



***PROTEIN DATA
BANK***

PDB



**O QUE É O
PDB?**

PROTEIN DATA BANK - PDB

- ✓ Um banco de dados de estrutura tridimensional (3-D) de macromoléculas, cujo acesso *on-line* é de domínio público
- ✓ Início: em 1971, contendo apenas 7 estruturas de proteínas!!!!
- ✓ Em 1999, já continha 10.000 estruturas depositadas
- ✓ Em 2021, com 50 anos de idade, o PDB conta com mais de 170.000 estruturas depositadas.

O PDB contém informações sobre a estrutura 3D de proteínas, ácidos nucleicos e diferentes complexos de biomoléculas.

PROTEIN DATA BANK - PDB

Como são gerados os dados estruturais depositados no PDB?

Métodos físicos e bioquímicos:

- ✓ Difração de Raio X
- ✓ Ressonância Magnética Nuclear (RMN)
- ✓ Crio-microscopia eletrônica

O PDB disponibiliza recursos educacionais voltados para Biologia estrutural e suas aplicações – RCSB Vídeos, imagens, jogos, entre outros.

The screenshot shows the RCSB PDB website homepage. At the top, there is a navigation bar with links for Deposit, Search, Visualize, Analyze, Download, Learn, More, Documentation, and Careers. The main header features the RCSB PDB logo, the text "186670 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education", and a search bar. Below the header, there are logos for PDB-101, Worldwide Protein Data Bank, and other partners. A banner for "Developers: Join the RCSB PDB Team" is visible. The main content area is divided into three sections: "Welcome" (a sidebar menu), "A Structural View of Biology" (text describing the resource's purpose and its role in the wwPDB), and "February Molecule of the Month" (featuring a 3D model of Oligosaccharyltransferase). At the bottom, there are promotional banners for "COVID-19 CORONAVIRUS Resources" and "Join the RCSB PDB Team". The Windows taskbar is visible at the very bottom of the image.



Para mais informações entre no link: <https://www.rcsb.org/pages/about-us/index>

Algumas estruturas 3D disponíveis:

The screenshot shows the RCSB PDB website interface. At the top, there is a navigation bar with links for Deposit, Search, Visualize, Analyze, Download, Learn, More, Documentation, and Careers. A search bar is located on the right side of the navigation bar. Below the navigation bar, the RCSB PDB logo is displayed, along with the text "186670 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education". A search bar with a magnifying glass icon is also present. Below the search bar, there are several logos for partner organizations: PDB-101, Worldwide PDB Protein Data Bank, EMDataResource, Nucleic Acid Database, and Worldwide Protein Data Bank Foundation. The main content area is titled "Visualize Related Features" and contains a section for "Mol* 3D Viewer". This section includes a paragraph: "Launch Mol* from the Structure Summary page for any entry. A standalone version of Mol* is available. Users can upload their custom files into this tool. A detailed Mol* User Guide is available." Below this text, there are three 3D protein structure visualizers. The first one is highlighted with a red box and is labeled "PDB ID: 4HHB". The second is labeled "PDB ID: 3J3Q" and the third is labeled "PDB ID: 1BTN". At the bottom of the page, there is a section for "Protein Feature View" which provides a graphical summary of biological and structural protein features. The bottom of the screenshot shows a Windows taskbar with various application icons and a system tray with the date and time (19:57, 06/02/2022).

RCSB PDB Deposit Search Visualize Analyze Download Learn More Documentation Careers MyPDB

RCSB PDB 186670 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

PDB Archive

Advanced Search | Browse Annotations Help

PDB-101 WORLDWIDE PDB PROTEIN DATA BANK EMDataResource NUCLEIC ACID DATABASE Worldwide Protein Data Bank Foundation

Visualize Related Features

Mol* 3D Viewer

Launch Mol* from the Structure Summary page for any entry.

A standalone version of Mol* is available. Users can upload their custom files into this tool.

[A detailed Mol* User Guide is available.](#)

PDB ID: 4HHB PDB ID: 3J3Q PDB ID: 1BTN

Protein Feature View

Provides a graphical summary of biological and structural protein features of PDB entities and how they correspond to UniProtKB sequences. It loads features from RCSB PDB webservices and third party resources such as UniProtKB, CATH or SCOPe.

