

Worldwide Protein Data Bank

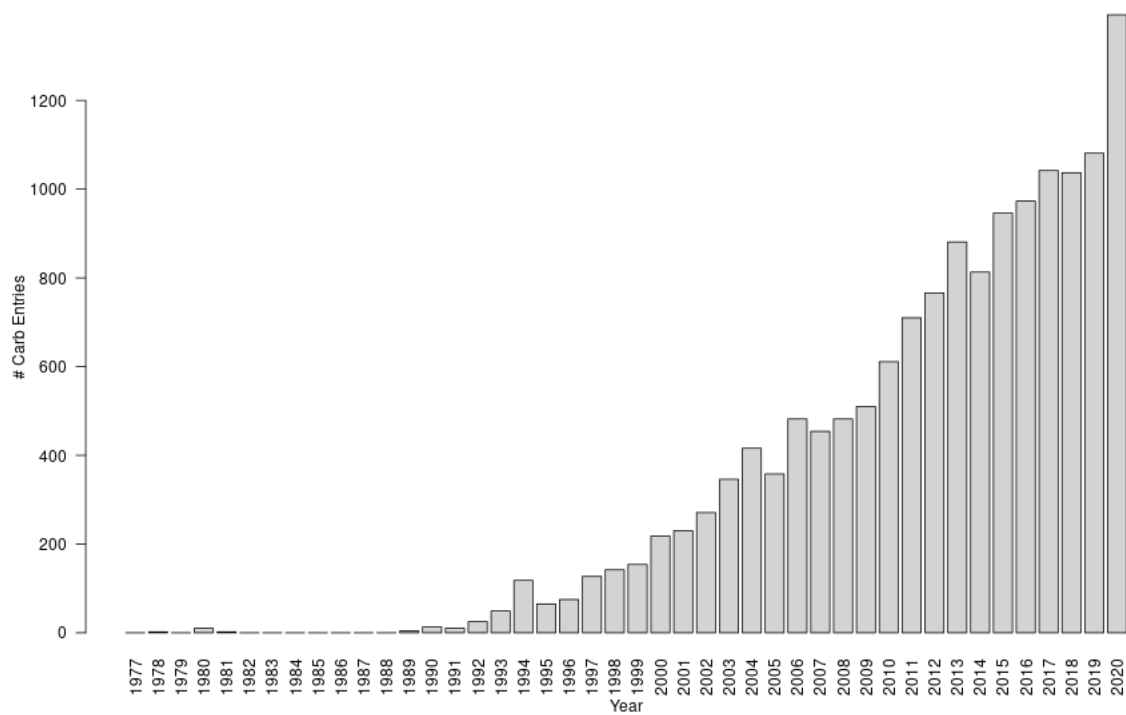
Supplementary Data: Modernized Uniform Representation of Carbohydrate Molecules in the Protein Data Bank

Chenghua Shao, Zukang Feng, John Westbrook, Ezra Peisach, John Berrisford, Yasuyo Ikegawa, Genji Kurisu, Sameer Velankar, Stephen K. Burley and Jasmine Y. Young

Table of Contents

Supplementary Figure S1: Carbohydrate-containing PDB Entries by Year.....	3
Supplementary Table SI: Cyclic Monosaccharides in the PDB.....	4
Supplementary Table SII: Glycosylation Types in the PDB.....	26
Supplementary Table SIII: Blood Group Antigens in BIRD	27
Supplementary Table SIV: Commonly Observed Oligosaccharides in the PDB.....	28
Supplementary Table SV: PDB Examples of Glycan Sequences at the Different Glycosylation Sites.....	31
Appendix I: Example of Remediated CCD definition of NAG.....	35
Appendix II: Example of Remediated PDB Entry 1B5F.....	39

Supplementary Figure S1: Carbohydrate-containing PDB Entries by Year



Supplementary Table S1: Cyclic Monosaccharides in the PDB

id	name	basic/ modified	parent	SNFG symbol	isomer	ring size	anomer	aldose/ ketose
289	D-glycero-alpha-D-manno-heptopyranose	basic		DDmanHep	D	pyranose	alpha	aldose
0MK	beta-L-ribose	basic		Rib	L	pyranose	beta	aldose
1GN	2-amino-2-deoxy-beta-D-galactopyranose	basic		GalN	D	pyranose	beta	aldose
1S4	alpha-muramic acid	basic		Mur	D	pyranose	alpha	aldose
32O	beta-L-ribofuranose	basic		Rib	L	furanose	beta	aldose
34V	beta-L-ribulofuranose	basic			L	furanose	beta	ketose
3MK	beta-L-altropyranose	basic		Alt	L	pyranose	beta	aldose
49T	2-acetamido-2-deoxy-alpha-D-fucopyranose	basic		FucNAc	D	pyranose	alpha	aldose
4GL	alpha-D-gulopyranose	basic		Gul	D	pyranose	alpha	aldose
4N2	beta-L-idopyranose	basic		Ido	L	pyranose	beta	aldose
64K	alpha-D-arabinopyranose	basic		Ara	D	pyranose	alpha	aldose
66O	alpha-L-6-deoxy-gulopyranose	basic		6dGul	L	pyranose	alpha	aldose
95Z	2-amino-2-deoxy-alpha-D-mannopyranose	basic		ManN	D	pyranose	alpha	aldose
A2G	2-acetamido-2-deoxy-alpha-D-galactopyranose	basic		GalNAc	D	pyranose	alpha	aldose
A5C	alpha-L-talofuranose	basic		Tal	L	furanose	alpha	aldose
ABE	alpha-D-Abequopyranose	basic		Abe	D	pyranose	alpha	aldose
ADA	alpha-D-galactopyranuronic acid	basic		GalA	D	pyranose	alpha	aldose
AFD	alpha-D-allopyranose	basic		All	D	pyranose	alpha	aldose
AHR	alpha-L-arabinofuranose	basic		Ara	L	furanose	alpha	aldose
ALL	beta-D-allopyranose	basic		All	D	pyranose	beta	aldose
AMU	N-acetyl-beta-muramic acid	basic		MurNAc	D	pyranose	beta	aldose
ARA	alpha-L-arabinopyranose	basic		Ara	L	pyranose	alpha	aldose
ARB	beta-L-arabinopyranose	basic		Ara	L	pyranose	beta	aldose
BDF	beta-D-fructopyranose	basic		Fru	D	pyranose	beta	ketose
BDP	beta-D-glucopyranuronic acid	basic		GlcA	D	pyranose	beta	aldose
BDR	beta-D-ribofuranose	basic		Rib	D	furanose	beta	aldose
BEM	beta-D-mannopyranuronic acid	basic		ManA	D	pyranose	beta	aldose
BGC	beta-D-glucopyranose	basic		Glc	D	pyranose	beta	aldose
BM3	2-acetamido-2-deoxy-alpha-D-mannopyranose	basic		ManNAc	D	pyranose	alpha	aldose
BM7	2-acetamido-2-deoxy-beta-D-mannopyranose	basic		ManNAc	D	pyranose	beta	aldose
BMA	beta-D-mannopyranose	basic		Man	D	pyranose	beta	aldose
BXX	beta-D-arabinofuranose	basic		Ara	D	furanose	beta	aldose
BXY	alpha-D-arabinofuranose	basic		Ara	D	furanose	alpha	aldose
DDA	beta-D-Olivopyranose	basic		Oli	D	pyranose	beta	aldose
FCA	alpha-D-fucopyranose	basic		Fuc	D	pyranose	alpha	aldose
FCB	beta-D-fucopyranose	basic		Fuc	D	pyranose	beta	aldose
FRU	beta-D-fructofuranose	basic		Fru	D	furanose	beta	ketose
FUB	beta-L-arabinofuranose	basic		Ara	L	furanose	beta	aldose
FUC	alpha-L-fucopyranose	basic		Fuc	L	pyranose	alpha	aldose
FUL	beta-L-fucopyranose	basic		Fuc	L	pyranose	beta	aldose

G6D	alpha-D-quinovopyranose	basic		Qui	D	pyranose	alpha	aldose
GAL	beta-D-galactopyranose	basic		Gal	D	pyranose	beta	aldose
GCS	2-amino-2-deoxy-beta-D-glucopyranose	basic		GlcN	D	pyranose	beta	aldose
GCU	alpha-D-glucopyranuronic acid	basic		GlcA	D	pyranose	alpha	aldose
GIV	beta-L-galactopyranose	basic		Gal	L	pyranose	beta	aldose
GL0	beta-D-gulopyranose	basic		Gul	D	pyranose	beta	aldose
GLA	alpha-D-galactopyranose	basic		Gal	D	pyranose	alpha	aldose
GLC	alpha-D-glucopyranose	basic		Glc	D	pyranose	alpha	aldose
GMH	L-glycero-alpha-D-manno-heptopyranose	basic		LDmanHep	D	pyranose	alpha	aldose
GTK	beta-D-galactofuranuronic acid	basic		GalA	D	furanose	beta	aldose
GTR	beta-D-galactopyranuronic acid	basic		GalA	D	pyranose	beta	aldose
GUP	alpha-L-gulopyranose	basic		Gul	L	pyranose	alpha	aldose
GXL	alpha-L-galactopyranose	basic		Gal	L	pyranose	alpha	aldose
GYE	beta-D-fucofuranose	basic		Fuc	D	furanose	beta	aldose
GZL	beta-D-galactofuranose	basic		Gal	D	furanose	beta	aldose
HSQ	2-acetyl-amino-2-deoxy-alpha-L-idopyranose	basic		IdoNAc	L	pyranose	alpha	aldose
HSY	alpha-L-xylopyranose	basic		Xyl	L	pyranose	alpha	aldose
IDR	alpha-L-idopyranuronic acid	basic		IdoA	L	pyranose	alpha	aldose
KDM	deamino-alpha-neuraminic acid	basic		Kdn	D	pyranose	alpha	ketose
KDN	deamino-beta-neuraminic acid	basic		Kdn	D	pyranose	beta	ketose
KDO	3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid	basic		Kdo	D	pyranose	alpha	ketose
LDY	alpha-D-lyxopyranose	basic		Lyx	D	pyranose	alpha	aldose
LFR	beta-L-fructofuranose	basic		Fru	L	furanose	beta	ketose
LGU	alpha-L-gulopyranuronic acid	basic		GulA	L	pyranose	alpha	aldose
LXB	2-acetamido-2-deoxy-beta-D-gulopyranose	basic		GulNAc	D	pyranose	beta	aldose
LXC	beta-L-xylopyranose	basic		Xyl	L	pyranose	beta	aldose
LXZ	2-acetamido-2-deoxy-alpha-D-idopyranose	basic		IdoNAc	D	pyranose	alpha	aldose
MAN	alpha-D-mannopyranose	basic		Man	D	pyranose	alpha	aldose
MAV	alpha-D-mannopyranuronic acid	basic		ManA	D	pyranose	alpha	aldose
MUB	N-acetyl-alpha-muramic acid	basic		MurNAc	D	pyranose	alpha	aldose
MUR	beta-muramic acid	basic		Mur	D	pyranose	beta	aldose
NAA	2-acetamido-2-deoxy-beta-D-allopyranose	basic		AlINAc	D	pyranose	beta	aldose
NAG	2-acetamido-2-deoxy-beta-D-glucopyranose	basic		GlcNAc	D	pyranose	beta	aldose
NDG	2-acetamido-2-deoxy-alpha-D-glucopyranose	basic		GlcNAc	D	pyranose	alpha	aldose
NGA	2-acetamido-2-deoxy-beta-D-galactopyranose	basic		GalNAc	D	pyranose	beta	aldose
NGC	N-glycolyl-alpha-neuraminic acid	basic		Neu5Gc	D	pyranose	alpha	ketose
NGE	N-glycolyl-beta-neuraminic acid	basic		Neu5Gc	D	pyranose	beta	ketose
NGZ	2-acetamido-2-deoxy-alpha-L-glucopyranose	basic		GlcNAc	L	pyranose	alpha	aldose
PA1	2-amino-2-deoxy-alpha-D-glucopyranose	basic		GlcN	D	pyranose	alpha	aldose
PSV	alpha-D-psicofuranose	basic		Psi	D	furanose	alpha	ketose
PZU	alpha-D-Paratopyranose	basic		Par	D	pyranose	alpha	aldose
RAE	alpha-L-Olivopyranose	basic		Oli	L	pyranose	alpha	aldose
RAM	alpha-L-rhamnopyranose	basic		Rha	L	pyranose	alpha	aldose

RIB	alpha-D-ribofuranose	basic		Rib	D	furanose	alpha	aldose
RIP	beta-D-ribopyranose	basic		Rib	D	pyranose	beta	aldose
RM4	beta-L-rhamnopyranose	basic		Rha	L	pyranose	beta	aldose
RUU	alpha-L-ribulofuranose	basic			L	furanose	alpha	ketose
SDY	beta-D-talopyranose	basic		Tal	D	pyranose	beta	aldose
SEJ	beta-D-arabinopyranose	basic		Ara	D	pyranose	beta	aldose
SF6	alpha-L-psicofuranose	basic		Psi	L	furanose	alpha	ketose
SF9	beta-L-psicofuranose	basic		Psi	L	furanose	beta	ketose
SHD	alpha-D-altropyranose	basic		Alt	D	pyranose	alpha	aldose
SIA	N-acetyl-alpha-neuraminic acid	basic		Neu5Ac	D	pyranose	alpha	ketose
SLB	N-acetyl-beta-neuraminic acid	basic		Neu5Ac	D	pyranose	beta	ketose
SOE	alpha-L-sorbopyranose	basic		Sor	L	pyranose	alpha	ketose
T6T	alpha-D-tagatopyranose	basic		Tag	D	pyranose	alpha	ketose
TTV	beta-D-psicofuranose	basic		Psi	D	furanose	beta	ketose
TYV	alpha-D-Tyvelopyranose	basic		Tyv	D	pyranose	alpha	aldose
UEA	beta-D-sorbofuranose	basic		Sor	D	furanose	beta	ketose
WO O	beta-L-allopyranose	basic		All	L	pyranose	beta	aldose
X0X	beta-D-talopyranuronic acid	basic		TalA	D	pyranose	beta	aldose
X1X	alpha-D-talopyranuronic acid	basic		TalA	D	pyranose	alpha	aldose
X6X	2-amino-2-deoxy-alpha-D-galactopyranose	basic		GalN	D	pyranose	alpha	aldose
XLF	beta-D-xylulofuranose	basic			D	furanose	beta	ketose
XXM	3-C-(hydroxymethyl)-alpha-D-erythrofuranose	basic		Api	D	furanose	alpha	aldose
XXR	alpha-D-rhamnopyranose	basic		Rha	D	pyranose	alpha	aldose
XYP	beta-D-xylopyranose	basic		Xyl	D	pyranose	beta	aldose
XYS	alpha-D-xylopyranose	basic		Xyl	D	pyranose	alpha	aldose
XYZ	beta-D-xylofuranose	basic		Xyl	D	furanose	beta	aldose
YYK	beta-D-quinovopyranose	basic		Qui	D	pyranose	beta	aldose
YYM	alpha-D-ribopyranose	basic		Rib	D	pyranose	alpha	aldose
YYQ	2-acetamido-2-deoxy-alpha-L-galactopyranose	basic		GalNAc	L	pyranose	alpha	aldose
Z0F	alpha-L-idopyranose	basic		Ido	L	pyranose	alpha	aldose
Z2D	alpha-L-allopyranose	basic		All	L	pyranose	alpha	aldose
Z3U	beta-D-Digitoxopyranose	basic		Dig	D	pyranose	beta	aldose
Z4W	beta-D-lyxopyranose	basic		Lyx	D	pyranose	beta	aldose
Z5J	beta-L-Olivopyranose	basic		Oli	L	pyranose	beta	aldose
Z6H	alpha-L-altropyranose	basic		Alt	L	pyranose	alpha	aldose
Z6J	alpha-L-ribofuranose	basic		Rib	L	furanose	alpha	aldose
Z8H	beta-L-gulopyranose	basic		Gul	L	pyranose	beta	aldose
Z8T	beta-L-glucopyranose	basic		Glc	L	pyranose	beta	aldose
Z9N	alpha-D-fructofuranose	basic		Fru	D	furanose	alpha	ketose
Z9W	2-acetamido-2-deoxy-beta-D-quinovopyranose	basic		QuiNAc	D	pyranose	beta	aldose
ZCD	alpha-D-idopyranose	basic		Ido	D	pyranose	alpha	aldose
ZEE	beta-L-talopyranose	basic		Tal	L	pyranose	beta	aldose
145	2-nitrophenyl beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose

147	4-nitrophenyl beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
149	D-galactonolactone	modified			D	pyranose		aldose
291	prop-2-en-1-yl 7-O-carbamoyl-L-glycero-alpha-D-manno-heptopyranoside	modified	GMH		D	pyranose	alpha	aldose
293	2-deoxy-beta-L-galacto-heptopyranose	modified			D	pyranose	alpha	aldose
445	N-[oxo(phenylamino)acetyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
475	N-[oxo(pyridin-2-ylamino)acetyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
491	2-acetamido-3-O-[(1R)-1-carboxyethyl]-2-deoxy-1-O-phosphono-alpha-D-glucopyranose	modified	NDG		D	pyranose	alpha	aldose
510	methyl (2S,4R)-1-[(2S,3R,4R,5S,6S)-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]sulfonyl-4-sulfamoyloxy-pyrrolidine-2-carboxylate	modified			L	pyranose	alpha	aldose
604	2-[(3-bromobenzene-1-carbonyl)amino]-6-[[4-carboxy-5-methylfuran-2-yl]sulfonyl]amino}-2,6-dideoxy-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
05L	heptyl 1-seleno-beta-D-glucopyranoside	modified			D	pyranose	beta	aldose
07E	(3S)-3-hydroxybutyl beta-D-xylopyranoside	modified	XYP		D	pyranose	beta	aldose
0HX	pentan-3-yl 2-acetamido-2,4-dideoxy-alpha-L-threo-hex-4-enopyranosiduronic acid	modified			L	dihydrofuran	alpha	aldose
0LP	5-acetamido-2,6-anhydro-3,5-dideoxy-3-[(2E)-3-phenylprop-2-en-1-yl]-D-glycero-L-altro-non-2-enonic acid	modified			L	dihydropyran		ketose
0NZ	2-deoxy-6-O-phosphono-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
0WK	1,5-anhydro-6-O-phosphono-D-glucitol	modified			D	pyranose		aldose
0XY	5-fluoro-N-acetyl-alpha-D-glucosamine	modified			D	pyranose	alpha	aldose
0YT	2-acetamido-2-deoxy-5-thio-beta-D-glucopyranose	modified			D	thiopyranose	beta	aldose
12E	N-[(2E)-2-(pyridin-4-ylmethylidene)hydrazino]carbonothioyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
14T	3,4-difluorophenyl 2-deoxy-2-[(difluoroacetyl)amino]-beta-D-glucopyranoside	modified	NAG		D	pyranose	beta	aldose
15L	D-galactaro-1,5-lactone	modified			D	pyranose		aldose
16F	N-[(2Z)-2-[(3-hydroxyphenyl)methylidene]hydrazino]carbonothioyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
16G	2-acetamido-2-deoxy-6-O-phosphono-alpha-D-glucopyranose	modified	NDG		D	pyranose	alpha	aldose
16O	N-[(2E)-2-[(4-bromophenyl)methylidene]hydrazino]carbonothioyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
17T	N-[(2E)-2-[(4-chlorophenyl)methylidene]hydrazino]carbonothioyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
18D	3,5-dideoxy-5-(propanoylamino)-D-glycero-alpha-D-galactonon-2-ulopyranosonic acid	modified	SIA		D	pyranose	alpha	ketose
18O	N-[(2E)-2-[(4-nitrophenyl)methylidene]hydrazino]carbonothioyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
1CF	2-hydroxyethyl 6-deoxy-beta-L-galactopyranoside	modified	FUL		L	pyranose	beta	aldose
1GL	2,6-dideoxy-4-O-methyl-alpha-D-galactopyranose	modified			D	pyranose	alpha	aldose
1S3	(2R,3aR,5R,6S,7S,7aR)-5-(hydroxymethyl)tetrahydro-3aH-[1,3,2]dioxaphospholo[4,5-b]pyran-2,6,7-triol 2-oxide	modified	GLC		D	pyranose	alpha	aldose
1SD	(1S)-1,5-anhydro-1-sulfamoyl-D-galactitol	modified			D	pyranose	beta	aldose
1X4	2,3-dideoxy-5-O-phosphono-alpha-D-ribofuranose	modified			D	furanose	alpha	aldose
20X	N-[(2E)-2-[(4-fluorophenyl)methylidene]hydrazino]carbonothioyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
22O	N-[(2E)-2-[(3-bromophenyl)methylidene]hydrazino]carbonothioyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose

22S	N-(((2E)-2-[(2-chlorophenyl)methylidene]hydrazino)carbonothioyl)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
23V	N-(((2E)-2-[(3-chlorophenyl)methylidene]hydrazino)carbonothioyl)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
24S	N-(((2Z)-2-[(2-nitrophenyl)methylidene]hydrazino)carbonothioyl)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
25E	N-(((2Z)-2-[(4-hydroxyphenyl)methylidene]hydrazino)carbonothioyl)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
26O	N-(((2E)-2-[(2-hydroxyphenyl)methylidene]hydrazino)carbonothioyl)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
27C	5-O-[(S)-butoxy(hydroxy)phosphoryl]-2-deoxy-2-fluoro-alpha-D-arabinofuranose	modified			D	furanose	alpha	aldose
2DG	2-deoxy-alpha-D-galactopyranose	modified			D	pyranose	alpha	aldose
2DR	2-deoxy-beta-D-erythro-pentofuranose	modified			D	furanose	beta	aldose
2F8	methyl 2-acetamido-2-deoxy-alpha-D-glucopyranoside	modified	NDG		D	pyranose	alpha	aldose
2FG	2-deoxy-2-fluoro-beta-D-galactopyranose	modified			D	pyranose	beta	aldose
2GL	4-O-acetyl-2,6-dideoxy-beta-D-galactopyranose	modified			D	pyranose	beta	aldose
2GS	2-O-methyl-alpha-D-galactopyranose	modified	GLA		D	pyranose	alpha	aldose
2H5	3-deoxy-3-fluoro-beta-D-galactopyranose	modified			D	pyranose	beta	aldose
2M5	methyl 7-deoxy-L-glycero-alpha-D-manno-heptopyranoside	modified	MAN		D	pyranose	alpha	aldose
2M8	(2R)-3-hydroxy-2-(alpha-D-mannopyranosyloxy)propanoic acid	modified	MAN		D	pyranose	alpha	aldose
2WP	S-ribosylhomocysteine	modified			D	furanose	alpha	aldose
3DO	3-deoxy-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
3FM	3-O-carbamoyl-alpha-D-mannopyranose	modified	MAN		D	pyranose	alpha	aldose
3HD	1,5-anhydro-3-O-methyl-D-mannitol	modified			D	pyranose		aldose
3J3	(1R)-1,5-anhydro-1-[[4-(sulfamoyloxy)piperidin-1-yl]sulfonyl]-D-galactitol	modified			D	pyranose	alpha	aldose
3J4	(6S)-2,6-anhydro-6-[[[(3R)-3-(sulfamoyloxy)pyrrolidin-1-yl]sulfonyl]-D-glucitol	modified			L	pyranose	alpha	aldose
3LJ	2-amino-2-deoxy-6-O-sulfo-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
3MG	3-O-methyl-beta-D-glucopyranose	modified	BGC		D	pyranose	beta	aldose
3R3	[[[(2R,3R,4S,5R)-3,4-bis(oxidanyl)-5-(phosphonooxymethyl)oxolan-2-yl]oxy-oxidanyl-phosphoryl]amino]phosphonic acid	modified	RIB		D	furanose	alpha	aldose
3S6	prop-2-en-1-yl beta-D-galactofuranoside	modified	GZL		D	furanose	beta	aldose
3YW	(2S)-2,3-dihydroxypropyl 2-acetamido-2-deoxy-alpha-D-glucopyranoside	modified	NDG		D	pyranose	alpha	aldose
42D	3,5-dideoxy-5-[(methoxycarbonyl)amino]-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid	modified			D	pyranose	alpha	ketose
44S	2-deoxy-6-O-phosphono-beta-D-lyxo-hexofuranose	modified			D	furanose	beta	aldose
46Z	(2R,3R,4S,5S)-4-fluoro-3,5-dihydroxytetrahydrofuran-2-yl 2-phenylethyl hydrogen (S)-phosphate	modified			D	furanose	alpha	aldose
49A	4,9-AMINO-2,4-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID	modified			D	dihydropyran		ketose
49S	2-acetamido-2-deoxy-beta-D-mannopyranuronic acid	modified			D	pyranose	beta	aldose
49V	2-acetamido-2,4-dideoxy-alpha-L-erythro-hex-4-enopyranuronic acid	modified			L	dihydropyran	alpha	ketose
4AM	4-AMINO-2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID	modified			D	dihydropyran		ketose
4GP	N-(carboxycarbonyl)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
4JA	(2S)-3-[(6-deoxy-beta-D-glucopyranosyl)oxy]-2-hydroxypropyl dihydrogen phosphate	modified	YYK		D	pyranose	beta	aldose

