

Supporting Information

Table 1. ¹H NMR chemical shifts^a and sequence-specific assignments of *Anabaena variabilis* plastocyanin^b

Residue	NH	α CH	β CH	Others
Glu 1		3.94	1.71, 2.00	γ CH ₂ 2.00, 2.18
Thr 2	8.62	5.40	3.73	γ CH ₃ 0.94
Tyr 3	8.74	4.67	2.96, 2.37	δ CH 6.97; ϵ CH 6.85
Thr 4	8.60	5.09	3.83	γ CH ₃ 1.12
Val 5	9.29	4.42	1.73	γ CH ₃ 1.22, 0.64
Lys 6	9.04	4.83	2.04, 1.79	γ CH ₂ 1.27; δ CH ₂ 1.72; ϵ CH ₂ 2.97
Leu 7	8.82	4.00	2.16, 0.92	γ CH 1.61; δ CH ₃ 0.90
Gly 8	7.64	4.62, 3.95		
Ser 9	8.65	4.56	3.68, 4.35	
Asp 10	9.45	4.26	2.68, 2.77	
Lys 11	7.47	4.36	1.53, 2.00	γ CH ₂ 1.41; δ CH ₂ 1.67; ϵ CH ₂ 2.99
Gly 12	8.29	4.11, 3.31		
Leu 13	7.43	4.44	1.65, 1.41	γ CH 1.40; δ CH ₃ 0.85, 0.78
Leu 14	8.38	4.07	1.71, 0.96	γ CH 1.55; δ CH ₃ 0.12, 0.69
Val 15	7.46	4.69	2.25	γ CH ₃ 0.82, 0.56
Phe 16	8.64	5.06	2.51, 3.14	δ CH 6.93; ϵ CH 7.04; ζ CH 7.21
Glu 17	8.97	4.92	2.08, 1.62	γ CH ₂ 2.13, 2.10
Pro 18		4.98	2.59, 2.36	γ CH ₂ 1.87, 2.15; δ CH ₂ 4.15, 3.71
Ala 19	8.08	4.40	1.74	
Lys 20	7.36	5.53	1.73	γ CH ₂ 1.40; δ CH ₂ 1.66; ϵ CH ₂ 2.96
Leu 21	7.73	4.54	1.34, 1.30	γ CH 1.26; δ CH ₃ 0.58, 0.50
Thr 22	8.22	5.28	3.83	γ CH ₃ 1.08
Ile 23	8.92	4.60	2.21	γ CH ₃ 0.11; γ CH ₂ 0.63, 0.14; δ CH ₃ -0.47
Lys 24	8.95	4.95	1.61	γ CH ₂ 1.54; δ CH ₂ 1.74; ϵ CH ₂ 3.03
Pro 25		3.85	2.47, 1.89	γ CH ₂ 2.19; δ CH ₂ 3.70, 3.55
Gly 26	7.10	4.32, 3.82		
Asp 27	7.90	4.97	3.19, 2.80	
Thr 28	8.60	5.24	4.04	γ CH ₃ 1.03
Val 29	9.18	4.54	1.64	γ CH ₃ 0.72, -0.06
Glu 30	9.18	4.51	1.62, 1.85	γ CH ₂ 2.00, 1.85
Phe 31	9.13	5.26	2.87, 2.74	δ CH 6.95; ϵ CH 6.30; ζ CH 6.87
Leu 32	8.93	4.59	1.63, 1.24	γ CH 1.34; δ CH ₃ 0.81
Asn 33	9.30	4.92	3.18, 2.59	δ NH ₂ 5.17, 6.42
Asn 34	8.77	5.14	3.53, 2.24	δ NH ₂ 7.72, 7.94
Lys 35	8.09	4.71	1.82, 1.70	γ CH ₂ 1.32, 1.29; δ CH ₂ 1.74; ϵ CH ₂ 3.06

Table 1. (continued)

