Report for the experiment 30-01-661

Pseudomonas aeruginosa is an opportunistic human pathogen which infects injured, immunodificient, or ortherwise compromised patients. Under iron-limited conditions, the bacterium secretes different siderophores such as the pyochelin (MM < 2000 Da). The pyochelin is transported across the outer membrane by the pyochelin receptor FptA (MM: 75000 Da). To date, the biochemistry of FptA is not very known contrary of the one of FpvA which is another siderophore receptor from *P. aeruginosa* also involved in the iron transport but using the pyoverdine.

During the first part of the experiment 30-01-661 (May 2004), 2 datasets were collected from two crystals grown in different crystallization conditions. The data were processed and scaled using Denzo/Scalepack and XDS. The crystallographic data are summarized in the Table 1.

Table 1: summary of the crystallographic data

	Crystal 1	Crystal 2
Data processing/scaling	Denzo/Scalepack	XDS
Wavelength (Å)	0.979784	0.979784
Resolution (Å)	3.2	2.6
Space group	P1	$P2_12_12_1$
Cell parameters (Å)	85.165 98.792 94.574 62.318 63.081 69.933	75.989 84.904 162.755
Number of reflections	41875	219192
Unique reflections	32410	33111
Completeness (%)	82	99.9
R_{sym} (%)	11.5	12.5

The second part of the experiment was performed in July (from 07/04 to 07/05). 6 data sets were collected at different wavelenghts from orthorhombic crystals ($P2_12_12_1$). The data were processed and scaled using Denzo/Scalepack and XDS. Only the statistics provided by XDS are given. For all the crystals used, the cell parameters are approximatly: a= 75, b= 84 and c= 162 Å. 1 molecule is in the asymmetric unit.

Table 2: FptA crystals soaked in $FeCl_3$

	Crystal 1	Crystal 2
Wavelength (Å)	0.979733	0.979733
Resolution (Å)	2.8	2.8
Number of reflections	125710	126421
Unique reflections	23549	25861
Completeness (%)	90.6	99.2
R_{sym} (%)	11.3	10.5

Table 3: FptA crystal soaked in $FeCl_3$. Data collection at the peak of the iron *K* edge.

Wavelength (Å)	1.738911
Resolution (Å)	2.97
Number of reflections	118381
Unique reflections	41194
Completeness (%)	99.3
R_{sym} (%)	6.5

Table 4: FptA crystals: data collection at the peak of the iron *K* edge.

Wavelength (Å)	1.738943
Resolution (Å)	3.2
Number of reflections	97880
Unique reflections	32821
Completeness (%)	99.9
R_{sym} (%)	13

Table 5: FptA crystals: data collection at the peak of the zinc *K* edge.

Wavelength (Å)	1.283472
Resolution (Å)	2.8
Number of reflections	147124
Unique reflections	49002
Completeness (%)	99.9
R_{sym} (%)	10.5

Table 6: FptA crystal: high resolution dataset.

Wavelength (Å)	0.979530
Resolution (Å)	2.0
Number of reflections	340859
Unique reflections	71021
Completeness (%)	99.7
R_{sym} (%)	6.5

The structure rebuilding is now underway using all the data between 29.3 and 2.0 Å resolution. The R_{free} and R_{cryst} are better than 25 %.