Supporting Information with

Redox state dependent complex formation between pseudoazurin and nitrite reductase

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Table S1: The pK_a values obtained by fitting with equations 7 or 8 the chemical shift changes of PAZ backbone amides (in ^{15}N or ^{1}H dimension) affected during a pH titration between pH 8.0 - 4.0. Buffer: 20 mM potassium phosphate. T = 295 K.

Residue	(^{15}N) pK_{a1}	(^{15}N) pK_{a2}	(^{1}H) pK_{a1}	(^{1}H) pK_{a2}
Glu 1	5.0 ± 0.1	7.2 ± 0.1	4.7 ± 0.1	7.2 ± 0.1
Glu 4	5.0 ± 0.1	7.2 ± 0.1		
Val 5	5.4 ± 0.2	7.3 ± 0.1	4.3 ± 0.1	7.2 ± 0.1
His 6	-	7.3 ± 0.2	5.2 ± 0.1	7.5 ± 0.5
Leu 8	5.9 ± 0.1		4.7 ± 0.1	
Lys 10	4.7 ± 0.1		5.0 ± 0.1	
Gly 11	4.7 ± 0.1			
Glu 13	4.5 ± 0.1		4.7 ± 0.1	
Val 17	5.0 ± 0.1		5.0 ± 0.1	7.7 ± 0.2
Glu19	4.5 ± 0.1	7.3 ± 0.1	5.0 ± 0.1	7.7 ± 0.2
Ala21	4.4 ± 0.2	7.4± 0.2		
Asn 26	5.0 ± 0.1		4.7 ± 0.1	
Asp 29	4.4 ± 0.1		5.0 ± 0.1	
Thr 30	5.6 ± 0.1		5.0 ± 0.1	7.0 ± 0.1
Ile 34		7.6 ± 0.2		7.5 ± 0.2
Val 36	5.0 ± 0.1			
Asp 37	4.7 ± 0.2	7.3 ± 0.1	4.3 ± 0.1	7.5 ± 0.2
Gly39	4.7± 0.2	7.3± 0.1	4.4 ± 0.2	7.2 ± 0.1
His 40		7.4 ± 0.1		7.5 ± 0.1
Lys 77	5.0 ± 0.1	-	5.0 ± 0.1	-
Cys 78	5.0 ± 0.1			
Thr 79	5.0 ± 0.1	7.5 ± 0.3	5.0 ± 0.1	7.5 ± 0.1
Tyr 82	5.0 ± 0.1	-	4.7 ± 0.2	
Ala 83	4.7 ± 0.3	-	5.0 ± 0.1	-
Met 84	4.7 ± 0.1		5.0 ± 0.1	
Met 86	5.0 ± 0.1	7.8 ± 0.1	4.7 ± 0.1	8.4 ± 0.2
Ala 88	5.0 ± 0.1	7.7 ± 0.1	5.0 ± 0.1	7.6 ± 0.1