Properties of amino acids

Amino acid residue	pK_a of ionizing side chain[a]	Average residue mass[b] (daltons)	Monoisotopic mass (daltons)[b]	Occurrence in proteins[c] (%)	Percent buried residues[d] (%)	V_r[e] (Å^3)	van der Waals volume[f] (Å^3)	Accessible surface area[g] (Å^2)	Ranking of amino acid polarities[h]
Alanine	–	71.0788	71.03711	7.5	38 (12)	92	67	67	9 (7)
Arginine	12.5 (>12)	156.1876	156.10111	5.2	0	225	148	196	15 (19)
Asparagine	–	114.1039	114.04293	4.6	10 (2)	135	96	113	16 (16)
Aspartic acid	3.9 (4.4–4.6)	115.0886	115.02694	5.2	14.5 (3)	125	91	106	19 (18)
Cysteine	8.3 (8.5–8.8)	103.1448	103.00919	1.8	47 (3)	106	86	104	7 (8)
Glutamine	–	128.1308	128.05858	4.1	6.3 (2.2)	161	114	144	17 (14)
Glutamic acid	4.3 (4.4–4.6)	129.1155	129.04259	6.3	20 (2)	155	109	138	18 (17)
Glycine	–	57.0520	57.02146	7.1	37 (10)	66	48		11 (9)
Histidine	6.0 (6.5–7.0)	137.1412	137.05891	2.2	19 (1.2)	167	118	151	10 (13)
Isoleucine	–	113.1595	113.08406	5.5	65 (12)	169	124	140	1 (2)
Leucine	–	113.1595	113.08406	9.1	41 (10)	168	124	137	3 (1)
Lysine	10.8 (10.0–10.2)	128.1742	128.09496	5.8	4.2 (0.1)	171	135	167	20 (15)
Methionine	–	131.1986	131.04049	2.8	50 (2)	171	124	160	5 (5)
Phenylalanine	–	147.1766	147.06841	3.9	48 (5)	203	135	175	2 (4)
Proline	–	97.1167	97.05276	5.1	24 (3)	129	90	105	13 (–)
Serine	–	87.0782	87.03203	7.4	24 (8)	99	73	80	14 (12)
Threonine	–	101.1051	101.04768	6.0	25 (5.5)	122	93	102	12 (11)
Tryptophan	–	186.2133	186.07931	1.3	23 (1.5)	240	163	217	6 (6)
Tyrosine	10.9 (9.6–10.0)	163.1760	163.06333	3.3	13 (2.2)	203	141	187	8 (10)
Valine	–	99.1326	99.06841	6.5	56 (15)	142	105	117	4 (3)

[a]The pK_a values in most cases are at 25°C. The expected pK_a values in proteins, shown in parentheses, are determined from model compounds in which titration of side chains is decoupled from charge effects of α-substituents. (Data from Cantor and Schimmel 1980.)

[b]Data from Burlingame and Carr (1996).

[c]Frequency of occurrence of each amino acid residue in the primary structures of 105,990 sequences in the nonredundant OWL protein database (release 26.0 e) (Trinquier and Sanejouand 1998).

[d]This column represents the tendency of an amino acid to be buried (defined as <5% of residue available to solvent) in the interior of a protein and is based on the structures of nine proteins (total of ~2000 individual residues studied, with 587 [29%] of these buried). Values indicate how often each amino acid was found buried, relative to the total number of residues of this amino acid found in the proteins (values in parentheses indicate the number of buried residues of this amino acid found relative to all buried residues in the proteins). (Data from Schien 1990; for other calculation methods with similar results, see Janin 1979 and Rose at al. 1985.)

[e]Average volume (V_r) of buried residues, calculated from the surface area of the side chain (Richards 1977; Baumann et al. 1989).

[f]Data from Darby and Creighton (1993).

[g]Total accessible surface area (ASA) of amino acid side chain for residue X in a Gly-X-Gly tripeptide with the main chain in an extended conformation (Miller et al. 1987). The ASA or cavity surface area is defined as the surface traced by the center of a sphere with the radius of a water molecule (0.15 mm) as it is rolled over the surface of a molecular model of the solution (Lee and Richards 1971).

[h]Values shown represent the mean ranking of amino acids according to the frequency of their occurrence at each sequence rank for 38 published hydrophobicity scales (Trinquier and Sanejouand 1998). Although the majority of these hydrophobicity scales are derived from experimental measurements of chemical behavior or physicochemical properties (e.g., solubility in water, partition between water and organic solvent, chromatographic migration, or effects on surface tension) of isolated amino acids, several "operational" hydrophobicity scales based on the known environment characteristics of amino acids in proteins, such as their solvent accessibility or their inclination to occupy the core of proteins (based on the position of residues in the tertiary structures as observed by X-ray crystallography or NMR) are included (Trinquier and Sanejouand 1998). The lower rankings represent the most hydrophobic amino acids, and higher values represent the most hydrophilic amino acids. For comparative purposes, the hydrophobicity scale of Radzicka and Wolfenden is shown in parentheses. This scale was derived from the measured hydration potential of amino acids that is based on their free energies of transfer from the vapor phase to cyclohexane, 1-octanol, and neutral aqueous solution (Radzicka and Wolfenden 1988).