Tertiary structure of protein

Semester II
b.Sc. Microbiology Core (MBIO CC203)
UNIT - 4

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Tertiary structure

- The overall three-dimensional arrangement of all atoms in a protein is referred to as the protein's **tertiary structure.** Again, it is the sequence of amino acids that specifies this final **three-dimensional structure**
- Once folded, the **three-dimensional, biologically active (native) conformation** of the protein is maintained by

  1) hydrophobic interactions

  2) electrostatic forces

  3) hydrogen bonding and, if present

  4) covalent disulfide bonds.

Salt Bridges

Vander Waals interaction

- The electrostatic forces include **salt bridges between oppositely charged groups** and the **multiple weak van der Waals interactions** between the tightly packed aliphatic side-chains in the interior of the protein.

Fibrous protein and Globular protein

Fibrous protein

- **Fibrous proteins,** having polypeptide chains arranged in long strands or sheets.
- Fibrous proteins usually consist largely of a single type of secondary structure.
- structures that provide support, shape, and external protection to vertebrates are made of fibrous proteins.
- Fibrous proteins share properties that give strength and/or flexibility to the structures in which they occur.
- In each case, the fundamental structural unit is a simple repeating element of secondary structure.
- All fibrous proteins are insoluble in water
- Alpha – keratin, collagen, silk fibrion

Globular protein

- **globular proteins,** having polypeptide chains folded into a spherical or globular shape.
- globular proteins often contain several type
- Globular proteins include enzymes, transport proteins, motor proteins, regulatory proteins, immunoglobulins, and proteins with many other functions.

Fibrous Protein

TABLE 4-1 Secondary Structures and Properties of Fibrous Proteins

Structure	*Characteristics*	*Examples of occurrence*
α Helix, cross-linked by disulfide bonds	Tough, insoluble protective structures of varying hardness and flexibility	α-Keratin of hair, feathers, and nails
β Conformation	Soft, flexible filaments	Silk fibroin
Collagen triple helix	High tensile strength, without stretch	Collagen of tendons, bone matrix

Alpha -keratin

- The -keratins have evolved for strength.
- Found in mammals, these proteins constitute almost the entire dry weight of hair, wool, nails, claws, quills, horns, hooves, and much of the outer layer of skin.
- The keratins are part of a broader family of proteins called intermediate filament (IF) proteins.
- The alpha -keratin helix is a right-handed helix
- The alpha- helices of keratin are arranged as a coiled coil.
- Two strands of Alpha – keratin, oriented in parallel (with their amino terminal at the same end) are wrapped about each other to form a super twisted coiled coil just like a rope.
- Alpha -keratin is rich in the hydrophobic residues Ala, Val, Leu, Ile, Met, and Phe.

- Coiled coils of this type are common structural elements in filamentous proteins and in the muscle protein myosin
- The quaternary structure of -keratin can be quite complex. Many coiled coils can be assembled into large supramolecular complexes, such as the arrangement of -keratin to form the intermediate filament of hair

