ESRF	**Experiment title:** Uppsala (II) BAG, LS-1665 (T. Alwyn Jones BAG) Cellulases; EG3	**Experiment number**: LS 1804
Beamline: ID 14:EH1	**Date of experiment**: from: 2 Dec 2000 to: 4 Dec 2000	**Date of report**:
Shifts: 1 (EG3: 1.0)	**Local contact(s)**: Stéphanie Monaco	*Received at ESRF:*

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Report:

Protein Name EG3: Endoglucanase 3 from *T. reesei*

Brief background and outline of project

(Cel12A, GH family 12). EG3 is a minor component in the cellulase system, but may nevertheless play an important role. It differs from the other cellulases in that it does not contain the additional cellulose binding module and linker typical for many cellulases. It is also smaller than other fungal cellolytic enzymes and subsequently appears to have a larger ability to penetrate the cellulose substrate. We have solved the native structure enzyme and reasently also the structure of two catalytic inactive mutants, with data collected on ID14:EH4. Our aim now is to obtain a ligand enzyme complexes structure with two new catalytic inactive mutants enzymes for understanding catalytic mechanism, substrate binding and specificity. Large crystals have been obtained for the catalytic inactive mutants that diffract to high resolution, and which could hopefully yield ligand enzyme complex structures at atomic resolution.

Datasets collected on ID14:EH1

Two datasets were collected at ID14:EH1, from the two new *T. reesei* EG3 catalytic inactive mutants, co-crystallized with a ligands. Booth datasets were of high quality and high completeness. The space-group of one of these two new datasets was a new one (P31) compared with the one (P21) previously always obtained from crystals of this enzyme

previously. Both the two new datasts had to bee solved by molecular replacement methods. These two new catalytic inactive mutants structures have now been solved and refined. Neither of these two structure did contain a ligand in the active site but these structures will also, together with previous mutant structures, be used in a manuscript where we try to explain the catalytic mechanism of the enzyme.

Data statistics for the datasets:

Dataset1:

Ligand: No
Mutation: C
Resolution: 19-1.7A
Space group: P31
Cell: x:70.99 y:70.99 z:69.23 , ? : 90, ? :90, ?:120
Completeness: 99%

Dataset 2:

Ligand: No
Mutation: B
Resolution: 20-1.5 A
Space group: P21
Cell: x:69.7 y:71.6 z:121.4, ? : 90 ? :118.5 ?:90
Completeness: 95%