

INTRODUCTION TO PROTEINS

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DIPARTIMENTO DI FISICA



SAPIENZA
UNIVERSITÀ DI ROMA

- SEQUENCE->STRUCTURE/UNSTRUCTURE->DYNAMICS-FUNCTIONS

JOURNALS

PROTEINS

PROTEIN SCIENCE

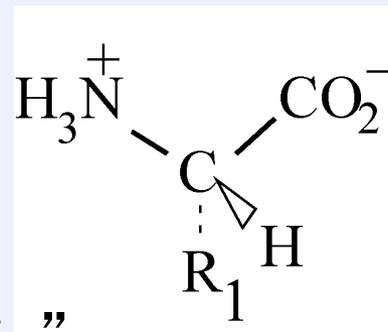
JOURNAL OF MOLECULAE BIOLOGY

Proteopedia https://proteopedia.org/wiki/index.php/Main_Page

Proteins

- From the Greek “proteios” meaning “of first importance”
- The basic building blocks of almost all living organisms
- Constitute the majority of the cell (see biology by numbers), and perform nearly all enzymatic activities
- Composed of 20 naturally occurring amino-acids

varying moiety
called “side chain”



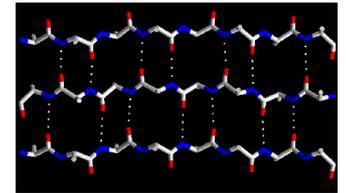
Hierarchy of Protein Structure

Primary 1°

AKSDQPWFAGLE

Linear chain made of 20 possible amino acids

Secondary 2°



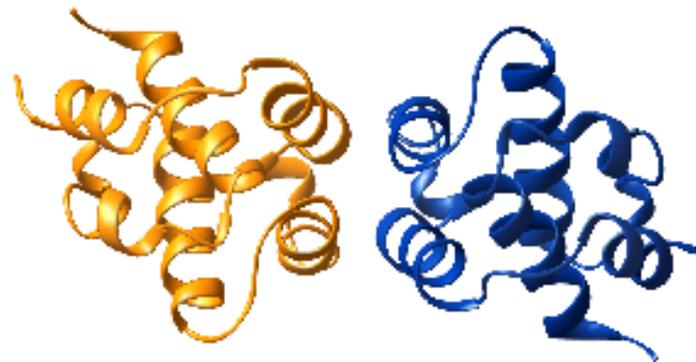
Alpha-helices, beta-sheets, turns

Tertiary 3°



Motifs, domains

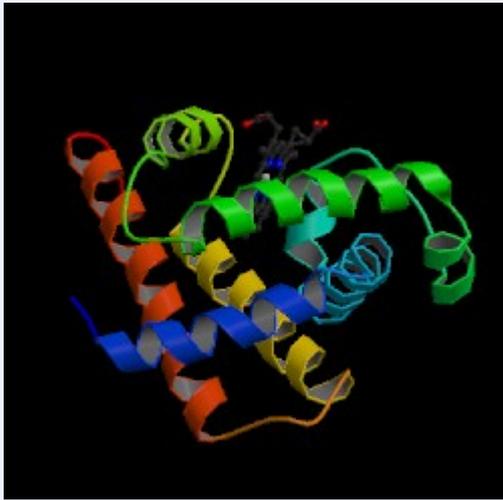
Quaternary 4°



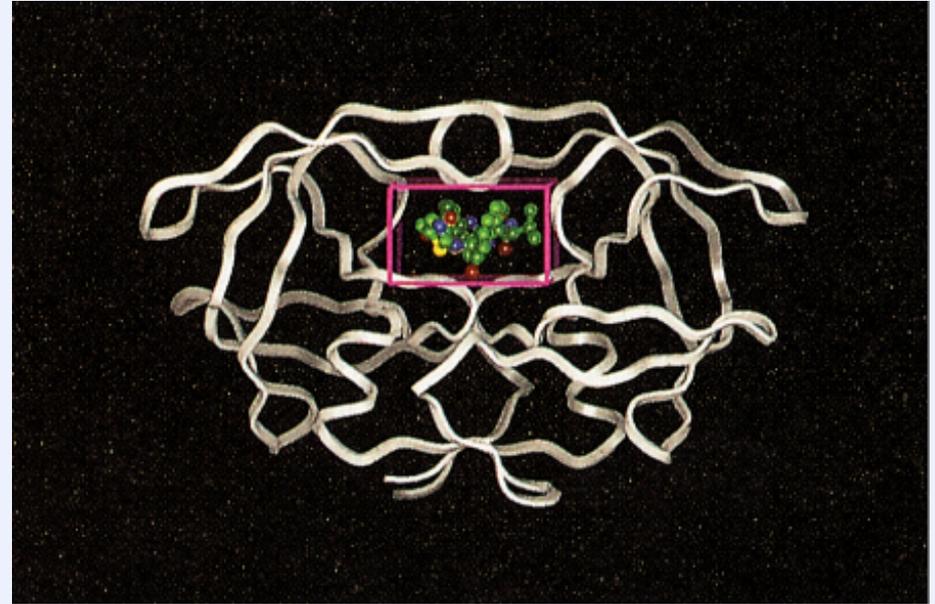
Oligomers, complexes

Structure/Unstructure

is quite basic in protein science



Myoglobin (1958) x-ray structure M.F. Perutz



Viral proteases are targets of the molecular design of inhibitor drugs such as Ritonavir, capable of blocking the active site of the enzyme and to contribute to the containment of HIV epidemics.

The Protein Data Bank (www.pdb.org)

The screenshot displays the RCSB Protein Data Bank website in a Microsoft Internet Explorer browser window. The address bar shows the URL <http://www.pdb.org/pdb/home/home.do>. The page features a blue header with the RCSB PDB logo and the text "An Information Portal to Biological Macromolecular Structures". Below the header, there is a search bar with options for "PDB ID or keyword" and "Author", and a "SEARCH" button. The main content area is divided into three columns. The left column contains a navigation menu with links such as "Home", "Tutorial About This Site", "Getting Started", "Download Files", "Deposit and Validate", "Structural Genomics", "Dictionaries & File Formats", "Software Tools", "General Education", "BioSync", "General Information", "Acknowledgements", "Frequently Asked Questions", "Known Problems", and "Report Bugs/Comments". The middle column is titled "Welcome to the RCSB PDB" and contains several paragraphs of text, including a "Molecule of the Month: Transposase" section with a molecular structure image. The right column is titled "NEWS" and features a "Complete News" section with a link to "RCSB PDB Poster Prize Awarded at AsCA" and a date of "19-December-2006". The browser's taskbar at the bottom shows the Windows Start button, several open applications, and the system clock displaying "3:05 PM".

RCSB PDB
PROTEIN DATA BANK

A MEMBER OF THE PDB

An Information Portal to Biological Macromolecular Structures

As of Tuesday Dec 19, 2006 there are 40749 Structures | PDB Statistics

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PDB ID or keyword Author SEARCH Advanced Search

Home Search

- Home
- Tutorial About This Site
- Getting Started
- Download Files
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- Structural Genomics
- Dictionaries & File Formats
- Software Tools
- General Education
- BioSync
- General Information
- Acknowledgements
- Frequently Asked Questions
- Known Problems
- Report Bugs/Comments

Welcome to the RCSB PDB

The RCSB PDB provides a variety of tools and resources for studying the structures of biological macromolecules and their relationships to sequence, function, and disease.

The RCSB is a member of the [wwPDB](#) whose mission is to ensure that the PDB archive remains an international resource with uniform data.

This site offers tools for browsing, searching, and reporting that utilize the data resulting from ongoing efforts to create a more consistent and comprehensive archive.

Information about compatible browsers can be found [here](#).

A [narrated tutorial](#) illustrates how to search, navigate, browse, generate reports and visualize structures using this new site. [This requires the [Macromedia Flash player download](#).]