4NN	N-[(5S,6R)-5-hydroxy-6-(hydroxymethyl)-2-oxo-5,6-dihydro-2H-pyran-3-yl]acetamide	modified			D	dihydropyran		aldose
4QY	2-acetamido-2-deoxy-6-O-phosphono-beta-D-glucopyranose	modified	NAG		D	pyranose	beta	aldose
4R1	2-amino-2-deoxy-6-O-phosphono-beta-D-glucopyranose	modified	GCS		D	pyranose	beta	aldose
4SG	4-thio-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
4UZ	2-[[[(benzyloxy)carbonyl]amino]-2-deoxy-beta-D-glucopyranose	modified	GCS		D	pyranose	beta	aldose
4V5	2-deoxy-2-[[3-(4-hydroxyphenyl)propanoyl]amino]-alpha-D-glucopyranose	modified	PA1		D	pyranose	alpha	aldose
50A	2-deoxy-2-fluoro-5-O-phosphono-alpha-D-ribofuranose	modified			D	furanose	alpha	aldose
51N	5-O-[(R)-hydroxy(phosphonoxy)phosphoryl]-1-O-phosphono-alpha-D-ribofuranose	modified	RIB		D	furanose	alpha	aldose
56N	phenyl beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
57S	4-O-[2-acetamido-2-deoxy-beta-D-glucopyranosyl]-5-O-phosphono-D-ribitol	modified	NAG		D	pyranose	beta	aldose
5DI	alpha-D-threo-hexo-2,5-diulo-2,6-pyranosyl fluoride	modified				pyranose		aldose
5GF	5-fluoro-beta-D-glucopyranose	modified	BGC		D	pyranose	beta	aldose
5KQ	(6R)-5-acetamido-6-[(1S,2S)-3-acetamido-1,2-dihydroxypropyl]-3,5-dideoxy-beta-L-threo-hex-2-ulopyranosonic acid	modified			L	pyranose	beta	ketose
5KV	2-deoxy-6-O-sulfo-2-(sulfoamino)-beta-D-glucopyranose	modified	GCS		D	pyranose	beta	aldose
5L2	methyl (2S,4R)-1-[(2S,3R,4R,5S,6S)-6-(acetyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]sulfonyl-4-sulfamoyloxy-pyrrolidine-2-carb oxylate	modified			D	pyranose	beta	aldose
5L3	(6R)-5-O-acetyl-2,6-anhydro-6-[[4-(sulfamoyloxy)piperidin-1-yl]sulfonyl]-L-glucitol	modified			D	pyranose	alpha	aldose
5LS	2,4-di-O-sulfo-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
5LT	3,4-di-O-sulfo-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
5N6	9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid	modified	SIA		D	pyranose	alpha	ketose
5QP	(1R,2R,3S,5R,6S)-2,3,5-trihydroxy-6-(hydroxymethyl)cyclohexyl alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose
5TH	[(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate	modified	GLC		D	pyranose	alpha	aldose
5TJ	[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate	modified	GLC		D	pyranose	alpha	aldose
5TK	(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol	modified	GLC		D	pyranose	alpha	aldose
5TM	[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate	modified	GLC		D	pyranose	alpha	aldose
61J	(6S)-2,6-anhydro-1-deoxy-6-(2-[[[S]-hydroxy(oxido)-lambda~5~-phosphanyl]oxy]ethyl)-D-galactitol	modified			D	pyranose		ketose
62I	(6R)-1-O-acetyl-2,6-anhydro-6-[[4-(sulfamoyloxy)piperidin-1-yl]sulfonyl]-L-glucitol	modified			D	pyranose	alpha	aldose
6BG	6-bromo-6-deoxy-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
6C2	methyl 2-acetamido-2-deoxy-beta-D-glucopyranosiduronic acid	modified			D	pyranose	beta	aldose
6GP	N-[methoxy(oxo)acetyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
6GR	2-(alpha-L-altropyranosyloxy)benzoic acid	modified	Z6H		L	pyranose	alpha	aldose
6K3	heptyl 4-deoxy-4-fluoro-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
6KH	heptyl 3-fluoro-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
6KL	methyl 4,5-bisacetamido-3,4,5-trideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid	modified			D	pyranose	alpha	ketose
6KS	heptyl 2-fluoro-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
6KU	heptyl 4-deoxy-4-deoxy-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
6KW	heptyl 3-deoxy-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
6LS	heptyl 2-deoxy-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose

6LW	(Z)-L-Arabinonhydroximo-1,4-lactone	modified			L	furanose		aldose
6MJ	methyl beta-D-xylopyranoside	modified	XYP		D	pyranose	beta	aldose
6MN	2-amino-2-deoxy-6-O-phosphono-alpha-D-mannopyranose	modified	95Z		D	pyranose	alpha	aldose
6PY	5-acetamido-2,6-anhydro-4-carbamimidamido-3,4,5-trideoxy-7-O-[(2-methoxyethyl)carbamoyl]-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
6PZ	5,7-bisacetamido-3,5,7,9-tetradeoxy-L-glycero-alpha-L-mannon-2-ulopyranosonic acid	modified			D	pyranose	beta	ketose
6S2	methyl 2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranoside	modified	NAG		D	pyranose	beta	aldose
6UD	5-acetamido-2,6-anhydro-3,5,9-trideoxy-9-triazan-1-yl-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
6Y6	2,6-anhydro-3,4,5-trideoxy-4-[4-(methoxymethyl)-1H-1,2,3-triazol-1-yl]-5-[(2-methylpropanoyl)amino]-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
6YR	methyl 1-seleno-2-O-methyl-beta-L-fucopyranoside	modified			L	pyranose	beta	aldose
6ZC	4-nitrophenyl 2-acetamido-2-deoxy-alpha-D-glucopyranoside	modified	PA1		D	pyranose	alpha	aldose
73E	(1S)-1,5-anhydro-1-(5-phenyl-4H-1,2,4-triazol-3-yl)-D-glucitol	modified			D	pyranose		aldose
79J	4-O-acetyl-5-acetamido-3,5-dideoxy-L-glycero-alpha-D-galacto-non-2-ulopyranosonic acid	modified			D	pyranose	alpha	ketose
7CV	6-deoxy-2,3-di-O-methyl-alpha-L-mannopyranose	modified	RAM		L	pyranose	alpha	aldose
7D1	1,5-anhydro-2-deoxy-D-arabino-hexitol	modified			D	pyranose		aldose
7GP	N-[ethoxy(oxo)acetyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
7JZ	2-deoxy-2,2-difluoro-beta-D-lyxo-hexopyranose	modified			D	pyranose	beta	aldose
7K2	[(3S,4R,5R)-4,5-dihydropiperidin-3-yl]methyl 1-thio-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
7K3	1-thio-alpha-D-mannopyranose	modified			D	pyranose	alpha	aldose
7NU	phenyl 6,7-anhydro-D-glycero-beta-D-galacto-heptopyranoside	modified	BGC		D	pyranose	beta	aldose
83Y	3-O-sulfo-alpha-L-rhamnopyranose	modified	RAM		L	pyranose	alpha	aldose
89Y	(3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-one	modified			D	furanose		aldose
8B9	2-acetamido-2,4-dideoxy-alpha-D-xylo-hexopyranose	modified			D	pyranose	alpha	aldose
8EX	2-acetamido-2-deoxy-4,6-di-O-sulfo-beta-D-galactopyranose	modified	NGA		D	pyranose	beta	aldose
8GA	5-Se-methyl-5-seleno-alpha-D-ribofuranose	modified			D	furanose	alpha	aldose
8GG	5-Se-methyl-5-seleno-beta-D-ribofuranose	modified			D	furanose	beta	aldose
8GP	N-[(cyclopropylamino)(oxo)acetyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
8LM	2,6-anhydro-3,5-dideoxy-5-[(2-methylpropanoyl)amino]-3-(4-phenyl-1H-1,2,3-triazol-1-yl)-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
8LR	2-hydroxyethyl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
8OQ	alpha-D-aceric acid	modified			D	furanose	alpha	aldose
8PK	4-O-[(1R)-1-hydroxyethyl]-2-O-methyl-alpha-L-fucopyranose	modified	FUC		L	pyranose	alpha	aldose
8S0	L-glucono-1,5-lactone	modified			L	pyranose		aldose
96O	(1-methyl-1H-1,2,3-triazol-4-yl)methyl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
9AM	9-AMINO-2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID	modified			D	dihydropyran		ketose
9C1	2-[[[(2E)-4-chlorobut-2-enoyl]amino]-2-deoxy-beta-D-glucopyranose	modified	GCS		D	pyranose	beta	aldose
9CD	2-[[[(2E)-but-2-enoyl]amino]-2-deoxy-beta-D-glucopyranose	modified	GCS		D	pyranose	beta	aldose
9GP	N-(hydroxyacetyl)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
9KJ	{[(2R,3R,4R,5R)-3-(alpha-D-glucopyranosyloxy)-4-hydroxy-2,5-bis(hydroxymethyl)pyrrolidin-1-yl]methyl}phosphonic acid	modified	GLC		D	pyranose	alpha	aldose

9MR	(3R,4R,5R)-3-hydroxy-5-(hydroxymethyl)piperidin-4-yl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
9OK	2-(3,4-dihydroxyphenyl)ethyl beta-D-fructofuranoside	modified	FRU		D	furanose	beta	ketose
9PG	4-nitrophenyl alpha-D-galactopyranoside	modified	GLA		D	pyranose	alpha	aldose
9QG	methyl 3-O-[(1R)-1-carboxyethyl]-beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
9S7	5-acetamido-2,6-anhydro-3,5,8-trideoxy-3-fluoro-D-threo-L-galacto-nononic acid	modified			D	pyranose		ketose
9SG	(2R,3R,5R,6R)-5-acetamido-2,3-bis(fluoranyl)-6-[(1R,2R)-1,2,3-tris(oxidanyl)propyl]oxane-2-carboxylic acid	modified			D	pyranose		ketose
9SJ	5-acetamido-2,6-anhydro-3,5,7-trideoxy-3-fluoro-D-threo-L-galacto-nononic acid	modified			D	pyranose		ketose
9SM	(2R,3R,4R,5R,6S)-5-acetamido-6-[(2S)-2,3-bis(oxidanyl)propyl]-2,3-bis(fluoranyl)-4-oxidanyl-oxane-2-carboxylic acid	modified			D	pyranose		ketose
9SP	(2R,3R,4R,5R,6R)-5-acetamido-6-[(1R)-1,3-bis(oxidanyl)propyl]-2,3-bis(fluoranyl)-4-oxidanyl-oxane-2-carboxylic acid	modified			D	pyranose		ketose
9T1	5-acetamido-2,6-anhydro-3,5,9-trideoxy-3-fluoro-D-erythro-L-glucos-4-ulosonic acid	modified			L	pyranose		ketose
9T7	(2R,3R,4R,5R,6R)-5-acetamido-6-[(1R,2R)-1,2-bis(oxidanyl)propyl]-2,3-bis(fluoranyl)-4-oxidanyl-oxane-2-carboxylic acid	modified			D	pyranose		ketose
9VP	5-acetamido-2,6-anhydro-3,4,5-trideoxy-3-fluoro-D-erythro-L-glucos-4-ulosonic acid	modified			D	pyranose		ketose
9WJ	4-acetamido-4,6-dideoxy-beta-D-mannopyranose	modified			D	pyranose	beta	aldose
9WN	(2R)-2-(alpha-D-glucopyranosyloxy)-3-hydroxypropanoic acid	modified	GLC		D	pyranose	alpha	aldose
9WZ	2-hydroxy-4-(2-hydroxyethyl)phenyl beta-D-fructofuranoside	modified	FRU		D	furanose	beta	ketose
9YW	(alpha-D-glucopyranosyloxy)acetic acid	modified	GLC		D	pyranose	alpha	aldose
A0K	1,3-dihydroxypropan-2-yl alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose
A1Q	methyl L-glycero-alpha-D-manno-heptopyranoside	modified	GMH		D	pyranose	alpha	aldose
A6P	6-O-phosphono-alpha-D-allopyranose	modified	AFD		D	pyranose	alpha	aldose
AAL	3,6-anhydro-alpha-L-galactopyranose	modified			L	pyranose	alpha	aldose
ABF	5-O-phosphono-beta-D-arabinofuranose	modified	BXX		D	furanose	beta	aldose
ABL	(2R,3R,4R,5R)-4,5-dihydroxy-2-(hydroxymethyl)-6-oxopiperidin-3-yl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
AC1	4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino]-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
AF1	4,6-dideoxy-4-[[[(1S,4S,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino]-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
AFO	octyl alpha-D-arabinofuranoside	modified	BXY		D	furanose	alpha	aldose
AFP	1,6-di-O-phosphono-alpha-D-fructofuranose	modified	Z9N		D	furanose	alpha	ketose
AFR	alpha-D-threo-hexo-2,5-diulo-5,1-pyranosyl fluoride	modified				pyranose		aldose
AGL	4-amino-4,6-dideoxy-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
AH2	1-deoxy-alpha-D-mannopyranose	modified			D	pyranose		aldose
AH8	(2R,3R,4R,5S)-2-azido-5-(hydroxymethyl)oxolane-3,4-diol	modified			L	furanose	alpha	aldose
AHG	2,5-anhydro-1,6-di-O-phosphono-D-glucitol	modified			D	furanose		
AHM	2,5-anhydro-1,6-di-O-phosphono-D-mannitol	modified			D	furanose		
AIG	hexyl 3-amino-3-deoxy-beta-D-galactopyranoside	modified			D	pyranose	beta	aldose
ALX	2-O-phosphono-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
AMG	methyl alpha-D-galactopyranoside	modified	GLA		D	pyranose	alpha	aldose
AMN	methyl 5-acetamido-9-amino-3,5,9-trideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid	modified			D	pyranose	alpha	ketose
AMV	methyl 2-acetamido-3-O-[(1R)-1-carboxyethyl]-2-deoxy-beta-D-glucopyranoside	modified	NAG		D	pyranose	beta	aldose

ANA	methyl 4-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid	modified	SIA		D	pyranose	alpha	ketose
AOG	octyl 3-amino-3-deoxy-beta-D-galactopyranoside	modified			D	pyranose	beta	aldose
AQA	4-deoxy-beta-L-threo-hex-4-enopyranuronic acid	modified			L	dihydropyran	beta	aldose
ARI	(2R,3R,6R)-6-hydroxy-2-methyltetrahydro-2H-pyran-3-yl acetate	modified			D	pyranose	beta	aldose
ARW	methyl beta-D-arabinopyranoside	modified	SEJ		D	pyranose	beta	aldose
ASC	ASCORBIC ACID	modified			L	dihydrofuran		aldose
ASG	2-acetamido-2-deoxy-4-O-sulfo-beta-D-galactopyranose	modified	NGA		D	pyranose	beta	aldose
ASO	1,5-anhydro-D-glucitol	modified			D	pyranose		aldose
AXP	(1S)-4-acetamido-1,5-anhydro-2,4-dideoxy-1-phosphono-D-glycero-D-galacto-octitol	modified			D	pyranose		ketose
AXR	methyl alpha-D-arabinofuranoside	modified	BXY		D	furanose	alpha	aldose
AY9	Ascopyrone M	modified			D	dihydropyran		aldose
AZC	N-(acetylcarbamoyle)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
B0D	(2R,3S,4R,5R,6R)-2,6-difluoro-2-(hydroxymethyl)tetrahydro-2H-pyran-3,4,5-triol	modified			L	pyranose		aldose
B16	1,6-di-O-phosphono-beta-D-glucopyranose	modified	BGC		D	pyranose	beta	aldose
B1H	(1S)-1,5-anhydro-1-(3-[4-[hydroxy(oxo)azaniumyl]phenyl]-1H-1,2,4-triazol-5-yl)-D-glucitol	modified			D	pyranose	beta	aldose
B1N	(1S)-1,5-anhydro-1-[3-(4-hydroxyphenyl)-1H-1,2,4-triazol-5-yl]-D-glucitol	modified			D	pyranose		aldose
B6D	2,4-bisacetamido-2,4,6-trideoxy-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
B7G	heptyl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
B8D	4-O-methyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
B9D	5-fluoro-alpha-L-idopyranose	modified			L	pyranose	alpha	aldose
BBK	2-acetamido-2-deoxy-5-thio-alpha-D-galactopyranose	modified			D	thiopyranose	alpha	aldose
BBV	benzyl 2-acetamido-2-deoxy-alpha-D-glucopyranoside	modified	NDG		D	pyranose	alpha	aldose
BDG	2,6-diamino-2,6-dideoxy-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
BFN	5-acetamido-9-(benzoylamino)-3,5,9-trideoxy-3-fluoro-D-erythro-alpha-L-manno-non-2-ulopyranosonic acid	modified			D	pyranose	beta	ketose
BG6	6-O-phosphono-beta-D-glucopyranose	modified	BGC		D	pyranose	beta	aldose
BG8	2-(benzoylamino)-2-deoxy-beta-D-glucopyranose	modified	GCS		D	pyranose	beta	aldose
BGL	2-O-octyl-beta-D-glucopyranose	modified	BGC		D	pyranose	beta	aldose
BGN	2-(butanoylamino)-2-deoxy-beta-D-glucopyranose	modified	GCS		D	pyranose	beta	aldose
BGP	6-O-phosphono-beta-D-galactopyranose	modified	GAL		D	pyranose	beta	aldose
BGS	(1S)-1,5-anhydro-1-(ethylsulfonyl)-D-glucitol	modified			D	pyranose	beta	aldose
BHG	hexyl beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
BMX	2-acetamido-2-deoxy-6-O-phosphono-alpha-D-mannopyranose	modified	BM3		D	pyranose	alpha	aldose
BND	methyl 5-acetamido-3,5,9-trideoxy-9-[(phenylcarbonyl)amino]-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid	modified			D	pyranose	alpha	ketose
BNG	nonyl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
BNX	2-O-phosphono-beta-D-glucopyranose	modified	BGC		D	pyranose	beta	aldose
BO1	N-(4-sulfamoylphenyl)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
BOG	octyl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
BQY	2-methoxyphenyl beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
BS7	8-hydroxyquinoline beta-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
BTG	ortho-biphenyl-2'-carboxyl N-acetyl-beta-galactosaminoside	modified	NGA		D	pyranose	beta	aldose

BWG	N-[5-[(1R)-1-hydroxyethyl]-1,3-thiazol-2-yl]-alpha-D-mannopyranosylamine	modified		D	pyranose	alpha	aldose
BXF	2-deoxy-2-fluoro-beta-D-xylopyranose	modified		D	pyranose	beta	aldose
BZD	N-[(phenylcarbonyl)carbamoyl]-beta-D-glucopyranosylamine	modified		D	pyranose	beta	aldose
C3B	4-amino-1-beta-D-glucopyranosylpyrimidin-2(1H)-one	modified		D	pyranose	beta	aldose
C3G	4-nitrophenyl beta-D-glucopyranosiduronic acid	modified	BDP	D	pyranose	beta	aldose
C3X	(2R)-oxiran-2-ylmethyl beta-D-xylopyranoside	modified	XYP	D	pyranose	beta	aldose
C4B	1-beta-D-glucopyranosyl-1,3,5-triazinane-2,4,6-trione	modified		D	pyranose	beta	aldose
C4W	1-azido-beta-N-acetyl-D-glucosamine	modified		D	pyranose	beta	aldose
C5X	3-[(2R)-oxiran-2-yl]propyl beta-D-xylopyranoside	modified	XYP	D	pyranose	beta	aldose
CBF	(2R,3R,4S,5S,6R)-2,3,4,5-tetrahydroxy-6-(hydroxymethyl)oxane-2-carboxamide	modified		D	pyranose	alpha	ketose
CDR	(2R,5S,6R)-6-methyltetrahydro-2H-pyran-2,5-diol	modified		D	pyranose	beta	aldose
CEG	4,6-O-[(1S)-1-carboxyethylidene]-beta-D-glucopyranose	modified	BGC	D	pyranose	beta	aldose
CEZ	4-O-beta-D-glucopyranosyl-D-gluconic acid	modified	BGC	D	pyranose	beta	aldose
CGF	C-(1-AZIDO-ALPHA-D-GLUCOPYRANOSYL) FORMAMIDE	modified		D	pyranose		aldose
CJB	1-beta-D-glucopyranosylpyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
CKB	1-beta-D-glucopyranosyl-5-methylpyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
CKP	6-O-phosphono-beta-D-psicofuranosonic acid	modified	PSV	D	furanose	alpha	ketose
CNP	2-propenyl-N-acetyl-neuraminic acid	modified		D	pyranose		ketose
CR1	N-(methoxycarbonyl)-beta-D-glucopyranosylamine	modified		D	pyranose	beta	aldose
CR6	1-DEOXY-1-ACETYLAMINO-BETA-D-GLUCO-2-HEPTULOPYRANOSONAMIDE	modified		D	pyranose	beta	aldose
CRA	1-DEOXY-1-METHOXYCARBAMIDO-BETA-D-GLUCO-2-HEPTULOPYRANOSONAMIDE	modified		D	pyranose	beta	aldose
D1M	5-ethynyl-1-(beta-D-glucopyranosyl)pyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
D5E	paromamine	modified	PA1	D	pyranose	alpha	aldose
D6G	2-deoxy-6-O-phosphono-alpha-D-glucopyranose	modified		D	pyranose	alpha	aldose
DAF	4,6-dideoxy-4-[[[(1S,5R,6S)-3-formyl-5,6-dihydroxy-4-oxocyclohex-2-en-1-yl]amino]-alpha-D-xylo-hex-5-enopyranose	modified		D	pyranose	alpha	aldose
DAG	4-amino-4,6-dideoxy-beta-D-glucopyranose	modified		D	pyranose	beta	aldose
DAN	2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID	modified		D	dihydropyran		ketose
DDL	2,6-dideoxy-beta-D-galactopyranose	modified		D	pyranose	beta	aldose
DEG	butyl alpha-D-mannopyranoside	modified	MAN	D	pyranose	alpha	aldose
DFR	3-deoxy-3-methyl-beta-D-fructofuranose	modified		D	furanose	beta	ketose
DFX	1,5-anhydro-2-deoxy-2-fluoro-D-xylitol	modified		D	pyranose		aldose
DGO	D-glucal	modified		D	dihydropyran		aldose
DGS	3,6-anhydro-2-O-sulfo-alpha-D-galactopyranose	modified		D	pyranose	alpha	aldose
DJB	3-O-acetyl-2-acetamido-2-deoxy-alpha-D-galactopyranuronic acid	modified		D	pyranose	alpha	aldose
DJE	2-acetamido-2-deoxy-alpha-D-galactopyranuronic acid	modified		D	pyranose	alpha	aldose
DK4	1-(3-deoxy-3-fluoro-beta-D-glucopyranosyl)-5-fluoropyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
DKX	1-(3-deoxy-3-fluoro-beta-D-glucopyranosyl)pyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
DKZ	4-amino-1-(3-deoxy-3-fluoro-beta-D-glucopyranosyl)pyrimidin-2(1H)-one	modified		D	pyranose	beta	aldose
DL6	N-(azidoacetyl)-beta-D-glucopyranosylamine	modified		D	pyranose	beta	aldose
DLF	2-deoxy-alpha-L-fucopyranose	modified		L	pyranose	alpha	aldose

