

ESRF	Experiment title: Structural Investigation of imidazole glycerol phosphate dehydratase	Experiment number: LS 1875
Beamline: BM30A	Date of experiment: from: 13 June 2001 to: 15 June 2001	Date of report : 30-8-2001
Shifts:	Local contact(s):	Received at ESRF:

Names and affiliations of applicants (* indicates experimentalists):

Dr. Richard KAHN

P.J.Baker *, D.Hargreaves *, S.Bailey *, J.B.Rafferty, P.J.Artymiuk & D.W.Rice. Krebs Institute, Dept. Molecular Biology and Biotechnology, University of Sheffield, Western Bank, Sheffield S10 2TN. U.K.

Report:

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Preliminary report on LS1875, BM30A:

Five shifts were allocated on station BM30A, primarily to collect selenomethionine multiple wavelength anomalous dispersion data on crystals of imidazole glycerol phosphate dehydratase (IGPD). We had previously shown that our crystals of this enzyme were perfectly twinned (see report LS1745) and, despite checking scores of crystals on our home detector, had been unable in the intervening time to grow any crystals that were not twinned. Crystals of four other proteins were thus taken to the ESRF to use this beam time. Each of these four proteins had an unknown structure. Two had been overexpressed in the presence of seleno methionine, one had been doped with mercury and for the other we had both mercury doped and gadolinium doped crystals. Crystals of each had been tested at Sheffield and were transported to the ESRF at 100K. Full MAD data sets were collected at three wavelengths for the two seleno-met grown crystals, corresponding to the peak, inflection and high energy remote wavelengths, as determined from a fluorescence scan of each

crystal. For the gadolinium doped protein, a fluorescence scan was undertaken at the Gd edge, which indicated the presence of Gd, and thus data were collected at the peak, inflection and high energy remote wavelengths for Gd. We also had mercury doped crystals of this protein and data were collected at the Hg peak position as well. The final three hours of beam time were used collecting a Hg peak wavelength data set for the fourth protein.

Using this data we have been successful in determining the structures of two of these four proteins. The structure of the Gd doped protein is fully refined, and a manuscript is in preparation. The selenium substructure of one of the Se-Met crystals has been determined and the protein model is undergoing refinement. It has thus far proved impossible to determine the selenium substructure of the other protein, possibly due to low level incorporation of selenium.

A full report will follow, once these structures have been fully refined.