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| | Experiment title: Data collection on VIM-2 beta-lactamase Test on PBP1a transpeptidase domain | Experiment number: LS-1794 |
| Beamline: ID14 EH4 | Date of experiment: from: 11-9-00 to: 12-9-00 | Date of report: 10-2-01 |
| Shifts: 3 | Local contact(s): E. GORDON | <i>Received at ESRF:</i> |
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Report:

A) Zn beta-lactamase

Analysis of VIM-2 beta-lactamase from *Pseudomonas aeruginosa* crystal co-crystallized with the inhibitor D-Captopril, grown in PEG, Sodium Acetate at pH 6.5. The crystal was frozen directly in the cryostream after brief soaking in 15% glycerol. Two data collection at 1.5 Å and 2.5 Å were collected (merged data 96% completeness). Crystals belong to the space group I222 and have unit cell parameters $a = 67.17 \text{ \AA}$ $b = 78.03 \text{ \AA}$ $c = 80.12 \text{ \AA}$.

Structure solution revealed no presence of inhibitor in the active site and strong oxydation of one cysteine located in the active site. The possible role of radiation on this oxydation is under consideration.

B) Transpeptidase domain

Beamline had problems with the beam touching the inside of the collimator, causing severe scattering and consequently images of lesser quality ; however, since the diffraction did not go much beyond 3.2 Å, scattering did not interfere with data processing with DENZO. The crystal showed some radiation damage. PBP1a TP crystals belong to space group C2221 and have unit cell parameters $a=114.2 \text{ \AA}$ $b= 185.7 \text{ \AA}$ $c= 51.9 \text{ \AA}$. There is one molecule per asymmetric unit and 45% solvent. Collected one 90% complete data set.