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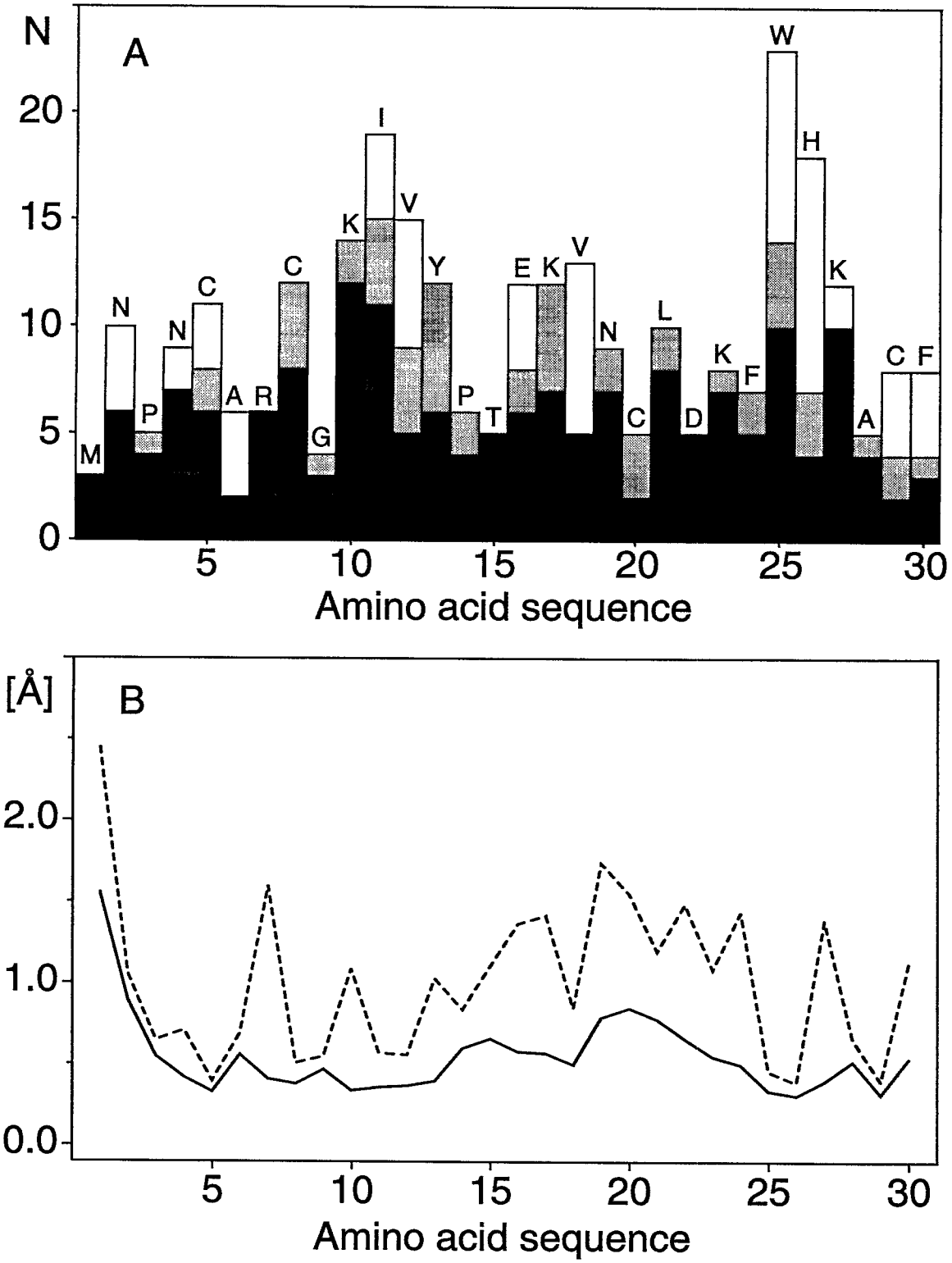
Table 1: Proton chemical shifts for ZF-1 in H_2O at 25 °C and pH 5.5.

