

Bio 37

Structural Biology

Williamson
Fall, 2009
The first day

Philosophy

- Molecular explanations of biological processes
- Hypotheses – no and yes
- Evolution and particulars
- Visual science

- A course in the making

The course: The pieces

The screenshot shows a web browser window with the title "Structural Biology | Amherst College - Mozilla Firefox". The address bar displays the URL "https://www.amherst.edu/academiclife/departments/courses/0910F/BIOL/BIOL-37-0910F". The browser's toolbar includes various icons for navigation and search. The page header features the Amherst College logo and the motto "TERRAS IRRADIANT". A navigation menu includes links for "About Amherst", "Academics", "Admission & Financial Aid", "Alumni", "Library", "Museums", and "Student Life". The main content area is titled "STRUCTURAL BIOLOGY" and includes a sidebar with links for "Announcements", "Syllabus", "Documents and Links", "E-reserves", "Lecture Notes", and "Class Roster". The main text area contains the following information:

Home » Academics » Areas of Study » Biology » Structural Biology

■ STRUCTURAL BIOLOGY

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Fall 2009 - [Get temporary access to course materials \(Amherst College and Five-college students only\)](#)

Structural Biochemistry

Listed in: [Biology](#), as BIOL-37

Faculty

[Patrick L. Williamson](#) (Section 01)

Description

This course will concentrate on the structure of proteins at the atomic level. It will include an introduction to methods of structure determination, to databases of structural information, and to publicly available visualization software. These tools will be used to study some class of specific structures, (such as membrane, nucleic acid binding, regulatory, structural, or metabolic proteins). These proteins will provide the framework for discussion of such concepts as domains, motifs, molecular motion, structural homology, etc., as well as addressing how specific biological problems are solved at the atomic level. Four classroom hours per week plus one hour discussion .

Requisite: Biology 19 and Chemistry 12; Chemistry 21 would be helpful but is not required. Limited to 20 students. Fall semester. Professor Williamson.

Details

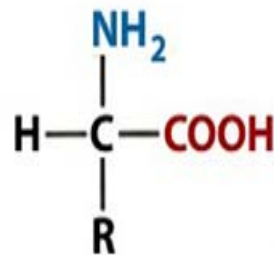
SECTION 01

LEC Tu 10:00 AM - 11:20 AM WEBS 102

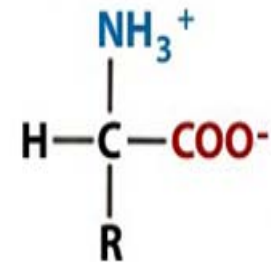
The Pregnant Pause...

Amino Acid Structure

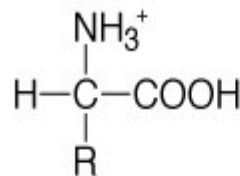
- α carbon and substituents
- Charged at amino and carboxyl terminal ends (of chains)
- Each aa residue is a dipole, and contributes to the dipole moment of the chain
- Water soluble as monomers, less so in polymer



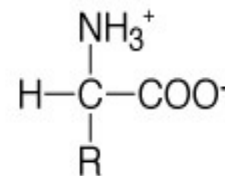
Un-ionized form of an amino acid



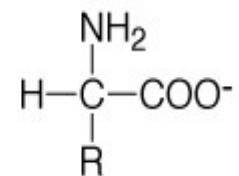
Dipolar ion (or zwitterion) form of an amino acid



Predominant form at pH 1



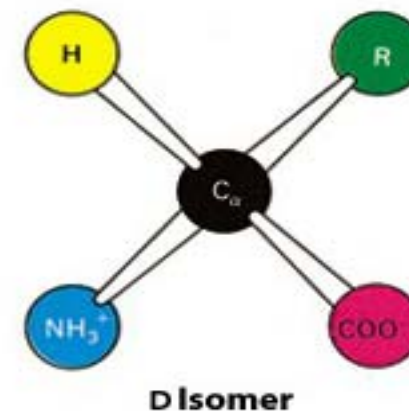
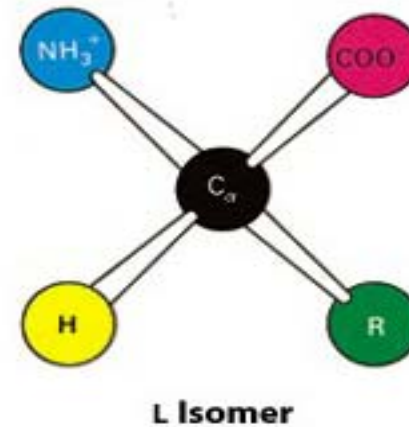
Predominant form at pH 7



