ESRF	**Experiment title:** FRANKFURT BAG: Quinol:fumarate reductase, a membrane protein complex from *Wolinella succinogenes*	**Experiment number**: LS-1930
Beamline: ID14-EH3	**Date of experiment**: from: 21-Apr-01 8:00 to: 23-Apr-01 7:00	**Date of report**: 30-Aug-2001
Shifts: 6	**Local contact(s)**: Dr. Hassan Belrhali	*Received at ESRF:*

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Report:

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 *Wolinella succinogenes* consists of three protein subunits, FrdA, FrdB, and FrdC. Crystals of this bioenergetically important 130 kDa membrane protein complex diffract up to at least 1.8 Å and have previously been shown to have two different unit cells, both of the monoclinic space group $P2_1$. The unit cell of crystal form "A" is a = 85.2 Å, b = 189.0 Å, c = 117.9 Å, and β = 104.5º. Crystal form "B" has the unit cell dimensions a = 118.4 Å, b = 85.1 Å, c = 188.9 Å, β =96.5º. There are four complexes per unit cell and thus two complexes in the asymmetric units of both unit cells. Using data collected earlier at ESRF BM14 (cf. experimental reports for LS-1369), the structure of crystal form A has been solved by multiple isomorphous replacement and anomalous scattering (MIRAS) and refined to 2.2 Å resolution, and that of crystal form B has been solved by molecular replacement (MR) and refined to 2.33 Å resolution [1]. The structure of the enzyme in a third crystal form, form "C", with cell dimensions a = 81.1 Å, b = 290.2 Å, c = 153.6 Å, β =95.7º and four heterotrimeric QFR complexes in the asymmetric unit, has also been solved by molecular replacement [2], and refined at 3.1 Å resolution [3]. Mechanistically interesting variant

enzymes have been obtained by site-directed mutagenesis. During the beam time available for this subproject, two data sets of form "A" crystals, one a high-resolution native data set, the other from a QFR enzyme-inhibitor complex could be collected (see Table) at T = 4°C from just one crystal each. These two structures are currently undergoing refinement. In addition, six partial data sets of variant QFR and QFR-inhibitor complexes could not be made complete due to lack of sufficient high quality crystals at the time.

Table. Diffraction data collected at ESRF ID14-EH3 on crystals of *W. succinogenes* QFR inhibitor complexes.

	resol. range [Å]	measured reflections	unique reflections	complete [%]	R_{sym} [%]
nat_93b04	28.8-1.78	769,713	295,439	85.8	7.1
	1.84-1.78	*30,025*	*20,289*	*59.0*	*31.6*
inh_56b06_1	30.0-2.50	538,310	128,310	99.2	8.7
	2.59-2.50	*42,254*	*12,068*	*93.3*	*34.2*

References

[1] CRD. Lancaster, A Kröger, M Auer, H Michel (1999) *Nature* **402,** 377-385.

[2] CRD Lancaster, R Gross, A Haas, M Ritter, W Mäntele, J Simon, A Kröger (2000). *Proc. Natl. Acad. Sci. U.S.A.* **97**, 13051-13056.

[3] CRD Lancaster, R Gross, J Simon (2001) *Eur. J. Biochem.* **268**, 1820-1827.