ESRF	**Experiment title:** Structural studies on prokaryotic Cu,Zn superoxide dismutase mutants from *P.leiognathi*	**Experiment number:** **LS1933**
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Shifts to BAG: 12	**Local contact(s):** Edward MITCHELL	*Received at ESRF:*

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Cu,Zn superoxide dismutases (Cu,Zn SODs) are a class of metallo-enzyme which catalyze the dismutation of superoxide radical into oxygen and hydrogen peroxide, protecting the cells from the oxidative damage.

The Cu,Zn SOD from *Photobacterium leiognathi* (PSOD) is one of the few prokaryotic Cu,Zn SODs to be biochemically characterized. PSOD is a hyper-efficient enzyme, showing a catalytic rate constant 2.5 times higher than the eukaryotic one, and displays a novel dimer interface, formed by β-strands 5e and 4f, instead of the highly conserved, in eukaryotic Cu,Zn SODs, 1a and 8h.

The dimer interface has a ring-shape, being built by 3 clusters of neighbouring residues.
The first cluster is centered on the side chain of Trp73 and involves several residues as Val28; the second is built by Met40 and Phe 86 and the third one is formed by Lys24, Tyr25 and Asp75.
Moreover, ordinated water molecules are trapped in the interface region of the PSOD dimer.

We are involved in a protein engineering study of the subunit-subunit interaction and og the role of residues involved in the 3 clusters; several PSOD mutants at the interface area are therefore being investigated.

In particular, a data set for the PSOD mutant Lys25→Asp, has been collected, at 1.75 Å resolution in this experiment.

Difference Fourier analysis, using the wild type PSOD atomin coordinates (without water molecules) allowed to recognize the mutated residue for Lys25→Asp mutant. The PSOD mutant structure has been refined with conventional restrained refinement cycles, using the program Refmac (see Table for data collection and refinement statistics).

Table: Summary of PSOD mutants data collection and refinement statistics:

Data collection statistics

	Lys25® Asp
Space Group	R32
Unit cell (Å)	$a=b=85.91$, $c=98.01$, $\gamma=120°$
Resolution (Å)	30-1.75
Completeness (%)	97.5
Rsym (%)	3.7
Mosaicity (°)	0.3

Refinement statistics

Refinement resolution range (Å)	30-1.75
Reflections used in refinement	14513
Protein atoms	1109
Cu,Zn atoms	2
Water molecules	91
Rfactor/Rfree (%)	18.3/23.1
Rmsd from ideal values:	
bond lengths (Å)	0.017
bond angles (°)	1.945

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