BIOCHEMISTRY
including biophysical chemistry & molecular biology
Biochemistry, 1998, 37(7), 1933-1940, DOI:10.1021/bi9718548

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Chemical shifts of the amino acids of as-pdα.

Residue	NH	$C^{\alpha}H$ (C^{α})	$C^{\beta}H$ (C^{β})	$C^{\gamma}H$ (C^{γ})	others
Asp3	8.16	4.65 (54.8)	2.64, 2.71 (41.5)		
Val4	7.86	4.11 (62.8)	2.06 (33.3)	0.91 (21.1, 21.9)	
Gln5	8.22	4.21 (n.d.)	1.98, n.d. (n.d.)	2.35 (34.4)	NHε: n.d. , n.d.
Asp6	7.92	4.57 (54.7)	2.63, 2.70 (41.5)		
Cys7					
Pro8	--	4.50*§			
Glu9	8.22*§	4.23 (57.7)	2.02 (30.2)	2.39 (36.2)	
Cys10	7.86	4.77	2.64, 2.71		
Thr11	8.65	4.46§	n.d.	1.19 (22.2)	
Leu12	7.59§	4.30	1.68	1.30 §	δ1: 0.59 (26.2); δ2: 0.77 (25.7)
Gln13	8.75	4.77 (54.4)	1.91, 2.22 (n.d.)	2.41 (n.d.)	NHε: n.d. , n.d.
Glu14	8.73	4.40	1.91, 2.06 (n.d.)	2.31 (n.d.)	
Asn15	9.13	4.93 (52.9)	2.4, 2.93		NHδ: n.d., 7.77§
Pro16	--	n.d.	n.d.	n.d., n.d.	
Phe17	7.66	4.23	2.48 (n.d.)		δ: 6.96 (n.d.); ε: n.d.; ζ: n.d.
Phe18	6.89	4.91	2.30, 3.48		δ: 7.09 (131.8); ε: 6.99; ζ: 6.72(n.d.)
Ser19	7.33	4.45 (58.7*)	3.88, 3.94		
Gln20	7.54	4.80 53.7)	1.78, 2.19 (31.4)	2.39 (34.2)	NHε: n.d., n.d.
Pro21	--	4.27	2.29, 1.94	2.15, 2.20	δ: 3.64, 3.76
Gly22	8.70	4.15, 3.83 (46.0)			
Ala23	8.27	4.78 50.8)	1.16 (19.5)		
Pro24	--	n.d.	n.d.	1.65*	δ: 3.59, 3.62
Ile25	8.46	4.40§	1.82	1.21, 1.48	γ2: 0.85 (17.8); δ: 0.52 (10.8)
Leu26	8.92	5.08	2.37	1.22	δ1: 0.72 (23.9); δ2: 0.88 (26.6*)
Gln27	9.45	4.69	1.81	2.18, 2.21	NHε: n.d. , n.d.
Cys28	11.64	4.86	2.75, 2.73		
Met29	9.22	4.70	1.85, 2.05 (37.8)	2.40, 2.48 (32.5)	1.92(18.0)*
Gly30	--	3.67* (n.d.)			
Cys31	8.84*§	4.71*§	n.d., n.d.		
Cys32	n.d.	n.d.	n.d., n.d.		
Phe33	8.32	4.69 (n.d.)	2.96, 3.19 (n.d.)		δ: 7.23(n.d.); ε: 7.32 (n.d.), ζ: (n.d.)
Ser34					
Arg35	8.03	4.28	1.78, 1.88 (31.2)	1.62 (27.8)	δ: 3.19 (43.9); NHε: 7.14
Ala36	n.d.	4.29* (52.5)	1.23* (20.2)		
Tyr37[a]	7.80	4.77 (n.d.)	2.80, 3.01 (39.1*)		δ: 7.04 (133.8); ε: 6.75 (n.d.)

