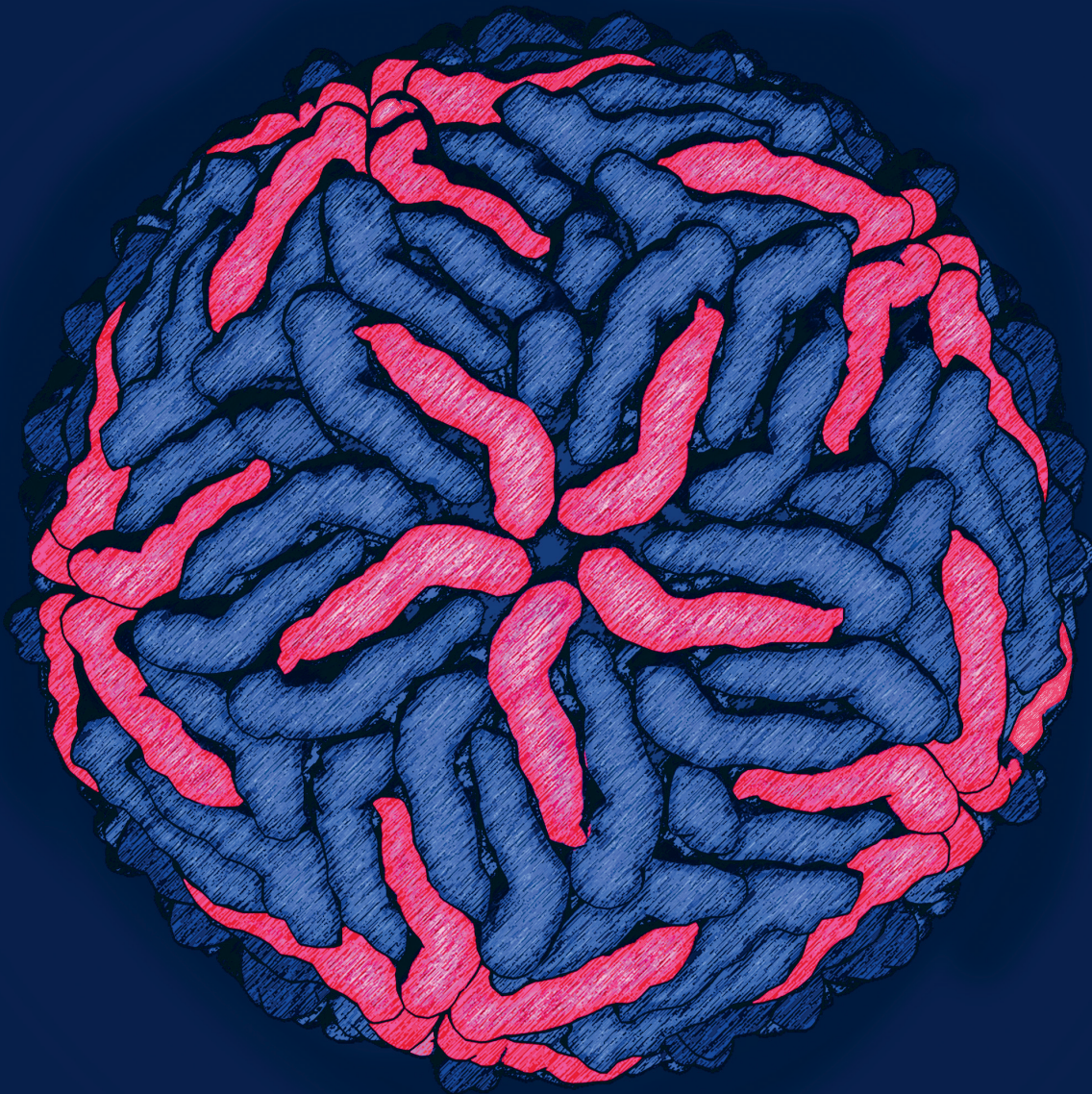


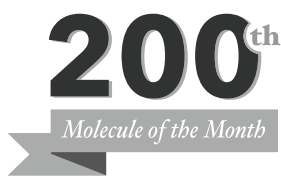
Coloring Molecular Machinery: A Tour of the Protein Data Bank



200th
Molecule of the Month

RCSB PDB-101

pdb101.rcsb.org



This is a molecular coloring book for all artists. Featured are selected highlights from the RCSB PDB's *Molecule of the Month* series, which is celebrating the release of its 200th article in August 2016.

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. Since 2000, the *Molecule of the Month* features have highlighted the structure and function of these important molecules and their relevance to human health and welfare.

Visit pdb101.rcsb.org to learn more about the PDB and the *Molecule of the Month*.



pdb101.rcsb.org

PDB-101 helps teachers, students, and the general public explore the 3D world of proteins and nucleic acids.

Learning about their diverse shapes and functions helps to understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease to biological energy.

All resources are freely available, including curricular materials, paper molecular models, posters, animations, and more. Resources are searchable as well as organized by topics such as Health and Disease, Molecules of Life, Biotech and Nanotech, and Structures and Structure Determination.

DNA

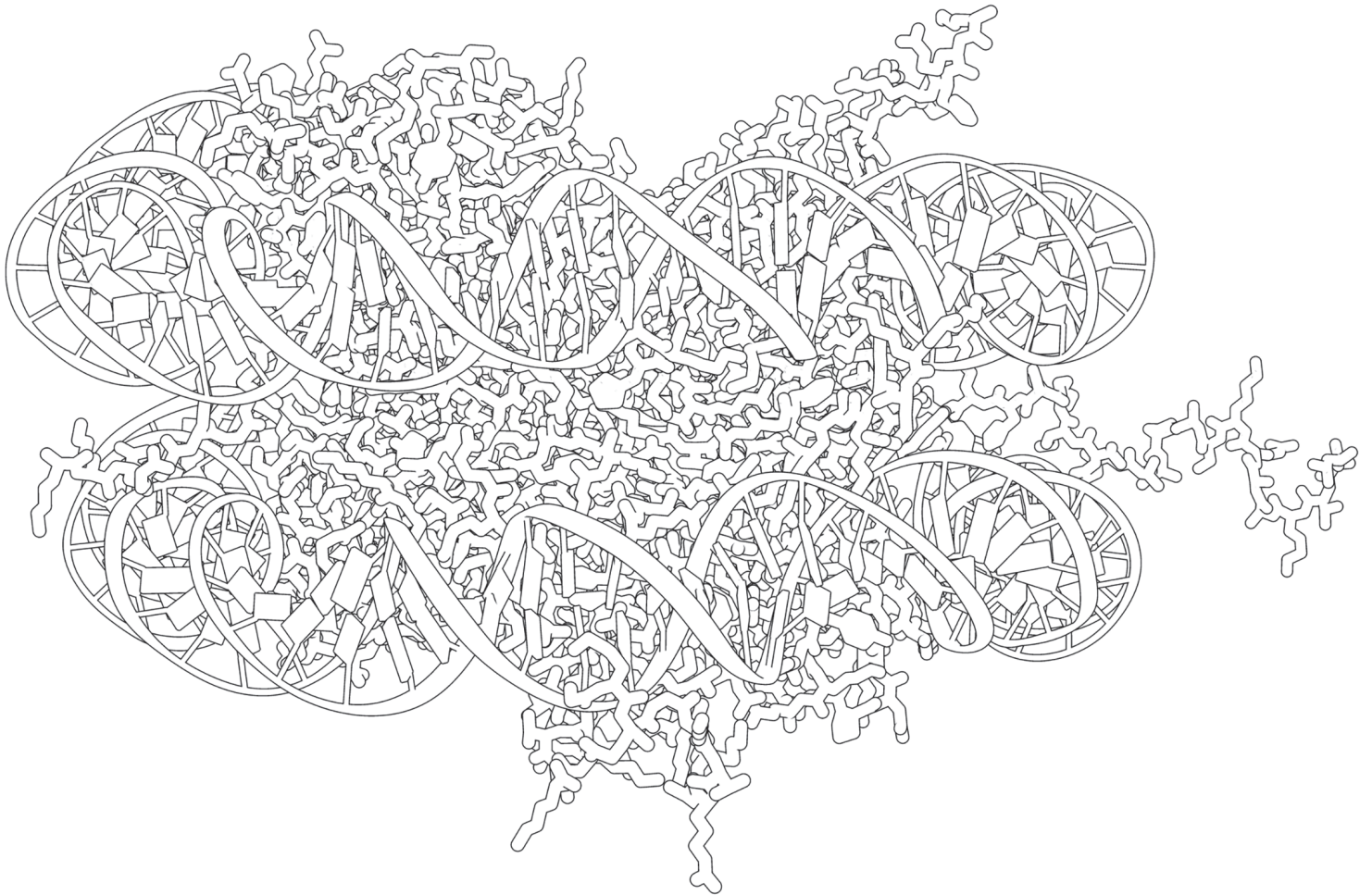
Atomic structures reveal how the iconic double helix encodes genomic information.



Nucleosome

(View 1)

The cell's genome is stored and protected by nucleosomes.



