

Supplementary Table 1 Data collection statistics of xylanase.

Crystal mount	capillary	capillary	capillary	cryoloop	cryoloop	cryoloop
Crystal size (mm)	0.13 × 0.07 × 0.04	0.15 × 0.08 × 0.04	0.11 × 0.07 × 0.03	0.13 × 0.06 × 0.04	0.10 × 0.07 × 0.04	0.13 × 0.07 × 0.04
Space group	<i>P2</i> ₁	<i>P2</i> ₁	<i>P2</i> ₁	<i>P2</i> ₁	<i>P2</i> ₁	<i>P2</i> ₁
Unit-cell parameters (Å)	<i>a</i> =56.7, <i>b</i> =38.9, <i>c</i> =81.2	<i>a</i> =56.8, <i>b</i> =38.9, <i>c</i> =81.4	<i>a</i> =56.7, <i>b</i> =38.9, <i>c</i> =81.2	<i>a</i> =56.7, <i>b</i> =38.8, <i>c</i> =81.3	<i>a</i> =56.5, <i>b</i> =38.9, <i>c</i> =81.1	<i>a</i> =56.7, <i>b</i> =38.8, <i>c</i> =81.3
(°)	<i>β</i> =94.8	<i>β</i> =94.8	<i>β</i> =94.8	<i>β</i> =94.8	<i>β</i> =94.9	<i>β</i> =94.8
Resolution range (Å)	20 – 1.66 (1.72–1.66)	20 – 1.64 (1.70–1.64)	20 – 1.74 (1.80–1.74)	20 – 1.66 (1.72–1.66)	20 – 1.84 (1.91–1.84)	20 – 1.80 (1.86–1.80)
No. of unique reflections	41342 (4038)	43875 (4311)	36670 (3657)	41388 (4011)	30836 (3026)	33096 (3250)
Redundancy	4.6 (4.6)	4.5 (4.5)	4.6 (4.5)	4.4 (3.9)	4.6 (4.5)	4.6 (4.4)
Completeness (%)	98.0 (96.4)	100 (100)	100 (100)	98.0 (95.4)	100 (99.7)	99.8 (99.0)
<i>R</i> _{sym} [†] (%)	5.1 (21.4)	4.8 (19.0)	7.0 (19.5)	6.4 (17.4)	7.4 (20.2)	5.0 (21.2)
< <i>I</i> /σ(<i>I</i>)>	11.5 (6.1)	13.2 (6.0)	9.9 (6.1)	10.3 (6.0)	8.2 (6.0)	11.5 (6.1)
Mosaicity (°)	0.37	0.39	0.34	0.41	0.39	0.54

[†] $R_{\text{sym}} = \sum_{hkl} \sum_i |I_i(hkl) - \langle I(hkl) \rangle| / \sum_{hkl} \sum_i I_i(hkl)$, where $\langle I(hkl) \rangle$ is the mean intensity of Bijvoet-equivalent observations $I_i(hkl)$.

Values in parentheses are for the outermost shell.