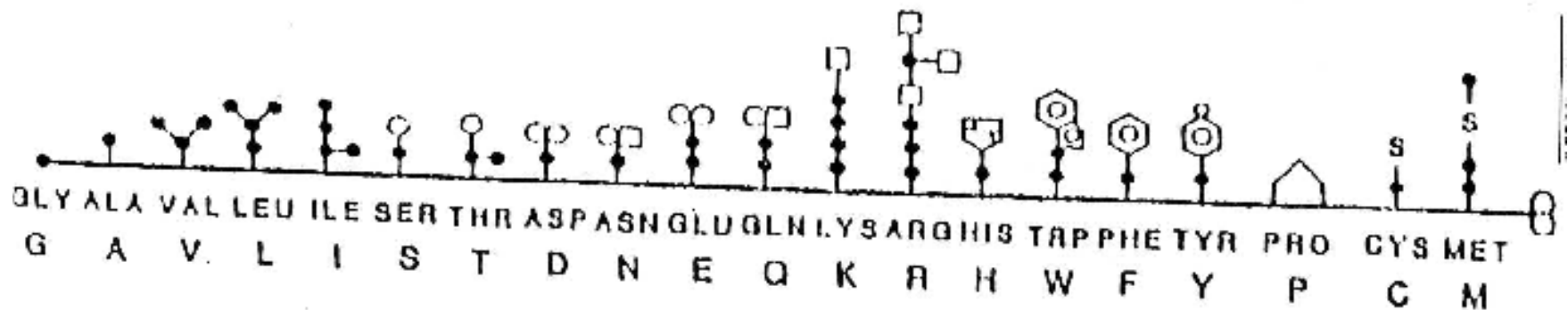
Predominant form at pH 11

The alpha carbon is a chiral center

- The α carbon of all amino acids (except glycine) are chiral (and possibly others in side chain as well.)
- Naturally occurring amino acids are the L stereoisomer.

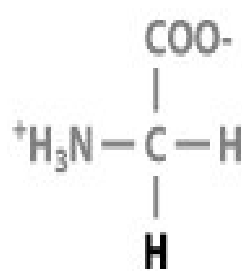


The sidechains: a quick summary (Thanks, Prof. O'Hara)

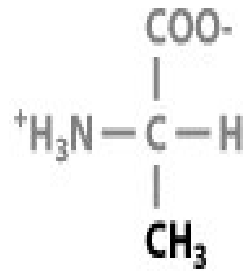


Short hand code for the structure of the individual amino acids

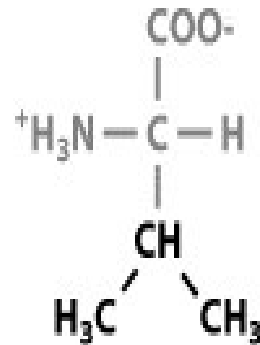
Aliphatic Side chains



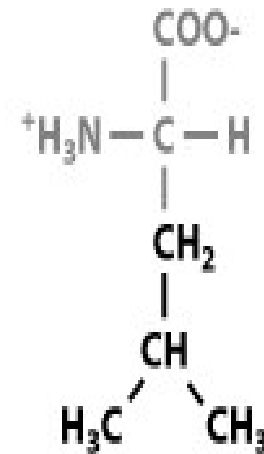
Glycine
(Gly, G)



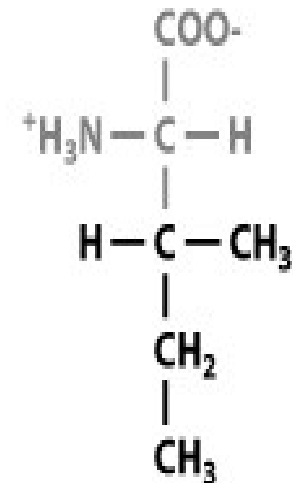
Alanine
(Ala, A)



