



**Experiment title: Collecting high resolution data from crystals of the ternary complex of tatronate semialdehyde reductase (TSAR), NADH and glycerate**

**Experiment number:**

<b>Beamline:</b>	<b>Date of experiment:</b> from: 30/11/04 to: 1/12/04	<b>Date of report:</b> 25/5/09
<b>Shifts:</b>	<b>Local contact(s):</b> Gordon Leonard	<i>Received at ESRF:</i>
<b>Names and affiliations of applicants (* indicates experimentalists):</b> <b>* Boaz Shaanan, *Hagay Shmueli, *Alexander Kaplun</b>		

**Report:** During the shift we recorded several data sets from crystal of complexes of tsar with D- and L-glycerate. The statistics of data collection are listed in the **table 1** below:

<i>Statistic</i>	<i>TSAR D</i>	<i>TSAR L</i>
Beamline	ESRF ID 14-4	
Wavelength (Å)	0.97926	0.93929
Range (Å) <sup>a</sup>	30-1.3 (1.4-1.3)	30-1.05 (1.2-1.05)
Space group	I222	
<i>a</i> (Å)	54.7	54.9
<i>b</i> (Å)	104.4	106.1
<i>c</i> (Å)	154.8	153.9
Total number of reflections	508203	1173079
Number of unique reflections	107636	196329
Completeness (%)	98.8 (98.9)	94.3 (89.7)
I/σ	12.8 (3.1)	17.1 (4.3)
<i>R</i> <sub>symm</sub> <sup>b</sup> (%)	6.1 (47.1)	5.8 (43.6)
<i>R</i> <sub>meas</sub> <sup>c</sup> (%)	6.9 (52.8)	6.3 (47.8)

Both complexes were refined (see table 2) but difficulties were encountered in interpreting the structure of the L-glycerate complex, which has delayed publication. Therefore, it was decided to include in our article only the description of the complex with D-glycerate which will be submitted for publication in a shortwhile.

**Table 2. Refinement and model quality statistics of GCL regulatory subunit.**

<i>Statistic</i>	<i>D-glycerate</i>	<i>L-glycerate</i>
<i>Refinement</i>		
Non-hydrogen atoms	2865	2630
Water molecules	664	500
$R_{\text{work}}^{\text{a}}$ (%)	12.1	11.7
$R_{\text{free}}^{\text{a}}$ (%)	16.2	14.0
Mean B-factor for all atoms ( $\text{\AA}^2$ )	16	11.2
B-factor estimated from Wilson plot ( $\text{\AA}^2$ )	18.6	11.8
<i>RMSD from ideality</i>		
Bond lengths ( $\text{\AA}$ )	0.018	0.023
Bond angles (deg.)	2.48	2.40
<i>Ramachandran analysis</i>		
Most-favored regions (%)	95.6	94.8
Additionally favored regions (%)	4.4	5.2
Generously favored regions (%)	0	0