

BINF 731

## Protein Structure Analysis

<http://binf.gmu.edu/vaisman/binf731/>

Iosif Vaisman

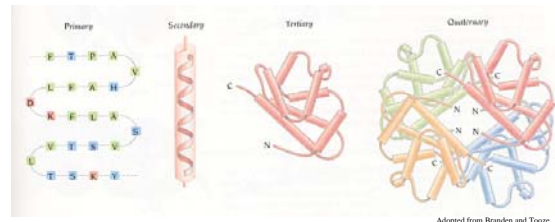
2009

### Secondary Structure: Computational Problems

#### Secondary structure characterization

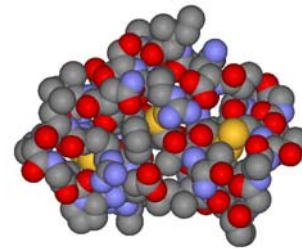
Secondary structure assignment  
Secondary structure prediction  
Protein structure classification

## Protein Structure Hierarchy

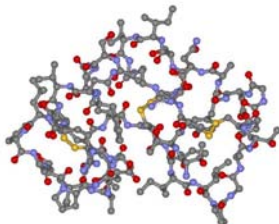


- Primary - the sequence of amino acid residues
- Secondary - ordered regions of primary sequence (helices, beta-sheets, turns)
- Tertiary - the three-dimensional fold of a protein subunit
- Quaternary - the arrangement of subunits in oligomers.

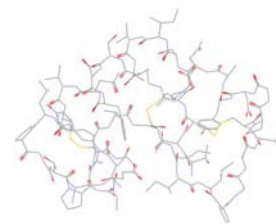
### Protein representations



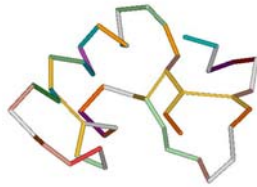
### Protein representations



### Protein representations



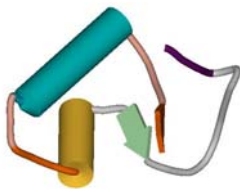
### Protein representations



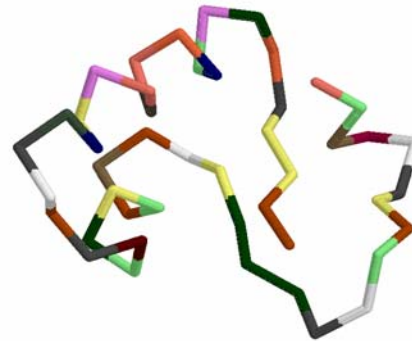
### Protein representations



### Protein representations

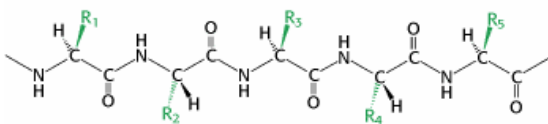


### Protein backbone

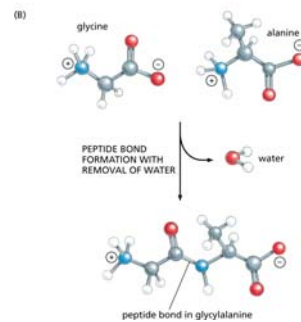
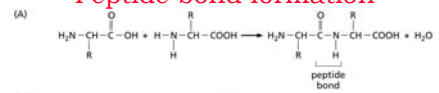


