ESRF	**Experiment title:** *E. coli* isomeroreductase and PBP2xR	**Experiment number**: LS-1655
Beamline: Id14-4	**Date of experiment**: from: 23-06-00 to: 24-06-00	**Date of report**: 24-07-00
Shifts:3	**Local contact(s)**:E. Gordon	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

*Biou Valérie (BAG IBS/LCM)
*Dessen Andrea

Report:

4 data sets were collected on three crystals and two crystal forms. Unfortunately, those crystals diffract weakly, probably because they have a high solvent content.

The crystals are hexagonal with unit cell dimensions 150.Å 150.Å 210Å, 90°. 90°. 120°.

Crystal 1 was large (400x100x100 microns) and 2 datasets were measured from it using 50 micron slits. However, the X-ray decay had obviously propagated because the second dataset was not better than the end of the first one.

Crystal 2 was highly mosaic and the data were not used.

Crystal 3 (form II) had a low mosaic spread. Unfortunately, it lasted only for 20 degrees in the beam.

Crystal 4 (form II) was slightly more mosaic but still nice. 115 degrees were collected, however for some unexplained reason (probably a bug in the data collection program), the last 70 degrees were not recorded.

Merging crystal 3 and 4 allowed to get a complete dataset.

Merging the data from crystals 3 and 4 yielded a complete dataset with statistics of a quality similar to those of the individual crystals. Tables 1 and 2 give data statistics

Table 1 **Crystal 1, first dataset. Processing : mosflm/scala.**

N	Dmin	Nmeas	Nref	%poss	Cm%poss	Mlplcty	Rmeas	Rmeas0	(Rsym)	PCV0
1	13.28	1378	509	76.9	76.9	2.7	0.100	0.100	0.080	0.129
2	9.39	3930	1177	97.3	90.1	3.3	0.074	0.074	0.063	0.085
3	7.67	5175	1530	98.2	93.8	3.4	0.094	0.094	0.079	0.108
4	6.64	6033	1802	98.7	95.5	3.3	0.104	0.104	0.088	0.120
5	5.94	6948	2071	99.2	96.6	3.4	0.142	0.142	0.119	0.165
6	5.42	7784	2274	98.9	97.1	3.4	0.165	0.165	0.140	0.193
7	5.02	8614	2466	99.3	97.6	3.5	0.176	0.176	0.149	0.206
8	4.70	9740	2682	99.6	98.0	3.6	0.186	0.186	0.159	0.219
9	4.43	10706	2830	99.6	98.2	3.8	0.225	0.225	0.195	0.270
10	4.20	11858	3008	99.8	98.4	3.9	0.273	0.273	0.238	0.332
Overall		72166	20349	98.4	98.4	3.5	0.116	0.157	0.157	
		Nmeas	Nref	%poss	Cm%poss	Mlplcty	Rmeas	Rmeas0	(Rsym)	

Table 2 **Crystals 3 and 4, processing : denzo/scalepack (scaling unmerged data)**

Lower limit	Upper Angstrom	Average I	Average error	Norm. stat.	Chi**2	Linear R-fac	Square R-fac	compl.
30.00	8.56	21726.6	2375.1	735.7	1.153	0.110	0.151	91.9
8.56	6.82	9093.8	1059.6	305.4	1.055	0.112	0.153	99.1
6.82	5.96	3724.7	549.5	175.6	1.033	0.136	0.158	99.6
5.96	5.42	2962.1	480.9	168.6	1.142	0.158	0.163	99.5
5.42	5.04	3206.4	600.0	188.7	1.049	0.165	0.177	99.6
5.04	4.74	3763.6	836.8	218.9	0.960	0.180	0.197	99.0
4.74	4.50	3771.9	857.1	235.4	1.275	0.191	0.181	98.8
4.50	4.31	3876.0	1049.9	230.1	1.171	0.236	0.258	99.4
4.31	4.14	2791.6	828.3	219.2	1.076	0.248	0.255	98.4
4.14	4.00	2314.6	738.4	218.9	1.075	0.273	0.265	99.0
All reflections		5645.1	929.8	267.2	1.097	0.151	0.161	98.4

Enzymes involved in peptidoglycan biosynthesis

Periplasmic enzymes

Two data sets were recently collected on PBP2xr of a β-lactam clinical resistant form of *Streptococcus pneumoniae* (ID14-4); however, crystals deteriorated very rapidly upon exposure to the beam, limiting the quality of the data sets. One data set to medium resolution was used for structure determination by molecular replacement (space group $P6_2$, a=146.15, b=146.15, c=132.2 Å, with two molecules per asymmetric unit). The structure at 3.2 Å is presently being refined, but a higher resolution data set will be necessary for project completion.