Structural Bioinformatics

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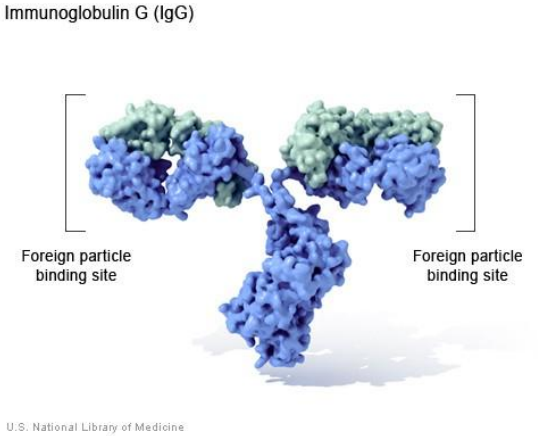
Introduction to Protein Structures

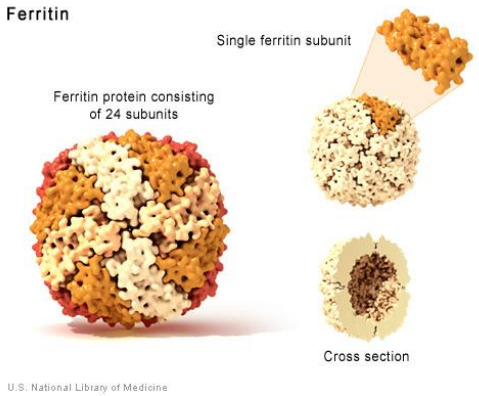
General principles

- Give three roles of proteins in an organism.
- How many amino acid types proteins are composed of? Name one polar amino acid, one aromatic, one negatively charged and one positively charged. Which amino acid has the smallest side chain?
- Describe the four levels of protein structure.
- Name three secondary structure elements. What are the protein main classes in SCOP classification?
- Describe 3 types of interactions that stabilize protein structure. What drives protein folding?

Protein functions

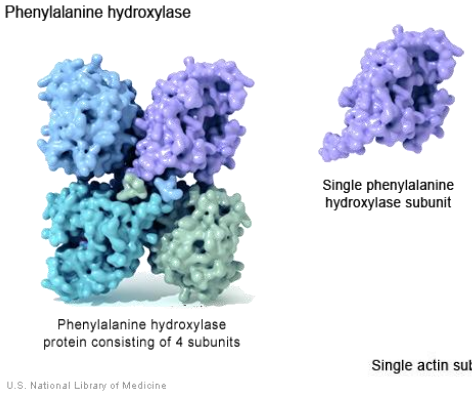


Antibodies bind to specific foreign particles, such as viruses and bacteria, to help protect the body.

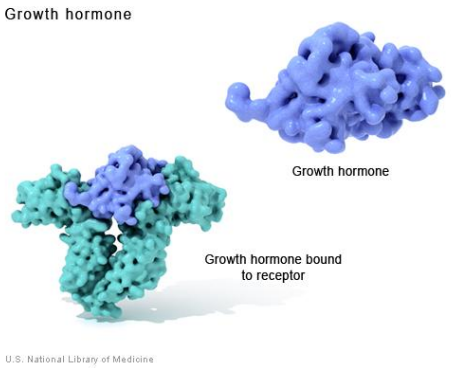


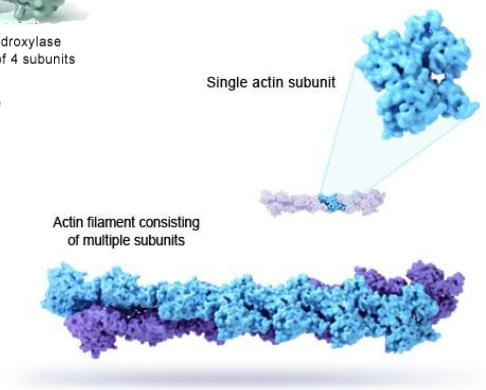
Transport/Storage proteins bind and carry atoms and small molecules within cells and throughout the body.

Enzymes carry out almost all of the thousands of chemical reactions that take place in cells. They also assist with the formation of new molecules by reading the genetic information stored in DNA.



