ESRF	**Experiment title:** FRANKFURT BAG: Quinol:fumarate reductase, a membrane protein complex from *Wolinella succinogenes*	**Experiment number**: LS-2189
Beamline: ID14-EH1	**Date of experiment**: from: 20-JUL-2002 to: 21-JUL-2002	**Date of report**: 5-AUG-2002
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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 $\beta = 104.5^{o}$. Crystal form "B" has the unit cell dimensions a = 118.4 Å, b = 85.1 Å, c = 188.9 Å, $\beta = 96.5^{o}$. 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, $\beta = 95.7^{o}$ 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 [2,3]. During the beam time

available for this subproject, four data sets of form “A” crystals from one enzyme-substrate, one enzyme-inhibitor, and two variant QFR enzyme complexes could be collected (see Table) at T = 4°C from just one crystal each. The resulting structures are currently undergoing refinement.

Table. Diffraction data collected at ESRF ID14-EH1 on crystals of two *W. succinogenes* QFR variants, one QFR-substrate and two QFR-inhibitor complexes.

	resol. range [Å]	measured reflections	unique reflections	complete [%]	R_{sym} [%]
sub_1220302_1	30.0-2.75	271,162	92,646	99.0	9.0
	2.85-2.75		*9,228*	*99.3*	*50.7*
inh_fr2002_3b05	30.0-2.70	312,025	97,128	98.2	9.1
	2.80-2.70		*9,747*	*99.1*	*39.9*
var50_117d01	30.0-2.80	189,161	70,855	79.9	9.4
	2.90-2.80		*7,264*	*82.3*	*48.4*
var75_117d01	30.0-3.20	94,015	47,234	78.4	11.4
	3.30-3.20		*3,592*	*60.0*	*24.6*

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.