DLG	hexyl 3-deoxy-beta-D-galactopyranoside	modified			D	pyranose	beta	aldose
DO8	3-deoxy-8-O-phosphono-alpha-D-manno-oct-2-ulopyranosonic acid	modified	KDO		D	pyranose	alpha	ketose
DPC	5-ACETYLAMINO-4-AMINO-6-(PHENETHYL-PROPYL-CARBAMOYL)-5,6-DIHYDRO-4H-PYRAN-2-CARBOXYLIC ACID	modified			L	dihydropyran		ketose
DRI	2,6-dideoxy-4-O-methyl-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
DSR	2,6-dideoxy-4-thio-beta-D-allopyranose	modified			D	pyranose	beta	aldose
DT6	2,4-bisacetamido-2,4-dideoxy-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
DVC	(2R,4S,6S)-4-azanyl-4,6-dimethyl-oxane-2,5,5-triol	modified			L	pyranose	alpha	aldose
DYM	(2R)-2,3-dihydroxypropyl 2-acetamido-2,4-dideoxy-alpha-L-threo-hex-4-enopyranosiduronic acid	modified			L	dihydropyran	alpha	ketose
E3M	(1R)-4-acetamido-3-amino-1,5-anhydro-2,3,4-trideoxy-1-sulfo-D-glycero-D-galacto-octitol	modified			D	pyranose		aldose
E5G	5-hydroxypentyl alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose
EAG	2-aminoethyl 2-acetamido-2-deoxy-beta-D-glucopyranoside	modified	NAG		D	pyranose	beta	aldose
EBG	2-[(2S)-oxiran-2-yl]ethyl alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose
EBQ	(3S)-3-hydroxybutyl alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose
EEN	2-deoxy-2-[(difluoroacetyl)amino]-alpha-D-galactopyranose	modified	A2G		D	pyranose	alpha	aldose
EEQ	2-deoxy-2-[(fluoroacetyl)amino]-alpha-D-galactopyranose	modified	A2G		D	pyranose	alpha	aldose
EGA	ethyl beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
EMP	2,4-dideoxy-4-(ethylamino)-3-O-methyl-alpha-L-threo-pentopyranose	modified			L	pyranose	alpha	aldose
EMZ	6-O-methyl-beta-D-galactopyranose	modified	GAL		D	pyranose	beta	aldose
EPG	(2R)-oxiran-2-ylmethyl alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose
EQP	(1R)-4-acetamido-1,5-anhydro-2,4-dideoxy-1-phosphono-D-glycero-D-galacto-octitol	modified			D	pyranose		ketose
EQV	Loganic acid	modified			D	pyranose	beta	aldose
ERE	4-epi-vancosamine	modified			L	pyranose	alpha	aldose
ERI	3-C-methyl-4-O-acetyl-alpha-L-Olivopyranose	modified	RAE		L	pyranose	alpha	aldose
ETT	5-acetamido-2,6-anhydro-3,5-dideoxy-3-[(2E)-3-(4-methylphenyl)prop-2-en-1-yl]-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
F1P	1-O-phosphono-beta-D-fructopyranose	modified	BDF		D	pyranose	beta	ketose
F1X	1-O-phosphono-beta-D-fructofuranose	modified	FRU		D	furanose	beta	ketose
F55	N-[(4-chlorophenyl)carbonyl]carbamoyle-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
F58	N-[(cyclohexylcarbonyl)carbamoyle]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
F6P	6-O-phosphono-beta-D-fructofuranose	modified	FRU		D	furanose	beta	ketose
FBP	1,6-di-O-phosphono-beta-D-fructofuranose	modified	FRU		D	furanose	beta	ketose
FDP	2,6-di-O-phosphono-beta-D-fructofuranose	modified	FRU		D	furanose	beta	ketose
FDQ	2,5-anhydro-1-deoxy-1-phosphono-6-O-phosphono-D-glucitol	modified			D	furanose		
FFX	(2R,3S,5R,6S)-2,6-DIFLUOROOXANE-3,4,5-TRIOLE	modified			D	pyranose		
FIF	2,6-anhydro-5-deoxy-5-fluoro-L-idonic acid	modified			L	pyranose		aldose
FK9	3-(propylsulfanyl)propyl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
FKD	3-deoxy-3-fluoro-D-erythro-alpha-L-manno-non-2-ulopyranosonic acid	modified			L	pyranose	alpha	ketose
FMF	2-deoxy-2-fluoro-beta-D-mannopyranosyl fluoride	modified			D	pyranose		aldose
FNG	5-aminocarbonyl-3-nitrophenyl alpha-D-galactopyranoside	modified	GLA		D	pyranose	alpha	aldose
FSA	1-S-(carboxymethyl)-1-thio-beta-D-fructopyranose	modified			D	pyranose	beta	ketose

FSI	5-acetamido-3,5-dideoxy-3-fluoro-D-erythro-alpha-L-mannono-2-ulopyranosonic acid	modified	SLB		D	pyranose	beta	ketose
FSR	(2S,3S,4R,5R,6R)-5-acetamido-2,3-bis(fluoranyl)-4-oxidanyl-6-[(1S,2S)-1,2,3-tris(oxidanyl)propyl]oxane-2-carboxylic acid	modified			L	pyranose		ketose
FSW	methyl 6-deoxy-2-Se-methyl-2-seleno-alpha-L-galactopyranoside	modified			L	pyranose	alpha	aldose
FUF	2-deoxy-2-fluoro-beta-L-fucopyranose	modified			L	pyranose	beta	aldose
FUY	beta-L-fucosyl-azide	modified			L	pyranose	beta	aldose
FVQ	3-(pyridin-3-yl)prop-2-yn-1-yl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
FX1	beta-D-threo-hexo-2,4-diulo-2,5-furanose	modified			D	furanose	beta	ketose
FYJ	phenyl 1-thio-beta-D-glucopyranosiduronic acid	modified			D	pyranose	beta	aldose
G0S	3-(beta-D-galactopyranosylthio)propanoic acid	modified			D	pyranose	beta	aldose
G16	1,6-di-O-phosphono-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
G1P	1-O-phosphono-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
G20	5-N-acetyl-4-guanidino-6-methyl(propyl) carboxamide-4,5-dihydro-2H-pyran-2-carboxylic acid	modified			L	dihydropyran		ketose
G28	5-N-acetyl-4-amino-6-diethyl carboxamide-4,5-dihydro-2H-pyran-2-carboxylic acid	modified			L	dihydropyran		ketose
G2F	2-deoxy-2-fluoro-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
G3F	3-deoxy-3-fluoro-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
G4D	4-deoxy-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
G4S	4-O-sulfo-beta-D-galactopyranose	modified	GAL		D	pyranose	beta	aldose
G6P	6-O-phosphono-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
G6S	6-O-sulfo-beta-D-galactopyranose	modified	GAL		D	pyranose	beta	aldose
G7P	6,7-dideoxy-7-phosphono-beta-D-gluco-heptopyranose	modified			D	pyranose	beta	aldose
G8Z	prop-2-en-1-yl 4-O-methyl-alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
GAA	3-nitrophenyl alpha-D-galactopyranoside	modified	GLA		D	pyranose	alpha	aldose
GAD	2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid	modified			L	dihydropyran		aldose
GAF	2-deoxy-2-fluoro-alpha-D-galactopyranose	modified			D	pyranose	alpha	aldose
GAT	4-aminophenyl alpha-D-galactopyranoside	modified	GLA		D	pyranose	alpha	aldose
GBH	2-{4-[2-(beta-D-glucopyranosyloxy)ethyl]piperazin-1-yl}ethanesulfonic acid	modified	BGC		D	pyranose	beta	aldose
GC1	2,6-anhydro-L-gulonic acid	modified			D	pyranose		aldose
GC4	4-deoxy-beta-D-glucopyranuronic acid	modified			D	pyranose	beta	aldose
GC9	2,6-anhydro-3,5-dideoxy-5-[(hydroxyacetyl)amino]-D-glycero-L-altro-non-2-enonic acid	modified			L	dihydropyran		ketose
GCB	(2S,3S,4S,5R)-3,4,5-trihydroxy-6-oxo-oxane-2-carboxylic acid	modified			D	pyranose		aldose
GCD	4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid	modified			L	dihydropyran	alpha	aldose
GCN	2-amino-2,3-dideoxy-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
GCT	2,6-anhydro-3-deoxy-L-xylo-hexonic acid	modified			D	pyranose		aldose
GCV	4-O-methyl-alpha-D-glucopyranuronic acid	modified	GCU		D	pyranose	alpha	aldose
GCW	4-O-methyl-beta-D-glucopyranuronic acid	modified	BDP		D	pyranose	beta	aldose
GDA	4-amino-4-deoxy-beta-D-glucopyranose	modified			D	pyranose	alpha	aldose
GDL	2-(acetylamido)-2-deoxy-D-glucono-1,5-lactone	modified			D	pyranose		aldose
GE1	2,6-diamino-2,3,4,6-tetradeoxy-alpha-D-erythro-hexopyranose	modified			D	pyranose	alpha	aldose
GE3	3-deoxy-4-C-methyl-3-(methylamino)-beta-L-arabinopyranose	modified			L	pyranose	beta	aldose
GFP	2-deoxy-2-fluoro-1-O-phosphono-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
GL1	1-O-phosphono-alpha-D-galactopyranose	modified	GLA		D	pyranose	alpha	aldose

GL2	(5S,7R,8S,9S,10R)-3-amino-8,9,10-trihydroxy-7-(hydroxymethyl)-6-oxa-1,3-diazaspiro[4.5]decane-2,4-dione	modified		D	pyranose		aldose
GL4	(5S,7R,8S,9S,10R)-8,9,10-trihydroxy-7-(hydroxymethyl)-2-thio-6-oxa-1,3-diazaspiro[4.5]decan-4-one	modified		D	pyranose		aldose
GL5	(5S,7R,8S,9S,10R)-3,8,9,10-tetrahydroxy-7-(hydroxymethyl)-6-oxa-1,3-diazaspiro[4.5]decane-2,4-dione	modified		D	pyranose		aldose
GL6	N-(dimethoxyphosphoryl)-beta-D-glucopyranosylamine	modified		D	pyranose	beta	aldose
GL7	8,9,10-TRIHYDROXY-7-HYDROXYMETHYL-3-METHYL-6-OXA-1,3-DIAZA-SPIRO[4.5]DECANE-2,4-DIONE	modified		D	pyranose		aldose
GL9	N-[(5S,7R,8S,9S,10R)-8,9,10-trihydroxy-7-(hydroxymethyl)-2,4-dioxo-6-oxa-1,3-diazaspiro[4.5]dec-3-yl]acetamide	modified		D	pyranose		aldose
GLD	4,6-dideoxy-alpha-D-xyllo-hexopyranose	modified		D	pyranose	alpha	aldose
GLF	alpha-D-glucopyranosyl fluoride	modified		D	pyranose		aldose
GLG	ALPHA-D-GLUCOPYRANOSYL-2-CARBOXYLIC ACID AMIDE	modified		D	pyranose		
GLP	2-amino-2-deoxy-6-O-phosphono-alpha-D-glucopyranose	modified	PA1	D	pyranose	alpha	aldose
GLS	BETA-D-GLUCOPYRANOSE SPIROHYDANTOIN	modified		D	pyranose	beta	aldose
GLT	5-thio-alpha-D-glucopyranose	modified		D	thiopyranose	alpha	aldose
GM0	4-O-phosphono-L-glycero-alpha-D-manno-heptopyranose	modified	GMH	D	pyranose	alpha	aldose
GMB	1,7-di-O-phosphono-L-glycero-beta-D-manno-heptopyranose	modified		D	pyranose	beta	aldose
GMT	(2S)-2-[[2-acetamido-2-deoxy-alpha-D-glucopyranosyl]oxy]butanedioic acid	modified	NDG	D	pyranose	alpha	aldose
GMZ	1,7-di-O-phosphono-D-glycero-beta-D-manno-heptopyranose	modified		D	pyranose	beta	aldose
GN1	2-acetamido-2-deoxy-1-O-phosphono-alpha-D-glucopyranose	modified	NDG	D	pyranose	alpha	aldose
GN4	2-acetamido-2-deoxy-4-O-phosphono-beta-D-glucopyranose	modified	BM7	D	pyranose	beta	aldose
GNS	2-deoxy-2-(sulfoamino)-alpha-D-glucopyranose	modified	PA1	D	pyranose	alpha	aldose
GNX	2-deoxy-3-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose	modified	PA1	D	pyranose	alpha	aldose
GP0	5-fluoro-1-[3-C-(hydroxymethyl)-beta-D-glucopyranosyl]pyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
GP1	2-amino-2-deoxy-1-O-phosphono-alpha-D-glucopyranose	modified	PA1	D	pyranose	alpha	aldose
GP4	2-amino-2-deoxy-4-O-phosphono-alpha-D-glucopyranose	modified		D	pyranose	alpha	aldose
GPH	4-O-phosphono-D-glycero-beta-D-manno-heptopyranose	modified		D	pyranose	beta	aldose
GPK	5-fluoro-1-(beta-D-glucopyranosyl)pyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
GPM	(1S)-1,5-anhydro-1-(phosphonomethyl)-D-glucitol	modified		D	pyranose		aldose
GPQ	5-chloro-1-(beta-D-glucopyranosyl)pyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
GPU	5-bromo-1-(beta-D-glucopyranosyl)pyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
GPV	1-(beta-D-glucopyranosyl)-5-iodopyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
GPW	1-(beta-D-glucopyranosyl)-5-(trifluoromethyl)pyrimidine-2,4(1H,3H)-dione	modified		D	pyranose	beta	aldose
GQ1	4-O-sulfo-alpha-D-glucopyranose	modified	GLC	D	pyranose	alpha	aldose
GRF	5-O-phosphono-beta-D-ribofuranosylamine	modified		D	furanose	beta	aldose
GRX	(1R)-1,5-anhydro-1-[(S)-fluoro(phosphono)methyl]-D-glucitol	modified		D	pyranose		
GS1	1-thio-beta-D-glucopyranose	modified		D	pyranose	beta	aldose
GS9	naphthalen-2-yl 1-thio-beta-D-galactopyranoside	modified		D	pyranose	beta	aldose
GTM	methyl 4-thio-beta-D-glucopyranoside	modified		D	pyranose	beta	aldose
GU0	2,3,6-tri-O-sulfonato-beta-D-glucopyranose	modified	BGC	D	pyranose	beta	aldose
GU1	2,3-di-O-methyl-beta-D-glucopyranuronic acid	modified	BDP	D	pyranose	beta	aldose
GU2	2,3-di-O-methyl-alpha-L-idopyranuronic acid	modified	ZOF	L	pyranose	alpha	aldose
GU3	methyl 3-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranoside	modified	GLC	D	pyranose	alpha	aldose

GU4	2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
GU5	2,3-di-O-methyl-6-O-sulfonato-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
GU6	2,3,6-tri-O-sulfo-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
GU8	2,3,6-tri-O-methyl-beta-D-glucopyranose	modified	BGC		D	pyranose	beta	aldose
GU9	2,3,6-tri-O-methyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
GUF	2-deoxy-2-fluoro-beta-D-glucopyranuronic acid	modified			D	pyranose	beta	aldose
GUL	(2R,3S,4R,5S)-2,6-difluoro-2-(hydroxymethyl)oxane-3,4,5-triol	modified			L	pyranose		aldose
GUZ	2-deoxy-2-fluoro-alpha-D-glucopyranuronic acid	modified			D	pyranose	alpha	aldose
GYG	(1R)-4-acetamido-1,5-anhydro-3-carbamimidamido-2,3,4-trideoxy-1-sulfo-D-glycero-D-galacto-octitol	modified			D	pyranose	beta	ketose
GYP	methyl alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose
GYU	2-acetamido-2-deoxy-1-O-(propylcarbamoyl)-alpha-D-glucopyranose	modified	PA1		D	pyranose	alpha	aldose
GYV	2-acetamido-1-O-carbamoyl-2-deoxy-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
H1M	methyl 2-deoxy-2-(2-hydroxyethyl)-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
H2P	1-deoxy-2-O-phosphono-alpha-D-gluco-hept-2-ulopyranose	modified	GLC		D	pyranose	alpha	aldose
H53	(1S)-1,5-anhydro-1-(2,5-dihydroxyphenyl)-D-glucitol	modified			D	pyranose		aldose
H6Q	2-O-[(R)-{[(2S)-1,1-dihydroxypropan-2-yl]oxy}(hydroxy)phosphoryl]-beta-D-glucopyranose	modified	BGC		D	pyranose	beta	aldose
H6Z	2-O-[(R)-{[(2S)-1,1-dihydroxypropan-2-yl]oxy}(hydroxy)phosphoryl]-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
HBZ	N-[[4-(4-hydroxyphenyl)carbonyl]carbamoyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
HD4	4-O-[2-acetamido-2-deoxy-beta-D-glucopyranosyl]-1-O-phosphono-D-ribitol	modified	NAG		D	pyranose	beta	aldose
HNV	3-(4-methoxyphenyl)prop-2-yn-1-yl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
HNW	4-(3-hydroxyprop-1-yn-1-yl)phenyl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
HSG	octyl alpha-L-altropyranoside	modified	Z6H		L	pyranose	alpha	aldose
HSH	octyl beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
HSJ	octyl beta-L-talopyranoside	modified	ZEE		L	pyranose	beta	aldose
HSX	5-O-phosphono-alpha-D-ribofuranose	modified	RIB		D	furanose	alpha	aldose
HTG	heptyl 1-thio-beta-D-glucopyranoside	modified			D	pyranose	beta	aldose
HTM	3-hydroxypropyl 2-acetamido-2,4-dideoxy-alpha-L-threo-hex-4-enopyranosiduronic acid	modified			L	dihydropyran	alpha	ketose
I57	2,6-anhydro-3,4,5-trideoxy-5-[(2-methylpropanoyl)amino]-4-(4-phenyl-1H-1,2,3-triazol-1-yl)-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
IDC	(5R,6R,7R,8S)-7,8-dihydroxy-5-(hydroxymethyl)-5,6,7,8-tetrahydroimidazo[1,2-a]pyridin-6-yl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
IDF	5-fluoro-alpha-L-idopyranosyluronic acid fluoride	modified			L	pyranose		aldose
IDG	2,6-diamino-2,6-dideoxy-beta-L-idopyranose	modified			L	pyranose	beta	aldose
IDS	2-O-sulfo-alpha-L-idopyranuronic acid	modified	IDR		L	pyranose	alpha	aldose
IDU	2-O-sulfo-beta-L-altropyranuronic acid	modified	3MK		L	pyranose	beta	aldose
IDX	2-O-sulfo-alpha-L-gulopyranuronic acid	modified	LGU		L	pyranose	alpha	aldose
IDY	1-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid	modified	IDR		L	pyranose	alpha	aldose
IEM	2-methylpropyl 2-acetamido-2,4-dideoxy-alpha-L-threo-hex-4-enopyranosiduronic acid	modified			L	dihydropyran	alpha	ketose
IN1	4-(beta-D-glucopyranosyloxy)-2,2-dihydroxybutyl propanoate	modified	BGC		D	pyranose	beta	aldose
IPT	1-methylethyl 1-thio-beta-D-galactopyranoside	modified			D	pyranose	beta	aldose
ISD	ISOASCORBIC ACID	modified			D	dihydrofuran		aldose
ISL	6-O-alpha-D-glucopyranosyl-D-fructose	modified	GLC		D	pyranose	alpha	aldose

ISX	(3R,4R,5R)-4-hydroxy-5-(hydroxymethyl)piperidin-3-yl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
IXD	4-deoxy-2-O-sulfo-beta-D-erythro-hex-4-enopyranuronic acid	modified			D	dihydropyran	beta	ketose
J5B	(3R)-3-hydroxybutyl alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose
JFZ	4-nitrophenyl 6-deoxy-alpha-L-galactopyranoside	modified	FUC		L	pyranose	alpha	aldose
JHM	2-deoxy-6-O-sulfo-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
JLT	3,7-anhydro-1,2,8-trideoxy-1,8-diphosphono-D-glycero-D-gulo-octitol	modified			D	pyranose		
JS2	5-O-[[[(R)-[[[(S)-[4-(8-amino-6-oxo-1,6-dihydro-9H-purin-9-yl)butoxy](hydroxy)phosphoryl]oxy](hydroxy)phosphoryl]-alpha-D-ribofuranose	modified	RIB		D	furanose	alpha	aldose
JV4	6-deoxy-6-fluoro-1-O-phosphono-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
JVA	2,6-anhydro-5,7-dideoxy-5-fluoro-7-phosphono-D-glycero-D-manno-heptitol	modified			D	pyranose		
JVS	1-deoxy-1-fluoro-2-O-phosphono-alpha-D-gluco-hept-2-ulopyranose	modified	GLC		D	pyranose	alpha	aldose
JZR	hexyl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
K5B	4,7-anhydro-3-deoxy-D-gluco-oct-2-ulosonic acid	modified			D	furanose		
K99	(2R,3R,4R,5R,6S)-2,3-bis(fluoranyl)-4,5-bis(oxidanyl)-6-[[[(1R,2R)-1,2,3-tris(oxidanyl)propyl]oxane-2-carboxylic acid	modified			D	pyranose		ketose
KBA	2-(1H-1,2,3-triazol-1-yl)ethyl 6-deoxy-alpha-L-galactopyranoside	modified	FUC		L	pyranose	alpha	aldose
KBG	beta-D-arabino-hexopyranos-2-ulose	modified			D	pyranose	beta	aldose
KD5	4,7-anhydro-3-deoxy-D-manno-oct-2-ulosonic acid	modified			D	furanose		
KDA	prop-2-en-1-yl 3-deoxy-alpha-D-manno-oct-2-ulopyranosidonic acid	modified	KDO		D	pyranose	alpha	ketose
KDB	3,4,5-trideoxy-alpha-D-erythro-oct-3-en-2-ulopyranosonic acid	modified			D	dihydropyran	alpha	ketose
KDD	2,6-anhydro-3,5-dideoxy-D-ribo-oct-2-enonic acid	modified			D	dihydropyran		ketose
KDE	prop-2-en-1-yl 3-deoxy-beta-L-gulo-oct-2-ulopyranosidonic acid	modified			D	pyranose	alpha	ketose
KDF	3-deoxy-alpha-D-erythro-hex-2-ulofuranosonic acid	modified			D	furanose	alpha	ketose
KDR	prop-2-en-1-yl 3-deoxy-alpha-D-manno-octos-2-ulopyranoside	modified			D	pyranose	alpha	ketose
KFN	2,6-anhydro-3-deoxy-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
KG1	propadienyl 6-deoxy-alpha-L-galactopyranoside	modified	FUC		L	pyranose	alpha	aldose
KGM	heptyl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
KHP	4-nitrophenyl alpha-L-arabinofuranoside	modified	AHR		L	furanose	alpha	aldose
KME	(1E)-prop-1-en-1-yl 3-deoxy-7-O-methyl-alpha-D-manno-oct-2-ulopyranosidonic acid	modified	KDO		D	pyranose	alpha	ketose
KO1	D-glycero-alpha-D-talo-oct-2-ulopyranosonic acid	modified			D	pyranose	alpha	ketose
KO2	prop-2-en-1-yl D-glycero-alpha-D-talo-oct-2-ulopyranosidonic acid	modified	KDO		D	pyranose	alpha	ketose
KOT	1-beta-D-glucopyranosyl-4-phenyl-1H-1,2,3-triazole	modified			D	pyranose	beta	aldose
KTU	prop-2-en-1-yl 3,5-dideoxy-alpha-D-threo-oct-5-en-2-ulopyranosidonic acid	modified			D	dihydropyran	alpha	ketose
L6S	6-O-sulfo-alpha-L-galactopyranose	modified	GXL		L	pyranose	alpha	aldose
LAH	2-O-[(R)-hydroxy(propan-2-yloxy)phosphoryl]-alpha-L-arabinopyranose	modified	ARA		L	pyranose	alpha	aldose
LAO	2-O-phosphono-alpha-L-arabinopyranose	modified	ARA		L	pyranose	alpha	aldose
LCN	1,5-anhydro-D-arabino-hex-1-enitol	modified			D	dihydropyran		aldose
LEC	4-nitrophenyl 2-acetamido-2-deoxy-beta-D-glucopyranoside	modified	NAG		D	pyranose	beta	aldose
LGC	D-glucono-1,5-lactone	modified			D	pyranose		aldose
LKA	5-thio-alpha-D-mannopyranosylamine	modified			D		alpha	aldose
LKS	N-[(1Z)-2-phenylethanimidoyl]-5-thio-alpha-D-mannopyranosylamine	modified			D	thiopyranose	alpha	aldose