Nucleosome

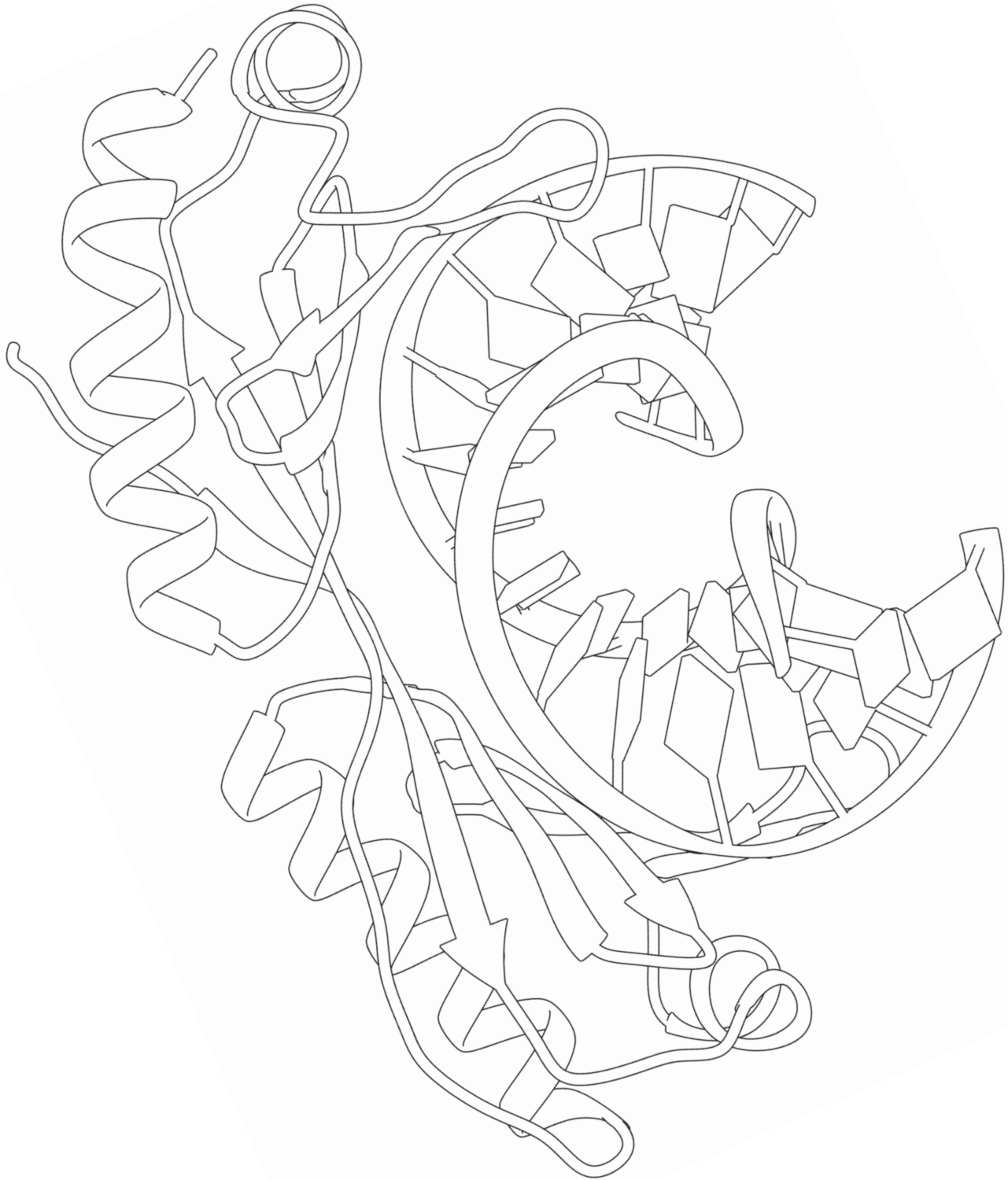
(View 2)

The long "tails" of nucleosomes interact with each other to control the accessibility of the genes to polymerases, thus regulating the gene transcription activity.



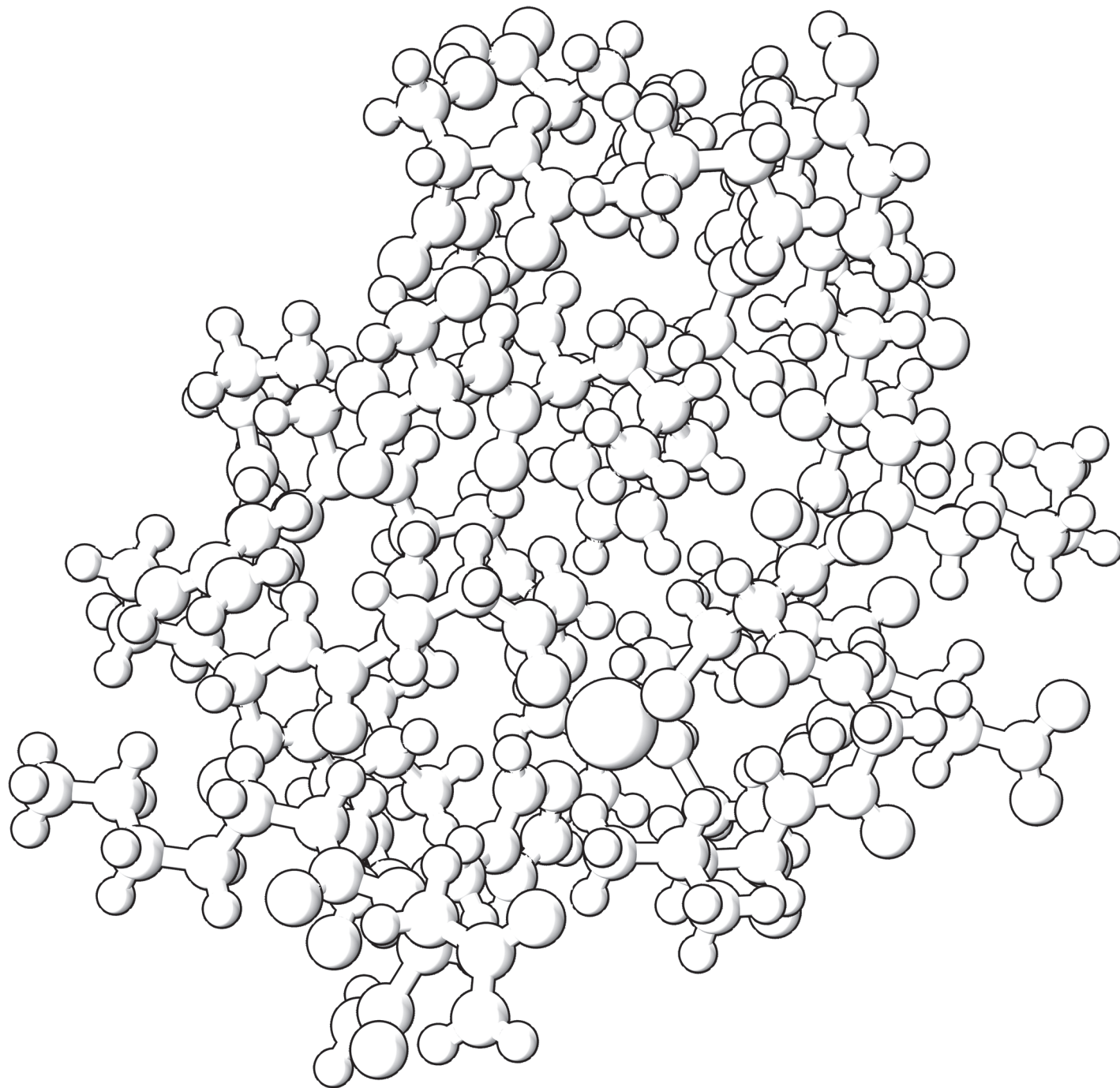
TATA-Binding Protein

TATA protein tells RNA polymerase where to get started on a gene.



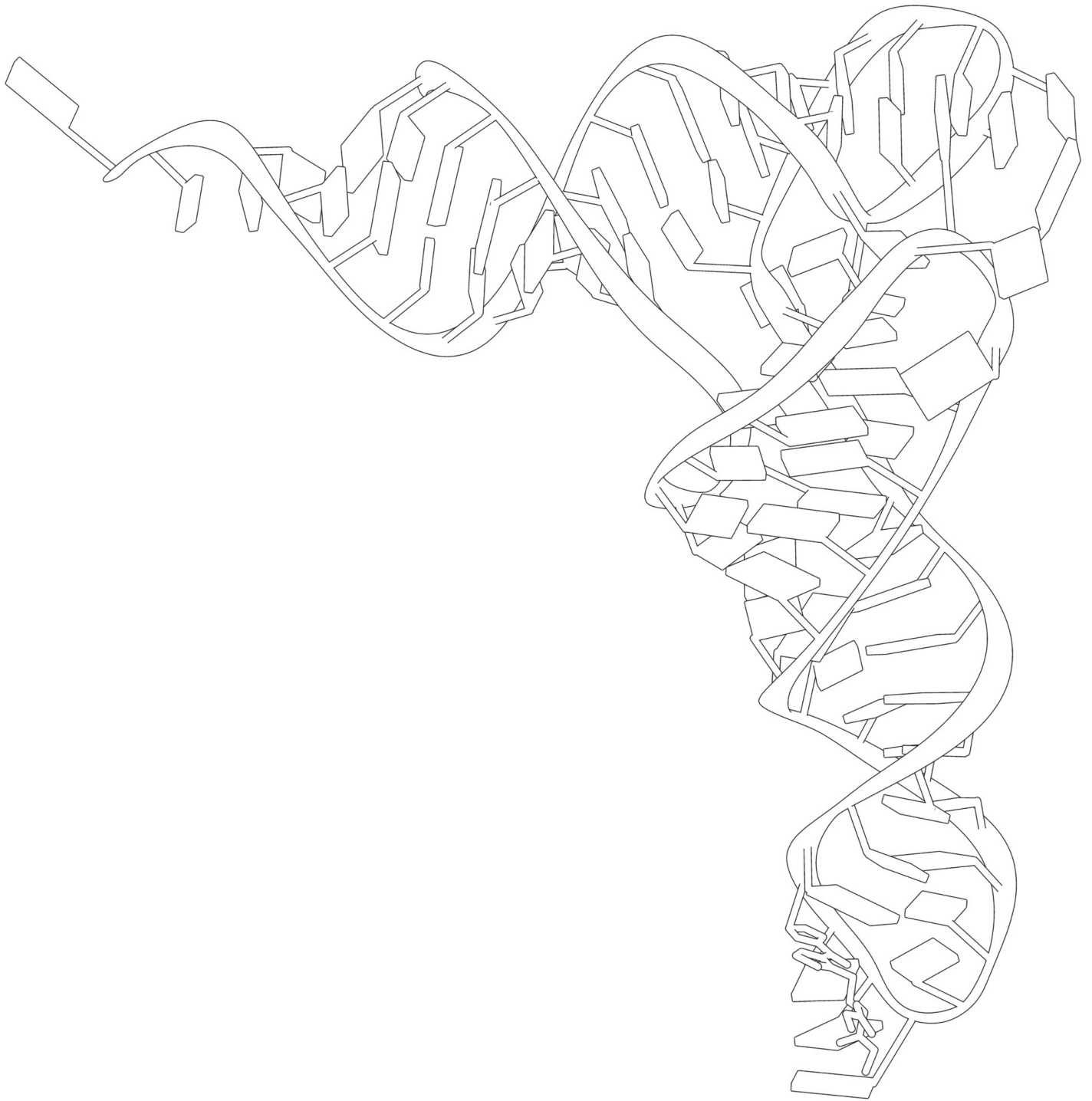
Zinc Fingers

Zinc ions are used to strengthen small protein modules that recognize DNA.



