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COLLEGE ON BIOPHYSICS: FROM MOLECULAR GENETICS TO STRUCTURAL BIOLOGY

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PROTEIN STRUCTURE AND FUNCTION:

An Introduction

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These are preliminary lecture notes, intended only for distribution to participants.









































Secondary structure = local regular conformations of the backbone











The beta sheet is held by back bone H-bonds

- The chain is elongated and the H/bonds form between sequentially distant amino acids.
- The H-bonds are the same as in α -helices:

 The sequence of the strands ("β-strands") is either parallel or antiparallel









Recognition of secondary structures: 3. H-patterns

- Recognize H-bonds by energy/geometry calculation
- A turn is a single H-bond between residues *n* and and *n*+*i*, *i*=3,4,5
- An α-helix is a series of 4-turns, 3/10 helix is a 3-turn.
- A bridge is a series of 3 H-bonds, between I-1, i, i+1, and j-1, j, j+1, respectively, parallel, or antiparallel
- β-sheets are series of bridges..

Kabsch-Sander approach, basis of most current methods.



Tertiary structure is the 3-D or space structure

The units of 3-d structures are the "folds" - these are independent structures, typically 50-200 aa long, one protein chain may contain several of these that may form "domains"..

A fold consist of α -helices and/or β -strands (sheets) and motifsbuilt up of these (e.g. β -hairpin-, β - α - β - and helix-loop-helix elements). Folds are connected usually via noncovalent bonds, often between side-chains.























