Supporting information with:

Structural comparison of crystal and solution states of the 138 kDa complex of methylamine dehydrogenase and amicyanin from *Paracoccus versutus*.

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Table S1. Assignment of *Paracoccus versutus* ¹⁵N-Zn- amicyanin, 20mM NaPi pH=7, T=300K (n.a.: not assigned)

Residue	¹⁵ N	¹ H ^N	Others				
0	Gly	n.a.	n.a.		53	Pro	-
1	Gln	n.a.	n.a.	NE2 111.69, HE21 7.48, HE22 6.73	54	His	n.a.
2	Asp	121.05	8.33		55	Asn	n.a.
3	Lys	120.13	8.61		56	Val	115.11
4	Ile	106.78	7.03		57	Ala	127.46
5	Thr	116.48	8.57		58	Phe	111.42
6	Val	128.05	8.87		59	Lys	122.38
7	Thr	122.54	7.76		60	Lys	120.92
8	Ser	114.31	7.72		61	Gly	111.21
9	Glu	125.65	8.77		62	Ile	120.14
10	Lys	115.17	7.68		63	Val	109.00
11	Pro	-	-		64	Gly	108.43
12	Val	115.97	8.76		65	Glu	118.31
13	Ala	123.29	8.59		66	Asp	115.59
14	Ala	123.99	8.23		67	Ala	123.27
15	Ala	117.07	8.15		68	Phe	120.61
16	Asp	115.69	7.77		69	Arg	130.01
17	Val	124.25	7.14		70	Gly	115.09
18	Pro	-	-		71	Glu	119.17
19	Ala	123.39	8.43		72	Met	118.14
20	Asp	113.65	8.21		73	Met	119.85
21	Ala	120.89	6.99		74	Thr	115.55
22	Val	123.67	8.74		75	Lys	120.36
23	Val	126.47	7.75		76	Asp	119.02
24	Val	130.27	9.28		77	Gln	116.89
25	Gly	113.39	8.76		78	Ala	121.24
26	Ile	119.13	7.93		79	Tyr	121.33
27	Glu	122.60	8.16		80	Ala	128.66
28	Lys	119.80	8.90		81	Ile	118.71
29	Met	107.96	8.98		82	Thr	124.48
30	Lys	113.98	7.29		83	Phe	125.75
31	Tyr	119.38	8.09		84	Asn	119.10
32	Leu	123.18	9.37		85	Glu	116.17
33	Thr	110.18	6.36		86	Ala	128.04
34	Pro	-	-		87	Gly	108.45
35	Glu	119.53	7.77		88	Ser	113.63
36	Val	122.31	7.70		89	Tyr	125.40
37	Thr	121.34	8.25		90	Asp	126.71
38	Ile	121.19	9.10		91	Tyr	119.80
39	Lys	118.93	8.63		92	Phe	119.25
40	Ala	121.93	8.34		93	Cys	119.59
41	Gly	111.20	9.40		94	Thr	127.41
42	Glu	120.10	8.05		95	Pro	-
43	Thr	116.65	8.16		96	His	116.12
44	Val	126.77	8.59		97	Pro	-
45	Tyr	122.70	8.37		98	Phe	111.48
46	Trp	123.93	9.66	NE1 123.25, HE1 8.65	99	Met	124.87
47	Val	118.27	8.14		100	Arg	121.35
48	Asn	124.92	8.81	ND2 108.74, HD21 7.43, HD22 6.32	101	Gly	108.33
49	Gly	116.32	9.37		102	Lys	119.23
50	Glu	120.17	8.41		103	Val	126.93
51	Val	112.40	7.73		104	Ile	130.40
52	Met	121.27	7.38		105	Val	127.21
					106	Glu	133.46

NE2 110.49, HE21 7.45, HE22 6.50

ND2 111.81, HD2 6.66

Table S2. Assignment of *Paracoccus versutus* ^{15}N - ^{13}C -Cu(I)- amicyanin, 300K, 10mM KPi pH 6.8 (n.a.: not assigned)