LNV	5-acetamido-2,6-anhydro-4-carbamimidamido-3,4,5-trideoxy-7-O-methyl-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
LOG	N-acetylglucosaminono-1,5-lactone (Z)-oxime	modified			D	pyranose		aldose
LOX	(2Z,3S,4S,5R)-2-hydroxyiminopiperidine-3,4,5-triol	modified			D			aldose
LRH	6-deoxy-beta-L-fructofuranose	modified			L	furanose	beta	ketose
LVO	5-acetamido-2,6-anhydro-4-carbamimidamido-3,4,5-trideoxy-7-O-methyl-9-O-octanoyl-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
LVZ	propan-2-yl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside	modified			D	pyranose	alpha	aldose
LZ0	[1-(2-oxoethyl)-1H-1,2,3-triazol-5-yl]methyl 6-deoxy-alpha-L-galactopyranoside	modified	FUC		L	pyranose	alpha	aldose
M1P	1-O-phosphono-alpha-D-mannopyranose	modified	MAN		D	pyranose	alpha	aldose
M2F	2,4-dinitrophenyl 2-deoxy-2-fluoro-beta-D-mannopyranoside	modified			D	pyranose	beta	aldose
M3N	4-(hydroxymethyl)-1-(alpha-D-mannopyranosyl)-1H-1,2,3-triazole	modified			D	pyranose	alpha	aldose
M55	benzyl alpha-D-glucopyranuronate	modified	GCU		D	pyranose	alpha	aldose
M6D	6-O-phosphono-beta-D-mannopyranose	modified	BMA		D	pyranose	beta	aldose
M6P	6-O-phosphono-alpha-D-mannopyranose	modified	MAN		D	pyranose	alpha	aldose
M7B	7-O-phosphono-D-glycero-beta-D-manno-heptopyranose	modified			D	pyranose	beta	aldose
M7P	7-O-phosphono-D-glycero-alpha-D-manno-heptopyranose	modified	289		D	pyranose	alpha	aldose
M8C	methyl alpha-D-galactopyranuronate	modified	ADA		D	pyranose	alpha	aldose
MA1	1,4-dithio-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
MA2	4-S-methyl-4-thio-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
MA3	methyl 4-thio-alpha-D-glucopyranoside	modified			D	pyranose	alpha	aldose
MA8	(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl 2-(L-cysteinylamino)-2-deoxy-alpha-D-glucopyranoside	modified	NDG		D	pyranose	alpha	aldose
MAF	2-deoxy-2-fluoro-alpha-D-mannopyranose	modified			D	pyranose	alpha	aldose
MAG	methyl 2-acetamido-2-deoxy-beta-D-glucopyranoside	modified	NAG		D	pyranose	beta	aldose
MAT	2,4-dideoxy-3-O-methyl-4-(propan-2-ylamino)-alpha-L-threo-pentopyranose	modified			L	pyranose	alpha	aldose
MAW	4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid	modified			L	dihydropyran	alpha	aldose
MBE	4-nitrophenyl beta-D-mannopyranoside	modified	BMA		D	pyranose	beta	aldose
MBF	2-deoxy-2-fluoro-beta-D-mannopyranose	modified			D	pyranose	beta	aldose
MBG	methyl beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
MCU	methyl 4-O-methyl-beta-D-glucopyranuronate	modified	BDP		D	pyranose	beta	aldose
MDA	2,6-dideoxy-3-C-methyl-beta-D-ribo-hexopyranose	modified			D	pyranose	beta	aldose
MDP	N-carboxyl-N-methyl-beta-muramic acid	modified	MUR		D	pyranose	beta	aldose
MFB	methyl beta-L-fucopyranoside	modified	FUL		L	pyranose	beta	aldose
MFU	methyl alpha-L-fucopyranoside	modified	FUC		L	pyranose	alpha	aldose
MG5	2,3,4-tri-O-propanoyl-6-O-sulfamoyl-beta-D-glucopyranose	modified	BGC		D	pyranose	beta	aldose
MGC	methyl 2-acetamido-2-deoxy-alpha-D-galactopyranoside	modified	A2G		D	pyranose	alpha	aldose
MGL	methyl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
MGS	methyl 4,6-dideoxy-4-[[[(2R)-2,4-dihydroxybutanoyl]amino]-2-O-methyl-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
MJJ	methyl 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid	modified	SIA		D	pyranose	alpha	ketose
MM A	methyl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
MNO	methyl 3,5-dideoxy-5-[(hydroxyacetyl)amino]-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid	modified	SIA		D	pyranose	alpha	ketose

MNA	2-O-methyl-5-N-acetyl-alpha-D-neuraminic acid	modified	SIA		D	pyranose	alpha	ketose
MQG	2-deoxy-2-[[[(S)-hydroxy(methyl)phosphoryl]amino]-beta-D-glucopyranose	modified	GCS		D	pyranose	beta	aldose
MQT	methyl 2-O-acetyl-3-O-(4-methylbenzoyl)-beta-D-talopyranoside	modified	SDY		D	pyranose	beta	aldose
MRH	4-acetamido-4,6-dideoxy-alpha-D-mannopyranose	modified			D	pyranose	alpha	aldose
MRP	3-O-methyl-alpha-L-rhamnopyranose	modified	RAM		L	pyranose	alpha	aldose
MSX	methyl 1,6-dithio-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
MXY	2-O-methyl-beta-L-fucopyranose	modified	FUL		L	pyranose	beta	aldose
MXZ	2-O-methyl-alpha-L-fucopyranose	modified	FUC		L	pyranose	alpha	aldose
MYG	(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl 2-amino-2-deoxy-alpha-D-glucopyranoside	modified	PA1		D	pyranose	alpha	aldose
N1L	2-amino-2-deoxy-beta-D-glucopyranuronic acid	modified			D	pyranose	beta	aldose
NA1	2-acetamido-2-deoxy-6-O-methyl-alpha-D-allopyranose	modified			D	pyranose	alpha	aldose
NBG	N-acetyl-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
NBX	N-[[[(4-aminophenyl)carbonyl]carbamoyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
NBY	N-[[[(4-nitrophenyl)carbonyl]carbamoyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
NFG	2,4-dinitrophenyl 2-deoxy-2-fluoro-beta-D-glucopyranoside	modified			D	pyranose	beta	aldose
NG1	2-acetamido-2-deoxy-1-O-phosphono-alpha-D-galactopyranose	modified	A2G		D	pyranose	alpha	aldose
NG6	2-acetamido-2-deoxy-6-O-sulfo-beta-D-galactopyranose	modified	NGA		D	pyranose	beta	aldose
NGK	2-acetamido-2-deoxy-4-O-sulfo-alpha-D-galactopyranose	modified	A2G		D	pyranose	alpha	aldose
NGS	2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose	modified	NAG		D	pyranose	beta	aldose
NGY	2-acetamido-2-deoxy-6-O-sulfo-alpha-D-glucopyranose	modified	NDG		D	pyranose	alpha	aldose
NHF	1,5-anhydro-D-fructose	modified			D	pyranose		aldose
NM6	2-acetamido-3-O-[(2R)-1-amino-1-oxopropan-2-yl]-2-deoxy-beta-D-glucopyranose	modified	NAG		D	pyranose	beta	aldose
NM9	methyl 2-acetamido-3-O-[(2R)-1-amino-1-oxopropan-2-yl]-2-deoxy-beta-D-glucopyranoside	modified	NAG		D	pyranose	beta	aldose
NNG	2-deoxy-2-[[[(S)-hydroxy(methyl)phosphoryl]amino]-6-O-phosphono-alpha-D-glucopyranose	modified	PA1		D	pyranose	alpha	aldose
NPF	2-nitrophenyl beta-D-fucopyranoside	modified	FCB		D	pyranose	beta	aldose
NSQ	4-nitrophenyl alpha-D-6-sulfoquinovoside	modified	G6D		D	pyranose	alpha	aldose
NTF	N-(trifluoroacetyl)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
NXD	methyl 5-acetamido-9-[[amino(oxo)acetyl]amino]-3,5,9-trideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid	modified			D	pyranose	alpha	ketose
O1G	3-deoxy-3-[(E)-{(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methylidene)amino]-6-O-phosphono-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
OAK	N-(phenylcarbonyl)-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
OEL	(6R)-2,6-anhydro-3,4,5-trideoxy-6-[(2S)-2,3-dihydroxypropanoyl]-3-fluoro-5-[(2-methylpropanoyl)amino]-4-triaza-1,2-dien-2-ium-1-yl-L-gulonic acid	modified			L	pyranose		ketose
OI7	1,7-di-O-phosphono-beta-D-altro-hept-2-ulofuranose	modified			D	furanose	beta	ketose
OPM	pentyl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
OTG	2-deoxy-2-[[[(2-methylphenyl)carbonyl]amino]-alpha-D-glucopyranose	modified	PA1		D	pyranose	alpha	aldose
OTN	2-nitrophenyl 1-thio-beta-D-galactopyranoside	modified			D	pyranose	beta	aldose
OTU	3-O-alpha-D-glucopyranosyl-D-fructose	modified	GLC		D	pyranose	alpha	aldose
OX2	(1R)-1,5-anhydro-1-(5-methyl-1,3,4-oxadiazol-2-yl)-D-glucitol	modified			D	pyranose		aldose

P53	2-(hydroxymethyl)phenyl 6-O-phosphono-beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
P6P	6-O-phosphono-alpha-D-fructofuranose	modified	Z9N		D	furanose	alpha	ketose
PAV	(2R,4S)-2-methyl-2,3,4-tetrahydroxytetrahydrofuran	modified			L	furanose	alpha	ketose
PDX	2,3-di-O-sulfo-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
PH5	benzyl 3,5-dideoxy-5-(propanoylamino)-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid	modified	SIA		D	pyranose	alpha	ketose
PKM	4-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid	modified	SIA		D	pyranose	alpha	ketose
PNA	4-nitrophenyl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
PNG	4-nitrophenyl alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose
PNJ	4-nitrophenyl 2-amino-2-deoxy-beta-D-glucopyranoside	modified			D	pyranose	beta	aldose
PNW	4-nitrophenyl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
PPC	1-O-[(R)-hydroxy(phosphonomethyl)phosphoryl]-5-O-phosphono-alpha-D-ribofuranose	modified	RIB		D	furanose	alpha	aldose
PRP	1-O-pyrophosphono-5-O-phosphono-alpha-D-ribofuranose	modified	RIB		D	furanose	alpha	aldose
PSG	4-nitrophenyl 1-thio-beta-D-glucopyranoside	modified			D	pyranose	beta	aldose
PUF	6-deoxy-alpha-L-psicofuranose	modified			L	furanose	alpha	ketose
QIF	1-deoxy-7-O-phosphono-alpha-D-gluco-hept-2-ulopyranose	modified	GLC		D	pyranose	alpha	aldose
R1P	1-O-phosphono-alpha-D-ribofuranose	modified	RIB		D	furanose	alpha	aldose
R1X	1,4-anhydro-D-ribitol	modified			D	furanose		aldose
R2B	1,4-anhydro-D-erythro-pent-1-enitol	modified			D	dihydrofuran		aldose
R2G	2,5-anhydro-4-deoxy-D-erythro-pent-4-enitol	modified			L	dihydrofuran		aldose
RAO	methyl 6-deoxy-alpha-L-rhamnopyranoside	modified	RAM		L	pyranose	alpha	aldose
RER	vancosamine	modified			L	pyranose	alpha	aldose
RF5	2-deoxy-2-fluoro-5-O-phosphono-alpha-D-arabinofuranose	modified			D	furanose	alpha	aldose
RGG	(2R)-2,3-dihydroxypropyl beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
RHA	6-deoxy-1-O-phosphono-alpha-L-rhamnopyranose	modified	RAM		L	pyranose	alpha	aldose
RHC	(2S)-2-amino-4-[[[(2S,3S,4R,5R)-3,4,5-trihydroxyoxolan-2-yl]methylsulfanyl]butanoic acid	modified			D	furanose	beta	aldose
RI2	1,5-di-O-phosphono-alpha-D-ribofuranose	modified	RIB		D	furanose	alpha	aldose
RP3	3-deoxy-5-O-phosphono-beta-D-ribofuranose	modified			D	furanose	beta	aldose
RP5	5-O-phosphono-beta-D-ribofuranose	modified	BDR		D	furanose	beta	aldose
RP6	5-acetamido-2,6-anhydro-3,5-dideoxy-3-prop-2-en-1-yl-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
RR7	2-deoxy-beta-D-arabino-hexopyranose	modified			D	pyranose	beta	aldose
RRJ	4-chloro-4-deoxy-alpha-D-galactopyranose	modified			D	pyranose	alpha	aldose
RRY	1,6-dichloro-1,6-dideoxy-beta-D-fructofuranose	modified			D	furanose	beta	ketose
RST	3-amino-2,3,6-trideoxy-alpha-L-ribo-hexopyranose	modified			L	pyranose	alpha	aldose
RTG	6-O-phosphono-alpha-L-idopyranose	modified	ZOF		L	pyranose	alpha	aldose
RTV	2-(acetylamino)-1,5-anhydro-2-deoxy-D-mannitol	modified			D	pyranose		aldose
RUG	1-beta-D-glucopyranosyl-4-(hydroxymethyl)-1H-1,2,3-triazole	modified			D	pyranose	beta	aldose
RVG	6-deoxy-2,3-di-O-methyl-beta-D-glucopyranose	modified	YYK		D	pyranose	beta	aldose
RVM	4,6-dideoxy-2,3-di-O-methyl-alpha-D-xylo-hexopyranose	modified			D	pyranose	alpha	aldose
RWI	(2S)-2-[(2-deoxy-2-[(hydroxycarbamoyl)amino]-alpha-D-glucopyranosyl)oxy]butanedioic acid	modified	PA1		D	pyranose	alpha	aldose
RY7	4,6-dideoxy-4-[[[(1S,2S,3S,4R,5R)-2,3,4-trihydroxy-5-(hydroxymethyl)cyclohexyl]amino]-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
RZM	(2R,3R,4R,5R)-4-hydroxy-2,5-bis(hydroxymethyl)pyrrolidin-3-yl alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose

S7P	1-C-(hydroxymethyl)-6-O-phosphono-beta-D-alfrofuranose	modified			D	pyranose	beta	ketose
S81	(1R,2R,3S,4R,6S)-4,6-diamino-2,3-dihydroxycyclohexyl 2,6-diamino-2,4,6-trideoxy-4-fluoro-alpha-D-glucopyranoside	modified			D	pyranose	alpha	aldose
SA0	2-(hydroxymethyl)phenyl beta-D-glucopyranoside	modified	BGC		D	pyranose	beta	aldose
SCG	Secologanin	modified			D	pyranose	beta	aldose
SFJ	(2R,3R,4R,5R,6R)-5-acetamido-2,3-difluoro-4-hydroxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]tetrahydro-2H-pyran-2-carboxylic acid	modified			D	pyranose		ketose
SFU	methyl 1-seleno-alpha-L-fucopyranoside	modified			L	pyranose	alpha	aldose
SG4	3,4-di-O-acetyl-6-O-sulfamoyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
SG5	2,3,4-tri-O-propanoyl-6-O-sulfamoyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
SG6	4-O-acetyl-6-O-sulfamoyl-alpha-D-galactopyranose	modified	GLA		D	pyranose	alpha	aldose
SG7	3,4-di-O-acetyl-6-O-sulfamoyl-alpha-D-mannopyranose	modified	MAN		D	pyranose	alpha	aldose
SGA	3-O-sulfo-beta-D-galactopyranose	modified	GAL		D	pyranose	beta	aldose
SGC	4-thio-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
SGD	6-thio-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
SGN	2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose	modified	PA1		D	pyranose	alpha	aldose
SHB	methyl beta-D-galactopyranuronate	modified	GAL		D	pyranose	beta	aldose
SHG	2-deoxy-2-fluoro-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
SID	methyl 9-S-acetyl-5-acetamido-3,5-dideoxy-9-thio-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid	modified			D	pyranose	alpha	ketose
SIO	methyl 4,9-di-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosidonic acid	modified	SIA		D	pyranose	alpha	ketose
SIZ	2-deoxy-2-[(difluoroacetyl)amino]-beta-D-galactopyranose	modified	NGA		D	pyranose	beta	aldose
SLM	(2S,4S,5R,6R)-5-acetamido-2,4-dihydroxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]oxane-2-carboxamide	modified			D	pyranose	beta	ketose
SN5	2-deoxy-2-(ethanethiolamino)-beta-D-glucopyranose	modified	GCS		D	pyranose	beta	aldose
SNG	methyl 2-acetamido-2-deoxy-1-seleno-beta-D-glucopyranoside	modified			D	pyranose	beta	aldose
SOG	octyl 1-thio-beta-D-glucopyranoside	modified			D	pyranose	beta	aldose
SR1	5-S-methyl-5-thio-alpha-D-ribofuranose	modified			D	furanose	alpha	aldose
SSG	1,4-dithio-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
STZ	Streptozotocin	modified	GCS		D	pyranose	beta	aldose
SUS	2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose	modified	PA1		D	pyranose	alpha	aldose
SZZ	Sinigrin	modified			D	pyranose	alpha	aldose
T68	N-[(pyridin-2-ylcarbonyl)carbamoyl]-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
TA6	6-O-phosphono-beta-D-tagatofuranose	modified			D	furanose	beta	ketose
TEU	1-O-alpha-D-glucopyranosyl-D-fructose	modified	GLC		D	pyranose	alpha	aldose
TFU	methyl 1-seleno-beta-L-fucopyranoside	modified			L	pyranose	beta	aldose
TGA	2-sulfanylethyl beta-D-galactopyranoside	modified	GAL		D	pyranose	beta	aldose
TGK	1-deoxy-beta-L-tagatopyranose	modified			L	pyranose	beta	ketose
TGR	1-deoxy-alpha-D-xylo-hex-3-ulofuranose	modified			D	furanose	alpha	aldose
TGY	1-deoxy-alpha-D-tagatopyranose	modified			D	pyranose	alpha	ketose
TH1	(1R)-1,5-anhydro-1-(5-methyl-1,3-benzothiazol-2-yl)-D-glucitol	modified			D	pyranose		aldose
TMR	2,6-dideoxy-4-S-methyl-4-thio-beta-D-ribo-hexopyranose	modified			D	pyranose	beta	aldose
TMX	2-deoxy-2-(trimethylammonio)-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
TNX	1,5-anhydro-2-deoxy-2-(ethanethiolamino)-D-arabino-hex-1-enitol	modified			D	dihydropyran		aldose
TOA	3-ammonio-3-deoxy-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose

TOC	2,6-diammonio-2,3,6-trideoxy-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
TQY	6-O-octanoyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
TRV	6-O-octanoyl-beta-D-fructofuranose	modified	FRU		D	furanose	beta	ketose
TS8	2,3,4,6-tetra-O-acetyl-1-thio-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
TT7	4-O-phosphono-beta-D-fructofuranose	modified	FRU		D	furanose	beta	ketose
TTZ	N-[(3aS,4R,5S,6S,6aS)-4,5,6-trihydroxy-4-(hydroxymethyl)-4,5,6,6a-tetrahydro-3aH-cyclopenta[d][1,3]thiazol-2-yl]-alpha-D-glucopyranosylamine	modified			D	pyranose	alpha	aldose
TU4	3-O-octanoyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
TUG	3,4-di-O-sulfo-alpha-D-altropyranose	modified	SHD		D	pyranose	alpha	aldose
TUJ	1,2,3,4-tetra-O-sulfo-alpha-D-allopyranose	modified	AFD		D	pyranose	alpha	aldose
TUP	3-deoxy-3-fluoro-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
TVD	N-acetyl-2-(acetylamino)-2-deoxy-beta-D-glucopyranosylamine	modified			D	pyranose	beta	aldose
TVG	propyl beta-D-galactofuranoside	modified	GZL		D	pyranose	beta	aldose
TVM	3-O-[(3-methoxyphenyl)methyl]-beta-D-galactopyranose	modified	GAL		D	pyranose	beta	aldose
TVS	prop-2-en-1-yl 2-(acetylamino)-2-deoxy-beta-D-glucopyranoside	modified	NAG		D	pyranose	beta	aldose
TVV	3-O-prop-2-yn-1-yl-beta-D-galactopyranose	modified	GAL		D	pyranose	beta	aldose
TVY	(1S)-2-amino-1-phenylethyl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
TW7	2-deoxy-2,2-difluoro-alpha-D-arabino-hexopyranosyl fluoride	modified			D	pyranose		aldose
TWA	2,3,4-tri-O-sulfo-beta-D-altropyranose	modified			D	pyranose	beta	aldose
TWD	2,3-di-O-sulfo-alpha-L-glucopyranose	modified			L	pyranose	alpha	aldose
TWJ	1-thio-beta-D-talopyranose	modified			D	pyranose	beta	aldose
TWY	4-thio-beta-D-xylopyranose	modified			D	pyranose	beta	aldose
TXB	4-deoxy-4-thio-alpha-D-xylopyranose	modified			D	pyranose	alpha	aldose
U1Y	methyl 6-thio-beta-D-glucopyranoside	modified			D	pyranose	beta	aldose
U2A	methyl 2-thio-beta-D-glucopyranoside	modified			D	pyranose	beta	aldose
U2D	6-O-decanoyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
U8V	6-O-butanoyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
U97	2-O-sulfo-beta-L-galactopyranuronic acid	modified			L	pyranose	beta	aldose
U9A	[(2R,3R,4R,5R,6R)-2,4,5-trihydroxy-6-(sulfooxy)tetrahydro-2H-pyran-3-yl]sulfamic acid	modified				pyranose		aldose
U9D	4-deoxy-2,3,6-tri-O-methyl-alpha-D-xylo-hexopyranose	modified			D	pyranose	alpha	aldose
U9G	2,3-di-O-methyl-6-O-sulfo-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
U9J	(2R,3R,4S,5S,6R)-6-(dihydroxymethyl)-3,4-dimethoxytetrahydro-2H-pyran-2,5-diol	modified			L	pyranose	alpha	aldose
U9M	(2R,3R,4S,5S,6S)-6-(dihydroxymethyl)-3,4-dimethoxytetrahydro-2H-pyran-2,5-diol	modified			D	pyranose	beta	aldose
UAP	4-deoxy-2-O-sulfo-alpha-L-threo-hex-4-enopyranuronic acid	modified			L	dihydropyran	alpha	ketose
UDC	2-acetamido-3-O-[(2S,3S)-2-carboxy-3,4-dihydroxybutan-2-yl]-2-deoxy-alpha-D-glucopyranose	modified	NDG		D	pyranose	alpha	aldose
V3M	2-deoxy-2-fluoro-alpha-D-arabinofuranose	modified			D	furanose	alpha	aldose
V3P	4-iodophenyl 1,4-dithio-beta-D-glucopyranoside	modified			D	pyranose	beta	aldose
V71	(1R,2R,3S,4R,6S)-4,6-diamino-2,3-dihydroxycyclohexyl 2,6-diamino-2,4,6-trideoxy-4-fluoro-alpha-D-galactopyranoside	modified			D	pyranose	alpha	aldose
VG1	ALPHA-D-GLUCOSE-1-PHOSPHATE-6-VANADATE	modified	GLC		D	pyranose	alpha	aldose
VTB	7-O-phosphono-alpha-L-galacto-hept-2-ulopyranose	modified			L	pyranose	alpha	ketose
WIA	methyl 6-thio-beta-D-galactopyranoside	modified			D	pyranose	beta	aldose

