



Protein Structure

Conformational Structure How does the polypeptide chain fold?

- 1) primary structure sequence of amino acids
- 2) secondary structure small units of repetitive structure
- 3) tertiary structure overall 3D shape
- 4) quaternary structure shape of ≥2 chains



Protein Structure-Secondary

The 4 S's for secondary structure:

Size-dependent on number of amino acidsSolubility-dependent on AA composition and shapeStability-complex and not well understoodShape

Why is there Secondary Structure?



Secondary Structure

Protein Structure-Secondary



In the early 1950's, Linus Pauling and Robert Corey predicted some rules that proteins should follow to find the lowest energy conformation.

- 1) The peptide bond must be planar without free rotation
- 2) The degree of H-bonding should be maximized to achieve the lowest energy state
 (unfolded)^{water} ⇒ (folded)^{water} transition]
- 3) The best H-bonds are linear
- 4) There should be repeating units of conformation (same) as you go from one residue to the next

Using these rules they predicted two basic structures: α-helix β-sheet

Protein Structure-Secondary



Kendrew (1917 - 1997)

There were no known protein structures until 1957, when Kendrew solved the structure of myoglobin:

Imagine the excitement when indeed there were the very helices Pauling predicted!

Iron atom













Residue P_{α} Propensition Ala 1.42 \Box Arg 0.98 \Box Asn 0.67 \neg prefer small, medium, hydrop Asp 1.01 \neg mo steric hindrance at C_{β} Cys 0.70 \neg Glu, Met, Ala, Leu, Lys, Phe, Glu 1.51 \bigcirc Gly 0.57 \neg Pro His 1.00 $-$ Pro Leu 1.21 \bigcirc Wet 1.45 \bigcirc Phe 1.13 \bigcirc Pro 0.57 \bigcirc Ser 0.77 \bigcirc	Table 6-1	Propensities of Amino Acid Conformations	Resid	lues for α Helical I NE α HEIIX:
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Residue	Ρα		Propensities
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Ala	1.42	0	Like [.]
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Arg	0.98	-	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Asn	0.67		-prefer small, medium, nydrophobic/cha
Cys 0.70 -Glu, Met, Ala, Leu, Lys, Phe, Gin 1.11 -Giu -Giu, Met, Ala, Leu, Lys, Phe, Giu 1.51 -Giu Don't Like: Giv 0.57 -Pro His 1.00 -Glu Ile 1.08 -Pro Leu 1.21 -Glu Met 1.45 -Glu Phe 1.13 -Pro Ser 0.77 -Glu	Asp	1.01		-no steric hindrance at C_{β}
Gin 1.11 Glu 1.51 Glv 0.57 His 1.00 Ile 1.08 Leu 1.21 Lys 1.16 Met 1.45 Pro 0.57 Ser 0.77	Cvs	0.70		-Glu Met Ala Leu Lvs Phe Gln
Glu 1.51 Don't Like: Gly 0.57 -Pro His 1.00 -Gly Leu 1.21 -Gly Lys 1.16 -Gly Phe 1.13 -Gly Pro 0.57 Ser 0.77	Gin	1.11	0	
Gly 0.57 -Pro His 1.00 -Gly Ile 1.08 -Gly Leu 1.21 - Lys 1.16 - Phe 1.13 - Pro 0.57 - Ser 0.77 -	Glu	1.51	÷	Don't Like:
His 1.00 -Gly Ile 1.08 -Gly Leu 1.21 Lys 1.16 Phe 1.13 Pro 0.57 Ser 0.77	Gly	0.57		-Pro
Ile 1.06 -Gily Leu 1.21 - Lys 1.16 - Met 1.45 - Phe 1.13 - Pro 0.57 - Ser 0.77 -	His	1.00		
Leu 1.21 Lys 1.16 Met 1.45 Phe 1.13 Pro 0.57 Ser 0.77	lle	1.08		-Gly
Lys 1.16 Met 1.45 Phe 1.13 Pro 0.57 Ser 0.77	Leu	1.21	4	
Met 1.45 Phe 1.13 Pro 0.57 Ser 0.77	Lys	1.16		T
Phe 1.13 Pro 0.57 Ser 0.77	Met	1.45	0	
Pro 0.57 Ser 0.77	Phe	1.13		
Ser 0.77	Pro	0.57		
	Ser	0.77		
Thr 0.83	Thr	0.83		C.A.
Trp 1.08	Trp	1.08		
Tyr 0.69	Tyr	0.69		Dra has fixed 4 CC
Val 1.06 PTO has lixe	Val	1.06		Pro has fixed $\varphi = -00$











































Protein Structure-Secondary							
The β Sheet: examples							
Fibrous Proteins: Silk fibroin (β -keratin)							
Silk all parallel β-sheet Sequence repeats:							
(GAGAGSGAAG(<mark>SGAGAG)₈Y)_{X (x>10)}</mark>							
 Gly is every-other residue, and Ala as well Recall the alternating R-groups Therefore, Gly is all on one side of sheet, and Ala on the other side of sheet 							













Protein Structure-Secondary									
	Structure	¢	Ψ	Rise (Dist/residue) (Å)	Residues/ Repeat	Pitch (Distance/repeat) (Å)	Diameter (Å)		
	α -helix	-57	-47	1.5	3.6	5.4	5.0		
	Anti- ដ β-sheet	-139	+135	3.4	2	6.8	-		
	Parallel ⇒ β-sheet	-119	+113	3.2	2	6.4	-		
	β -turn-Type I				4	0	-		
	<i>i</i> + 1	-60	-30	-					
	<i>i</i> + 2	-90	0	-					
	β -turn-Type II		<u> </u>		4	0	-		
	i+1	-60	120	-					
	i + 2	80	0	-					
	Start and s	top with	same a	ingles					









Protein Structure What is happe	-Secondary ening?						
 Different pieces of 2° structure are mixing together. 							
 These are called "Motifs" or Super-secondary Structures 							
 What are the structures an 	d names of some of						
the most common motifs?	βαβRossmann Fold						
	 β-hairpin 						
	• αα						
	 Greek key 						
	 β-meander β-barrel αβ-barrel 						

