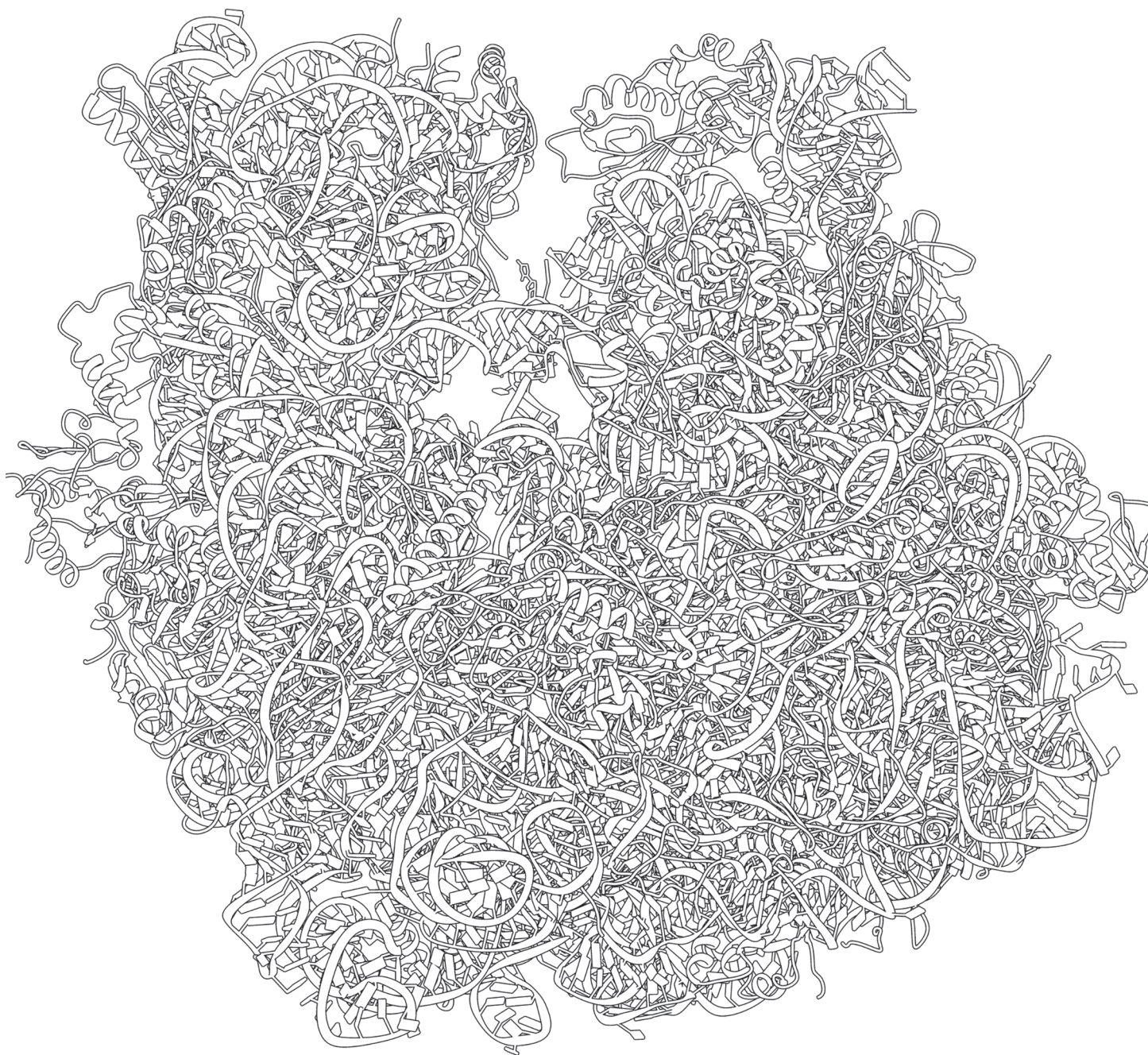
Transfer RNA

Transfer RNA translates the language of the genome into the language of proteins



Ribosome

Ribosomes are complex molecular machines that build proteins.



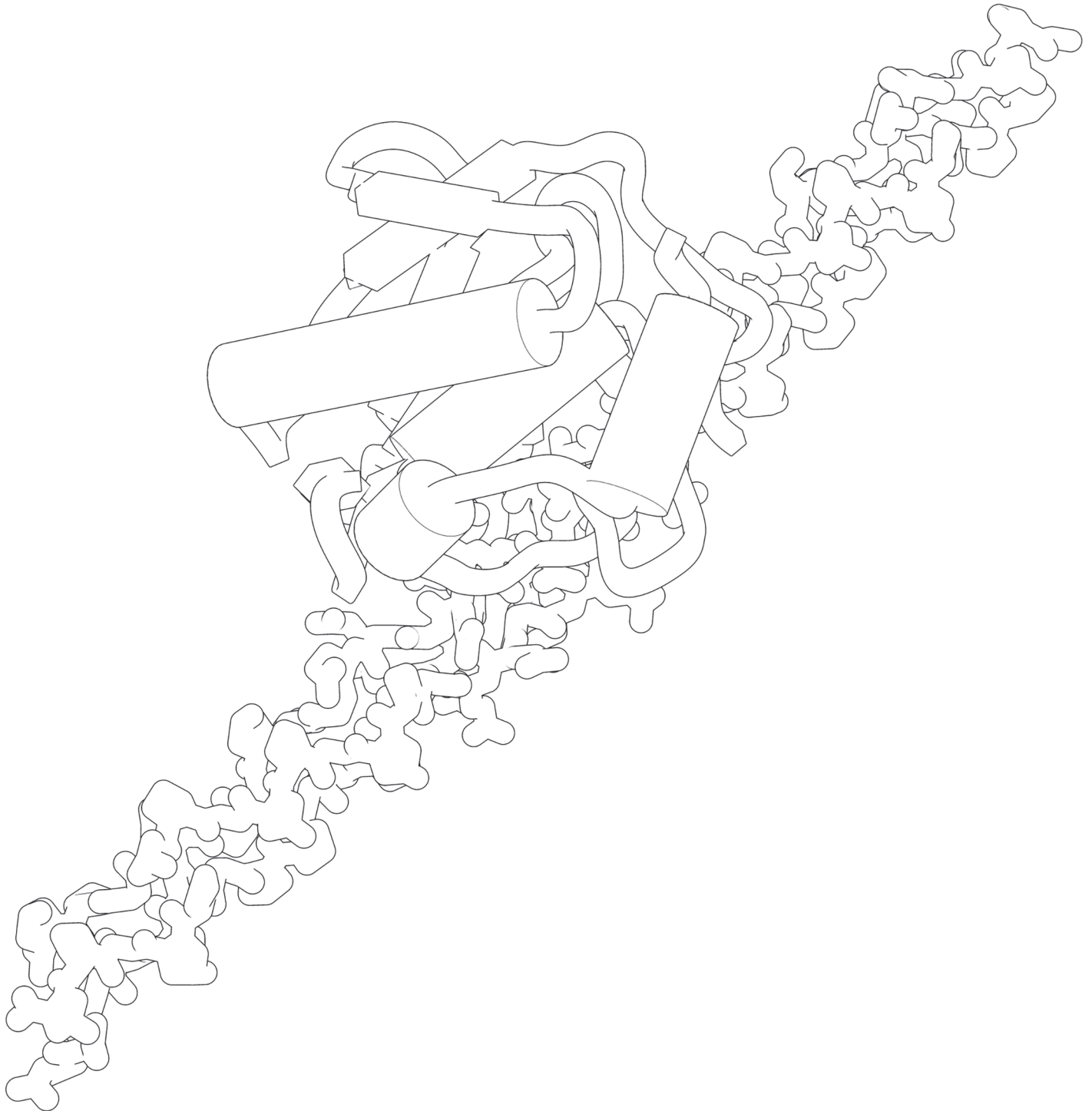
Insulin

The hormone insulin helps control the level of glucose in the blood.



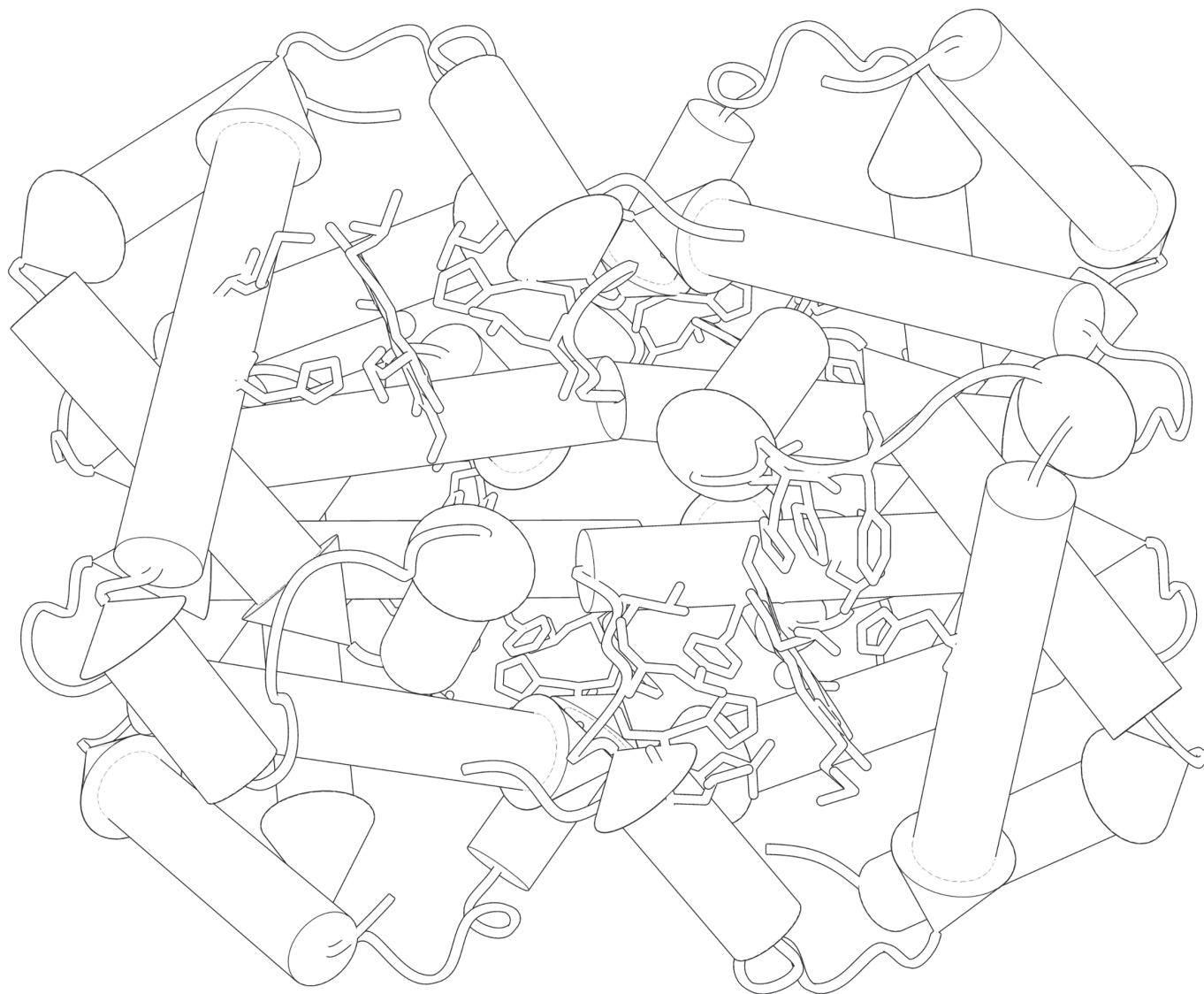
Collagen with Bound Metalloproteinase

Long, sturdy fibers of collagen give structure to our bodies. Metalloproteinase is a small enzyme (shown center) that creates lesions in the fibrils that are necessary for tissue remodeling.