WUN	2-amino-4-O-(4-chlorobenzyl)-2-deoxy-alpha-D-glucopyranose	modified	PA1		D	pyranose	alpha	aldose
X1P	1-O-phosphono-alpha-D-xylopyranose	modified	XYS		D	pyranose	alpha	aldose
X2F	2-deoxy-2-fluoro-alpha-D-xylopyranose	modified			D	pyranose	alpha	aldose
XDX	(2R)-2-(alpha-D-glucopyranosyloxy)-3-(phosphonoxy)propanoic acid	modified	GLC		D	pyranose	alpha	aldose
XGP	1-O-phosphono-beta-D-glucopyranose	modified	BGC		D	pyranose	beta	aldose
XIL	(3S,4R)-3-hydroxy-2-oxopiperidin-4-yl beta-D-xylopyranoside	modified	XYP		D	pyranose	beta	aldose
XM M	5-bromo-4-chloro-1H-indol-3-yl alpha-D-mannopyranoside	modified	MAN		D	pyranose	alpha	aldose
XXX	(1R,2R,3S,4R,6S)-4,6-diamino-2,3-dihydroxycyclohexyl 2,6-diamino-2,6-dideoxy-alpha-D-glucopyranoside	modified			D	pyranose	alpha	aldose
XYF	5(R)-fluoro-beta-D-xylopyranose	modified			D	pyranose	beta	aldose
YIO	1-thio-beta-D-galactopyranose	modified			D	pyranose	beta	aldose
YKR	2-amino-4-O-benzyl-2-deoxy-alpha-D-glucopyranose	modified	PA1		D	pyranose	alpha	aldose
YO5	(1R)-1,5-anhydro-1-(phosphonomethyl)-D-glucitol	modified			D	pyranose		
YX0	[(3E)-3-(1-hydroxyethylidene)-2,3-dihydroisoxazol-5-yl]methyl alpha-L-fucopyranoside	modified	FUC		L	pyranose	alpha	aldose
YX1	2-deoxy-2-[[2-hydroxy-1-methylhydrazino]carbonylamino]-beta-D-glucopyranose	modified			D	pyranose	beta	aldose
YYB	1,5-anhydro-3-O-methyl-2,6-di-O-sulfo-D-glucitol	modified			D	pyranose		aldose
YYH	7-deoxy-L-glycero-alpha-D-manno-heptopyranose	modified	MAN		D	pyranose	alpha	aldose
YYJ	1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose	modified	FRU		D	furanose	beta	ketose
YZ0	methyl beta-D-mannopyranoside	modified	BMA		D	pyranose	beta	aldose
Z15	(1S)-1,5-anhydro-1-(4-chloro-2,5-dihydroxyphenyl)-D-glucitol	modified			D	pyranose		aldose
Z16	(1S)-1,5-anhydro-1-(3-chloro-2,5-dihydroxyphenyl)-D-glucitol	modified			D	pyranose		aldose
Z2T	(1S)-1,5-anhydro-1-(3-chloro-2-hydroxy-5-methoxyphenyl)-D-glucitol	modified			D	pyranose		aldose
Z3K	(1S)-2,3,6-tri-O-acetyl-1,5-anhydro-1-sulfamoyl-D-glucitol	modified			D	pyranose	beta	aldose
Z3L	2,3,4,6-tetra-O-acetyl-beta-D-galactopyranose	modified	GAL		D	pyranose	beta	aldose
Z3Q	2-azidoethyl 2-acetamido-2-deoxy-beta-D-glucopyranoside	modified	NAG		D	pyranose	beta	aldose
Z4K	2-O-sulfo-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
Z4R	methyl 3-thio-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
Z4S	1,6-anhydro-N-acetyl-beta-D-glucopyranosamine	modified			D	pyranose	beta	aldose
Z4U	methyl 4-thio-alpha-D-xylopyranoside	modified			D	pyranose	alpha	aldose
Z4V	4-thio-beta-L-ribopyranose	modified			L	pyranose	beta	aldose
Z4Y	6-thio-alpha-D-mannopyranose	modified			D	pyranose	alpha	aldose
Z57	(1S)-1,5-anhydro-1-(4-bromo-2,5-dihydroxyphenyl)-D-glucitol	modified			D	pyranose		aldose
Z5L	methyl 2-thio-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
Z61	2-deoxy-alpha-D-arabino-hexopyranose	modified			D	pyranose	alpha	aldose
Z6W	(5R)-5-[(2R)-2-hydroxynonyl]-beta-D-xylulofuranose	modified			D	furanose	beta	ketose
Z9D	4-deoxy-beta-D-xylo-hexopyranose	modified			D	pyranose	beta	aldose
Z9E	1-thio-alpha-D-glucopyranose	modified			D	pyranose	alpha	aldose
Z9H	3,4-di-O-methyl-2,6-di-O-sulfo-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
Z9K	3-O-methyl-2-O-sulfo-alpha-L-idopyranuronic acid	modified	ZOF		L	pyranose	alpha	aldose
Z9L	methyl 2,3,6-tri-O-sulfo-alpha-D-glucopyranoside	modified	GLC		D	pyranose	alpha	aldose
Z9M	2-amino-2-deoxy-4-O-phosphono-beta-D-glucopyranose	modified	GCS		D	pyranose	beta	aldose
ZB0	2,3-di-O-methyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose

ZB1	3-O-methyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
ZB2	2-O-methyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
ZB3	2,6-di-O-methyl-alpha-D-glucopyranose	modified	GLC		D	pyranose	alpha	aldose
ZCZ	4,6-dideoxy-4-[[{(2R)-2,4-dihydroxybutanoyl]amino}-2-O-methyl-alpha-D-mannopyranose	modified			D	pyranose	alpha	aldose
ZD0	methyl 4,6-dideoxy-4-[[{(2R)-2,4-dihydroxybutanoyl]amino}-alpha-D-mannopyranoside	modified			D	pyranose	alpha	aldose
ZDC	3,7-anhydro-2,8-dideoxy-L-glycero-D-gluco-octonic acid	modified			D	pyranose		
ZDO	methyl 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranoside	modified	PA1		D	pyranose	alpha	aldose
ZEL	methyl beta-D-altropyranoside	modified			D	pyranose	beta	aldose
ZGE	5-acetamido-2,6-anhydro-4-carbamimidamido-3,4,5-trideoxy-3-fluoro-D-glycero-D-galacto-non-2-enonic acid	modified			D	dihydropyran		ketose
ZMR	ZANAMIVIR	modified			D	dihydropyran		ketose

Supplementary Table SII: Glycosylation Types in the PDB

Type	Site	Monosaccharide Symbols	CCD ID
N-Glycosylation	ASN	b-D-GlcpNAc	NAG
	ASN	b-D-Glcp	BGC
	ARG	b-D-GlcpNAc	NAG
O-Glycosylation	SER	a-D-GalpNAc	A2G
	SER	b-D-6-deoxy-GlcpNAc4NAc	B6D
	SER	b-D-Glcp	BGC
	SER	a-L-Fucp	FUC
	SER	a-D-Galp	GLA
	SER	a-D-Glcp	GLC
	SER	a-D-Manp	MAN
	SER	b-D-GlcpNAc	NAG
	THR	a-D-GalpNAc	A2G
	THR	a-L-Fucp	FUC
	THR	a-D-Glcp	GLC
	THR	a-D-Manp	MAN
	THR	b-D-GlcpNAc	NAG
	THR	a-D-GlcpNAc	NDG
	THR	b-D-GalpNAc	NGA
	TYR	b-D-Glcp	BGC
	TYR	a-D-Glcp	GLC
	TYR	a-D-GlcpNAc	NDG
S-Glycosylation	CYS	a-D-GalpNAc	A2G
	CYS	b-D-Glcp	BGC
	CYS	b-D-GlcpNAc	NAG
C-Mannosylation	TRP	a-D-Manp	MAN

Supplementary Table SIII: Blood Group Antigens in BIRD

BIRD ID	Molecule Name	Glycam Condensed Sequence	PDB ID
PRD_900129	Lewis A antigen, beta anomer	DGalpb1-3[LFucpa1-4]DGlcNACb1-ROH	3UET
PRD_900130	Lewis A antigen, alpha anomer	DGalpb1-3[LFucpa1-4]DGlcNAca1-ROH	4RM0
PRD_900119	Lewis X antigen, beta anomer	LFucpa1-3[DGalpb1-4]DGlcNACb1-ROH	2OX9
PRD_900120	Lewis X antigen, alpha anomer	LFucpa1-3[DGalpb1-4]DGlcNAca1-ROH	1SL6
PRD_900121	Sialyl-Lewis X antigen, beta anomer	DNeup5Aca2-3DGalpb1-4[LFucpa1-3]DGlcNACb1-ROH	2R61
PRD_900122	Sialyl-Lewis X antigen, alpha anomer	DNeup5Aca2-3DGalpb1-4[LFucpa1-3]DGlcNAca1-ROH	2RDG
PRD_900123	Lewis B antigen, beta anomer	LFucpa1-2DGalpb1-3[LFucpa1-4]DGlcNACb1-ROH	4GWJ
PRD_900085	Lewis B antigen, alpha anomer	LFucpa1-2DGalpb1-3[LFucpa1-4]DGlcNAca1-ROH	3LEK
PRD_900054	Lewis Y antigen, beta anomer	LFucpa1-2DGalpb1-4[LFucpa1-3]DGlcNACb1-ROH	4GWI
PRD_900124	Lewis Y antigen, alpha anomer	LFucpa1-2DGalpb1-4[LFucpa1-3]DGlcNAca1-ROH	1S3K
PRD_900049	H type 1 antigen, beta anomer	LFucpa1-2DGalpb1-3DGlcNACb1-ROH	1Z15
PRD_900036	H type 2 antigen, beta anomer	LFucpa1-2DGalpb1-4DGlcNACb1-ROH	1Z13
PRD_900125	H type 2 antigen, alpha anomer	LFucpa1-2DGalpb1-4DGlcNAca1-ROH	217M
PRD_900126	Blood group A Lewis B antigen, beta anomer	LFucpa1-2[DGalpNaca1-3]DGalpb1-3[LFucpa1-4]DGlcNACb1-ROH	5F7N
PRD_900127	Blood group A Lewis Y antigen, beta anomer	LFucpa1-2[DGalpNaca1-3]DGalpb1-4[LFucpa1-3]DGlcNACb1-ROH	2WMK
PRD_900128	Blood group A Lewis Y antigen, alpha anomer	LFucpa1-2[DGalpNaca1-3]DGalpb1-4[LFucpa1-3]DGlcNAca1-ROH	5ELE
PRD_900131	Blood group A H type 1 antigen, beta anomer	LFucpa1-2[DGalpNaca1-3]DGalpb1-3DGlcNACb1-ROH	3ASP
PRD_900132	Blood group A H type 2 antigen, beta anomer	LFucpa1-2[DGalpNaca1-3]DGalpb1-4DGlcNACb1-ROH	4DS0
PRD_900133	Blood group A H type 2 antigen, alpha anomer	LFucpa1-2[DGalpNaca1-3]DGalpb1-4DGlcNAca1-ROH	5XFD
PRD_900134	Blood group B H type 2 antigen, beta anomer	LFucpa1-2[DGalpa1-3]DGalpb1-4DGlcNACb1-ROH	2YGM

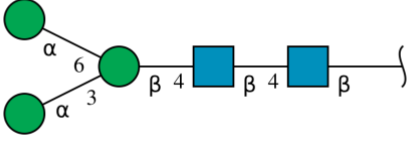
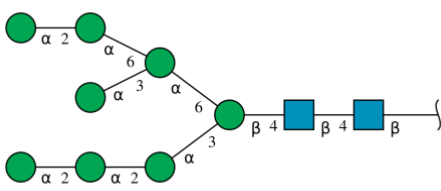
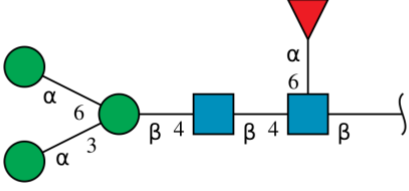
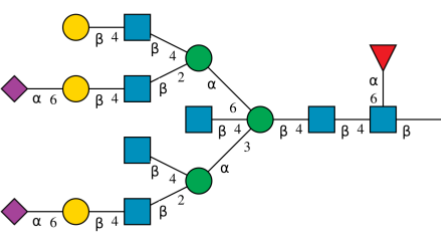
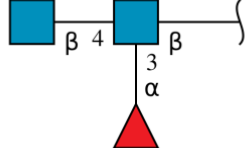
Each row records BIRD ID, the name of the blood group antigen, the Glycam Condensed Sequence and the PDB ID of representing entry. These blood group antigens are terminal patterned groups in complex with the target protein. Since the free reducing end hemiacetal may adopt either alpha or beta anomeric form, there are usually pairs of both, and the free hemiacetal group is represented by '1-ROH' in the Glycam Condensed Sequence.

Supplementary Table SIV: Commonly Observed Oligosaccharides in the PDB

#PDB Entries	Composition by CCD ID	Type of Descriptor	Descriptor
3124	NAG,NAG	PDB Systematic Name	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
		Glycam Condensed Sequence	DGlcNac1-4DGlcNac1-
		LINUXS	[]{[(4+1)][b-D-GlcNac]{[(4+1)][b-D-GlcNac]{}}}
		WURCS	WURCS=2.0/1,2,1/[a2122h-1b_1-5_2*NCC/3=O]/1-1/a4-b1
1056	NAG,NAG,BMA	PDB Systematic Name	beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
		Glycam Condensed Sequence	DManpb1-4DGlcNac1-4DGlcNac1-
		LINUXS	[]{[(4+1)][b-D-GlcNac]{[(4+1)][b-D-GlcNac]{[(4+1)][b-D-Manp]{}}}]
		WURCS	WURCS=2.0/2,3,2/[a2122h-1b_1-5_2*NCC/3=O][a1122h-1b_1-5]/1-1-2/a4-b1_b4-c1
431	NAG,NAG,BMA,MAN,MAN	PDB Systematic Name	alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
		Glycam Condensed Sequence	DManpa1-3[DManpa1-6]DManpb1-4DGlcNac1-4DGlcNac1-
		LINUXS	[]{[(4+1)][b-D-GlcNac]{[(4+1)][b-D-GlcNac]{[(4+1)][b-D-Manp]{[(3+1)][a-D-Manp]{[(6+1)][a-D-Manp]{}}}]}}}
		WURCS	WURCS=2.0/3,5,4/[a2122h-1b_1-5_2*NCC/3=O][a1122h-1b_1-5][a1122h-1a_1-5]/1-1-2-3/a4-b1_b4-c1_c3-d1_c6-e1
425	NAG,NAG,BMA,MAN	PDB Systematic Name	alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
		Glycam Condensed Sequence	DManpa1-3DManpb1-4DGlcNac1-4DGlcNac1-
		LINUXS	[]{[(4+1)][b-D-GlcNac]{[(4+1)][b-D-GlcNac]{[(4+1)][b-D-Manp]{[(3+1)][a-D-Manp]{}}}]}}}
		WURCS	WURCS=2.0/3,4,3/[a2122h-1b_1-5_2*NCC/3=O][a1122h-1b_1-5][a1122h-1a_1-5]/1-1-2-3/a4-b1_b4-c1_c3-d1
356	NAG,NAG,FUC	PDB Systematic Name	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose
		Glycam Condensed Sequence	DGlcNac1-4[LFucpa1-6]DGlcNac1-
		LINUXS	[]{[(4+1)][b-D-GlcNac]{[(4+1)][b-D-GlcNac]{[(6+1)][a-L-Fucp]{}}}]
		WURCS	WURCS=2.0/2,3,2/[a2122h-1b_1-5_2*NCC/3=O][a1221m-1a_1-5]/1-1-2/a4-b1_a6-c1
356	GLC,GLC	PDB Systematic Name	alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose
		Glycam Condensed Sequence	DGlcpa1-4DGlcpa1-ROH
		LINUXS	[]{[a-D-Glc]{[(4+1)][a-D-Glc]{}}}
		WURCS	WURCS=2.0/1,2,1/[a2122h-1a_1-5]/1-1/a4-b1
264	GLC,FRU	PDB Systematic Name	beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose
		Glycam Condensed Sequence	DFrufb2-1DGlcpa
		LINUXS	[]{[b-D-Fruf]{[(2+1)][a-D-Glc]{}}}
		WURCS	WURCS=2.0/2,2,1/[ha122h-2b_2-5][a2122h-1a_1-5]/1-2/a2-b1
233	NAG,FUC	PDB Systematic Name	alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose
		Glycam Condensed Sequence	LFucpa1-6DGlcNac1-
		LINUXS	[]{[(4+1)][b-D-GlcNac]{[(6+1)][a-L-Fucp]{}}}]
		WURCS	WURCS=2.0/2,2,1/[a2122h-1b_1-5_2*NCC/3=O][a1221m-1a_1-5]/1-2/a6-b1
232	NAG,NAG,MAN	PDB Systematic Name	alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
		Glycam Condensed Sequence	DManpa1-4DGlcNac1-4DGlcNac1-
		LINUXS	[]{[(4+1)][b-D-GlcNac]{[(4+1)][b-D-GlcNac]{[(4+1)][b-D-Manp]{}}}]
		WURCS	WURCS=2.0/2,3,2/[a2122h-1b_1-5_2*NCC/3=O][a1122h-1a_1-5]/1-1-2/a4-b1_b4-c1

171	NAG,NAG,BMA, MAN	PDB Systematic Name	alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
		Glycam Condensed Sequence	DManpa1-6DManpb1-4DGlcNACb1-4DGlcNACb1-
		LINUXS	[]{[(4+1)][b-D-GlcNAC]{[(4+1)][b-D-GlcNAC]{[(4+1)][b-D-Manp]{[(6+1)][a-D-Manp]{}}}}}
		WURCS	WURCS=2.0/3,4,3/[a2122h-1b_1-5_2*NCC/3=O][a1122h-1b_1-5][a1122h-1a_1-5]/1-1-2-3/a4-b1_b4-c1_c6-d1
129	BGC,GAL	PDB Systematic Name	beta-D-galactopyranose-(1-4)-beta-D-glucopyranose
		Glycam Condensed Sequence	DGalpb1-4DGlcpb1-ROH
		LINUXS	[]{[b-D-Glc]{[(4+1)][b-D-Galp]{}}
		WURCS	WURCS=2.0/2,2,1/[a2122h-1b_1-5][a2112h-1b_1-5]/1-2/a4-b1
122	NAG,NAG,BMA,F UC	PDB Systematic Name	beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose
		Glycam Condensed Sequence	DManpb1-4DGlcNACb1-4[LFucpa1-6]DGlcNACb1-
		LINUXS	[]{[(4+1)][b-D-GlcNAC]{[(4+1)][b-D-GlcNAC]{[(4+1)][b-D-Manp]{}}}{[(6+1)][a-L-Fucp]{}}
		WURCS	WURCS=2.0/3,4,3/[a2122h-1b_1-5_2*NCC/3=O][a1122h-1b_1-5][a1221m-1a_1-5]/1-1-2-3/a4-b1_a6-d1_b4-c1
116	NAG,NAG,NAG	PDB Systematic Name	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
		Glycam Condensed Sequence	DGlcNACb1-4DGlcNACb1-4DGlcNACb1-ROH
		LINUXS	[]{[b-D-GlcNAC]{[(4+1)][b-D-GlcNAC]{[(4+1)][b-D-GlcNAC]{}}
		WURCS	WURCS=2.0/1,3,2/[a2122h-1b_1-5_2*NCC/3=O]/1-1-1/a4-b1_b4-c1
111	BGC,BGC	PDB Systematic Name	beta-D-glucopyranose-(1-4)-beta-D-glucopyranose
		Glycam Condensed Sequence	DGlcpb1-4DGlcpb1-ROH
		LINUXS	[]{[b-D-Glc]{[(4+1)][b-D-Glc]{}}
		WURCS	WURCS=2.0/1,2,1/[a2122h-1b_1-5]/1-1/a4-b1

Supplementary Table SV: PDB Examples of Glycan Sequences at the Different Glycosylation Sites

Index	Site	Symbol of Monosaccharide connecting to protein	CCD ID	PDB Example	Observed pattern
N1	ASN	b-D-GlcpNAc	NAG	1INX	
N2	ASN	b-D-GlcpNAc	NAG	5ACO	
N3	ASN	b-D-GlcpNAc	NAG	6WPS	
N4	ASN	b-D-GlcpNAc	NAG	5T3X	
N5	ASN	b-D-GlcpNAc	NAG	1BCR	

N6	ASN	b-D-Glcp	BGC	5TIP	
O1	SER	a-D-GalpNac	A2G	5KDU	
O2	SER	a-D-GalpNac	A2G	4B1Q	
O3	SER	b-D-6-deoxy-GlcpNac4NAc	B6D	5VXX	

O4	SER	b-D-Glcp	BGC	5VYG	
O5	SER	a-L-Fucp	FUC	6RUS	
O6	SER	a-D-Manp	MAN	1HMU	
O7	SER	b-D-GlcpNAc	NAG	1AY2	
O8	THR	a-D-GalpNAc	A2G	6ROX	
O9	THR	a-L-Fucp	FUC	6RUR	

O10	THR	α -D-Manp	MAN	2FUQ	
O11	THR	β -D-GlcpNAc	NAG	4DUR	
O12	THR	α -D-GlcpNAc	NDG	1QDD	
O13	THR	β -D-GalpNAc	NGA	1G15	
O14	TYR	β -D-Glcp	BGC	5V2J	
O15	TYR	α -D-Glcp	GLC	3U2V	

The examples selected are relatively complete glycan sequences for the relevant glycosylation sites, confirmed by either the publication of the structures or the supporting experimental data. Most glycosylation glycans in the PDB archive are fragments of these examples, and majority of the glycosylation sites have only a monosaccharide modeled. N1-N6 are examples of N-Glycosylation, and O1-O15 are examples of O-Glycosylation. N1-N5 all have β -D-GlcpNAc (NAG) connected to ASN residue but have sequences of different types and lengths: N1 is the common 5-monomer N-glycan core; N2 is the near-complete oligomannose-type N-glycan; N3 is the commonly 1-6 fucosylated N-glycan core; N4 is the complex-type N-glycan; N5 has 1-3 fucosylation. Most of the N-glycans in the PDB entries are fragments of N1-N5. O1 and O2 both have α -D-GalpNAc (A2G) connected to SER residue.