Residue	^{15}N	$^1\text{H}^{\text{N}}$	C^{α}	C^{β}	CO	Others
0 Gly	n.a.	n.a.	n.a.	n.a.	n.a.	
1 Gln	n.a.	n.a.	56.07	29.81	172.42	CG 34.10, NE2 112.19, HE21 7.47, HE22 6.72
2 Asp	121.48	8.33	55.09	41.68	174.44	
3 Lys	120.52	8.60	59.40	33.81	172.90	
4 Ile	107.06	7.00	58.48	42.25	171.76	
5 Thr	116.89	8.54	62.11	72.61	169.88	
6 Val	128.41	8.85	62.78	32.48	173.14	
7 Thr	123.11	7.74	65.65	68.87	171.52	
8 Ser	114.68	7.71	55.91	64.69	170.91	
9 Glu	126.04	8.76	59.24	30.22	174.27	
10 Lys	115.41	7.66	53.06	33.09	171.07	
11 Pro	-	-	63.85	n.a.	n.a.	
12 Val	116.30	8.73	59.24	34.43	172.19	
13 Ala	123.63	8.56	52.85	19.08	176.21	
14 Ala	124.38	8.24	55.28	18.73	176.62	
15 Ala	117.51	8.15	54.06	19.00	174.66	
16 Asp	115.96	7.74	54.71	41.05	173.36	
17 Val	124.70	7.12	61.45	32.53	171.16	
18 Pro	-	-	63.29	32.79	174.04	
19 Ala	123.80	8.43	54.50	18.95	175.17	
20 Asp	113.99	8.19	53.40	39.91	172.42	
21 Ala	121.26	6.96	52.21	21.58	174.41	
22 Val	124.03	8.71	64.24	31.35	171.06	
23 Val	126.82	7.73	60.44	35.80	173.35	
24 Val	130.76	9.27	62.02	32.21	172.31	
25 Gly	113.65	8.70	45.17	-	n.a.	
26 Ile	119.51	7.86	61.09	41.35	172.64	
27 Glu	122.89	8.00	56.85	34.57	171.63	
28 Lys	120.65	9.02	-	29.85	173.04	
29 Met	109.11	9.02	-	29.03	171.28	
30 Lys	114.09	7.10	55.78	36.19	172.05	
31 Tyr	120.24	7.95	57.98	37.84	174.82	
32 Leu	123.70	9.36	58.22	42.18	174.74	
33 Thr	110.40	6.32	58.72	70.26	169.73	
34 Pro	-	-	65.35	-	172.61	
35 Glu	120.04	7.75	56.59	32.75	171.24	
36 Val	122.76	7.68	60.16	35.87	169.70	
37 Thr	121.69	8.24	61.75	70.32	171.16	
38 Ile	121.57	9.08	59.59	42.48	171.57	
39 Lys	119.21	8.61	54.36	34.28	173.76	
40 Ala	122.30	8.31	54.55	17.68	175.44	
41 Gly	111.59	9.39	44.83	-	n.a.	
42 Glu	120.39	8.02	57.09	31.31	171.08	
43 Thr	116.97	8.14	62.36	71.56	169.97	
44 Val	127.13	8.56	61.87	34.57	170.40	
45 Tyr	123.01	8.33	56.74	41.13	171.74	
46 Trp	124.53	9.62	58.42	33.12	173.21	NE1 123.78, HE1 8.61
47 Val	118.53	8.10	61.26	35.45	172.56	
48 Asn	125.23	8.73	53.58	38.41	172.92	ND2 109.54, HD21 7.51, HD22 6.28
49 Gly	116.59	9.170	45.61	-	n.a.	
50 Glu	121.27	8.60	54.20	34.06	169.46	
51 Val	112.30	7.63	64.04	32.25	174.48	
52 Met	122.03	7.35	53.40	32.62	168.95	
53 Pro	-	-	n.a.	n.a.	n.a.	
54 His	117.17	7.64	n.a.	n.a.	n.a.	

