wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 06:22 AM EDT

PDB ID	:	2GK1
Title	:	X-ray crystal structure of NGT-bound HexA
Authors	:	Lemieux, M.J.; Mark, B.L.; Cherney, M.M.; Withers, S.G.; Mahuran, D.J.; James, M.N.
Deposited on	:	2006-03-31
Resolution	:	3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

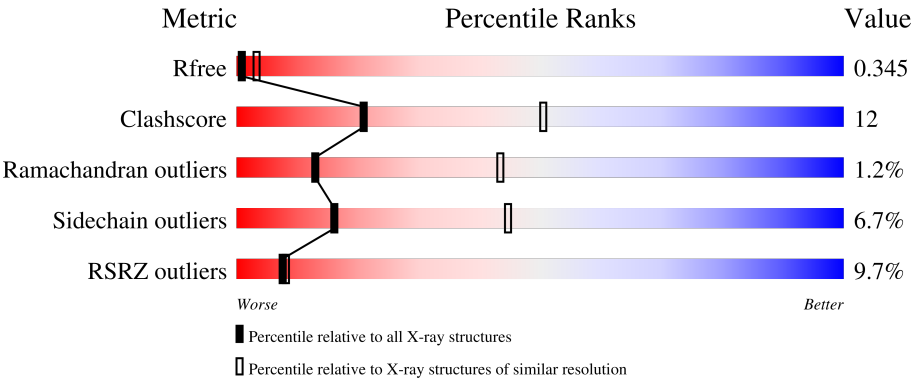
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	52	52% 37% 12%
1	C	52	2% 54% 42% ·
1	E	52	10% 62% 35% ·
1	G	52	4% 52% 44% ·
2	I	440	2% 66% 30% ·

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Mol	Chain	Length	Quality of chain
2	J	440	5% 71% 25%
2	K	440	11% 71% 26%
2	L	440	14% 67% 30%
3	B	58	2% 76% 10% 7% 7%
3	D	58	2% 83% 10% 7%
3	F	58	21% 66% 26% 7%
3	H	58	28% 59% 33% 7%
4	M	190	6% 73% 26%
4	O	190	4% 75% 23%
4	Q	190	15% 65% 34%
4	S	190	16% 79% 21%
5	N	237	4% 76% 23%
5	P	237	4% 69% 28%
5	R	237	11% 71% 27%
5	T	237	32% 75% 24%
6	U	3	100%
6	V	3	100%
6	W	3	100%
6	Y	3	33% 67%
6	d	3	33% 67%
7	X	2	50% 50%
7	Z	2	100%
7	a	2	100%
7	b	2	50% 50%
7	c	2	100%

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Mol	Chain	Length	Quality of chain
7	e	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	Y	1	-	-	X	-
6	NAG	Y	2	X	-	-	-
6	BMA	Y	3	-	-	-	X
6	NAG	d	2	X	-	-	-
7	NAG	X	1	-	-	-	X
7	NAG	X	2	-	-	-	X
7	NAG	Z	1	X	-	-	-
7	NAG	Z	2	X	-	-	-
7	NAG	a	1	X	-	-	-
7	NAG	a	2	X	-	-	X
7	NAG	b	1	X	-	-	-
7	NAG	b	2	X	-	-	-
7	NAG	c	2	X	-	-	X
7	NAG	e	2	X	-	-	-
8	NGT	A	21	-	-	X	-
8	NGT	C	530	-	-	X	-
8	NGT	E	530	-	-	X	-
8	NGT	G	533	-	-	X	-
8	NGT	H	28	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 32011 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-hexosaminidase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	52	Total	C	N	O	S	0	0	0
			441	286	73	81	1			
1	C	52	Total	C	N	O	S	0	0	0
			441	286	73	81	1			
1	E	52	Total	C	N	O	S	0	0	0
			441	286	73	81	1			
1	G	52	Total	C	N	O	S	0	0	0
			441	286	73	81	1			

- Molecule 2 is a protein called Beta-hexosaminidase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	440	Total	C	N	O	S	0	0	0
			3565	2312	577	663	13			
2	J	440	Total	C	N	O	S	0	0	0
			3565	2312	577	663	13			
2	K	440	Total	C	N	O	S	0	0	0
			3565	2312	577	663	13			
2	L	440	Total	C	N	O	S	0	0	0
			3565	2312	577	663	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	436	VAL	ILE	variant	UNP P06865
J	436	VAL	ILE	variant	UNP P06865
K	436	VAL	ILE	variant	UNP P06865
L	436	VAL	ILE	variant	UNP P06865

- Molecule 3 is a protein called Beta-hexosaminidase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	54	Total	C	N	O	S	0	0	0
			428	281	71	74	2			
3	D	54	Total	C	N	O	S	0	0	0
			428	281	71	74	2			
3	F	54	Total	C	N	O	S	0	0	0
			428	281	71	74	2			
3	H	54	Total	C	N	O	S	0	0	0
			428	281	71	74	2			

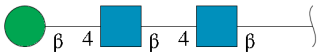
- Molecule 4 is a protein called Beta-hexosaminidase subunit beta chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	190	Total	C	N	O	S	0	0	0
			1528	982	256	286	4			
4	O	189	Total	C	N	O	S	0	0	0
			1522	979	255	284	4			
4	Q	190	Total	C	N	O	S	0	0	0
			1528	982	256	286	4			
4	S	190	Total	C	N	O	S	0	0	0
			1528	982	256	286	4			

- Molecule 5 is a protein called Beta-hexosaminidase subunit beta chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	236	Total	C	N	O	S	0	0	0
			1921	1242	316	356	7			
5	P	236	Total	C	N	O	S	0	0	0
			1921	1242	316	356	7			
5	R	236	Total	C	N	O	S	0	0	0
			1921	1242	316	356	7			
5	T	236	Total	C	N	O	S	0	0	0
			1921	1242	316	356	7			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	U	3	Total	C	N	O	0	0	0
			39	22	2	15			

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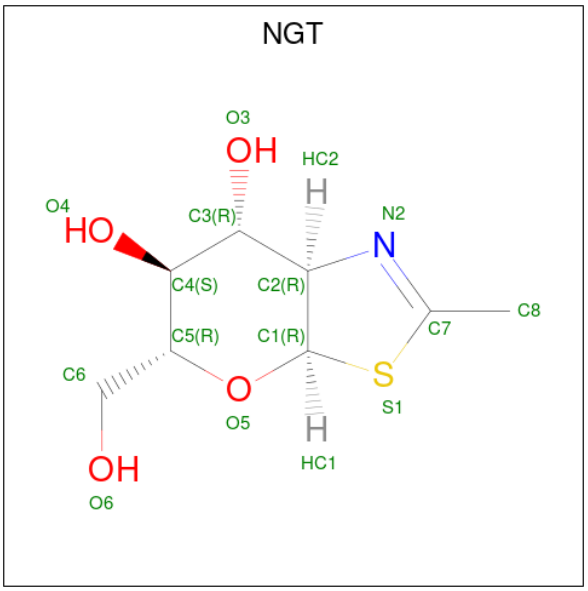
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	V	3	Total C N O 39 22 2 15	0	0	0
6	W	3	Total C N O 39 22 2 15	0	0	0
6	Y	3	Total C N O 39 22 2 15	0	0	0
6	d	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	X	2	Total C N O 28 16 2 10	0	0	0
7	Z	2	Total C N O 28 16 2 10	0	0	0
7	a	2	Total C N O 28 16 2 10	0	0	0
7	b	2	Total C N O 28 16 2 10	0	0	0
7	c	2	Total C N O 28 16 2 10	0	0	0
7	e	2	Total C N O 28 16 2 10	0	0	0

- Molecule 8 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (three-letter code: NGT) (formula: $C_8H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O S 14 8 1 4 1	0	0
8	B	1	Total C N O S 14 8 1 4 1	0	0
8	C	1	Total C N O S 14 8 1 4 1	0	0
8	D	1	Total C N O S 14 8 1 4 1	0	0
8	E	1	Total C N O S 14 8 1 4 1	0	0
8	F	1	Total C N O S 14 8 1 4 1	0	0
8	G	1	Total C N O S 14 8 1 4 1	0	0
8	H	1	Total C N O S 14 8 1 4 1	0	0

- Molecule 9 is water.

