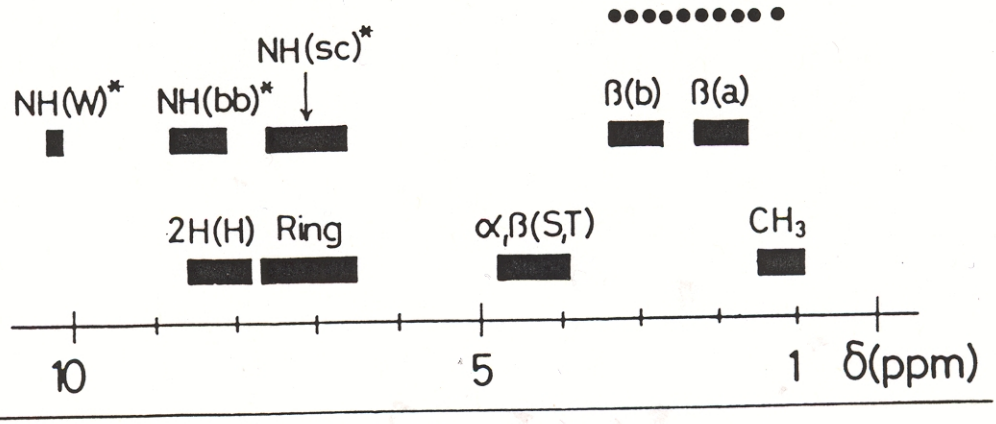
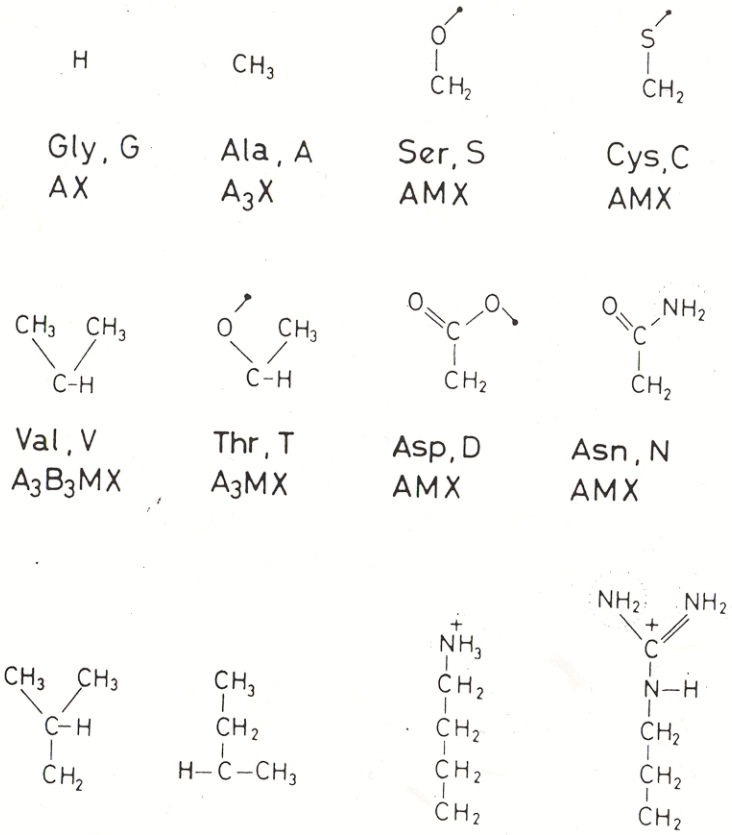
TABLE 2.4. Groups of Hydrogen Atoms in the Common Amino Acid Residues with Similar Random Coil ^{1}H Chemical Shifts[a]



Code	δ (ppm)	Comments
CH_3	0.9-1.4	
β(a)	1.6-2.3	βH of V,I,L,E,Q,M,P,R,K
β(b)	2.7-3.3	βH of C,D,N,F,Y,H,W
••••	1.2-3.3	Other Aliphatic CH
α,β(S,T)	3.9-4.8	All αH, βH of S and T
Ring	6.5-7.7	Aromatic CH of F,Y,W; 4H of H
2H(H)	7.7-8.6	2H of H in the pH range 1-11
NH(sc)*	6.6-7.6	Side Chain NH of N,Q,K,R
NH(bb)*	8.1-8.8	Backbone NH
NH(W)*	10.2	Indole NH of W

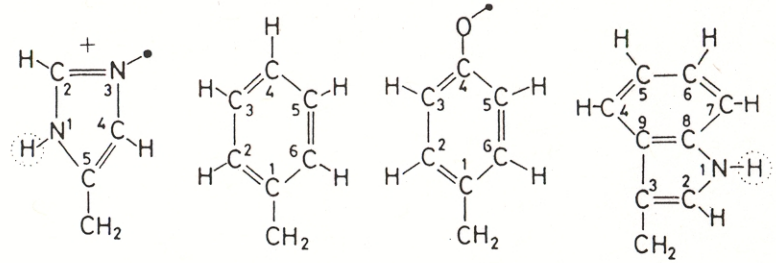
[a] In model peptides the labile protons (identified by *) are only observed in H_2O solution. The singlet resonance of εCH_3 in Met is at 2.13 ppm (Table 2.3).

