



	Experiment title: BAG-Frankfurt Cytochrome <i>bc</i> ₁ complex from <i>S. cerevisiae</i> , Complex I from <i>Yarrowia lipolytica</i>	Experiment number: MX336
Beamline: ID14EH3	Date of experiment: from: 6.11 to: 8.11.2004	Date of report: 1.2.05
Shifts: 2	Local contact(s): Dr. Celia Romao	<i>Received at ESRF:</i>
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Report:

In respiration, the mobile electron carrier cytochrome *c* shuttles electrons from the cytochrome *bc*₁ complex (QCR) to cytochrome *c* oxidase. We determined the structure of the mitochondrial membrane protein QCR with its substrate cytochrome *c* bound (Lange et Hunte 2002) at 3Å resolution. The crystals and the data collection strategy has been optimized during previous visits. All structures of the electron transfer complex determined so far display ordered binding of only one molecule of cytochrome *c* to one of the two binding sites. One of the major open questions is, why the second site is not occupied. To address this question, we examine dependency of cytochrome *c* binding on the redox states and substrate-Q_i-site occupancy. One of our goals was to occupy the Q_i site with the inhibitor Antimycin A1. During the experiment, two datasets of cytochrome *bc*₁ complex with cytochrome *c* and the Q_i site inhibitor Antimycin A1 at 2.5Å/ 3Å resolution were collected (Dataset 1: Resolution 2.5 Å, Completeness 94.8%, R_{merge} 6.9%, I/σI 12.8; Dataset 2: Resolution 3.1 Å, Completeness 96%, R_{merge} 12.3%, I/σI 12.3). Refinement of the structures is in progress and

the binding of the inhibitor Antimycin A1 has been confirmed (Dataset 1: R_{free} 27.8%, R_{cryst} 27.5% ; Dataset 2: R_{free} , 27.1%, R_{cryst} 21.6% ;).

Complex I is the largest and least understood enzyme of the respiratory chain. Structural information is limited to low resolution and is based on electron microscopy of single particles and 2 D crystals. We have obtained crystals of complex I from the strictly aerobic yeast *Yarrowia lipolytica* under several different crystallization conditions. Crystals are small and diffraction cannot be screened at the home source. A screen of additives had been performed and the diffraction quality of the crystals was tested. It had been planned to use the sample changer on this beamline. However, this approach had to be abandoned due to incompatibility with our pins. About 50 crystals could be measured in manual mode and the best crystals diffracted up to 6-7 Å.