

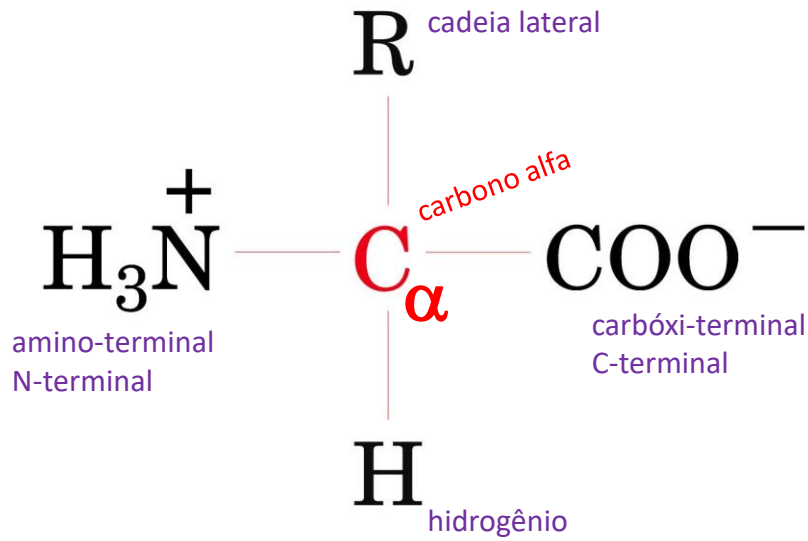
Bioinformática I

Estrutura Secundária

Profa. Dra. Iñez Caracelli

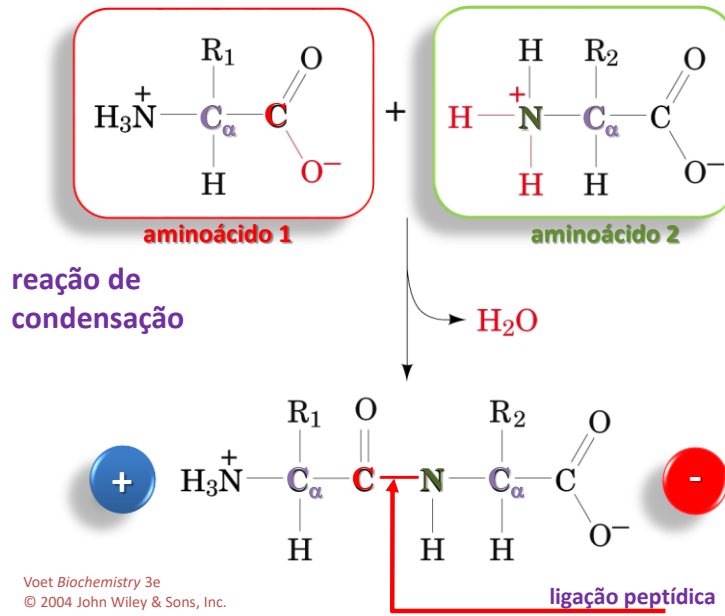
bit.603@gmail.com

O aminoácido em sua forma ionizada forma zwitteriônica

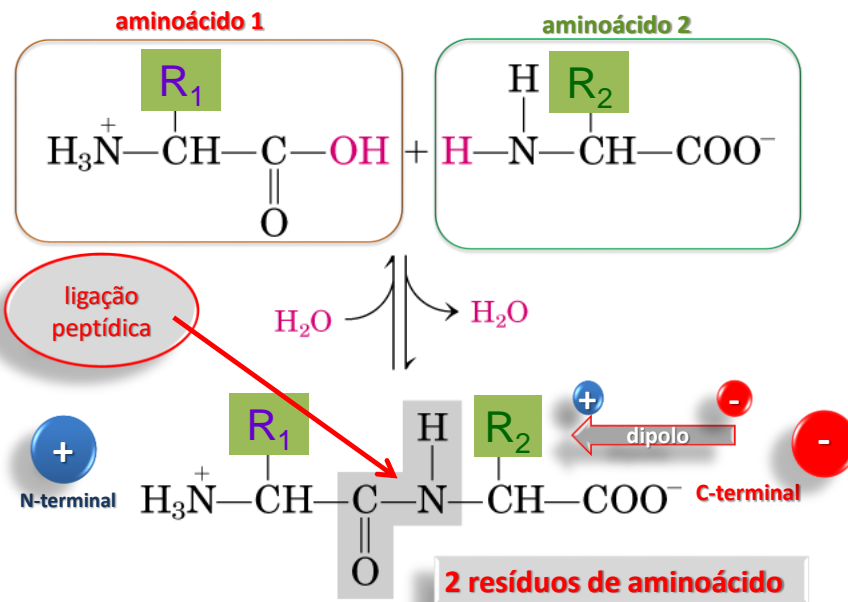


Voet Biochemistry 3e
© 2004 John Wiley & Sons, Inc.

