

In non-fibrous proteins, many segments of a polypeptide chain may have  $\alpha$  helical structure as shown in Fig 9-11 for myoglobin.

The second most common secondary structure found in proteins is the  $\beta$ -pleated sheet.

There are two  $\beta$  sheet conformations referred to as parallel and antiparallel.

The parallel  $\beta$  sheet conformation results from  $\Phi = -119^\circ$  and  $\Psi = 113^\circ$  while the antiparallel  $\beta$  sheet conformation results from  $\Phi = -139^\circ$  and  $\Psi = 135^\circ$  as shown in the Ramachandran plot.

Fig 7-16 shows the H-bonding arrangement in the antiparallel and parallel  $\beta$  sheet structures.

Let's redraw these structures to show the atoms in the peptide backbone

Note that the alignment ( $C \leftarrow N$ ) of the two peptide segments in the parallel  $\beta$  sheet is the same as shown in Fig 7-16.

In the antiparallel  $\beta$  sheet, the alignment of one segment is  $C \leftarrow N$  while that of the other segment is  $N \rightarrow C$ .

In the  $\beta$  sheet, the H-bonds are approximately perpendicular to the long axis of the chain.

The antiparallel  $\beta$  sheet comprises most of the polypeptide chains in silk fibroin, the protein found in silk fiber.

In silk, the H-bonds are between polypeptide chains (interpeptide) as shown in the handout.

The sheet results from several polypeptide chains H-bonded to each other.

Sheets are closely packed on top of each other as shown in Fig 7-29 to yield a three dimensional structure.

Note that the methyl groups of ala residues on one face of a sheet are nestled between the methyl groups of ala residues on one face of a neighboring sheet.

Likewise the H atoms of gly residues on the other face of a sheet nestle between the H atoms of gly residues the other neighboring sheet.

The close packing of sheets in this manner is dependent on particular a.a. composition and sequence.

The R groups must be small to prevent steric interaction between chains in a sheet.

The following three a. a. make up ~86% of the a.a. in silk fibroin:

45% gly

29% ala

12% ser

The primary structure has long regions of the repeating sequence

$(\text{gly-ser-gly-ala-gly-ala})_n$

consistent with a composition of gly, ala and ser in the ratio of 3: 2: 1.

The sequence has the effect of placing all methyl (ala) or hydroxymethyl (ser) groups on one side of a sheet and H atoms (gly) on the other side of the sheet so that close packing of sheets can occur.

Silk fiber is thought to be less extensible than wool fiber because the polypeptide chains in the  $\beta$  sheet are nearly fully extended.

Many proteins have both  $\alpha$ -helix and  $\beta$ -sheet structures as indicated in Figs. 2-10 and 2-11, for the secondary structure of glyceraldehyde-3-phosphate dehydrogenase.

As indicated earlier, the overall structure of non-fibrous proteins are globular.

As observed for myoglobin and glyceraldehydes-3-phosphate dehydrogenase, segments of  $\alpha$ -helix and  $\beta$ -sheet are interrupted by non-helical regions.

These non-helical regions are often characterized as turns, changes in the direction of the polypeptide chain that are brought about by a particular set of three or four amino acids as described in Figs 6.18 and 6.19.

There are two types of  $\beta$  turns characterized by four amino acids in which the C=O of the first amino acid is H-bonded to the N-H of the fourth amino acid.

Note that in the Type I and Type II turns the orientation of the peptide bond between the 2<sup>nd</sup> and 3<sup>rd</sup> amino acids is different.

The third amino acid in these turns is most often a glycine residue because an amino acid with a larger R group would result in steric interactions.

The turn involves three amino acids, the second of which is proline.

In this turn, the C=O of the first amino acid is H-bonded to the N-H of the third amino acid.

Lastly consider the secondary structure characteristic of collagen.

Collagen is the major protein component of teeth, bones, cartilage, tendons and ligaments and thus the most abundant protein in vertebrates.

A single collagen molecule is composed of three polypeptide chains each with about 1000 residues.

About one third of the residues are gly and 15-30% are pro and 4-hydroxyproline (hyp).

Each polypeptide chain forms a left-handed helix characterized by  $\Phi$  and  $\Psi$  angles of  $-51^\circ$  and  $153^\circ$  respectively with  $n = 3.3$  and  $p = 10.0 \text{ \AA}$ .