

## **Supplementary Data**

**Application of a serial crystallography to incomplete macromolecular crystallography datasets to generate a complete dataset**

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**Table S1.** Resource of the diffraction images used for data processing in this study.

Datasets	DOI	No. of total images	No. of used images	PDB	Ref.
Data I	10.5281/zenodo.13948740	300	No. 1-50	9K73	This study
Data II	10.5281/zenodo.8424379 (data name: Data III)	140	No. 1-50	8WFV	[1,2]
Data III	10.5281/zenodo.8424379 (data name: Data IV)	200	No. 1-50	8FWF	[1,2]
Data IV	10.5281/zenodo.13733646 (data name: TsaBgl-Tris Data I )	360	No. 1-50	8XPC	[3]
Data V	10.5281/zenodo.13733646 (data name: TsaBgl-Tris Data II )	360	No. 1-50	8XPD	[3]
Data VI	10.5281/zenodo.13733646 (data name: TsaBgl-Tris Data III)	360	No. 1-50	8XPE	[3]

**Table S2.** Data processing script and information.

Data processing	Script
Indexing script (Indexamajig)	\$indexamajig -i <b>input.lst</b> -o <b>output.stream</b> -p TsaBgl.pdb -g detector.geom --peaks=zaef --indexing=method -j 72
Unit cell information	a= 65.210 Å, b= 71.120 Å, c= 99.490 Å $\alpha=\beta=\gamma=90.00^\circ$ Space group: P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Geometry file	photon_energy = 12659 adu_per_eV = 0.0001 clen = 0.29955 res = 5814.0 ; 172 micron pixel size  0/min_fs = 0 0/max_fs = 2462 0/min_ss = 0 0/max_ss = 2526 0/corner_x = -1234.64 0/corner_y = -1264.35 0/fs = +1.000000x -0.001029y 0/ss = +0.001029x +1.000000y  rigid_group_q0 = 0 rigid_group_a0 = 0  rigid_group_collection_quadrants = q0 rigid_group_collection_asics = a0

During data indexing, the input file name input.lst (image list) and output file name output.stream (indexing results) were specified for each dataset. In the data merging test, the indexing method was set to MOSFLM. For a comparison of indexing algorithms, the indexing methods MOSFLM, DirAx, Taketwo, and XGANDAFL were selected.

**Table S3.** Data collection and refinement statistics for TsaBgl from the complete dataset of Data I.

<b>Data collection</b>	<b>TsaBgl (Data I)</b>
X-ray Source	11C beamline, PLS II
X-ray energy (eV)	14820
Processing image number	300
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Cell dimension	
a, b, c (Å)	64.68, 71.54, 98.67
α, β, γ (°)	90.0, 90.0, 90.0
Resolution (Å)	50.0-1.80 (1.83-1.80)
Unique reflections	4244 (1998)
Completeness (%)	98.5 (95.4)
Redundancy	7.5 (4.5)
I/σ	21.12 (2.98)
R <sub>merge</sub>	0.157 (0.534)
R <sub>meas</sub>	0.166 (0.590)
R <sub>pim</sub>	0.054 (0.244)
CC1/2	0.990 (0.513)
CC*	0.997 (0.824)
<b>Refinement</b>	
Resolution (Å)	49.34-1.80
R <sub>work</sub> <sup>a</sup>	0.1437
R <sub>free</sub> <sup>b</sup>	0.1779
R.m.s. deviations	
Bonds (Å)	0.007
Angles (°)	0.870
B factors (Å <sup>2</sup> )	
Protein	15.87
Water	30.15
Ramachandran plot	
Favoured (%)	97.71
Allowed (%)	2.29
Outliers (%)	0

Values for the outer shell are given in parentheses.

## References

1. Nam, K.H. The Conformational Change of the L3 Loop Affects the Structural Changes in the Substrate Binding Pocket Entrance of  $\beta$ -Glucosidase. *Molecules* **2023**, *28*, 7807, doi:10.3390/molecules28237807.
2. Nam, K.H. Data on the crystal structures of  $\beta$ -glucosidase from *Thermoanaerobacterium saccharolyticum*. *Data in Brief* **2024**, *57*, 111019, doi:10.1016/j.dib.2024.111019.
3. Nam, K.H. Structural analysis of Tris binding in  $\beta$ -glucosidases. *Biochem. Biophys. Res. Commun.* **2024**, *700*, 149608, doi:10.1016/j.bbrc.2024.149608.