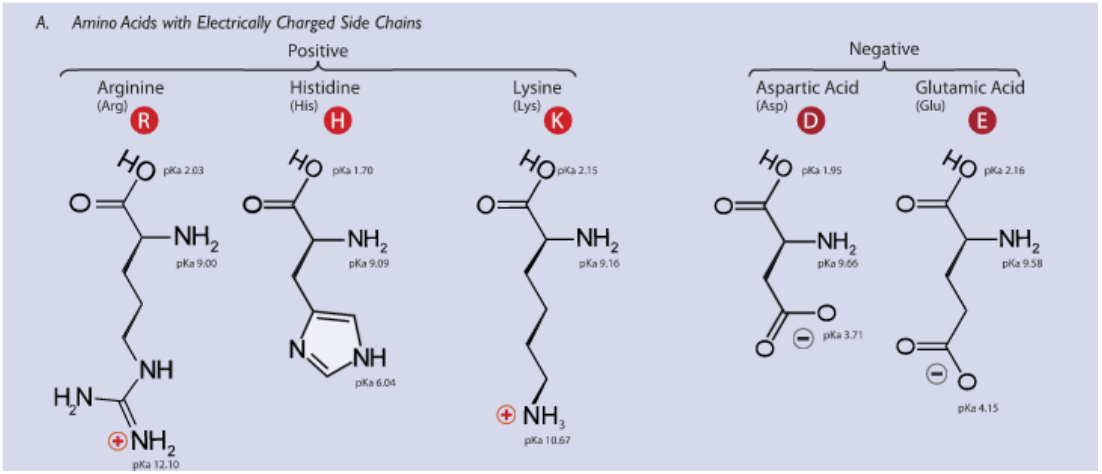
Messenger proteins, such as some types of hormones, transmit signals to coordinate biological processes between different cells, tissues, and organs.