4235.A Lysophosphatidic acid receptor 1, Soluble cytochrome b562 - homo sapiens, Escherichia coli

PDB INSTANCE SEQ. 4235.A

19:57 06/02/2022

Visualização disponível na própria plataforma:

RCSB PDB Deposit Search Visualize Analyze Download Learn More

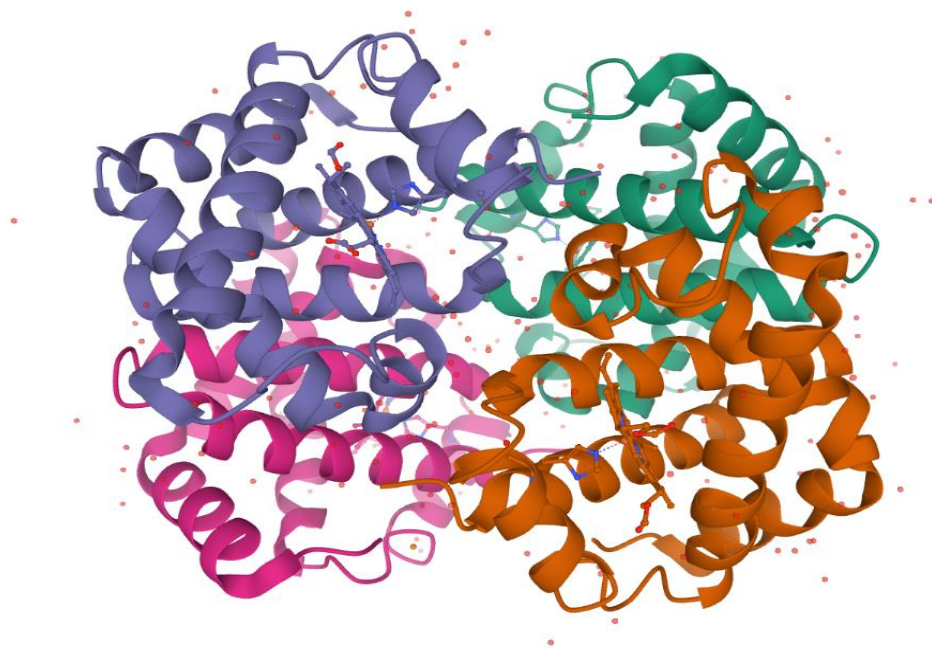
4HHB

Display Files Download Files

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Sequence of 4HHB | THE CR... 1: Hemoglobin ε A

```
1 11 21 31 41 51 61 71 81 91 101 111
VLSPADKTNVKAAWGKVGAAHAGEYGAEALERMFLSFPTTKTYFPHFDLSHGSAQVKGHGKKVADALTNAVAHVDDMPNALSALSDLHAHKLRVDPVNFKLLSHCLLVTLAAHL
121 131 141
PAEFTPAVHASLDRKFLASVSTVLTISKYR
```



Structure

4HHB | THE CRYSTAL STRUCTU...

Type Assembly

Asm Id 1: Author And Softwa.

Nothing Focused

Measurements

Components 4HHB

Preset	+ Add	≡	4
Polymer	Cartoon	👁	🗑
Ligand	Ball & Stick	👁	🗑
Water	Ball & Stick	👁	🗑
Ion	Ball & Stick	👁	🗑

Unit Cell P 1 21 1

Density

Assembly Symmetry

Ampliando uma região da proteína (zoom):

