

Supplementary material

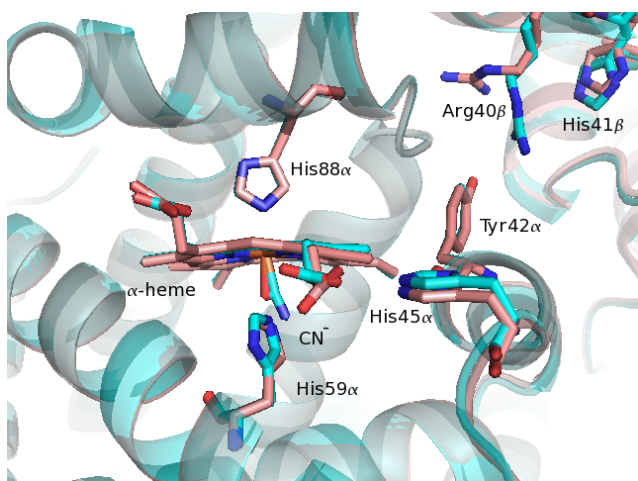


Fig. S1 Inset from Figure 3. Structural modifications of HbTb structure upon cyanidation at the α heme.

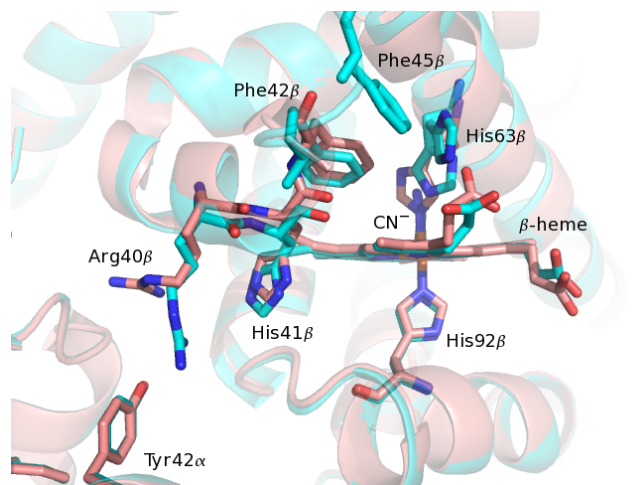


Fig. S2 Inset from Figure 3. Structural modifications of HbTb structure upon cyanidation at the β heme

Table S1 Data collection and refinement statistics.

<i>Diffraction data</i>	
Space group	C2
Cell parameters	
a (Å)	86.88
b (Å)	87.88
c (Å)	55.25
β (°)	99.66
Resolution range (Å)	30.00-1.54 (1.60-1.54)*
No. of unique reflections	61743
Completeness (%)	98.8 (96.7)*
Rmerge (%)	4.2 (22.3)*
$I/\sigma(I)$	22.9 (3.8)
Redundancy	5
<i>Refinement</i>	
Resolution range (Å)	30.00-1.54
R (%)	16.5
R_{free} (%)	19.7
No. of atoms	2320
No. of water molecules	405
<i>r.m.s. deviation</i>	
Bond lengths (Å)	0.016
Bond angles (°)	1.529
<i>Ramachandran statistics</i>	
Residues in favoured region (%)	93.8
Residues in allowed region (%)	6.2
Residues in generously allowed/outlier region (%)	0/0

55 *)The numbers in parentheses refer to the outermost shell

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