Crystal structure of the LH1-RC complex in bacterial photosynthesis

Carbon, which is one of the most important elements for life, is taken up into biological system by photosynthesis. Purple bacteria have a simpler photosynthetic system than plants: the chromatophore vesicle of photosynthetic bacteria contains several protein components such as core antenna (LH1), peripheral antenna (LH2), reaction center (RC) and the high-potential iron-sulfur protein (HiPIP) (Fig. 1). LH1 and RC form a supramolecular complex (LH1-RC) to utilize sunlight energy in a highly efficient manner. Therefore, it is indispensable to know the atomic structure of the LH1-RC, including the arrangement of cofactors, to understand the mechanism of energy and electron transfer. However, only low-resolution structures of LH1-RC have been hitherto reported [1,2].

High quality crystals were obtained for the LH1-RC complex purified from a thermophilic bacterium, *Thermochromatium tepidum* (ttLH1-RC). The diffraction data were collected at beamlines **BL41XU** and **BL44XU** of SPring-8 and BL1A, BL17A, and NE3A of the Photon Factory. The phases were calculated with the multiple isomorphous replacement method with anomalous scattering (MIRAS) assisted by the molecular replacement (MR) method. Correction of diffraction anisotropy and multi-crystal averaging of the electron densities significantly improved electron density maps. The structures of LH1-RC in the two crystal forms ($P2_1$ and $C2$) were refined at 3.0 Å resolution [3].

The ttLH1-RC complex is composed of cytochrome, L, M and H subunits for RC, $\alpha_{16}\beta_{16}$ subunits for LH1, and ~80 cofactors. The RC complex is completely surrounded by 16 αβ-heterodimers that form an elliptical ring (Fig. 2(a)). The distances of its major and minor axes are 82 Å and 73 Å for the inner ring and 105 Å and 96 Å for the outer ring, respectively. The RC portion in the ttLH1-RC complex is almost identical to its isolated RC complex [4], but the ubiquinone molecule is bound to the binding site of RC in the ttLH1-RC complex (Fig. 2(b)). Each αβ-heterodimer contains two bacteriochlorophyll (BChl), one spirilloxanthin (Spx), and one calcium ion. The two BChl molecules are bound to α-His36 and β-His36 in LH1 (Fig. 3(a)). BChl of the α-subunit forms a hydrogen bond with α-Trp46, whereas that of the β-subunit forms with β-Trp45. In addition, this BChl interacts with α-Gln28 and β-Trp28. BChl's bound to the α1, β1, α9, and β9 subunits are almost parallel to the special pair BChl's (Fig. 2(a)). These parallel BChl's may play an important role in the efficient transfer of the excitation energy from LH1 to the special pair.

It has been revealed that the binding of calcium ions regulates the thermostability of the ttLH1-RC complex. In addition, an absorption maximum at 915 nm (Q_y transition of BChls in LH1), which is approximately 30 nm red-shifted from that of other purple bacteria, is also resulted by calcium ions. In the ttLH1-RC structure, each calcium ion in LH1 is coordinated by five oxygen atoms from α-Trp46, α-Asp49, α-Asn50, and the C-terminal carboxyl group of β-Leu46 in the adjacent subunit (Fig. 3(b)). The magnesium-magnesium distance of two BChl's is shortest in the bacterial light-harvesting antennas.

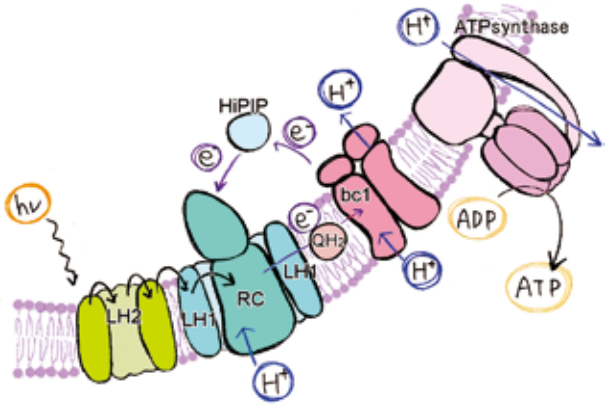

Fig. 1. Schematic representation of the chromatophore vesicle in photosynthetic purple bacteria. Only a part of the vesicle is shown. Vesicle contains photosynthetic proteins such as LH1-RC, LH2, cytochrome bc_1 complex (bc1), ATP synthase and HiPIP. Reduced ubiquinone molecule (QH_2) is transferred from RC to bc1 beyond the LH1 ring.