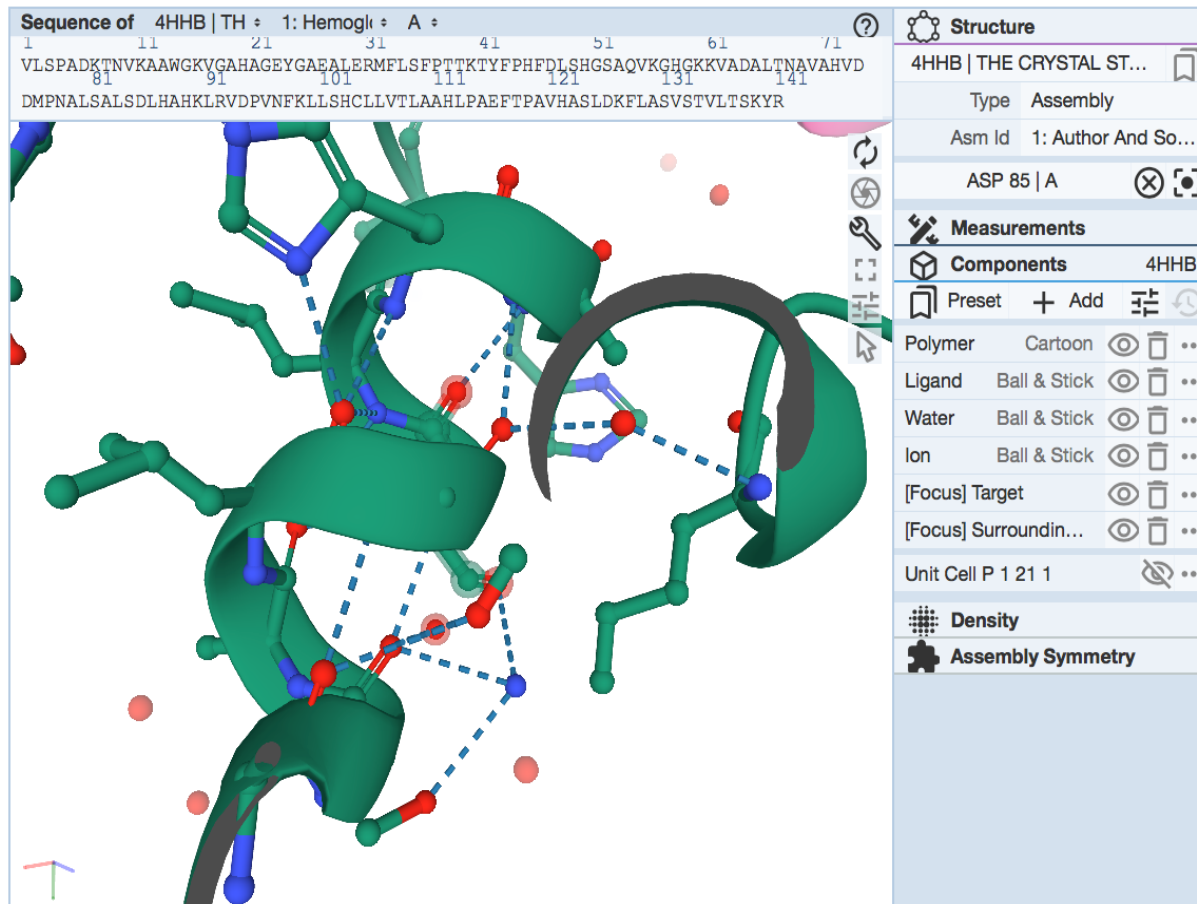
4HHB

Display Files -

Download Files -

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Help



Pontes de hidrogênio formadas entre os aminoácidos da alfa hélice.