NWVLSTAADMQGVVTDGMASGLDKD

### Protein backbone

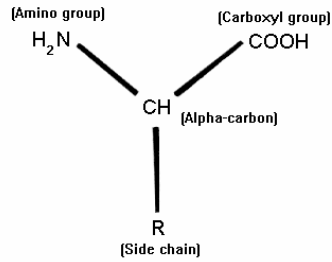


### Peptide bond formation

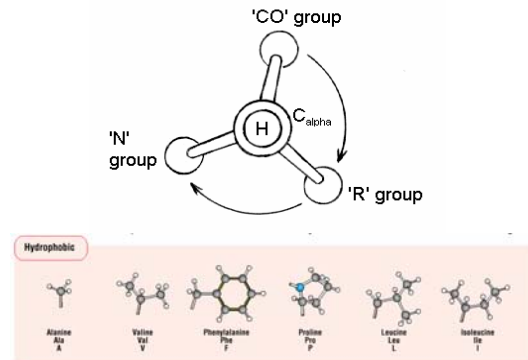


Adopted from Zvelebil, Baum, 2008

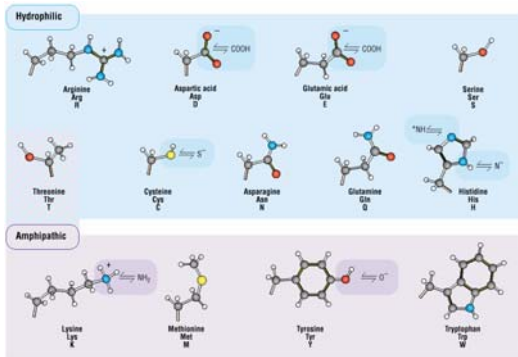
## Amino Acid Residue



## Amino Acid Residue

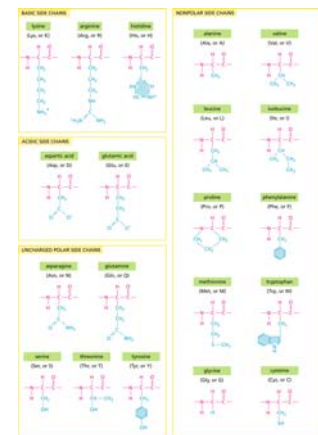


## Amino Acids



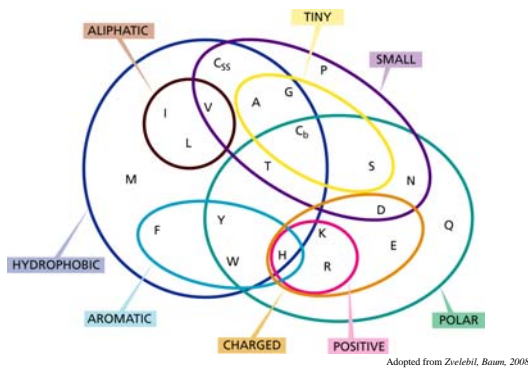
Adopted from: Gregory Pasko and Dagmar Ringo  
Protein Structure and Function: From Sequence to Consequence

