

	Experiment title: E. coli isomeroreductase heavy atom phasing	Experiment number: 30-01-313
Beamline: bm30	Date of experiment: from: 4 Mai 2001 to: 5 Mai 2001	Date of report: 22 mai 02 <i>Received at ESRF:</i>
Shifts: 1	Local contact(s): R. Kahn	
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Report:

E. coli isomeroreductase crystallizes in an hexagonal space group and molecular replacement has been unsuccessful to this date. We tried soaking crystals with Gd compounds and collected data on those crystals. However, the already weak diffraction of the native crystals was made worse by the soaks and we could only get data to 6Å. In spite of a definite Gd site, the merging between native and derivative was too bad and we could not get any phase extension.

Summary of data collection

Wavelength 1.711Å; distance 200 mm (4.5Å resolution at detector edge).

Number of images : 173; unit cell : 148Å, 148Å, 211Å, 90°, 90°, 120°.

Processing using denzo/scalepack :

R-sym = 6.9% (36.5% at 6.15Å)

R-ano = 7.7% (19% at 6.15Å).

Program SOLVE found 2 sites and phased molecular replacement allowed for space group to be identified as $P6_22$ (in contrast to $P6_422$ that did not give a solution). However, merging with native data gave R-merge of 25% and did not allow useful phase extension.

