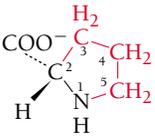


**Table 4-1. Key to Structure.** Covalent Structures and Abbreviations of the “Standard” Amino Acids of Proteins, Their Occurrence, and the pK Values of Their Ionizable Groups

| Name,<br>Three-letter Symbol,<br>and One-letter Symbol | Structural<br>Formula <sup>a</sup>  | Residue<br>Mass<br>(D) <sup>b</sup> | Average<br>Occurrence<br>in Proteins (%) <sup>c</sup> | pK <sub>1</sub><br>α-COOH <sup>d</sup> | pK <sub>2</sub><br>α-NH <sub>3</sub> <sup>+</sup> <sup>d</sup> | pK <sub>R</sub><br>Side Chain <sup>d</sup> |
|--|---|-------------------------------------|---|--|--|--|
| <b>Amino acids with nonpolar side chains</b>           |   |                                     |   |  |  |  |
| Glycine<br>Gly<br>G                                    | $\begin{array}{c} \text{COO}^- \\   \\ \text{H}-\text{C}-\text{H} \\   \\ \text{NH}_3^+ \end{array}$  | 57.0                                | 7.2   | 2.35                                   | 9.78   |  |
| Alanine<br>Ala<br>A                                    | $\begin{array}{c} \text{COO}^- \\   \\ \text{H}-\text{C}-\text{CH}_3 \\   \\ \text{NH}_3^+ \end{array}$   | 71.1                                | 7.8   | 2.35                                   | 9.87   |  |
| Valine<br>Val<br>V                                     | $\begin{array}{c} \text{COO}^- \\   \\ \text{H}-\text{C}-\text{CH} \\   \quad   \\ \text{NH}_3^+ \quad \text{CH}_3 \\ \quad \quad   \\ \quad \quad \text{CH}_3 \end{array}$                                     | 99.1                                | 6.6   | 2.29                                   | 9.74   |  |
| Leucine<br>Leu<br>L                                    | $\begin{array}{c} \text{COO}^- \\   \\ \text{H}-\text{C}-\text{CH}_2-\text{CH} \\   \quad \quad   \\ \text{NH}_3^+ \quad \quad \text{CH}_3 \\ \quad \quad \quad   \\ \quad \quad \quad \text{CH}_3 \end{array}$ | 113.2                               | 9.1   | 2.33                                   | 9.74   |  |
| Isoleucine<br>Ile<br>I                                 | $\begin{array}{c} \text{COO}^- \\   \\ \text{H}-\text{C}-\text{C}^*-\text{CH}_2-\text{CH}_3 \\   \quad   \\ \text{NH}_3^+ \quad \text{H} \\ \quad \quad   \\ \quad \quad \text{CH}_3 \end{array}$               | 113.2                               | 5.3   | 2.32                                   | 9.76   |  |
| Methionine<br>Met<br>M                                 | $\begin{array}{c} \text{COO}^- \\   \\ \text{H}-\text{C}-\text{CH}_2-\text{CH}_2-\text{S}-\text{CH}_3 \\   \\ \text{NH}_3^+ \end{array}$  | 131.2                               | 2.2   | 2.13                                   | 9.28   |  |
| Proline<br>Pro<br>P                                    |    | 97.1                                | 5.2   | 1.95                                   | 10.64  |  |
| Phenylalanine<br>Phe<br>F                              | $\begin{array}{c} \text{COO}^- \\   \\ \text{H}-\text{C}-\text{CH}_2-\text{C}_6\text{H}_5 \\   \\ \text{NH}_3^+ \end{array}$  | 147.2                               | 3.9   | 2.20                                   | 9.31   |  |
| Tryptophan<br>Trp<br>W                                 | $\begin{array}{c} \text{COO}^- \\   \\ \text{H}-\text{C}-\text{CH}_2-\text{C}_8\text{H}_6\text{N} \\   \\ \text{NH}_3^+ \end{array}$  | 186.2                               | 1.4   | 2.46                                   | 9.41   |  |

<sup>a</sup>The ionic forms shown are those predominating at pH 7.0 although residue mass is given for the neutral compound. The C<sub>α</sub> atoms, as well as those atoms marked with an asterisk, are chiral centers with configurations as indicated according to Fischer projection formulas. The standard organic numbering system is provided for heterocycles.

<sup>b</sup>The residue masses are given for the neutral residues. For the molecular masses of the parent amino acids, add 18.0 D, the molecular mass of H<sub>2</sub>O, to the residue masses. For side chain masses, subtract 56.0 D, the formula mass of a peptide group, from the residue masses.

<sup>c</sup>Calculated from a database of nonredundant proteins containing 300,688 residues as compiled by Doolittle, R.F. in Fasman, G.D. (Ed.), *Predictions of Protein Structure and the Principles of Protein Conformation*, Plenum Press (1989).

<sup>d</sup>Data from Dawson, R.M.C., Elliott, D.C., Elliott, W.H., and Jones, K.M., *Data for Biochemical Research* (3rd ed.), pp. 1–31, Oxford Science Publications (1986).

<sup>e</sup>The three- and one-letter symbols for asparagine or aspartic acid are Asx and B, whereas for glutamine or glutamic acid they are Glx and Z. The one-letter symbol for an undetermined or “nonstandard” amino acid is X.

<sup>f</sup>Both neutral and protonated forms of histidine are present at pH 7.0, since its pK<sub>R</sub> is close to 7.0.