Residue	NH	α CH	β CH	Others
Val 36	8.92	3.66	2.41	γ CH ₃ 0.70, 0.93
Pro 37		3.64	2.18, 1.94	γ CH ₂ 1.75, 1.51; δ CH ₂ 3.51, 3.23
Pro 38		4.90	2.39, 1.81	γ CH ₂ 1.81, 1.74; δ CH ₂ 3.53
His 39	7.16	5.96	3.54, 2.58	δ CH 7.50; ϵ CH 7.05; ϵ NH 11.52
Asn 40	9.83	4.61	2.69, 3.68	δ NH ₂ 7.12, 7.66
Val 41	6.92	4.26	1.46	γ CH ₃ 0.26, -0.23
Val 42	9.40	4.00	1.48	γ CH ₃ 0.77, 0.73
Phe 43	8.69	4.31	3.29, 2.95	δ CH 7.21; ϵ CH 6.93; ζ CH 6.63
Asp 44	8.36	4.49	2.78, 2.47	
Ala 45	8.60	3.72	1.43	
Ala 46	8.42	4.42	1.42	
Leu 47	8.64	4.60	1.80, 1.68	γ CH 1.64; δ CH ₃ 0.91, 0.80
Asn 48	8.03	5.25	3.46, 2.22	δ NH ₂ 6.39, 7.18
Pro 49		4.30	2.53, 1.50	γ CH ₂ 1.67, 1.51; δ CH ₂ 2.57, 2.27
Ala 50	6.96	4.53	1.38	
Lys 51	7.92	3.86	1.98	γ CH ₂ 1.45; δ CH ₂ 1.67; ϵ CH ₂ 3.06
Ser 52	8.20	4.90	3.77, 3.66	
Ala 53	9.18	4.23	1.51	
Asp 54	8.40	4.36	2.62, 2.43	
Leu 55	8.12	4.08	1.81, 1.60	γ CH 1.42; δ CH ₃ 1.10, 0.85
Ala 56	7.54	3.74	1.38	
Lys 57	8.52	4.00	1.99, 1.61	γ CH ₂ 1.46; δ CH ₂ 1.71; ϵ CH ₂ 2.97
Ser 58	7.71	4.24	3.96	
Leu 59	6.86	3.97	0.75, 0.06	γ CH 1.44; δ CH ₃ -0.08, -0.47
Ser 60	6.93	4.38	4.09, 4.15	γ OH 5.80
His 61	9.60	4.71	3.34, 2.93	δ CH 6.76; ϵ CH 8.49
Lys 62	8.76	3.87	1.79	γ CH ₂ 1.42, 1.48; δ CH ₂ 1.69; ϵ CH ₂ 3.00
Gln 63	8.36	4.09	2.02	γ CH ₂ 2.49, 2.45
Leu 64	8.19	4.18	1.73, 1.15	γ CH 1.81; δ CH ₃ 0.86, 0.66
	8.24	4.21	1.65, 1.07	
Leu 65	9.46	4.40	1.83, 1.18	γ CH 1.76; δ CH ₃ 0.74, 0.67
Met 66	8.07	4.46	2.09	γ CH ₂ 2.69, 2.50; ϵ CH ₃ 2.04
Ser 67	8.34	5.09	3.84, 3.63	
Pro 68		4.03	2.25, 1.77	γ CH ₂ 2.43, 1.99; δ CH ₂ 3.77, 3.94
Gly 69	8.98	4.46, 3.65		

Table 1. (continued)

Residue	NH	α CH	β CH	Others
Gln 70	7.50	4.43	2.16, 2.22	γ CH ₂ 2.48, 2.57; δ NH ₂ 7.18, 7.65
Ser 71	8.63	5.74	3.80, 3.70	
Thr 72	8.70	4.62	3.75	γ CH ₃ 0.83
Ser 73	8.13	5.68	3.60, 3.64	
Thr 74	9.49	4.71	4.10	γ CH ₃ 0.86
Thr 75	9.10	4.88	3.79	γ CH ₃ 0.97
Phe 76	9.15	4.05	3.08, 2.36	δ CH 6.72; ϵ CH 6.10; ζ CH 6.63
Pro 77	4.40	4.40	2.37, 2.09	γ CH ₂ 1.91, 2.00; δ CH ₂ 3.29, 3.79
Ala 78	8.82	3.75	1.39	
Asp 79	7.97	4.58	2.94, 2.44	
Ala 80	7.53	4.39	1.49	
Pro 81		4.34	2.31, 1.77	γ CH ₂ 1.93, 2.00; δ CH ₂ 3.93, 3.84
Ala 82	8.35	4.14	1.39	
Gly 83	8.82	4.70, 3.82		
Glu 84	8.46	4.98	1.92, 1.87	γ CH ₂ 2.25
Tyr 85	10.14	5.23	3.68, 3.17	δ CH 7.35; ϵ CH 6.69; η OH 9.54
Thr 86	8.60	5.03	4.26	γ CH ₃ 1.29
Phe 87	8.54	5.07	1.51, 1.08	δ CH 6.22; ϵ CH 5.89; ζ CH 6.58
Tyr 88	8.91	5.31	3.21, 3.06	δ CH 6.62; ϵ CH 6.74
Cys 89	7.72	5.28	3.33, 2.88	
Glu 90	9.99	4.27	2.47, 2.05	γ CH ₂ 2.70, 2.37
Pro 91		4.11	1.78, 1.08	γ CH ₂ 1.65, 1.58; δ CH ₂ 3.33, 5.26
His 92	8.55	5.14	3.40, 3.80	δ CH 7.12; ϵ CH 7.57
Arg 93	8.43	3.90	2.43	γ CH ₂ 1.40, 1.16; δ CH ₂ 2.60, 2.16; ϵ NH 6.66
Gly 94	9.07	3.85		
Ala 95	7.51	4.57	1.61	
Gly 96	8.04	4.49, 3.76		
Met 97	7.60	4.50	2.17, 1.37	γ CH ₂ 1.89, 1.44; ϵ CH ₃ 0.76
Val 98	7.92	4.87	1.92	γ CH ₃ 1.02, 0.97
Gly 99	8.93	4.65, 2.51		
Lys 100	8.23	5.34	1.69, 1.60	γ CH ₂ 1.34; δ CH ₂ 1.60, 1.49; ϵ CH ₂ 2.82, 2.86
Ile 101	9.45	4.94	1.77	γ CH ₃ 0.38; γ CH ₂ 1.17; δ CH ₃ 0.76
Thr 102	9.22	5.05	4.11	γ CH ₃ 1.03
Val 103	9.30	4.17	2.35	γ CH ₃ 0.65, 0.32
Ala 104	9.22	4.42	1.28	
Gly 105	7.78	3.82, 3.69		

^a Chemical shifts are expressed relative to 1,4-dimethyl-4-silapentane-1-sulfonate. The chemical shifts are generally accurate to 0.02 ppm.

^b At pH 7.0 and 298 K.