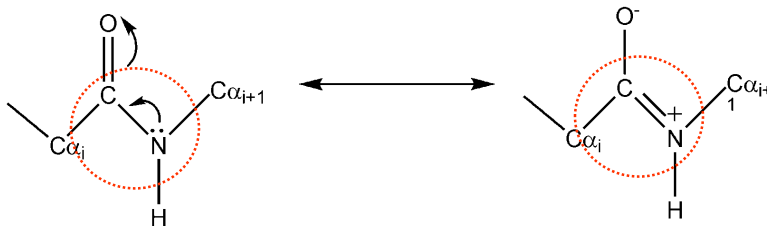
Ligação peptídica



A ligação peptídica



A ligação peptídica

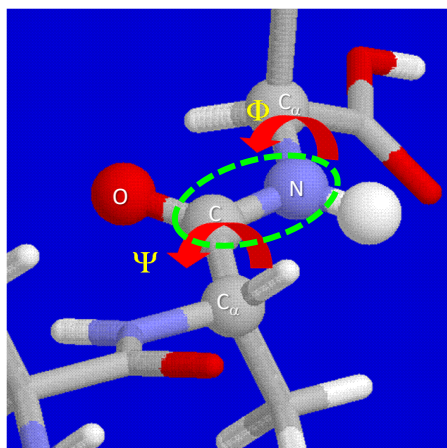


C — N 1,49 Å
C = N 1,27 Å

ligação peptídica
C — N 1,32 Å

A ligação peptídica

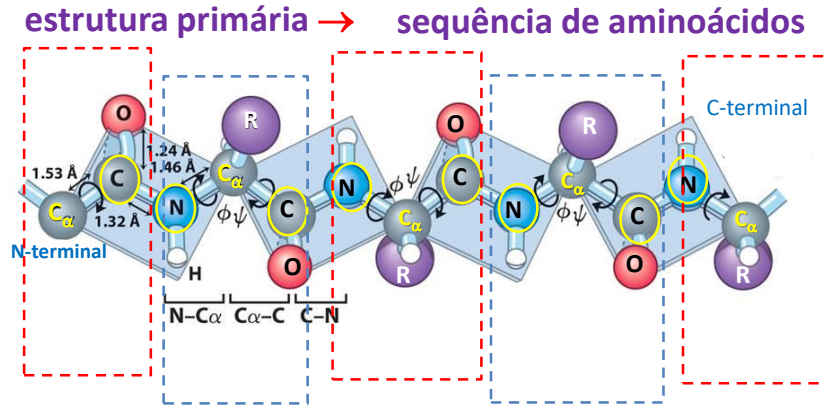
ligação peptídica → estrutura primária



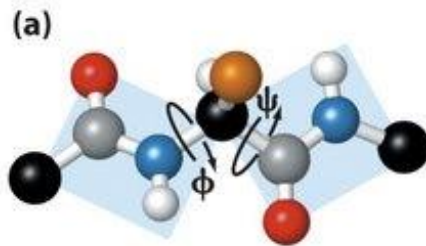
ângulos de
conformação ϕ e ψ

C — N 1,32 Å

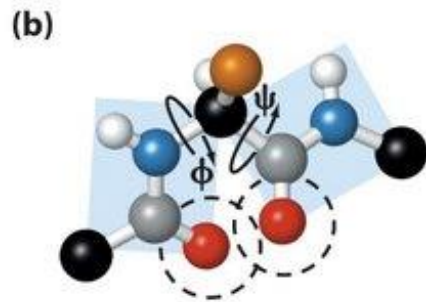
A ligação peptídica



Estrutura Primária

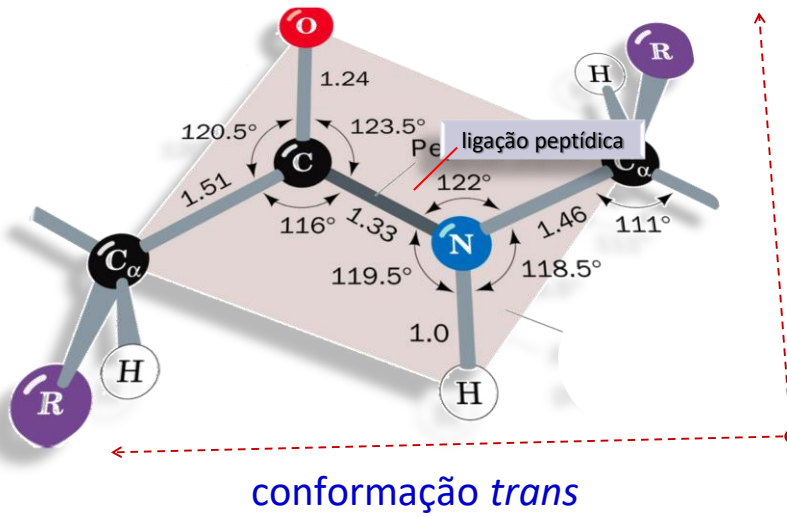


Os ângulos ϕ (phi) e ψ (psi) têm “livre” rotação

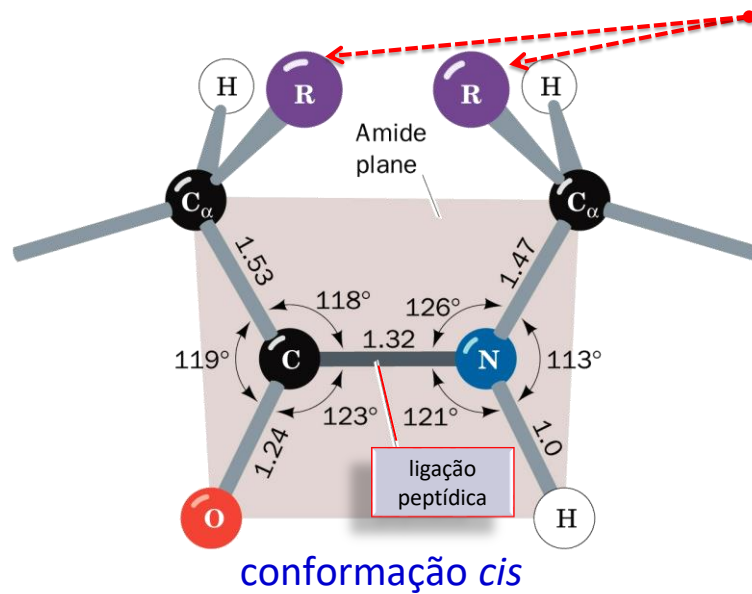


- α -carbon
- Carbonyl carbon
- Hydrogen
- Nitrogen
- Oxygen
- Side chain

A ligação peptídica

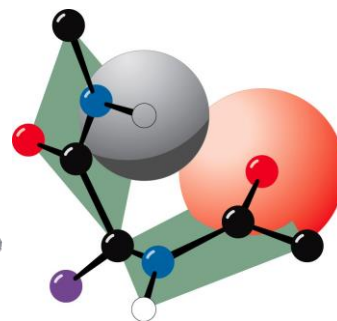
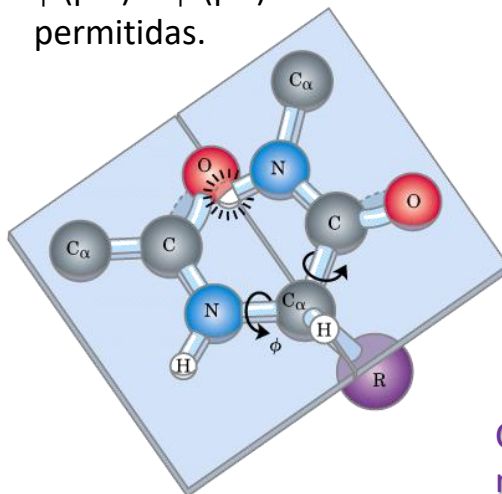


A ligação peptídica



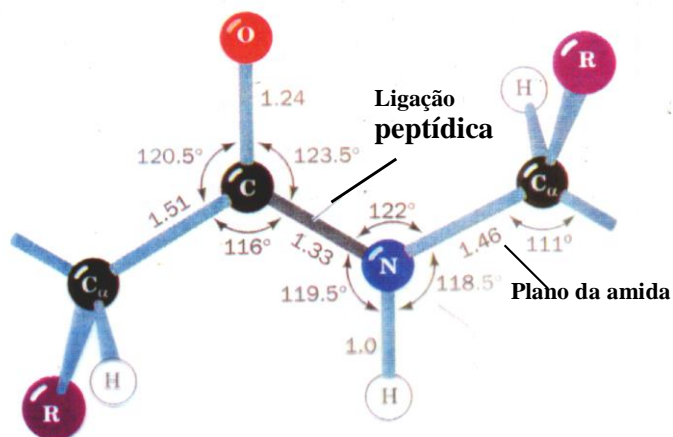
Estrutura Primária

Algumas combinações dos ângulos ϕ (phi) e ψ (psi) não são permitidas.



Colisões estéricas não-favoráveis

O grupo peptídico

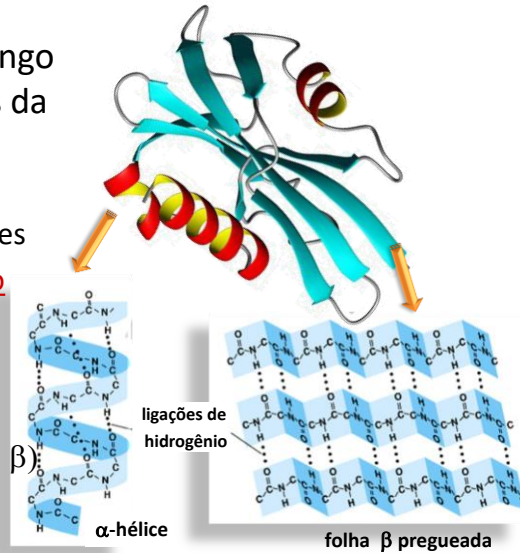


Estrutura secundária das proteínas

“folding local”

enovelamento ao longo de pequenas seções da cadeia polipeptídica

- interação entre aminoácidos adjacentes
- ligações de hidrogênio entre grupos R
 - α -hélice
 - folha β (constituída de fitas β)



Estrutura Secundária

- hélice alfa
- fita beta → folha beta
- “turns”



