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Computational Studies of Proteins¹

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MultiConformation Continuum Electrostatics (MCCE), calculated acidic and basic residue ionization and sidechain positions in bacteriorhodopsin (BR) and halorhodopsin (HR). BR pumps protons out of the cell while HR pumps chlorides in. Comparison of BR ionization states in ground and late M state structures show retinal isomerization moves the protonated Schiff base away from the ionized Asp85 and 212 shifting the proton so only one acid is ionized. A proton is released from the Glu194/204 cluster because the acids separate and Arg 82 moves closer to them. In HR Asp 96 and 85 and Glu 204, important in BR proton transfers are replaced with small residues. In Monte Carlo sampling Cl⁻ are bound near the deleted Asp 85 and Glu 204 in the ground state and released in an intermediate modeled by isomerization retinal from trans to cis and Arg movement toward the extracellular cluster. The charge shifts are similar to those found in BR. Thus, in BR H⁺ is the mobile charge Asp's and Glu's are fixed. In HR mobile Cl⁻ substitutes for the deleted acids. Proton pumping in BR and chloride pumping in HR are driven by the same electrostatic forces.

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