

Supplement to the "Water Molecules and Hydrogen-Bonded Networks in Bacteriorhodopsin - Molecular Dynamics Simulations of the Ground State and the M Intermediate"

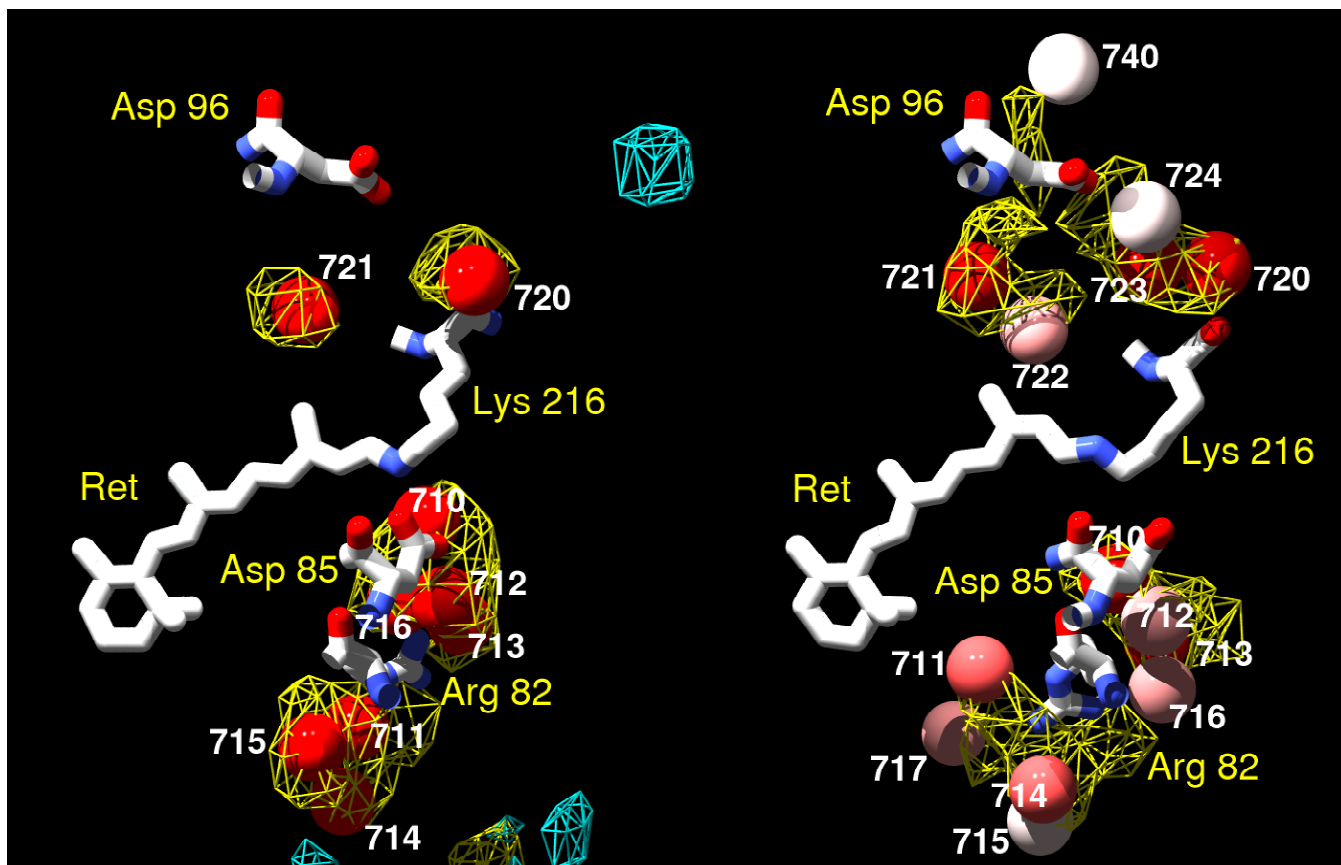


FIG. 1: Trapped water molecules for G (left) and M (right) states are shown in a different saturation of red colour between white and dark-red according to their mobility. The more saturated the red colour, the more immobile is the corresponding water molecule. The surfaces of the volumes for trapped and diffusive water molecules are represented by yellow and blue triangulated nets, respectively, and mark the double σ width of a Gaussian approximation of the radial distribution function (see Fig. 5 in the paper). The red balls represent the locations of trapped water molecules as identified by crystallographic studies (Sass et al., 2000). Those positions of diffusive water molecules are presented, which have high occupancies.