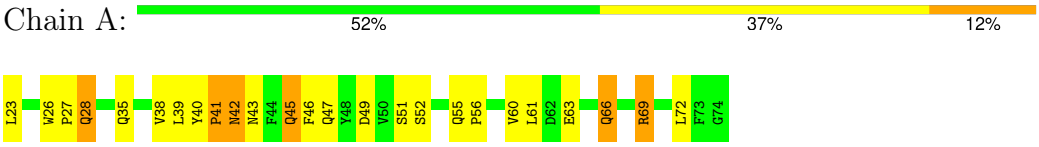
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	5	Total O 5 5	0	0
9	B	1	Total O 1 1	0	0
9	C	2	Total O 2 2	0	0
9	D	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

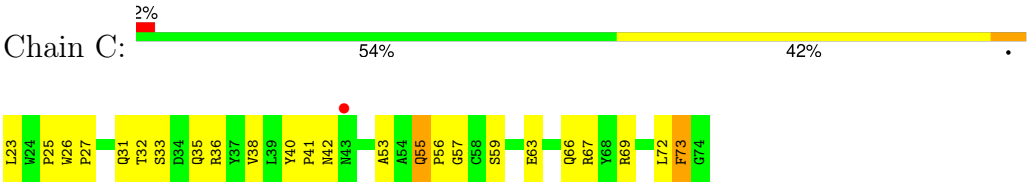
• Molecule 1: Beta-hexosaminidase subunit alpha

Chain A:



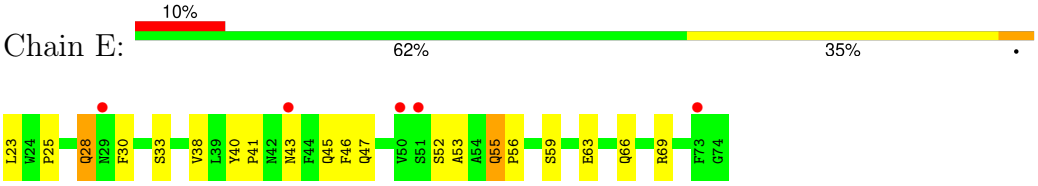
• Molecule 1: Beta-hexosaminidase subunit alpha

Chain C:



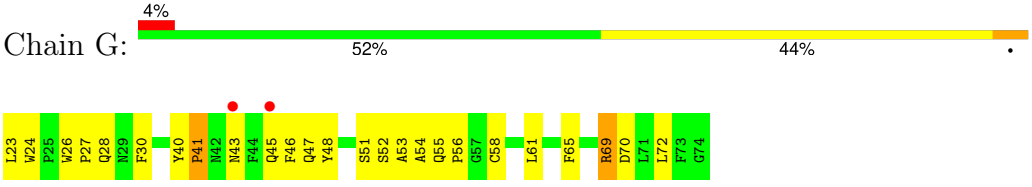
• Molecule 1: Beta-hexosaminidase subunit alpha

Chain E:



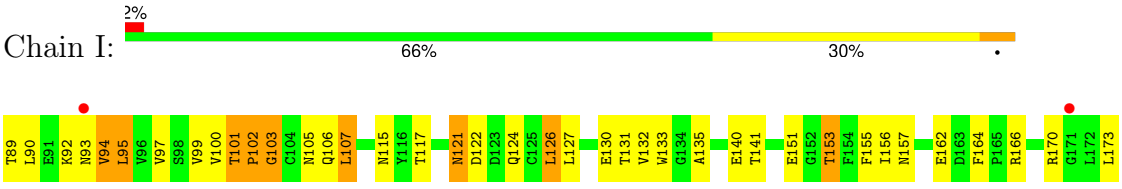
• Molecule 1: Beta-hexosaminidase subunit alpha

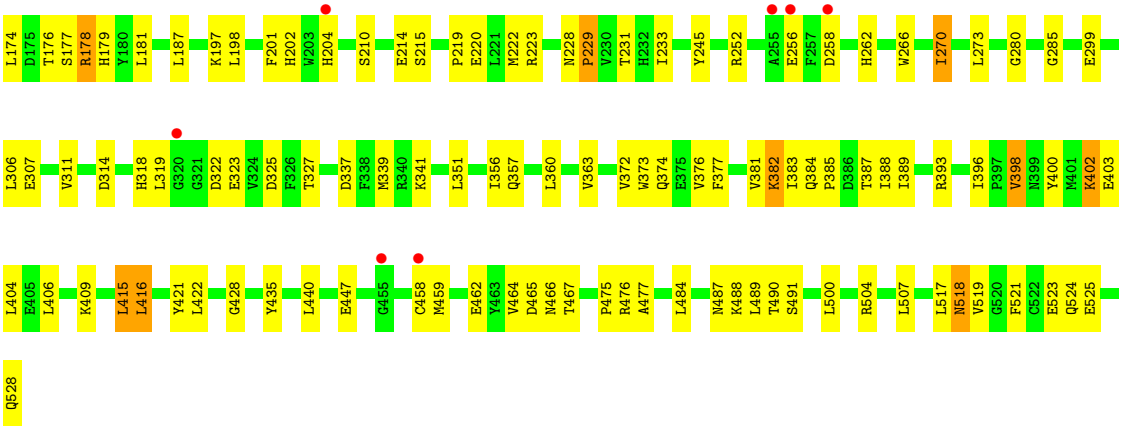
Chain G:



• Molecule 2: Beta-hexosaminidase subunit alpha

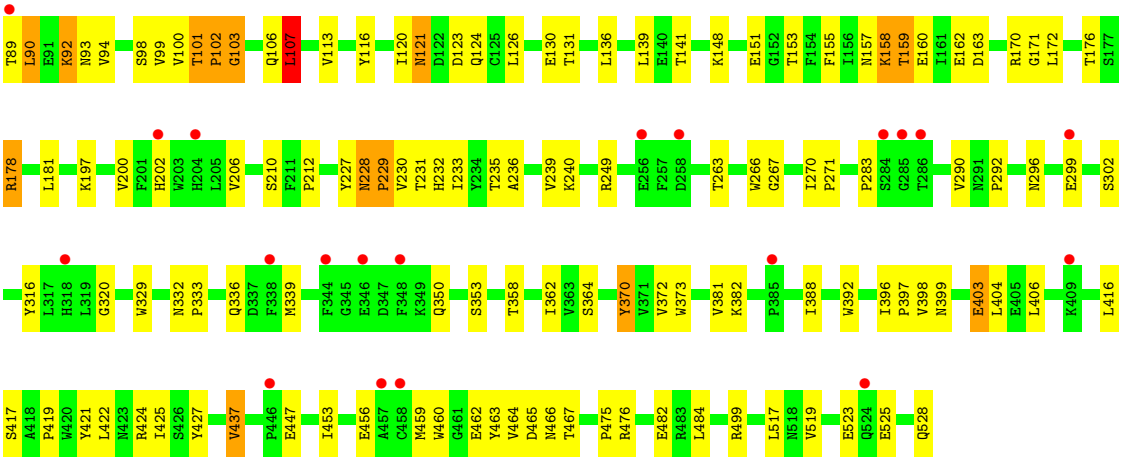
Chain I:





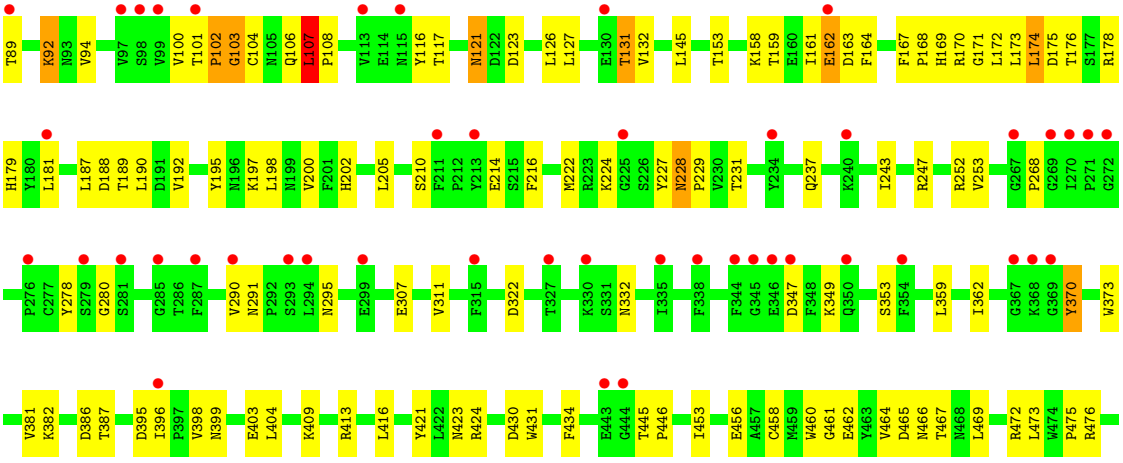
• Molecule 2: Beta-hexosaminidase subunit alpha

