Table 4. Paramagnetic relaxation enhancements used in the structure calculation of the metal site of *A.v.* plastocyanin

Nucleus	R_{1p}, ms^{-1}*	ν, MHz	$k^{\pm}_{prlx}$ †
His-39 H$^{\beta_1}$	0.62 ± 0.09	800	500
His-39 H$^{\varepsilon_1}$	3.30 ± 0.20	800	50
His-39 H$^{\delta_2}$	0.31 ± 0.02	800	500
Asn-40 H$^{\alpha}$	0.12 ± 0.02	800	500
Cys-89 H$^{\alpha}$	1.53 ± 0.23	800	500
Cys-89 H^{N}	0.36 ± 0.12‡	500	500
His-92 H$^{\varepsilon_1}$	3.30 ± 0.20	800	50
His-92 H$^{\delta_2}$	0.31 ± 0.02	800	500
Met-97 H$^{\gamma_1}$	0.70 ± 0.04	800	500
Met-97 H$^{\gamma_2}$	0.30 ± 0.02	800	500
Cys-89 H$^{\beta_2}$	64 ± 10§	800	50

* Obtained from the relaxation recoveries (*e.g.* Fig. 6) in signal eliminating relaxation filter (SERF) experiments (1), as described previously (2), except for Cys-89 H^{N} and Cys-89 H$^{\beta_2}$, see text and below. The uncertainties used in the structure calculation correspond to approximately three times the uncertainty obtained from the experimental data, however larger than 0.020 ms^{-1}. This lower limit prevents overflow in the structure calculation during the high temperature dynamics.

† The force constant used for the different restraints. The unit is kcal·mol^{-1} for k^{-}_{prlx} while kcal·mol^{-1}·Å^{-2} for k^{+}_{prlx}.

‡ This restraint was obtained previously from one-dimensional NMR experiments on a partly oxidized sample (3).

§ This value corresponds to the dipolar transverse paramagnetic relaxation enhancement R_{2p}, which is obtained from Fig. 4.

1. Hansen, D. F. & Led, J. J. (2001) *J. Magn. Reson.* **151,** 339–346.
2. Hansen, D. F. & Led, J. J. (2004) *J. Am. Chem. Soc.* **126,** 1247–1253.
3. Jensen, M. R., Hansen, D. F. & Led, J. J. (2002) *J. Am. Chem. Soc.* **124,** 4093–4096.