ESRF	**Experiment title:** Frankfurt BAG	**Experiment number**: LS-1800
Beamline: BM14	**Date of experiment**: from: 22-Nov-2000 to: 23-Nov-2000	**Date of report**: 28-Feb-2001
Shifts: 3	**Local contact(s)**: Dr. Sigrid Stuhrmann	*Received at ESRF:*

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Report:

Quinol:fumarate reductase, a membrane protein complex from *Wolinella succinogenes*

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 three different unit cells, all 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]. A third monoclinic crystal form, form "C", ($P2_1$; a = 81.1 Å, b= 290.2 Å, c = 153.6 Å, β = 95.7°) has four heterotrimeric QFR complexes in the asymmetric unit [2,3].

These crystals exhibit a high degree of anisotropy in the diffraction pattern (<2.8 Å resolution along the b* and c* axes, ~3.8 Å along the a* axis). The structure of crystal form C has been solved by molecular replacement (MR) [2] and refined to 3.1 Å resolution. It displays functionally important structural differences compared to the previous crystal forms. These can be attributed to alternate crystal packing contacts [3].

During the beam time allocated to this subproject, one higher quality data set and a medium-resolution data set for a variant QFR could be collected (both for crystal form A). Due to the optimum conditions for data collection at BM14 first established in November 1998 (cf. our previous reports for LS-1137 and LS-1369), only one crystal was required for each data set. Structures for the two data sets are currently being refined.

Table: *W. succinogenes* QFR diffraction data collected at ESRF BM14 (22-23 November 2000)

	resol. range [Å]	measured reflections	unique reflections	complete [%]	I/σ(I)	>2σ [%]	R_{sym}* [%]
inhibitor complex							
proj47/56a03_1	40.0-2.25	645,852	157,618	99.1	11.0	87.8	9.8
	2.30-2.25	*42,086*	*10,558*	*100.0*	*5.1*	*72.4*	*38.4*
mutant							
mut1/47a03_2	40.0-3.50	124,067	36,384	93.4	10.0	73.3	7.7
	3.58-3.50	*7,954*	*2385*	*91.4*	*2.9*	*44.6*	*37.7*

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.*, in press.