Appendix I: Example of Remediated CCD definition of NAG

Updates from PDB carbohydrate remediation are highlighted in yellow.

```
#
data_NAG
#
_chem_comp.id                NAG
_chem_comp.name              2-acetamido-2-deoxy-beta-D-glucopyranose
_chem_comp.type              "D-saccharide, beta linking"
_chem_comp.pdbx_type         ATOMS
_chem_comp.formula           "C8 H15 N O6"
_chem_comp.mon_nstd_parent_comp_id ?
_chem_comp.pdbx_formal_charge 0
_chem_comp.pdbx_initial_date 1999-07-08
_chem_comp.pdbx_modified_date 2020-07-17
_chem_comp.pdbx_ambiguous_flag N
_chem_comp.pdbx_release_status REL
_chem_comp.pdbx_replaced_by   ?
_chem_comp.pdbx_replaces     ?
_chem_comp.formula_weight     221.208
_chem_comp.one_letter_code    ?
_chem_comp.three_letter_code  NAG
_chem_comp.pdbx_model_coordinates_details ?
_chem_comp.pdbx_model_coordinates_missing_flag N
_chem_comp.pdbx_ideal_coordinates_details Corina
_chem_comp.pdbx_ideal_coordinates_missing_flag N
_chem_comp.pdbx_model_coordinates_db_code 8PCH
_chem_comp.pdbx_subcomponent_list ?
_chem_comp.pdbx_processing_site RCSB
# #
loop_
  pdbx_chem_comp_synonyms.ordinal
  pdbx_chem_comp_synonyms.comp_id
  pdbx_chem_comp_synonyms.name
  pdbx_chem_comp_synonyms.provenance
  pdbx_chem_comp_synonyms.type
1  NAG  N-acetyl-beta-D-glucosamine      PDB  ?
2  NAG  2-acetamido-2-deoxy-beta-D-glucose  PDB  ?
3  NAG  2-acetamido-2-deoxy-D-glucose        PDB  ?
4  NAG  2-acetamido-2-deoxy-glucose          PDB  ?
5  NAG  N-ACETYL-D-GLUCOSAMINE               PDB  ?
# #
loop_
_chem_comp_atom.comp_id
_chem_comp_atom.atom_id
_chem_comp_atom.alt_atom_id
_chem_comp_atom.type_symbol
_chem_comp_atom.charge
_chem_comp_atom.pdbx_align
_chem_comp_atom.pdbx_aromatic_flag
_chem_comp_atom.pdbx_leaving_atom_flag
_chem_comp_atom.pdbx_stereo_config
_chem_comp_atom.model_Cartn_x
_chem_comp_atom.model_Cartn_y
_chem_comp_atom.model_Cartn_z
_chem_comp_atom.pdbx_model_Cartn_x_ideal
_chem_comp_atom.pdbx_model_Cartn_y_ideal
```

	<u>_chem_comp_atom.pdbx_model_Cartn_z_ideal</u>																
	<u>_chem_comp_atom.pdbx_component_atom_id</u>																
	<u>_chem_comp_atom.pdbx_component_comp_id</u>																
	<u>_chem_comp_atom.pdbx_ordinal</u>																
1	NAG	C1	C1	C	0	1	N	N	R	7.396	28.163	26.662	0.185	1.082	-0.421	C1	NAG
2	NAG	C2	C2	C	0	1	N	N	R	6.973	29.233	27.644	0.790	-0.220	0.112	C2	NAG
3	NAG	C3	C3	C	0	1	N	N	R	7.667	29.055	29.000	-0.124	-1.390	-0.265	C3	NAG
4	NAG	C4	C4	C	0	1	N	N	S	7.573	27.588	29.490	-1.526	-1.129	0.294	C4	NAG
5	NAG	C5	C5	C	0	1	N	N	R	7.902	26.592	28.373	-2.042	0.207	-0.246	C5	NAG
6	NAG	C6	C6	C	0	1	N	N	N	7.599	25.173	28.797	-3.417	0.504	0.355	C6	NAG
7	NAG	C7	C7	C	0	1	N	N	N	6.291	31.299	26.595	3.197	0.157	0.076	C7	NAG
8	NAG	C8	C8	C	0	1	N	N	N	6.684	32.649	26.036	4.559	-0.052	-0.533	C8	NAG
9	NAG	N2	N2	N	0	1	N	N	N	7.268	30.545	27.089	2.114	-0.422	-0.480	N2	NAG
10	NAG	O1	O1	O	0	1	N	Y	N	6.676	28.363	25.419	1.003	2.185	-0.024	O1	NAG
11	NAG	O3	O3	O	0	1	N	N	N	7.038	29.909	29.947	0.395	-2.600	0.291	O3	NAG
12	NAG	O4	O4	O	0	1	N	N	N	8.494	27.358	30.574	-2.405	-2.180	-0.114	O4	NAG
13	NAG	O5	O5	O	0	1	N	N	N	7.104	26.875	27.206	-1.130	1.248	0.113	O5	NAG
14	NAG	O6	O6	O	0	1	N	N	N	6.232	25.040	29.165	-3.949	1.691	-0.236	O6	NAG
15	NAG	O7	O7	O	0	1	N	N	N	5.114	30.936	26.562	3.074	0.845	1.067	O7	NAG
16	NAG	H1	H1	H	0	1	N	N	N	8.477	28.257	26.481	0.133	1.040	-1.509	H1	NAG
17	NAG	H2	H2	H	0	1	N	N	N	5.888	29.146	27.803	0.879	-0.163	1.197	H2	NAG
18	NAG	H3	H3	H	0	1	N	N	N	8.729	29.321	28.892	-0.174	-1.478	-1.350	H3	NAG
19	NAG	H4	H4	H	0	1	N	N	N	6.544	27.403	29.831	-1.483	-1.091	1.382	H4	NAG
20	NAG	H5	H5	H	0	1	N	N	N	8.971	26.674	28.128	-2.123	0.154	-1.332	H5	NAG
21	NAG	H61	H61	H	0	1	N	N	N	7.816	24.492	27.961	-4.088	-0.333	0.157	H61	NAG
22	NAG	H62	H62	H	0	1	N	N	N	8.232	24.910	29.657	-3.320	0.645	1.431	H62	NAG
23	NAG	H81	H81	H	0	1	N	N	N	5.791	33.159	25.646	4.560	0.320	-1.558	H81	NAG
24	NAG	H82	H82	H	0	1	N	N	N	7.136	33.258	26.833	5.305	0.490	0.050	H82	NAG
25	NAG	H83	H83	H	0	1	N	N	N	7.411	32.511	25.222	4.799	-1.115	-0.532	H83	NAG
26	NAG	HN2	HN2	H	0	1	N	N	N	8.210	30.881	27.079	2.212	-0.973	-1.273	HN2	NAG
27	NAG	HO1	HO1	H	0	1	N	Y	N	6.933	27.696	24.793	0.679	3.044	-0.328	HO1	NAG

NAG	HO3	HO3	H	0	1	N	Y	N	7.459	29.809	30.793	-0.135	-3.384	0.091	HO3	NAG
28																
NAG	HO4	HO4	H	0	1	N	Y	N	8.425	26.456	30.863	-3.312	-2.079	0.206	HO4	NAG
29																
NAG	HO6	HO6	H	0	1	N	Y	N	6.060	24.143	29.428	-4.822	1.940	0.099	HO6	NAG
30																

#

loop_

_chem_comp_bond.comp_id
_chem_comp_bond.atom_id_1
_chem_comp_bond.atom_id_2
_chem_comp_bond.value_order
_chem_comp_bond.pdbx_aromatic_flag
_chem_comp_bond.pdbx_stereo_config
_chem_comp_bond.pdbx_ordinal

NAG	C1	C2	SING	N	N	1
NAG	C1	O1	SING	N	N	2
NAG	C1	O5	SING	N	N	3
NAG	C1	H1	SING	N	N	4
NAG	C2	C3	SING	N	N	5
NAG	C2	N2	SING	N	N	6
NAG	C2	H2	SING	N	N	7
NAG	C3	C4	SING	N	N	8
NAG	C3	O3	SING	N	N	9
NAG	C3	H3	SING	N	N	10
NAG	C4	C5	SING	N	N	11
NAG	C4	O4	SING	N	N	12
NAG	C4	H4	SING	N	N	13
NAG	C5	C6	SING	N	N	14
NAG	C5	O5	SING	N	N	15
NAG	C5	H5	SING	N	N	16
NAG	C6	O6	SING	N	N	17
NAG	C6	H61	SING	N	N	18
NAG	C6	H62	SING	N	N	19
NAG	C7	C8	SING	N	N	20
NAG	C7	N2	SING	N	N	21
NAG	C7	O7	DOUB	N	N	22
NAG	C8	H81	SING	N	N	23
NAG	C8	H82	SING	N	N	24
NAG	C8	H83	SING	N	N	25
NAG	N2	HN2	SING	N	N	26
NAG	O1	HO1	SING	N	N	27
NAG	O3	HO3	SING	N	N	28
NAG	O4	HO4	SING	N	N	29
NAG	O6	HO6	SING	N	N	30

#

loop_

_pdbx_chem_comp_descriptor.comp_id
_pdbx_chem_comp_descriptor.type
_pdbx_chem_comp_descriptor.program
_pdbx_chem_comp_descriptor.program_version
_pdbx_chem_comp_descriptor.descriptor

NAG	SMILES	ACDLabs	12.01	"O=C(NC1C(O)C(O)C(OC1O)CO)C"
NAG	InChI	InChI	1.03	"InChI=1S/C8H15NO6/c1-3(11)9-5-7(13)6(12)4(2-10)15-8(5)14/h4-8,10,12-14H,2H2,1H3,(H,9,11)/t4-,5-,6-,7-,8-/m1/s1"
NAG	InChIKey	InChI	1.03	OVRNDRQMDRJTHS-FMDGEEDCSA-N
NAG	SMILES_CANONICAL	CACTVS	3.370	"CC(=O)N[C@H]1[C@H](O)O[C@H](CO)[C@@H](O)[C@@H]1O"

```

NAG SMILES CACTVS 3.370
"CC(=O)N[CH]1[CH](O)O[CH](CO)[CH](O)[CH]1O"
NAG SMILES_CANONICAL "OpenEye OEToolkits" 1.7.6
"CC(=O)N[C@@H]1[C@H]([C@@H]([C@H](O[C@H]1O)CO)O)O"
NAG SMILES "OpenEye OEToolkits" 1.7.6 "CC(=O)NC1C(C(C(OC1O)CO)O)O"
# #
loop_
_pdbx_chem_comp_identifier.comp_id
_pdbx_chem_comp_identifier.type
_pdbx_chem_comp_identifier.program
_pdbx_chem_comp_identifier.program_version
_pdbx_chem_comp_identifier.identifier
NAG "SYSTEMATIC NAME" ACDLabs 12.01 "2-
(acetylamino)-2-deoxy-beta-D-glucofuranose"
NAG "SYSTEMATIC NAME" "OpenEye OEToolkits" 1.7.6 "N-
[(2R,3R,4R,5S,6R)-6-(hydroxymethyl)-2,4,5-tris(oxidanyl)oxan-3-yl]ethanamide"
NAG "CONDENSED IUPAC CARBOHYDRATE SYMBOL" GMML 1.0 DGlcPNAcb
NAG "COMMON NAME" GMML 1.0 N-acetyl-b-D-
glucopyranosamine
NAG "IUPAC CARBOHYDRATE SYMBOL" PDB-CARE 1.0 b-D-GlcPNAc
NAG "SNFG CARBOHYDRATE SYMBOL" GMML 1.0 GlcNAc
# #
loop_
_pdbx_chem_comp_feature.comp_id
_pdbx_chem_comp_feature.type
_pdbx_chem_comp_feature.value
_pdbx_chem_comp_feature.source
_pdbx_chem_comp_feature.support
NAG "CARBOHYDRATE ISOMER" D PDB ?
NAG "CARBOHYDRATE RING" pyranose PDB ?
NAG "CARBOHYDRATE ANOMER" beta PDB ?
NAG "CARBOHYDRATE PRIMARY CARBONYL GROUP" aldose PDB ?
# #
loop_
_pdbx_chem_comp_audit.comp_id
_pdbx_chem_comp_audit.action_type
_pdbx_chem_comp_audit.date
_pdbx_chem_comp_audit.processing_site
NAG "Create component" 1999-07-08 RCSB
NAG "Modify descriptor" 2011-06-04 RCSB
NAG "Modify leaving atom flag" 2011-07-01 RCSB
NAG "Modify leaving atom flag" 2012-11-26 RCSB
NAG "Other modification" 2019-08-12 RCSB
NAG "Other modification" 2019-12-19 RCSB
NAG "Other modification" 2020-07-03 RCSB
NAG "Modify name" 2020-07-17 RCSB
NAG "Modify synonyms" 2020-07-17 RCSB
##

```

Appendix II: Example of Remediated PDB Entry 1B5F

```

# Updates from PDB carbohydrate remediation are highlighted in yellow.
#
data_1B5F
#
_entry.id    1B5F
#
...
#
loop_
_entity.id
_entity.type
_entity.src_method
_entity.pdbx_description
_entity.formula_weight
_entity.pdbx_number_of_molecules
_entity.pdbx_ec
_entity.pdbx_mutation
_entity.pdbx_fragment
_entity.details
...
3 branched man
;alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-
glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose
;
894.823    1    ?    ? ? ?
4 branched man
;beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-
fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose
;
732.682    2    ?    ? ? ?
5 branched man
;alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-
acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-
deoxy-beta-D-glucopyranose
;
1056.964    1    ?    ? ? ?
#
...
#
loop_
_chem_comp.id
_chem_comp.type
_chem_comp.mon_nstd_flag
_chem_comp.name
_chem_comp.pdbx_synonyms
_chem_comp.formula
_chem_comp.formula_weight
ALA 'L-peptide linking'          y ALANINE                ? 'C3 H7 N
O2'          89.093
ARG 'L-peptide linking'          y ARGININE                ? 'C6 H15 N4
O2 1' 175.209
ASN 'L-peptide linking'          y ASPARAGINE              ? 'C4 H8 N2
O3'          132.118
ASP 'L-peptide linking'          y 'ASPARTIC ACID'        ? 'C4 H7 N
O4'          133.103

```

BMA 'D-saccharide, beta linking'	. beta-D-mannopyranose	'beta-D-
mannose; D-mannose; mannose'	'C6 H12 O6'	
180.156		
CYS 'L-peptide linking'	y CYSTEINE	? 'C3 H7 N
O2 S'	121.158	
FUC 'L-saccharide, alpha linking'	. alpha-L-fucopyranose	
'alpha-L-fucose; 6-deoxy-alpha-L-galactopyranose; L-fucose; fucose'	'C6 H12 O5'	
164.156		
GLN 'L-peptide linking'	y GLUTAMINE	? 'C5 H10 N2
O3'	146.144	
GLU 'L-peptide linking'	y 'GLUTAMIC ACID'	? 'C5 H9 N
O4'	147.129	
GLY 'peptide linking'	y GLYCINE	? 'C2 H5 N
O2'	75.067	
HIS 'L-peptide linking'	y HISTIDINE	? 'C6 H10 N3
O2 1'	156.162	
HOH non-polymer	. WATER	? 'H2 O'
18.015		
ILE 'L-peptide linking'	y ISOLEUCINE	? 'C6 H13 N
O2'	131.173	
LEU 'L-peptide linking'	y LEUCINE	? 'C6 H13 N
O2'	131.173	
LYS 'L-peptide linking'	y LYSINE	? 'C6 H15 N2
O2 1'	147.195	
MAN 'D-saccharide, alpha linking'	. alpha-D-mannopyranose	'alpha-D-
mannose; D-mannose; mannose'	'C6 H12 O6'	
180.156		
MET 'L-peptide linking'	y METHIONINE	? 'C5 H11 N
O2 S'	149.211	
NAG 'D-saccharide, beta linking'	. 2-acetamido-2-deoxy-beta-D-glucopyranose	
;N-acetyl-beta-D-glucosamine; 2-acetamido-2-deoxy-beta-D-glucose; 2-acetamido-2-deoxy-D-	glucose; 2-acetamido-2-deoxy-glucose; N-ACETYL-D-GLUCOSAMINE	
;		
'C8 H15 N O6'	221.208	
PHE 'L-peptide linking'	y PHENYLALANINE	? 'C9 H11 N
O2'	165.189	
PRO 'L-peptide linking'	y PROLINE	? 'C5 H9 N
O2'	115.130	
SER 'L-peptide linking'	y SERINE	? 'C3 H7 N
O3'	105.093	
THR 'L-peptide linking'	y THREONINE	? 'C4 H9 N
O3'	119.119	
TRP 'L-peptide linking'	y TRYPTOPHAN	? 'C11 H12
N2 O2'	204.225	
TYR 'L-peptide linking'	y TYROSINE	? 'C9 H11 N
O3'	181.189	
VAL 'L-peptide linking'	y VALINE	? 'C5 H11 N
O2'	117.146	
#		
...		
#		
loop_		
pdbx_chem_comp_identifier.comp_id		
pdbx_chem_comp_identifier.type		
pdbx_chem_comp_identifier.program		
pdbx_chem_comp_identifier.program_version		
pdbx_chem_comp_identifier.identifier		
BMA 'CONDENSED IUPAC CARBOHYDRATE SYMBOL'	GMML	1.0 DManpb
BMA 'COMMON NAME'	GMML	1.0 b-D-mannopyranose


```

BMA 'IUPAC CARBOHYDRATE SYMBOL' PDB-CARE 1.0 b-D-Manp
BMA 'SNFG CARBOHYDRATE SYMBOL' GMLL 1.0 Man
FUC 'CONDENSED IUPAC CARBOHYDRATE SYMBOL' GMLL 1.0 LFucpa
FUC 'COMMON NAME' GMLL 1.0 a-L-fucopyranose
FUC 'IUPAC CARBOHYDRATE SYMBOL' PDB-CARE 1.0 a-L-Fucp
FUC 'SNFG CARBOHYDRATE SYMBOL' GMLL 1.0 Fuc
MAN 'CONDENSED IUPAC CARBOHYDRATE SYMBOL' GMLL 1.0 DManpa
MAN 'COMMON NAME' GMLL 1.0 a-D-mannopyranose
MAN 'IUPAC CARBOHYDRATE SYMBOL' PDB-CARE 1.0 a-D-Manp
MAN 'SNFG CARBOHYDRATE SYMBOL' GMLL 1.0 Man
NAG 'CONDENSED IUPAC CARBOHYDRATE SYMBOL' GMLL 1.0 DGlcNac
NAG 'COMMON NAME' GMLL 1.0 N-acetyl-b-D-glucofuranosamine
NAG 'IUPAC CARBOHYDRATE SYMBOL' PDB-CARE 1.0 b-D-GlcNac
NAG 'SNFG CARBOHYDRATE SYMBOL' GMLL 1.0 GlcNac
#
...
#
loop_
  pdbx_entity_branch.entity_id
  pdbx_entity_branch.type
3 oligosaccharide
4 oligosaccharide
5 oligosaccharide
#
loop_
  pdbx_entity_branch_descriptor.ordinal
  pdbx_entity_branch_descriptor.entity_id
  pdbx_entity_branch_descriptor.descriptor
  pdbx_entity_branch_descriptor.type
  pdbx_entity_branch_descriptor.program
  pdbx_entity_branch_descriptor.program_version
1 3 'DManpa1-3DManpb1-4DGlcNac1-4[LFucpa1-3]DGlcNac1-' 'Glycam Condensed Sequence'
GMLL 1.0
2 3 'WURCS=2.0/4,5,4/[a2122h-1b_1-5_2*NCC/3=0][a221m-1a_1-5][a1122h-1b_1-5][a1122h-1a_1-5]/1-2-1-3-4/a3-b1_a4-c1_c4-d1_d3-e1'
WURCS PDB2Glycan 1.1.0
3 3 '[[[(4+1)][b-D-GlcNac]][(3+1)][a-L-Fucp]][(4+1)][b-D-GlcNac]][(4+1)][b-D-Manp]][(3+1)][a-D-Manp]]]' LINUCS PDB-CARE
?
4 4 'DManpb1-4DGlcNac1-4[LFucpa1-3]DGlcNac1-' 'Glycam Condensed Sequence' GMLL
1.0
5 4 'WURCS=2.0/3,4,3/[a2122h-1b_1-5_2*NCC/3=0][a221m-1a_1-5][a1122h-1b_1-5]/1-2-1-3/a3-b1_a4-c1_c4-d1' WURCS PDB2Glycan 1.1.0
6 4 '[[[(4+1)][b-D-GlcNac]][(3+1)][a-L-Fucp]][(4+1)][b-D-GlcNac]][(4+1)][b-D-Manp]]]' LINUCS PDB-CARE
?
7 5 'DManpa1-3[DManpa1-6]DManpb1-4DGlcNac1-4[LFucpa1-3]DGlcNac1-' 'Glycam Condensed Sequence' GMLL 1.0
8 5
'WURCS=2.0/4,6,5/[a2122h-1b_1-5_2*NCC/3=0][a221m-1a_1-5][a1122h-1b_1-5][a1122h-1a_1-5]/1-2-1-3-4-4/a3-b1_a4-c1_c4-d1_d3-e1_d6-f1'
WURCS PDB2Glycan 1.1.0
9 5 '[[[(4+1)][b-D-GlcNac]][(3+1)][a-L-Fucp]][(4+1)][b-D-GlcNac]][(4+1)][b-D-Manp]][(3+1)][a-D-Manp]][(6+1)][a-D-Manp]]]'
LINUCS PDB-CARE ?
#
loop_
  pdbx_entity_branch_list.entity_id
  pdbx_entity_branch_list.comp_id