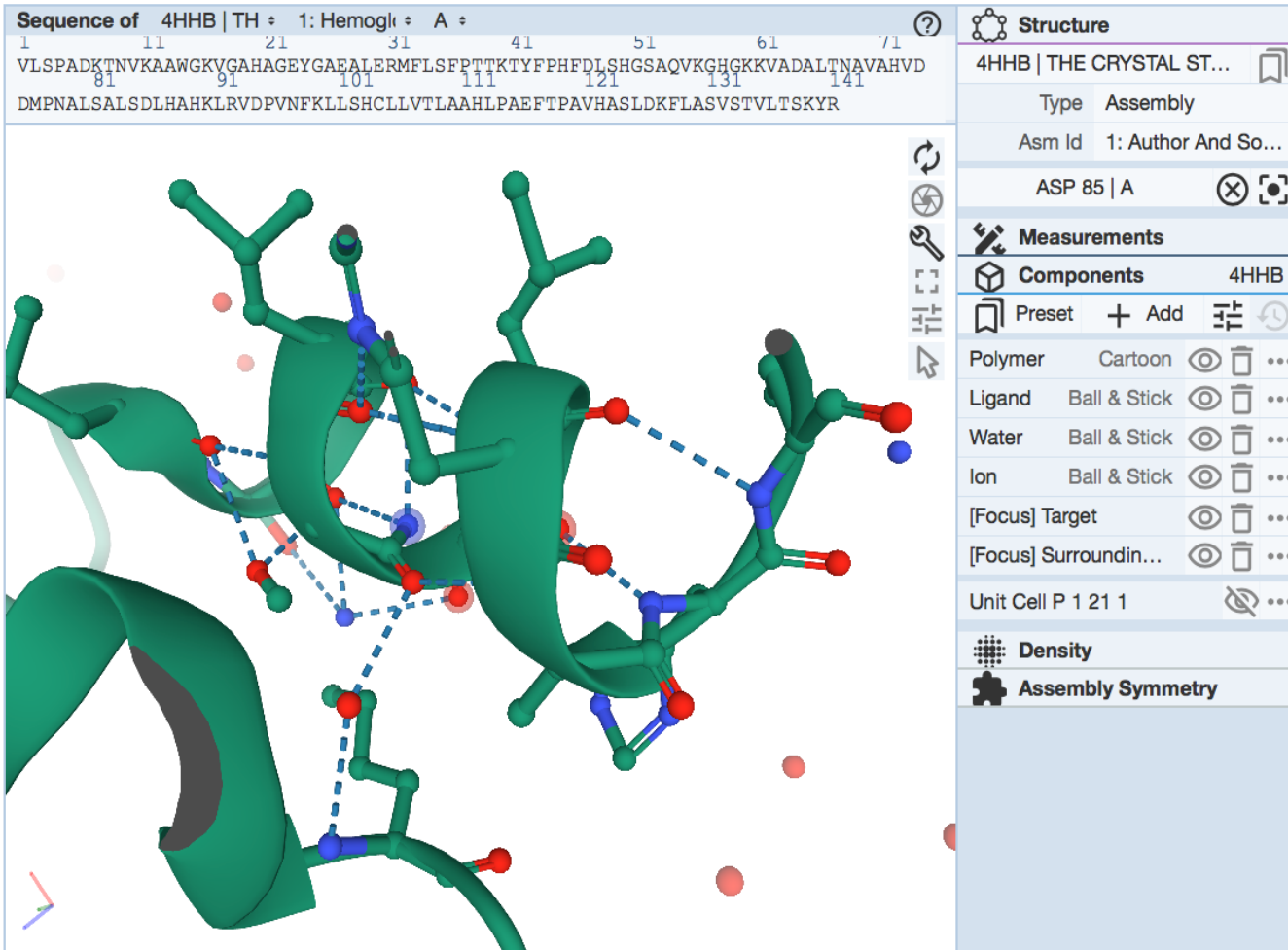
4HHB

Display Files

Download Files

THE CRYSTAL STRUCTURE OF HUMAN DEOXYHAEMOGLOBIN AT 1.74 ANGSTROMS RESOLUTION

Help

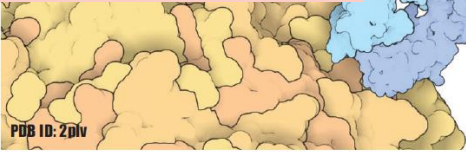
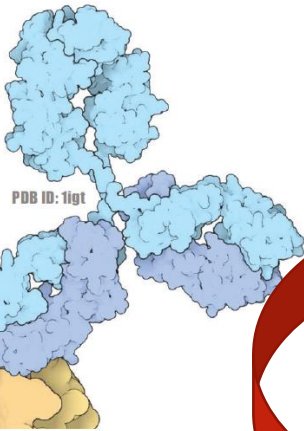


Select a different viewer Mol* (Javascript)

Ponte de hidrogênio entre o H do nitrogênio da Lisina com o O da Serina de outra alfa hélice

DEFESA

Anticorpo -
Reconhece e se
liga a moléculas
estranhas ao
organismo.