Table 2. ^{13}C NMR Chemical Shifts^a of *A.v.* Plastocyanin^b.

Residue	CO	C $_{\alpha}$	C $_{\beta}$	Others
Glu 1	172.1	55.9	31.0	γ :35.8
Thr 2	173.1	61.2	70.4	γ :21.4
Tyr 3	174.3	56.7	42.5	δ :133.4 ; ϵ :117.7
Thr 4	174.0	62.6	70.5	γ :21.9
Val 5	175.2	61.3	34.9	γ :21.8(1.22),22.1(0.64)
Lys 6	177.3	56.7	34.3	γ :25.9 ; δ :29.6 ; ϵ :42.0
Leu 7	174.9	54.2	40.4	γ :27.0; δ :25.9
Gly 8	173.9	43.6		
Ser 9		56.8	65.3	
Asp 10		57.8	39.8	
Lys 11	176.4	55.7	32.3	γ :25.4 ; δ :28.8 ; ϵ :42.0
Gly 12	173.2	45.5		
Leu 13	177.5	54.1	42.1	γ :27.8; δ :25.0(0.85),22.5(0.79)
Leu 14	174.6	52.9	38.9	γ :25.2; δ :25.5(0.70),21.6(0.14)
Val 15	179.4	58.1	35.7	γ :22.2(0.83),18.8(0.57)
Phe 16	175.8	57.5	40.6	δ :131.7 ; ϵ :132.3 ; ζ :129.2
Glu 17		52.6	33.7	γ :36.6
Pro 18	173.2	63.8	34.9	γ :24.9 ; δ :50.5
Ala 19	177.0	52.6	19.4	
Lys 20	175.0	54.5	35.4	γ :24.8 ; δ :29.6 ; ϵ :42.1
Leu 21	174.8	55.0	46.3	γ :26.9; δ :25.8(0.59),25.4(0.50)
Thr 22		61.5	69.8	γ :21.6
Ile 23	173.2	58.8	40.5	γ Me:17.2 ; γ :25.4 ; δ :13.2
Lys 24		53.2	32.3	γ :24.8 ; δ :29.0 ; ϵ :42.0
Pro 25	177.6	64.6	28.0	γ :26.5 ; δ :50.4
Gly 26	174.9	45.0		
Asp 27	174.8	55.2	42.3	
Thr 28		62.0	71.5	γ :21.7
Val 29		60.7	33.3	γ :21.7(0.73),22.2(-0.06)
Glu 30	173.6	54.5	31.3	γ :36.3
Phe 31	173.9	56.8	39.0	δ :132.0 ; ϵ :128.5 ; ζ :130.6
Leu 32	175.6	53.2	45.2	γ :27.4; δ :25.6(0.82),23.6(0.82)
Asn 33	172.9	54.3	38.8	
Asn 34	173.6	55.3	41.1	
Lys 35		53.9	38.5	γ :25.8 ; δ :28.4 ; ϵ :42.5

Table 2. (continued)

Residue	CO	α C	β C	Others
Val 36		62.0	31.3	γ :23.7(0.93),20.7(0.71)
Pro 37		61.6	31.2	γ :27.0 ; δ :50.5
Pro 38	173.1	62.0	37.5	γ :24.7; δ :51.0 γ :24.2 ^c
His 39	175.5	54.5	38.6	δ :119.7; ϵ :138.0
Asn 40	171.5	52.7	39.4	
Val 41	173.7	61.8	34.8	γ :20.1(0.26),20.4(-0.22)
Val 42	174.2	61.7	34.5	γ :21.7(0.77),21.5(0.73)
Phe 43		57.4	37.6	δ :132.0 ; ϵ :130.7 ; ζ :127.8
Asp 44	177.2	55.3	45.3	
Ala 45	176.1	54.9	19.7	
Ala 46	175.4	52.4	20.6	
Leu 47	175.3	53.2	39.3	γ :25.9; δ :25.9(0.91),22.3(0.81)
Asn 48		51.3	40.3	
Pro 49	176.8	65.5	32.8	γ :28.8; δ :49.5
Ala 50	175.5	50.8	20.1	
Lys 51	175.2	57.2	30.3	γ :25.0 ; δ :29.5 ; ϵ :42.4
Ser 52		55.3	64.5	
Ala 53	180.5	54.6	18.4	
Asp 54	178.8	57.4	40.5	
Leu 55	179.3	57.3	41.6	γ :27.3; δ :26.4(1.11),21.6(0.85)
Ala 56	181.0	55.6	18.5	
Lys 57	179.9	60.2	32.3	γ :25.0 ; δ :28.4; ϵ :42.5
Ser 58	174.7	61.2	63.1	
Leu 59	176.4	54.6	42.2	γ :25.0; δ :26.2(-0.47),20.0(-0.08)
Ser 60	172.0	60.6	65.9	
His 61	175.1	54.5	29.4	δ :119.1; ϵ :137.5
Lys 62	177.2	57.7	33.3	γ :25.5; δ :29.1 ; ϵ :42.0
Gln 63	175.7	56.7	28.1	γ :33.8
Leu 64	177.9	55.7	42.2	γ :28.1; δ :25.4(0.87),22.6(0.68)
		55.6 ^d		
Leu 65	176.8	55.2	41.2	γ :27.0; δ :25.8(0.75),24.3(0.68)
Met 66	177.3	56.2	33.5	γ :31.9 ; ϵ :16.3
Ser 67		56.1	63.8	
Pro 68	177.1	63.9	31.8	γ :30.3; δ :51.6
Gly 69	174.6	45.2		