55	Asn	n.a.	n.a.	n.a.	42.20	168.89	
56	Val	114.00	6.56	62.61	34.71	169.84	
57	Ala	127.62	8.32	50.63	22.47	170.86	
58	Phe	111.40	8.76	56.16	44.37	174.40	
59	Lys	122.76	9.55	56.56	34.08	173.51	
60	Lys	121.33	8.79	58.81	33.36	172.67	
61	Gly	111.66	7.20	46.87	-	172.07	
62	Ile	120.45	7.82	63.06	38.37	174.02	
63	Val	109.3	8.69	60.55	31.56	171.15	
64	Gly	108.89	7.40	44.68	-	168.93	
65	Glu	118.63	8.59	59.40	30.43	174.72	
66	Asp	115.91	8.13	53.06	43.20	174.25	
67	Ala	123.64	8.82	53.16	20.06	172.47	
68	Phe	121.08	8.52	57.66	43.95	170.67	
69	Arg	107.89	8.05	55.07	32.64	170.56	
70	Gly	115.60	8.46	44.98	-	171.41	
71	Glu	119.30	6.43	56.84	31.32	172.57	
72	Met	118.23	8.24	55.15	31.20	173.31	
73	Met	120.53	8.99	54.95	39.31	174.46	
74	Thr	115.54	8.62	60.45	69.57	170.01	
75	Lys	120.32	7.87	59.24	33.44	174.31	
76	Asp	119.44	9.14	57.03	38.98	172.12	
77	Gln	117.18	7.87	55.36	32.52	170.47	NE2 110.74, HE21 7.41, HE22 6.44
78	Ala	121.44	9.25	50.14	25.98	172.77	
79	Tyr	121.88	9.15	58.53	44.36	170.00	
80	Ala	104.98	7.56	50.71	22.52	173.48	
81	Ile	119.02	8.46	61.58	42.77	170.87	
82	Thr	124.77	8.48	62.26	69.93	170.19	
83	Phe	126.11	8.01	57.56	41.17	172.13	
84	Asn	119.46	8.21	55.29	40.36	171.61	ND2 112.30, HD2 6.64
85	Glu	116.51	7.74	55.00	34.08	172.38	
86	Ala	128.42	8.87	53.12	19.51	173.63	
87	Gly	108.85	8.99	45.16	-	183.16	
88	Ser	114.00	7.79	57.68	64.57	170.95	
89	Tyr	125.80	9.29	57.65	39.96	171.25	
90	Asp	127.04	8.27	55.22	42.71	171.51	
91	Tyr	120.27	8.61	55.89	42.45	171.65	
92	Phe	120.52	8.92	55.91	42.43	182.41	
93	Cys	121.32	6.79	57.61	31.54	n.a.	
94	Thr	125.36	9.79	70.01	65.76	n.a.	
95	Pro	-	-	n.a.	n.a.	172.50	
96	His	118.50	7.26	n.a.	n.a.	170.47	
97	Pro	-	-	n.a.	n.a.	172.70	
98	Phe	114.50	6.66	57.13	37.96	173.86	
99	Met	126.99	8.62	57.16	32.28	n/a	
100	Arg	120.56	7.69	54.87	35.64	172.45	
101	Gly	109.05	7.38	44.59	-	168.38	
102	Lys	119.64	8.58	56.39	37.81	172.71	
103	Val	127.37	8.88	62.06	34.84	171.12	
104	Ile	130.71	9.39	61.90	38.31	170.51	
105	Val	127.53	9.12	60.52	33.21	173.14	
106	Glu	133.75	9.13	57.74	32.81	177.65	

Table S3. Shift perturbations (ppm) for *P.versutus* Cu(I) and Zn-substituted amicyanin bound to MADH (d:disappeared, n.a.: not assigned)