Comments? info@rcsb.org

Molecule of the Month: Transposase

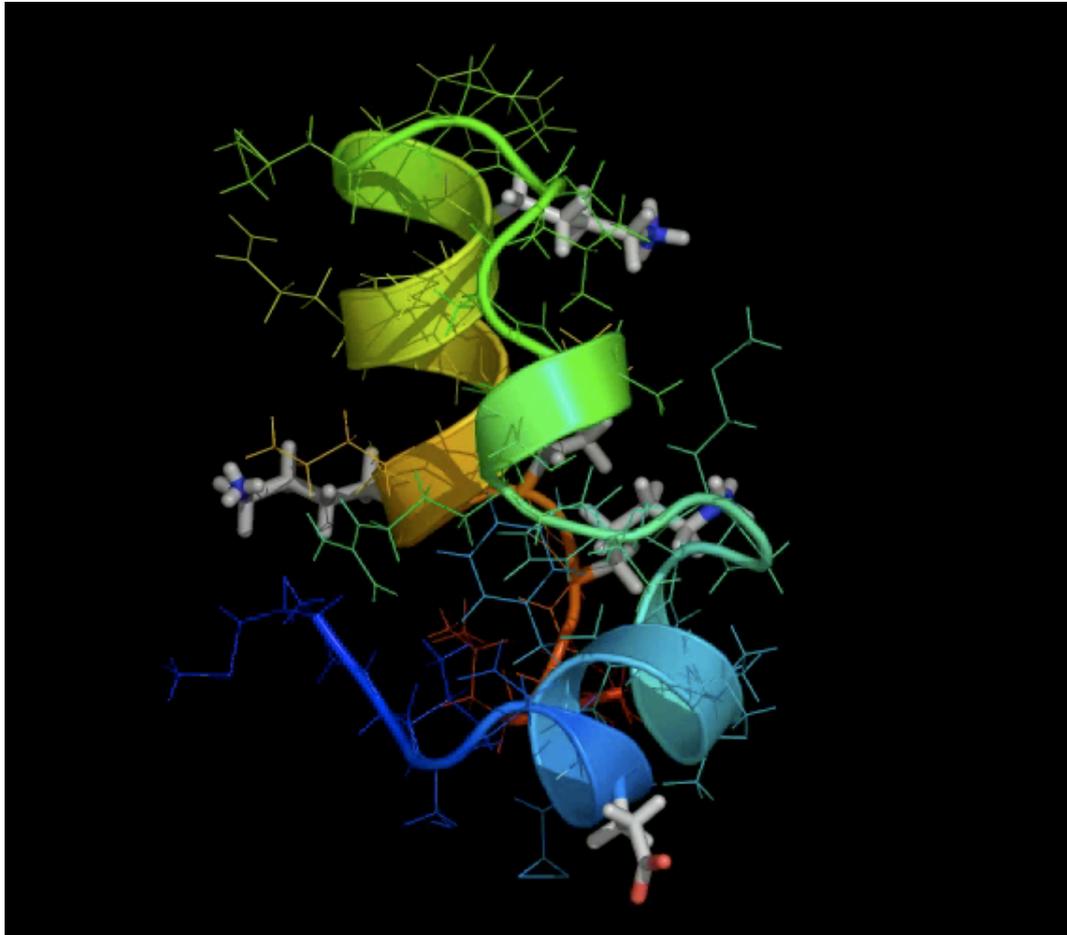
In the 1940's, Barbara McClintock discovered that

NEWS

- Complete News
- Newsletter
- Discussion Forum

19-December-2006
RCSB PDB Poster Prize Awarded at AsCA

Thanks to everyone who participated in the recent competition for best student poster related to macromolecular crystallography at the Joint Conference of the Asian Crystallographic Association and the Crystallographic Society of Japan (AsCA; November 20-23 in Tsukuba, Japan).



Sequence->Structure->Function
Sequence->Function-> Structure
AND/OR DYNAMICS

Pioneers:

H. Frauenfelder, G. Careri,
G. Weber, (early seventies)
M. Karplus (1977)

Early review

[Nature. 1990 Oct 18;347\(6294\):631-9.](#)

[Molecular dynamics simulations in biology.](#)

[Karplus M, Petsko GA..](#)

[*Molecular dynamics--the science of simulating the motions of a system of particles--applied to biological macromolecules gives the fluctuations in the relative positions of the atoms in a protein or in DNA as a function of time. Knowledge of these motions provides insights into biological phenomena such as the role of flexibility in ligand binding and the rapid solvation of the electron transfer state in photosynthesis. Molecular dynamics is also being used to determine protein structures from NMR, to refine protein X-ray crystal structures faster from poorer starting models, and to calculate the free energy changes resulting from mutations in proteins.*](#)

Domain Boundaries, Reliability of
Present Methods and Promising
Avenues, Suggested Reading

Problem 3 Function Prediction
Introduction to the Problem, The
Definition of Biological Function,
The Function Vocabulary, Protein
Names, Text Mining, Transferring
Functional Annotations by
Similarity, Transcriptomics,
Proteomics, Promising Avenues,
Suggested Reading

Problem 4 Protein Structure
Prediction
Introduction to the Problem,
Energetic Calculations of Protein
Structures (Energy Calculation,

Water forms a hydration shell around proteins.

The properties of this bound water are still the subject of many experimental and theoretical investigations.