Table 2. (continued)

Residue	CO	α C	β C	Others
Gln 70	174.5	56.8	31.0	γ :35.0
Ser 71	173.6	56.4	67.4	
Thr 72	171.9	60.6	69.2	γ :19.1
Ser 73	173.6	57.5	66.0	
Thr 74	173.2	62.2	72.5	γ :24.0
Thr 75	174.2	61.9	69.6	γ :21.4
Phe 76		56.5	38.2	δ :130.7 ; ϵ :130.6 ; ζ :129.1
Pro 77	177.3	62.1	32.7	γ :27.5 ; δ :50.4
Ala 78	176.8	54.5	18.1	
Asp 79	176.0	51.6	39.5	
Ala 80		50.7	17.3	
Pro 81		62.3	32.1	γ :27.5 ; δ :50.4
Ala 82	177.3	52.3	19.0	
Gly 83	172.5	43.6		
Glu 84	176.1	56.7	36.3	γ :37.3
Tyr 85	175.9	57.1	39.4	
Thr 86	173.5	64.0	69.6	γ :21.0
Phe 87		54.7	40.3	δ :131.8 ; ϵ :129.7 ; ζ :126.9
Tyr 88	171.9	55.3	40.8	δ :133.1 ; ϵ :117.3
Cys 89	178.5	56.9	33.4	
Glu 90		61.8	27.5	γ :39.7
Pro 91	179.5	66.2	30.4	γ :27.7 ; δ :49.7
His 92	177.2	56.0	32.9	δ :116.2 ; ϵ :138.6
Arg 93		61.0	30.2	γ :26.2 δ :43.5
Gly 94	174.5	46.2		
Ala 95	178.1	51.4	19.5	
Gly 96	174.1	45.1		
Met 97	171.9	57.9	30.8	γ :37.2 ϵ :19.2
Val 98	175.3	60.9	36.5	γ :21.2(1.02),20.9(0.97)
Gly 99	171.6	44.1		
Lys 100		55.4	37.0	γ :24.7 ; δ :29.3 ; ϵ :42.0
Ile 101	175.3	59.1	42.3	γ Me:18.1 ; γ :29.8 ; δ :14.3
Thr 102	173.3	61.9	69.8	γ :21.0
Val 103	176.0	61.1	32.0	γ :21.3(0.66),23.8(0.32)
Ala 104	175.5	52.0	20.5	
Gly 105		45.9		

^a Chemical shifts are expressed relative to 1,4-dimethyl-4-silapentane-1-sulfonate. The chemical shifts are generally accurate to 0.1 ppm.

^b At pH 7.0 and 298 K.

^c The assignment of the second folded conformation of *cis*Pro 38 - His 39 peptide bond.

^d The assignment of the second conformation of Leu 64.

Table 3. ^{15}N NMR Chemical Shifts^a and Sequence-Specific Assignments of *Anabaena variabilis* Plastocyanin^b

Residue	Backbone	Sidechain	Residue	Backbone	Sidechain
Glu 1			Thr 28	115.9	
Thr 2	120.3		Val 29	127.3	
Tyr 3	127.4		Glu 30	129.5	
Thr 4	119.3		Phe 31	126.6	
Val 5	130.6		Leu 32	126.0	
Lys 6	127.2		Asn 33	128.0	δ 105.5
Leu 7	122.7		Asn 34	130.6	δ 116.1
Gly 8	115.4		Lys 35	117.6	
Ser 9	120.3		Val 36	116.0	
Asp 10	121.6		Pro 37		
Lys 11	116.6		Pro 38		
Gly 12	109.7		His 39	113.3	ϵ 165.0
Leu 13	118.1		Asn 40	123.8	δ 106.6
Leu 14	125.7		Val 41	109.7	
Val 15	113.3		Val 42	129.1	
Phe 16	120.6		Phe 43	126.2	
Glu 17	122.9		Asp 44	124.9	
Pro 18			Ala 45	128.9	
Ala 19	117.6		Ala 46	118.2	
Lys 20	116.5		Leu 47	123.9	
Leu 21	122.2		Asn 48	115.2	δ 116.1
Thr 22	122.0		Pro 49		
Ile 23	121.6		Ala 50	116.2	
Lys 24	120.1		Lys 51	121.2	
Pro 25			Ser 52	110.5	
Gly 26	114.6		Ala 53	134.8	
Asp 27	121.6		Asp 54	120.8	

Table 3. (continued)

residue	Backbone	Sidechain	residue	Backbone	Sidechain
Leu 55	124.4		Pro 81		
Ala 56	120.3		Ala 82	125.3	
Lys 57	121.6		Gly 83	108.1	
Ser 58	115.9		Glu 84	120.5	
Leu 59	121.3		Tyr 85	126.2	
Ser 60	111.8		Thr 86	122.2	
His 61	122.0		Phe 87	127.1	
Lys 62	123.8		Tyr 88	116.0	
Gln 63	120.9	ϵ 113.3	Cys 89	125.9	
Leu 64	122.29,122.24 ^c		Glu 90	126.3	
Leu 65	125.6		Pro 91		
Met 66	122.6		His 92	116.4	
Ser 67	114.3		Arg 93	130.1	ϵ 85.6
Pro 68			Gly 94	108.3	
Gly 69	113.6		Ala 95	122.4	
Gln 70	120.6	ϵ 112.2	Gly 96	107.1	
Ser 71	116.7		Met 97	125.1	
Thr 72	116.9		Val 98	126.6	
Ser 73	118.6		Gly 99	118.7	
Thr 74	121.9		Lys 100	118.3	
Thr 75	127.8		Ile 101	128.3	
Phe 76	132.3		Thr 102	126.7	
Pro 77			Val 103	129.4	
Ala 78	123.9		Thr 104	134.4	
Asp 79	113.8		Gly 105	114.6	
Ala 80	125.2				

^a The chemical shifts are generally accurate to 0.1 ppm.