Residue	Cu(I)-amicyanin +5eq of MADH			Zn-amicyanin +3eq of MADH			
	¹⁵ N	¹ H ^N	Δδ _{avg}	¹⁵ N	¹ H ^N	Δδ _{avg}	
0	Gly						
1	Gln	n.a.	n.a.	n.a.	n.a.	n.a.	
2	Asp	0.28	0.006	0.040	0.29	0.001	0.041
3	Lys	0.36	0.055	0.064	0.33	0.062	0.064
4	Ile	0.19	0.048	0.043	0.27	0.053	0.054
5	Thr	0.09	0.006	0.013	0.13	0.023	0.025
6	Val	0.11	0.003	0.016	0.12	0.017	0.021
7	Thr	0.28	0.007	0.040	0.48	0.015	0.069
8	Ser	0.35	0.004	0.050	0.40	0.003	0.057
9	Glu	0.09	0.052	0.039	0.33	0.009	0.047
10	Lys	0.06	0.012	0.012	0.06	0.014	0.013
11	Pro	-	-	-	-	-	-
12	Val	0.21	0.069	0.057	0.36	0.070	0.071
13	Ala	0.02	0.015	0.011	0.06	0.017	0.015
14	Ala	0.02	0.011	0.008	0.05	0.003	0.007
15	Ala	0.14	0.046	0.038	0.14	0.042	0.036
16	Asp	0.07	0.025	0.020	0.02	0.015	0.011
17	Val	0.18	0.032	0.034	0.15	0.020	0.025
18	Pro	-	-	-	-	-	-
19	Ala	0	0.014	0.010	0.03	0.006	0.006
20	Asp	0.01	0.012	0.009	0.01	0.001	0.002
21	Ala	0.03	0.023	0.017	0.02	0.010	0.008
22	Val	0.02	0.005	0.004	0.02	0.016	0.012
23	Val	0.12	0.024	0.024	0.05	0.002	0.007
24	Val	0.15	0.024	0.027	0.08	0.028	0.023
25	Gly	0.12	0.015	0.020	0.04	0.000	0.006
26	Ile	0.17	0.034	0.034	0.09	0.003	0.013
27	Glu	0.01	0.09	0.064	0.04	0.034	0.025
28	Lys	d	d	d	0.56	0.164	0.140
29	Met	d	d	d	1.84	0.167	0.286
30	Lys	d	d	d	0.14	0.032	0.030
31	Tyr	0.2	0.009	0.029	0.15	0.046	0.039
32	Leu	0.02	0.011	0.008	0.05	0.001	0.007
33	Thr	0	0.019	0.013	0.13	0.008	0.019
34	Pro	-	-	-	-	-	-
35	Glu	0.06	0.01	0.011	0.13	0.002	0.018
36	Val	0.23	0.01	0.033	0.23	0.001	0.033
37	Thr	0.01	0.001	0.002	0.06	0.011	0.012
38	Ile	0.04	0.019	0.015	0.00	0.005	0.004
39	Lys	0.03	0.02	0.015	0.02	0.005	0.005
40	Ala	0.03	0.019	0.014	0.01	0.011	0.008
41	Gly	0.01	0.011	0.008	0.01	0.000	0.001
42	Glu	0.02	0.015	0.011	0.00	0.004	0.003
43	Thr	0.01	0.003	0.002	0.01	0.014	0.010
44	Val	0.04	0.02	0.015	0.02	0.007	0.006
45	Tyr	0.13	0.035	0.031	0.06	0.016	0.014
46	Trp	0.2	0.01	0.029	0.20	0.012	0.030
47	Val	0.65	0.039	0.096	0.58	0.012	0.082
48	Asn	0.46	0.014	0.066	0.53	0.018	0.076
49	Gly	d	d	d	0.02	0.122	0.086
50	Glu	0.29	0.066	0.062	0.14	0.006	0.020
51	Val	d	d	d	2.47*	0.130*	0.361*
52	Met	d	d	d	2.56	0.002	0.362
53	Pro	-	-	-	-	-	-
54	His	d	d	d	n.a.	n.a.	n.a.
55	Asn	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