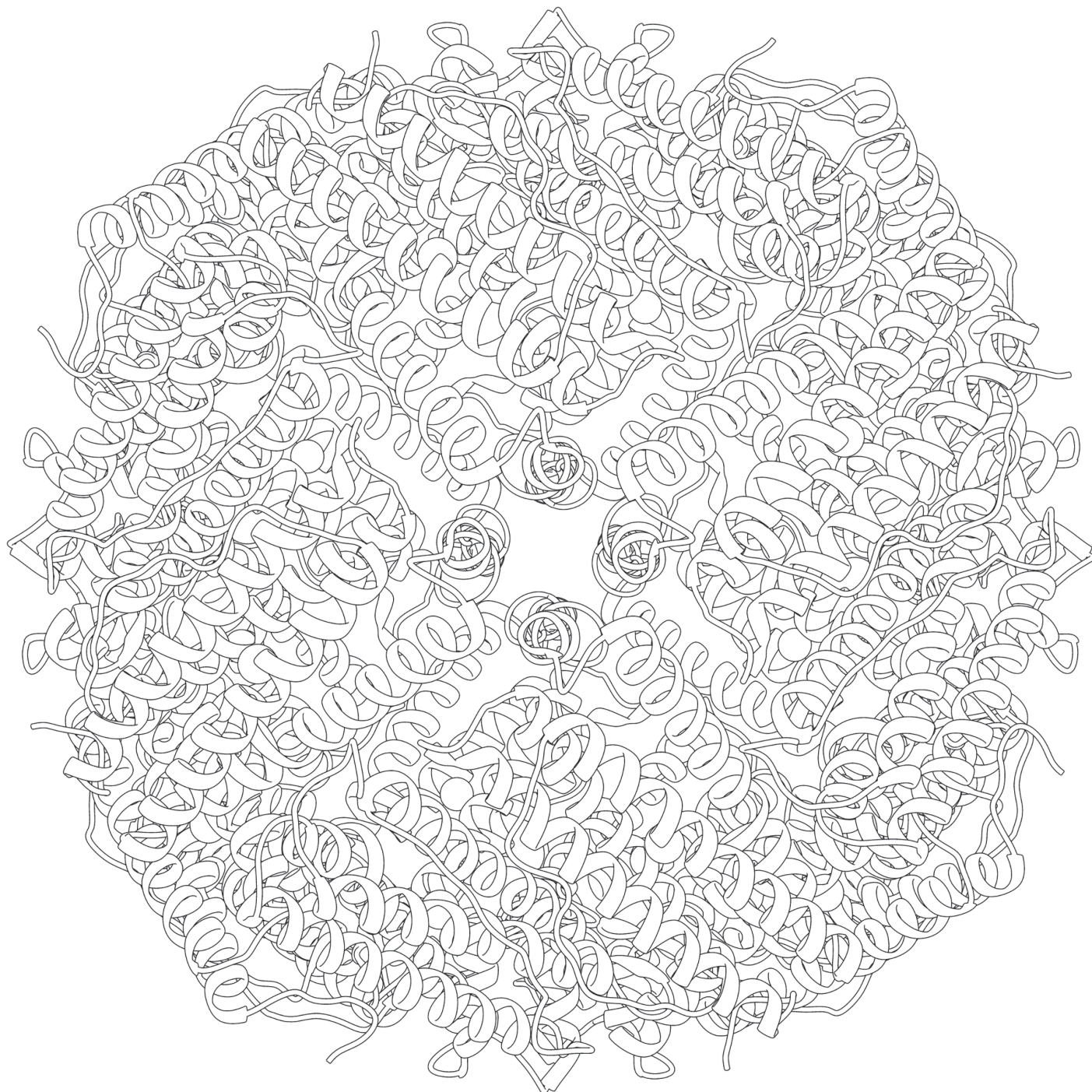
Hemoglobin

Hemoglobin carries oxygen from the lungs to the body's tissues.



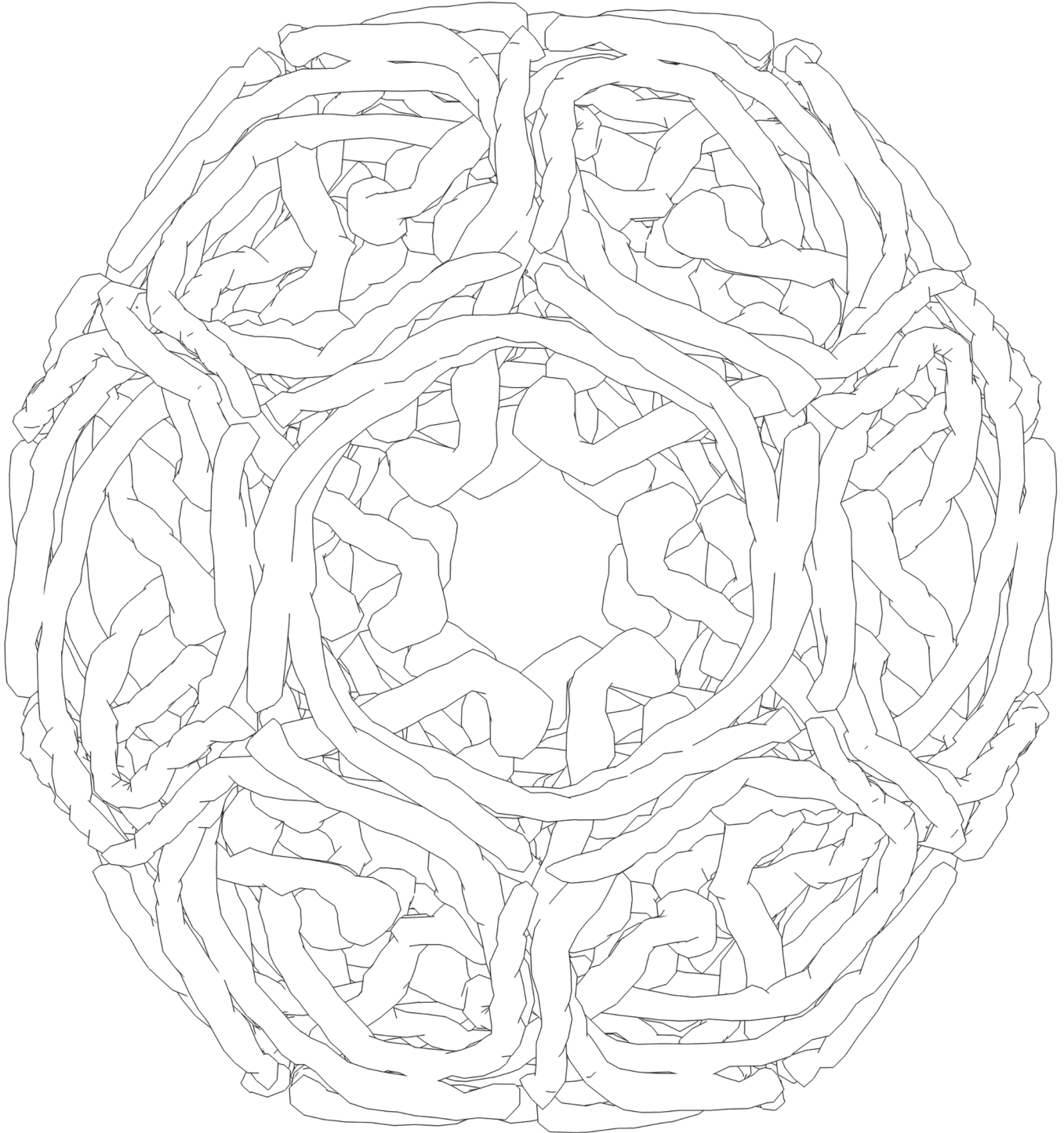
Ferritin

Ferritin forms a hollow shell that stores iron from our food.



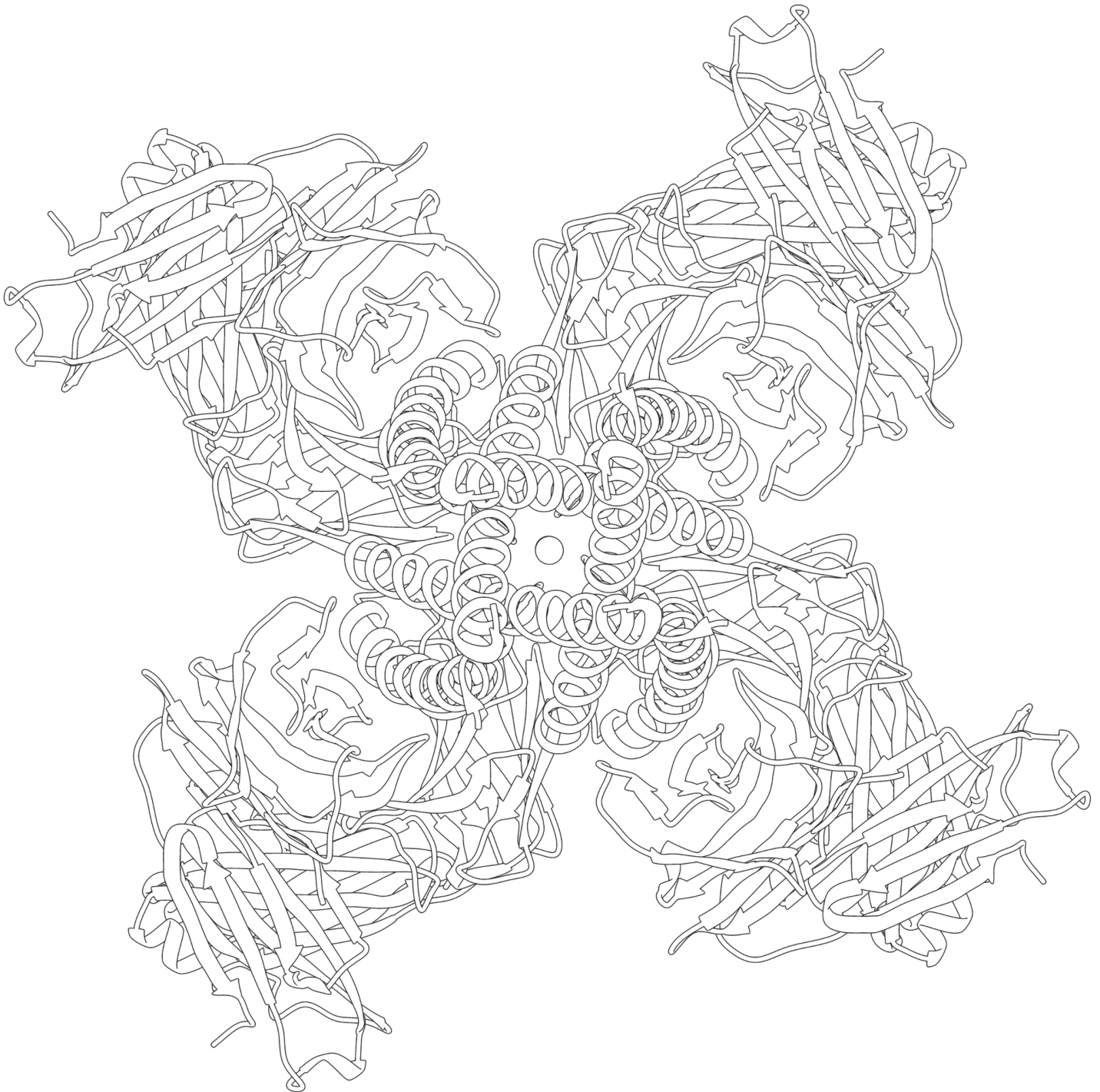
Clathrin

Three-armed clathrin triskelions are used to build molecular cages involved in transport.