^b At pH 7.0 and 298 K.

^c Assignment of the second conformation of Leu 64.

Table 4. Relaxation parameters for ^{15}N of A.v. PCu at 11.7 T and 298 K^a.

Residue	R_1/s^{-1}	esd	R_2/s^{-1}	esd	NOE	esd	S^2	esd	S^2	esd	S_f^2	esd	τ_i/ps	esd	R_{zz}/s^{-1}	esd	$\chi^{2,b}$
3	2.136	0.004	7.930	0.070	0.748	0.022	0.797	0.013	0.857	0.009	2251.7	1053.6	23.3	2.3	0.41	0.04	0.00
4	1.955	0.005	7.361	0.039	0.709	0.007	0.750	0.002									0.00
5	2.192	0.010	7.320	0.100	0.765	0.023	0.860	0.004									79.92*
6	2.250	0.005	7.758	0.029	0.739	0.017	0.823	0.006	0.877	0.007	1805.5	663.3					0.00
7	2.258	0.006	7.790	0.040	0.760	0.011	0.874	0.002									80.40*
8	2.104	0.005	8.250	0.060	0.756	0.011	0.823	0.003			12.8	4.7			0.55	0.06	0.00
10	2.116	0.009	8.930	0.090	0.698	0.012	0.818	0.004			40.9	5.3			1.24	0.09	0.00
11	2.010	0.060	11.760	0.230	0.720	0.024	0.800	0.024			27.4	10.2			4.01	0.34	0.00
12	2.150	0.007	8.460	0.110	0.722	0.008	0.849	0.003			36.9	4.4			0.33	0.11	0.00
13	2.164	0.007	8.470	0.070	0.703	0.005	0.829	0.003	0.821	0.004	2263.2	1327.1	40.9	2.3	0.79	0.08	0.00
14	2.103	0.006	7.462	0.028	0.764	0.011	0.794	0.007			21.8	4.3					0.00
15	2.160	0.005	8.076	0.039	0.747	0.008	0.851	0.002							0.25	0.04	0.13
16	2.230	0.007	8.546	0.035	0.750	0.009	0.883	0.003									69.76*
17	2.203	0.007	7.726	0.041	0.738	0.009	0.855	0.002							0.18	0.02	6.71*
20	2.013	0.004	7.524	0.012	0.720	0.024	0.790	0.002									0.00
21	2.085	0.003	7.740	0.050	0.725	0.008	0.795	0.009	0.844	0.003	1190.4	243.6			0.39	0.06	0.00
22	1.988	0.005	7.720	0.050	0.663	0.008	0.769	0.002			43.4	2.7			0.18	0.06	0.00
23	2.199	0.008	8.100	0.050	0.765	0.009	0.856	0.004			10.4	5.3					0.00
24	2.188	0.008	8.210	0.040	0.757	0.007	0.865	0.003			17.4	4.4					0.16
26	2.211	0.005	7.530	0.070	0.735	0.006	0.755	0.013	0.858	0.005	2891.8	391.5			0.24	0.07	0.00
27	2.249	0.005	8.360	0.060	0.755	0.018	0.875	0.004			19.5	13.0			0.58	0.08	0.00
28	2.181	0.007	8.480	0.080	0.767	0.012	0.853	0.003									1.59
29	2.199	0.007	8.280	0.050	0.766	0.016	0.875	0.003									34.25*
30	2.235	0.005	7.710	0.060	0.776	0.021	0.870	0.002									1.92
31	2.188	0.008	7.720	0.060	0.737	0.017	0.842	0.004			29.2	8.9					14.31*
32	2.208	0.007	7.642	0.035	0.761	0.046	0.825	0.004			91.1	14.4					0.00
33	2.271	0.007	7.810	0.130	0.768	0.026	0.813	0.040	0.871	0.010	5172.2	2794.9					0.00
34	2.198	0.007	7.630	0.050	0.760	0.010	0.799	0.014	0.850	0.005	3255.2	1622.8					0.00
39	2.162	0.008	7.900	0.130	0.737	0.010	0.836	0.004			23.5	5.5					1.53
40	2.162	0.007	7.640	0.060	0.752	0.007	0.817	0.012	0.847	0.004	1499.9	607.7					0.00
41	2.196	0.008	7.660	0.110	0.766	0.006	0.810	0.030	0.849	0.007	3524.9	2195.5					0.00
42	2.189	0.009	7.850	0.080	0.752	0.024	0.856	0.003									3.11
43	2.265	0.009	8.090	0.050	0.745	0.012	0.860	0.013	0.894	0.015	1248.6	748.8					0.00
44	2.244	0.009	8.690	0.090	0.760	0.010	0.891	0.004			20.3	8.5			0.20	0.10	0.00
45	2.089	0.011	8.360	0.080	0.738	0.008	0.814	0.005			20.7	3.6			0.74	0.09	0.00
46	2.017	0.005	8.510	0.060	0.787	0.009	0.821	0.002			10.6	2.7			0.51	0.06	0.00
47	1.901	0.006	7.560	0.050	0.747	0.009	0.740	0.003							0.66	0.05	0.00
48	2.076	0.004	7.886	0.030	0.776	0.007	0.823	0.002							0.13	0.04	1.10
50	2.050	0.005	8.070	0.050	0.738	0.006	0.814	0.002			21.3	2.8			0.26	0.05	0.00