Valine
(Val, V)



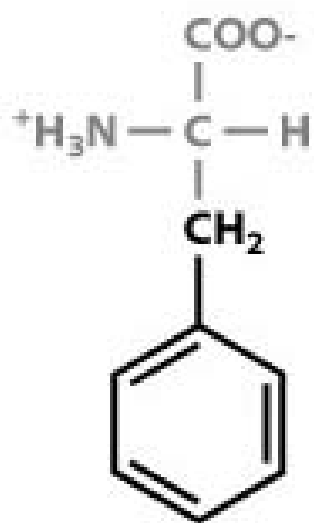
Leucine
(Leu, L)



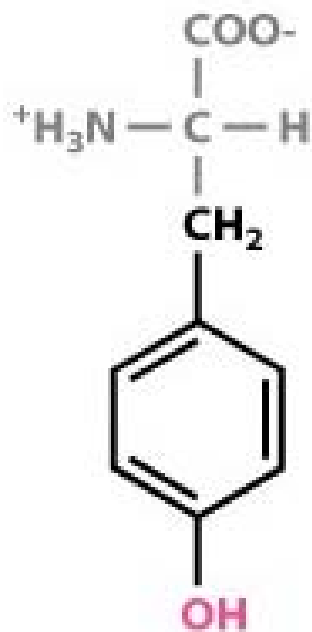
Isoleucine
(Ile, I)

Val, Leu, and Ile are strongly hydrophobic amino acids

Aromatic Side chains



Phenylalanine
(Phe, F)

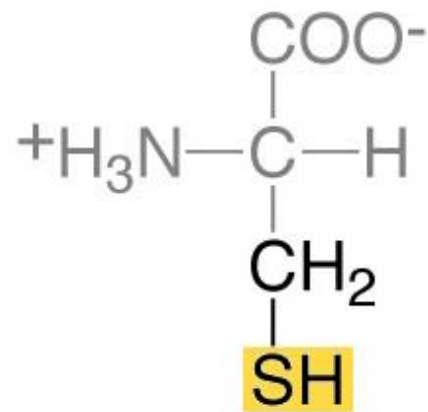


Tyrosine
(Tyr, Y)

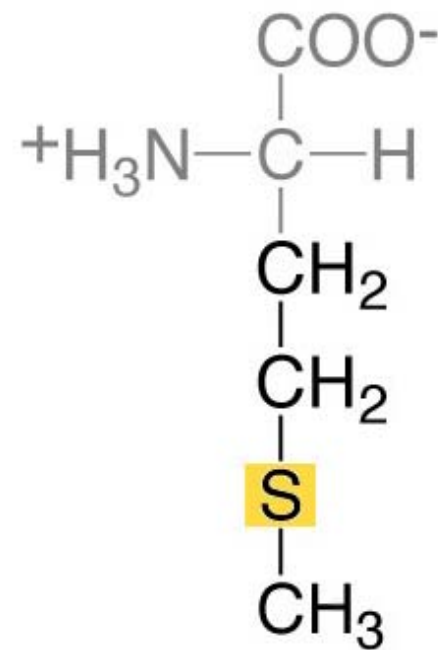


Tryptophan
(Trp, W)

Sulfur-containing sidechains

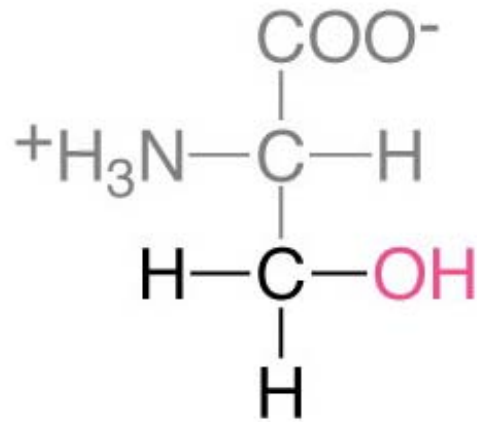


Cysteine
(Cys, C)