Estrutura Secundária: hélice α

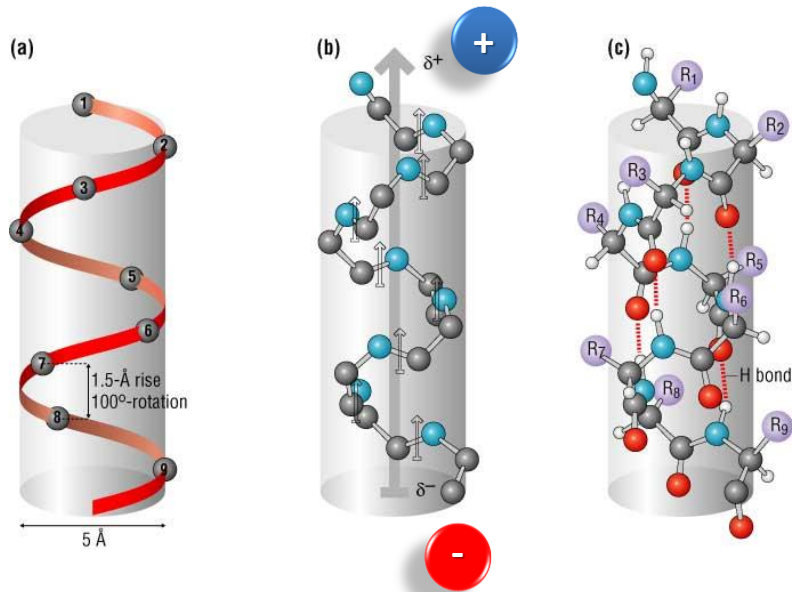
hélice α

3,6 aminoácidos por volta
 passo = 5.4 Å
 1 Å = 10^{-10} m

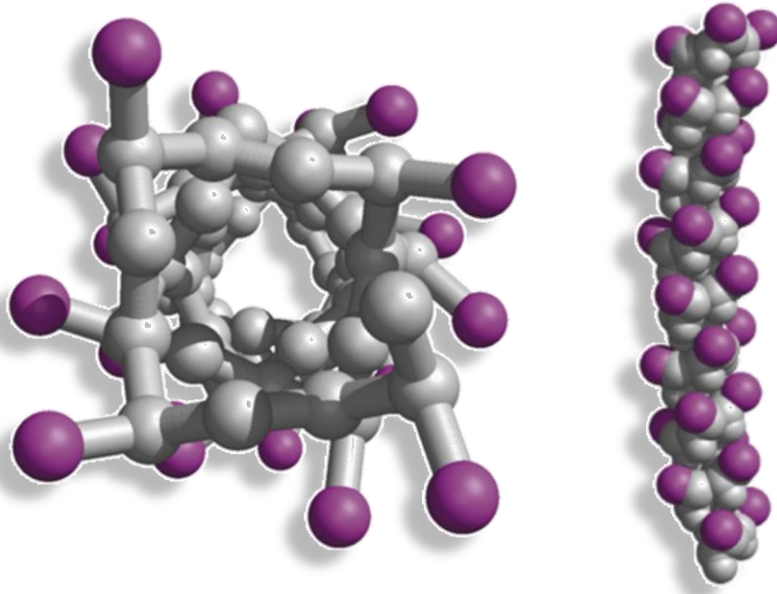
grupos-R → para fora

ligações de H entre
 (1) C=O...H-N (4)

Estrutura Secundária: hélice α



Estrutura Secundária: hélice α

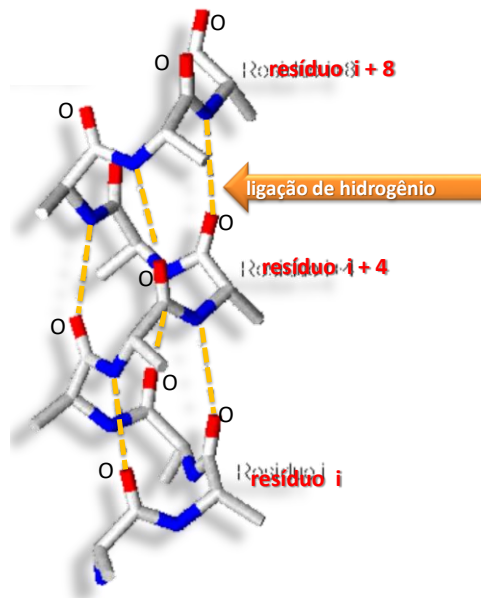


Estrutura Secundária: hélice α

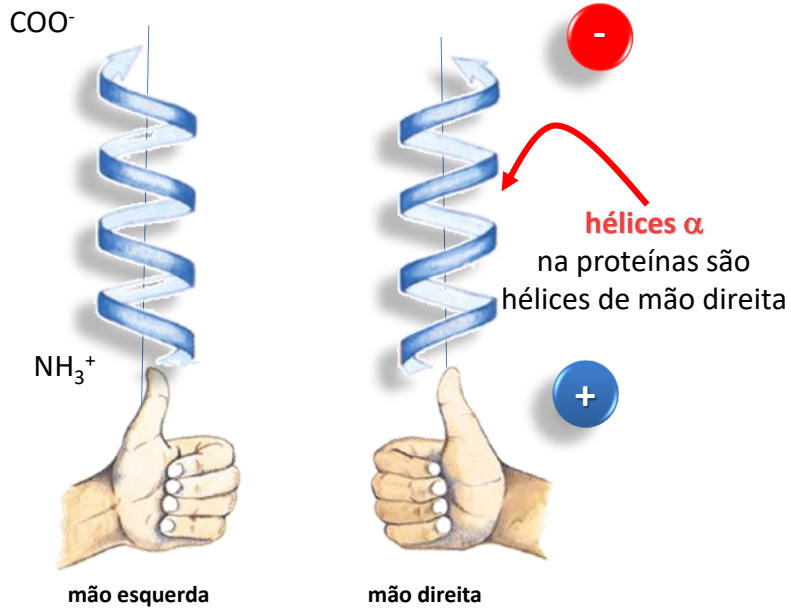
hélice alfa de mão direita

a ligação de hidrogênio está representada por linhas pontilhadas

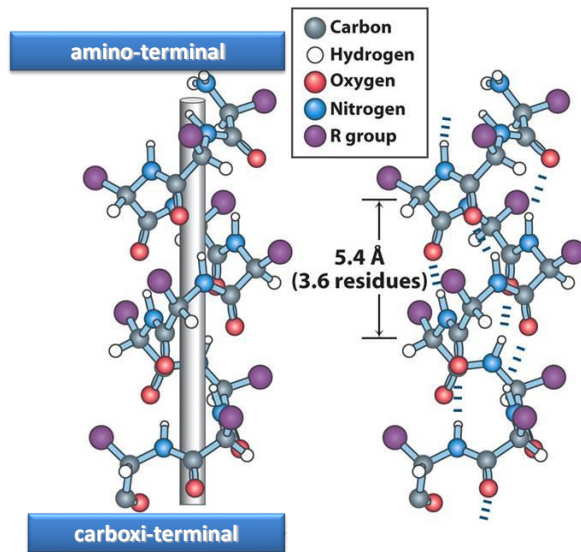
as ligações de hidrogênio ocorrem dentro de uma sequência de resíduos de aminoácidos



Estrutura Secundária: hélice α

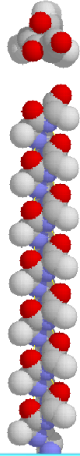


Estrutura Secundária: hélice α



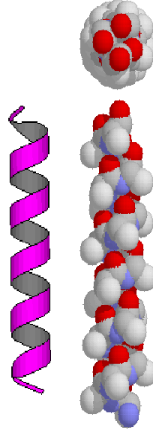
Estrutura Secundária: hélices

Hélice 3_{10}



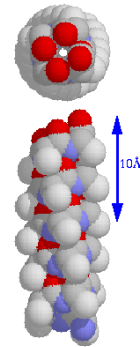
3,0 aa/volta
passo = 4,8Å

Hélice α



3,6 aa/volta
passo = 5,4 Å

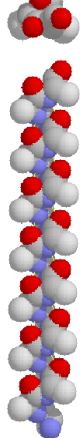
Hélice π



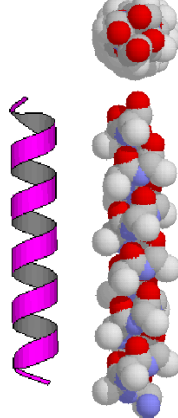
4,0 aa/volta
passo = 6,0 Å

Estrutura Secundária: hélices

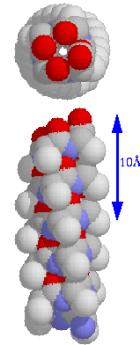
Hélice 3_{10}



Hélice α



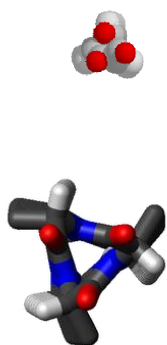
Hélice π



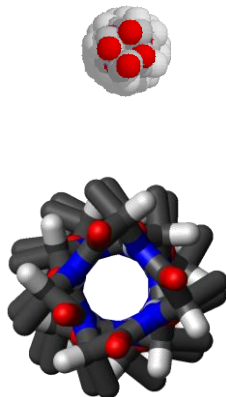
Conformation	Phi	Psi	Omega	Residues per turn	Translation per residue
Alpha helix	-57	-47	180	3.6	1.5
3-10 helix	-49	-26	180	3.0	2.0
Pi-helix	57	-70	180	4.4	1.15