Residue	R_1/s^{-1}	esd	R_2/s^{-1}	esd	NOE	S^2	esd	S^2	esd	S^2	esd	S^2	esd	τ_i/ps	esd	R_{ex}/s^{-1}	esd	$\chi^{2,b}$
51	2.233	0.004	8.460	0.080	0.748	0.022	0.871	0.002	0.859	0.005	1966.1	448.7	0.43	0.08	2.25			
52	2.158	0.007	7.860	0.080	0.746	0.006	0.807	0.013	0.859	0.005	1966.1	448.7	1.27	0.21	0.00			
53	2.255	0.027	10.000	0.180	0.779	0.008	0.908	0.011	0.859	0.005	1966.1	448.7	1.60	0.15	0.61			
54	2.132	0.022	9.810	0.110	0.802	0.068	0.857	0.009	0.859	0.005	1966.1	448.7	1.60	0.15	0.06			
55	2.209	0.004	8.870	0.070	0.775	0.008	0.875	0.002	0.859	0.005	1966.1	448.7	0.62	0.07	1.09			
56	2.205	0.006	8.710	0.090	0.756	0.011	0.882	0.003	0.859	0.005	1966.1	448.7	0.21	0.10	0.00			
57	2.172	0.006	8.570	0.050	0.783	0.032	0.884	0.002	0.859	0.005	1966.1	448.7	0.17	0.06	1.59			
58	2.130	0.003	8.240	0.340	0.783	0.007	0.863	0.001	0.859	0.005	1966.1	448.7	0.17	0.06	0.26			
59	2.265	0.005	8.380	0.060	0.777	0.006	0.886	0.002	0.859	0.005	1966.1	448.7	0.17	0.06	0.55			
60	2.085	0.008	8.150	0.080	0.779	0.006	0.841	0.003	0.859	0.005	1966.1	448.7	0.15	0.07	1.80			
61	2.174	0.007	8.180	0.060	0.763	0.011	0.855	0.004	0.859	0.005	1966.1	448.7	0.15	0.07	0.00			
62	2.131	0.017	9.020	0.090	0.765	0.012	0.836	0.006	0.859	0.005	1966.1	448.7	1.25	0.10	2.10			
63	2.072	0.006	8.530	0.090	0.757	0.079	0.822	0.003	0.859	0.005	1966.1	448.7	0.78	0.10	0.11			
64	2.070	0.003	7.420	0.080	0.717	0.013	0.797	0.003	0.859	0.005	1966.1	448.7	0.36	0.06	0.11			
65	2.186	0.006	7.290	0.070	0.723	0.012	0.755	0.013	0.846	0.006	2234.8	428.2	0.36	0.06	0.00			
66	2.035	0.007	7.290	0.017	0.752	0.012	0.764	0.004	0.802	0.005	1935.4	748.4	0.36	0.06	0.00			
67	1.914	0.007	7.588	0.037	0.702	0.007	0.769	0.002	0.802	0.005	1935.4	748.4	0.36	0.06	1.95			
69	2.085	0.008	6.794	0.040	0.669	0.007	0.680	0.007	0.818	0.004	1837.7	126.0	0.36	0.06	0.00			
70	2.071	0.004	7.870	0.060	0.712	0.010	0.801	0.003	0.831	0.003	497.9	126.9	0.36	0.06	0.00			
71	2.078	0.006	7.289	0.019	0.680	0.007	0.782	0.003	0.831	0.003	497.9	126.9	0.36	0.06	0.00			
72	2.221	0.008	8.020	0.050	0.736	0.008	0.860	0.003	0.831	0.003	497.9	126.9	0.36	0.06	0.00			
73	1.938	0.008	8.260	0.090	0.704	0.007	0.745	0.003	0.831	0.003	497.9	126.9	0.36	0.06	2.75			
74	2.160	0.008	8.330	0.060	0.738	0.017	0.843	0.004	0.831	0.003	497.9	126.9	0.36	0.06	0.00			
75	2.096	0.009	7.970	0.060	0.735	0.014	0.809	0.004	0.831	0.003	497.9	126.9	0.36	0.06	0.00			
76	2.230	0.009	8.060	0.060	0.765	0.006	0.883	0.003	0.831	0.003	497.9	126.9	0.36	0.06	0.00			
78	2.078	0.009	7.450	0.070	0.752	0.009	0.806	0.003	0.831	0.003	497.9	126.9	0.36	0.06	0.00			
79	2.086	0.007	7.288	0.030	0.743	0.020	0.731	0.008	0.816	0.007	2918.5	1006.6	0.36	0.06	0.00			
80	2.130	0.004	7.600	0.070	0.747	0.023	0.797	0.014	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
82	1.966	0.003	7.840	0.060	0.768	0.008	0.783	0.002	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
83	2.190	0.004	7.420	0.050	0.775	0.008	0.865	0.002	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
84	2.050	0.005	7.500	0.060	0.779	0.068	0.808	0.002	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
85	2.145	0.006	7.820	0.040	0.749	0.008	0.832	0.003	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
86	2.099	0.009	9.070	0.090	0.751	0.043	0.833	0.004	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
87	2.271	0.008	8.480	0.070	0.780	0.036	0.889	0.003	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
89	2.254	0.007	8.462	0.023	0.770	0.031	0.880	0.003	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
90	2.270	0.004	7.840	0.070	0.774	0.008	0.889	0.002	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
92	2.082	0.010	9.470	0.060	0.741	0.011	0.804	0.004	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
93	2.267	0.008	8.410	0.090	0.782	0.010	0.885	0.003	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
94	2.350	0.050	10.310	0.150	0.753	0.006	0.922	0.019	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			
95	2.081	0.006	8.010	0.060	0.757	0.040	0.818	0.002	0.840	0.009	1750.6	1157.1	0.36	0.06	0.00			

