

**Experiment title:**

Structure determination of L-aspartate oxidase in complex with FAD and the substrate.

**Experiment number:****LS-1517****Beamline:**  
ID14-EH1**Date of experiment:** 14/02/2000**Date of report:**  
29.02.00**Shifts:** 2**Local contact(s):** H.Belrhali*Received at ESRF:***Names and affiliations of applicants (\* indicates experimentalists):**

(\*)Claudio Lina and Andrea Mattevi

Dept. Genetics and Microbiology,  
University of Pavia (Italy).

**Report:Background:** L-aspartate oxidase catalyses the first step in the bacterial *de novo* biosynthesis of NAD<sup>+</sup>. This biosynthetic pathway is present in bacteria but not in eukaryotes and represents a target for drug design studies. We have solved the crystal structure of the *E. coli* enzyme in the FAD-free apoform. The wild type protein could never be crystallised in the active holo-form.

**Experiments carried out at the ESRF:** The mutant Arg386Leu of *E. coli* L-aspartate oxidase crystallises in a different form with respect to the wild type crystals. A 2.9 Å data set has been collected on ID14-EH1 with the following statistics: n° measurements=82176, n° reflections=17836, R<sub>sym</sub>=12.2% (34.2% in the highest resolution shell), completeness=99.6% (95.3%), I/σ=7.7 (2.4).

**Results:** Yellow crystals of the Arg386Leu mutant belong to space group P4<sub>1</sub>2<sub>1</sub>2 with unit cell parameters  $a=b=73$  Å and  $c=311$  Å (the data were measured only two weeks ago).