Estrutura Secundária: hélices

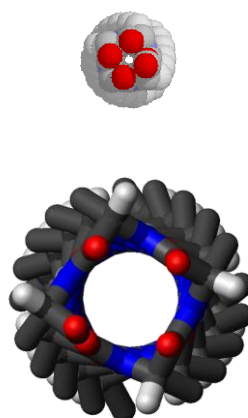
Hélice 3_{10}



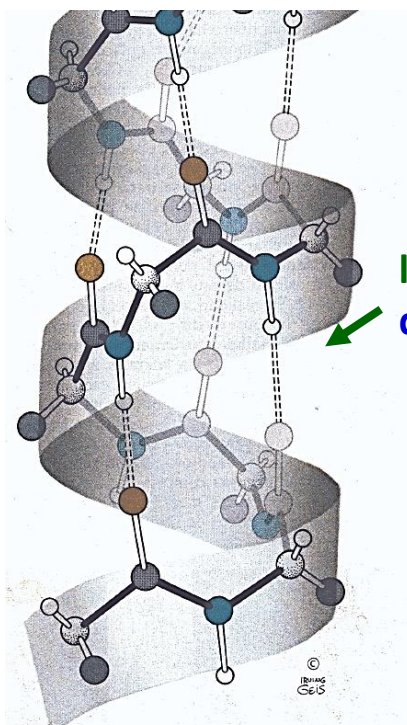
Hélice α



Hélice π



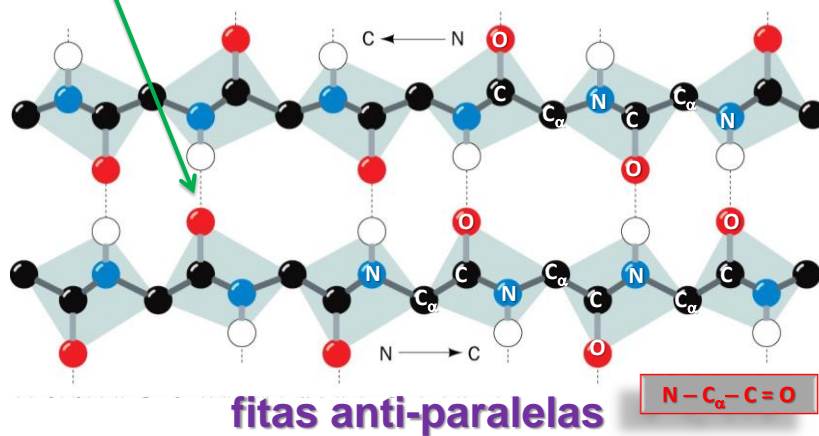
Estruturas Secundárias: hélice α



ligação de hidrogênio
dentro da mesma hélice

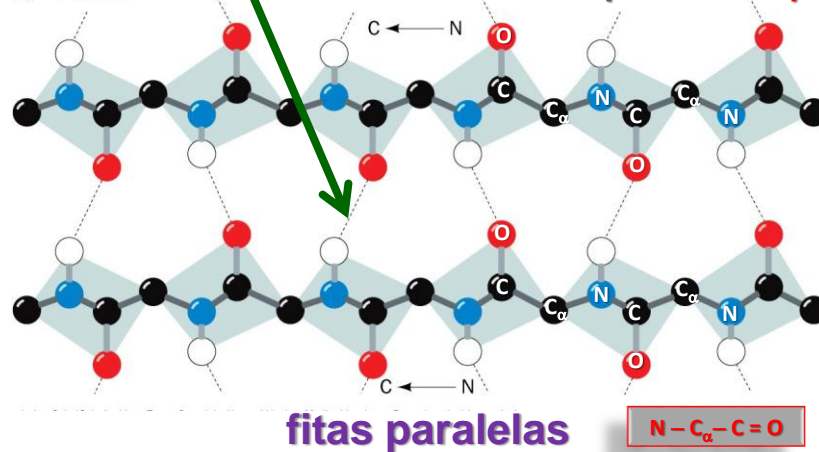
Estruturas Secundárias: folhas β

ligação de hidrogênio (entre fitas $\beta \rightarrow$ folha β)



Estruturas Secundárias: folhas β

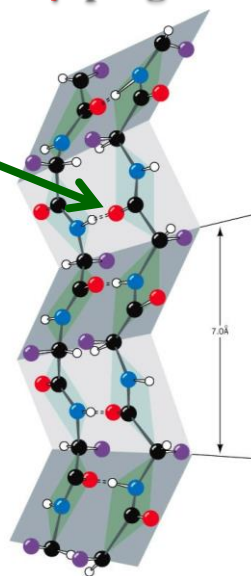
ligação de hidrogênio (entre fitas $\beta \rightarrow$ folha β)



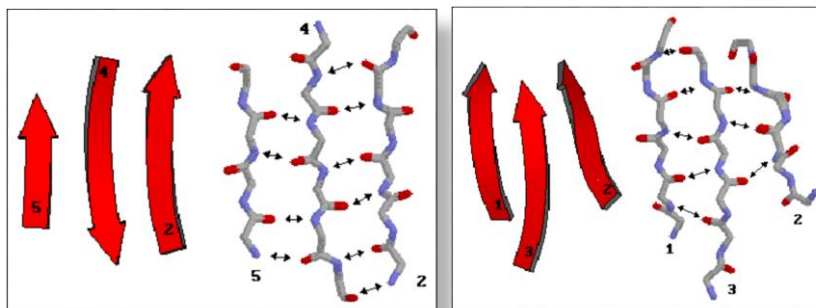
Estruturas Secundárias: folhas β pregueadas

ligação de hidrogênio
(entre fitas $\beta \rightarrow$ folha β)

