

**Experiment title:**

High resolution data collection from a
thiolase crystal

**Experiment
number:**

LS226 Commissioning

Beamline:

102

Date of Experiment:

from: ⁵February, 1995 to: ⁵ February, 1995

Date of Report:

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Shifts:

2

Local contact(s):

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Report:

During this visit a 1.8 Å dataset was collected from acryofrozen peroxisomal yeast thiolase crystal. Previous to this visit the thiolase structure had already been solved and refined at 2.8Å resolution. Subsequently this structure was further refined against the 1.8Å ESRF dataset. The refinement was done with X-PLOR and TNT. Currently the R-factor is 18.7% with good geometry. A manuscript, describing the refined structure, including a hypothesis for the thiolase reaction mechanism is in preparation.

I have delayed writing this manuscript because so far I was not happy with the refinement status; several attempts have been made to improve the quality of the refinement, most importantly:

1. The data collected at the ESRF was reprocessed with the help of Dr. Lamzin (EMBL-Hamburg), which showed that the low resolution data was not good and also indicated problems with the overloads. The crystallographic R-factor dropped by 1% with the reprocessed data (using the same model). This dataset is 98.9% complete between 10Å and 1.8Å. The Rmerge is 4.770.

2. The dataset was anisotropic. After scaling the Fcalc and Fobs with anisotropic B-factors, the R-factor dropped by 1.170.