Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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Inhibition of the family 20 glycoside hydrolase catalytic modules in the *Streptococcus pneumoniae exo*-β-D-*N*-acetylglucosaminidase, StrH

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Table 1: Data and refinement statistics for GH20A.

	GH20A		GH20AGG
	NGT	PUGNAc	PUGNAc
Data Collection			
Beamline	MM-002	SSRL BL9-2	SSRL BL9-2
Wavelength (Å)	1.54180	0.97934	0.97884
Space Group	I222	I222	$P3_121$
Cell Dimensions			
a, *b*, *c* (Å)	78.5, 110.1, 112.2	78.3, 109.6, 112.6	90.1, 90.1, 101.6
Resolution (Å)	21.99-1.73 (1.82-1.73)	28.81-1.36 (1.43-1.36)	45.03-2.10 (2.21-2.10)
R_{merge}	0.069 (0.399)	0.071 (0.381)	0.088 (0.386)
I/σI	14.9 (3.3)	19.1 (4.0)	18.8 (6.5)
Completness (%)	97.3 (95.0)	90.1 (57.7)	100.0 (100.0)
Redundancy	4.9 (4.7)	9.8 (5.5)	10.7 (10.1)
No. of reflections	244,440	912,052	302,144
No. Unique	49,487	93,267	28,340
Refinement			
Resolution (Å)	21.99-1.73	28.81-1.36	45.03-2.10
R_{work}/R_{free}	0.16/0.19	0.12/0.14	0.17/0.21
No. Of atoms			
Protein	3627	3757	3270
Ligand	23 (PEG), 14 (NGT), 4 (MG), 12 (EDO)	20 (PEG), 25 (PUGNAc), 12 (EDO)	20 (SO4), 50 (PUGNAc), 20 (EDO)
Water	674	652	298
B-factors			
Protein	14.8	13.3	25.8
Ligand	34.3 (PEG), 12.0 (NGT), 22.8 (MG), 45.5 (EDO)	34.5 (PEG), 13.6 (PUGNAc), 30.0 (EDO)	37.1 (SO4), 20.2 (PUGNAc), 48.0 (EDO)
Water	28.8	31.7	34.2
r.m.s.d			
Bond lenghts (Å)	0.014	0.010	0.009
Bond angles (°)	1.351	1.360	1.109
Ramachandran (%)			
Preferred	98.6	98.6	96.8
Generously allowed	1.4	1.4	3.2
Disallowed	0.3	0	0

Data for highest resolution shell are shown in parentheses

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Table 2: Data and refinement statistics for GH20B.

	GH20B		GH20BWY
	NGT	PUGNAc	PUGNAc
Data Collection			
Beamline	SSRL BL9-2	SSRL BL9-2	SSRL BL9-2
Wavelength (Å)	0.97946	0.97946	0.95369
Space Group	$P2_1$	$P2_12_12_1$	$P2_1$
Cell Dimensions			
a, *b*, *c* (Å)	67.2, 115.6, 132.0 (β=99.4°)	66.7, 115.2, 129.9	67.1, 116.1, 69.6 (β=109.6°)
Resolution (Å)	52.81-2.09 (2.20-2.09)	30.0-2.40 (2.53-2.40)	57.1-1.98 (2.09-1.98)
R_{merge}	0.104 (0.399)	0.117 (0.401)	0.133 (0.357)
I/σI	9.8 (3.5)	15.4 (5.4)	6.4 (3.2)
Completness (%)	100.0 (100.0)	99.1 (97.3)	97.8 (97.1)
Redundancy	4.3 (4.3)	10.0 (9.3)	4.3 (4.1)
No. of reflections	503,094	396,066	294,022
No. Unique	117,532	39,589	68,111
Refinement			
Resolution (Å)	52.81-2.09	30.0-2.40	57.1-1.98
R_{work}/R_{free}	0.19/0.24	0.19/0.25	0.24/0.30
No. Of atoms			
Protein	3346 (A), 3399 (B), 3374 (C), 3357 (D)	3347 (A), 3329 (B)	3293 (A), 3319 (B)
Ligand	14 (NGT-E), 14 (NGT-F), 14 (NGT-G), 14 (NGT-H), 16 (EDO), 8 (MG)	25 (PUGNAc-C), 25 (PUGNAc-D), 36 (EDO), 24 (ACT)	25 (PUGNAc-C), 25 (PUGNAc-D), 4 (BR), 24 (EDO), 33 (BCN)
Water	2057	546	1148
B-factors			
Protein	17.8 (A), 22.5 (B), 18.1 (C), 23.2 (D)	18.9 (A), 19.7 (B)	16.3 (A), 16.3 (B)
Ligand	10.8 (NGT-E), 19.3 (NGT-F), 14.6 (NGT-G), 19.9 (NGT-H), 47.4 (EDO), 19.0 (MG)	22.1 (PUGNAc-C), 21.2 (PUGNAc-D), 33.2 (EDO), 41.4 (ACT)	13.4 (PUGNAc-C), 13.3 (PUGNAc-D), 52.1 (BR), 26.9 (EDO), 36.6 (BCN)
Water	31.4	24.4	27.0
r.m.s.d			
Bond lenghts (Å)	0.010	0.010	0.007
Bond angles (°)	1.165	1.369	1.168
Ramachandran (%)			
Preferred	96.6	95.1	97.2
Generously allowed	3.4	4.7	2.8
Disallowed	0	0.2	0

Data for highest resolution shell are shown in parentheses