	Experiment title: STRUCTURAL DETERMINATION OF AN EARLY PHOTO-INTERMEDIATE OF BACTERIORHODOPSIN	**Experiment number:** LS 1317
Beamline: ID14-EH3	**Date of experiment:** from: 17 Feb. 99 to: 20 Feb. 99	**Date of report:** 29 Aug. 99
Shifts: 9	**Local contact(s):** Wilhelm Burmeister	*Received at ESRF:* U 2 SEP. 1999

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Report

This experiment was conducted in Feb. 1999. It was a continuation of preliminary experiments that were conducted on beamline ID14, EH3 under experiment LS-1106 in Dec 98 (see experiment report LS-1106 by R. Neutze).

The experiment resulted in the first high-resolution X-ray structure of an early photocycle intermediate of wild type bacteriorhodopsin. A manuscript describing these findings has been accepted for publication in *Nature*:

Karl Edman, Peter Nollert, Antoine Royant, Hassan Belrhali, Eva Pebay-Peyroula, Janos Hajdu, Richard Neutze & Ehud M. Landau
HIGH RESOLUTION X-RAY STRUCTURE OF AN EARLY INTERMEDIATE IN THE BACTERIORHODOPSIN PHOTOCYCLE, *Nature*, in press

Abstract: Bacteriorhodopsin (bR) is the simplest known photon-driven proton pump and as such provides a paradigm for the study of a basic function in bioenergetics. Its seven transmembrane helices encompass a proton translocation pathway containing the

chromophore, a retinal molecule covalently bound to Lys216 *via* a protonated Schiff base, and a series of proton donors and acceptors. Photoisomerisation of the all-*trans* retinal to the 13-*cis* configuration initiates the vectorial translocation of a proton from the Schiff base, the primary proton donor, to the extracellular side, followed by reprotonation of the Schiff base from the cytoplasm. Here we report the high resolution X-ray structure of an early intermediate in the photocycle of bacteriorhodopsin, formed directly after photoexcitation. A key water molecule is dislocated enabling the primary proton acceptor, Asp85, to move. Movement of main chain Lys216 locally disrupts the hydrogen bonding network of helix G, facilitating structural changes in later stages of the photocycle.