

Amino Acids Structure

General Structure

- Central α -carbon
- Amino group ($-\text{NH}_2$)
- Carboxyl group ($-\text{COOH}$)
- Variable R group (side chain)

Classification

- Nonpolar/hydrophobic
- Polar uncharged
- Positively charged (basic)
- Negatively charged (acidic)

Chirality

- All are L-amino acids in proteins
- D-amino acids rare in nature
- Asymmetric α -carbon
- Mirror image isomers

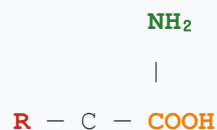
Ionization States

- pKa values determine charge
- Zwitterion at physiological pH
- Affects protein interactions
- Important for enzyme catalysis

Detailed Structure Examples

1. General Structure

Basic Amino Acid Structure



Key Features

The central α -carbon is bonded to four different groups, making it a chiral center (except glycine). This tetrahedral arrangement is fundamental to amino acid structure.



α -carbon (chiral center)

Components:

- Amino group
- Carboxyl group
- Variable R group
- Hydrogen atom

Tetrahedral geometry

Chiral center

Zwitterion Form

At physiological pH (~7.4), amino acids exist as zwitterions with NH_3^+ and COO^- groups, carrying both positive and negative charges.

pH dependent

Amphoteric

• 2. Classification by R Group Properties

Example R Groups

Nonpolar:

$-\text{CH}_3$ (Alanine)

$-\text{CH}(\text{CH}_3)_2$ (Valine)

Polar uncharged:

$-\text{CH}_2\text{OH}$ (Serine)

$-\text{CH}_2\text{CONH}_2$ (Asparagine)

Positive (+):

$-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{NH}_3^+$

Nonpolar/Hydrophobic

Examples: Alanine, Valine, Leucine, Isoleucine, Methionine, Phenylalanine, Tryptophan, Proline

These amino acids have hydrocarbon R groups that avoid water. They're typically found in protein interiors and membrane proteins.

Hydrophobic effect

Protein core

Polar Uncharged

Examples: Serine, Threonine, Cysteine, Asparagine, Glutamine, Tyrosine

Contain polar groups (OH, SH, NH_2 , C=O) that can form hydrogen bonds but don't ionize at physiological pH.

H-bonding

Surface residues

(Lysine)

Negative (-):

$-\text{CH}_2 - \text{COO}^-$

(Aspartate)

Charged Amino Acids

Basic (+): Lysine, Arginine, Histidine (pKa ~6-12.5)

Acidic (-): Aspartate, Glutamate (pKa ~3.5-4.5)

These residues are ionized at physiological pH and participate in salt bridges and electrostatic interactions.

Ionic interactions

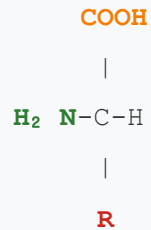
Active sites

- 3. Chirality (Optical Isomerism)

L vs D Configuration

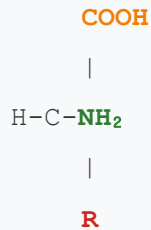
L-Amino Acid

(Natural)



D-Amino Acid

(Rare)



Mirror images (enantiomers)

Non-superimposable

Fischer Projection

Vertical lines = away from viewer

Horizontal lines = toward viewer

L-Configuration Dominance

All amino acids in proteins are L-isomers. The L/D notation is based on the configuration relative to L-glyceraldehyde. In L-amino acids, the amino group is on the left in Fischer projection.

Biological selectivity

Homochirality

Glycine Exception

Glycine (R = H) is the only achiral amino acid because its α -carbon has two hydrogen atoms attached, making it superimposable on its mirror image.

Achiral

No optical activity

D-Amino Acids in Nature

D-amino acids are rare but found in bacterial cell walls, some antibiotics (e.g., gramicidin), and as neurotransmitters in mammals. They're not incorporated into proteins by ribosomes.

Bacterial walls

Specialized roles

4. Ionization States and pKa Values

pH-Dependent Forms

Henderson-Hasselbalch Equation

$$\text{pH} = \text{pKa} + \log\left(\frac{[\text{A}^-]}{[\text{HA}]}\right)$$

This equation determines the ionization state of amino acids at different pH values. At pH = pKa, 50% of molecules are protonated.

Buffer capacity

pI calculation

Low pH (<2)



(+1 charge)

Cationic

Neutral pH (~7)



(0 net charge)

Zwitterion

High pH (>11)



(-1 charge)

Anionic

Typical pKa Values:

α -COOH: ~2.2

α -NH₃⁺: ~9.4

Side chains: 3.5-12.5

Isoelectric Point (pI)

The pH at which an amino acid has no net charge (zwitterion form predominates). For simple amino acids: $pI = (pK_{a1} + pK_{a2})/2$

Examples:

- Alanine: $pI \approx 6.0$
- Lysine: $pI \approx 9.7$ (basic)
- Aspartate: $pI \approx 2.8$ (acidic)

Electrophoresis

Protein purification

Functional Significance

Ionization states control:

- Enzyme catalytic mechanisms (His, Asp, Glu in active sites)
- Protein-protein interactions via salt bridges
- Protein solubility and stability
- Signal transduction through protonation changes

Catalysis

Regulation

Binding