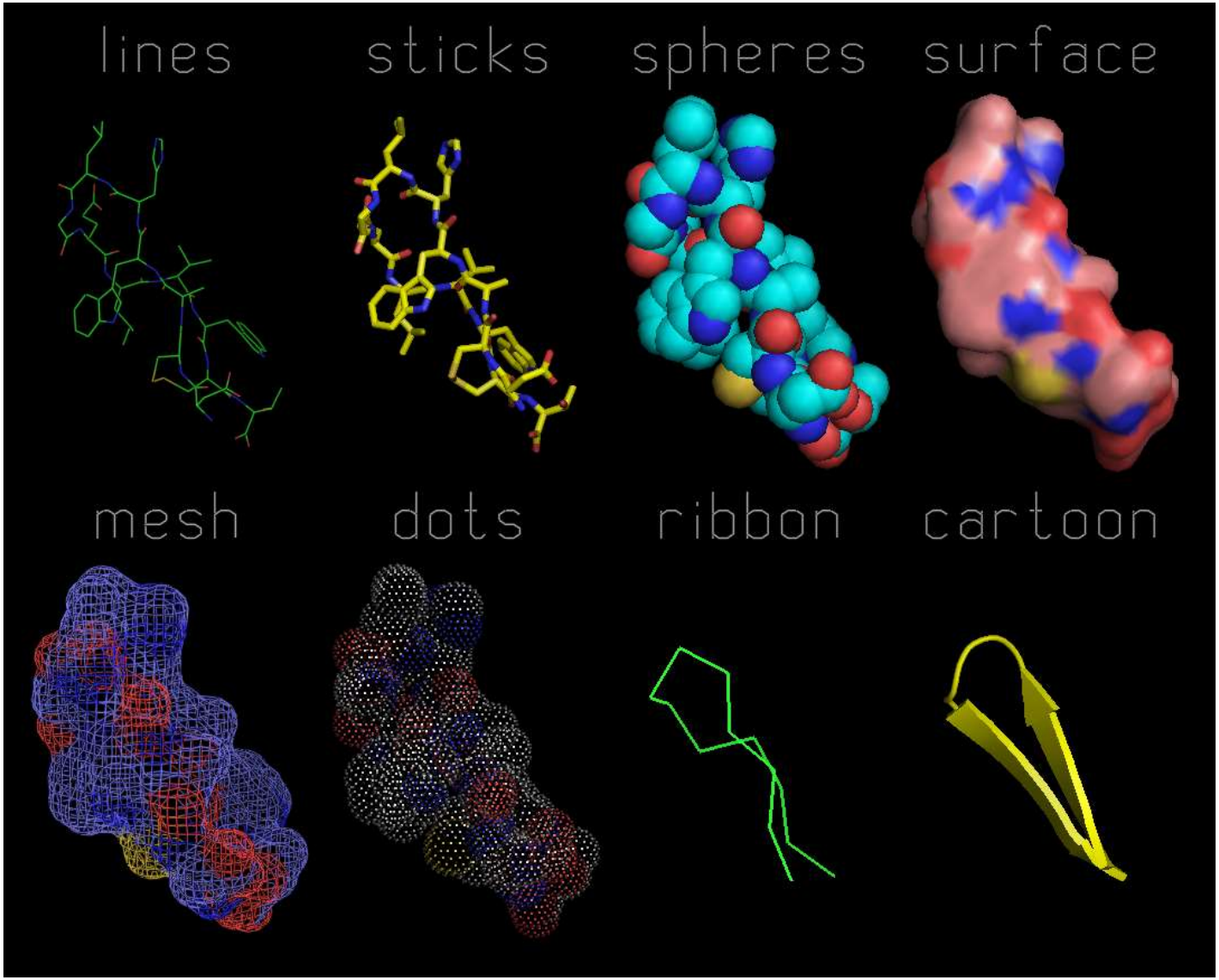
Mesh



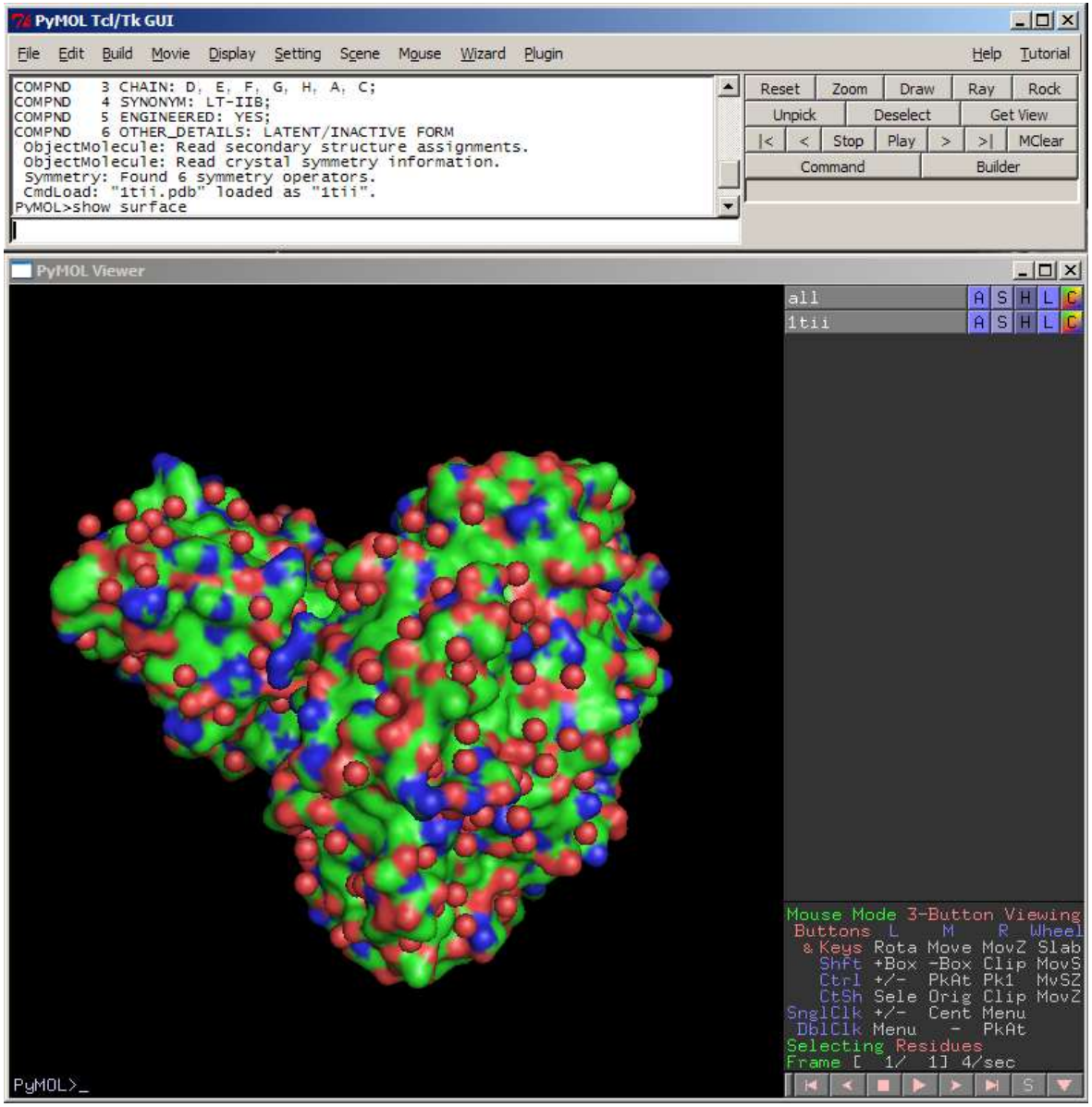
Surface



Modos de representação de estruturas



PyMOL (www.pymol.org)



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