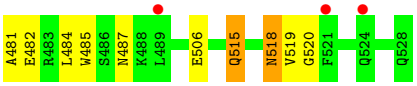
Chain J:



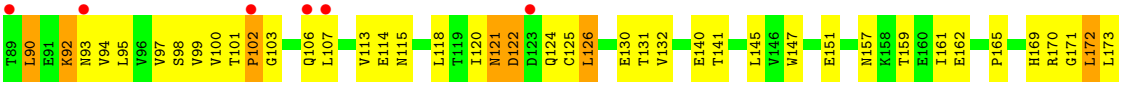
• Molecule 2: Beta-hexosaminidase subunit alpha

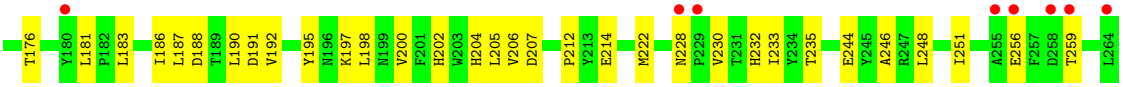
Chain K:

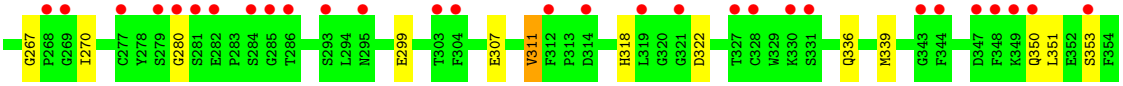


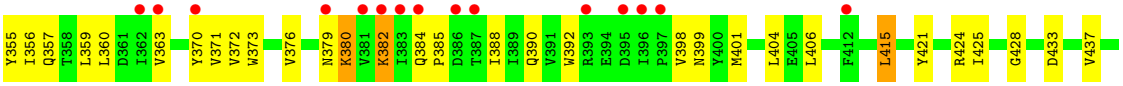


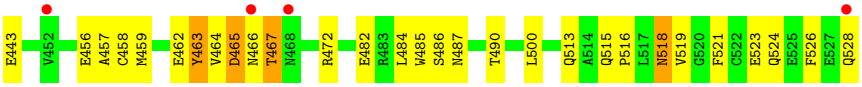
• Molecule 2: Beta-hexosaminidase subunit alpha



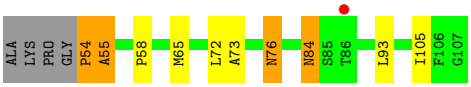




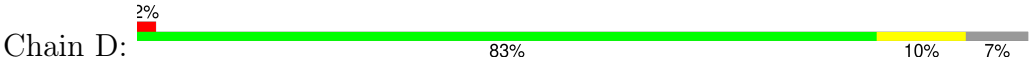


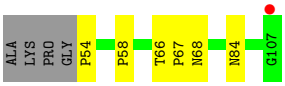


• Molecule 3: Beta-hexosaminidase subunit beta

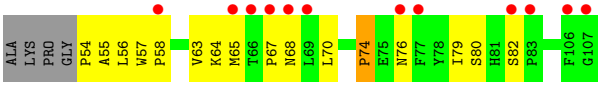


• Molecule 3: Beta-hexosaminidase subunit beta

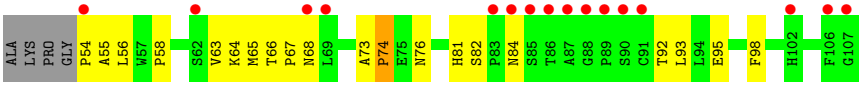




• Molecule 3: Beta-hexosaminidase subunit beta

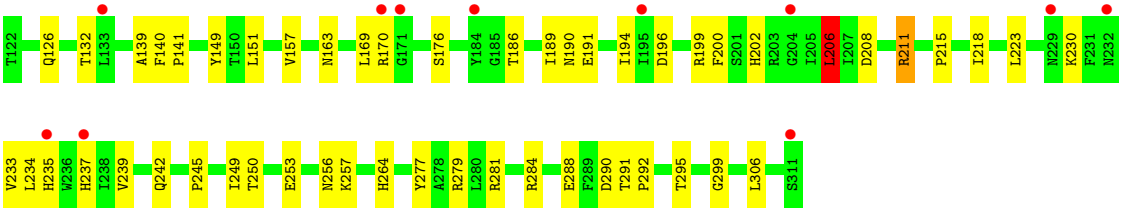


• Molecule 3: Beta-hexosaminidase subunit beta



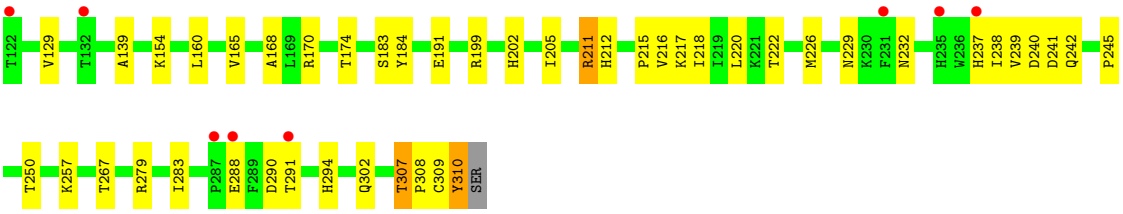
• Molecule 4: Beta-hexosaminidase subunit beta chain B

Chain M:



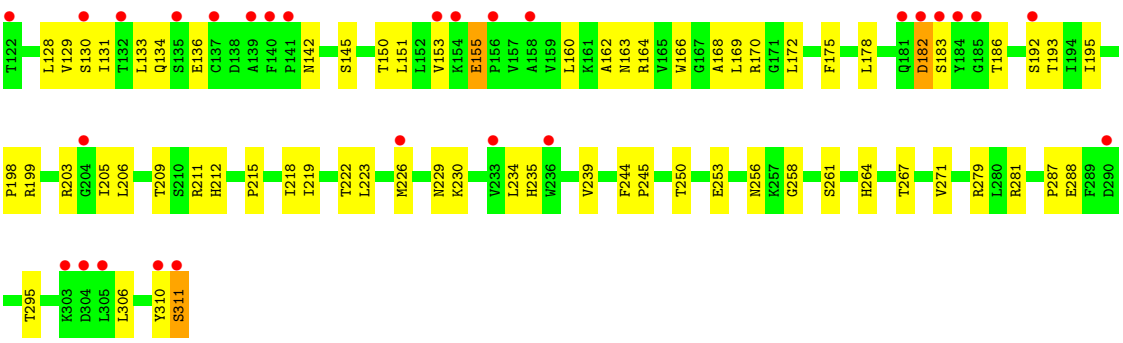
• Molecule 4: Beta-hexosaminidase subunit beta chain B

Chain O:



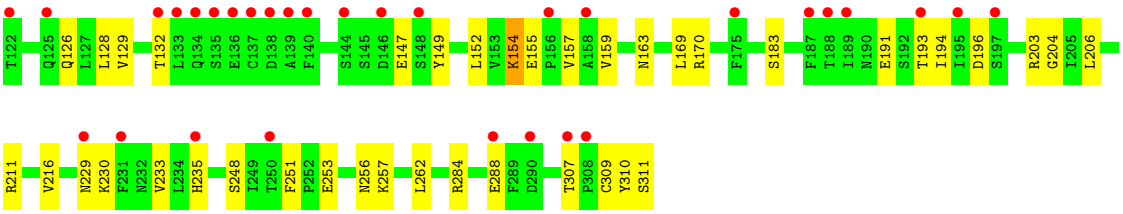
• Molecule 4: Beta-hexosaminidase subunit beta chain B

Chain Q:



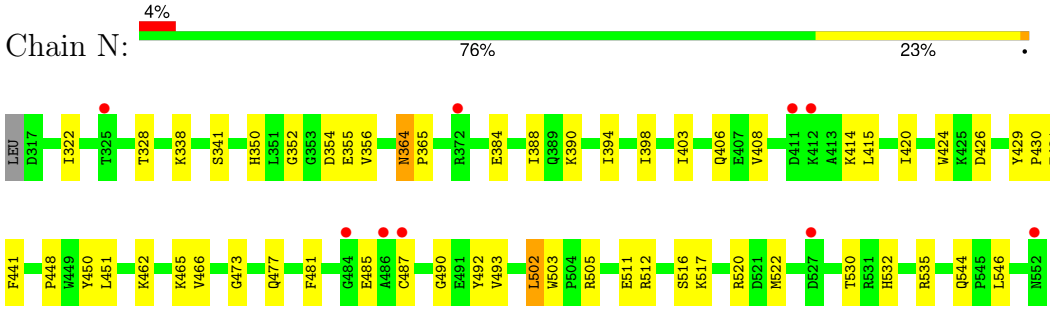
• Molecule 4: Beta-hexosaminidase subunit beta chain B

Chain S:



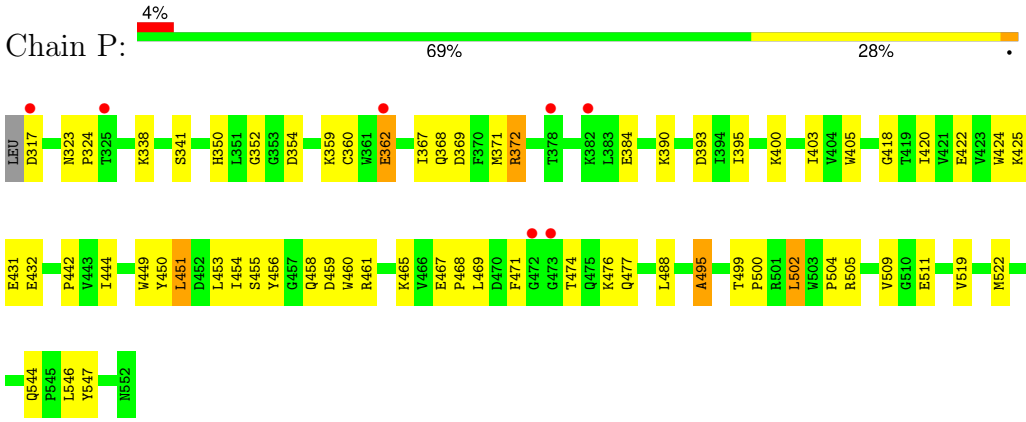
• Molecule 5: Beta-hexosaminidase subunit beta chain A

Chain N:



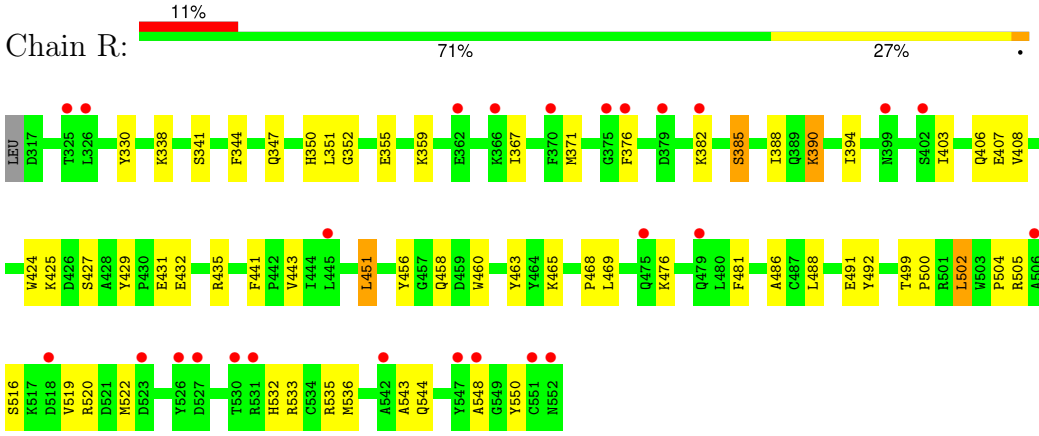
• Molecule 5: Beta-hexosaminidase subunit beta chain A

Chain P:



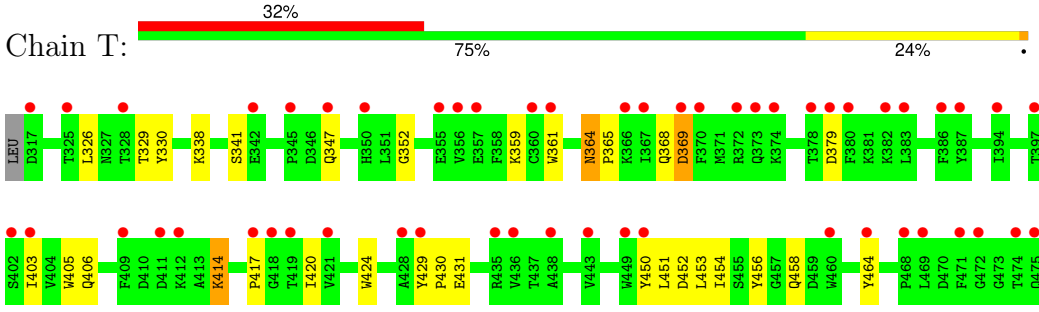
• Molecule 5: Beta-hexosaminidase subunit beta chain A

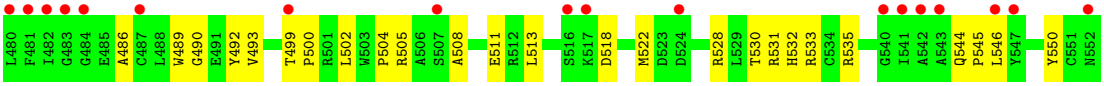
Chain R:



• Molecule 5: Beta-hexosaminidase subunit beta chain A

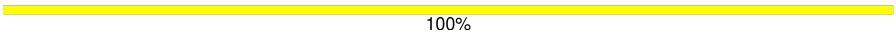
Chain T:





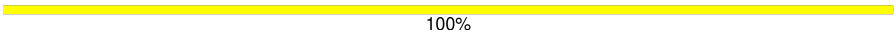
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



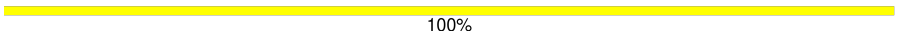
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

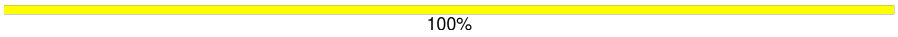
Chain d:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

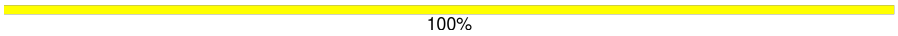
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

