	Experiment title: SseA	**Experiment number**: MX-129
Beamline:	**Date of experiment**: 5-6/ 08/03	**Date of report**: 26/08/03
Shifts: 12 h	**Local contact:** C. Petosa	*Received at ESRF:*

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Report:

Introduction

3-mercaptopyruvate sulfurtransferases are widespread enzyme which catalyse, in vitro, the transfer of a sulfur atom from 3-mercaptopyruvate to cyanide according to the general scheme:

$HS\text{-}CH_2\text{-}COO^- + CN^- \rightarrow CH_3\text{-}COO^- + CNS^-$

E. coli SseA, a member of 3-mercaptopyruvate sulfurtransferase family, was cocrystallized with a substrate analogue (3-bromo pyruvate) in order to have structural information about the catalytic mechanism of the 3-mercaptopyruvate-dependent sulfurtransfer reaction. Moreover a soaking with cyanide anion, the *in vitro* sulfur acceptor of the reaction, was tried.

Data sets collected

	3-Brpyr	**3-Brpyr / CN^-**
Space group	P4(3)	P4(3)
Unit cell (Å)	$a = b = 150.79$	a = b = 150.56,
	$c = 39.56$	$c = 39.57$
Mosaicity (°)	1.1	1.0
Resolution (Å)	3.2	3.0
Measurements	279,114	390,792
Unique reflections	15,207	19,346
Completeness (%)	94	99.8
Rsym (%)	9.6	10.3

Results achieved

The quality of the data together with the intrinsic flexibility of the enzyme active site loop, do not allowed a clear observation of the covalent modification of the catalytic residue.