Investigation of the Bacteriochlorin rings and its environment in Fenna-Matthews-Olsen antenna complex revealed by neutron and ultra-high resolution X-ray crystallography

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Photosynthesis is initiated by the capture of a photon by a pigment in an antenna complex to form an exciton, followed by its transfer to the reaction center, where charge separation takes place. In green sulfur bacteria, Fenna-Matthews-Olson (FMO) protein functions as an energy transfer wire between chlorosome and reaction center. The efficiency of the energy transfer is mediated by the specific local environment around the pigments and their optimal geometry. To understand the efficient energy transfer designed by nature and be able to apply the knowledge to fabricating bio hybrid systems for light-harvesting, uncovering the atomic details of antenna complexes has been desirable. Here we report the neutron structure and the highest resolution X-ray structures (at cryogenic and room temperature) of FMO.

We have crystallized FMO from *Prosthecochloris. aestuarii* in a new crystal form consisting of two FMO monomers in the asymmetric unit. Those monomers belong to two separate trimers, which show distinct occupancies for the eighth Bacteriochlorophyll (BChl). Large single crystals were obtained for room temperature neutron diffraction experiment, and an all-atom structure has been refined to 2.2 Å. The X-ray resolution has been improved to 0.99 Å for cryogenic temperature and 1.25 Å for room temperature, representing the highest resolution structures of FMO. The ultra-high resolution X-ray data allowed more precise and detailed conformational analysis of the protein-pigment complex, while the neutron structure explicitly reveals the protonation states of key protein residues. We also investigated the degrees of BChl ring deformation and the factors contributing to them in the FMO crystal structure using a normal coordination structural decomposition procedure.