Overview of Beta-Pleated Sheet Secondary Structure

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Like the α-helix, **beta-pleated sheet** (**β-sheet**) structures are a common feature of protein three-dimensional conformations and, again by analogy, the prevalence of β-beta sheets is most likely attributed to the inherent stability of these structures. Namely, the geometry of the β-beta sheet **polypeptide backbone** is such that H-bonding atoms are aligned for nearly perfect H-bond formation. Moreover, close internal packing of the backbone atoms in β-beta sheet structures serves to optimize **van der Waals interactions** and minimize energetically unfavorable **hydrophobic interactions** between nonpolar protein groups and water molecules in the environment. Collectively, these factors help reduce the net free energy of the β-beta sheet thereby increasing its stability relative to other structures.

When viewed in a wireframe representation, the basic design of the β-sheet resembles that of a pleated skirt. Typically, β-sheets are formed from several adjacent, almost fully-extended **polypeptide backbone strands** which together weave the "fabric" of the skirt. In proteins, β-sheets can be composed of **parallel**, **anti-parallel,** or mixtures of **parallel** and **anti-parallel** adjacent polypeptide segments. By convention, the orientations of adjacent strands of a β-sheet are defined by the relative ***N*** » *C* orientations of their **primary** AA sequences. For example, in parallel β-sheets the ***N*** » *C* orientations of the AA sequences of adjacent strands run in a parallel direction. Occasionally, one "isolated" segment of the polypeptide backbone of a protein will adopt either the parallel or anti-parallel β-sheet conformation itself without flanking a β-sheet strands; technically, this also counts as a "β-sheet" conformation.

The parallel and anti-parallel β-sheet conformations are very similar but differ subtly in their respective polypeptide backbone conformations and in the geometry of the H-bonds formed between adjacent β-sheet segments. However, both types of β-sheet appear to be "pleated" as the result of uniformly-spaced and parallel polypeptide backbone kinks in adjacent strands. These backbone kinks are structurally **reiterated every two residues** along the AA sequence of each segment and the kinks of adjacent segments tend to be aligned in more-or-less parallel fashion giving rise to the overall pleated appearance of β-sheet structures. The repeated backbone motif of parallel and anti-parallel β-sheet conformations classify them as protein **secondary structures**.

When viewed in spacefilling representation, where the atomic **van der Waals** radii are taken into account and each atom is viewed as "**spacefilled**" hard sphere, the backbone of the β-sheet takes on the appearance of a slightly-distorted "flat" surface or "plane" whereas the **sidechain groups** of the constituent strands emerge almost **orthogonal to the plane of the sheet** and appear to "coat" two sides of a surface created by the backbone. A particularly significant feature of the sidechain groups of **adjacent residues** in the β-sheet is that they **project on opposite sides** of the plane surface created by the β-sheet backbone. Thus, the sidechains of successive AA residues appear to alternate from one side of the sheet to the other as one moves down the peptide sequence. This feature results in structures with the sidechain groups of **every second AA residue** located on the **same side** of the sheet. Thus, the combined chemical properties of every second AA residue of the β-sheet strands define the chemical properties of side of the β-sheet.

In proteins, the sidechain groups lining one surface of a β-sheet frequently exhibit uniform chemical properties, *e.g.*, nonpolar, polar, charged, *etc*. Because the β-sheet naturally defines two surfaces, β-sheets can simultaneously make stable interaction with quite different physical environments, akin to

the α-helix.

The simple repeating structure of the β-sheet is noteworthy from a genetic standpoint because fairly minimal genetic information is needed to specify a chemically-defined, β-sheet surface.

The **minimum genetic criteria** for polypeptides to adopt the β-sheet conformation are two-fold:

1. The gene encoding a polypeptide segment must specify a linear sequence of AA residues that together will spontaneously adopt an β-sheet conformation. For example, certain AA residues or combinations of residues will interfere with or prevent proper spontaneous formation of the β-sheet.
2. The exact sequence of the encoded polypeptide segment must be organized such that every **second AA residue** conforms to the particular biological function served by a given "side" of the two β-sheet surfaces. For example, one side of the sheet may function to produce **intramolecular** interactions or **intermolecular** interactions stabilizing a protein's overall three-dimensional conformation whereas the opposite side of the same β-sheet surface may interact with the aqueous environment surrounding a protein
3. Finally, the intervening polypeptide backbone between two β-sheet strands must be such that adjacent β-sheet strands are suitably oriented to form β-sheet.

In contrast to the β-sheet conformation, it seems intuitively logical that considerably more genetic information would be required in order to create similar physical surfaces from "irregular" polypeptide sequences. For example, an "irregular" polypeptide sequence would have be longer (i.e., require more genetic code) in order position the same group of AA sidechains in the same spatial orientations as produced with an β-sheet.

In summary, the statistical prevalence of β-sheet segments in proteins stems not only from their inherent structural stability but also from the economy of genetic information required to encode the biologically functional surfaces presented by a β-sheet.

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