



Experiment title: Structural studies on a transcription activator in *Rhizobium meliloti*:FixJ

Experiment number:
LS-1192

Beamline:
ID14-EH3

Date of experiment:

from 19 Oct 1998 7:00 h to 20 Oct. 1998 7:00 h
from: 22 Nov 1998 7:00 h to: 23 Nov 1998 7:00 h

Date of report:

Shifts:
6

Local contact(s):

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Report

Several crystal forms of regulatory domain of FixJ (FixJ-N) were obtained from various crystallization conditions. They have been analysed in the first three shifts. Native data sets were collected as well as some heavy atom derivatives. After data analysis, the three next shifts were dedicated to the monoclinic and to the triclinic crystals. The crystals were small (20 μm x 20 μm x 100 μm) and flash-frozen. Complete native data sets on both crystal forms have been measured. Diffraction data for several heavy atom derivatives data have were collected on the (best diffracting) triclinic form (2.4 \AA). A compromise between time available and resolution which would guarantee completeness and redundancy, despite the low symmetry of the lattice, was decided. Among the several derivatives, the dispersive and anomalous contributions of the platinum and of the samarium derivatives allowed phase determination. The structure of the triclinic form (2 molecules in the a.u.) was then used to solve the structure of FixJ-N in the monoclinic form (2 molecules in the a.u.) by molecular replacement. This work was presented as a poster at the User Meeting in March 1999. After refinement (monoclinic 2.8 \AA , triclinic 2.4 \AA) we found that each protomer, in each crystal form present different structural features in the active site area. The conformations in the different protomers illustrate different functional status of the regulatory domain. These observations were used to design experiments in both crystal forms that would illustrate how conformational transitions from latent to catalytically functional species occur. The data have been collected on ID14 EH4 on February 25-27 1999 (project LS-1339). The resolution has been improved to 1.8 \AA resolution (phone report). A manuscript is in preparation.