56	Val	d	d	d	0.27	0.101	0.081
57	Ala	0.35	0.042	0.058	0.00	0.084	0.059
58	Phe	0.56	0.108	0.110	0.17	0.039	0.037
59	Lys	0.38	0.053	0.065	0.06	0.024	0.019
60	Lys	0.15	0.088	0.066	0.15	0.093	0.069
61	Gly	0.65	0.013	0.092	0.61	0.026	0.088
62	Ile	0.01	0.012	0.009	0.17	0.022	0.029
63	Val	0.28	0.083	0.071	d	d	d
64	Gly	0.11	0.014	0.018	0.10	0.005	0.015
65	Glu	0.03	0.004	0.005	0.06	0.002	0.009
66	Asp	0.22	0.052	0.048	0.22	0.071	0.059
67	Ala	0.08	0.033	0.026	0.10	0.031	0.026
68	Phe	0.47	0.063	0.080	0.46	0.108	0.100
69	Arg	0.06	0.016	0.014	0.66	0.128	0.130
70	Gly	d	d	d	1.43	0.059	0.206
71	Glu	d	d	d	0.30	0.389	0.278
72	Met	d	d	d	0.41	0.162	0.128
73	Met	d	d	d	0.13	0.100	0.073
74	Thr	2.09	0.036	0.297	1.85	0.010	0.262
75	Lys	0.11	0.014	0.018	0.27	0.041	0.048
76	Asp	0.3	0.074	0.067	0.52	0.077	0.092
77	Gln	0.08	0.018	0.017	0.18	0.025	0.031
78	Ala	0.04	0.024	0.018	0.01	0.006	0.004
79	Tyr	0.24	0.004	0.034	0.19	0.010	0.028
80	Ala	0.34	0.104	0.088	0.23	0.090	0.071
81	Ile	0.05	0.01	0.010	0.01	0.014	0.010
82	Thr	0.06	0.029	0.022	0.03	0.012	0.009
83	Phe	0	0.005	0.003	0.05	0.021	0.016
84	Asn	0.03	0.023	0.017	0.01	0.015	0.011
85	Glu	0.03	0.021	0.015	0.04	0.008	0.008
86	Ala	0.06	0.001	0.008	0.09	0.007	0.014
87	Gly	0.04	0.018	0.014	0.04	0.004	0.006
88	Ser	0.09	0.012	0.015	0.06	0.002	0.009
89	Tyr	0.22	0.02	0.034	0.18	0.009	0.026
90	Asp	0.19	0.036	0.037	0.12	0.087	0.064
91	Tyr	0.27	0.025	0.042	0.39	0.006	0.055
92	Phe	d	d	d	0.48	0.003	0.068
93	Cys	d	d	d	0.57	0.186	0.154
94	Thr	d	d	d	0.83	0.137	0.152
95	Pro	-	-	-	-	-	-
96	His	d	d	d	2.99*	0.100*	0.429*
97	Pro	-	-	-	-	-	-
98	Phe	d	d	d	3.09*	0.430*	0.532*
99	Met	d	d	d	0.35*	0.532*	0.379*
100	Arg	d	d	d	1.10	0.000	0.156
101	Gly	0.31	0.006	0.044	0.27	0.036	0.046
102	Lys	0.67	0.031	0.097	0.71	0.033	0.103
103	Val	0.24	0.006	0.034	0.18	0.002	0.025
104	Ile	0.03	0.011	0.009	0.07	0.008	0.011
105	Val	0.03	0.011	0.009	0.01	0.007	0.005
106	Glu	0.05	0.021	0.016	0.04	0.002	0.006

* These are the minimum shifts because assignment was not possible

Table S4. Interface contacts (<4 Å) between chain A (amicyanin) and chains L and H (MADH) in the *P. versutus* complex.

CHAIN	RES	ATOM	:	CHAIN	RES	ATOM	:	DISTANCE
A	29 (MET)	CE	:	L	101 (GLU)	CG	:	3.21
			:	L	101 (GLU)	CD	:	3.83
			:	L	101 (GLU)	OE1	:	3.95
A	51 (VAL)	CG1	:	L	129 (LYS)	C	:	3.92
			:	L	129 (LYS)	O	:	2.96
A	51 (VAL)	C	:	L	71 (LEU)	CD2	:	3.98
A	51 (VAL)	O	:	L	71 (LEU)	CD2	:	3.98
A	52 (MET)	SD	:	L	58 (VAL)	CG2	:	3.72
A	52 (MET)	CE	:	L	101 (GLU)	CB	:	3.45
			:	L	102 (PHE)	CE2	:	3.86
			:	L	102 (PHE)	CZ	:	3.60
			:	L	58 (VAL)	CG2	:	3.76
A	53 (PRO)	CD	:	L	58 (VAL)	CG1	:	3.85
A	53 (PRO)	CG	:	L	127 (VAL)	CG1	:	3.81
A	69 (ARG)	NE	:	L	54 (THR)	OG1	:	3.59
			:	L	111 (GLY)	CA	:	3.90
A	69 (ARG)	CZ	:	L	111 (GLY)	CA	:	3.86
			:	L	111 (GLY)	O	:	3.88
A	69 (ARG)	NH1	:	L	111 (GLY)	CA	:	3.92
A	69 (ARG)	NH2	:	L	111 (GLY)	O	:	3.67
A	72 (MET)	CG	:	L	54 (THR)	O	:	3.44
A	74 (THR)	CB	:	L	127 (VAL)	O	:	3.95
A	74 (THR)	OG1	:	L	127 (VAL)	O	:	3.35
A	74 (THR)	CG2	:	L	127 (VAL)	O	:	3.98
A	94 (THR)	CG2	:	L	110 (PHE)	CB	:	3.88
			:	L	55 (ALA)	CB	:	3.82
A	95 (PRO)	CD	:	L	55 (ALA)	CB	:	3.82
A	95 (PRO)	CB	:	L	55 (ALA)	CB	:	3.47
A	95 (PRO)	CG	:	L	55 (ALA)	CB	:	3.90
A	95 (PRO)	O	:	L	108 (TRP)	CZ3	:	3.87
			:	L	108 (TRP)	CH2	:	3.71
A	96 (HIS)	CD2	:	L	101 (GLU)	CG	:	3.68
A	96 (HIS)	NE2	:	L	101 (GLU)	CA	:	3.92
			:	L	101 (GLU)	CB	:	3.56
			:	L	101 (GLU)	CG	:	3.59
A	98 (PHE)	CD2	:	L	100 (PRO)	CG	:	3.94
A	98 (PHE)	CE2	:	L	100 (PRO)	CG	:	3.44
A	98 (PHE)	CZ	:	L	101 (GLU)	CG	:	3.78
			:	L	101 (GLU)	CD	:	3.96
			:	L	101 (GLU)	OE2	:	3.81
A	59 (LYS)	CG	:	H	198 (PRO)	CB	:	3.93
A	59 (LYS)	NZ	:	H	198 (PRO)	CB	:	3.68
			:	H	198 (PRO)	C	:	3.65
			:	H	198 (PRO)	O	:	3.46
			:	H	199 (ALA)	CB	:	3.28
A	92 (PHE)	CD2	:	H	198 (PRO)	O	:	3.67
A	92 (PHE)	CE2	:	H	198 (PRO)	O	:	3.72
A	92 (PHE)	CZ	:	H	198 (PRO)	CB	:	3.89
A	95 (PRO)	O	:	H	196 (PHE)	CE2	:	3.76
			:	H	196 (PHE)	CZ	:	3.53
A	97 (PRO)	CD	:	H	196 (PHE)	CE2	:	3.77
			:	H	196 (PHE)	CE1	:	3.96
			:	H	196 (PHE)	CZ	:	3.36
A	97 (PRO)	CB	:	H	196 (PHE)	O	:	3.70
			:	H	198 (PRO)	O	:	3.69
A	97 (PRO)	CG	:	H	196 (PHE)	O	:	3.66
			:	H	196 (PHE)	CE2	:	3.54

