ESRF	**Experiment title:** FRANKFURT BAG: Quinol:fumarate reductase, a membrane protein complex from *Wolinella succinogenes*	**Experiment number**: LS-1930
Beamline: ID14-EH1	**Date of experiment**: from: 06-OCT-2001 8:00 to: 07-OCT-2001 7:00	**Date of report**: 21-Feb-2002
Shifts: 3	**Local contact(s)**: Dr. Stéphanie Monaco	*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 [2,3]. During the beam time available for this

subproject, five data sets of form "A" crystals from two variant QFR enzymes, one enzyme-substrate, and two enzyme-inhibitor 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} [%]
var_117c02_1	50.0-2.20	970,241	182,229	99.8	9.2
	2.25-2.20		*12,145*	*100*	*35.6*
sub_12201_0501	50.0-2.20	516,921	179,041	98.1	8.0
	2.25-2.20		*11,854*	*97.6*	*74.4*
inh_122_11_0401	50.0-2.20	435,603	166,389	91.2	9.9
	2.25-2.20		*10,495*	*86.4*	*27.0*
inh_120_04_04_2	50.0-2.20	492,754	171,300	93.9	9.8
	2.25-2.20		*10,872*	*89,5*	*24.5*
var_118d05_1	50.0-2.20	586,975	171,993	94.2	8.6
	2.25-2.20		*11,071*	*91.1*	*25.8*

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.