ESRF	**Experiment title:** **ROO - Rubredoxin oxygen oxidoreductase**	**Experiment number**: LS-1093
Beamline: ID14 3	**Date of experiment:** from: 16.12.98 to: 17.12.98	**Date of report:** 25.02.1999
Shifts: 3 (BAG)	Local contact(s)**:** Laurence Dumon	*Received at ESRF:*

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Report: ROO crystals were grown from a new protein batch. A preliminary screen of crystals with a rotating anode X-ray generator and a MarResearch imaging plate led to two crystal specimens with potential diffraction capabilities. The crystals were transported to ESRF in a liquid nitrogen container. Rotation images had revealed a substantial increase in the resolution limits, 2.4 Å on a conventional source. However, at station ID14 3 with the highly collimated beam, both crystals revealed to suffer from twinning: at different rotation zones a high percentage of spots showed an irregular shape or a satellite. The resolution, however, was indeed remarkably higher then ever before, better then 1.6 Å (to compare with 2.3 Å, the highest resolution previously obtained on a synchrotron source). A 100° rotation data collection was performed with the best crystal, and data processed trying to isolate each spot from its satellite by limiting the spot mask. However, depending on the particular crystal orientation, 'spot' and 'satellite' were interchangeable or even overlapped. The R_{merge} was about 15-18% throughout the resolution band until 1.7 Å.

The residual collection time was used to collect diffraction data from a backup project, the 7Fe-dicluster-ferredoxin from *Acidianus ambivalens*. A frozen, needle like crystal was used to collect a diffraction data set to 1.98 Å resolution. Data statistics are presented below. Inspection of the cummulative Wilson distribution indicates a possible merohedric twin, but the self rotation function does not reveal any additional rotation axis at a special orientation. A molecular replacement search using the ferredoxin from *Sulfolobus* with program AmoRe enabled the definitive space-group determination, $P3_121$. The structure was solved using three molecules in the asymmetric unit (calculated solvent content 50%).

Data statistics:

Space group	$P3_121$
Cell dimensions	a=b=116.76, c=51.04 Å
Resolution range	30.6 - 1.98
Number of unique intensities	26493
Overall redundancy	6.2
Completeness	94.3 %
$R_{merge}(I)$	9.0 %
$I/\sigma(I)$	17.8

Outer shell (2.03-1.98 Å)

Completeness	73.7 %
$R_{merge}(I)$	37.7 %
$I/\sigma(I)$	2.1

AmoRe molecular replacement solution:

Correlation-factor 50.0, R-factor 38.7