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Supporting information for article:

Crystal structure of highly glycosylated human leukocyte elastase in complex with an S2′-site binding inhibitor

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Validation results for pyranose sugars:

Name	Chain	Q[1]	Phi	Theta	Anomer	D/L[2]	Conformation	RSCC[3]	<Bfactor>	Diagnostic
NAG	A	0.570	348.043	2.58004	beta	D	$^4C_1$	0.89	78.2229	Ok
FUC	A	0.543	313.205	177.325	alpha	L	$^1C_4$	0.84	68.95	Ok
NAG	A	0.569	16.6432	3.13505	beta	D	$^4C_1$	0.86	103.065	Ok
BMA	A	0.567	323.701	6.60432	beta	D	$^4C_1$	0.64	125.148	Ok
MAN	A	0.558	244.052	5.37527	alpha	D	$^4C_1$	0.78	116.972	Ok
NAG	A	0.567	16.303	2.61201	beta	D	$^4C_1$	0.84	87.3879	Ok
FUC	A	0.542	31.2478	173.59	alpha	L	$^1C_4$	0.85	96.214	Ok
NAG	A	0.572	239.803	0.7168	beta	D	$^4C_1$	0.75	119.181	Ok
BMA	A	0.571	323.719	4.72404	beta	D	$^4C_1$	0.32	169.553	Ok
NAG	B	0.566	20.704	2.20162	beta	D	$^4C_1$	0.85	92.61	Ok
FUC	B	0.547	13.2909	176.32	alpha	L	$^1C_4$	0.86	83.218	Ok
NAG	B	0.559	42.5295	5.40987	beta	D	$^4C_1$	0.78	103.629	Ok
BMA	B	0.492	356.781	22.0816	beta	D	$^4C_1$	0.68	150.725	Ok
MAN	B	0.556	221.248	11.0071	alpha	D	$^4C_1$	0.73	134.063	Ok
MAN	B	0.573	99.8756	9.42077	alpha	D	$^4C_1$	0.57	184.451	Ok
NAG	B	0.570	37.453	3.10993	beta	D	$^4C_1$	0.83	74.6264	Ok
FUC	B	0.547	9.43823	173.53	alpha	L	$^1C_4$	0.79	92.44	Ok
NAG	B	0.565	5.99907	2.93145	beta	D	$^4C_1$	0.85	103.509	Ok
BMA	B	0.567	340.575	4.40551	beta	D	$^4C_1$	0.50	133.261	Ok

[1]Q is the total puckering amplitude, measured in Angstroems.

[2]Whenever N is displayed in the D/L column, it means that Privateer has been unable to determine the handedness based solely on the structure.

[3]RSCC, short for Real Space Correlation Coefficient, measures the agreement between model and positive omit density. A RSCC below 0.8 is tipically considered poor.

▼ Summary and information for Table 1

Stereochemical problems	0
Unphysical puckering amplitude	0
In unlikely ring conformation	0

Figure S1 Output of the carbohydrate validation of the final HLE/CQH co-crystal structure with PRIVATEER (Agirre, Iglesias-Fernández *et al.*, 2015). The angle definitions and conformation symbols are explained in Agirre (2017).