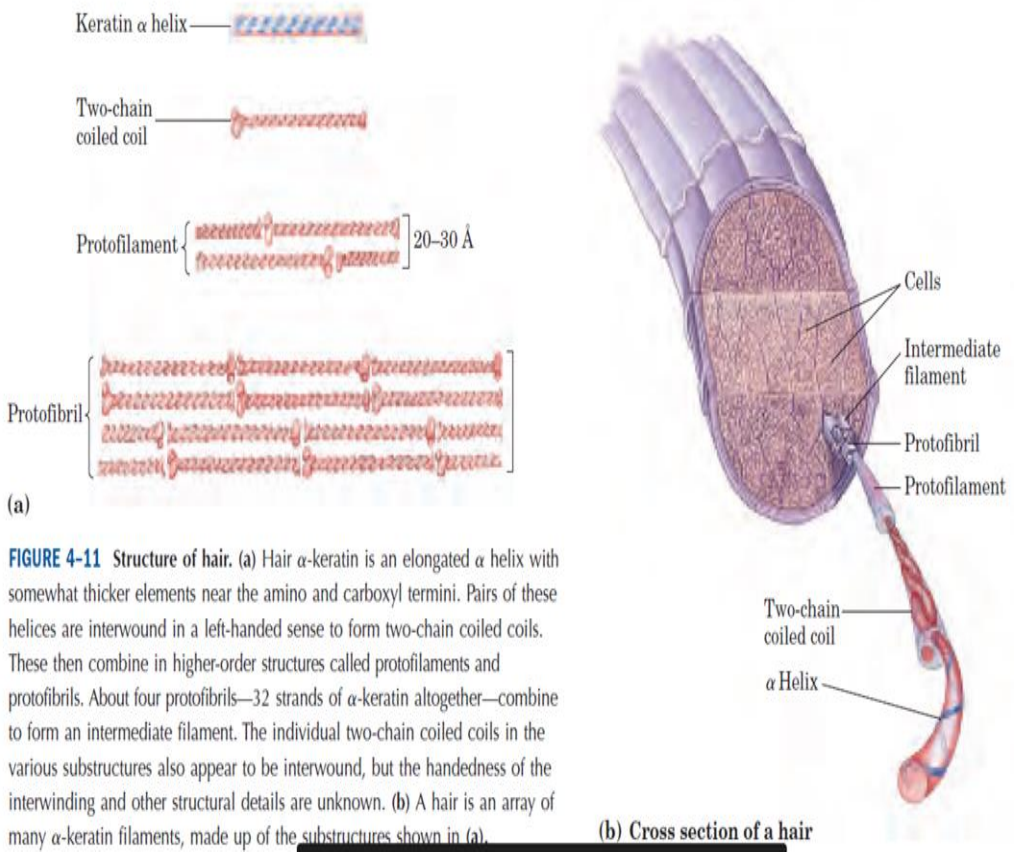

FIGURE 4-11 Structure of hair. (a) Hair α-keratin is an elongated α helix with somewhat thicker elements near the amino and carboxyl termini. Pairs of these helices are interwound in a left-handed sense to form two-chain coiled coils. These then combine in higher-order structures called protofilaments and protofibrils. About four protofibrils—32 strands of α-keratin altogether—combine to form an intermediate filament. The individual two-chain coiled coils in the various substructures also appear to be interwound, but the handedness of the interwinding and other structural details are unknown. (b) A hair is an array of many α-keratin filaments, made up of the substructures shown in (a).

Collagen

- **Collagen**, which is present in all multicellular organisms, is **<u>not one protein but diversity a family of structurally related proteins.</u>** It is the most abundant protein in mammals and is present in most organs of the body, where it serves to hold cells together in discrete units. It is also the major **fibrous element** of skin, bones, tendons, cartilage, blood vessels, cornea of eye and teeth.
- The collagen helix is a unique secondary structure quite distinct from the helix. It is left-handed and has three amino acid residues per turn.
- The super helical twisting is right-handed in collagen, opposite in sense to the left-handed helix of the chains.
- The chain of collagen has a repeating secondary structure unique to this protein. The repeating tripeptide sequence Gly–X–Pro or Gly–X–4-Hyp adopts a left-handed helical structure with three residues per turn.
- Typically they contain about 35% Gly, 11% Ala, and 21% Pro and 4-Hyp (4- hydroxyproline, an uncommon amino acid;

Silk Fibres

- Protein of silk is called as **Fibroin.**
- Its polypeptide chains are predominantly in the conformation. Fibroin is rich in Ala and Gly residues, permitting a close packing of sheets and an interlocking arrangement of R groups.
- The overall structure is stabilized by extensive hydrogen bonding between all peptide linkages in the polypeptides of each sheet and by the optimization of van der Waal interactions between sheets.
- Silk does not stretch, because the conformation is already highly extended.

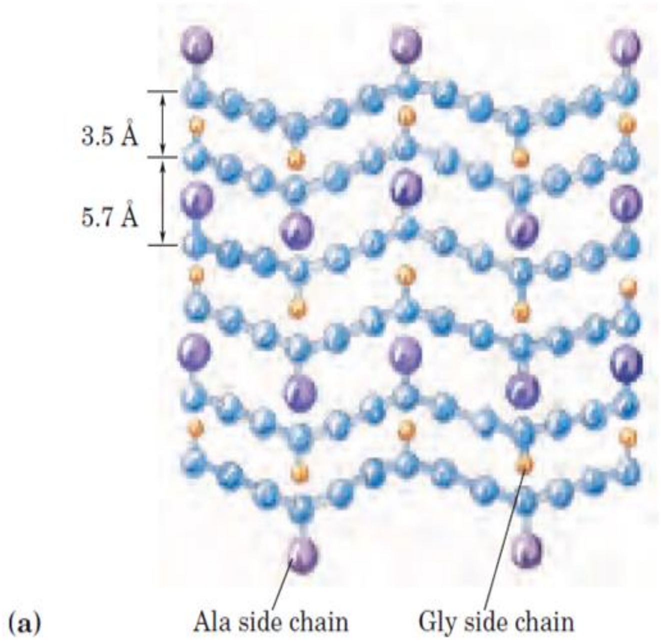

FIGURE 4–14 Structure of silk. The fibers used to make silk cloth or a spider web are made up of the protein fibroin. **(a)** Fibroin consists of layers of antiparallel β sheets rich in Ala (purple) and Gly (yellow) residues. The small side chains interdigitate and allow close packing

Globular Proteins

- Myoglobin
- Haemoglobin
- Immunoglobulin

Globular proteins

- In a globular protein, different segments of a polypeptide chain (or multiple polypeptide chains) fold back on each other.
- The folding also provides the structural diversity necessary for proteins to carry out a wide array of biological functions.
- Protein Data Bank (PDB; www.rcsb.org/pdb), an archive of experimentally determined three-dimensional structures of biological macromolecules.

