ESRF	**Experiment title:** Uppsala (II) BAG, LS-1665 (T. Alwyn Jones BAG) Cellulases; EG3	Experiment number: LS 1665
Beamline: ID 14:EH1	**Date of experiment:** from: 26-Feb 2000 to: 28 Feb 2000	**Date of report:**
Shifts: 6 (Eg3: 2)	**Local contact(s):** Hassan Belrhali	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

T. Alwyn Jones, Uppsala University, alwyn@xray.bmc.uu.se
Sherry L. Mowbray, Swedish Univ. Agric. Sciences, mowbray@alpha2.bmc.uu.se
Jerry Ståhlberg, Swedish Univ. Agric. Sciences, Jerry. Stahlberg@molbio.slu.se
* Mats Sandgren, Uppsala University, mats@alpha2.bmc.uu.se
* Emma Jakobsson, Uppsala University, emma@alpha2.bmc.uu.se
* Martin Hällberg, Uppsala University, martin-h@alpha2.bmc.uu.se
* EvaLena Andersson Uppsala University, evalena@alpha2.bmc.uu.se

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 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 A) and which could hopefully yield structures at atomic resolution.

Datasets collected on ID14:EH1

Three datasets were collected on protein crystals with catalytic inactive mutant T. reesei EG3. The crystals were co-crystallized with three different sugar substrate analogs: G3S, G5 and G6. All three datasets had high completeness and were of high quality and gave very nice density maps. Non of the three datasets had any ligand bound in the catalytic active cleft of the protein.

Data statistics for the datasets:

Dataset1:

Ligand: G6 20 mM
Resolution: 40-1.7A
Space group: P21
Cell: a:43.2, b:104.3, c:45.4, ? : 90, ? :118.5, ?:90
Completeness: 98%

Dataset 2:

Ligand: G5 20 mM
Resolution: 40-1.4A
Space group: P21
Cell: a:43.2, b:104.1, c:45.5, ? : 90, ? :118.3, ?:90
Completeness: 96%

Dataset 3:

Ligand: G3S 20 mM
Resolution: 40-1.4A
Space group: P21
Cell: a:43.98, b:104.9, c:45.3, ? : 90, ? :118.2, ?:90
Completeness: 98%