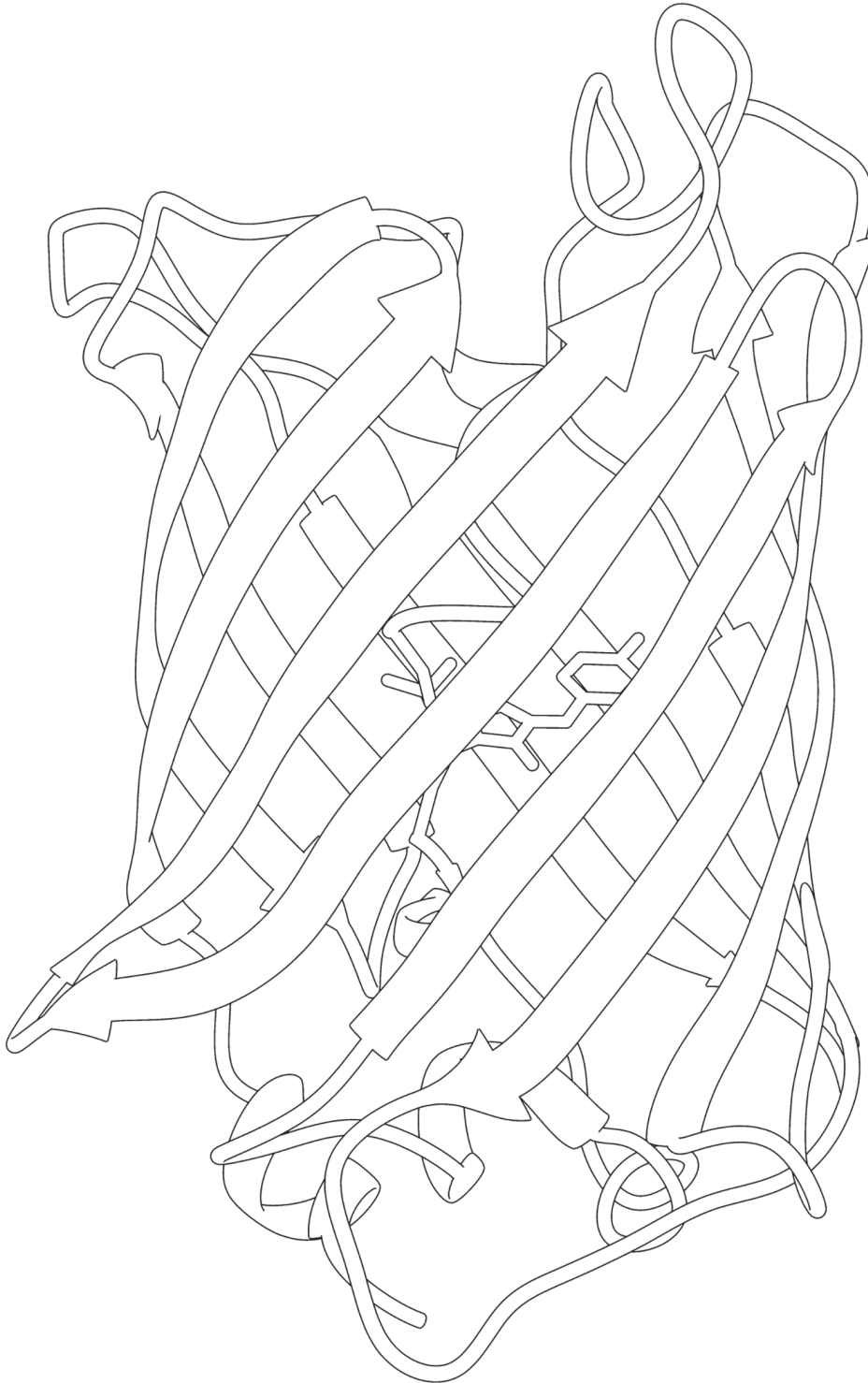
Potassium Channels

Potassium channels allow potassium ions to pass, but block the smaller sodium ions.



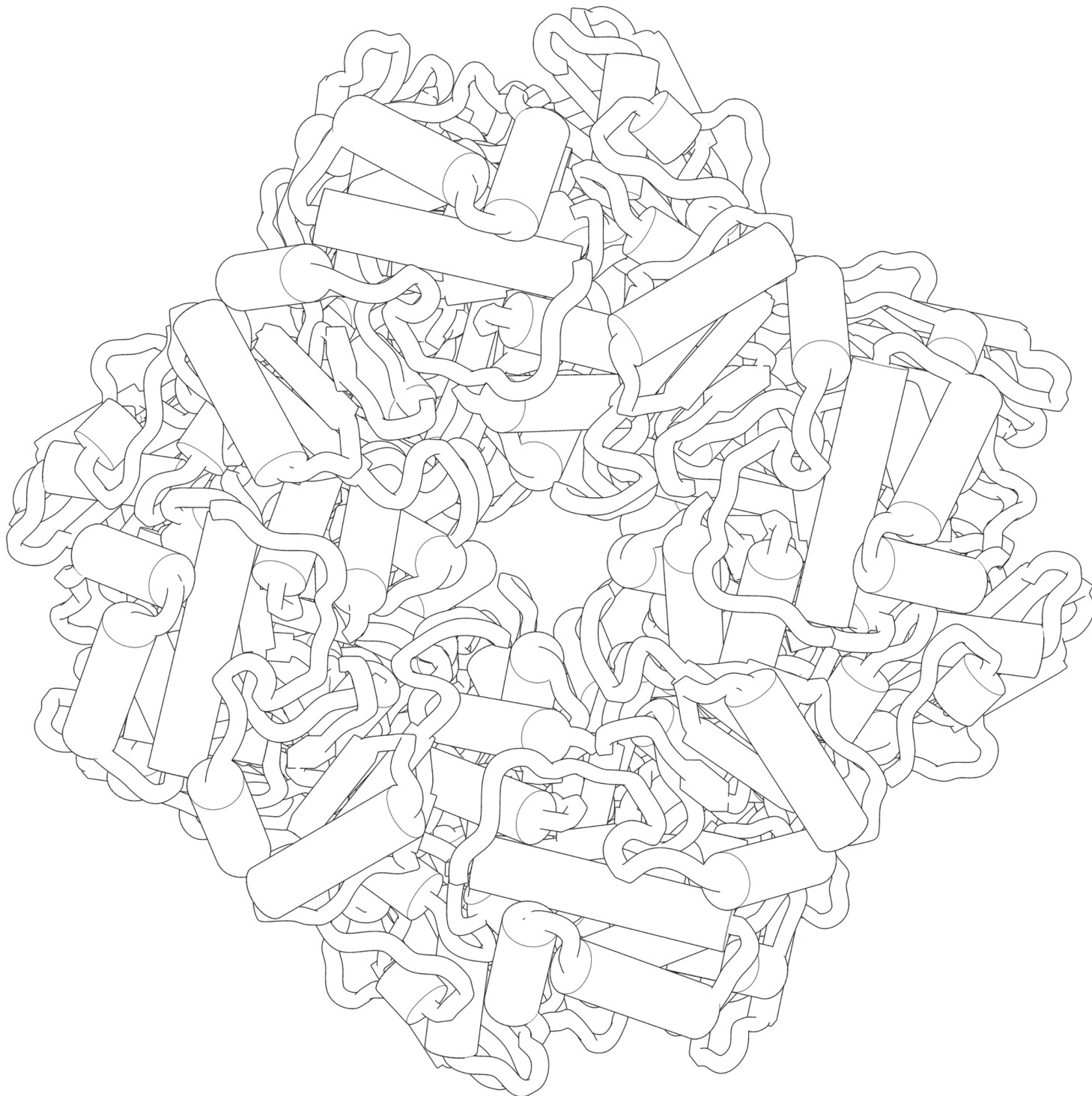
Green Fluorescent Protein (GFP)

GFP is a tiny protein from jellyfish that glows when exposed to ultraviolet light.