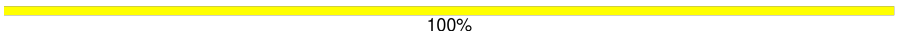


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

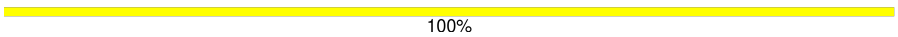
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	322.25Å 109.80Å 132.76Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	29.99 – 3.25 29.98 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.99-3.25) 97.8 (29.98-3.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.274 , 0.322 0.305 , 0.345	Depositor DCC
R_{free} test set	3599 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	89.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 15.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	32011	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, NGT, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.54	0/457	0.63	0/624
1	C	0.43	0/457	0.52	0/624
1	E	0.37	0/457	0.48	0/624
1	G	0.40	0/457	0.51	0/624
2	I	0.38	0/3671	0.56	0/5004
2	J	0.40	0/3671	0.53	1/5004 (0.0%)
2	K	0.40	0/3671	0.54	1/5004 (0.0%)
2	L	0.40	0/3671	0.54	0/5004
3	B	2.59	4/445 (0.9%)	0.78	1/609 (0.2%)
3	D	0.32	0/445	0.49	0/609
3	F	0.39	0/445	0.51	0/609
3	H	0.38	0/445	0.50	0/609
4	M	0.36	0/1567	0.55	1/2134 (0.0%)
4	O	0.39	0/1561	0.59	1/2126 (0.0%)
4	Q	0.39	0/1567	0.54	0/2134
4	S	0.35	0/1567	0.49	0/2134
5	N	0.40	0/1976	0.52	0/2680
5	P	0.41	0/1976	0.54	0/2680
5	R	0.45	0/1976	0.54	0/2680
5	T	0.36	0/1976	0.47	0/2680
All	All	0.50	4/32458 (0.0%)	0.54	5/44196 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	O	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	54	PRO	N-CA	42.00	2.18	1.47
3	B	54	PRO	N-CD	32.56	1.93	1.47
3	B	55	ALA	CA-CB	7.07	1.67	1.52
3	B	54	PRO	CG-CD	5.16	1.67	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	54	PRO	CA-N-CD	-12.34	94.23	111.50
4	O	309	CYS	N-CA-C	8.31	133.45	111.00
2	K	107	LEU	CA-CB-CG	5.67	128.33	115.30
2	J	107	LEU	CA-CB-CG	5.21	127.28	115.30
4	M	206	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	O	308	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	441	0	397	28	0
1	C	441	0	397	20	0
1	E	441	0	397	21	0
1	G	441	0	397	27	0
2	I	3565	0	3442	118	0
2	J	3565	0	3441	102	0
2	K	3565	0	3441	94	0
2	L	3565	0	3438	101	1
3	B	428	0	416	10	0
3	D	428	0	416	5	0
3	F	428	0	416	8	0
3	H	428	0	416	18	0
4	M	1528	0	1511	38	0
4	O	1522	0	1504	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	1528	0	1509	46	0
4	S	1528	0	1509	27	0
5	N	1921	0	1857	39	0
5	P	1921	0	1857	59	0
5	R	1921	0	1857	52	0
5	T	1921	0	1857	42	1
6	U	39	0	34	5	0
6	V	39	0	34	1	0
6	W	39	0	34	1	0
6	Y	39	0	33	7	0
6	d	39	0	34	0	0
7	X	28	0	25	1	0
7	Z	28	0	25	2	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
7	e	28	0	25	0	0
8	A	14	0	13	6	0
8	B	14	0	13	3	0
8	C	14	0	13	12	0
8	D	14	0	13	4	0
8	E	14	0	13	6	0
8	F	14	0	13	2	0
8	G	14	0	13	8	0
8	H	14	0	13	6	0
9	A	5	0	0	1	0
9	B	1	0	0	0	0
9	C	2	0	0	1	0
9	D	2	0	0	0	0
All	All	32011	0	30898	743	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 743 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:157:ASN:HD21	6:Y:1:NAG:C1	1.16	1.58
2:I:115:ASN:HD21	6:U:1:NAG:C1	1.18	1.53
2:I:157:ASN:HD21	6:V:1:NAG:C1	1.34	1.40
3:B:54:PRO:N	3:B:54:PRO:CD	1.93	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:530:NGT:HC62	2:K:462:GLU:OE1	1.19	1.29

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:424:ARG:NH2	5:T:369:ASP:OD1[2_456]	1.93	0.27

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	50/52 (96%)	46 (92%)	3 (6%)	1 (2%)	7 33
1	C	50/52 (96%)	48 (96%)	2 (4%)	0	100 100
1	E	50/52 (96%)	48 (96%)	2 (4%)	0	100 100
1	G	50/52 (96%)	44 (88%)	5 (10%)	1 (2%)	7 33
2	I	438/440 (100%)	400 (91%)	30 (7%)	8 (2%)	8 35
2	J	438/440 (100%)	402 (92%)	29 (7%)	7 (2%)	9 37
2	K	438/440 (100%)	402 (92%)	31 (7%)	5 (1%)	14 46
2	L	438/440 (100%)	404 (92%)	25 (6%)	9 (2%)	7 32
3	B	52/58 (90%)	42 (81%)	8 (15%)	2 (4%)	3 19
3	D	52/58 (90%)	42 (81%)	10 (19%)	0	100 100
3	F	52/58 (90%)	45 (86%)	4 (8%)	3 (6%)	1 10
3	H	52/58 (90%)	45 (86%)	6 (12%)	1 (2%)	8 34
4	M	188/190 (99%)	177 (94%)	10 (5%)	1 (0%)	29 62
4	O	187/190 (98%)	175 (94%)	12 (6%)	0	100 100
4	Q	188/190 (99%)	170 (90%)	17 (9%)	1 (0%)	29 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	S	188/190 (99%)	178 (95%)	10 (5%)	0	100 100
5	N	234/237 (99%)	215 (92%)	19 (8%)	0	100 100
5	P	234/237 (99%)	213 (91%)	16 (7%)	5 (2%)	7 32
5	R	234/237 (99%)	210 (90%)	22 (9%)	2 (1%)	17 50
5	T	234/237 (99%)	217 (93%)	15 (6%)	2 (1%)	17 50
All	All	3847/3908 (98%)	3523 (92%)	276 (7%)	48 (1%)	13 43

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	103	GLY
3	B	55	ALA
2	J	102	PRO
2	J	103	GLY
2	K	102	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	47/47 (100%)	39 (83%)	8 (17%)	2 9
1	C	47/47 (100%)	42 (89%)	5 (11%)	6 25
1	E	47/47 (100%)	41 (87%)	6 (13%)	4 18
1	G	47/47 (100%)	43 (92%)	4 (8%)	10 34
2	I	393/394 (100%)	364 (93%)	29 (7%)	13 40
2	J	393/394 (100%)	359 (91%)	34 (9%)	10 34
2	K	393/394 (100%)	371 (94%)	22 (6%)	21 52
2	L	393/394 (100%)	362 (92%)	31 (8%)	12 37
3	B	47/49 (96%)	45 (96%)	2 (4%)	29 59
3	D	47/49 (96%)	45 (96%)	2 (4%)	29 59
3	F	47/49 (96%)	44 (94%)	3 (6%)	17 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	H	47/49 (96%)	45 (96%)	2 (4%)	29 59
4	M	174/174 (100%)	168 (97%)	6 (3%)	37 64
4	O	173/174 (99%)	161 (93%)	12 (7%)	15 43
4	Q	174/174 (100%)	169 (97%)	5 (3%)	42 68
4	S	174/174 (100%)	168 (97%)	6 (3%)	37 64
5	N	205/206 (100%)	192 (94%)	13 (6%)	18 47
5	P	205/206 (100%)	188 (92%)	17 (8%)	11 36
5	R	205/206 (100%)	191 (93%)	14 (7%)	16 44
5	T	205/206 (100%)	195 (95%)	10 (5%)	25 55
All	All	3463/3480 (100%)	3232 (93%)	231 (7%)	16 45

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	P	360	CYS
5	T	338	LYS
2	K	162	GLU
4	S	309	CYS
2	L	336	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	47	GLN
4	Q	126	GLN
4	S	302	GLN
2	K	106	GLN
2	K	448	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

27 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	U	1	6,2	14,14,15	0.75	0	17,19,21	0.62	0
6	NAG	U	2	6	14,14,15	0.59	0	17,19,21	1.26	1 (5%)
6	BMA	U	3	6	11,11,12	0.62	0	15,15,17	1.33	2 (13%)
6	NAG	V	1	6,2	14,14,15	0.53	0	17,19,21	0.61	0
6	NAG	V	2	6	14,14,15	0.58	0	17,19,21	1.22	1 (5%)
6	BMA	V	3	6	11,11,12	0.76	0	15,15,17	2.17	3 (20%)
6	NAG	W	1	6	14,14,15	0.59	0	17,19,21	0.62	0
6	NAG	W	2	6	14,14,15	0.64	0	17,19,21	1.13	1 (5%)
6	BMA	W	3	6	11,11,12	2.26	2 (18%)	15,15,17	3.09	6 (40%)
7	NAG	X	1	7,2	14,14,15	0.65	0	17,19,21	0.89	1 (5%)
7	NAG	X	2	7	14,14,15	0.53	0	17,19,21	0.77	0
6	NAG	Y	1	6,2	14,14,15	1.02	2 (14%)	17,19,21	0.63	0
6	NAG	Y	2	6	14,14,15	1.14	2 (14%)	17,19,21	4.11	6 (35%)
6	BMA	Y	3	6	11,11,12	0.61	0	15,15,17	1.79	2 (13%)
7	NAG	Z	1	7,4	14,14,15	0.48	0	17,19,21	0.62	0
7	NAG	Z	2	7	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
7	NAG	a	1	7,2	14,14,15	2.76	5 (35%)	17,19,21	0.77	1 (5%)
7	NAG	a	2	7	14,14,15	1.20	1 (7%)	17,19,21	1.93	3 (17%)
7	NAG	b	1	7,4	14,14,15	0.64	0	17,19,21	0.61	0
7	NAG	b	2	7	14,14,15	0.69	0	17,19,21	1.22	2 (11%)
7	NAG	c	1	7,2	14,14,15	2.01	3 (21%)	17,19,21	0.64	0
7	NAG	c	2	7	14,14,15	0.66	0	17,19,21	1.34	3 (17%)
6	NAG	d	1	6,2	14,14,15	0.58	0	17,19,21	0.61	0
6	NAG	d	2	6	14,14,15	0.63	0	17,19,21	1.23	2 (11%)
6	BMA	d	3	6	11,11,12	0.62	0	15,15,17	0.98	1 (6%)
7	NAG	e	1	7,4	14,14,15	1.07	1 (7%)	17,19,21	0.61	0
7	NAG	e	2	7	14,14,15	0.65	0	17,19,21	1.21	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	U	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	4/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	NAG	V	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	3/6/23/26	0/1/1/1
6	BMA	V	3	6	-	1/2/19/22	0/1/1/1
6	NAG	W	1	6	-	2/6/23/26	0/1/1/1
6	NAG	W	2	6	-	5/6/23/26	0/1/1/1
6	BMA	W	3	6	-	2/2/19/22	0/1/1/1
7	NAG	X	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	X	2	7	-	5/6/23/26	0/1/1/1
6	NAG	Y	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	Y	2	6	1/1/5/7	4/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	2/2/19/22	0/1/1/1
7	NAG	Z	1	7,4	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	a	1	7,2	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	a	2	7	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	b	1	7,4	1/1/5/7	6/6/23/26	0/1/1/1
7	NAG	b	2	7	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	c	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	1/1/5/7	3/6/23/26	0/1/1/1
6	NAG	d	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	d	2	6	1/1/5/7	5/6/23/26	0/1/1/1
6	BMA	d	3	6	-	0/2/19/22	0/1/1/1
7	NAG	e	1	7,4	-	3/6/23/26	0/1/1/1
7	NAG	e	2	7	1/1/5/7	4/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	3	BMA	O2-C2	6.61	1.57	1.43
7	a	1	NAG	O4-C4	-6.22	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	1	NAG	C2-N2	6.17	1.56	1.46
7	a	1	NAG	C1-C2	4.48	1.58	1.52
7	a	1	NAG	O5-C1	-4.37	1.36	1.43

