Figure EV1. A cross-section of surface structures of CcO and Cyt.c–CcO complex.

Cyt.c and CcO are shown as surface representation each colored in red and green, respectively. The cross-section of the surface representation indicates that Cyt.c fits closely with the concave surface.
Figure EV2. Comparison of the Cyt.c-CcO complex with caa₃-type CcO (Lyons et al, 2012).

A, B Arrangement of redox cofactors in the Cyt.c-CcO complex (A) and caa₃-type CcO (B). Heme groups (c, a, a, a, and a₃) are shown as black sticks. Copper and magnesium ions are represented by orange and blue spheres, respectively. Distances from iron of heme c to Cuₐ are indicated.

C Comparison of ET pathways from iron of heme c to Cuₐ between the Cyt.c-CcO complex (cyan sticks and yellow lines) and caa₃-type CcO (magenta sticks and green lines). Both structures are superposed with their Cuₐ-containing domains. Solid and dashed lines represent through-bond and through-space processes, respectively.
Figure EV3. Structure of waters around the direct interaction region between Cyt.c and CcO. Stick models of Cyt.c and CcO are drawn in the same colors as in Fig 3C. Water is shown by a sphere.

A Stereoscopic view of the 2(Fo–Fc) map of the Cyt.c–CcO complex, drawn at the 1.0 σ level. Each water molecule is clearly assigned in the map.

B Stereoscopic view of water structure. Each water molecule is drawn in the same color as in Fig 4A. Hydrogen bond networks consisting of water molecules including non-interacting waters link Cyt.c and CcO.
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Figure EV4. Distribution of B-factors of Cyt.c molecules.

A–F Stick representations of ferri-Cyt.c (A; PDB 3O1Y), ferro-Cyt.c (B; PDB 3O20), Cyt.c portion of yeast Cyt.b–Cyt.c complex (C; PDB 3CXS), yeast iso-1 Cyt.c (D; PDB 1YCC), Cyt.c portion of Leishmania major Cyt.c–CcP complex (E; PDB 4GED), and Leishmania major Cyt.c (F; PDB 4DY9). All structures are viewed from the same direction. The B-factor color scale is provided below in Å^2 unit. Heme c atoms of each Cyt.c have lower B-factors than those of peripheral residues.