



	Experiment title: Uppsala (II) BAG, LS-1665 (T. Alwyn Jones BAG) Cellulases; EG3	Experiment number: LS 1804
Beamline: ID 29	Date of experiment: from: 9 Feb 2001 to: 11 Feb 2001	Date of report: <i>Received at ESRF:</i>
Shifts: 6 (Eg3: 1)	Local contact(s): Bill Shepard	
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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 recently solved the structure and now aim at obtaining homologous protein structures, ligand complexes with wild-type and mutated enzymes for understanding catalytic mechanism, substrate binding and specificity. Very large crystals have been obtained that diffract to very high resolution (0.9-1.0 Å) and which could hopefully yield structures at atomic resolution.

Datasets collected on ID14:EH1

Two datasets were collected. One on a crystal from a catalytic inactive mutant of *T. reesei* EG3, co-crystallized with a sugar substrate analogs: G3S. The second dataset was collected on a crystal from a homologous *T. reesei* EG3 protein. The two datasets had high completeness and were of high quality and gave very nice density maps. The dataset from the ligand soaked crystal had no ligand bound in the catalytic active cleft of the protein. The second dataset from the homologous protein has now been solved by molecular replacement methods, and will be published as a new homologous EG3 structure.

Data statistics for the datasets:

Dataset 1:

Ligand: No

Mutation: A

Resolution: 40-1.7A

Space group: P21

Cell: a:62.5, b:77.6, c:83.4, ? : 90, ?:98.46, ?:90

Completeness: 96%

Dataset 2:

Homologue Jes

Ligand: No

Resolution: 50-1.6A

Space group: P43

Cell: a:49.2, b:49.2, c:165.5, ? : 90, ?:90, ?:90

Completeness: 98%