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Y	2	NAG	O5-C5-C6	10.51	128.11	107.66
6	Y	2	NAG	O5-C1-C2	10.45	127.45	111.29
6	W	3	BMA	C1-C2-C3	6.51	119.12	109.64
6	W	3	BMA	C1-O5-C5	-5.99	104.16	112.19
7	a	2	NAG	C1-O5-C5	5.93	120.13	112.19

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	Y	2	NAG	C5
6	d	2	NAG	C1
7	Z	1	NAG	C1
7	Z	2	NAG	C1
7	a	1	NAG	C1

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	2	NAG	C1-C2-N2-C7
6	V	2	NAG	C3-C2-N2-C7
6	W	2	NAG	C3-C2-N2-C7
6	W	2	NAG	C8-C7-N2-C2
6	W	2	NAG	O7-C7-N2-C2

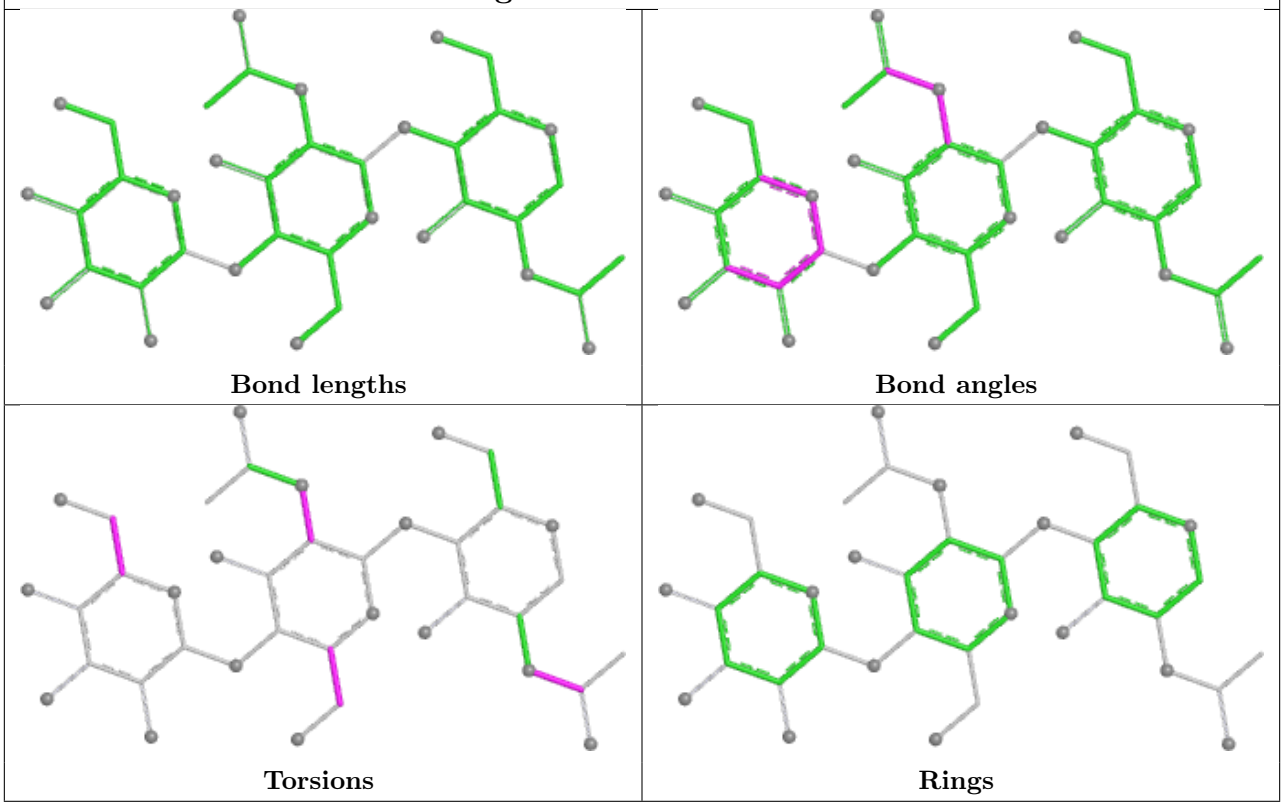
There are no ring outliers.

7 monomers are involved in 17 short contacts:

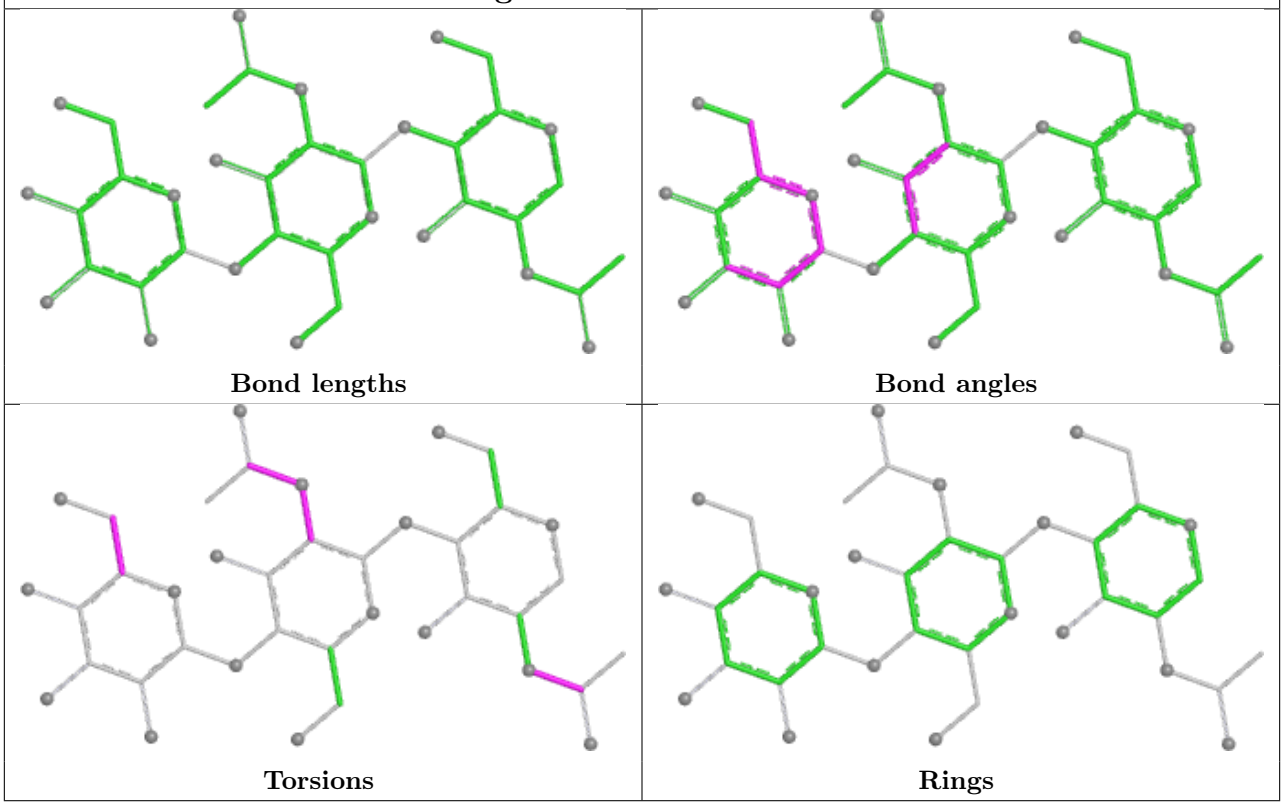
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Y	1	NAG	7	0
6	W	1	NAG	1	0
7	X	1	NAG	1	0
7	Z	1	NAG	2	0
6	Y	2	NAG	1	0
6	U	1	NAG	5	0
6	V	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