Myoglobin

- It was the first protein to have its **three dimensional structure** determined by **X-ray crystallography** by John Kendrew in 1957.
- Myoglobin is a typical **globular protein** in that it is a highly folded compact structure with most of the hydrophobic amino acid residues buried in the interior and many of the polar residues on the surface.
- Myoglobin is a relatively small protein of mass 17.8 kDa made up of 153 amino acids in a single polypeptide chain.
- Myoglobin is a relatively small (Mr 16,700), oxygen-binding protein of muscle cells. It functions both to store oxygen and to facilitate oxygen diffusion in rapidly contracting muscle tissue.

Contd.

- X-ray crystallography revealed that the single polypeptide chain of myoglobin consists entirely of **-helical secondary structure**. In fact there are eight –helices (labeled A–H) in myoglobin.
- Myoglobin contains a single polypeptide chain of 153 amino acid residues of known sequence and a single iron protoporphyrin, or heme, group.
- Within a hydrophobic crevice formed by the folding of the polypeptide chain is the **heme prosthetic group**.
- This non-polypeptide unit is noncovalently bound to myoglobin and is essential for the biological activity of the protein (i.e. the binding of O_2).

3- D Structure of Myoglobin

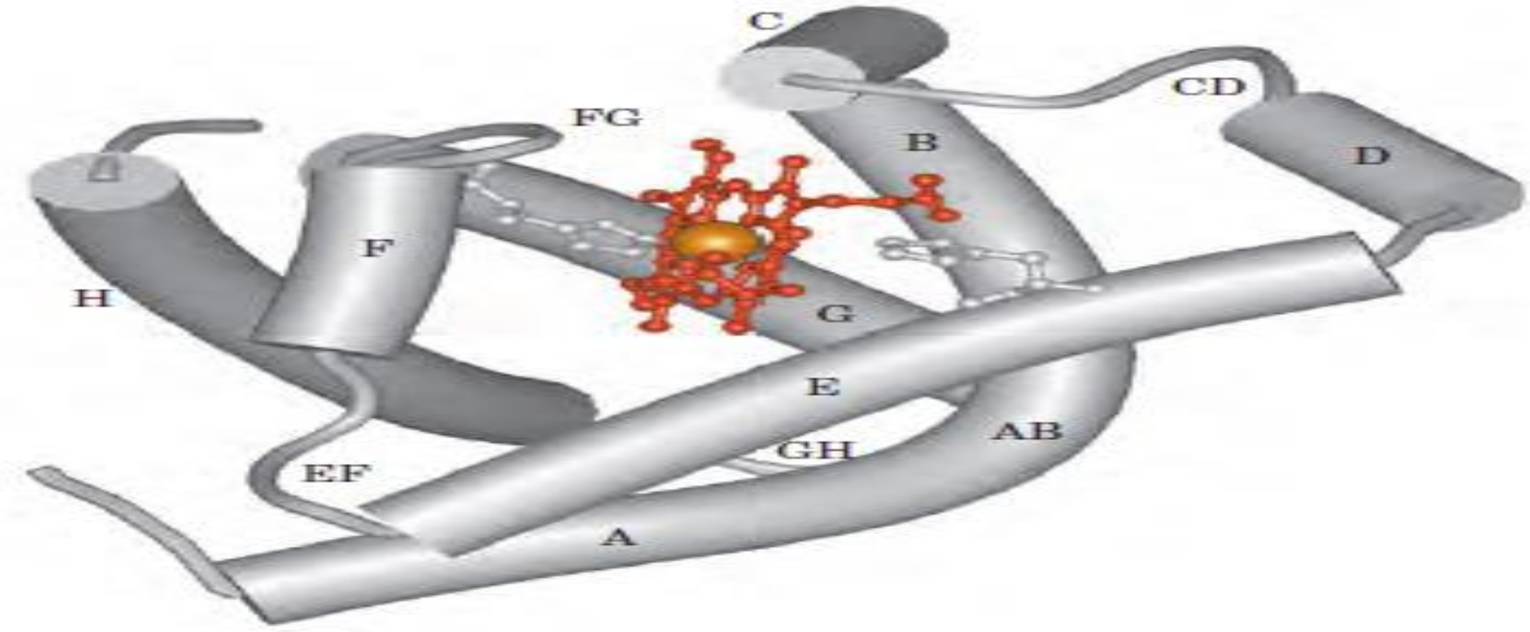

FIGURE 5–3 The structure of myoglobin. (PDB ID 1MBO) The eight α-helical segments (shown here as cylinders) are labeled A through H. Nonhelical residues in the bends that connect them are labeled AB, CD, EF, and so forth, indicating the segments they interconnect. A few bends, including BC and DE, are abrupt and do not contain any residues; these are not normally labeled. (The short segment visible between D and E is an artifact of the computer representation.) The heme is bound in a pocket made up largely of the E and F helices, although amino acid residues from other segments of the protein also participate.

- Myoglobin is abundant in the muscles of diving mammals such as the whale, seal, and porpoise, whose muscles are so rich in this protein that they are brown.
- Storage and distribution of oxygen by muscle myoglobin permit these animals to remain submerged for long periods of time.