Table S1. Data Collection and Refinement Statistics

	MeOH	EtOH
Wavelength (Å)	0.970	0.980
Space group	$P2_12_12_1$	$P2_12_12_1$
Cell dimensions		
a (Å)	70.7	71.4
b (Å)	171.3	172.4
c (Å)	221.3	221.1
Resolution (Å)	30–2.05	30–1.96
Total observations	1,528,378	2,094,314
Unique reflections	163,616	192,245
$I/\sigma(I)$ [a]	16.6 (4.1)	17.8 (3.6)
R_{sym} (%) [a,b]	6.8 (35.8)	6.4 (44.2)
Completeness (%) [a]	96.8 (81.5)	98.1 (87.4)
Resolution range (Å)	30–2.05	30–1.96
Reflections used	150,517	176,692
R_{cryst} [c]	0.218	0.214
R_{free} [d]	0.243	0.255
Rms deviations		
Bond lengths (Å)	0.014	0.006
Bond angles (°)	1.76	1.16
Dihedral angles (°)	20.6	20.1
Improper angles (°)	1.06	1.16
Avg B-value (Å^2) (all atoms)	35.5	39.3

[a] Values in parentheses are for the highest resolution shells. [b] $R_{sym} = \Sigma|I - \langle I\rangle|/\Sigma I$, where I is the observed intensity and $\langle I\rangle$ is the average intensity over all observations of symmetry-related reflections. [c] $R_{cryst} = \Sigma||F_{obs}| - |F_{calc}||/\Sigma|F_{obs}|$, where $|F_{obs}|$ and $|F_{calc}|$ are the observed and calculated structure factor amplitudes, respectively. [d] R_{free} was calculated from a randomly chosen subset of 3.5% of the reflections.

The structure of the oxidized protein without water molecules or the side chain of Glu243 was used as a starting model for rigid body refinement in CNS.15 After one cycle of simulated annealing refinement to remove previous model bias and a cycle of grouped *B*-factor refinement, the protein was manually inspected in O and minor adjustments were made. The model was then subjected to cycles of positional and individual *B*-factor refinement followed by an automated water picking routine. Only peaks $\geq$3.0s in the difference Fourier maps located between 2.5 and 3.3 Å from the protein with *B*-factors <60 $Å^2$ were written to a file. The peaks in this list were then examined manually in O, and those having no obvious hydrogen bonding partners, or no corresponding electron density in the $2F_{obs} - F_{calc}$ maps, were rejected. Five cycles of water picking were required to locate all 1128 and 1086 water molecules in the methanol- and ethanol-soaked MMOH structures, respectively. The bridging alcohols were added only after the models were nearly complete. The final models had $R_{cryst} = 0.218$ ($R_{free} = 0.243$) and $R_{cryst} = 0.214$ ($R_{free} = 0.255$) for the methanol and ethanol structures, respectively. Simulated annealing omit maps were also calculated to verify the observed electron density feature bridging the iron atoms.