ESRF	**Experiment title:** Marseille BAG	**Experiment number:** LS1508
Beamline: ID14-2	**Date of experiment:** from: 16/11/99 to: 17/11/99	**Date of report:** Feb 00
Shifts: 3	**Local contact(s):** Ed Mitchell	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Kieron BROWN
Mariella TEGONI
Christian CAMBILLAU

Report:

Nitrous Oxide Reductase

Complete datasets have been collected from crystals of nitrous oxide reductase soaked in the presence of inhibitors; thiocyanate (SCN-) and nitrite (NO_2-), as well as from the substrate-free oxidised enzyme, see table 1.

	Oxidised Substrate-free	SCN-	NO_2-
Rsym (%)	5.9 (36)	8.7 (34.7)	9.4 (29.7)
Ranom (%)	5.7 (23.1)	6.5 (29.4)	7.6 (26.6)
I/sigI	10.1 (1.9)	4.8 (2.1)	5.0 (2.8)
Completeness (%)	98 (99)	95 (96)	93 (94)
Rwork		24.3	22.3
Rfree		25.9	27.1

Table 1: Processing/refinement statistics for nitrous oxide reductase from *Pseudomonas nautica*. Values in parentheses are for the outer resolution shell.

These data were refined against the model of the reduced structure (Brown *et al. Nat. Struct. Biol.*, in press) by CNS (Brunger *et al. Acta Cryst.* **A46** 467 (1990)), using rigid body and group B-factor protocols, and 2Fo-Fc and Fo-Fc Fourier maps calculated in the vicinity of the CuA and CuZ copper clusters.

No conformational changes were observed in residues neighbouring the copper centres. Furthermore, there was no evidence that inhibitor binding had been successful, since no difference Fourier could be observed. However, upon superimposing the oxidised structure and the reduced structure, a displacement of monomer B of the dimer was observed (rmsd 0.6A), see figure 1. This displacement brought about an enlargement of the solvent channel between monomer A and B of the homodimer.

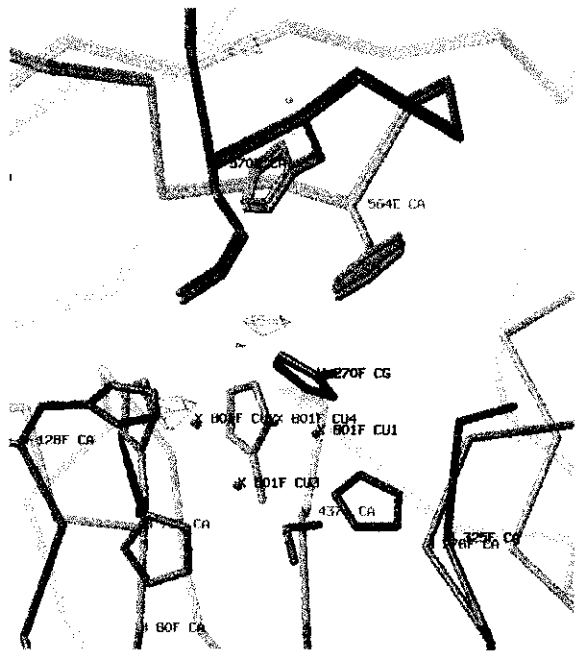

Figure 1. Superposition of the oxidised structure of nitrous oxide reductase on the reduced structure, in the vicinity of the CuZ copper centre.