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Biochemistry, 1996, 35(39), 12723-12732, DOI:[10.1021/bi961149j](https://doi.org/10.1021/bi961149j)

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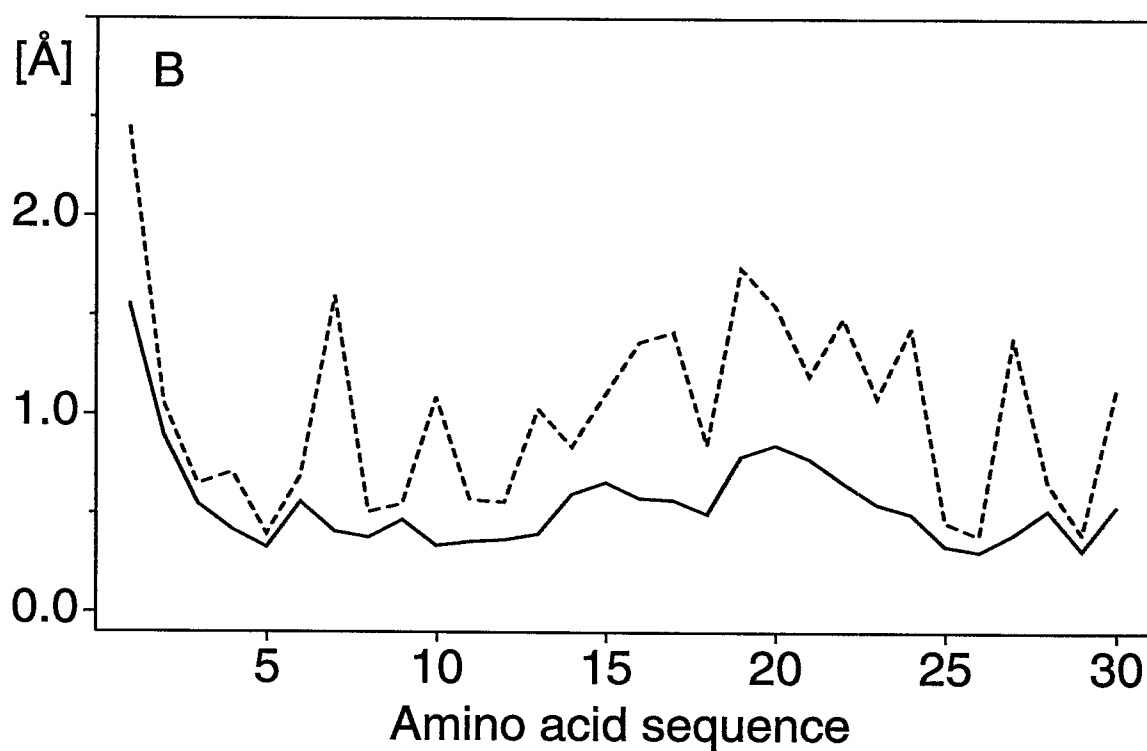
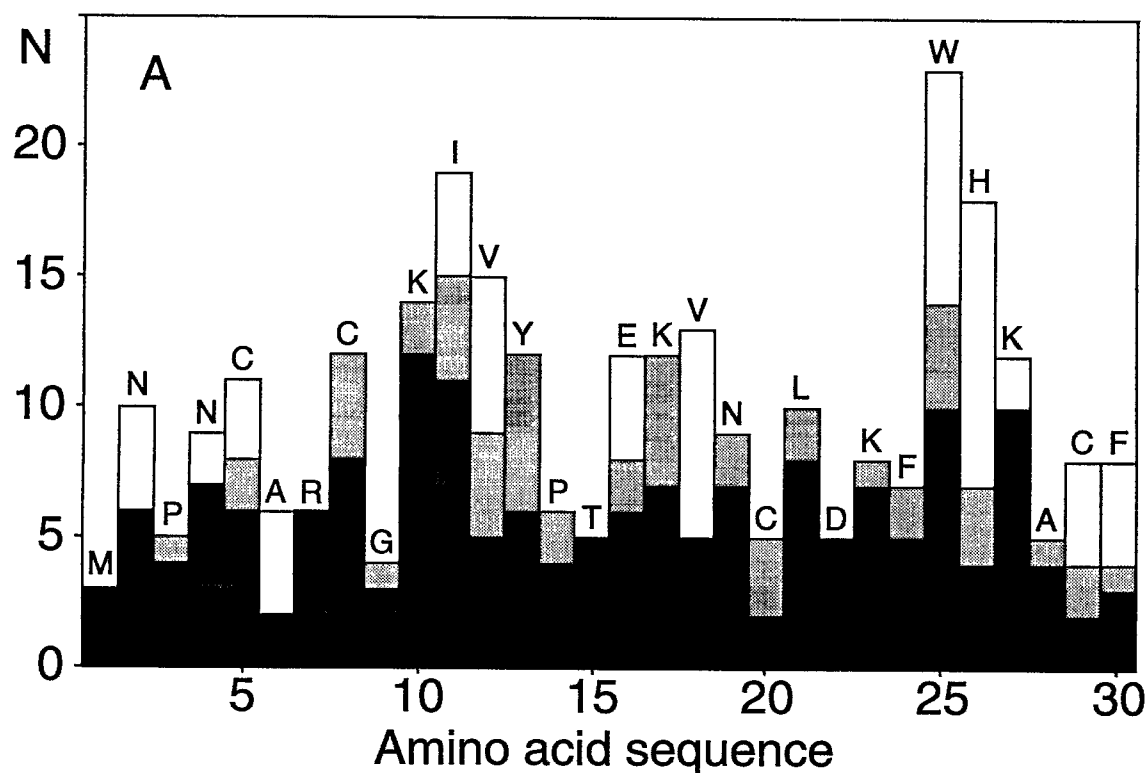
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Table 1: Proton chemical shifts for ZF-1 in H₂O at 25 °C and pH 5.5.

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

^a For methylene groups two chemical shifts are given only when both resonances are resolved or the existence 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.