## Amino Acids



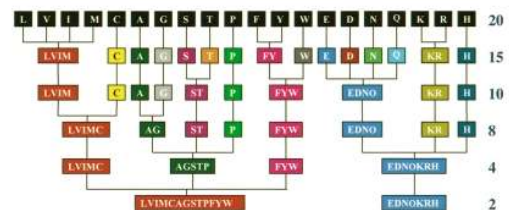
Adopted from Zvelebil, Baum, 2008

## Amino Acid Residue Clustering

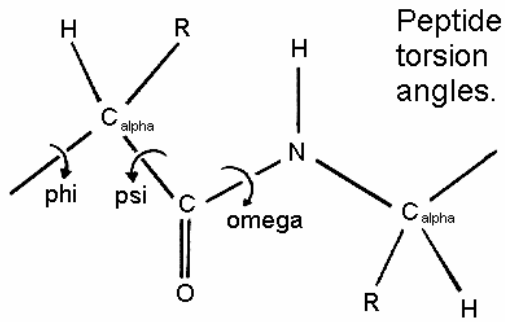


Adopted from Zvelebil, Baum, 2008

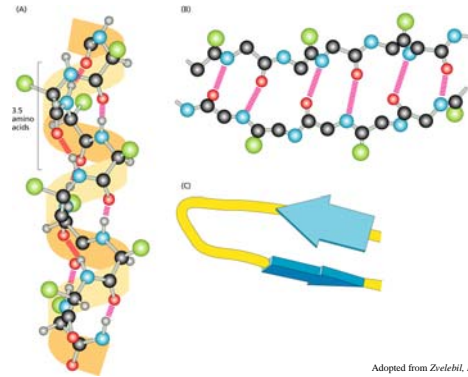
## Amino Acid Residue Clustering



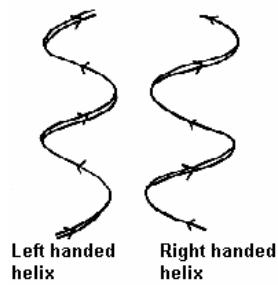
Adopted from: L.R.Murphy et al., 2000



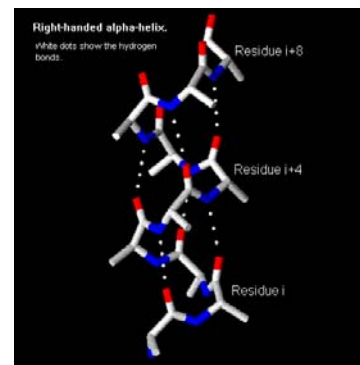
## Secondary Structures



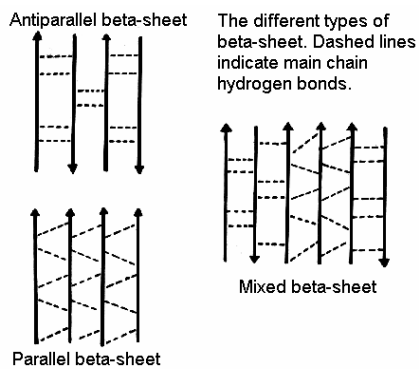
## Secondary Structure (Helices)



## Helix

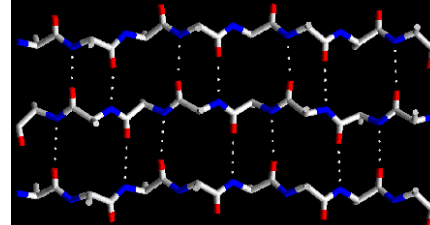


## Secondary Structure (Beta-sheets)

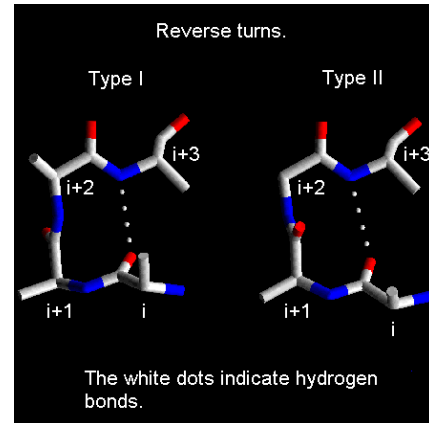
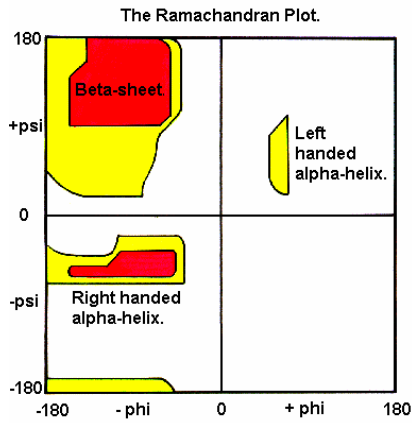


## Antiparallel Beta-Sheet

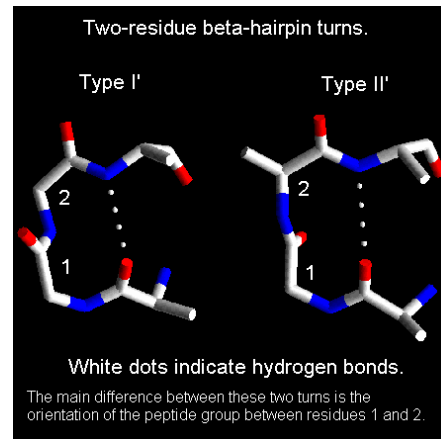
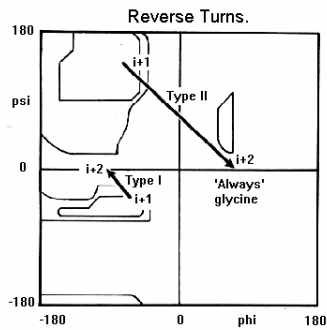
(White dots indicate hydrogen bonds)



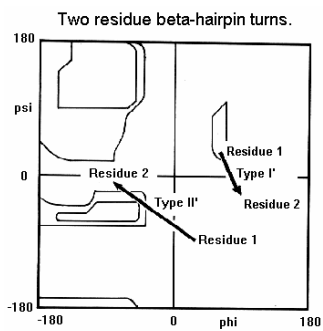
Can you identify the amino- and carboxy- termini of the strands?