```

```

_pdbx_entity_branch_list.num
_pdbx_entity_branch_list.hetero
3 NAG 1 n
3 NAG 2 n
3 BMA 3 n
3 MAN 4 n
3 FUC 5 n
4 NAG 1 n
4 NAG 2 n
4 BMA 3 n
4 FUC 4 n
5 NAG 1 n
5 NAG 2 n
5 BMA 3 n
5 MAN 4 n
5 MAN 5 n
5 FUC 6 n
#
loop_
_pdbx_entity_branch_link.link_id
_pdbx_entity_branch_link.entity_id
_pdbx_entity_branch_link.entity_branch_list_num_1
_pdbx_entity_branch_link.comp_id_1
_pdbx_entity_branch_link.atom_id_1
_pdbx_entity_branch_link.leaving_atom_id_1
_pdbx_entity_branch_link.entity_branch_list_num_2
_pdbx_entity_branch_link.comp_id_2
_pdbx_entity_branch_link.atom_id_2
_pdbx_entity_branch_link.leaving_atom_id_2
_pdbx_entity_branch_link.value_order
_pdbx_entity_branch_link.details
1 3 2 NAG C1 O1 1 NAG O4 HO4 sing ?
2 3 3 BMA C1 O1 2 NAG O4 HO4 sing ?
3 3 4 MAN C1 O1 3 BMA O3 HO3 sing ?
4 3 5 FUC C1 O1 1 NAG O3 HO3 sing ?
5 4 2 NAG C1 O1 1 NAG O4 HO4 sing ?
6 4 3 BMA C1 O1 2 NAG O4 HO4 sing ?
7 4 4 FUC C1 O1 1 NAG O3 HO3 sing ?
8 5 2 NAG C1 O1 1 NAG O4 HO4 sing ?
9 5 3 BMA C1 O1 2 NAG O4 HO4 sing ?
10 5 4 MAN C1 O1 3 BMA O3 HO3 sing ?
11 5 5 MAN C1 O1 3 BMA O6 HO6 sing ?
12 5 6 FUC C1 O1 1 NAG O3 HO3 sing ?
#
loop_
_pdbx_branch_scheme.asym_id
_pdbx_branch_scheme.entity_id
_pdbx_branch_scheme.mon_id
_pdbx_branch_scheme.num
_pdbx_branch_scheme.pdb_asym_id
_pdbx_branch_scheme.pdb_mon_id
_pdbx_branch_scheme.pdb_seq_num
_pdbx_branch_scheme.auth_asym_id
_pdbx_branch_scheme.auth_mon_id
_pdbx_branch_scheme.auth_seq_num
_pdbx_branch_scheme.hetero
E 3 NAG 1 E NAG 1 E NAG 401 n
E 3 NAG 2 E NAG 2 E NAG 403 n
E 3 BMA 3 E BMA 3 E MAN 404 n

```

```
E 3 MAN 4 E MAN 4 E MAN 405 n
E 3 FUC 5 E FUC 5 E FUC 402 n
F 4 NAG 1 F NAG 1 F NAG 501 n
F 4 NAG 2 F NAG 2 F NAG 503 n
F 4 BMA 3 F BMA 3 F MAN 504 n
F 4 FUC 4 F FUC 4 F FUC 502 n
G 5 NAG 1 G NAG 1 G NAG 401 n
G 5 NAG 2 G NAG 2 G NAG 403 n
G 5 BMA 3 G BMA 3 G MAN 404 n
G 5 MAN 4 G MAN 4 G MAN 405 n
G 5 MAN 5 G MAN 5 G MAN 406 n
G 5 FUC 6 G FUC 6 G FUC 402 n
H 4 NAG 1 H NAG 1 H NAG 501 n
H 4 NAG 2 H NAG 2 H NAG 503 n
H 4 BMA 3 H BMA 3 H MAN 504 n
H 4 FUC 4 H FUC 4 H FUC 502 n
```

```
#
```

```
...
```

```
#
```

```
loop_
```

```
_struct_asym.id
```

```
_struct_asym.pdbx_blank_PDB_chainid_flag
```

```
_struct_asym.pdbx_modified
```

```
_struct_asym.entity_id
```

```
_struct_asym.details
```

```
A N N 1 ?
```

```
B N N 2 ?
```

```
C N N 1 ?
```

```
D N N 2 ?
```

```
E N N 3 ?
```

```
F N N 4 ?
```

```
G N N 5 ?
```

```
H N N 4 ?
```

```
I N N 6 ?
```

```
J N N 6 ?
```

```
K N N 6 ?
```

```
L N N 6 ?
```

```
#
```

```
...
```

```
#
```

```
loop_
```

```
_struct_conn.id
```

```
_struct_conn.conn_type_id
```

```
_struct_conn.pdbx_leaving_atom_flag
```

```
_struct_conn.pdbx_PDB_id
```

```
_struct_conn.ptnr1_label_asym_id
```

```
_struct_conn.ptnr1_label_comp_id
```

```
_struct_conn.ptnr1_label_seq_id
```

```
_struct_conn.ptnr1_label_atom_id
```

```
_struct_conn.pdbx_ptnr1_label_alt_id
```

```
_struct_conn.pdbx_ptnr1_PDB_ins_code
```

```
_struct_conn.pdbx_ptnr1_standard_comp_id
```

```
_struct_conn.ptnr1_symmetry
```

```
_struct_conn.ptnr2_label_asym_id
```

```
_struct_conn.ptnr2_label_comp_id
```

```
_struct_conn.ptnr2_label_seq_id
```

```
_struct_conn.ptnr2_label_atom_id
```

```
_struct_conn.pdbx_ptnr2_label_alt_id
```

```
_struct_conn.pdbx_ptnr2_PDB_ins_code
```

```

_struct_conn.ptnr1_auth_asym_id
_struct_conn.ptnr1_auth_comp_id
_struct_conn.ptnr1_auth_seq_id
_struct_conn.ptnr2_auth_asym_id
_struct_conn.ptnr2_auth_comp_id
_struct_conn.ptnr2_auth_seq_id
_struct_conn.ptnr2_symmetry
_struct_conn.pdbx_ptnr3_label_atom_id
_struct_conn.pdbx_ptnr3_label_seq_id
_struct_conn.pdbx_ptnr3_label_comp_id
_struct_conn.pdbx_ptnr3_label_asym_id
_struct_conn.pdbx_ptnr3_label_alt_id
_struct_conn.pdbx_ptnr3_PDB_ins_code
_struct_conn.details
_struct_conn.pdbx_dist_value
_struct_conn.pdbx_value_order
_struct_conn.pdbx_role
disulf1  disulf ?    ? A CYS 46  SG  A ? ? 1_555 A CYS 52  SG  A ? A CYS 45  A CYS 50
1_555 ? ? ? ? ? ? ? 2.027 ? ?
disulf2  disulf ?    ? A CYS 46  SG  B ? ? 1_555 A CYS 52  SG  B ? A CYS 45  A CYS 50
1_555 ? ? ? ? ? ? ? 2.032 ? ?
disulf3  disulf ?    ? A CYS 207 SG  ? ? ? 1_555 A CYS 211 SG  ? ? A CYS 206 A CYS 210
1_555 ? ? ? ? ? ? ? 2.067 ? ?
disulf4  disulf ?    ? B CYS 7   SG  ? ? ? 1_555 B CYS 44  SG  ? ? B CYS 249 B CYS 282
1_555 ? ? ? ? ? ? ? 2.078 ? ?
disulf5  disulf ?    ? C CYS 46  SG  ? ? ? 1_555 C CYS 52  SG  ? ? C CYS 45  C CYS 50
1_555 ? ? ? ? ? ? ? 2.037 ? ?
disulf6  disulf ?    ? C CYS 207 SG  ? ? ? 1_555 C CYS 211 SG  ? ? C CYS 206 C CYS 210
1_555 ? ? ? ? ? ? ? 2.060 ? ?
disulf7  disulf ?    ? D CYS 7   SG  ? ? ? 1_555 D CYS 44  SG  ? ? D CYS 249 D CYS 282
1_555 ? ? ? ? ? ? ? 2.056 ? ?
covale1  covale one  ? A ASN 69  ND2 ? ? ? 1_555 E NAG .  C1 ? ? A ASN 67  E NAG 1
1_555 ? ? ? ? ? ? ? 1.471 ? N-Glycosylation
covale2  covale one  ? B ASN 15  ND2 ? ? ? 1_555 F NAG .  C1 ? ? B ASN 257 F NAG 1
1_555 ? ? ? ? ? ? ? 1.450 ? N-Glycosylation
covale3  covale one  ? C ASN 69  ND2 ? ? ? 1_555 G NAG .  C1 ? ? C ASN 67  G NAG 1
1_555 ? ? ? ? ? ? ? 1.483 ? N-Glycosylation
covale4  covale one  ? D ASN 15  ND2 ? ? ? 1_555 H NAG .  C1 ? ? D ASN 257 H NAG 1
1_555 ? ? ? ? ? ? ? 1.456 ? N-Glycosylation
covale5  covale both ? E NAG .  04 ? ? ? 1_555 E NAG .  C1 ? ? E NAG 1  E NAG 2
1_555 ? ? ? ? ? ? ? 1.387 ? ?
covale6  covale both ? E NAG .  03 ? ? ? 1_555 E FUC .  C1 ? ? E NAG 1  E FUC 5
1_555 ? ? ? ? ? ? ? 1.430 ? ?
covale7  covale both ? E NAG .  04 ? ? ? 1_555 E BMA .  C1 ? ? E NAG 2  E BMA 3
1_555 ? ? ? ? ? ? ? 1.396 ? ?
covale8  covale both ? E BMA .  03 ? ? ? 1_555 E MAN .  C1 ? ? E BMA 3  E MAN 4
1_555 ? ? ? ? ? ? ? 1.408 ? ?
covale9  covale both ? F NAG .  04 ? ? ? 1_555 F NAG .  C1 ? ? F NAG 1  F NAG 2
1_555 ? ? ? ? ? ? ? 1.385 ? ?
covale10 covale both ? F NAG .  03 ? ? ? 1_555 F FUC .  C1 ? ? F NAG 1  F FUC 4
1_555 ? ? ? ? ? ? ? 1.425 ? ?
covale11 covale both ? F NAG .  04 ? ? ? 1_555 F BMA .  C1 ? ? F NAG 2  F BMA 3
1_555 ? ? ? ? ? ? ? 1.389 ? ?
covale12 covale both ? G NAG .  04 ? ? ? 1_555 G NAG .  C1 ? ? G NAG 1  G NAG 2
1_555 ? ? ? ? ? ? ? 1.388 ? ?
covale13 covale both ? G NAG .  03 ? ? ? 1_555 G FUC .  C1 ? ? G NAG 1  G FUC 6
1_555 ? ? ? ? ? ? ? 1.427 ? ?
covale14 covale both ? G NAG .  04 ? ? ? 1_555 G BMA .  C1 ? ? G NAG 2  G BMA 3
1_555 ? ? ? ? ? ? ? 1.399 ? ?

```

```

covale15 covale both ? G BMA . 03 ? ? ? 1_555 G MAN . C1 ? ? G BMA 3 G MAN 4
1_555 ? ? ? ? ? ? ? 1.406 ? ?
covale16 covale both ? G BMA . 06 ? ? ? 1_555 G MAN . C1 ? ? G BMA 3 G MAN 5
1_555 ? ? ? ? ? ? ? 1.410 ? ?
covale17 covale both ? H NAG . 04 ? ? ? 1_555 H NAG . C1 ? ? H NAG 1 H NAG 2
1_555 ? ? ? ? ? ? ? 1.390 ? ?
covale18 covale both ? H NAG . 03 ? ? ? 1_555 H FUC . C1 A ? H NAG 1 H FUC 4
1_555 ? ? ? ? ? ? ? 1.424 ? ?
covale19 covale both ? H NAG . 03 ? ? ? 1_555 H FUC . C1 B ? H NAG 1 H FUC 4
1_555 ? ? ? ? ? ? ? 1.416 ? ?
covale20 covale both ? H NAG . 04 ? ? ? 1_555 H BMA . C1 ? ? H NAG 2 H BMA 3
1_555 ? ? ? ? ? ? ? 1.391 ? ?
#
...
#
loop_
_atom_site.group_PDB
_atom_site.id
_atom_site.type_symbol
_atom_site.label_atom_id
_atom_site.label_alt_id
_atom_site.label_comp_id
_atom_site.label_asym_id
_atom_site.label_entity_id
_atom_site.label_seq_id
_atom_site.pdbx_PDB_ins_code
_atom_site.Cartn_x
_atom_site.Cartn_y
_atom_site.Cartn_z
_atom_site.occupancy
_atom_site.B_iso_or_equiv
_atom_site.pdbx_formal_charge
_atom_site.auth_seq_id
_atom_site.auth_comp_id
_atom_site.auth_asym_id
_atom_site.auth_atom_id
_atom_site.pdbx_PDB_model_num
...

```

HETATM	5072	C	C1	.	NAG	E	3	.	?	35.913	20.650	4.893	1.00	22.56	?	1	NAG	E	C1	1
HETATM	5073	C	C2	.	NAG	E	3	.	?	37.104	21.268	5.555	1.00	30.15	?	1	NAG	E	C2	1
HETATM	5074	C	C3	.	NAG	E	3	.	?	38.299	20.356	5.576	1.00	30.02	?	1	NAG	E	C3	1
HETATM	5075	C	C4	.	NAG	E	3	.	?	37.901	18.990	6.097	1.00	27.08	?	1	NAG	E	C4	1
HETATM	5076	C	C5	.	NAG	E	3	.	?	36.704	18.416	5.335	1.00	26.79	?	1	NAG	E	C5	1
HETATM	5077	C	C6	.	NAG	E	3	.	?	36.168	17.108	5.930	1.00	25.93	?	1	NAG	E	C6	1
HETATM	5078	C	C7	.	NAG	E	3	.	?	37.278	23.649	5.795	1.00	37.04	?	1	NAG	E	C7	1
HETATM	5079	C	C8	.	NAG	E	3	.	?	37.049	24.933	5.037	1.00	53.78	?	1	NAG	E	C8	1
HETATM	5080	N	N2	.	NAG	E	3	.	?	37.473	22.581	5.018	1.00	36.08	?	1	NAG	E	N2	1
HETATM	5081	O	O3	.	NAG	E	3	.	?	39.195	20.903	6.586	1.00	36.65	?	1	NAG	E	O3	1
HETATM	5082	O	O4	.	NAG	E	3	.	?	39.010	18.099	6.001	1.00	34.37	?	1	NAG	E	O4	1
HETATM	5083	O	O5	.	NAG	E	3	.	?	35.614	19.356	5.369	1.00	24.51	?	1	NAG	E	O5	1
HETATM	5084	O	O6	.	NAG	E	3	.	?	36.104	17.215	7.365	1.00	21.96	?	1	NAG	E	O6	1
HETATM	5085	O	O7	.	NAG	E	3	.	?	37.284	23.608	7.022	1.00	53.48	?	1	NAG	E	O7	1
HETATM	5086	C	C1	.	NAG	E	3	.	?	39.385	17.481	7.185	1.00	36.71	?	2	NAG	E	C1	1
HETATM	5087	C	C2	.	NAG	E	3	.	?	40.647	16.688	7.073	1.00	31.39	?	2	NAG	E	C2	1
HETATM	5088	C	C3	.	NAG	E	3	.	?	40.931	16.001	8.392	1.00	35.05	?	2	NAG	E	C3	1
HETATM	5089	C	C4	.	NAG	E	3	.	?	40.967	16.962	9.541	1.00	32.61	?	2	NAG	E	C4	1
HETATM	5090	C	C5	.	NAG	E	3	.	?	39.666	17.783	9.563	1.00	28.91	?	2	NAG	E	C5	1
HETATM	5091	C	C6	.	NAG	E	3	.	?	39.666	18.963	10.521	1.00	35.91	?	2	NAG	E	C6	1
HETATM	5092	C	C7	.	NAG	E	3	.	?	40.571	15.771	4.825	1.00	47.69	?	2	NAG	E	C7	1

HETATM	5093	C	C8	NAG E 3	?	41.437	14.692	4.234	1.00	41.34	?	2	NAG E	C8	1
HETATM	5094	N	N2	NAG E 3	?	40.415	15.590	6.124	1.00	38.22	?	2	NAG E	N2	1
HETATM	5095	O	O3	NAG E 3	?	42.095	15.183	8.215	1.00	43.65	?	2	NAG E	O3	1
HETATM	5096	O	O4	NAG E 3	?	41.151	16.298	10.790	1.00	35.78	?	2	NAG E	O4	1
HETATM	5097	O	O5	NAG E 3	?	39.390	18.346	8.265	1.00	33.88	?	2	NAG E	O5	1
HETATM	5098	O	O6	NAG E 3	?	38.344	19.254	10.997	1.00	51.88	?	2	NAG E	O6	1
HETATM	5099	O	O7	NAG E 3	?	40.073	16.681	4.178	1.00	79.63	?	2	NAG E	O7	1
HETATM	5100	C	C1	BMA E 3	?	42.097	16.784	11.695	1.00	42.84	?	3	BMA E	C1	1
HETATM	5101	C	C2	BMA E 3	?	41.865	16.288	13.096	1.00	43.10	?	3	BMA E	C2	1
HETATM	5102	C	C3	BMA E 3	?	42.943	16.985	13.980	1.00	47.36	?	3	BMA E	C3	1
HETATM	5103	C	C4	BMA E 3	?	44.290	16.424	13.474	1.00	44.98	?	3	BMA E	C4	1
HETATM	5104	C	C5	BMA E 3	?	44.507	16.889	12.052	1.00	49.37	?	3	BMA E	C5	1
HETATM	5105	C	C6	BMA E 3	?	45.841	16.392	11.476	1.00	50.83	?	3	BMA E	C6	1
HETATM	5106	O	O2	BMA E 3	?	42.156	14.859	13.168	1.00	38.32	?	3	BMA E	O2	1
HETATM	5107	O	O3	BMA E 3	?	42.845	16.435	15.311	1.00	49.32	?	3	BMA E	O3	1
HETATM	5108	O	O4	BMA E 3	?	45.320	16.945	14.296	1.00	54.09	?	3	BMA E	O4	1
HETATM	5109	O	O5	BMA E 3	?	43.409	16.440	11.229	1.00	50.64	?	3	BMA E	O5	1
HETATM	5110	O	O6	BMA E 3	?	46.044	14.956	11.468	1.00	60.64	?	3	BMA E	O6	1
HETATM	5111	C	C1	MAN E 3	?	42.913	17.368	16.363	1.00	51.69	?	4	MAN E	C1	1
HETATM	5112	C	C2	MAN E 3	?	42.977	16.574	17.663	1.00	60.04	?	4	MAN E	C2	1
HETATM	5113	C	C3	MAN E 3	?	41.902	15.496	17.476	1.00	63.95	?	4	MAN E	C3	1
HETATM	5114	C	C4	MAN E 3	?	40.526	16.156	17.379	1.00	60.30	?	4	MAN E	C4	1
HETATM	5115	C	C5	MAN E 3	?	40.528	17.198	16.298	1.00	56.41	?	4	MAN E	C5	1
HETATM	5116	C	C6	MAN E 3	?	39.257	18.005	16.043	1.00	54.83	?	4	MAN E	C6	1
HETATM	5117	O	O2	MAN E 3	?	42.775	17.477	18.789	1.00	46.92	?	4	MAN E	O2	1
HETATM	5118	O	O3	MAN E 3	?	41.959	14.538	18.533	1.00	79.05	?	4	MAN E	O3	1
HETATM	5119	O	O4	MAN E 3	?	39.525	15.184	17.115	1.00	49.74	?	4	MAN E	O4	1
HETATM	5120	O	O5	MAN E 3	?	41.655	18.094	16.369	1.00	52.25	?	4	MAN E	O5	1
HETATM	5121	O	O6	MAN E 3	?	39.368	18.974	14.965	1.00	49.83	?	4	MAN E	O6	1
HETATM	5122	C	C1	FUC E 3	?	40.249	21.729	6.085	1.00	49.04	?	5	FUC E	C1	1
HETATM	5123	C	C2	FUC E 3	?	41.031	22.463	7.181	1.00	43.14	?	5	FUC E	C2	1
HETATM	5124	C	C3	FUC E 3	?	41.925	21.537	7.988	1.00	54.66	?	5	FUC E	C3	1
HETATM	5125	C	C4	FUC E 3	?	42.813	20.733	7.029	1.00	54.35	?	5	FUC E	C4	1
HETATM	5126	C	C5	FUC E 3	?	41.910	19.991	6.016	1.00	55.62	?	5	FUC E	C5	1
HETATM	5127	C	C6	FUC E 3	?	42.663	19.219	4.977	1.00	42.57	?	5	FUC E	C6	1
HETATM	5128	O	O2	FUC E 3	?	40.136	23.111	8.077	1.00	47.37	?	5	FUC E	O2	1
HETATM	5129	O	O3	FUC E 3	?	42.691	22.301	8.922	1.00	86.06	?	5	FUC E	O3	1
HETATM	5130	O	O4	FUC E 3	?	43.646	21.632	6.310	1.00	60.09	?	5	FUC E	O4	1
HETATM	5131	O	O5	FUC E 3	?	41.100	20.948	5.251	1.00	56.15	?	5	FUC E	O5	1
HETATM	5132	C	C1	NAG F 4	?	20.063	-22.064	24.947	1.00	29.49	?	1	NAG F	C1	1
HETATM	5133	C	C2	NAG F 4	?	20.028	-23.128	25.994	1.00	41.96	?	1	NAG F	C2	1
HETATM	5134	C	C3	NAG F 4	?	18.875	-22.872	26.925	1.00	47.29	?	1	NAG F	C3	1
HETATM	5135	C	C4	NAG F 4	?	18.905	-21.466	27.475	1.00	49.79	?	1	NAG F	C4	1
HETATM	5136	C	C5	NAG F 4	?	18.973	-20.463	26.305	1.00	36.92	?	1	NAG F	C5	1
HETATM	5137	C	C6	NAG F 4	?	19.081	-19.020	26.758	1.00	32.87	?	1	NAG F	C6	1
HETATM	5138	C	C7	A NAG F 4	?	21.077	-25.259	25.482	0.72	43.79	?	1	NAG F	C7	1
HETATM	5139	C	C7	B NAG F 4	?	19.216	-24.662	24.244	0.28	43.98	?	1	NAG F	C7	1
HETATM	5140	C	C8	A NAG F 4	?	21.165	-26.191	24.296	0.72	50.88	?	1	NAG F	C8	1
HETATM	5141	C	C8	B NAG F 4	?	17.734	-24.925	24.341	0.28	32.44	?	1	NAG F	C8	1
HETATM	5142	N	N2	A NAG F 4	?	20.008	-24.476	25.448	0.72	43.09	?	1	NAG F	N2	1
HETATM	5143	N	N2	B NAG F 4	?	19.821	-24.455	25.401	0.28	43.57	?	1	NAG F	N2	1
HETATM	5144	O	O3	NAG F 4	?	18.920	-23.795	28.041	1.00	57.75	?	1	NAG F	O3	1
HETATM	5145	O	O4	NAG F 4	?	17.730	-21.261	28.248	1.00	54.51	?	1	NAG F	O4	1
HETATM	5146	O	O5	NAG F 4	?	20.165	-20.790	25.534	1.00	29.19	?	1	NAG F	O5	1
HETATM	5147	O	O6	NAG F 4	?	20.257	-18.838	27.554	1.00	35.82	?	1	NAG F	O6	1
HETATM	5148	O	O7	A NAG F 4	?	21.933	-25.266	26.359	0.72	38.83	?	1	NAG F	O7	1
HETATM	5149	O	O7	B NAG F 4	?	19.793	-24.653	23.159	0.28	54.77	?	1	NAG F	O7	1
HETATM	5150	C	C1	NAG F 4	?	17.810	-20.607	29.466	1.00	51.07	?	2	NAG F	C1	1
HETATM	5151	C	C2	NAG F 4	?	16.427	-20.315	29.968	1.00	40.53	?	2	NAG F	C2	1