fitas anti-paralelas



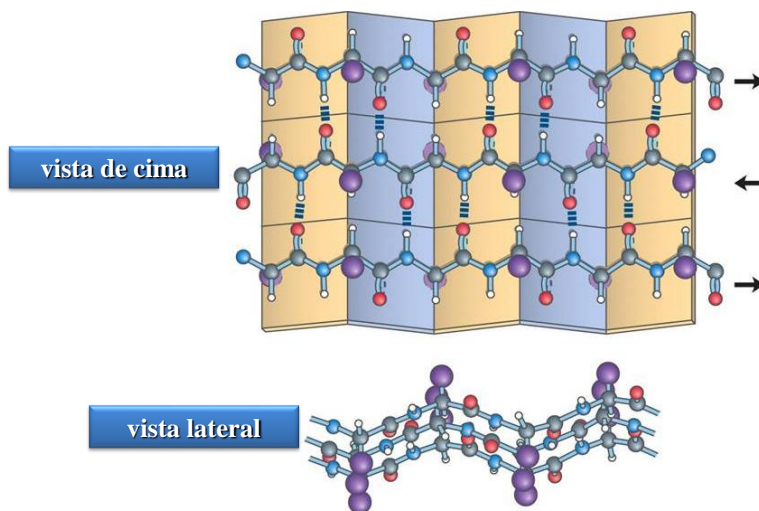
Folha β : paralelas e antiparalelas



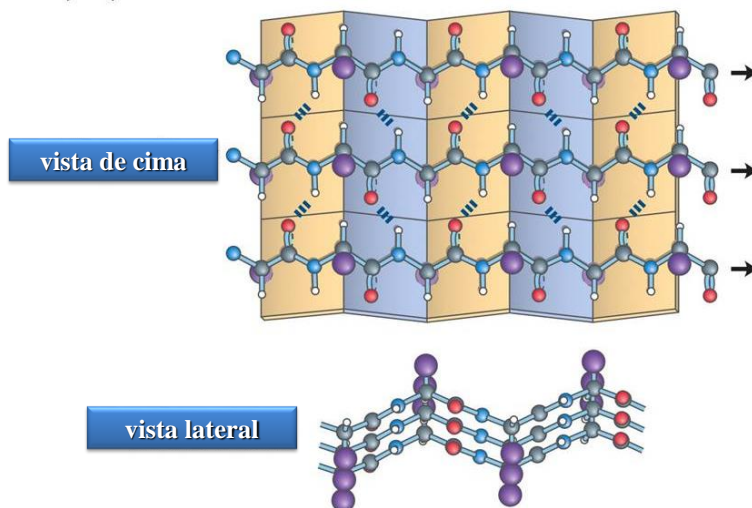
antiparalelas

paralelas

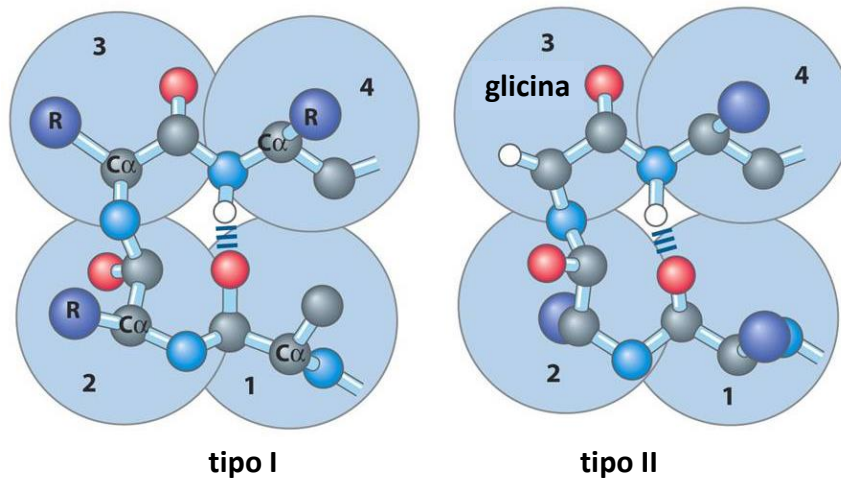
Estruturas Beta Anti-paralelas



Estruturas Beta Paralelas

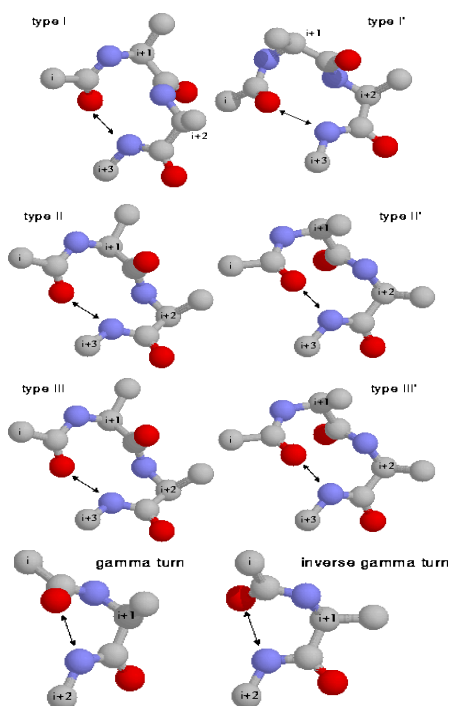


Estruturas "β turns"

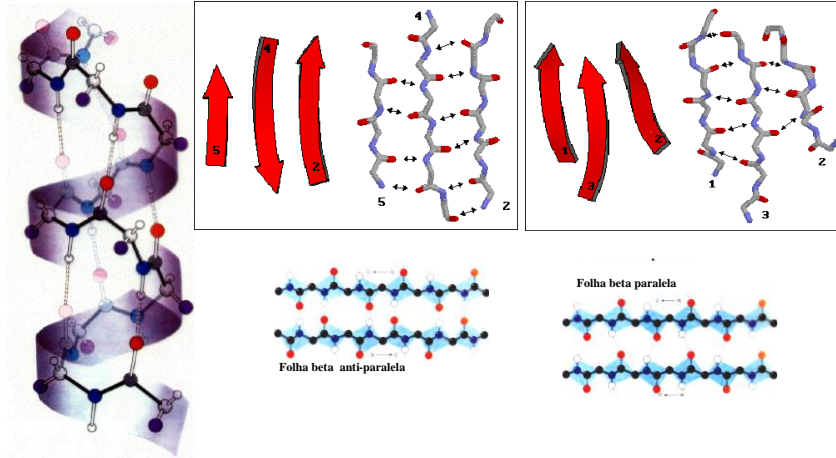


Lehninger Principios de Bioquímica
David L. Nelson y Michael M. Cox

Estruturas "turns"



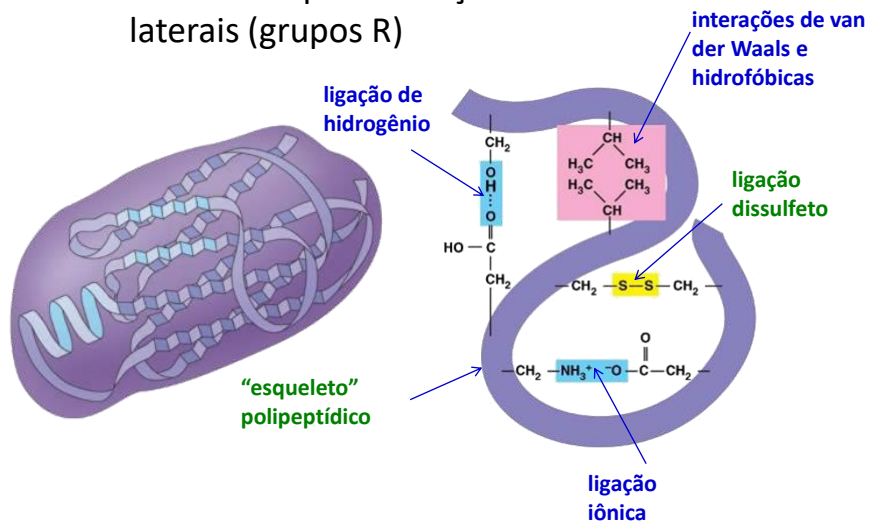
Principais Elementos de Estrutura Secundária



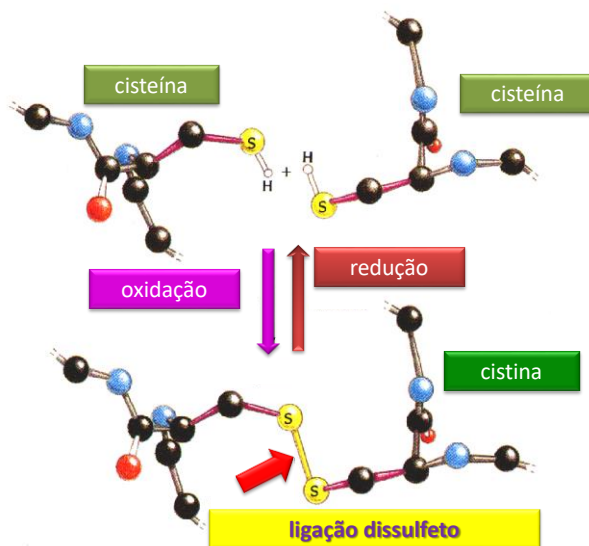
Estrutura Terciária

“Folding global”