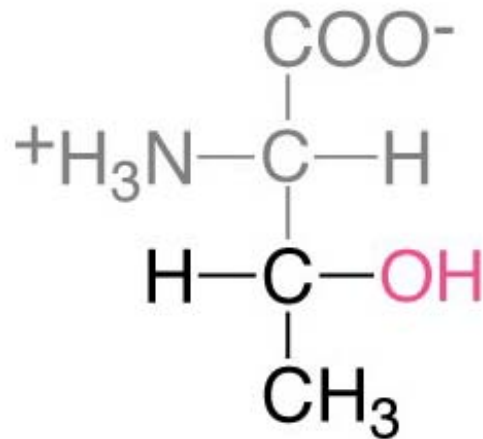


Methionine
(Met, M)

Hydroxyl sidechains



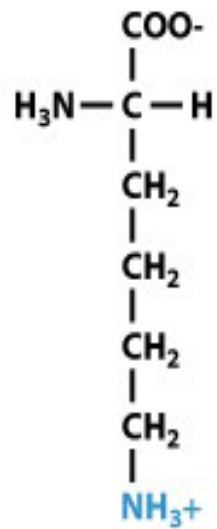
Serine
(Ser, S)



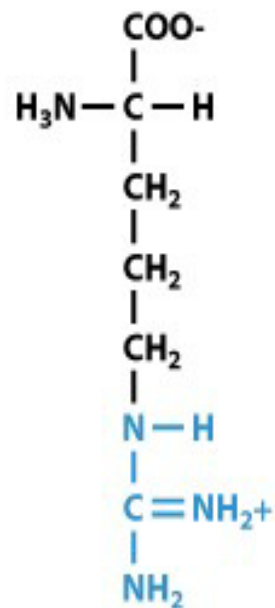
Threonine
(Thr, T)

...and tyrosine as well

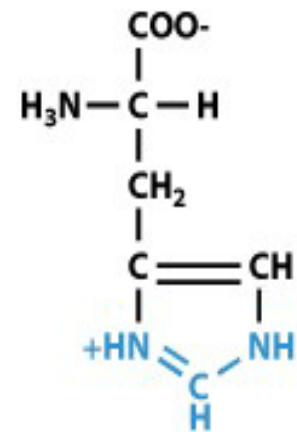
Basic Side chains



Lysine
(Lys, K)

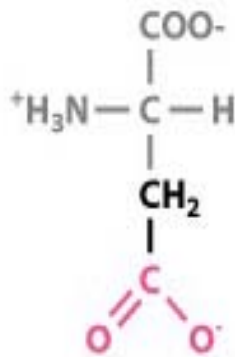


Arginine
(Arg, R)

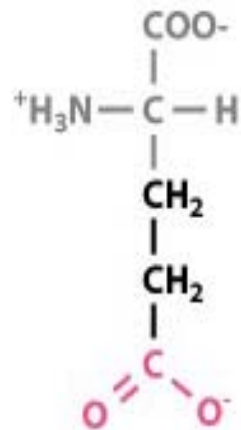


Histidine
(His, H)

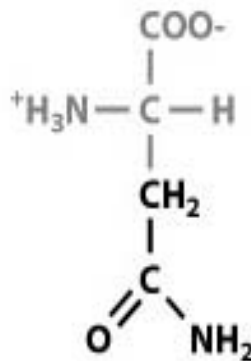
Anionic Side Chains & relations



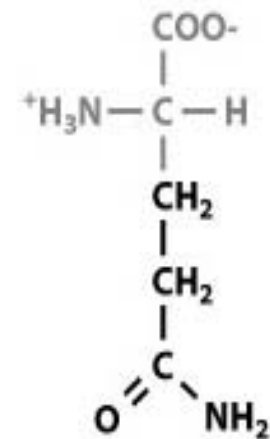
Aspartate
(Asp, D)



Glutamate
(Glu, E)



Asparagine
(Asn, N)



Glutamine
(Gln, Q)

ACIDIC AND BASIC AMINO ACIDS

| Name | Polarity | Hydropathy | pK ₁ | pK ₂ | pK _r |
|----------------------------|----------|------------|-----------------|-----------------|-----------------|
| Aspartate Asp- D | +0.80 | -3.5 | 2.09 | 9.82 | 3.86 (3.65) |
| Glutamate Glu- E | +0.77 | -3.5 | 2.19 | 9.67 | 4.25 |
| Lysine Lys- K | +1.18 | -3.9 | 2.18 | 8.95 | 10.53 |
| Histidine His- H | -0.49 | -3.2 | 1.82 | 9.17 | 6.00 |
| Arginine Arg- R | +0.84 | -4.5 | 2.17 | 9.04 | 12.5 |

Polarity Scale: Found in Aqueous environment (+ values)
 Found in Hydrophobic environment (- values)
 H.R. Guy (1984) Biophys. J. 47 61-70.

