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Supporting information for article:

Structure of bovine cytochrome *c* oxidase in the ligand-free reduced state at neutral pH

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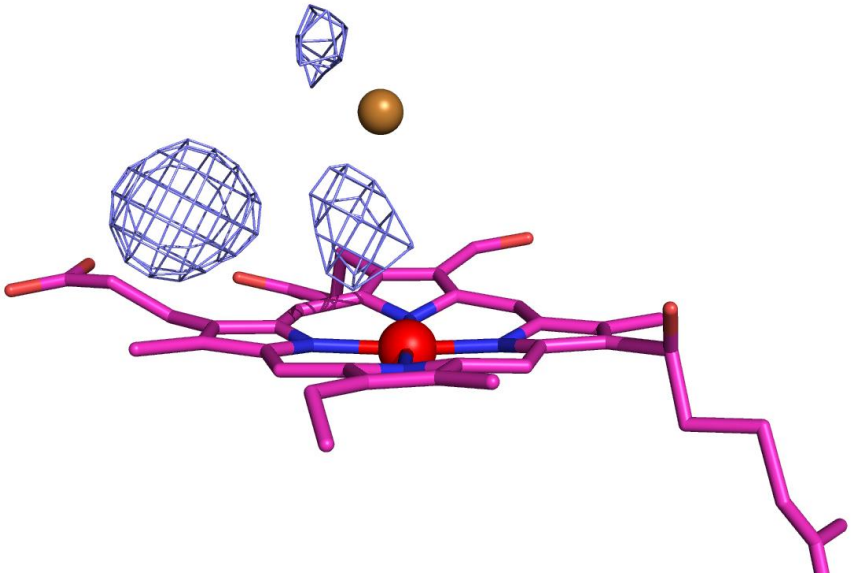

Figure S1 Difference maps calculated with coefficients (|*F*o| - |*F*c|)exp(*i*α_c). Heme *a*3 are drawn as stick models, with C, N and O atoms coloured purple, blue and red, respectively. Fe_{a3} and Cu_B are shown as red and brown spheres, respectively. All difference maps were drawn at the 2.0 σ level. The electron density between Fe_{a3} and Cu_B indicates the density of a peroxide anion of the fully oxidized CcO. The large density between two propionates is the density of a water molecule that is not included in the structure refinement. The peak height of the peroxide is 33% of that of the water. The ccupancy of the peroxide converged to 0.20 in the structure refinement. Thus the present reduced crystal contains the fully oxidized CcO at 20%.