	Experiment title: Conformational study of plurimodular cellulases.	**Experiment number**: LS-1435
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Shifts: 9	**Local contact(s)**: Pierre Panine	*Received at ESRF:*

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Report:

Cellulase Cel45 from *Humicola insolens* has a modular structure with a catalytic module and a cellulose-binding module (CBM) separated by a 36 amino acid, glycosylated, linker peptide. The solution conformation of the entire two-domain Cel45 protein as well as the effect of the length and flexibility of the linker on the spatial arrangement of the constitutive modules were studied by small angle X-ray scattering combined with the known 3-D structure of the individual modules. Measurements of the radii of gyration and the distance distribution functions show that the linker exhibits an extended conformation leading to a maximum extension between the two centres of mass of each module corresponding to about 4 cellobiose units of similar orientation on a cellulose chain. The glycosylation of the linker is the key-factor defining its extended conformation, and a 5-proline stretch mutation on the linker was found to confer a higher rigidity to the enzyme. Our study shows that even though the linker is rather flexible and extended, its structure most likely influences the respective positioning of the catalytic module and the CBM onto the insoluble substrate. The combination of these results with calculation of the shape of the full length enzyme is consistent with a model where cellulases can move on the surface of cellulose with a caterpillar-like displacement with free energy restrictions.

V. Receveur, M. Czjzek, M. Schülein, P. Panine , B. Henrissat (2002) Dimension, shape and conformational flexibility of a two-domain fungal cellulase in solution probed by small angle X-ray scattering, submitted.