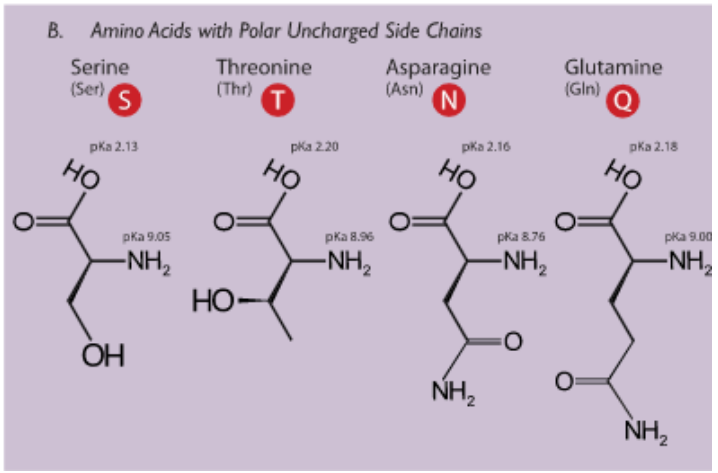


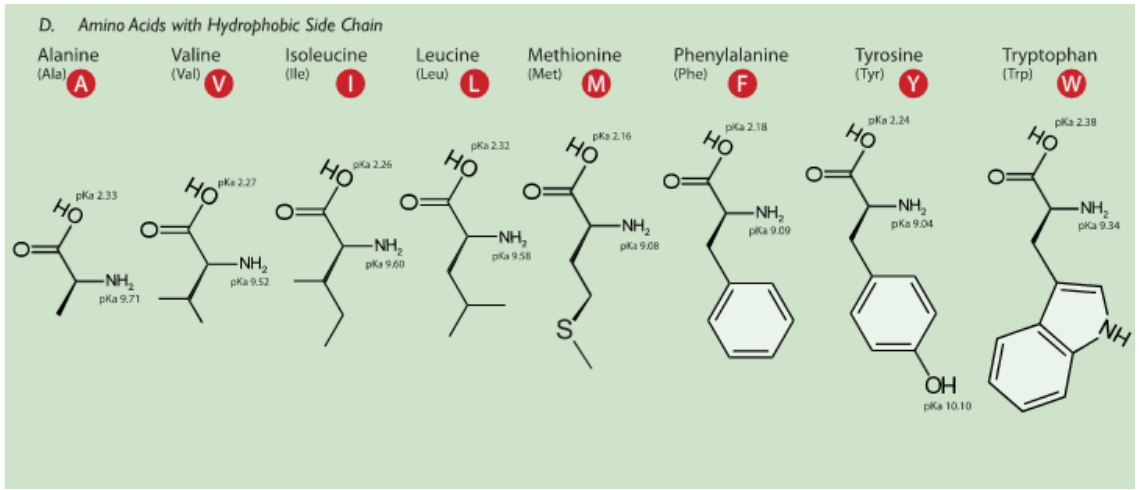


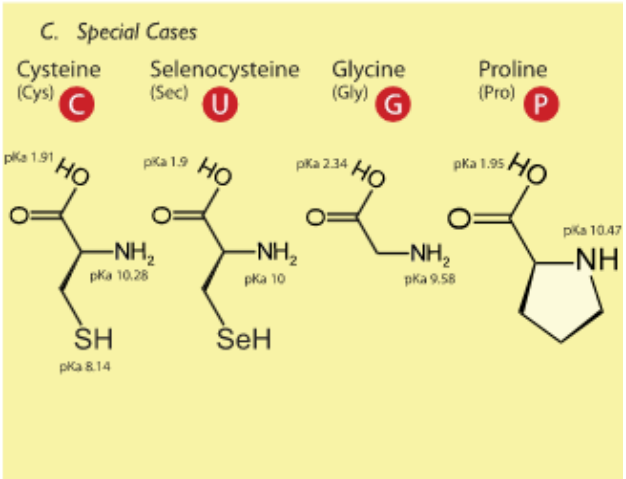
Structural proteins provide structure and support for cells. On a larger scale, they also allow the body to move.