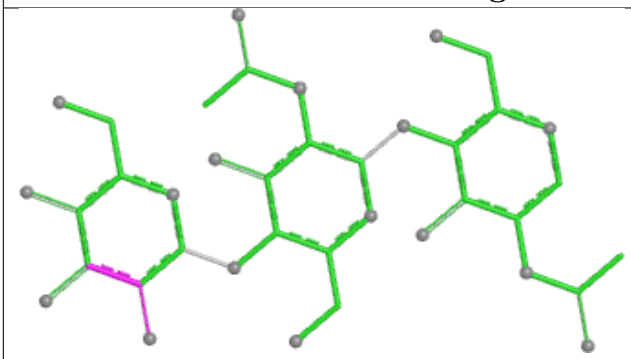
Oligosaccharide Chain U



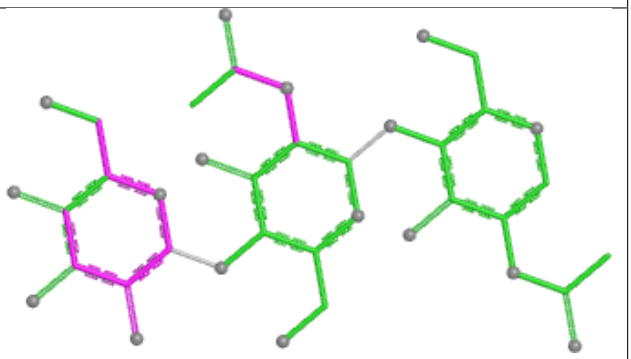
Oligosaccharide Chain V



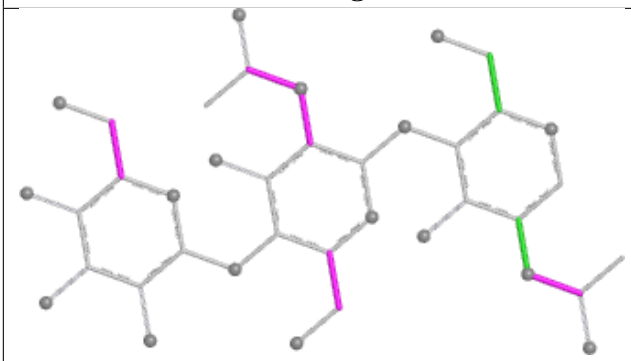
Oligosaccharide Chain W



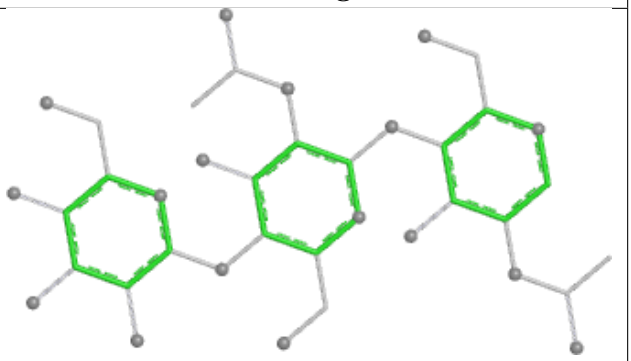
Bond lengths



Bond angles

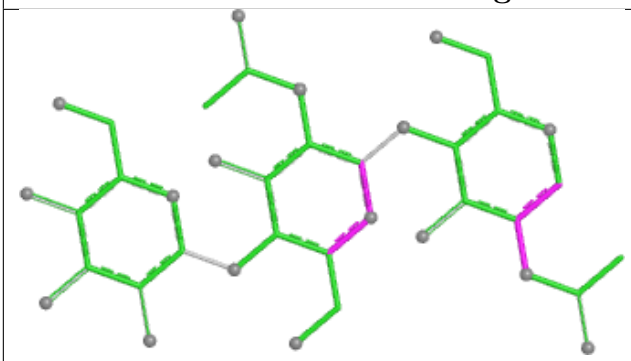


Torsions

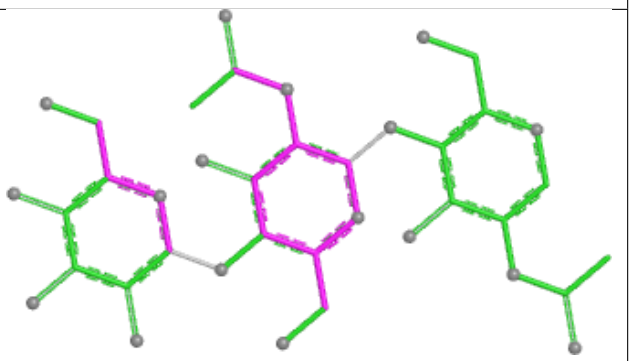


Rings

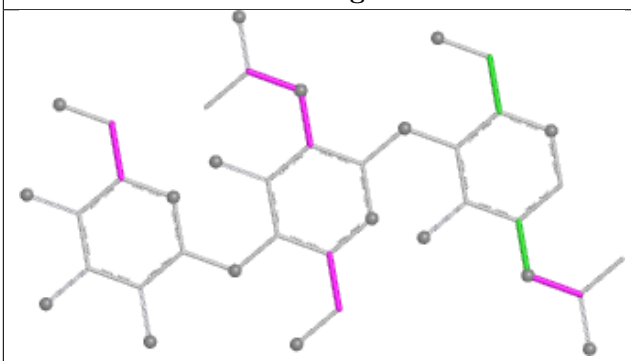
Oligosaccharide Chain Y



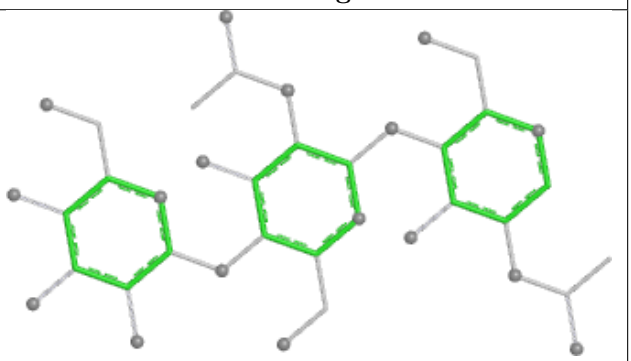
Bond lengths



Bond angles

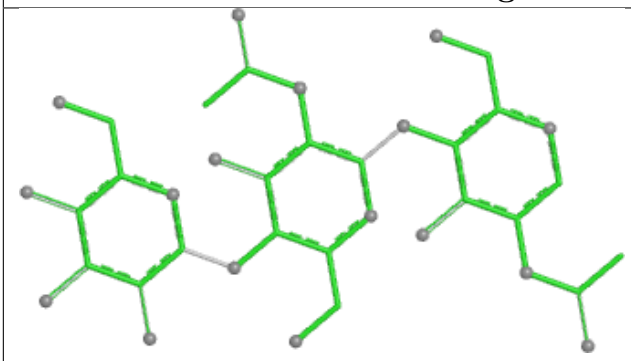


