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Report:

Mutant H369A nitrite reductase

Data were collected to 2.8Å resolution from the H369A mutant enzyme of nitrite reductase from *Pseudomonas aeruginosa*. Green crystals of size 500x30x30um were flash frozen in 30% glycerol in mother liquor, and mounted on the beamline. After an initial diffraction image, from which the optimal oscillation range was calculated using program STRATEGY, a complete dataset was recorded, see table 1.

Space group	P41212
Cell	93.6 93.6 158.2 90 90 90
Rsym (%)	3.8 (28.8)
I/sigI	13.1 (2.1)
Completeness (%)	98 (98)

Table 1: Processing statistics for H369A mutant of Nitrite reductase from *Pseudomonas aeruginosa*. Values in parentheses are for the outer resolution shell.

These data were refined by CNS (Brunger *et al. Acta Cryst.* **A46** 467 (1990)) against the reduced structure (Nurizzo *et al.* (1998) **37**, 13987) using rigid and group B-factor protocols. Fourier difference maps were calculated in the vicinity of the c-heme and d1-heme, which demonstrated that the c-heme domain had a different position compared with the reduced and oxidised structures. Furthermore, the position of the C-terminal arm, which had previously been seen to be responsible for the domain exchange phenomenon, was not visible. In consequence the presence of the Tyr10 distal ligand of the d1-heme through an OH- ioncould not be confirmed. The mutant enzyme forms crystals in space group P41212, unlike the wild-type which forms crystals belonging to the space group P21212. This difference is manifested as only one molecule per asymmetric unit instead of two, an intriguing result considering the homodimeric nature of the functional enzyme in solution. In order to elucidate the position of the cytochrome c domain in the structure of the H369A mutant enzyme, we propose using the MAD technique, exploiting the Fe heme ion.