

**Experiment title:**

The mechanism of isopenicillin N synthase

Experiment**number:**

LS 1387

Beamline:

ID14 EH3

Date of experiment: 9-5-1999

from:

to:

Date of report:

20-3-2000

Shifts:

1 (16 hr)

Local contact(s):*Received at ESRF:***Names and affiliations of applicants (* indicates experimentalists):**

Dr P. L. Roach*

Dr I. J. Clifton*

J. M. Elkins*

J. M. Ogle*

P. J. Rutledge

Professor Sir Jack Baldwin

Report:

With this allocation of beamtime we have continued our time resolved studies on isopenicillin N synthase. Data was collected from crystals of Fe-IPNS with two substrate analogues, δ -(L- α -aminoadipoyl)-L-cysteinyl-D-cyclopropylglycine (ACcpG) and δ -(L- α -aminoadipoyl)-L-cysteine D- α -hydroxy isovaleryl ester (ACoV).

The crystals had been subjected to high-pressure oxygen gas prior to freezing and data collection in the attempt to bring about turnover in the active site.

Specifically, datasets were collected from IPNS:Fe²⁺:ACcpG crystals that had been exposed for 120 min, 320 min and 360 min, and from crystals of IPNS:Fe²⁺:ACoV pressurised for 2 min, 4 min, 5 min and 10 min. Seven datasets were collected in all.