



**Experiment title:** Cytochrome *bc*<sub>1</sub> complex from *S. cerevisiae*, BAG Frankfurt

**Experiment number:**  
MX-336

<b>Beamline:</b> ID14 EH1	<b>Date of experiment:</b> from: 03.03.2005 at 8.00 to: 03.03.2005 at 23.59	<b>Date of report:</b> 03.02.06
<b>Shifts:</b> 2	<b>Local contact(s):</b> Dr. Celia Romao and Dr. Stephanie Monaco	<i>Received at ESRF:</i>
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## Report:

In the mitochondrial respiratory chain, the soluble protein cytochrome *c* shuttles electrons from the cytochrome *bc*<sub>1</sub> complex (QCR) to cytochrome *c* oxidase. QCR from yeast is a mitochondrial transmembrane complex with a molecular weight of 466 kDa. The structure of QCR with its substrate cytochrome *c* bound was previously determined at 3 Å resolution (Lange and Hunte, 2002). We were recently able to improve the structure of the electron transfer complex to 1.9 Å resolution. With the results from this structure, structure-function analysis studies were initiated, which focus on mutagenesis of the main interacting residues and crystal contacts. During the beamtime, two datasets were collected of the QCR complex with a H45A cytochrome *c* variant bound. First dataset: resolution 3.0 Å,  $R_{\text{sym}}$  7.5 %,  $I/\sigma I$  14.9, completeness 95.1 %, space group  $P2_1$ , unit cell dimensions 147.4 165.17 194.65 90 104.16 90. The structure of the electron transfer complex was refined at 3.0 Å,  $R_{\text{free}}$  = 28 %  $R_{\text{cryst}}$  = 23%. Second data set: resolution 3.0 Å,  $R_{\text{sym}}$  5.4 %,  $I/\sigma I$  16.3, completeness 91.7 %, space group  $P2_1$ , unit cell dimensions 146.3 164.3 195.2 90 104.3 90. The structure of the electron transfer complex was refined at 3.0 Å,  $R_{\text{free}}$  = 26.9 %  $R_{\text{cryst}}$  = 21.7%. The data collection was hampered by the substantially lower quality of the variant crystals compared to the wild type crystals.

Another major project is the study of redox-dependent conformational changes of the electron transfer complex. For this purpose, datasets at various redox states have been already

collected (ascorbate-reduced, native, oxidized). To complement the studies, a dataset of an oxidized crystal, which was cocrystallized and soaked with ferricyanide, was collected (Resolution 3.4 Å,  $R_{\text{sym}}$  10.1 %,  $I/\sigma I$  12.8 , completeness 95.6 %, space group  $P2_1$ , unit cell dimensions 145.2 165.9 195.0 90 104.145 90). The structure has been refined to 3.4 Å,  $R_{\text{free}}=28$  %  $R_{\text{cryst}}=22$ %.