

 <b>ESRF</b>	<b>Experiment title:</b> Structure determination of glutamate mutase	<b>Experiment number:</b> <b>LS 1132</b>
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Report:

We have prepared a Krypton-derivative by exposing crystals of glutamate mutase to a gas pressure of 100 bar for several minutes and subsequent flash-freezing. On these crystals, we collected anomalous diffraction data at three wavelenghts around and at the krypton K-shell edge at 14 3339 eV (pk), 14 3306 eV (pi) and 16 000 ev (re).

Spacegroup P2<sub>1</sub>: a = 64, b= 112, c = 108 and  $\beta$  = 96.

For a complete data set for spacegroup P2<sub>1</sub> with the crystal in its orientation, we should have collected over 180° at each wavelength. Due to the limited beamtime, the data set at pk was collected over 175°, at pi over 155° and re over 84°. The uncompleteness makes it more difficult to find the krypton site, which we so far have been unable to do. However, this data set might still be of use in combination with data from another heavyatom derivative.

## Data Statistics for Krypton-loaded Glutamate mutase crystals

Wavelength (Å)	Reflections <sup>a</sup> (Nr)	Redundancy <sup>b</sup> (%)	Completeness <sup>c</sup> (%)	R <sub>square</sub> <sup>d</sup> (%)
0.864977 (pk)	557631/ 93635	67.5	99.4 (98.5)	3.5
0.865177 (pi)	550022/ 99461	64.9	97.8 (96.8)	4.0
0.775000 (re)	295998/ 99867	23.3	64.1 (64.0)	4.2

<sup>a</sup> measured/unique

<sup>b</sup> % of reflections with four observations

<sup>c</sup> 30-2.05 Å (last shell 2.10-2.05 Å)

<sup>d</sup>  $\Sigma(I-\langle I \rangle)^2 / \Sigma I^2$