Table 2. Hydrogen bond distances in *Clostridium pasteurianum* rubredoxin (*Cp*Rd) variants derived from the ^{15}N chemical shifts in Table 1 by theoretical Eqs. 1 and 2 (main text)

Oxidized (Fe^{III}) proteins *

*Cp*Rd variant	Reduction potential, mV (1)	Predicted $H^N\cdots S^\gamma$ bond lengths, Å †			
		44 $H^N\cdots S^\gamma$ 42	8 $H^N\cdots S^\gamma$ 6	11 $H^N\cdots S^\gamma$ 9	41 $H^N\cdots S^\gamma$ 39
V44G	0	2.40	2.71	2.57	2.65
V44A	-24	2.58	2.69	2.54	2.63
V44I	-53	2.76	2.68	2.59	2.64
Wild type	-77	2.87	2.68	2.57	2.67
V44L	-87	2.76	2.76	2.60	2.68
V8G	-7	2.89	2.42	2.38	2.58
V8A	-44	2.85	2.65	2.51	2.64
Wt	-77	2.87	2.68	2.57	2.67
V8I	-81	2.87	2.68	2.56	2.66
V8L	-82	2.87	2.70	2.56	2.66
V8G/V44G	+39	2.67/2.49		2.47	2.58

Reduced (Fe^{II}) proteins †

*Cp*Rd variant	Reduction potential, mV (1)	Predicted $H^N\cdots S^\gamma$ bond lengths, Å †			
		44 $H^N\cdots S^\gamma$ 42	8 $H^N\cdots S^\gamma$ 6	11 $H^N\cdots S^\gamma$ 9	41 $H^N\cdots S^\gamma$ 39
V44G	0	2.21	2.32	2.39	2.33
V44A	-24	2.50	2.23	2.46	2.28
V44I	-53	2.62	2.16	2.53	2.33
Wild type	-77	2.80	2.20	2.47	2.36
V44L	-87	2.65	2.21	2.52	2.30
V8G	-7	2.85	2.04	2.47	2.15
V8A	-44	2.87	2.24	2.50	2.29
Wt	-77	2.80	2.20	2.47	2.36
V8I	-81	2.80	2.20	2.45	2.37
V8L	-82	2.83	2.23	2.46	2.36
V8G/V44G	+39	2.47/2.30		2.44	2.14

*Fermi contact spin densities were calculated as a function of the H–S distance for the oxidized and reduced models described in the main text. These values were converted to hyperfine shifts by multiplication with 2.6743×10^5 for oxidized *Cp*Rd and 2.2923×10^5 for reduced *Cp*Rd (2). The relationship between the hyperfine shifts and the H–S distance was investigated by linear regression analysis. The values obtained for the oxidized model were indistinguishable from those reported in ref. 2. In the notation used, 44 $H^N\cdots S^\gamma$ 42 denotes the H^N of residue 44 H-bonded to the S^γ of residue 42.

†No high-resolution x-ray structure is available for reduced *Cp*Rd that could be used to compare model distances with theoretical values in the reduced state.

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