Amino acid types



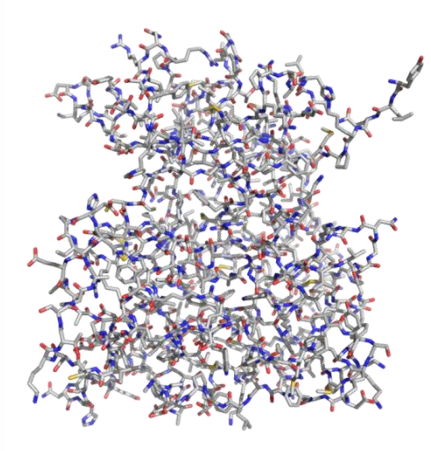


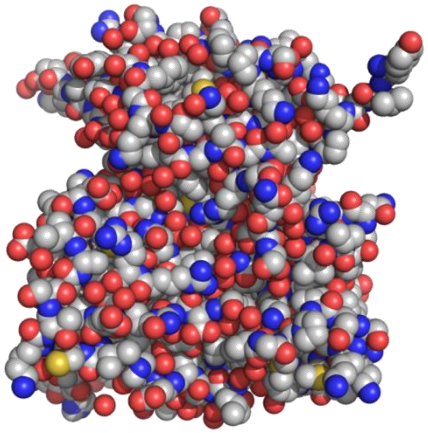




Protein structure

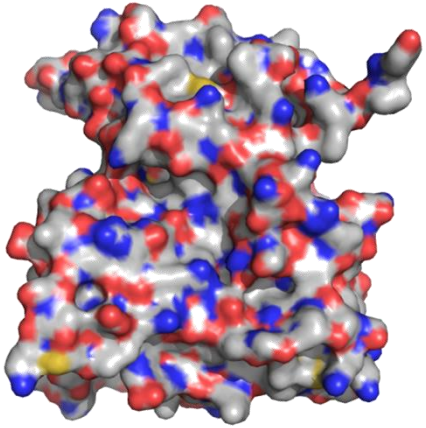
sticks





spheres

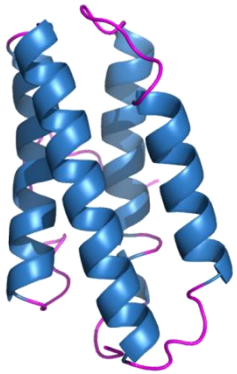
surface



cartoon

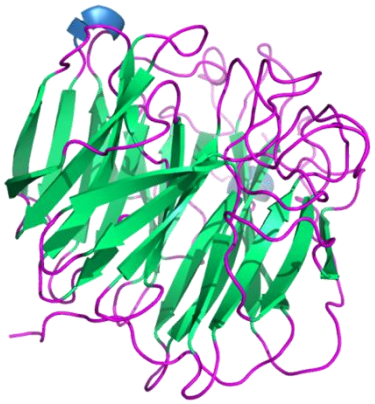
Protein classes

All Alpha
All Beta
Alpha/Beta
Alpha+Beta



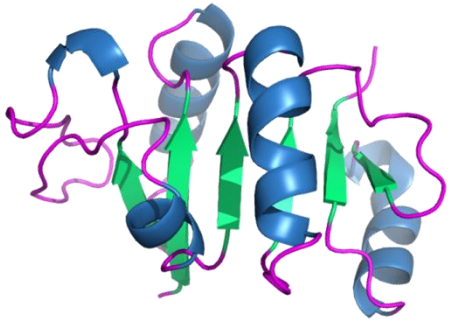
myohemerythrin

All Alpha



Neuraminidase
Beta Propeller

All Beta

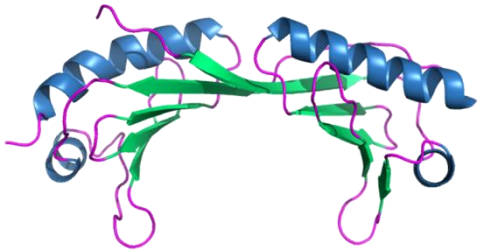


Aspartate Semi-
Aldehyde
Dehydrogenase

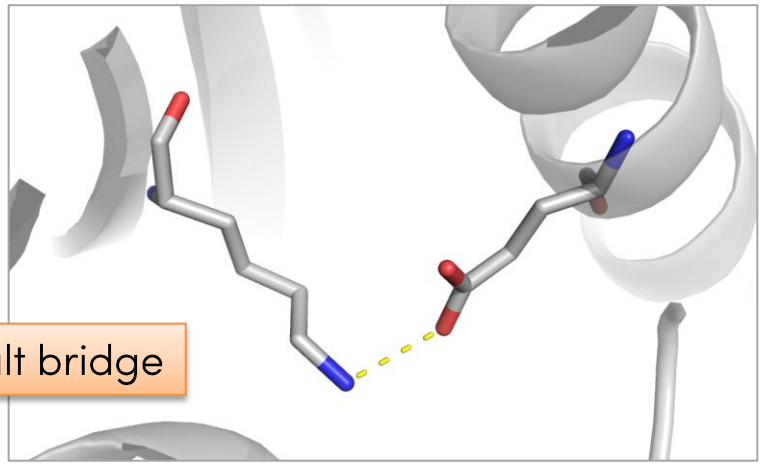
Alpha/Beta

TATA Binding
Protein

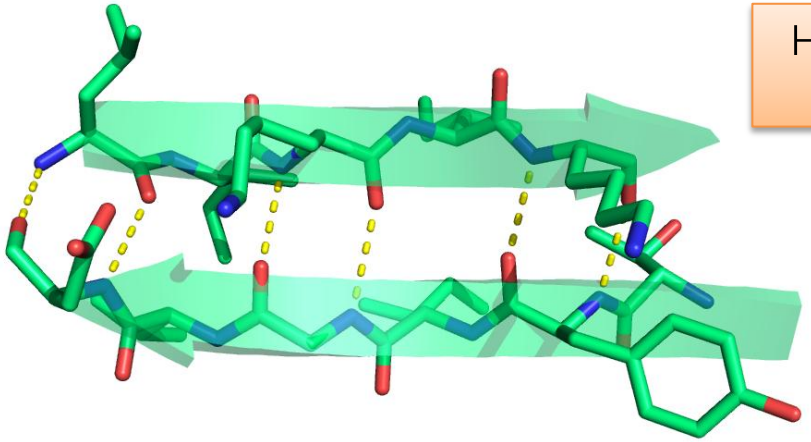
Alpha+Beta



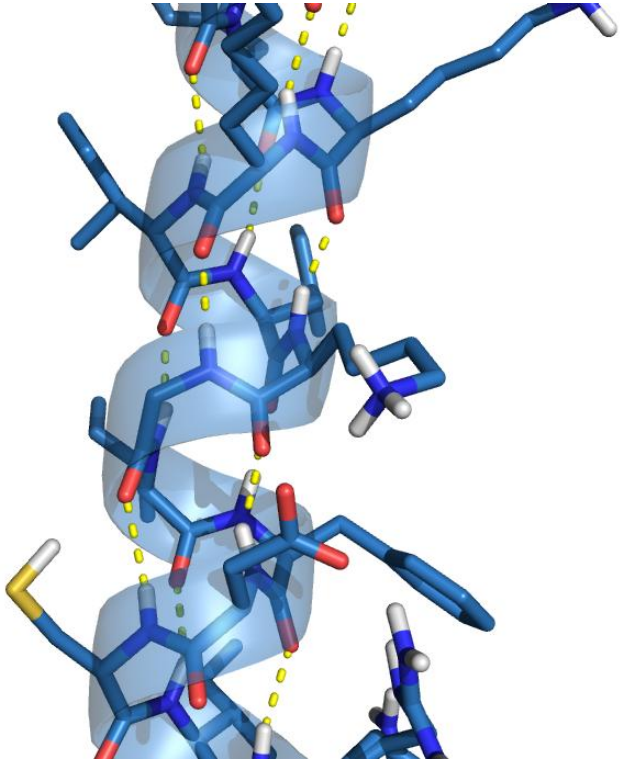
Protein interactions



Salt bridge

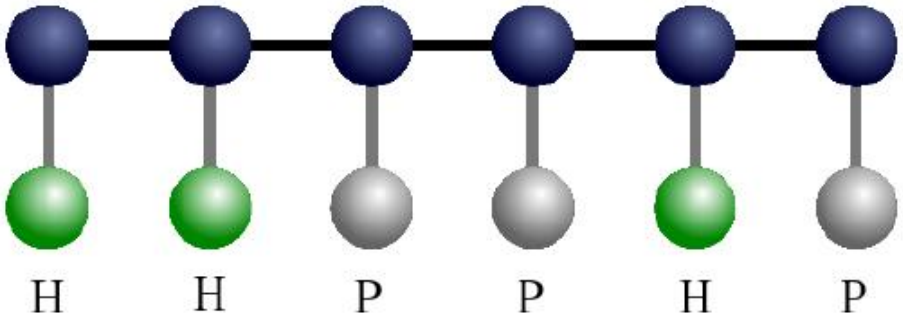


Hydrogen-bonds



Protein folding

A lattice protein in the Side-Chain HP-model within the 2D square lattice looks like this:



Each aa residue is represented via 2 monomers: 1 for the side chain and 1 for the backbone. The energy of stability of the lattice protein is evaluated as the opposite value of the number of H-H contacts.

a. Define the set of neighboring vectors N_{L2} for the 2D square lattice L^2. This set N_{L2} contains all vectors of minimal length between coordinates of the lattice
b. Define the Side-Chain HP-model for a given HP-sequence *S* of length *n*, an arbitrary lattice *L* and its set of neighboring vectors *NL*
c. Construct the best-energy structure of a Side-Chain HP-model protein in the 2D square lattice for the sequences: 1) HHHHPPPPHHHHP 2) HHHHPPHHHH

Secondary structures: α-helices

These three sequence regions fold as α-helices:

Leu – Ser – Phe – Ala – Ala –Ala – Met – Asn – Gly – Leu – Ala

Ile – Asn – Glu – Gly – Phe –Asp –Leu – Leu – Arg – Ser – Gly

Lys – Glu – Asp – Ala – Lys – Gly – Lys – Ser – Glu – Glu –Glu

- Draw representations of the helices as 2D wheels where residues are displayed as beads colored differently depending on whether they are hydrophobic, polar or charged
- Describe how the helices appear as different using this representation. What is the distibution of the polar and charged residues?