Rubisco

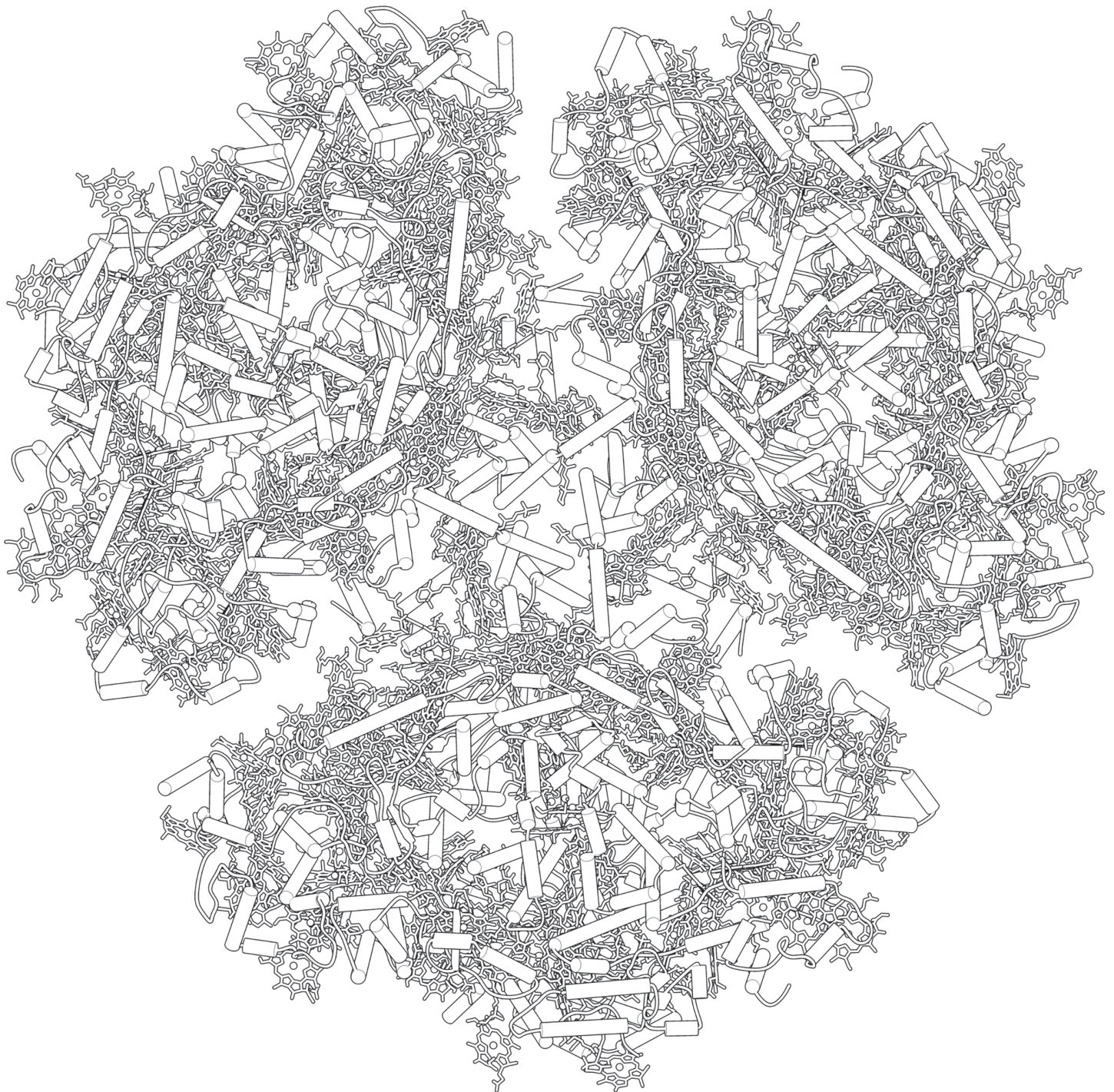
Rubisco fixes atmospheric carbon dioxide into bioavailable sugar molecules.



Photosystem I

(View 1)

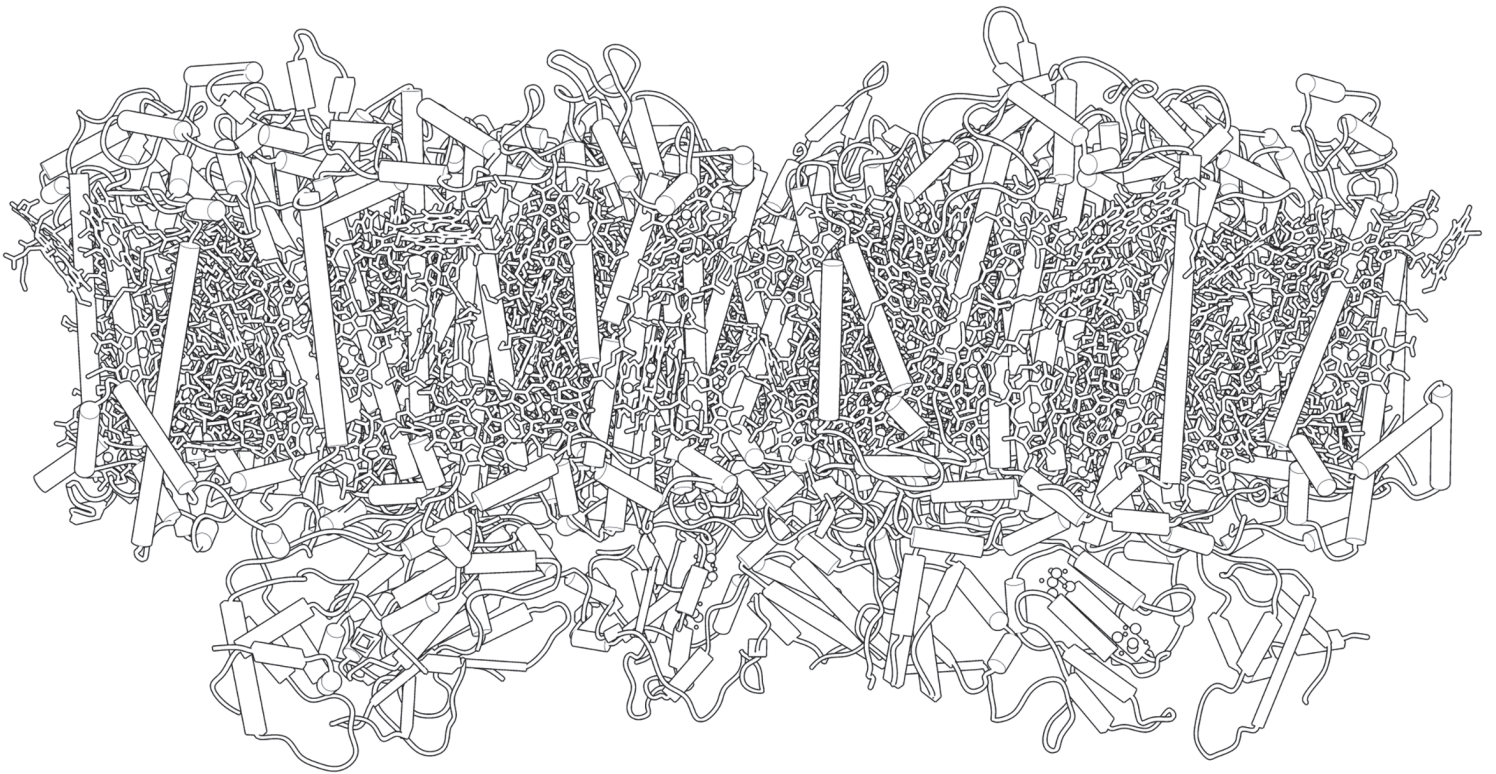
Photosystem I captures the energy in sunlight.



Photosystem I

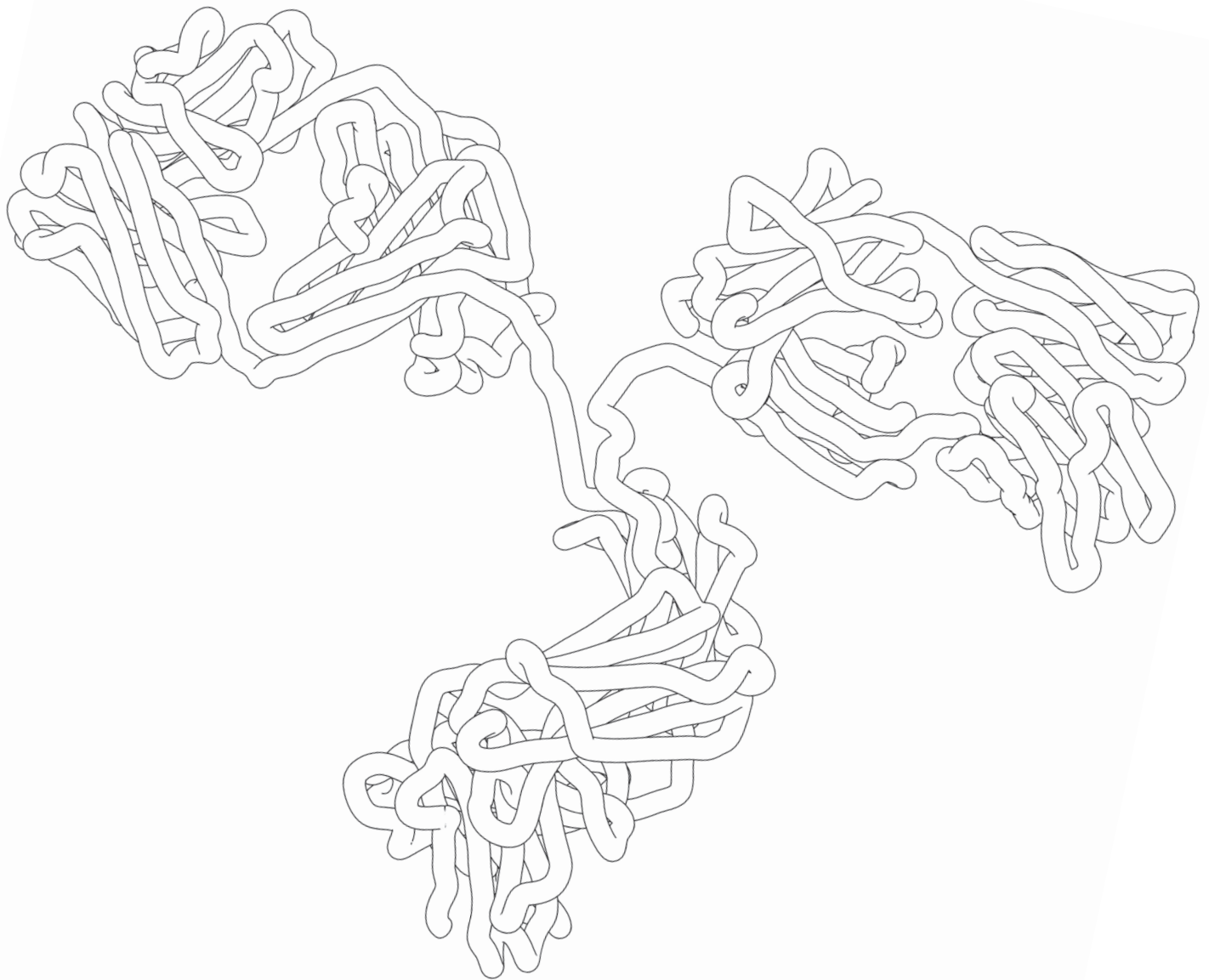
(View 2)

Photosystem I is a trimeric complex that forms a large disk. In cells, the complex floats in a membrane with the large flat faces exposed above and below the membrane.



Antibodies

Antibodies search for foreign molecules in the blood.