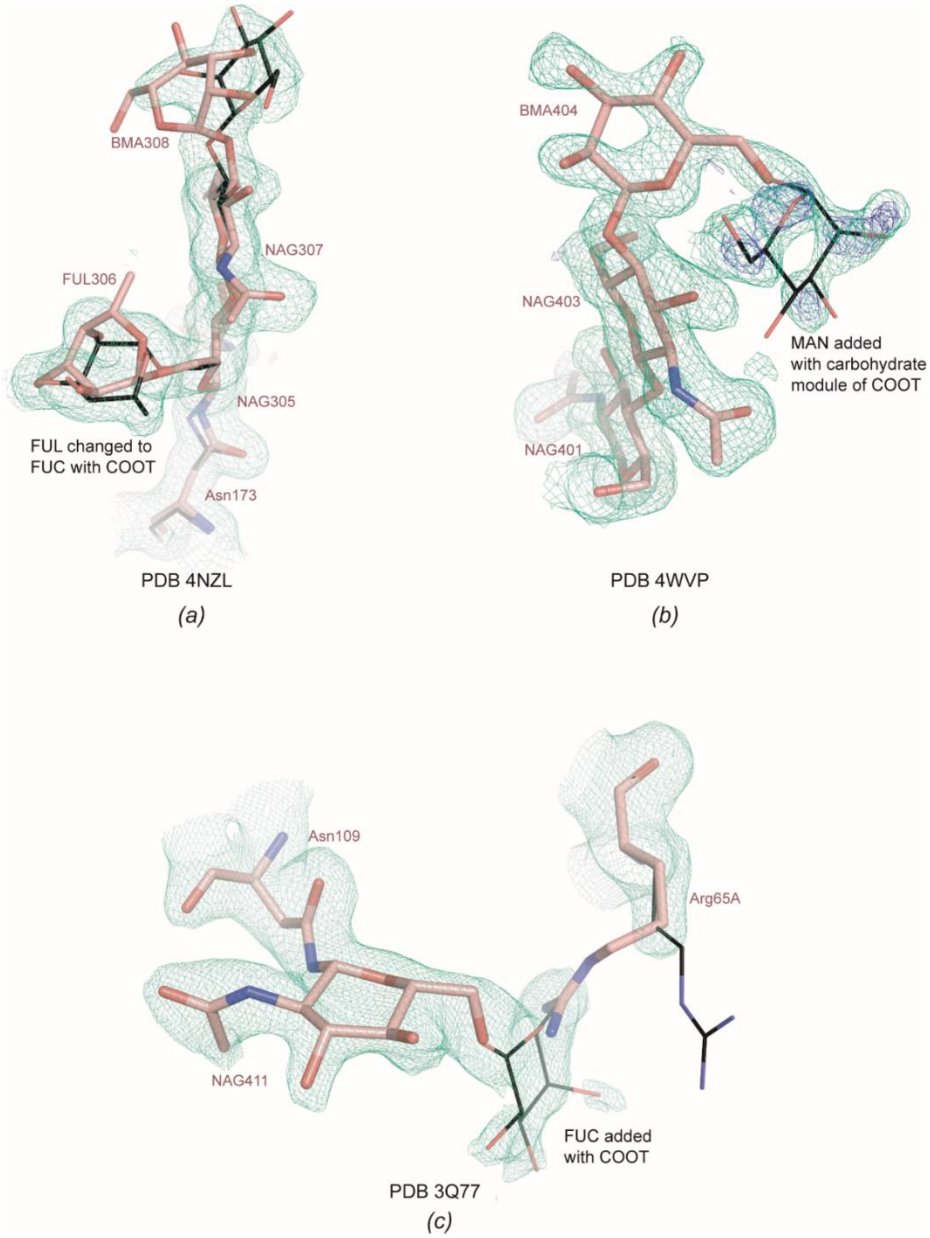

Figure S2 Cases of local errors or incomplete modelling in N-glycan chains of existing HLE structures that could be easily corrected and supplemented with COOT (Emsley *et al.*, 2010) on the basis of the published electron densities and difference Fourier densities. a) An N-glycan in 4NZL (Stapels *et al.*, 2014) with a β-L-fucose (FUL) rather than an α-L-fucose (FUC) residue and with a wrongly orientated terminal β-mannose (BMA) moiety; the electron density was drawn with a cutoff level of 1 σ. b) In 4WVP (Lechtenberg *et al.*, 2015) one of the N-glycans can be supplemented by a terminal α-mannose residue (MAN) (cutoff levels: 0.7 σ for the electron density in green and 3.0 σ for the difference Fourier density in blue). c) In 3Q77 (Hansen *et al.*, 2011) a neighbouring Arg side chain (with black C-atoms after re-modelling) extends into the space which is correctly occupied by α-*L*-fucose (FUC); the electron density was drawn with a cutoff level of 0.7 σ. All parts of the figure were prepared with Pymol (Schrödinger).