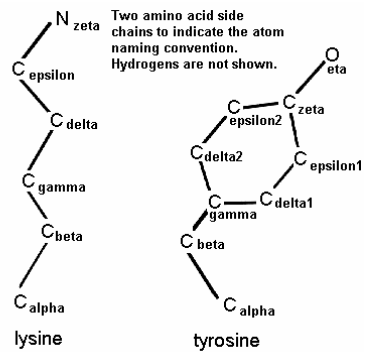
## Reverse Turns on a Ramachandran Plot



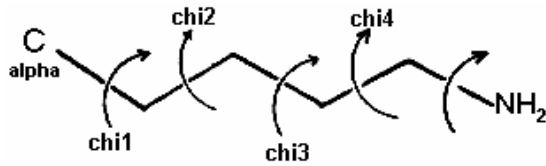
## Beta-hairpin Turns on a Ramachandran Plot



## Side-Chain Atom Nomenclature



## Side-Chain Torsional Angles



## Secondary Structure: Computational Problems

Secondary structure characterization

**Secondary structure assignment**

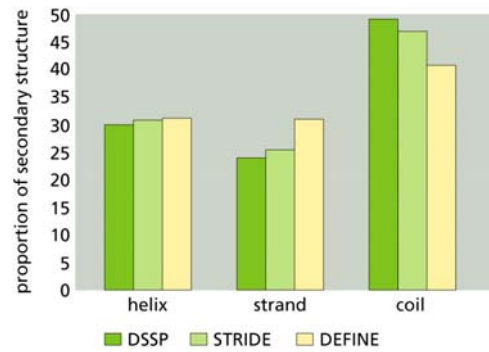
Secondary structure prediction

Protein structure classification

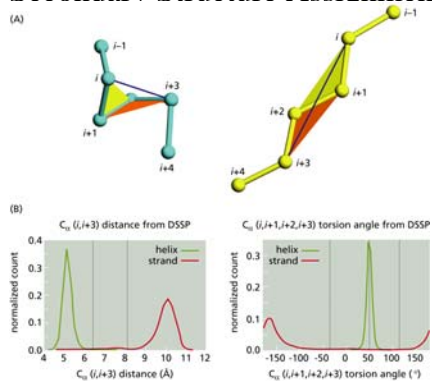
## Secondary Structure Conformations

	$\phi$	$\psi$
alpha helix	-57	-47
alpha-L	57	47
3-10 helix	-49	-26
$\pi$ helix	-57	-80
type II helix	-79	150
$\beta$ -sheet parallel	-119	113
$\beta$ -sheet antiparallel	-139	135

## Secondary Structure Assignment



## Secondary Structure Assignment



Adapted from Zvelebil, Baum, 2008

## Secondary Structure Assignment

```

.....1.....2.....3.....4.....5.....6.....7.....
-- sequential resnumber, including chain breaks as extra residues
-- original PDB resname, not nec. sequential, may contain letters
-- amino acid sequence in one letter code
-- secondary structure summary based on columns 19-38
xxxxxxx recommend columns for secstruc details
-- 3-turns/helix
-- 4-turns/helix
-- 5-turns/helix
-- geometrical bend
-- chirality
-- beta bridge label
-- beta bridge label
-- beta bridge partner resnum
-- beta bridge partner resnum
-- beta sheet label
-- solvent accessibility
# RESIDUE AA STRUCTURE BP1 BP2 ACC
35 47 I E + 0 0 2
36 48 R E > S- K 0 39C 97
37 49 Q T 3 S+ 0 0 86 (example from 1EST)
38 50 N T 3 S+ 0 0 34
39 51 W E < -KL 36 98C 6
    
```