Residue	R_1/s^{-1}	esd	R_2/s^{-1}	esd	NOE	esd	S^2	esd	S_I^2	esd	τ_i/ps	esd	R_{zz}/s^{-1}	esd	$\chi^{2,b}$
96	2.161	0.008	8.050	0.090	0.775	0.006	0.841	0.003			3.2	3.1	0.29	0.10	0.00
97	2.194	0.006	8.964	0.038	0.777	0.031	0.877	0.002					0.61	0.05	0.05
98	2.163	0.005	8.470	0.050	0.749	0.009	0.845	0.003			19.2	4.8	0.57	0.06	0.00
99	2.243	0.007	8.370	0.050	0.764	0.007	0.881	0.003			14.7	5.7	0.11	0.06	0.00
100	2.135	0.005	8.167	0.027	0.723	0.008	0.831	0.003			31.5	4.7	0.35	0.03	0.00
101	2.165	0.008	7.640	0.070	0.720	0.022	0.831	0.004			40.0	10.2			2.80
102	2.157	0.007	8.230	0.070	0.769	0.017	0.862	0.003							1.03
103	2.207	0.006	7.670	0.100	0.765	0.023	0.863	0.002							12.21*
104	2.205	0.007	7.940	0.080	0.782	0.008	0.881	0.003							47.17*
105	1.043	0.002	2.658	0.023	-0.595	0.006	0.240	0.004	0.564	0.004	384.9	18.3			0.00

^a Model-free parameters were calculated with the overall rotational diffusion properties given in the manuscript. ^b Residues for which the χ^2 value exceeded the $\alpha = 0.05$ critical value for all models were parametrized with the most appropriate of models 1, 2 and 3 according to F-statistics testing and are indicated by a (*) after the χ^2 value.

Table 5. Relaxation parameters for backbone $^{13}\text{C}_\alpha$ of A.v.PCu at 11.7 T and 298 K^a.

Residue	R_1/s^{-1}	esd	R_2/s^{-1}	esd	NOE	esd	S^2	esd	S^2	esd	τ_1/ps	esd	R_{ex}/s^{-1}	esd	χ^2
4	1.750	0.180	22.700	1.400	1.261	0.116	0.863	0.051							1.84
6	2.070	0.230	27.800	3.000	1.683	0.251	0.879	0.081			242.2	330.4			2.51
10	1.650	0.110	29.800	2.200	1.185	0.326	0.969	0.046							4.02
11	1.550	0.075	19.000	1.200	1.116	0.162	0.778	0.030							5.64
13	1.522	0.140	20.500	2.000	1.289	0.156	0.791	0.050							1.16
14	1.630	0.140	30.700	3.000	1.383	0.107	0.776	0.084			43.6	21.5	9.46	3.61	0.00
16	1.990	0.120	25.600	2.900	1.406	0.203	0.905	0.065			236.9	316.3			0.10
17	2.200	0.240	23.600	2.700	1.191	0.114	0.991	0.074							4.02
18	1.451	0.076	25.400	2.200	1.252	0.080	0.820	0.039							4.01
19	1.845	0.048	24.500	0.800	1.171	0.058	0.960	0.018							6.44*
21	1.780	0.130	23.500	1.200	1.128	0.162	0.896	0.036							1.51
22	1.760	0.270	21.100	2.100	1.328	0.296	0.818	0.065							1.49
23	1.690	0.150	21.800	1.500	1.095	0.059	0.841	0.047							2.52
24	1.910	0.230	26.500	2.100	1.494	0.111	0.826	0.069			121.7	112.7	3.71	2.88	0.00
25	1.440	0.130	22.800	1.800	1.105	0.103	0.814	0.049							0.62
27	1.700	0.120	23.200	0.800	1.353	0.124	0.868	0.029							3.40
28	1.900	0.120	28.100	2.200	1.356	0.080	0.932	0.037							1.74
30	1.986	0.046	26.100	1.300	1.174	0.297	0.954	0.032			191.5	161.8			0.00
32	1.694	0.070	24.400	0.800	1.195	0.056	0.908	0.022			977.7	977.6			0.63
34	1.484	0.059	26.800	2.600	1.095	0.100	0.826	0.031							3.62
36	1.468	0.042	28.100	2.500	1.539	0.079	0.630	0.042							0.00
37	1.468	0.042	28.100	2.500	1.539	0.079	0.630	0.039			40.0	5.7	10.71	2.75	0.00
38	1.620	0.100	24.500	1.800	1.276	0.102	0.891	0.038			40.0	5.3	10.71	2.76	0.00
39	1.530	0.180	29.200	3.000	1.163	0.075	0.940	0.076							1.40
40	1.699	0.061	24.800	1.400	1.144	0.095	0.922	0.026							2.75
41	1.710	0.060	25.600	1.500	1.268	0.122	0.934	0.028							0.04
42	1.620	0.120	20.600	1.900	1.095	0.076	0.825	0.049							0.85
43	1.686	0.100	26.100	0.800	1.206	0.118	0.953	0.026							2.30
45	1.380	0.080	23.600	2.300	1.063	0.375	0.776	0.040							0.71
46	1.845	0.048	24.500	0.800	1.171	0.058	0.960	0.020							1.65
47	1.694	0.070	24.400	0.800	1.195	0.056	0.908	0.021							6.44*
49	1.344	0.090	24.700	2.200	1.055	0.054	0.779	0.045							0.63
50	1.450	0.080	22.800	2.500	1.424	0.140	0.799	0.043							7.28*
52	1.660	0.110	23.400	0.900	1.342	0.087	0.873	0.029							3.87
53	1.692	0.067	24.400	1.000	1.141	0.092	0.911	0.028							4.72
54	1.772	0.110	26.500	0.500	1.200	0.120	0.977	0.016			22.3	9.4	9.16	2.74	0.18
55	1.430	0.110	28.300	1.900	1.338	0.078	0.701	0.068							0.17
56	1.100	0.046	26.400	2.900	1.060	0.170	0.599	0.026							0.00
57	1.560	0.150	27.800	1.600	1.074	0.054	0.965	0.048							0.34
															5.53