Pro38	--	n.d.	n.d., n.d.		δ: n.d., n.d.
Thr39	7.87	4.58 60.5)	4.19 (n.d.)	1.24 (22.1)	
Pro40	--	n.d.	n.d., n.d.	n.d.	δ: n.d., 3.82
Leu41	7.95	4.30	1.60	1.60	δ1: 0.85 (24.3); δ2: 0.89 (25.4)
Arg42	~Arg35*				NHε: 7.11*
Ser43					
Lys44					
Lys45(/51)	8.10	4.33*	1.74*, 1.85* (33.8*)	1.52 (25.4*)	δ: 1.63; ε: 3.10 (n.d.)
Thr46	7.79	4.31 (62.5)	4.20	1.19 (22.2)	
Met47	8.05	4.47	2.00, 2.08 (33.7)	2.50, 2.56 (32.7)	2.06 (17.7)*
Leu48	7.95	4.31*	1.59 (42.9)	1.59 (27.6)	δ1: 0.83 (24.2), δ2: 0.89 (25.4)
Val49	7.77	4.11 (62.8)	2.06 (33.3)	0.90	
Gln50	8.11	4.35	1.96, 2.08 (30.0)	2.32 (34.4)	NHε: n.d., n.d.
Lys51(/45)	8.07	4.32	1.76, 1.86 (33.5)	~1.43 (25.2*)	δ: 1.68 (29.5); ε: 3.00 (42.5)
Asp52	n.d.	4.64*§	n.d., n.d.		
Val53	7.90	4.20 (62.9)	2.15 (33.1)	0.90	
Thr54	8.00	4.49	4.21 (n.d.)	1.16 (22.4)	
Ser55					
Glu56	8.25	4.34	1.96, 2.07	2.32, 2.32 (n.d.)	
Ser57					
Thr58	n.d.	n.d.	3.90*	1.06 (23.0)	
Cys59	8.89	4.85	2.72, 2.97		
Cys60	8.54	4.75	2.75		
Val61	8.81	4.76			
Ala62	8.13	4.94 (53.0)	0.51 (16.7)		
Lys63	8.62	3.98	0.93, 1.00 (n.d.)	1.17 (n.d.)	δ:1.25,1.29 (29.6); ε: 2.77 (42.1)
Ser64	7.27	4.53	3.64		
Tyr65	7.91	5.39	2.88, 3.24		δ: 6.58 (133.5); ε: 6.73 (118.7)
Asn66	8.82	5.07	2.69, 2.81 (42.4)		NHδ: n.d., n.d.
Arg67	8.80	5.01 (56.9)	1.71, 1.83 (31.5)	1.50, 1.71 (28.9)	3.25 (44.0)
Val68	8.79	4.65 (60.1)	2.05 (35.9)	0.71 (20.9); 0.85 (22.3)	
Thr69	8.21	4.90 (62.6)	3.94 (n.d.)	1.07 (22.4)	
Val70	8.64	4.65 (60.1)	2.33 (35.4)	0.77 (20.1); 0.84 (23.0)	
Met71	8.42	4.11 (57.8)	2.11, 2.23 (32.7)	2.61 (32.9)	2.06 (17.7)*
Gly72	8.40	3.68, 4.21 (46.1)			
Gly73	8.01	3.63, 4.08 (46.1)			
Phe74	7.30	4.61	2.86, 2.96(n.d.)		δ:7.17 (132.3); ε: 7.30 (132.1); ζ: n.d.

Lys75	8.11	5.04	1.45§, 1.68§	1.29§, 1.37§ (25.6)	δ:1.54 (29.7); ε:2.92 (42.6)
Val76	8.64	4.36 (n.d.)	1.63 (35.9)	0.29 (21.6), 0.40 (20.8)	
Glu77	8.09	4.49	1.58, 1.99	2.09	
Asn78	9.06	5.28 (51.8)	2.28, 3.18 (n.d.)		NHδ: 8.52
His79	8.54	4.90	2.89§, 3.09§		δ: 6.56; ε: 8.01
Thr80	8.14	4.54 (61.6)	4.30 (n.d.)	1.12 (22.4)	
Ala81	7.62	4.49 (53.4)	1.44 (22.3)		
Cys82	8.82	5.55 (54.4)	2.42, 3.04		
His83	9.24	4.85	3.21§, 3.41§		δ: 7.02; ε: 8.21
Cys84	8.35	5.22	2.72, 2.95		
Ser85	8.80	4.54	2.86, 3.24		
Thr86			n.d.		
Cys87					
Tyr88[a]			n.d.		δ: 6.94 (133.8); ε: 6.72 (n.d.)
Tyr89[a]		n.d.	n.d., n.d.		δ: 7.04 (133.8); ε: 6.82 (118.9)
His90		n.d.	3.15, 3.27 (30.4)		δ: 7.24 (120.5); ε: 8.43*

^{13}C chemical shifts were referenced to the α-anomeric chemical shift of ^{13}C-labelled glucose (δ_C 94.8 versus 2,2-dimethyl-2-silapentane-5-sulfonic acid) at 328K, pH 5.1. ^{13}C chemical shift-assignment is based on chemical shift data of the intact α-subunit (15). * indicates tentative assignment. n.d. stands for 'not determined'. § indicates value taken from the spectrum recorded at the Varian Unity Plus 750 MHz spectrometer. [a] In our previous list (15) the chemical shift values of δ and ε have been interchanged accidentally.