ESRF	**Experiment title:** MAD data collection on MurE synthetase from *E.coli*	**Experiment number:** LS1506
Beamline: BM14	**Date of experiment:** from: 25 to: 26 november 1999	**Date of report:** 28-2-2000
Shifts: 1	**Local contact(s):** Gordon Leonard	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Elspeth Gordon*

Report:

MAD data collection on MurE

MurE belongs to a family of ligases which are involved in the biosynthesis of the the muropeptide, the precursor of the bacterial cell wall. The protein is a possible target for antibacterial drug therapy.

The protein crystallises readily in several different crystal forms. For structure determination we used a monoclinic form. Crystals are small but diffract to high resolution. The space group is $C222_1$ with a=93.27 Å, b=99.51 Å, c=234.34Å

A MAD experiment was carried out at the Selenium edge on BM14 using the MAR CCD detector. Data were collected to only 2.8Å because the long cell axis compromised the data collection. Data were collected at 3 wavelengths, inflection point (0.9791Å), peak (0.9790Å) and remote (0.8550Å). Data were processed using DENZO. 24 Selenium positions (out of 26 expected) were found using SOLVE, the phasing to 2.8Å had a figure of merit of 0.81 and a score of 181.52.

MAD phases were extended to 2Å by solvent flattening and averaging of the molecules in the asymmetric unit (DM). The high resolution data set, to 2Å, was collected on ID14 EH2 (λ=0.933Å) using the MAR CCD. Rsym 6.6% (in outer shell 22.0%). This allowed ARP to be used to obtain an automatic tracing of the polypeptide chain. The structure has been refined to 2.0Å, with R=20% and Rfree=23%.