Residue	R_1/s^{-1}	esd	R_2/s^{-1}	esd	NOE	esd	S^2	esd	S^2	esd	τ_i/ps	esd	R_{ex}/s^{-1}	esd	χ^2 ^b
58	1.735	0.049	26.800	2.200	1.106	0.091	0.948	0.024							0.61
59	1.607	0.068	30.000	3.500	1.175	0.137	0.892	0.036							3.02
60	1.920	0.080	21.700	2.200	1.430	0.174	0.817	0.064			120.6	36.6			0.38
62	1.570	0.080	23.700	2.000	1.341	0.159	0.860	0.039							1.38
67	1.540	0.140	23.100	0.600	1.212	0.070	0.851	0.020							0.63
68	1.480	0.074	17.800	1.700	1.035	0.059	0.762	0.036							8.28*
70	1.740	0.120	23.800	1.600	1.395	0.185	0.909	0.042							2.23
72	1.820	0.140	26.900	1.800	1.306	0.122	0.992	0.048							1.46
73	2.020	0.190	25.800	1.300	1.186	0.069	0.978	0.044							1.82
74	1.770	0.130	21.200	2.100	0.982	0.078	0.881	0.048							8.01*
75	1.620	0.100	23.200	2.000	1.276	0.102	0.873	0.042							1.41
76	1.810	0.070	23.300	1.300	1.293	0.045	0.886	0.029							0.74
77	1.389	0.061	23.300	1.700	0.935	0.164	0.779	0.030			64.6	23.9			4.01
78	1.422	0.047	21.600	2.400	1.293	0.158	0.776	0.025							0.79
79	1.643	0.062	22.700	1.300	1.046	0.062	0.875	0.027							4.13
80	1.621	0.044	22.200	2.100	1.254	0.245	0.877	0.024							0.75
81	1.388	0.073	23.900	2.100	1.049	0.128	0.782	0.034							2.85
82	1.330	0.110	26.100	2.900	1.354	0.124	0.646	0.070			19.0	11.0	8.46	3.33	0.00
84	1.412	0.120	25.500	3.900	1.048	0.080	0.798	0.060							3.11
85	1.710	0.100	29.000	1.500	1.360	0.077	0.826	0.060							0.00
86	1.489	0.061	25.300	2.300	1.264	0.074	0.827	0.031							3.86
87	1.610	0.130	16.400	4.200	0.845	0.253	0.829	0.063							4.06
88	2.020	0.140	22.300	1.200	1.205	0.050	0.893	0.037							10.71*
89	1.760	0.080	28.600	1.900	1.295	0.072	0.985	0.036							5.03
90	1.710	0.060	25.600	1.500	1.268	0.122	0.934	0.028							0.85
91	1.580	0.090	25.000	1.300	1.178	0.056	0.892	0.035							0.96
92	1.630	0.110	23.110	0.290	1.212	0.069	0.854	0.010							0.92
93	1.440	0.089	24.800	1.900	1.121	0.064	0.826	0.038							2.73
95	1.643	0.062	22.700	1.300	1.046	0.062	0.875	0.028							4.13
97	1.550	0.160	26.700	3.500	1.269	0.123	0.888	0.069							1.64
100	2.020	0.140	22.300	1.200	1.205	0.050	0.893	0.035							10.71*
101	1.880	0.180	21.900	2.200	0.880	0.059	0.896	0.063							25.40*
102	1.640	0.200	19.400	2.300	1.164	0.169	0.783	0.069							1.63
103	1.502	0.050	24.400	2.300	1.018	0.190	0.825	0.025							1.41
104	2.419	0.057	14.100	1.300	1.953	0.204	0.473	0.046			179.5	15.8			0.57

^a Model-free parameters were calculated with the overall rotational diffusion properties given in the manuscript. ^b Residues for which the χ^2 value exceeded the $\alpha = 0.05$ critical value for all models were parametrized with the most appropriate of models 1, 2 and 3 according to F-statistics testing and are indicated by a (*) after the χ^2 value.