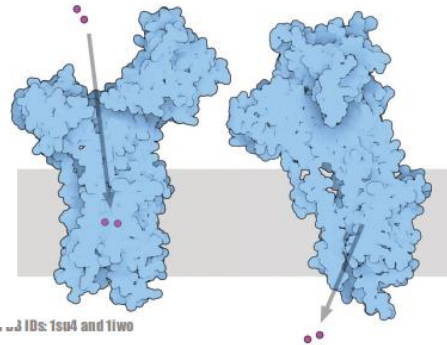
COMUNICAÇÃO

Insulina – pequena,
estável – mantém sua
forma ao atravessar o
corpo pelo sangue
para regular a
quantidade de
açúcar



ENZIMÁTICA (CATALISADOR)

Amilase – enzima com sítio
catalítico que começa a
quebrar os carboidratos na
nossa saliva

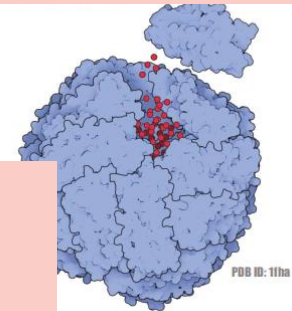


ESTRUTURAL

Colágeno forma uma fibra tripla de hélices forte e flexível
que é usada em várias partes do corpo para suporte.

ARMAZENAMENTO

Ferritina forma um buraco que
armazena ferro da nossa
alimentação



TRANSPORTE

A bomba de cálcio move íons pelas
membrana da célula permitindo a
contração muscular



PARA SABER MAIS.... FOLDER

Cells build many complex molecular machines that perform the biological jobs needed for life. Some of these machines are molecular scissors that cut food into digestible pieces. Others then use these pieces to build new molecules when cells grow or tissues need to be repaired. Some molecular machines form sturdy beams that support cells, and others are motors that use energy to crawl along these beams. Some recognize attackers and mobilize defenses against infection.



Researchers around the world are studying these molecules at the atomic level. These 3D structures are freely available at the Protein Data Bank (PDB), the central storehouse of biomolecular structures. A few examples from the ~100,000 structures held in the PDB are shown here at a magnification of about 3,500,000 times, with each atom represented as a small sphere. The enormous range of molecular sizes is illustrated here, from the water molecule (H₂O) with only three atoms (shown at the left) to the ribosomal subunits with hundreds of thousands of atoms.

Digestive Enzymes: breaking food into small nutrient molecules

1. Amylase 1smd
2. Phospholipase 1poe
3. Deoxyribonuclease 2dnj
4. Lysozyme 1ltt
5. Pepsin 5pep
6. Trypsin 2ptt
7. Carboxypeptidase 3cpa
8. Ribonuclease 5rsa

Blood Plasma Proteins: transporting nutrients and defending against injury

9. Factor X 1xka, 1lod
10. Thrombin 1tpb
11. Fibrin 1mij, 2baf
12. Serum Albumin 1e7f

Viruses and Antibodies: engaging in constant battle in the bloodstream

13. Antibody 1igt
14. Rhinovirus 4rhv

Hormones: carrying molecular messages through blood

15. Glucagon 1gcn
16. Insulin 2hiu
17. Epidermal Growth Factor 1egf

Channels, Pumps and Receptors: getting back and forth across the membrane

18. Ras Protein 5p2i
19. Beta2-Adrenergic Receptor/Gs Protein 3sn6
20. Acetylcholine Receptor 2b9g
21. Epidermal Growth Factor Receptor 1tvo, 2jwa, 2z66
22. Rhodopsin 1f88
23. P-glycoprotein 4m2t
24. Potassium Channel 3lut
25. Calcium Pump 1su4
26. Cyclooxygenase 1pnh

Photosynthesis: harvesting energy from the sun

27. Photosystem II 1ssi
28. Light-harvesting Complex 1twt
29. Photosynthetic Reaction Center 1prc

Scale:

1nm 5nm 10nm

1nm (nanometer) = 10⁻⁹ millimeters

Energy Production: powering the processes of the cell

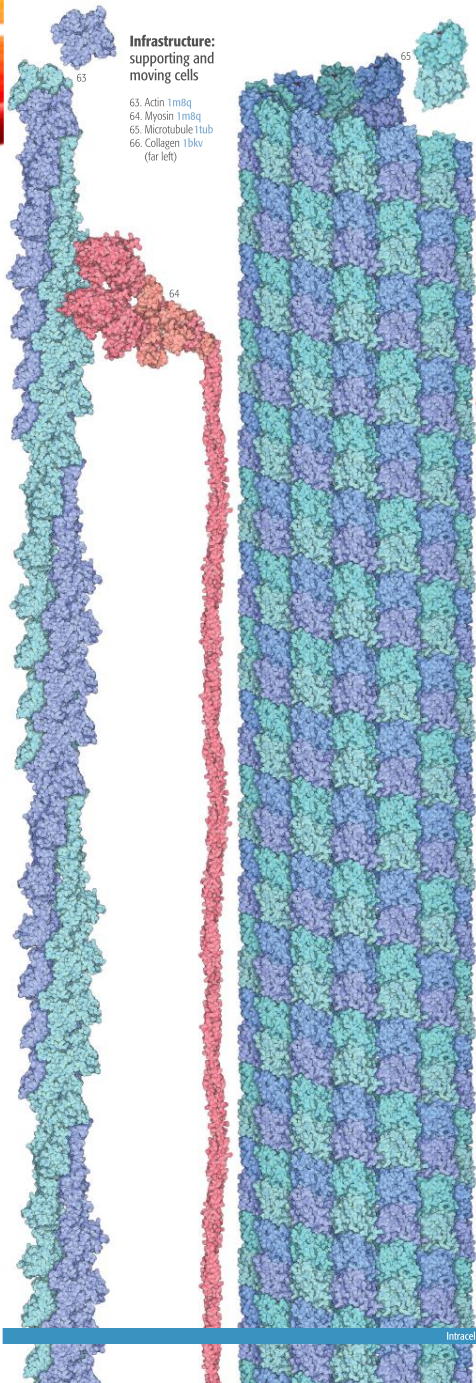
30. Cytochrome c Oxidase (Complex IV) 1oco
31. Cytochrome c 3cvt
32. Cytochrome bc1 (Complex III) 1tby
33. Succinate Dehydrogenase (Complex II) 1nek
34. NADH-Quinone Oxidoreductase (Complex I) 5mfs, 3rko
35. ATP Synthase 1e79, 1c17, 1l2p, 2a7u
36. Myoglobin 1mbd
37. Hemoglobin 4hhb

Storage: containing nutrients for future consumption

38. Ferritin 1hrs

Enzymes: cutting and joining the molecules of life

39. Fatty Acid Synthase 2uvb, 2uvc
40. RubisCo: Ribulose Biphosphate Carboxylase/Oxygenase 1rcc
41. Green Fluorescent Protein 1gfl
42. Luciferase 2d1s
43. Glutamine Synthetase 2gls
44. Alcohol Dehydrogenase 2ohx
45. Dihydrofolate Reductase 1dhf
46. Nitrogenase 1n2c
47. Leucine Aminopeptidase 1lap
48. beta-Lactamase 4blm
49. Catalase 1cqv
50. Thymidylate Synthase 2tsc
51. Tryptophan Synthase 1wsy
52. Aspartate Carboxyltransferase 4at1
53. Hexokinase 1d6k
54. Phosphoglucose Isomerase 1thx
55. Phosphofructokinase 4pflk
56. Aldolase 1ald
57. Triosephosphate Isomerase 2tpi
58. Glyceraldehyde-3-phosphate Dehydrogenase 3gpd
59. Phosphoglycerate Kinase 3pgk
60. Phosphoglycerate Mutase 3pgm
61. Enolase 5eml
62. Pyruvate Kinase 1a3w

