Collection of X-ray diffraction data from the crystals of *Bucillus circulans* chitinase D using various X-ray optics

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We have collected X-ray diffraction data by a Weissenberg method from an orthorhombic crystal ($P2_12_12_1$, a=51.13Å, b=77.31Å, c=178.83Å) of *Bacillus circulans* chitinase D (Watanabe *et al.*, *J. Bacteriol.* **174**, 408-414 (1992)) at the beamline 41XU. A flat detector with a large size (400 X 800 mm^2) imaging plate was used and a total of 30 images was collected. The rotation angle and the coupling constant for a frame were 3° and 0.4°/mm, respectively. This diffraction data was processed with the software suite developed and installed on the workstation at the beamline by Dr. Higashi of Rigaku. Some experimental conditions and the statistics of the data are summarized in the column of the data set number 1 in the right table. The data sets number 2 and 3 were collected at the Photon Factory and the data set number 4 was collected by an R-AXIS IIc diffractometer with a conventional X-ray generator. As shown in the table, we have collected the best X-ray diffraction data from the chitinase D at the BL41XU. The resolution, the overall S/N ratio (<*I*>/<s>), and the number of observed reflections of the data set number 1 are better than those of the other data sets.

Data set number	1	2
Experimental conditions		
X-ray source	BL41XU SPring-8	BL-6A PF
Temperature (K)	299	293
Method	Weissenberg	Weissenberg
IP size (mm2)	400 X 800	200 X 400
Detector distance (mm)	560.0	286.5
Wavelength (A)	0.708	1.000
Resolution limit (A)	2.00	2.50
Integration	INTEG	DENZO
Scaling	SCALE	SCALA
Data statistics		
Overall		
Resolution range (A)	58.4 - 2.00	44.6 - 2.50
R-merge on *I*	0.098	0.065
Completeness	0.900	0.804
<*I*/s>	11.2*	3.0
Multiplicity	**	4.0
# Independent reflections	44,050	21,933
Highest resolution shell		
Resolution range (A)	2.06 - 2.00	2.56 - 2.50
R-merge on *I*	0.382	0.177
Completeness	0.875	0.601
<*I*/s>	2.1	2.6
Multiplicity	**	3.3

Data set number	3	4
Experimental conditions		
X-ray source	BL-6B PF	Monochromater Rotating anode
Temperature (K)	293	293
Method	Weissenberg	Oscillation
IP size (mm2)	400 X 800	200 X 200
Detector distance (mm)	573	129.2
Wavelength (A)	1.000	1.542
Resolution limit (A)	2.50	2.45
Integration	DENZO	PROCESS
Scaling	SCALA	SCALE
Data statistics		
Overall		
Resolution range (A)	46.6 - 2.50	52.0 - 2.45
R-merge on *I*	0.105	0.099
Completeness	0.748	0.929
<*I*/s>	5.5	6.8*
Multiplicity	4.1	**
# Independent reflections	19,692	23,514
Highest resolution shell		
Resolution range (A)	2.56 - 2.50	2.60 - 2.45
R-merge on *I*	0.306	0.206
Completeness	0.663	0.879
<*I*/s>	1.8	2.5
Multiplicity	3.7	**

* <*I*>/<s>
**Not specified.