Supplementary material for Blindauer *et al*. (August 7, 2001) *Proc. Natl. Acad. Sci. USA*, 10.1073/pnas.171120098

Table 2. ^{1}H NMR chemical shifts

Residue*	NH	CH(α)	CH(β)	CH(γ)	CH(δ)	CH(ε)
Thr-5	8.10	4.25	4.06	1.12		
Leu-6	7.86	4.68	1.11	1.54	0.76; 0.63	
Val-7	8.74	4.50	2.05	0.82; 0.74		
Lys-8	8.35	4.43	2.00; 1.82	1.51; 1.38	1.71	†
Cys-9	8.93	3.96	2.97; 2.92			
Ala-10	8.01	4.07	0.98			
Cys-11	7.95	4.63	3.69; 3.05			
Glu-12	9.29	4.12	2.18; 2.27	2.38		
Pro-13	—	4.48	2.19; 1.65	1.43; 1.32	3.64	
Cys-14	8.07	4.16	3.50; 3.32			
Leu-15	8.51	4.42	1.76	1.98	0.99; 0.89	
Cys-16	8.16	3.81	2.86; 2.79			
Asn-17	8.49	5.32	2.55; 2.26		7.22; 6.68	
Val-18	9.64	4.52	1.84	0.54; 0.42		
Asp-19	8.50	4.93	2.73; 2.40			
Pro-20	—	3.98/3.76‡	1.84	1.40; 1.10	3.24	
Ser-21	8.26	4.23	3.89; 3.83			
Lys-22	7.81	4.59	1.98; 1.60	1.35; 1.28	1.68	2.97
Ala-23	7.44	4.56	1.35			
Ile-24	7.72	4.03	1.66	1.15; 0.78	0.69	
Asp-25	8.46	5.27	2.74; 2.48			
Arg-26	8.94	4.57	1.79	1.56; 1.49	3.22; 3.04	
Asn-27	9.22	4.32	3.07; 2.80		7.58;6.87	
Gly-28	8.91	3.95; 3.41				
Leu-29	7.29	4.18	1.76	1.49	0.91; 0.84	
Tyr-30	7.45	5.37	2.45		6.87	6.74
Tyr-31	9.20	5.84	2.97; 2.59		6.79; 6.89§	6.49
Cys-32	10.09	4.68	3.57; 2.72			
Ser-33	8.42	4.80	4.39; 4.18			
Glu-34	9.41	3.78	1.97; 1.90	2.26		
Ala-35	8.13	3.87	1.14			
Cys-36	7.24	3.71	3.36; 2.89			
Ala-37	7.52	1.73	0.84			
Asp-38	7.83	4.46	2.63			
Gly-39	7.43	4.03; 3.94				
His-40	8.59	3.82	3.48; 3.11		6.69	7.78
Thr-41	7.39	4.15	4.08	1.25		
Gly-42	¶					
Gly-43	8.38	4.11; 3.97				
Ser-44	7.20	4.33	4.01; 3.88			
Lys-45	8.41	4.77	1.74; 1.68	1.44; 1.30	1.62	2.92
Gly-46	9.02	4.54; 3.87				

Cys-47	8.61	4.91	3.55; 2.83			
Gly-48	8.36	3.82; 3.63				
His-49	6.91	5.17	3.21; 2.80		7.27	8.10
Thr-50	¶					
Gly-51	¶					
Cys-52	7.54	4.60	3.28; 2.83			
Asn-53	8.62	5.17	2.92; 2.60		7.50	6.77
Cys-54	8.14	3.98	3.12; 2.87			
His-55	6.02	3.79	3.20; 3.10		7.28	8.31
Gly-56	8.54	4.22; 3.69				

* The numbering refers to the full-length protein; residue M1 was not present in the recombinant protein; NH resonances for residues T2–T4 were not observable; crosspeaks for remaining protons of these residues were unassignable because of overlap and absence of interresidue NOEs.

† Unassigned due to crosspeak overlap.

‡ Two shifts were observed for CH(α), possibly due to cis/trans-isomerism. The major peak at 3.76 ppm was used in the structure determination, but use of the minor peak led to only minor local changes in the structure.

§ Two resonances for the δ protons are observed due to hindered rotation [CH/π interaction with CH(α) of Ala-37].

¶ Unassigned; no NH resonance observed, no interresidue NOEs detected.