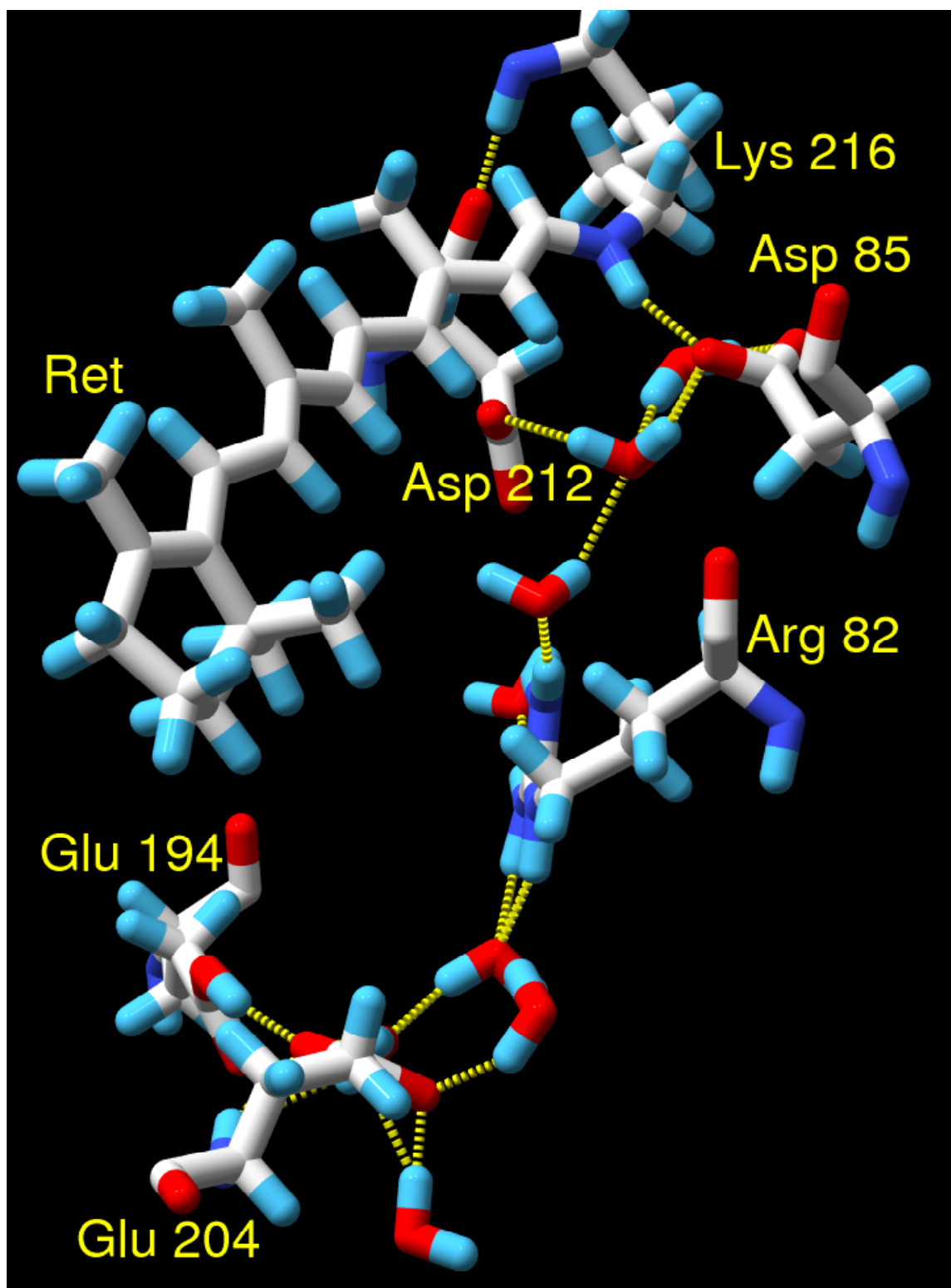


FIG. 2: A snapshot taken from the G state simulation representing a hydrogen-bonded network in the extracellular side of the protein. Several key residues involved in a hydrogen-bonding network are shown. The hydrogen bonds are depicted with yellow broken lines.