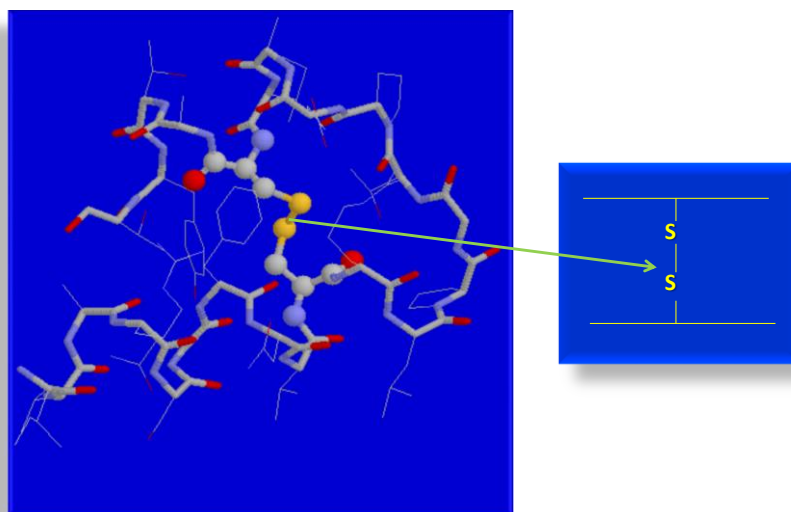
determinada por interações entre as cadeias laterais (grupos R)



A ligação dissulfeto



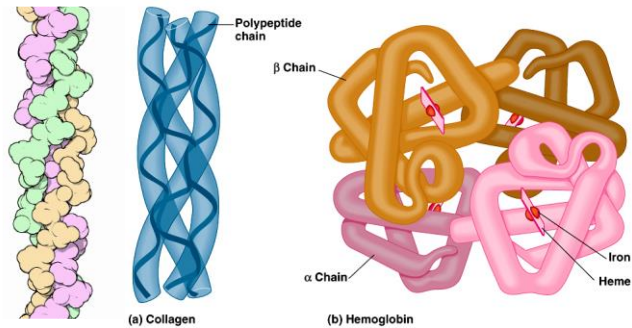
A ligação dissulfeto



Estrutura quaternária

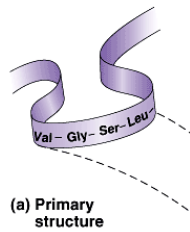
- Mais que uma cadeia polipeptídica
juntas por
– interações fracas

colágeno



hemoglobina

Estrutura de Proteínas (review)

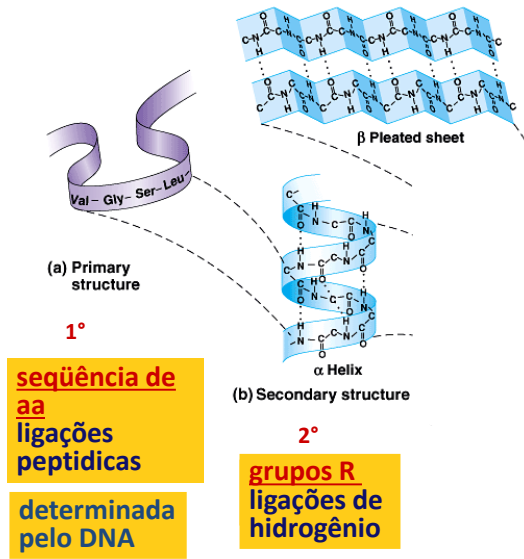


1°

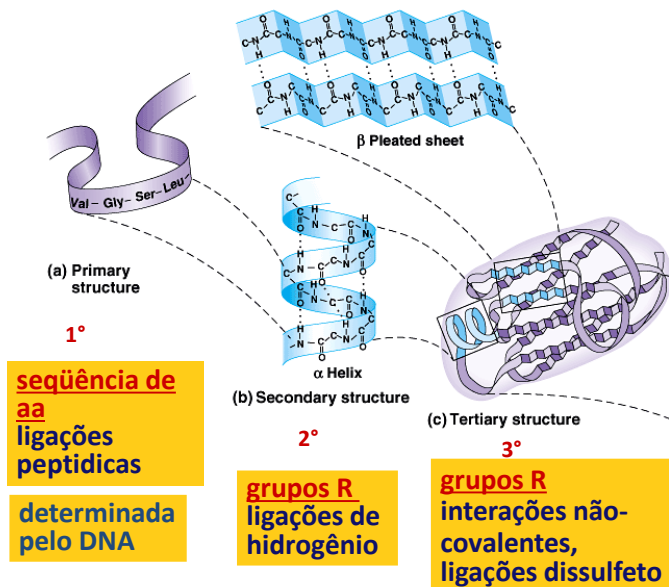
seqüência de
aa
ligações
peptídicas

determinada
pelo DNA

Estrutura de Proteínas (review)

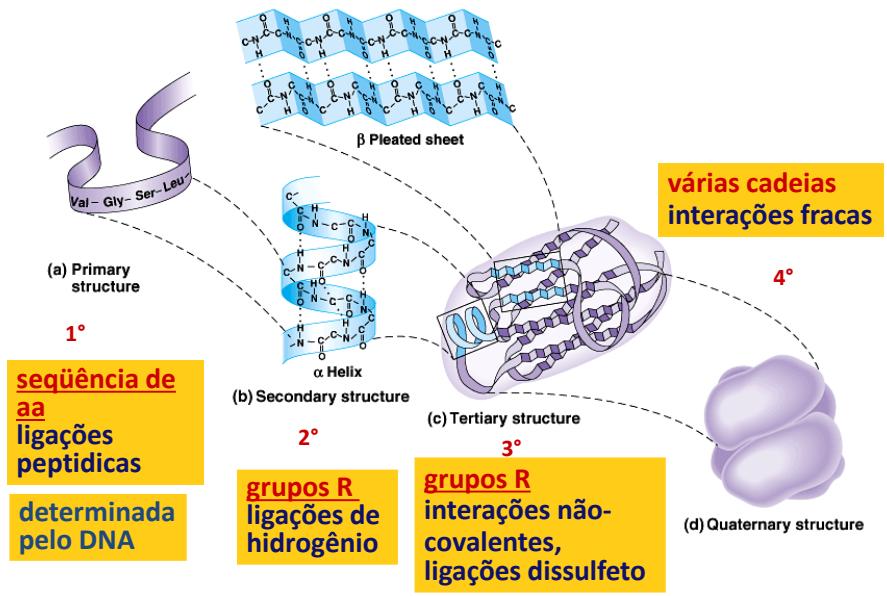


Estrutura de Proteínas (review)

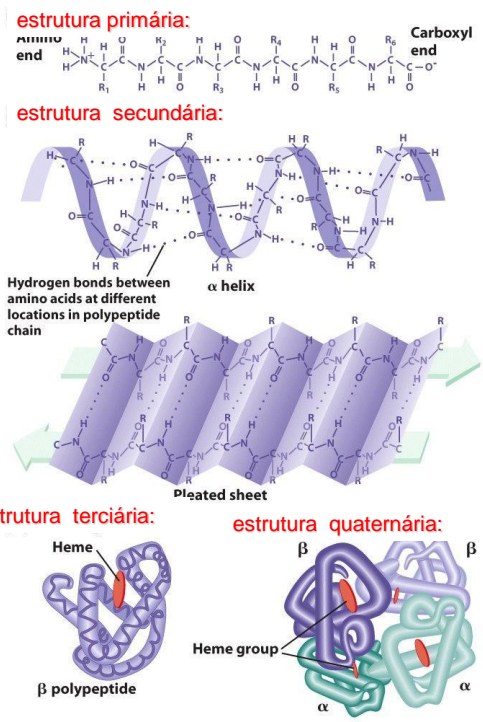


Estrutura de Proteínas (review)