HETATM	5152	C	C3	NAG	F	4	?	16.433	-19.728	31.351	1.00	55.87	?	2	NAG	F	C3	1
HETATM	5153	C	C4	NAG	F	4	?	17.457	-20.308	32.283	1.00	72.14	?	2	NAG	F	C4	1
HETATM	5154	C	C5	NAG	F	4	?	18.824	-20.530	31.611	1.00	64.24	?	2	NAG	F	C5	1
HETATM	5155	C	C6	NAG	F	4	?	19.812	-21.311	32.464	1.00	60.22	?	2	NAG	F	C6	1
HETATM	5156	C	C7	NAG	F	4	?	14.740	-19.582	28.390	1.00	52.83	?	2	NAG	F	C7	1
HETATM	5157	C	C8	NAG	F	4	?	13.557	-20.004	29.229	1.00	74.85	?	2	NAG	F	C8	1
HETATM	5158	N	N2	NAG	F	4	?	15.831	-19.294	29.090	1.00	43.93	?	2	NAG	F	N2	1
HETATM	5159	O	O3	NAG	F	4	?	15.101	-19.840	31.894	1.00	42.65	?	2	NAG	F	O3	1
HETATM	5160	O	O4	NAG	F	4	?	17.650	-19.445	33.404	1.00	87.58	?	2	NAG	F	O4	1
HETATM	5161	O	O5	NAG	F	4	?	18.603	-21.292	30.394	1.00	59.45	?	2	NAG	F	O5	1
HETATM	5162	O	O6	NAG	F	4	?	20.317	-22.435	31.717	1.00	94.45	?	2	NAG	F	O6	1
HETATM	5163	O	O7	NAG	F	4	?	14.682	-19.508	27.167	1.00	75.95	?	2	NAG	F	O7	1
HETATM	5164	C	C1	BMA	F	4	?	16.933	-19.668	34.572	1.00	99.27	?	3	BMA	F	C1	1
HETATM	5165	C	C2	BMA	F	4	?	17.871	-19.717	35.751	1.00	104.96	?	3	BMA	F	C2	1
HETATM	5166	C	C3	BMA	F	4	?	16.994	-19.988	36.964	1.00	110.16	?	3	BMA	F	C3	1
HETATM	5167	C	C4	BMA	F	4	?	15.947	-18.899	37.144	1.00	108.29	?	3	BMA	F	C4	1
HETATM	5168	C	C5	BMA	F	4	?	15.086	-18.833	35.895	1.00	104.58	?	3	BMA	F	C5	1
HETATM	5169	C	C6	BMA	F	4	?	13.989	-17.767	35.968	1.00	103.25	?	3	BMA	F	C6	1
HETATM	5170	O	O2	BMA	F	4	?	18.763	-18.571	35.743	1.00	101.38	?	3	BMA	F	O2	1
HETATM	5171	O	O3	BMA	F	4	?	17.722	-20.215	38.168	1.00	136.64	?	3	BMA	F	O3	1
HETATM	5172	O	O4	BMA	F	4	?	15.100	-19.168	38.249	1.00	112.48	?	3	BMA	F	O4	1
HETATM	5173	O	O5	BMA	F	4	?	15.926	-18.651	34.736	1.00	101.95	?	3	BMA	F	O5	1
HETATM	5174	O	O6	BMA	F	4	?	13.025	-17.905	37.043	1.00	99.55	?	3	BMA	F	O6	1
HETATM	5175	C	C1	FUC	F	4	?	18.016	-24.895	27.976	1.00	66.14	?	4	FUC	F	C1	1
HETATM	5176	C	C2	FUC	F	4	?	18.391	-26.026	28.949	1.00	75.03	?	4	FUC	F	C2	1
HETATM	5177	C	C3	FUC	F	4	?	18.087	-25.634	30.390	1.00	81.78	?	4	FUC	F	C3	1
HETATM	5178	C	C4	FUC	F	4	?	16.620	-25.193	30.481	1.00	82.20	?	4	FUC	F	C4	1
HETATM	5179	C	C5	FUC	F	4	?	16.301	-24.071	29.472	1.00	74.09	?	4	FUC	F	C5	1
HETATM	5180	C	C6	FUC	F	4	?	14.832	-23.751	29.393	1.00	75.55	?	4	FUC	F	C6	1
HETATM	5181	O	O2	FUC	F	4	?	19.789	-26.283	28.871	1.00	68.49	?	4	FUC	F	O2	1
HETATM	5182	O	O3	FUC	F	4	?	18.334	-26.787	31.210	1.00	80.98	?	4	FUC	F	O3	1
HETATM	5183	O	O4	FUC	F	4	?	15.789	-26.312	30.235	1.00	89.82	?	4	FUC	F	O4	1
HETATM	5184	O	O5	FUC	F	4	?	16.670	-24.466	28.106	1.00	65.17	?	4	FUC	F	O5	1
HETATM	5185	C	C1	NAG	G	5	?	-13.900	13.276	22.185	1.00	36.70	?	1	NAG	G	C1	1
HETATM	5186	C	C2	NAG	G	5	?	-14.663	12.946	23.436	1.00	49.77	?	1	NAG	G	C2	1
HETATM	5187	C	C3	NAG	G	5	?	-15.606	14.030	23.879	1.00	46.58	?	1	NAG	G	C3	1
HETATM	5188	C	C4	NAG	G	5	?	-14.780	15.297	24.100	1.00	47.28	?	1	NAG	G	C4	1
HETATM	5189	C	C5	NAG	G	5	?	-14.026	15.645	22.800	1.00	47.34	?	1	NAG	G	C5	1
HETATM	5190	C	C6	NAG	G	5	?	-13.042	16.799	22.962	1.00	44.03	?	1	NAG	G	C6	1
HETATM	5191	C	C7	NAG	G	5	?	-15.088	10.737	24.319	1.00	65.77	?	1	NAG	G	C7	1
HETATM	5192	C	C8	NAG	G	5	?	-16.332	9.965	24.695	1.00	87.14	?	1	NAG	G	C8	1
HETATM	5193	N	N2	NAG	G	5	?	-15.319	11.648	23.377	1.00	64.56	?	1	NAG	G	N2	1
HETATM	5194	O	O3	NAG	G	5	?	-16.170	13.616	25.149	1.00	53.92	?	1	NAG	G	O3	1
HETATM	5195	O	O4	NAG	G	5	?	-15.608	16.387	24.448	1.00	32.21	?	1	NAG	G	O4	1
HETATM	5196	O	O5	NAG	G	5	?	-13.268	14.522	22.323	1.00	41.57	?	1	NAG	G	O5	1
HETATM	5197	O	O6	NAG	G	5	?	-12.143	16.581	24.056	1.00	40.14	?	1	NAG	G	O6	1
HETATM	5198	O	O7	NAG	G	5	?	-14.003	10.517	24.850	1.00	58.28	?	1	NAG	G	O7	1
HETATM	5199	C	C1	NAG	G	5	?	-15.295	17.230	25.505	1.00	33.64	?	2	NAG	G	C1	1
HETATM	5200	C	C2	NAG	G	5	?	-16.412	18.217	25.730	1.00	33.61	?	2	NAG	G	C2	1
HETATM	5201	C	C3	NAG	G	5	?	-16.141	19.057	26.949	1.00	29.99	?	2	NAG	G	C3	1
HETATM	5202	C	C4	NAG	G	5	?	-15.883	18.211	28.154	1.00	24.21	?	2	NAG	G	C4	1
HETATM	5203	C	C5	NAG	G	5	?	-14.802	17.183	27.852	1.00	33.88	?	2	NAG	G	C5	1
HETATM	5204	C	C6	NAG	G	5	?	-14.480	16.209	28.968	1.00	38.02	?	2	NAG	G	C6	1
HETATM	5205	C	C7	NAG	G	5	?	-16.994	18.707	23.414	1.00	62.96	?	2	NAG	G	C7	1
HETATM	5206	C	C8	NAG	G	5	?	-17.550	19.840	22.579	1.00	70.93	?	2	NAG	G	C8	1
HETATM	5207	N	N2	NAG	G	5	?	-16.524	19.118	24.584	1.00	40.34	?	2	NAG	G	N2	1
HETATM	5208	O	O3	NAG	G	5	?	-17.235	19.962	27.174	1.00	33.43	?	2	NAG	G	O3	1
HETATM	5209	O	O4	NAG	G	5	?	-15.514	19.002	29.276	1.00	29.85	?	2	NAG	G	O4	1
HETATM	5210	O	O5	NAG	G	5	?	-15.070	16.451	26.649	1.00	33.97	?	2	NAG	G	O5	1

HETATM	5211	O	O6	NAG	G	5	?	-13.118	15.749	28.826	1.00	64.06	?	2	NAG	G	O6	1
HETATM	5212	O	O7	NAG	G	5	?	-16.990	17.544	23.020	1.00	80.38	?	2	NAG	G	O7	1
HETATM	5213	C	C1	BMA	G	5	?	-16.074	18.667	30.514	1.00	31.63	?	3	BMA	G	C1	1
HETATM	5214	C	C2	BMA	G	5	?	-15.133	18.955	31.638	1.00	27.34	?	3	BMA	G	C2	1
HETATM	5215	C	C3	BMA	G	5	?	-15.788	18.591	32.973	1.00	39.35	?	3	BMA	G	C3	1
HETATM	5216	C	C4	BMA	G	5	?	-17.120	19.322	33.095	1.00	39.33	?	3	BMA	G	C4	1
HETATM	5217	C	C5	BMA	G	5	?	-18.000	19.123	31.894	1.00	42.73	?	3	BMA	G	C5	1
HETATM	5218	C	C6	BMA	G	5	?	-19.236	20.029	31.974	1.00	56.20	?	3	BMA	G	C6	1
HETATM	5219	O	O2	BMA	G	5	?	-14.706	20.342	31.653	1.00	33.11	?	3	BMA	G	O2	1
HETATM	5220	O	O3	BMA	G	5	?	-14.979	19.159	34.045	1.00	37.28	?	3	BMA	G	O3	1
HETATM	5221	O	O4	BMA	G	5	?	-17.786	18.900	34.277	1.00	36.16	?	3	BMA	G	O4	1
HETATM	5222	O	O5	BMA	G	5	?	-17.320	19.358	30.648	1.00	35.83	?	3	BMA	G	O5	1
HETATM	5223	O	O6	BMA	G	5	?	-20.225	19.889	30.948	1.00	89.67	?	3	BMA	G	O6	1
HETATM	5224	C	C1	MAN	G	5	?	-14.582	18.227	35.020	1.00	34.71	?	4	MAN	G	C1	1
HETATM	5225	C	C2	MAN	G	5	?	-14.044	18.946	36.239	1.00	30.57	?	4	MAN	G	C2	1
HETATM	5226	C	C3	MAN	G	5	?	-12.989	19.926	35.693	1.00	38.15	?	4	MAN	G	C3	1
HETATM	5227	C	C4	MAN	G	5	?	-11.864	19.143	35.024	1.00	40.70	?	4	MAN	G	C4	1
HETATM	5228	C	C5	MAN	G	5	?	-12.414	18.193	33.968	1.00	37.86	?	4	MAN	G	C5	1
HETATM	5229	C	C6	MAN	G	5	?	-11.308	17.232	33.476	1.00	40.28	?	4	MAN	G	C6	1
HETATM	5230	O	O2	MAN	G	5	?	-13.495	17.899	37.111	1.00	29.24	?	4	MAN	G	O2	1
HETATM	5231	O	O3	MAN	G	5	?	-12.451	20.740	36.748	1.00	34.14	?	4	MAN	G	O3	1
HETATM	5232	O	O4	MAN	G	5	?	-10.959	19.998	34.331	1.00	27.31	?	4	MAN	G	O4	1
HETATM	5233	O	O5	MAN	G	5	?	-13.502	17.408	34.513	1.00	30.22	?	4	MAN	G	O5	1
HETATM	5234	O	O6	MAN	G	5	?	-11.830	16.068	32.789	1.00	44.16	?	4	MAN	G	O6	1
HETATM	5235	C	C1	MAN	G	5	?	-20.331	20.912	29.984	1.00	115.47	?	5	MAN	G	C1	1
HETATM	5236	C	C2	MAN	G	5	?	-20.866	22.174	30.641	1.00	123.89	?	5	MAN	G	C2	1
HETATM	5237	C	C3	MAN	G	5	?	-22.040	21.692	31.470	1.00	128.01	?	5	MAN	G	C3	1
HETATM	5238	C	C4	MAN	G	5	?	-23.073	20.912	30.692	1.00	130.39	?	5	MAN	G	C4	1
HETATM	5239	C	C5	MAN	G	5	?	-22.480	19.922	29.723	1.00	127.13	?	5	MAN	G	C5	1
HETATM	5240	C	C6	MAN	G	5	?	-23.452	19.277	28.732	1.00	123.05	?	5	MAN	G	C6	1
HETATM	5241	O	O2	MAN	G	5	?	-21.022	23.223	29.652	1.00	135.93	?	5	MAN	G	O2	1
HETATM	5242	O	O3	MAN	G	5	?	-22.585	22.686	32.333	1.00	124.59	?	5	MAN	G	O3	1
HETATM	5243	O	O4	MAN	G	5	?	-23.939	20.197	31.572	1.00	137.56	?	5	MAN	G	O4	1
HETATM	5244	O	O5	MAN	G	5	?	-21.347	20.483	29.023	1.00	125.42	?	5	MAN	G	O5	1
HETATM	5245	O	O6	MAN	G	5	?	-22.907	18.874	27.455	1.00	105.59	?	5	MAN	G	O6	1
HETATM	5246	C	C1	FUC	G	5	?	-17.464	13.018	25.220	1.00	54.35	?	6	FUC	G	C1	1
HETATM	5247	C	C2	FUC	G	5	?	-17.792	12.498	26.647	1.00	57.72	?	6	FUC	G	C2	1
HETATM	5248	C	C3	FUC	G	5	?	-17.742	13.637	27.649	1.00	64.98	?	6	FUC	G	C3	1
HETATM	5249	C	C4	FUC	G	5	?	-18.766	14.703	27.199	1.00	65.03	?	6	FUC	G	C4	1
HETATM	5250	C	C5	FUC	G	5	?	-18.490	15.115	25.744	1.00	60.69	?	6	FUC	G	C5	1
HETATM	5251	C	C6	FUC	G	5	?	-19.491	16.053	25.149	1.00	80.94	?	6	FUC	G	C6	1
HETATM	5252	O	O2	FUC	G	5	?	-16.849	11.494	26.982	1.00	50.50	?	6	FUC	G	O2	1
HETATM	5253	O	O3	FUC	G	5	?	-18.078	13.200	28.971	1.00	54.76	?	6	FUC	G	O3	1
HETATM	5254	O	O4	FUC	G	5	?	-20.055	14.118	27.295	1.00	81.13	?	6	FUC	G	O4	1
HETATM	5255	O	O5	FUC	G	5	?	-18.477	13.953	24.851	1.00	53.54	?	6	FUC	G	O5	1
HETATM	5256	C	C1	NAG	H	4	?	15.231	53.524	28.709	1.00	32.98	?	1	NAG	H	C1	1
HETATM	5257	C	C2	NAG	H	4	?	16.081	54.651	29.212	1.00	46.15	?	1	NAG	H	C2	1
HETATM	5258	C	C3	NAG	H	4	?	17.445	54.135	29.615	1.00	54.21	?	1	NAG	H	C3	1
HETATM	5259	C	C4	NAG	H	4	?	17.346	52.965	30.565	1.00	54.63	?	1	NAG	H	C4	1
HETATM	5260	C	C5	NAG	H	4	?	16.463	51.859	29.959	1.00	42.67	?	1	NAG	H	C5	1
HETATM	5261	C	C6	NAG	H	4	?	16.115	50.722	30.907	1.00	33.70	?	1	NAG	H	C6	1
HETATM	5262	C	C7	NAG	H	4	?	15.766	56.820	28.185	1.00	65.39	?	1	NAG	H	C7	1
HETATM	5263	C	C8	NAG	H	4	?	16.043	57.665	26.964	1.00	55.43	?	1	NAG	H	C8	1
HETATM	5264	N	N2	NAG	H	4	?	16.318	55.612	28.115	1.00	56.22	?	1	NAG	H	N2	1
HETATM	5265	O	O3	NAG	H	4	?	18.200	55.208	30.239	1.00	65.63	?	1	NAG	H	O3	1
HETATM	5266	O	O4	NAG	H	4	?	18.640	52.459	30.857	1.00	62.00	?	1	NAG	H	O4	1
HETATM	5267	O	O5	NAG	H	4	?	15.186	52.436	29.589	1.00	39.48	?	1	NAG	H	O5	1
HETATM	5268	O	O6	NAG	H	4	?	15.077	51.123	31.814	1.00	43.49	?	1	NAG	H	O6	1
HETATM	5269	O	O7	NAG	H	4	?	15.093	57.226	29.130	1.00	66.70	?	1	NAG	H	O7	1

HETATM	5270	C	C1	.	NAG	H	4	.	?	19.037	52.162	32.156	1.00	76.62	?	2	NAG	H	C1	1
HETATM	5271	C	C2	.	NAG	H	4	.	?	20.525	51.977	32.184	1.00	85.78	?	2	NAG	H	C2	1
HETATM	5272	C	C3	.	NAG	H	4	.	?	21.106	51.954	33.573	1.00	101.90	?	2	NAG	H	C3	1
HETATM	5273	C	C4	.	NAG	H	4	.	?	20.605	53.113	34.402	1.00	110.98	?	2	NAG	H	C4	1
HETATM	5274	C	C5	.	NAG	H	4	.	?	19.065	53.062	34.400	1.00	100.71	?	2	NAG	H	C5	1
HETATM	5275	C	C6	.	NAG	H	4	.	?	18.401	54.188	35.178	1.00	103.95	?	2	NAG	H	C6	1
HETATM	5276	C	C7	.	NAG	H	4	.	?	20.521	50.341	30.335	1.00	72.00	?	2	NAG	H	C7	1
HETATM	5277	C	C8	.	NAG	H	4	.	?	20.672	51.386	29.258	1.00	88.76	?	2	NAG	H	C8	1
HETATM	5278	N	N2	.	NAG	H	4	.	?	20.869	50.704	31.553	1.00	79.69	?	2	NAG	H	N2	1
HETATM	5279	O	O3	.	NAG	H	4	.	?	22.542	52.004	33.450	1.00	127.35	?	2	NAG	H	O3	1
HETATM	5280	O	O4	.	NAG	H	4	.	?	21.060	53.035	35.744	1.00	125.41	?	2	NAG	H	O4	1
HETATM	5281	O	O5	.	NAG	H	4	.	?	18.596	53.143	33.041	1.00	87.62	?	2	NAG	H	O5	1
HETATM	5282	O	O6	.	NAG	H	4	.	?	17.010	53.860	35.371	1.00	122.67	?	2	NAG	H	O6	1
HETATM	5283	O	O7	.	NAG	H	4	.	?	20.112	49.210	30.080	1.00	62.68	?	2	NAG	H	O7	1
HETATM	5284	C	C1	.	BMA	H	4	.	?	22.246	53.639	36.148	1.00	136.26	?	3	BMA	H	C1	1
HETATM	5285	C	C2	.	BMA	H	4	.	?	23.066	52.621	36.921	1.00	142.24	?	3	BMA	H	C2	1
HETATM	5286	C	C3	.	BMA	H	4	.	?	22.318	52.451	38.242	1.00	147.60	?	3	BMA	H	C3	1
HETATM	5287	C	C4	.	BMA	H	4	.	?	22.509	53.674	39.117	1.00	147.23	?	3	BMA	H	C4	1
HETATM	5288	C	C5	.	BMA	H	4	.	?	22.624	54.900	38.238	1.00	144.03	?	3	BMA	H	C5	1
HETATM	5289	C	C6	.	BMA	H	4	.	?	24.038	55.533	38.121	1.00	144.35	?	3	BMA	H	C6	1
HETATM	5290	O	O2	.	BMA	H	4	.	?	24.462	53.047	36.956	1.00	134.70	?	3	BMA	H	O2	1
HETATM	5291	O	O3	.	BMA	H	4	.	?	22.584	51.226	38.918	1.00	153.42	?	3	BMA	H	O3	1
HETATM	5292	O	O4	.	BMA	H	4	.	?	21.366	53.871	40.008	1.00	148.18	?	3	BMA	H	O4	1
HETATM	5293	O	O5	.	BMA	H	4	.	?	21.917	54.767	36.989	1.00	139.91	?	3	BMA	H	O5	1
HETATM	5294	O	O6	.	BMA	H	4	.	?	24.761	55.511	39.424	1.00	138.93	?	3	BMA	H	O6	1
HETATM	5295	C	C1	A	FUC	H	4	.	?	19.608	55.038	30.371	0.73	75.86	?	4	FUC	H	C1	1
HETATM	5296	C	C1	B	FUC	H	4	.	?	17.854	55.552	31.568	0.27	69.15	?	4	FUC	H	C1	1
HETATM	5297	C	C2	A	FUC	H	4	.	?	20.453	55.853	29.374	0.73	80.15	?	4	FUC	H	C2	1
HETATM	5298	C	C2	B	FUC	H	4	.	?	18.459	56.850	32.152	0.27	74.61	?	4	FUC	H	C2	1
HETATM	5299	C	C3	A	FUC	H	4	.	?	20.328	57.346	29.643	0.73	81.58	?	4	FUC	H	C3	1
HETATM	5300	C	C3	B	FUC	H	4	.	?	17.512	58.003	32.379	0.27	73.01	?	4	FUC	H	C3	1
HETATM	5301	C	C4	A	FUC	H	4	.	?	20.864	57.558	31.075	0.73	83.11	?	4	FUC	H	C4	1
HETATM	5302	C	C4	B	FUC	H	4	.	?	16.202	57.483	32.993	0.27	68.53	?	4	FUC	H	C4	1
HETATM	5303	C	C5	A	FUC	H	4	.	?	20.049	56.702	32.073	0.73	78.94	?	4	FUC	H	C5	1
HETATM	5304	C	C5	B	FUC	H	4	.	?	15.604	56.414	32.054	0.27	65.73	?	4	FUC	H	C5	1
HETATM	5305	C	C6	A	FUC	H	4	.	?	20.612	56.725	33.464	0.73	71.65	?	4	FUC	H	C6	1
HETATM	5306	C	C6	B	FUC	H	4	.	?	14.316	55.827	32.552	0.27	45.47	?	4	FUC	H	C6	1
HETATM	5307	O	O2	A	FUC	H	4	.	?	20.073	55.579	28.043	0.73	103.13	?	4	FUC	H	O2	1
HETATM	5308	O	O2	B	FUC	H	4	.	?	19.513	57.294	31.306	0.27	79.01	?	4	FUC	H	O2	1
HETATM	5309	O	O3	A	FUC	H	4	.	?	21.100	58.085	28.683	0.73	54.89	?	4	FUC	H	O3	1
HETATM	5310	O	O3	B	FUC	H	4	.	?	18.135	58.945	33.265	0.27	82.48	?	4	FUC	H	O3	1
HETATM	5311	O	O4	A	FUC	H	4	.	?	22.204	57.082	31.089	0.73	105.44	?	4	FUC	H	O4	1
HETATM	5312	O	O4	B	FUC	H	4	.	?	16.511	56.873	34.237	0.27	72.74	?	4	FUC	H	O4	1
HETATM	5313	O	O5	A	FUC	H	4	.	?	20.053	55.283	31.699	0.73	79.70	?	4	FUC	H	O5	1
HETATM	5314	O	O5	B	FUC	H	4	.	?	16.523	55.284	31.929	0.27	66.98	?	4	FUC	H	O5	1

...
#

...
#

_database_PDB_caveat.id 1

_database_PDB_caveat.text 'BMA H 3 HAS WRONG CHIRALITY AT ATOM C1'

#