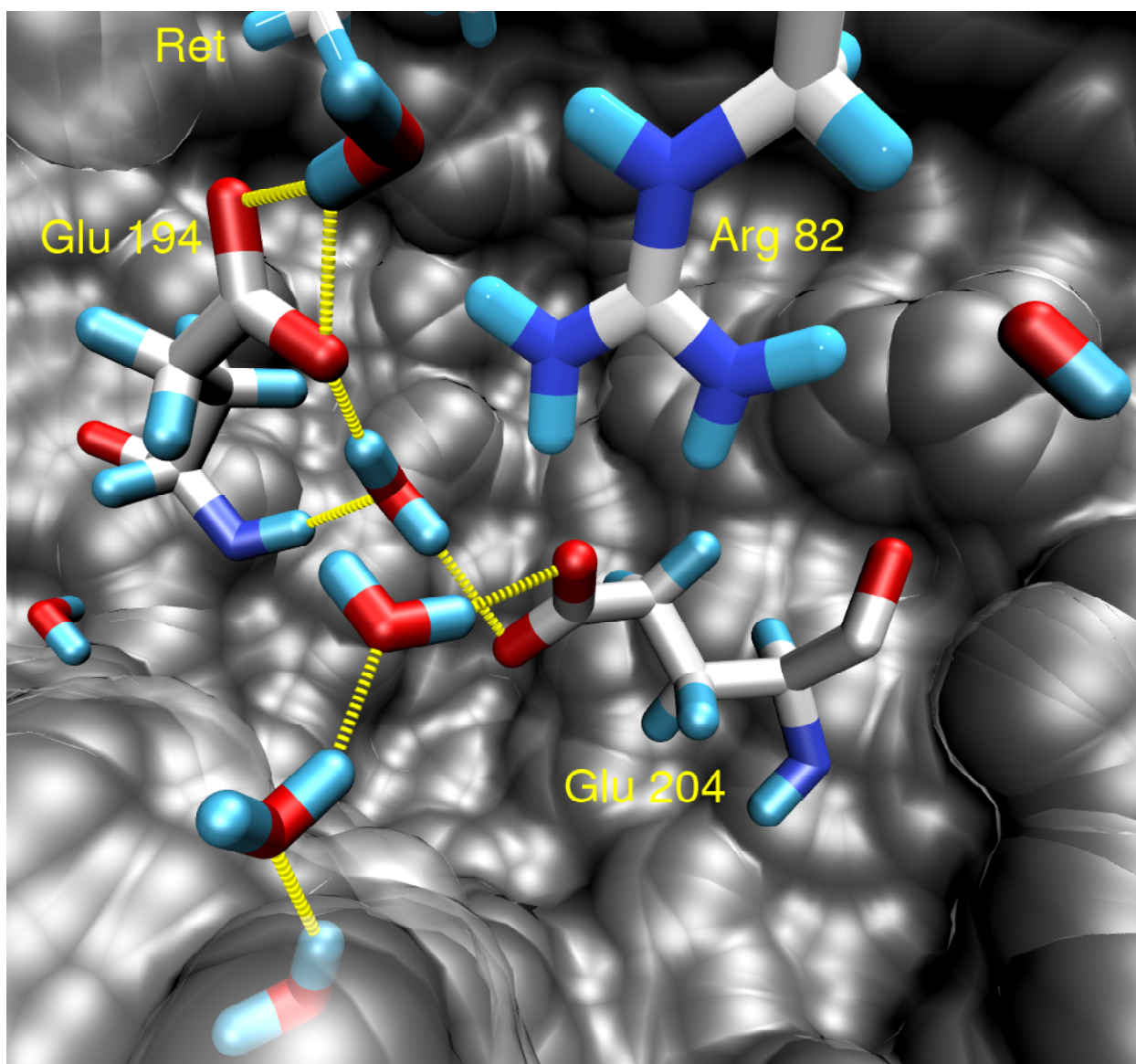


FIG. 3: A snapshot taken from the late M state simulation represents a possible hydrogen-bonded pathway from Glu204 to the bulk water. Several key residues involved in a hydrogen-bonding network are shown. The hydrogen bonds depicted with yellow broken lines. Protein water accessible surface is shown in gray color. The snapshot is taken from the interior of the protein.

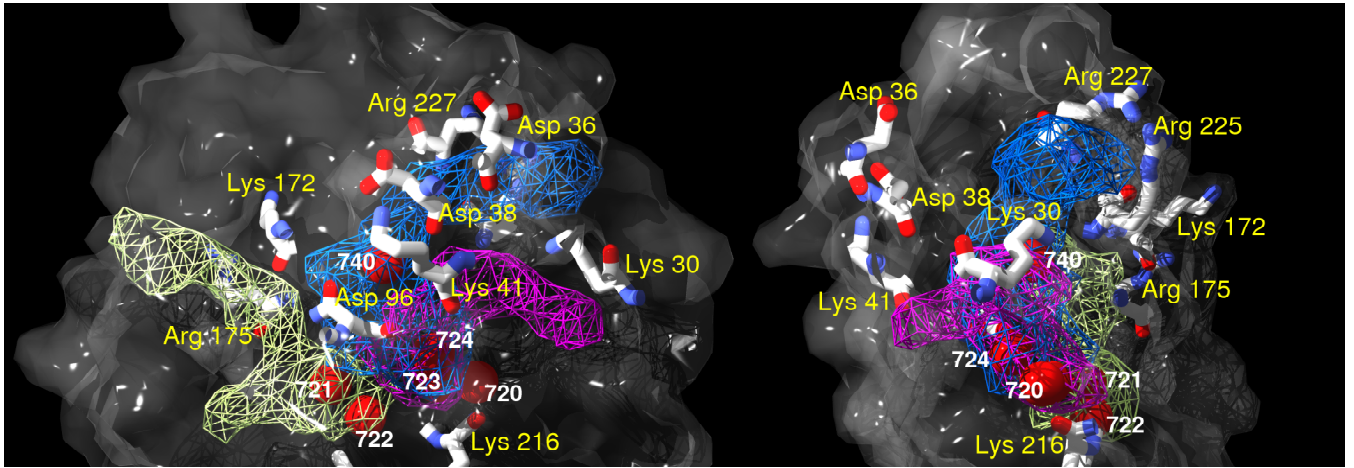


FIG. 4: Three channels for diffusive water molecules in the M state are shown with triangulated nets. Two projections are represented (left and right), the right-hand side of the figure was obtained by rotating the structure in the left-hand side of the figure by the angle of 90° . Three different nets identified from their colours, represent three different channels for water molecules. The red balls represent the locations of trapped water molecules as identified by crystallographic studies (Sass et al., 2000). The escape pathways for the water molecule 740, which escaped from the protein in two monomers, turned out to be the same and are represented by the blue meshed surface. The escape pathway for the water molecule 722, which escaped from the protein in one monomer, is represented by the yellow meshed surface. The penetration of a bulk water molecule towards the cytoplasmic side of the protein (up to water molecules 720, 723, 724) is represented by the magenta meshed surface. It should be noted that the yellow and magenta pathways end up in the polar lipid head groups environment. Nothing prevents water molecules at the end of the yellow channel from escape to the bulk. However it may seem less probable for water to penetrate from the bulk into the magenta channel. Although water population in the region, where the channel ends up is smaller compared to the bulk, it is not negligible and there might occur water penetration to the channel on a longer time scale.