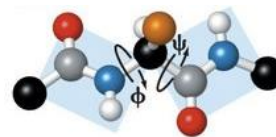
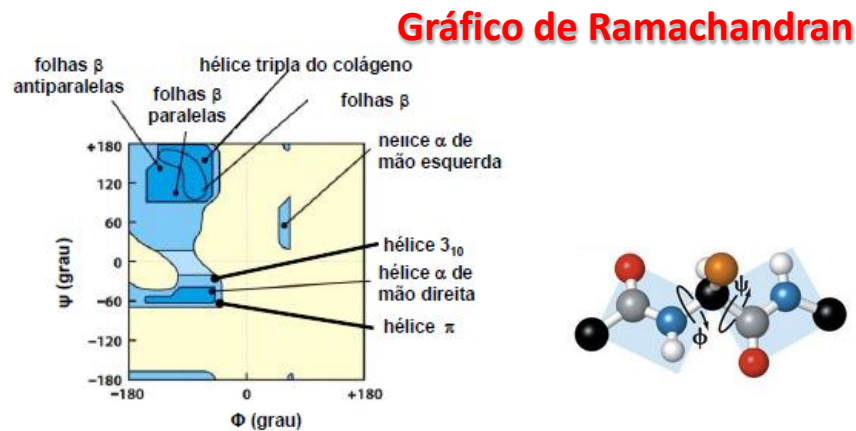
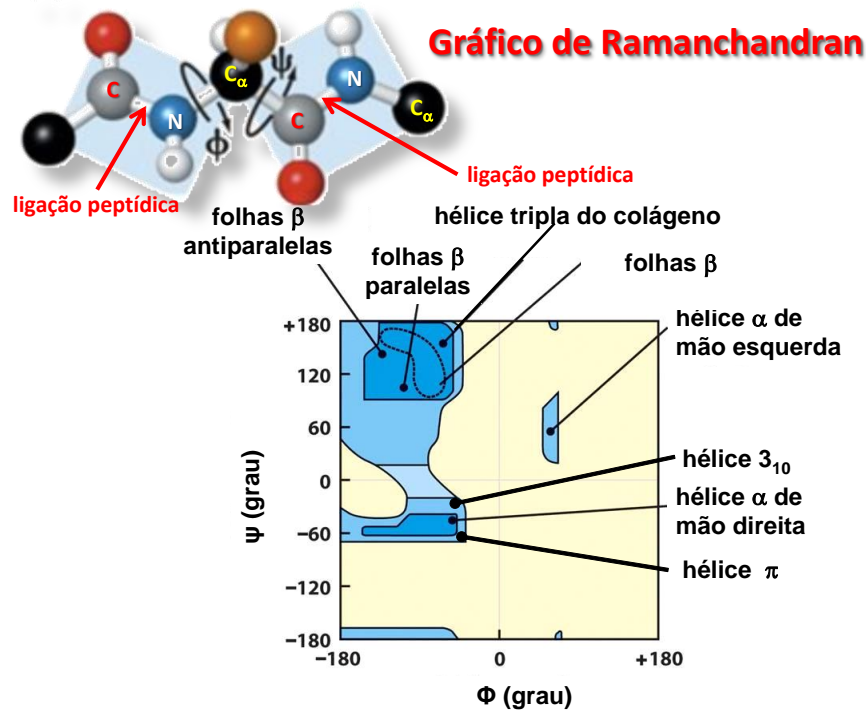
UFPA BIT 768 BIOINFORMÁTICA I   Ignéz Caracelli & Julio Zukerman



Níveis estruturais nas proteínas



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Estrutura Secundária	ϕ ($^{\circ}$)	ψ ($^{\circ}$)
hélice α de mão direita (α)	-57	-47
folha β pregueada paralela ($\uparrow\uparrow$)	-119	113
folha β pregueada anti-paralela ($\uparrow\downarrow$)	-139	135
hélice de mão direita 3_{10} (3)	-49	-26
hélice de mão direita π (π)	-57	-70
colágeno (C)	-51	153
hélice α de mão esquerda (α_L)	57	47

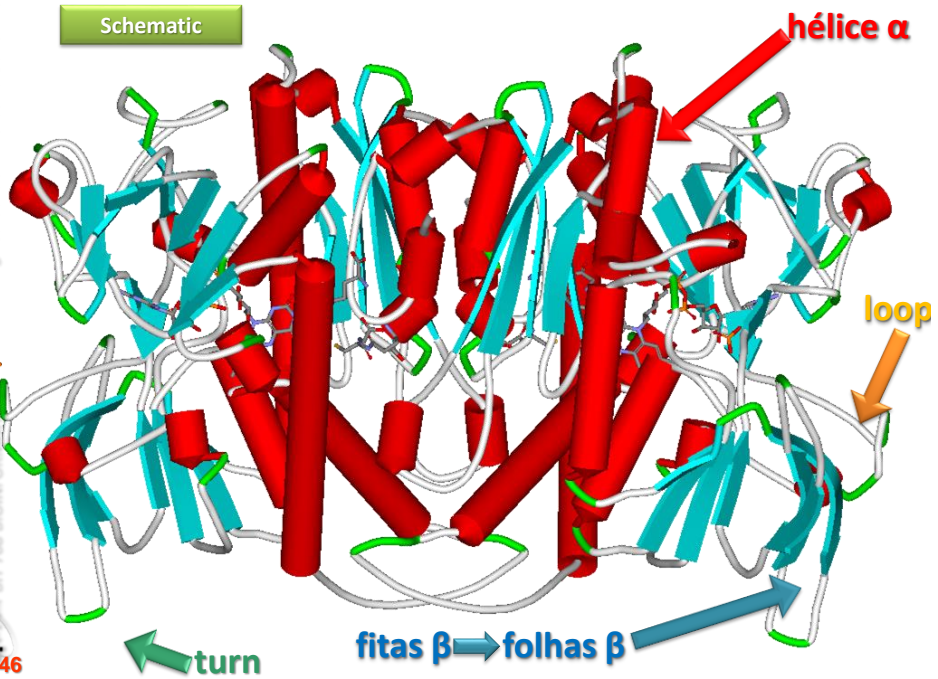
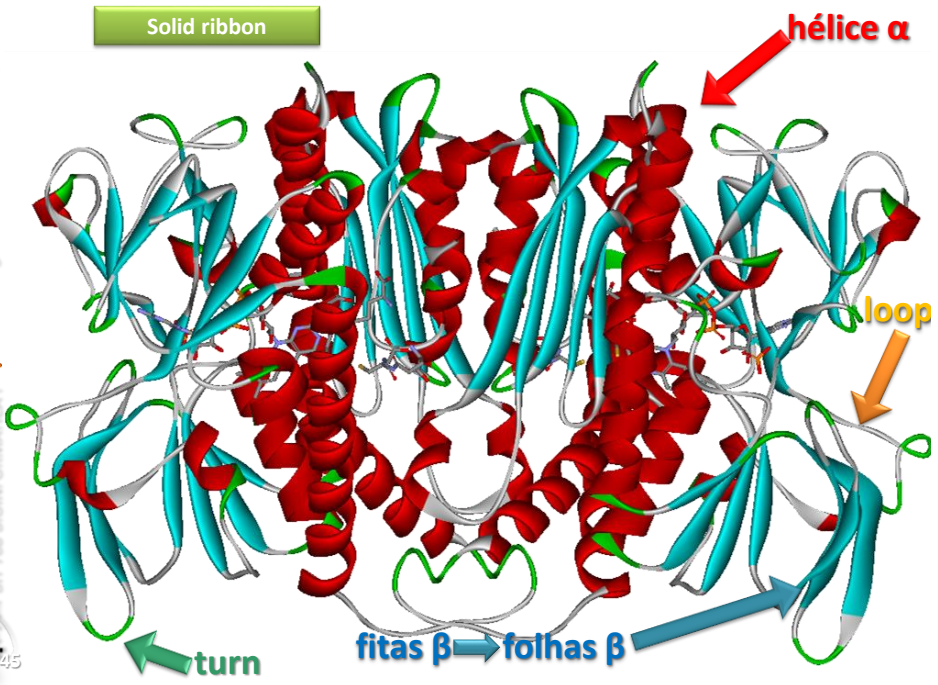
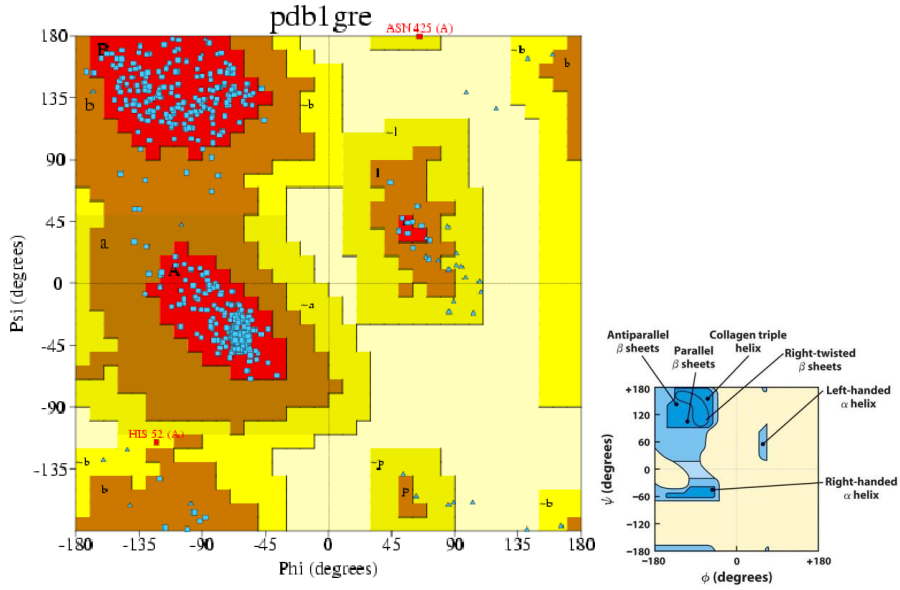