TABLE . Side Chains R (see Fig. 2.1) and Three-Letter and One Letter Symbols for the 20 Common Amino Acids, and Spin Systems of the Nonlabile Hydrogen Atoms in the Molecular Fragments H–αC–R[a,b]



Gly, G	Ala, A	Ser, S	Cys, C
AX	A_3X	AMX	AMX
Val, V	**Thr, T**	**Asp, D**	**Asn, N**
A_3B_3MX	A_3MX	AMX	AMX
Leu, L	**Ile, I**	**Lys, K**	**Arg, R**
A_3B_3MPTX	$A_3MPT(B_3)X$	$A_2(F_2T_2)MPX^c$	$A_2(T_2)MPX^c$
Glu, E	**Gln, Q**	**Met, M**	**Pro, P[d]**
AM(PT)X	AM(PT)X	AM(PT)X+A$_3$	$A_2(T_2)MPX^c$

TABLE 2.2. (Continued)



His, H	Phe, F	Tyr, Y	Trp, W
AMX + AX[e]	AMX + AMM'XX'	AMX + AA'XX'	AMX + A(X)MP + A

[a] Also indicated is the numeration used for the aromatic ring atoms. Not indicated is the standard identification of the other side chain heavy atoms by lower case Greek letters, with βC being next to αC (IUPAC–IUB Commission on Biochemical Nomenclature, 1970).

[b] Labile protons that can under certain conditions be observed by NMR in aqueous solution are shown in dotted circles. Those labile protons, which are not usually observed, are indicated by small filled circles.

[c] For simplicity the spin systems for Arg, Lys, and Pro were written with the assumption that with the exception of the β position, each methylene group gives rise to a single two-proton resonance.

[d] The structure for Pro includes the backbone atoms αCH and N.

[e] In His, 2H and 4H appear often as two singlet lines, but the connectivity through the small four-bond coupling of approximately 1 Hz was observed in several proteins. 2H can be exchanged with deuterium of the solvent, D_2O, within a period of several hours to several months.

TABLE 2.3. Random Coil ^1H Chemical Shifts for the 20 Common Amino Acid Residues[a]

Residue	NH	αH	βH	Others
Gly	8.39	3.97		
Ala	8.25	4.35	1.39	
Val	8.44	4.18	2.13	γCH_3 0.97, 0.94
Ile	8.19	4.23	1.90	γCH_2 1.48, 1.19
				γCH_3 0.95
				δCH_3 0.89
Leu	8.42	4.38	1.65,1.65	γH 1.64
				δCH_3 0.94, 0.90
Pro[b]		4.44	2.28,2.02	γCH_2 2.03, 2.03
				δCH_2 3.68, 3.65
Ser	8.38	4.50	3.88,3.88	
Thr	8.24	4.35	4.22	γCH_3 1.23
Asp	8.41	4.76	2.84,2.75	
Glu	8.37	4.29	2.09,1.97	γCH_2 2.31, 2.28
Lys	8.41	4.36	1.85,1.76	γCH_2 1.45, 1.45
				δCH_2 1.70, 1.70
				εCH_2 3.02, 3.02
				εNH_3^+ 7.52
Arg	8.27	4.38	1.89,1.79	γCH_2 1.70, 1.70
				δCH_2 3.32, 3.32
				NH 7.17, 6.62
Asn	8.75	4.75	2.83,2.75	γNH_2 7.59, 6.91
Gln	8.41	4.37	2.13,2.01	γCH_2 2.38, 2.38
				δNH_2 6.87, 7.59
Met	8.42	4.52	2.15,2.01	γCH_2 2.64, 2.64
				εCH_3 2.13
Cys	8.31	4.69	3.28,2.96	
Trp	8.09	4.70	3.32,3.19	2H 7.24
				4H 7.65
				5H 7.17
				6H 7.24
				7H 7.50
				NH 10.22
Phe	8.23	4.66	3.22,2.99	2,6H 7.30
				3,5H 7.39
				4H 7.34
Tyr	8.18	4.60	3.13,2.92	2,6H 7.15
				3,5H 6.86
His	8.41	4.63	3.26,3.20	2H 8.12
				4H 7.14

[a] Data for the nonterminal residues X in tetrapeptides GGXA, pH 7.0, 35°C [from Bundi and Wüthrich (1979a), except that more precise data were obtained for Leu, Pro, Lys, Arg, Met and Phe using new measurements at 500 MHz].

[b] Data for *trans*-Pro.