	Experiment title:	Experiment number:
	X-RAY study of C1s calcium binding N-terminal domain	Ls1656
Beamline: ID14EH1	**Date of experiment:** from: 13/4/00 to: 14/4/00	**Date of report:**
Shifts: <1	**Local contact(s):** Hassan Belrhali	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Christine GABORIAUD, LCCP/IBS *
Lynn GREGORY, LCCP/IBS
Juan Carlos FONTECILLA-CAMPS, LCCP/IBS

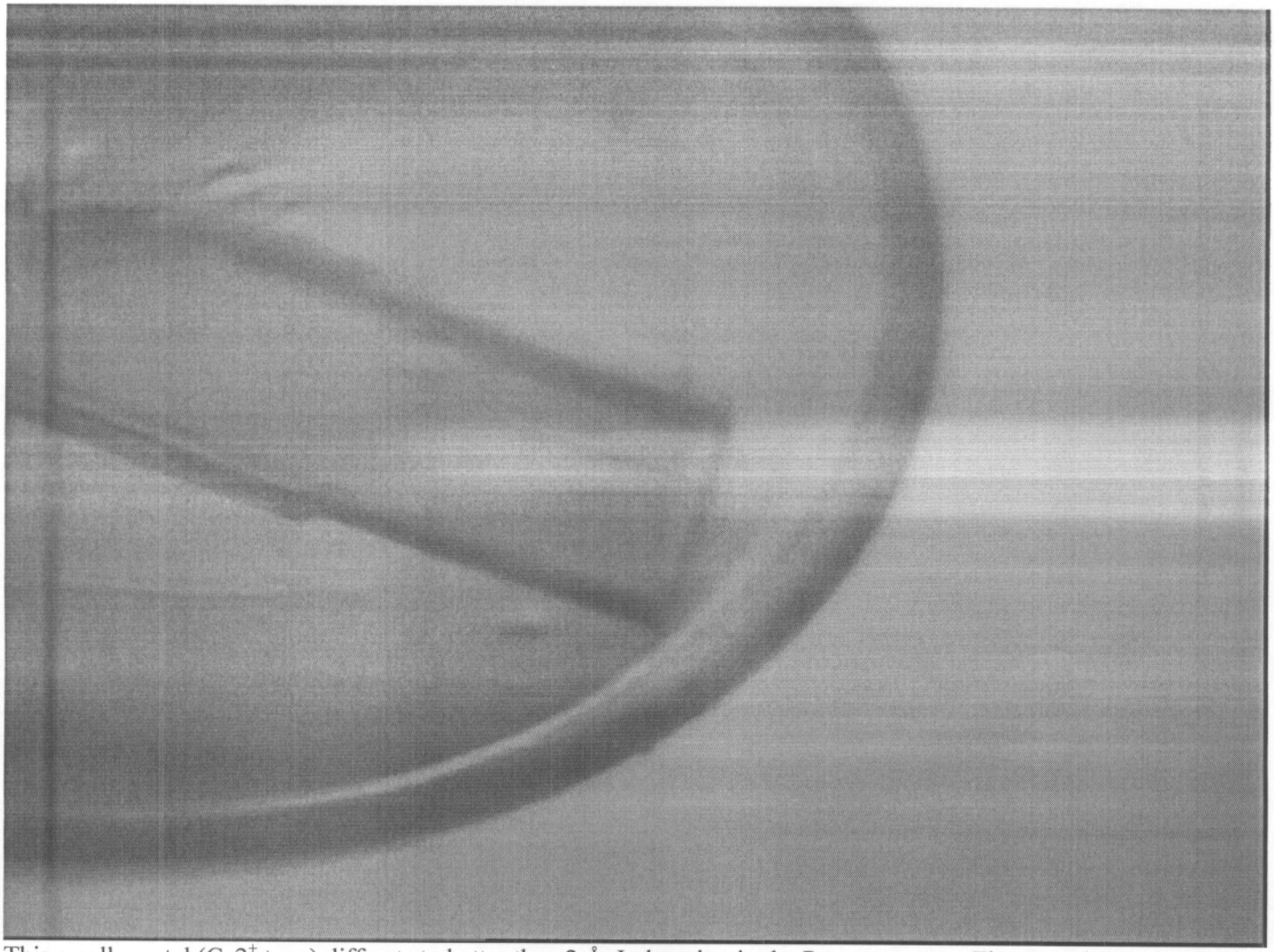
Report:

The complement system constitutes an important part of the innate immune system that is designed to eliminate "harmful" substances from the body.
C1 triggers the complement system by the classical pathway. The catalytic domain of C1 consists of a tetramer of the complex modular proteases C1s and C1r. We have recently solved the structure of the C-terminal catalytic domain of C1s (" Crystal structure of the catalytic domain of human complement C1s: a serine protease with a handle ." C. Gaboriaud, V. Rossi, I. Bally, G. Arlaud, and J.C. Fontecilla-Camps. EMBO J., 19, 1755-1765 (2000).
The association of the C1s-C1r-C1r-C1s tetramer is calcium dependant, and essential for the catalytic activity of C1. The structure of this calcium binding domain, which forms a dimer in the presence of calcium, will give the first pieces of knowledge at the atomic level about this unknown mechanism of calcium dependant association.

Crystals of the recombinant human C1s calcium binding domain have been grown with PEG and different cations (Mg2+, Ca2+). These crystals show very different diffraction potentials and variable cell and space group. Here the experiments were carried out on two very different crystals.

A "big" crystal (0.45 x 0.2 x 0.15 mm3) with Mg2+ was very nicely diffracting in some directions (about 1.7 Å) but very badly in other direction. Moreover, the indexation of the spots in the "good" direction is difficult because many spots are not predicted. Trouble with ice formation were also encountered because the nitrogen flux was not perfectly settled.

A "small" crystal (picture taken with the microdiffractometer setup).



This small crystal ($Ca2^+$ type) diffracts to better than 2 Å. Indexation in the P_1 space group. The crystal was not optimally centered and control of the diffractometer was lost in the middle of the night, just after this nice view has been taken.

At least, a clear indication of the more regular order in the crystal of the $Ca2^+$ type was obtained from this experiment, which was of great help to enhance further the quality of the crystals. Good statictics (Rsym 4%) are obtained in the first 210 frames.