Gráfico de Ramachandran

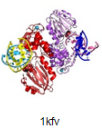


<http://www.ebi.ac.uk/pdbsum/>

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 1ktv

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PDBsum

PDB code (4 chars) Example: "1ktv" 

PDBsum provides an at-a-glance overview of every macromolecular structure deposited in the Protein Data Bank (PDB), giving schematic diagrams of the molecules in each structure and of the interactions between them.

Text and sequence searches

Text search
Scans all TITLE, HEADER, COMPND, SOURCE and AUTHOR records in the PDB (eg to find a given protein by name).

Search by sequence
Perform FASTA search vs all sequences in the PDB to get a list of the closest matches.

Notes

You can use the **Generate** option on the left to submit your own structure and get a password protected PDBsum analysis generated for it.

The development of PDBsum has been partly funded by the [Wellcome Trust](#)

Contents

PDBsum contains 74,767 entries, including 1,551 superseded
 Last update: 20 March, 2011

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- EC-POB**
Enzyme 3D structures organized by the E.C. numbering hierarchy.
- DrugPort**
Structures of drugs and their target proteins in the PDB.
- S&S**
Searches sequence against all PDB sequences and structurally annotates alignment.
- ProFunc**
Prediction of protein function from 3D structure.
- Arch Schema**
NEW Graphs of protein sequences having related Plam domain architectures.

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PDBsum Go to PDB code:

[Top page](#) | [Protein](#) | [Ligands](#) | [Prot-prot](#) | [Links](#)

Oxygen transport PDB id: **1hbs**



PDB id: 1hbs [Links](#)

Name: Oxygen transport

Title: Refined crystal structure of deoxyhemoglobin s. I. Restrained least-squares refinement at 3.0-angstroms resolution

Structure: Hemoglobin s (deoxy) (alpha chain). Chain: a, c, e, g. Engineered: yes.
Hemoglobin s (deoxy) (beta chain). Chain: b, d, f, h. Engineered: yes

Source: Homo sapiens. Human. Organism_taxid: 9606. Organism_taxid: 9606

Biol. unit: Tetramer (from PQS)


Resolution: 3.00Å **R-factor:** 0.254

Authors: E.A.Padlan,W.E.Love

Key ref: E.A.Padlan and W.E.Love (1985). Refined crystal structure of deoxyhemoglobin S. I. Restrained least-squares refinement at 3.0-A resolution. *J Biol Chem*, 260, 8272-8279. **PubMed id:** 4008491

Date: 02-Jun-82 **Release date:** 29-Jul-82

PROCHECK



Headers

References

Contents

- Protein chains
 - A 141 a.a.
 - B 146 a.a.
- Ligands
 - HEM x8

* Residue conservation analysis

Protein chains [P69905 \(HBA_HUMAN\) - Hemoglobin subunit alpha](#)

Seq:  142 a.a.
 Struc:  141 a.a.

Protein chains [P69871 \(HBB_HUMAN\) - Hemoglobin subunit beta](#)

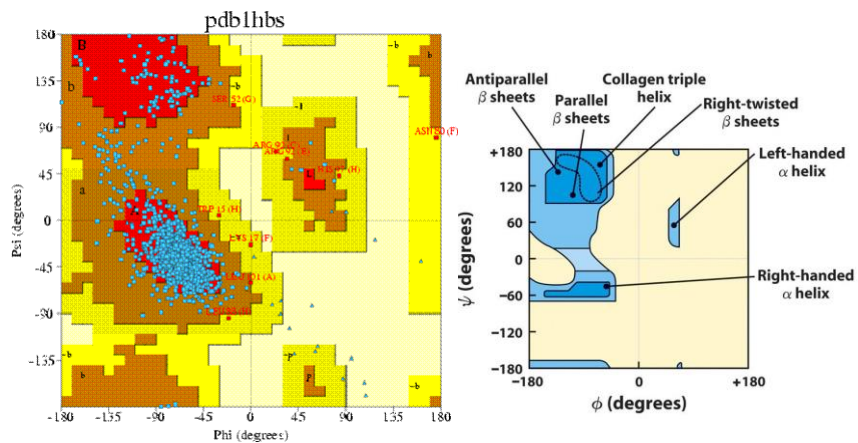
Seq:  147 a.a.
 Struc:  146 a.a.

Key: PfamA domain Secondary structure CATH domain
 * PDB and UniProt seqs differ at 1 residue position (black cross)

Gene Ontology (GO) functional annotation

	Cellular component	hemoglobin complex	2 terms
	Biological process	transport	6 terms
	Biochemical function	protein binding	7 terms

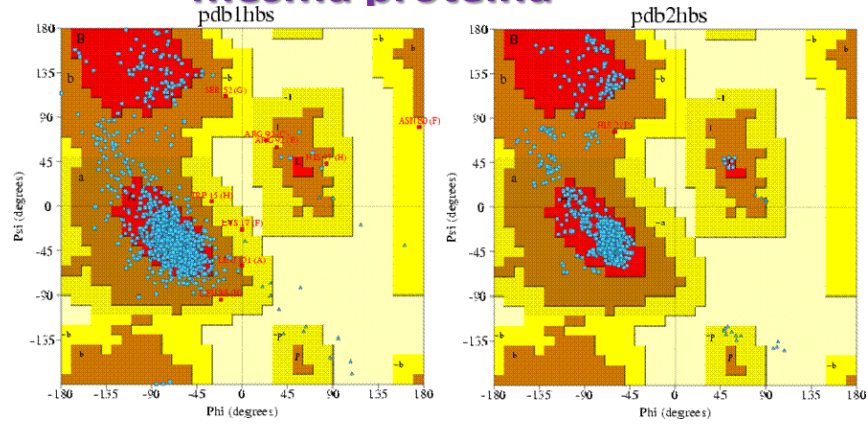
Gráfico de Ramachandran



1hbs – 3,00 Å
baixa resolução

Gráfico de Ramachandran

mesma proteína

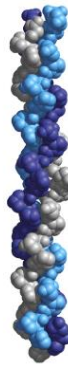
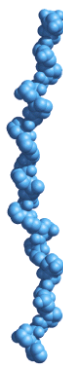


1hbs – 3,00 Å
baixa resolução

2hbs - 2,05Å
alta resolução

Principais formas tridimensionais

fibrosas
exemplo: colágeno



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Principais formas tridimensionais

globulares
exemplo: mioglobina

