ESRF	Experiment title: FRANKFURT BAG: ATOMIC MECHANISMS OF MEMBRANE PROTEINS	Experiment number: MX-135
Beamline: ID14-EH2	Date of experiment : from: 31-JUL-2004 8:30 to: 02-AUG-2004 8:00	Date of report : 15-Feb-2005
Shifts:	Local contact(s): Dr. Elena MICOSSI	Received at ESRF:

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Report:

Outer Membrane Protein Complex Aq1862 from the Hyperthermophilic Eubacterium Aquifex aeolicus

(Guohong Peng*, Jürgen Koepke, Verena Linhard, Ulrike Wedemeyer, Hartmut Michel)

Aq1862 crystals were screened for lower mosaicity and higher resolution, two native datasets at 2.0 Å and 1.85 Å resolution, respectively, were collected.

Table 1. Diffraction data set collected at ESRF ID14-EH1 on a crystal of Aquifex aeolicus (R3, na1: a = b =110.36Å, c = 539.02 Å, na52:a=b=109.3, c=237.89)

	resol. range [Å]	measured reflections	unique reflections	complete [%]	R _{sym} [%]
na1	20.0-2.00	937,111	165.237	99.9(100)	14.3(4.2)
na52	20.0-1.85	544,949	199,506	98.9 <i>(95.2)</i>	10.0(3.96)

Variant Photosynthetic Reaction Center from *Rhodopseudomonas viridis* (H. Juhnke*, C.R.D. Lancaster)

Two shifts of beam time were devoted to recording (ultimately) four data sets of a variant photosynthetic reaction center from *Rhodopseudomonas viridis*. The best data set is summarized in Table 2. However, the resolution of the resulting electron density maps was

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still insufficient to reliable discuss any differences to the wild-type structure, so higher resolution data are required.

Table 2. Best of four diffraction data sets collected at ESRF ID14-EH1 on a crystal of a variant *Rp. viridis* RC $(P4_32_12, a = b = 223.5 \text{ Å}, c = 113.6 \text{ Å})$

	resol. range [Å]	measured reflections	unique reflections	complete [%]	R _{sym} [%]
pH7_AS195_1	50.0-2.50	478,663	99,099	98.5	8.8
	2.56-2.50	<i>27,170</i>	<i>6,456</i>	<i>98.0</i>	<i>47.6</i>

Quinol:Fumarate Reductase from Campylobacter jejuni (M. Mileni*, C.R.D. Lancaster)

Quinol:fumarate reductase (QFR), couples the reduction of fumarate to succinate to the oxidation of quinol to quinone, in a reaction opposite to that catalysed by mitochondrial complex II (succinate dehydrogenase). QFR from the anaerobic bacterium *Campylobacter jejuni* consists of three protein subunits, FrdA, FrdB, and FrdC. Crystals of this bioenergetically important membrane protein complex have previously been obtained in space group P1 with unit cell dimensions of a = 130.1 Å, b = 130.9 Å, c = 164.2 Å, and α = 108.6°, β = 90.6°, and γ = 118.5° and complete diffraction data to 3.9 Å has been collected in February 2003 at ID14 EH1 (see earlier report). More recently, a new crystal form of space group P2₁ with the unit cell dimensions a = 117.2 Å, b = 130.7 Å, c = 132.9 Å, β =108.0° has been obtained. The remaining shift of beamtime was devoted to (ultimately unsuccesful) attempts to improve the previously recorded data set of this crystal form at 3.24 Å resolution (see May 2004 EH1 report).

Complex I from Yarrowia lipolytica

(Volker Zickermann*, Carola Hunte)

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* with a monoclonal antibody fragment. Crystals are small and diffraction cannot be screened at the home source. 20 crystals were tested for diffraction. A few crystals diffracted up to 18-12 Å resolution. The pattern indicated a stability and/or a freezing problem. Optimization of crystallization conditions is in progress.

One (night) shift was lost due to ProDC interface problems (Vasundara Srinivasan*)