

Table S1. Data collection and crystallographic refinement statistics

Data set	Reduced BST2(47-152)	Oxidized BST2(51-151)
PDB code	3nwh	2xg7
Space group	$P2_1$	$P2_12_12_1$
Cell dimensions (Å,°)	$a = 26.6$ $b = 59.6$ $c = 159.5$ $\beta = 91.6$	$a = 28.86$ $b = 91.86$ $c = 146.96$
Solvent content (%)	57	70
Resolution (Å)	50.00-2.60 (2.69-2.60)	38.95-3.45 (3.64-3.45)
Completeness (%)	97.5 (93.2)	99.4 (97.6)
$I/\sigma(I)$	17.2 (4.0)	8.9 (2.5)
Multiplicity	3.6 (3.3)	6.8 (6.5)
R_{sym} (%) *	5.8 (26.9)	11.3 (70.9)
# Unique reflections	15,096	5,576
Wilson B (Å ²)	46.9	133.4
R factor (%)	26.0	26.9
R_{free} (%) †	28.7	29.8
# of protein atoms	3,266	1,209
# water molecules	18	0
# sugar molecules	-	2
$\langle B \rangle$ (Å ²)		
protein atoms	16.4	126.6
water molecules	37.4	-
sugar molecules		181.5
RMSD from ideality		
Bonds (Å)	0.018	0.012
Angles (°)	1.64	1.38
Phi/Psi angles:		
Favored (%)	98	98.04
Allowed (%)	2.0	1.96
Disallowed (%)	0.0	0.0

Values in parentheses are for the highest-resolution shell.

* $R_{\text{sym}} = \sum |I - \langle I \rangle| / \sum I$, where $\langle I \rangle$ is the average intensity from multiple observations of equivalent reflections.

† $R_{\text{factor}} = 100 \times \sum \|F_o\| - |F_c| / \sum |F_o|$. R_{free} is the R_{factor} computed from the 7.6% of reflections in the case of 3nwh and 4.5% in the case of 2xg7 that were chosen randomly and excluded from the refinement calculations.