ESRF	Experiment title: Mannanase	Experiment number: LS1383
Beamline: ID14.4	<b>Date of experiment:</b> From: 22/02/99 to: 25/02/99	Date of report:
Shifts: BAG	Local contact(s):	Received at ESRF:

Names and affiliations of applicants (\* indicates experimentalists):

E. Sabini

J.P. Turkenburg\*

K.S. Wilson

M. Siika-Aho

M. Penttila

York Structural Biology Laboratory, Chemistry Department, University of York, Heslington, York, YO10 5DD, UK

## Report:

This work was published in Acta Cryst D, and only the abstract and full reference are included here:

The crystal structure of the catalytic core domain of  $\beta$ -mannanase from the fungus Trichoderma reesei has been determined at a resolution of 1.5Å. The structure was solved using the anomalous scattering from a single non-isomorphous platinum complex with two heavy-metal sites in space group P2<sub>1</sub>. The map computed with the experimental phases was enhanced by the application of an automated model building and refinement procedure using the amplitudes and experimental phases as observations. This approach is expected to be of more general application. The structure of the native enzyme and complexes with tris-HCl and mannobiose are also reported: the mannobiose binds in subsites +1 and +2. The structure is briefly compared with that of the homologous  $\beta$ -mannanase from the bacterium Thermomonospora fusca.

## Published in:

E. Sabini, H. Schubert, G. Murshudov, K.S. Wilson, M. Siika-Aho and M. Penttila

"The three-dimensional structure of a *Trichoderma reesei* b-mannanase from glycoside hydrolase family 5"

Acta Crystallographica (2000) D56, pag 3-13.