				H 196 (PHE)	CE1	:	3.96
				H 196 (PHE)	CZ	:	3.52
A	98 (PHE)	N	:	H 220 (ASP)	OD1	:	3.98
A	98 (PHE)	CA	:	H 220 (ASP)	CG	:	3.60
				H 220 (ASP)	OD1	:	3.16
				H 220 (ASP)	OD2	:	3.81
A	98 (PHE)	CB	:	H 220 (ASP)	CB	:	3.84
				H 220 (ASP)	CG	:	3.30
				H 220 (ASP)	OD1	:	3.30
				H 220 (ASP)	OD2	:	3.60
A	98 (PHE)	CG	:	H 237 (ARG)	NE	:	3.74
A	98 (PHE)	CD1	:	H 237 (ARG)	NE	:	3.78
				H 237 (ARG)	CZ	:	3.77
				H 237 (ARG)	NH2	:	3.88
A	98 (PHE)	CD2	:	H 237 (ARG)	NE	:	3.91
				H 237 (ARG)	NH2	:	3.64
A	98 (PHE)	CE1	:	H 237 (ARG)	CZ	:	3.52
				H 237 (ARG)	NH1	:	3.91
				H 237 (ARG)	NH2	:	3.34
A	98 (PHE)	CE2	:	H 237 (ARG)	CZ	:	3.86
				H 237 (ARG)	NH2	:	3.05
A	98 (PHE)	CZ	:	H 237 (ARG)	CZ	:	3.56
				H 237 (ARG)	NH2	:	2.87
A	98 (PHE)	O	:	H 220 (ASP)	OD2	:	3.88
A	100 (ARG)	CZ	:	H 220 (ASP)	OD1	:	3.33
				H 220 (ASP)	OD2	:	3.88
A	100 (ARG)	NH1	:	H 220 (ASP)	CG	:	3.89
				H 220 (ASP)	OD1	:	3.56
				H 220 (ASP)	OD2	:	3.35
A	100 (ARG)	NH2	:	H 200 (PRO)	CD	:	3.82
				H 200 (PRO)	CG	:	3.88
				H 220 (ASP)	CG	:	3.24
				H 220 (ASP)	OD1	:	2.35
				H 220 (ASP)	OD2	:	3.47

Figure S2 ^{15}N -HSQC spectrum of *P. versutus* Zn(II)-amicyanin.