



	<b>Experiment title: PETN Reductase</b>	<b>Experiment number:</b> LS1684
<b>Beamline:</b> ID14-4	<b>Date of experiment:</b> from: Feb 18, 2000 to: Feb 19, 2000	<b>Date of report:</b> Aug 2000
<b>Shifts: 3</b>	<b>Local contact(s):</b> Dr Raimond Ravelli	<i>Received at ESRF:</i>

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**Report:**

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Crystals of PETN reductase were obtained from a solution containing 25 % w/v PEG 3000, 0.1 M trisodium citrate, 0.1 M cacodylic acid pH 6.2, 17% w/v iso-propanol using sitting-drop vapour diffusion method. PETN reductase in complexes with substrates ( picric acid, 2-cyclohexen-1-one ) and inhibitors ( 2,4-dinitrophenol, picolinic acid) were prepared by co-crystallization using 10-fold excess of ligands. The crystals belong to space group P212121 with cell dimensions  $a=59\text{\AA}$   $b=68\text{\AA}$   $c=89\text{\AA}$  and contain one molecule per asymmetric unit. The structures of the enzyme-substrate and enzyme-inhibitor complexes has given valuable information for explaining the substrate specificity. The atomic resolution structure of PETN reductase in complex with picric acid has revealed a different redox-state of the bound substrate.

Data collection statistics				
Ligands	2,4-DNP	picolinic acid	2-cyclohexen-1-one	picric acid
Total reflections	2207687	938630	150283	1089263
Unique reflections	184989	108776	24003	138671
Cell (Å)	56.59 68.411 88.35	56.69 68.70 88.66	56.70 68.58 88.834	56.43 68.34 88.13
Resolution (Å)	1.0	1.2	1.8	1.1
Completeness (%)	98.7	95.2	94.4	86.0
R <sub>merge</sub> (%)	0.08	0.04	0.041	0.046
Outer shell	0.52	0.09	0.044	0.31
overall I/sig(I)	10.4	19.1	33.9	13.5

Needle-like crystals of NodL (the rizobial *nodL* gene product) were grown from conditions 100mM Tris, pH8.0, 12% PEG 600, 1% Dioxane, 0.1% BOG. A native data set was collected to 2.7Å resolution. The crystal was found to have symmetry P6<sub>3</sub>22 with unit cell a=b=75.7Å c=160.9Å. The data were 98.5% complete and had a merging R factor of 7% with a multiplicity of 2.0.