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Supporting Information

Regulating the Coordination State of a Heme Protein by a Designed Distal Hydrogen-Bonding Network

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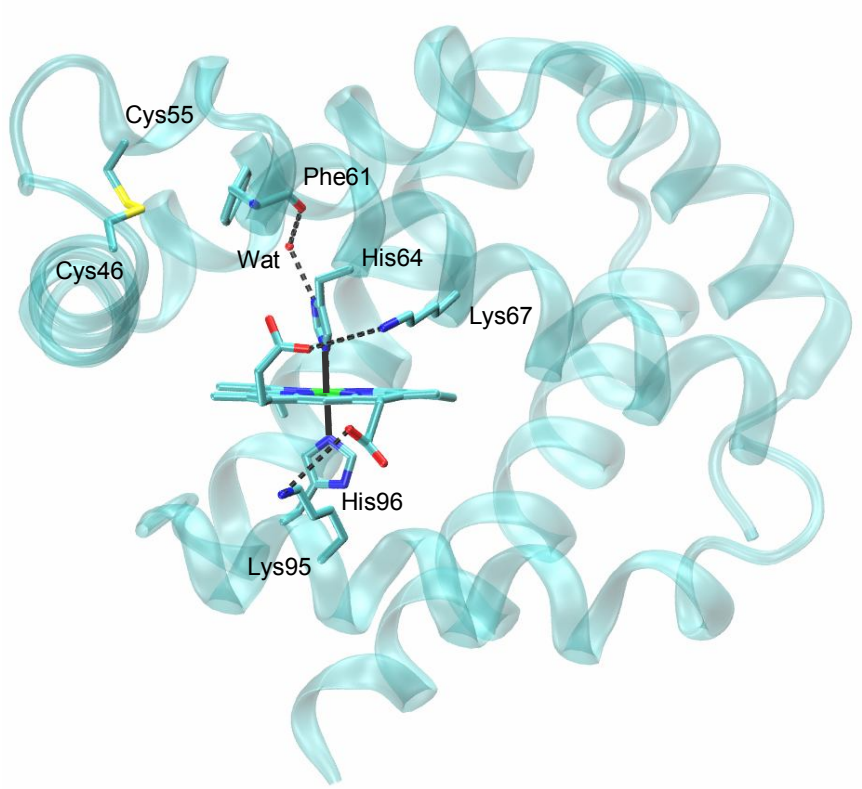

Fig. S1. X-ray structure of human Ngb (PDB code 4MPM, Guimarães *et al. Acta. Cryst.* **2014**, *D70*, 1005-1014), showing the bis-His coordination state and the hydrogen-bonding interactions in the heme active site.

Table S1. X-ray crystallography data collection and refinement statistics

	L29E Mb	**F43H Mb**	**L29E/F43H Mb**
Wavelength	0.9792	0.9792	0.9792
Space group	$P2_12_12_1$	$P2_12_12_1$	$P2_12_12_1$
Unit-cell dimensions (Å, °)	a = 39.866, b = 48.640, c =78.694; $\alpha=\beta=\gamma$= 90	a = 39.808, b = 48.055, c =77.210; $\alpha=\beta=\gamma$= 90	a =33.968, b = 60.898, c =75.356; $\alpha=\beta=\gamma$=90
Resolution (Å)	1.45	1.50	1.95
No. of observations	205235	207454	69709
No. of unique reflections[a]	27782(1397)	23101(1125)	12082 (615)
Completeness (%)	99.7(99.9)	95.3(94.9)	100.0 (100.0)
<I>/ (I)	23.7(6.8)	32.1(5.9)	18.5 (5.8)
Redundancy	7.4(7.5)	9.0(9.3)	5.8 (5.8)
R_{sym}[b]	0.089(0.441)	0.063(0.484)	0.100 (0.447)
R_{cryst}[c](%)/R_{free}[d](%)	0.1839/0.2069	0.1811/0.2087	0.1817/0.2188
RMSD bonds (Å)/angles (°)	0.006/1.015	0.007/1.173	0.009/1.169
Ramachandran plot, residues in:			
Most favored regions (%)	98	98	98.4
Additional allowed regions (%)	1.6	1.6	1.6
Generously allowed regions (%)	0.4	0.4	0.0
Disallowed regions (%)	0.0	0.0	0.0
PDB code	4PQ6	4PQC	4PQB

[a] Numbers in parentheses represent values in the highest resolution shell (Å).

[b] $R_{sym} = \Sigma|I_j-\langle I\rangle|/\Sigma I_j$, where I_j is the observed integrated intensity, <I> is the average integrated intensity obtained from multiple measurements, and the summation is over all observed reflections.

[c] $R_{cryst} = \Sigma||F_{obs}|-|F_{calc}||/\Sigma|F_{obs}|$, F_{obs} and F_{calc} are observed and calculated structure factor amplitudes, respectively.

[d] R_{free} calculated with randomly selected reflections (5%).