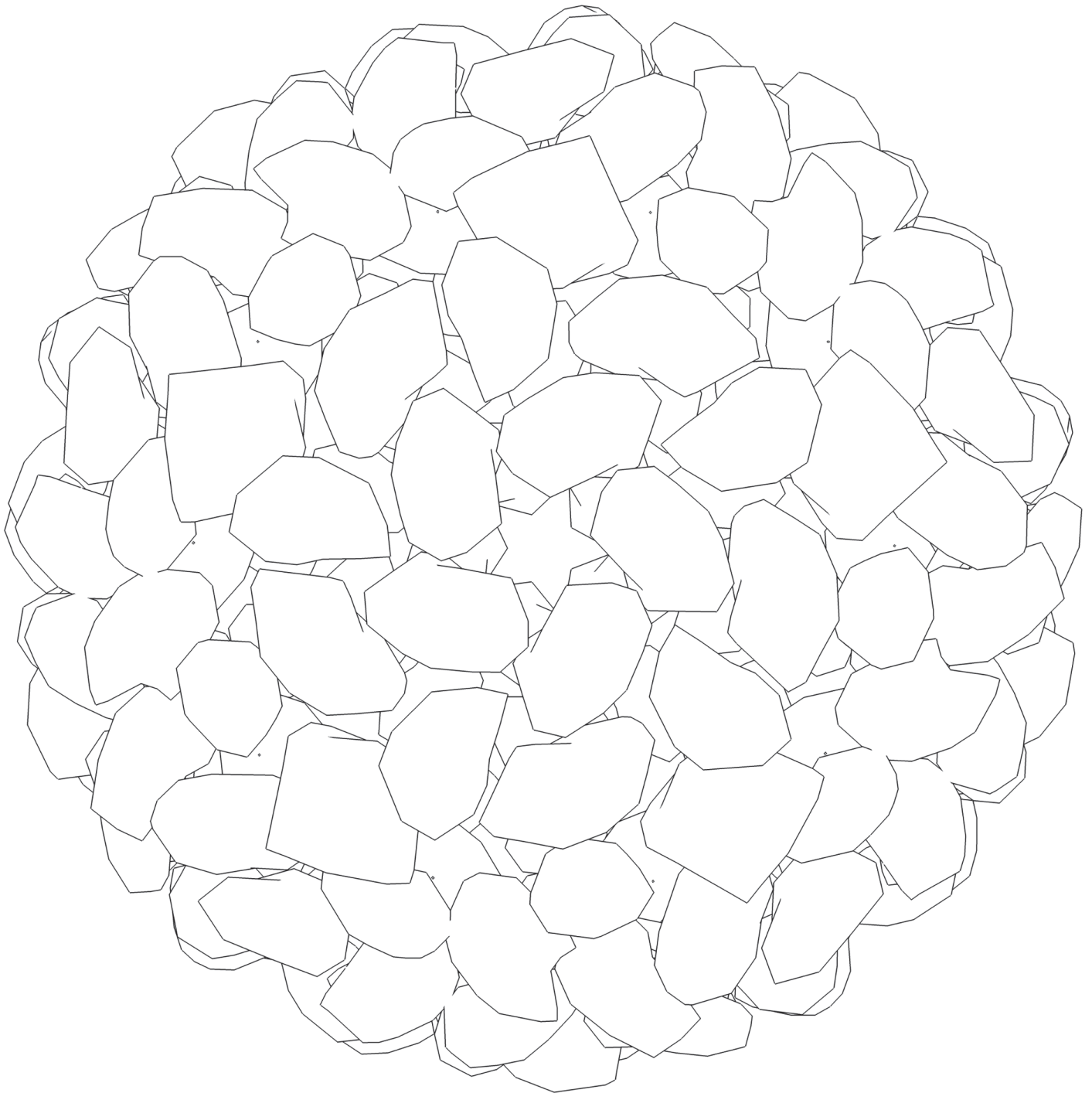
New Delhi Metallo-Beta-Lactamase

The New Delhi Metallo-Beta-Lactamase, shown as a stereoscopic image, is an enzyme found in some bacteria that inactivates a wide range of penicillin-like antibiotics.



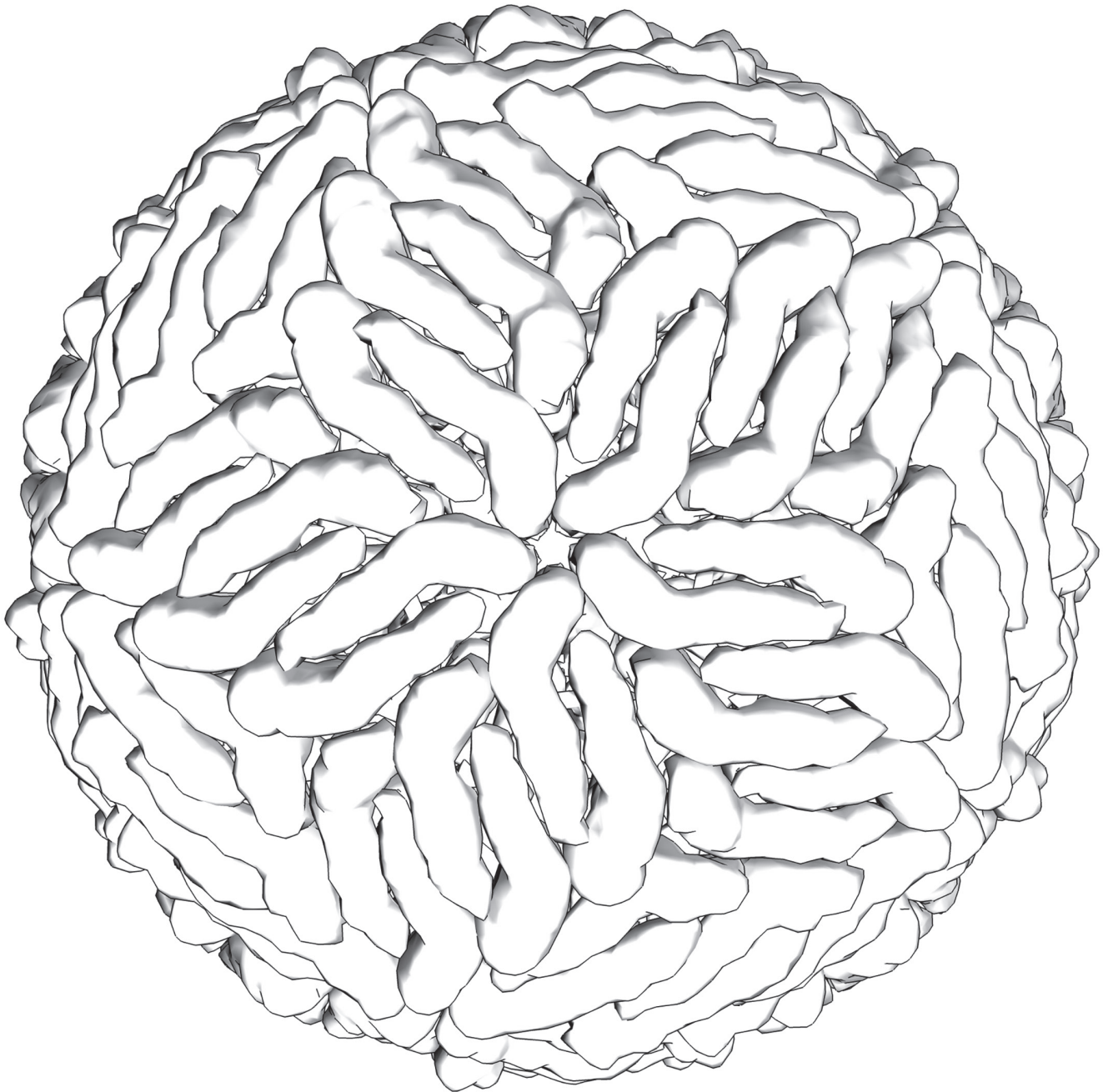
Rhinovirus

Rhinovirus is a picornavirus, or "little RNA virus". These viruses are composed of a protein shell surrounding a short piece of RNA.



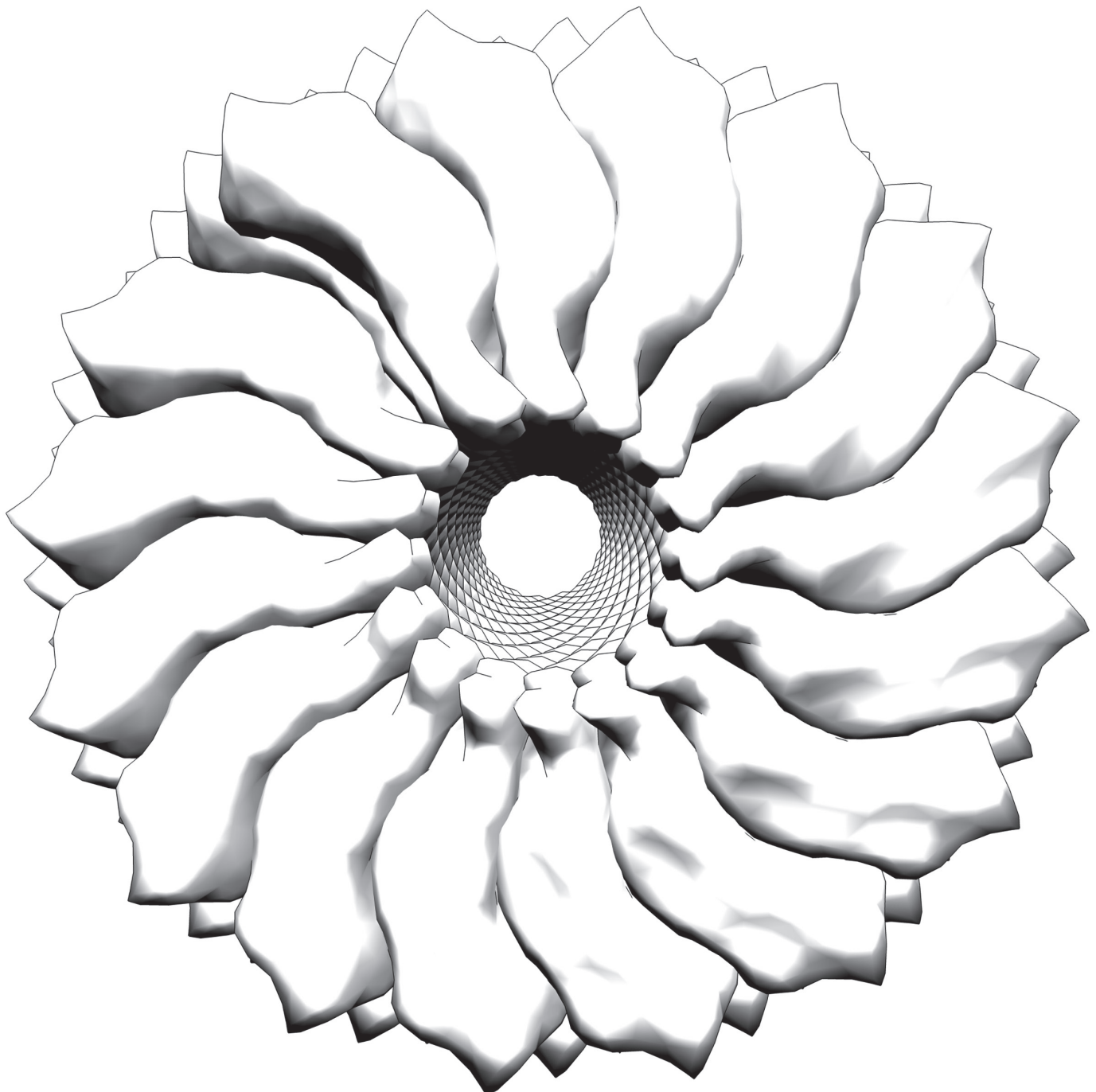
Zika Virus

Cryo-electron microscopy reveals the structure of Zika virus.