Hydropathy Scale: Found in Aqueous environment (- values)
 Found in Hydrophobic environment (+ values).
 Kyte & Doolittle (1982) J. Mol. Bio. 157, 105-132.

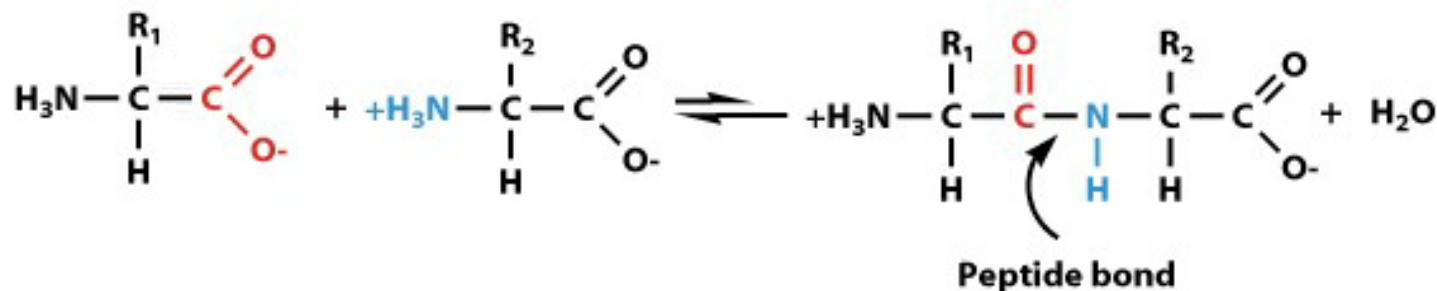
PREDICTED HYDROPHOBIC AMINO ACIDS

| Name | Polarity | Hydropathy | pK ₁ | pK ₂ | pK _r |
|--------------------------------|----------|------------|-----------------|-----------------|-----------------|
| Alanine Ala- A | +0.06 | +1.8 | 2.34 | 9.69 | |
| Valine Val- V | -1.09 | +4.2 | 2.32 | 9.62 | |
| Leucine Leu- L | -1.21 | +3.8 | 2.36 | 9.60 | |
| Isoleucine Ile- I | -1.31 | +4.5 | 2.36 | 9.68 | |
| Proline Pro- P | +0.70 | -1.6 | 1.99 | 10.96 | |
| Phenylalanine Phe- F | -1.68 | +2.8 | 1.83 | 9.13 | |
| Tryptophan Trp- W | -0.88 | -0.9 | 2.38 | 9.39 | |
| Methionine Met- M | -1.23 | +1.9 | 2.38 | 9.21 | |

PREDICTED HYDROPHILIC AMINO ACIDS

| Name | Polarity | Hydropathy | pK₁ | pK₂ | pK_r |
|-----------------------------|-----------------|-------------------|-----------------------|-----------------------|-----------------------|
| Glycine Gly- G | +0.41 | -0.4 | 2.34 | 9.60 | |
| Serine Ser- S | +0.50 | -0.8 | 2.21 | 9.15 | 13.60 |
| Threonine Thr- T | +0.27 | -0.7 | 2.63 (2.11) | 10.4 (9.62) | 13.60 |
| Cysteine Cys- C | -1.36 | +2.5 | 1.71 (1.96) | 10.8 (8.18) | 8.3 (10.28) |
| Tyrosine Tyr- Y | -0.33 | -1.3 | 2.20 | 9.11 | 10.5 |
| Asparagine Asn- N | +0.48 | -3.5 | 2.02 | 8.80 | |
| Glutamine Gln- Q | +0.73 | -3.5 | 2.17 | 9.13 | |

The peptide bond



- Two amino acids combine to form a dipeptide, three to form a tripeptide, several to form an oligopeptide, many to form a polypeptide, or protein
- Forward reaction is a dehydration, backward reaction is an hydrolysis
- Note energetics