		Chemical shift, δ (ppm)[a]		
Residue	NH	αH	βH	Others
1 Met	8.28	4.33	1.97, 1.90	γCH_2 2.49, 2.53; εCH_2 2.08; acetyl CH_3 2.00
2 Asn	8.21	4.99	2.36, 2.50	δNH_2 7.59, 7.30
3 Pro		4.38	1.76, 1.64	γCH_2 1.13, 0.93; δCH_2 3.71, 3.39
4 Asn	8.17	4.67	2.40, 2.14	δNH_2 7.31, 6.73
5 Cys	8.45	4.01	2.43, 3.41	
6 Ala	8.85	3.93	0.38	
7 Arg	9.16	4.71	2.38, 2.35	γCH_2 1.85; δCH_2 3.53, 3.49; εNH_2 7.57
8 Cys	8.29	4.99	3.40, 3.05	
9 Gly	8.05	3.87, 4.24		
10 Lys	8.33	4.66	2.04, 2.18	γCH_2 1.63; 1.56; δCH_2 1.75; εCH_2 3.08
11 Ile	8.31	3.91	1.56	γCH 0.34; γCH_2 1.39, 0.85; δCH_3 0.78
12 Val	8.38	4.01	1.47	γCH_3 0.09, 0.70
13 Tyr	9.24	4.51	2.81, 3.38	δH 7.28; εH 6.83
14 Pro		4.15	2.50, 2.09	γCH_2 2.29, 2.15; δCH_2 4.06
15 Thr	7.86	4.26	4.47	γCH_3 1.35
16 Glu	7.75	4.73	2.65, 2.44	γCH_2 2.51
17 Lys	7.06	4.39	2.00	γCH_2 1.64, 1.47; δCH_2 1.33; εCH_2 2.82
18 Val	9.10	4.37	1.93	γCH_3 0.53, 0.82
19 Asn	8.75	5.44	2.74, 2.59	δNH_2 6.74, 6.51
20 Cys	8.48	4.52	2.63, 2.57	
21 Leu	9.50	4.01	2.23	γCH 1.74; δCH_3 1.06, 0.97
22 Asp	8.76	4.28	2.86, 2.86	
23 Lys	7.63	4.30	1.59, 1.18	γCH_2 1.41, 1.28; δCH_2 1.58; εCH_2 3.03
24 Phe	8.22	5.53	2.59, 2.59	δH 7.12; εH 7.34; ζH 7.33 ;
25 Trp	8.98	5.85	2.78, 3.58	δ^1H 7.03; ε^1NH 10.17; ε^3H 7.49; ζ^2H 7.38; ζ^3H 6.98; η^2H 7.21
26 His	8.45	4.98	3.80, 3.80	δH 7.63; εH 7.32; εNH 11.89
27 Lys	9.25	4.01	1.99, 1.90	γCH_2 1.46; δCH_2 1.76; εCH_2 3.00
28 Ala	8.98	4.38	1.56	
29 Cys	7.91	4.44	3.46, 3.46	
30 Phe	7.32	3.66	2.54, 2.81	δH 6.24; εH 6.71; ζH 6.96

[a] For methylene groups two chemical shifts are given only when both resonances are resolved or the existance of two degenerate resonances was confirmed using a double quantum spectrum. Stereospecifically assigned resonances are identified by underlined chemical shift values where the first number corresponds to the proton with the lower branch number, *e.g.* the β_2 proton.



(A) Number of ROE distance constraints per residue, N, used for the solution structure calculation of the ZF-1 peptide complexed with zinc. Black: intraresidual; dark grey: sequential; light grey: medium range constraints, (*i*, *i*+2) to (*i*, *i*+5); white: long range ROE constraints, (*i*, *i*>5). The amino acid sequence is given in the one letter code.

(B) Average r.m.s.d. *versus* the amino acid sequence for the backbone (N, C^{α} and C', solid line) and sidechain heavy atoms (dashed line) of the 20 refined conformers. The backbone atoms of residues 3 to 30 were superimposed for the r.m.s.d. calculation.