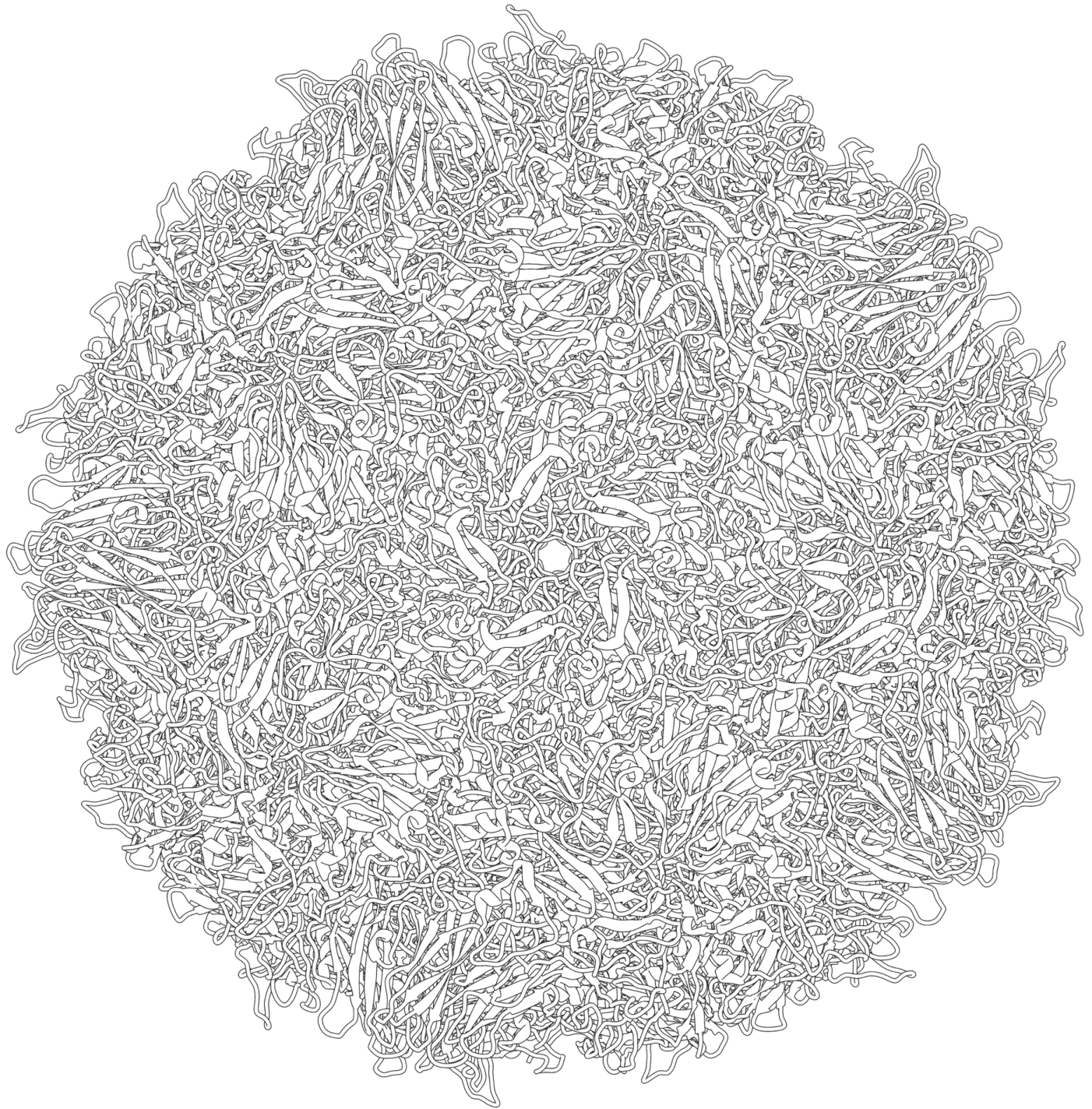
Tobacco Mosaic Virus

A cylindrical arrangement of proteins protects a long strand of RNA in TMV.



Poliovirus

Crystallographic structures reveal the atomic details of viruses and how to fight them.



Acknowledgments

The RCSB PDB *Molecule of the Month*¹ series by David S. Goodsell (RCSB PDB-Rutgers and The Scripps Research Institute) presents short accounts on molecules from the Protein Data Bank.

The molecular images in this booklet were created by Brian Hudson using UCSF Chimera².

1. David S. Goodsell, Shuchismita Dutta, Christine Zardecki, Maria Voigt, Helen M. Berman, Stephen K. Burley. (2015) The RCSB PDB "Molecule of the Month": Inspiring a Molecular View of Biology. *PLoS Biol* **13**: e1002140.
2. E. F. Pettersen, T. D. Goddard, C. C. Huang, G. S. Couch, D. M. Greenblatt, E. C. Meng, T. E. Ferrin. (2004) UCSF Chimera—a visualization system for exploratory research and analysis. *J Comput Chem.* **25**(13):1605-12.

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Antibodies (page 20)

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doi:10.2210/rcsb_pdb/mom_2001_9

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Clathrin (page 14)

April 2007, David Goodsell and Graham T. Johnson

doi:10.2210/rcsb_pdb/mom_2007_4

PDB ID 3iyv: A. Fotin, Y. Cheng, P. Sliz, N. Grigorieff, S. C. Harrison, T. Kirchhausen, T. Walz. (2004) Molecular model for a complete clathrin lattice from electron cryomicroscopy. *Nature* **432**: 573-579.

Collagen (page 11)

April 2000, David Goodsell

doi:10.2210/rcsb_pdb/mom_2000_4

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DNA (page 3)

November 2001, David Goodsell

doi:10.2210/rcsb_pdb/mom_2001_11

PDB ID 1bna: H. R. Drew, R. M. Wing, T. Takano, C. Broka, S. Tanaka, K. Itakura, R. E. Dickerson. (1981) Structure of a B-DNA dodecamer: conformation and dynamics. *Proc. Natl. Acad. Sci. U.S.A.* **78**: 2179-2183.

Ferritin (page 13)

November 2002, David Goodsell

doi:10.2210/rcsb_pdb/mom_2002_11

PDB ID 1fha: D. M. Lawson, P. J. Artymiuk, S. J. Yewdall, J. M. Smith, J. C. Livingstone, A. Treffry, A. Luzzago, S. Levi, P. Arosio, G. Cesareni, *et al.* (1991) Solving the structure of human H ferritin by genetically engineering intermolecular crystal contacts. *Nature* **349**: 541-544.

Green Fluorescent Protein (page 16)

June 2003, David Goodsell

doi:10.2210/rcsb_pdb/mom_2003_6

PDB ID 1ema: M. Ormo, A. B. Cubitt, K. Kallio, L. A. Gross, R. Y. Tsien, S. J. Remington. (1996) Crystal structure of the *Aequorea victoria* green fluorescent protein. *Science* **273**: 1392-1395.

Hemoglobin (page 12)

May 2003, David Goodsell and Shuchismita Dutta

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PDB ID 4hhb: G. Fermi, M. F. Perutz, B. Shaanan, R. Fourme (1984) The crystal structure of human deoxyhaemoglobin at 1.74 Å resolution. *J.Mol.Biol.* **175**: 159-174.

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February 2001, David Goodsell

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New Delhi Metallo-Beta-Lactamase (page 21)

July 2015, David Goodsell

doi:10.2210/rcsb_pdb/mom_2015_7

PDB ID 4eyl: D. T. King, L. J. Worrall, R. Gruninger, N. C. Strynadka (2012) New Delhi Metallo-Beta-Lactamase: Structural Insights into Beta-Lactam Recognition and Inhibition. *J.Am.Chem.Soc.* **134**: 11362-11365.

Nucleosome (page 4 & 5)

July 2000, David Goodsell

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PDB ID 1aoi: K. Luger, A. W. Mader, R. K. Richmond, D. F. Sargent, T. J. Richmond. (1997) Crystal structure of the nucleosome core particle at 2.8Å resolution. *Nature* **389**: 251-260.

Photosystem 1 (page 18 & 19)

October 2001, David Goodsell

doi:10.2210/rcsb_pdb/mom_2001_10

PDB ID 1jbo: P. Jordan, P. Fromme, H. T. Witt, O. Klukas, W. Saenger, N. Krauss. (2001) Three-dimensional structure of cyanobacterial photosystem I at 2.5 Å resolution. *Nature* **411**: 909-917.

Poliovirus (page 25)

August 2001, David Goodsell

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PDB ID 1hxs: S. T. Miller, J. M. Hogle, D. J. Filman. (2001) *Ab initio* phasing of high-symmetry macromolecular complexes: successful phasing of authentic poliovirus data to 3.0 Å resolution. *J Mol Biol* **307**: 499-512.

Potassium Channels (page 15)

February 2003, David Goodsell and Shuchismita Dutta

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PDB ID 1k4c: Y. Zhou, J. H. Morais-Cabral, A. Kaufman, R. MacKinnon. (2001) Chemistry of ion coordination and hydration revealed by a K⁺ channel-Fab complex at 2.0 Å resolution. *Nature* **414**: 43-48.

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Rubisco (page 17)

November 2000, David Goodsell

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Ribosome (page 9)

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PDB ID 3jci: T. Sprink, D. J. Ramrath, H. Yamamoto, K. Yamamoto, J. Loerke, J. Ismer, P. W. Hildebrand, P. Scheerer, J. Burger, T. Mielke, C. M. Spahn. (2016) Structures of ribosome-bound initiation factor 2 reveal the mechanism of subunit association. *Sci Adv* **2**: e1501502.

TATA-Binding Protein (page 6)

July 2005, David Goodsell

doi:10.2210/rcsb_pdb/mom_2005_7

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Tobacco Mosaic Virus (page 24)

January 2009, David Goodsell

doi:10.2210/rcsb_pdb/mom_2009_1

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Transfer RNA (page 8)

March 2001, David Goodsell

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Zika Virus (page 23)

May 2016, David Goodsell

doi:10.2210/rcsb_pdb/mom_2016_5

PDB ID 5ire: D. Sirohi, Z. Chen, L. Sun, T. Kloese, T. C. Pierson, M. G. Rossmann, R. J. Kuhn. (2016) The 3.8 Å resolution cryo-EM structure of Zika virus. *Science* **352**: 467-470.

Zinc Fingers (page 7)

March 2007, David Goodsell

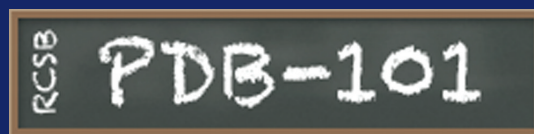
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The RCSB PDB is managed by the members of the
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