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Structures of Photosynthetic Reaction Center Mutants that Influence Proton Transfer. M. Schiffer, D.K. Hanson, P. Laible, S. Ginell, P.R. Pokkuluri, Biosciences Div., Argonne National Laboratory, Argonne, IL 60439.

When acidic residues L212Glu and L213Asp near Q_B of the reaction center (RC) are mutated to Ala, the proton transfer to the secondary quinone, Q_B is interrupted. We have determined the structures of *R. sphaeroides* RCs derived from photocompetent revertants of the photosynthetically incompetent double mutant L212Ala-L213Ala (AA). The revertants are AA+M5Asn \rightarrow Asp where an acidic residue was added, and AA+M233Arg \rightarrow Leu where a basic residue was removed. Our previously determined AA structure was used in rigid body refinement for the structure determination. Because the hand fitting of ~ 840 residue structure is tedious and could introduce operator-bias we adapted the computer program RSref (Acta Cryst. D58, 761, 2002) for rebuilding; it works well with relatively low resolution data. The maps show that in AA+M5D, the location of M5 changed that led to the reorientation of H194Q; in AA+M233L, side chains of residues M236Glu and H177Arg shifted by ~ 5 Å. We have predicted that these and other charged residues will reorient as part of the “electrostatic dominoes”. The mutation sites are 15 Å from Q_B , the effect of the mutation is transmitted to Q_B , through changes in side chain, main chain orientations and water positions.

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