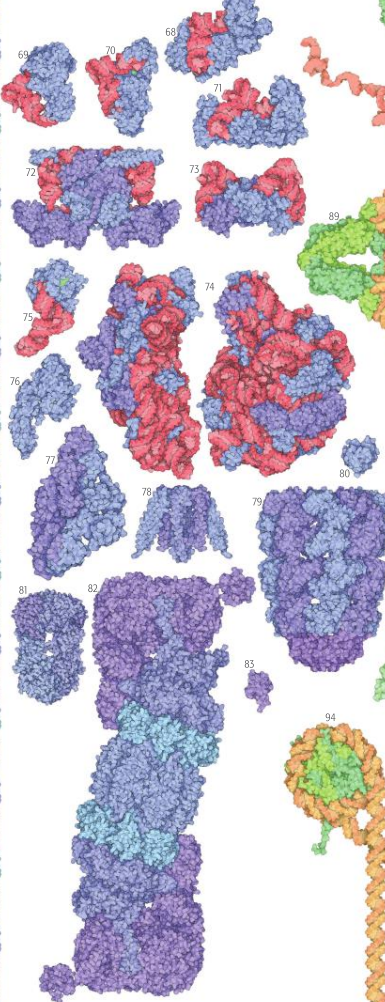


Infrastructure:
supporting and moving cells

- 63. Actin 1m8q
- 64. Myosin 1m8q
- 65. Microtubule 1tub
- 66. Collagen 1bkv (far left)

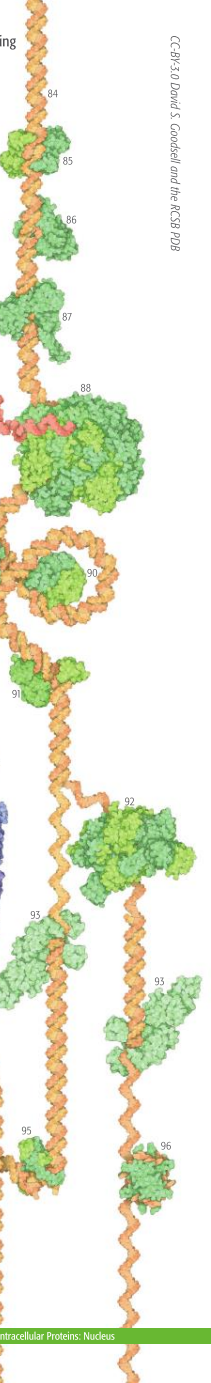
Protein Synthesis: building new molecular machines

- 67. Transfer RNA 4tna
- 68. Valyl-tRNA Synthetase 1gax
- 69. Threonyl-tRNA Synthetase 1qf6
- 70. Glutamyl-tRNA Synthetase 1euq
- 71. Isoleucyl-tRNA Synthetase 1ffy
- 72. Phenylalanyl-tRNA Synthetase 1eyi
- 73. Aspartyl-tRNA Synthetase 1asy
- 74. Ribosome 1j5e, 1ij2
- 75. Elongation Factor Tu/tRNA 1itt
- 76. Elongation Factor G 1dar
- 77. Elongation Factor Ts and Tu 1efu
- 78. Prefoldin 1tkk
- 79. Chaperonin GroEL/ES 1aon
- 80. Proline cis/trans isomerase 2cpl
- 81. Heat Shock Protein Hsp90 2c99
- 82. Proteasome 4b4t
- 83. Ubiquitin 1ubq



DNA: storing and reading genetic information

- 84. DNA 1bna
- 85. Restriction Endonuclease EcoRI 1eri
- 86. DNA Photolyase 1tez
- 87. Topoisomerase 1a36
- 88. RNA Polymerase 2eci
- 89. lac Repressor 1lhb 1efa
- 90. Catabolite Gene Activator Protein 1cgp
- 91. TATA-binding Protein/Transcription Factor IIB 1ais
- 92. DNA Helicase 4esv
- 93. DNA Polymerase 1tau
- 94. Nucleosome 1aon
- 95. HU Protein 1p51
- 96. Single-stranded DNA-binding Protein 3as5u



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PARA SABER MAIS.... VÍDEOS

COVID-19/SARS-CoV-2 Recursos.

<https://www.rcsb.org/news?year=2020&article=5e74d55d2d410731e9944f52&feature=true>

Vídeo explicativo sobre como o sabão pode matar o vírus.

<http://pdb101.rcsb.org/learn/videos/fighting-coronavirus-with-soap>

Vídeo mostrando como os anticorpos neutralizam o vírus, e como uma gotícula respiratória transposta o vírus.

<http://pdb101.rcsb.org/browse/coronavirus>