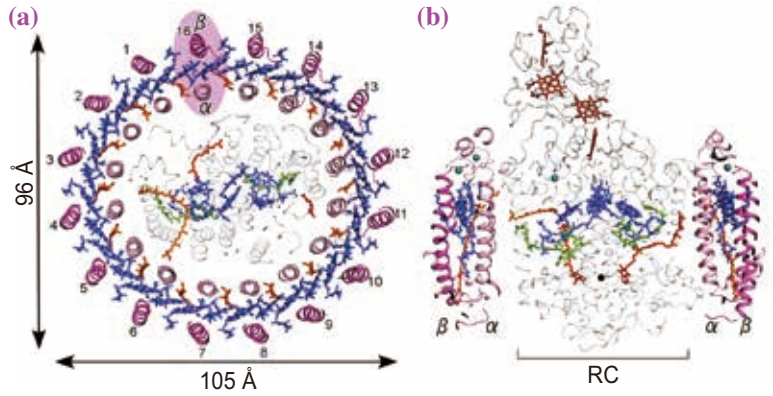

Fig. 2. Overall structure of ttLH1-RC. **(a)** Top view from the periplasmic side. The α and β-apoproteins in the LH1 ring are represented as light pink and pink ribbons, respectively. The subunits in RC are shown in grey. In addition, cofactors are represented in following colors: hemes, brown; calcium ions, green; BChl's, violet; bacteriopheophytin, yellow green; Spx, orange; quinones, red; and non-heme iron, black. A single αβ-heterodimer is shaded in pink. **(b)** Side view of (a) rotated by 90° around the horizontal axis.

These observations indicate that the tight association of the α- and β-apoproteins mediated by the calcium ions has a critical contribution to thermostability and the large red-shift.

The LH1 ring has channels at the interface between adjacent αβ-heterodimers. The channels and the ubiquinone binding site in RC are almost on the same level in the transmembrane region (Fig. 3(c)). The size of the channels is comparable to that of the benzoquinone head group of ubiquinone. Therefore, the channels can play a role of passages for ubiquinone shuttling through the closed LH1 ring.

The structural information of ttLH1-RC enables us to understand the molecular mechanism of the excited energy transfer from LH1 to RC and the ubiquinone shuttling. In addition, the calcium-binding manner indicates the structural basis for the unique properties of ttLH1-RC.

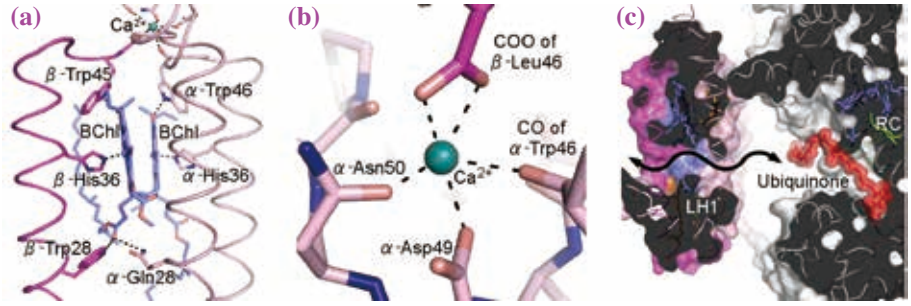

Fig. 3. Detailed views of ttLH1-RC. **(a)** Interactions around the BChl molecules in the LH1 ring. **(b)** Calcium binding site in the LH1 ring. **(c)** Cross section of ttLH1-RC at the ubiquinone transfer pathway.

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