Torsions

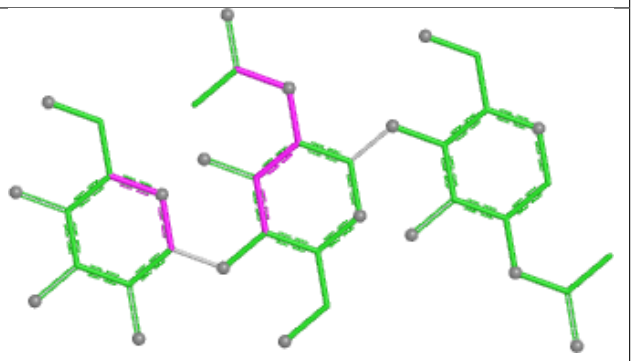


Rings

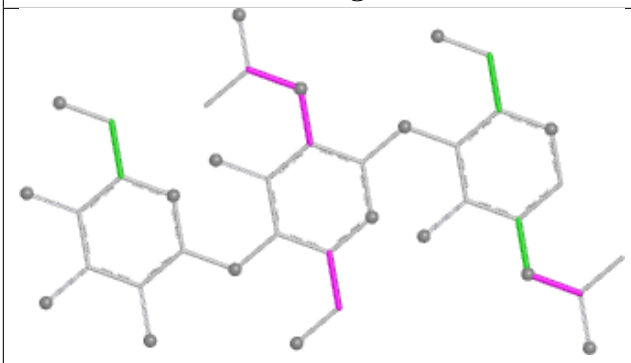
Oligosaccharide Chain d



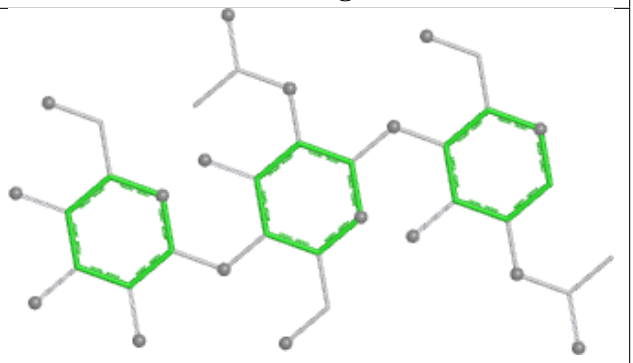
Bond lengths



Bond angles

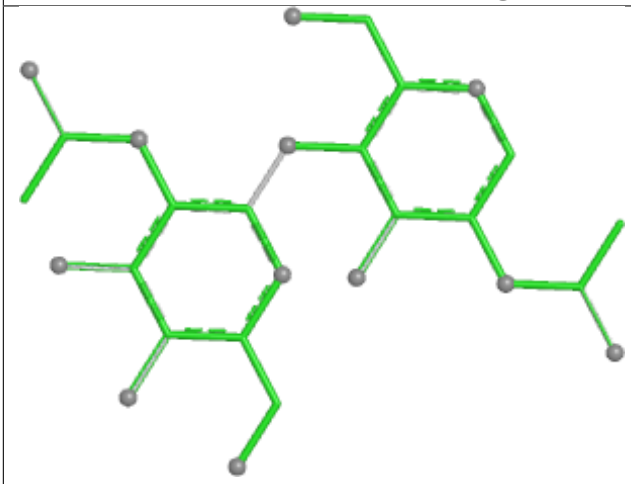


Torsions

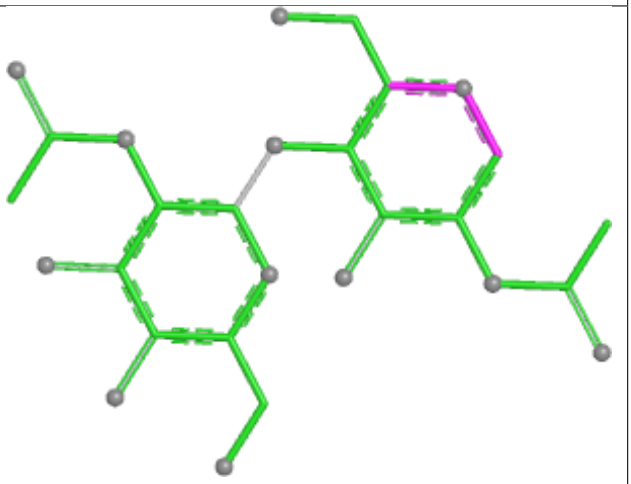


Rings

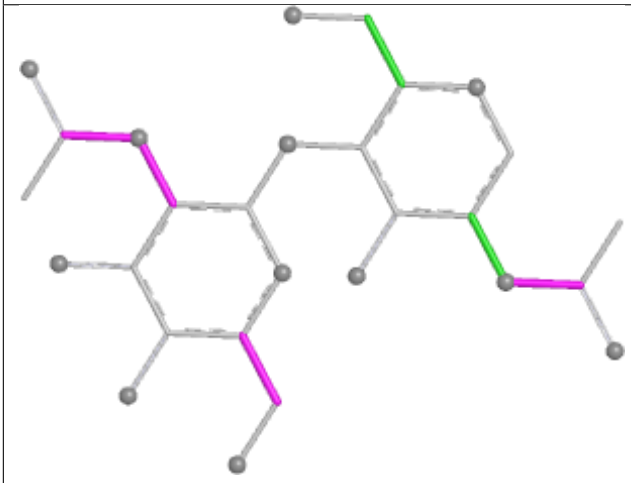
Oligosaccharide Chain X



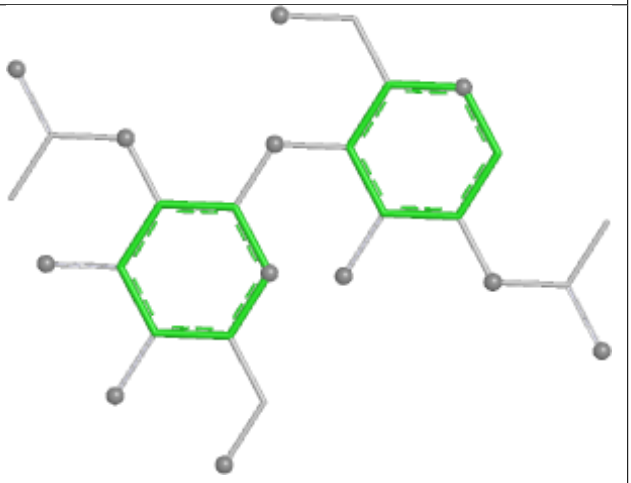
Bond lengths



Bond angles

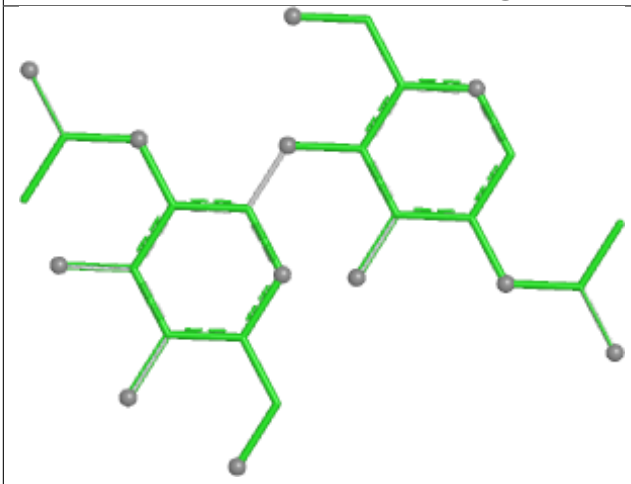


Torsions

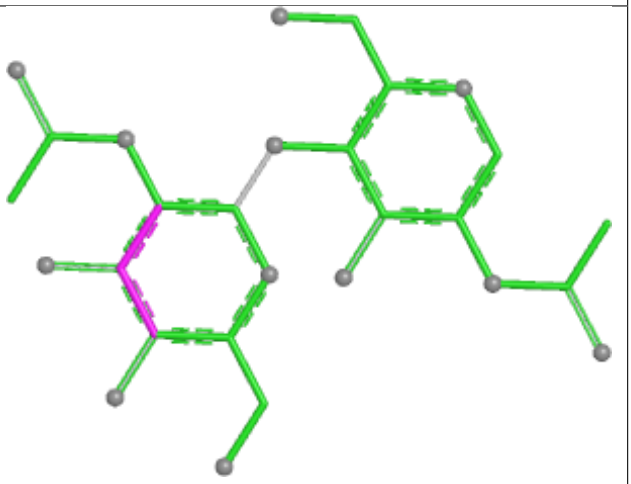


Rings

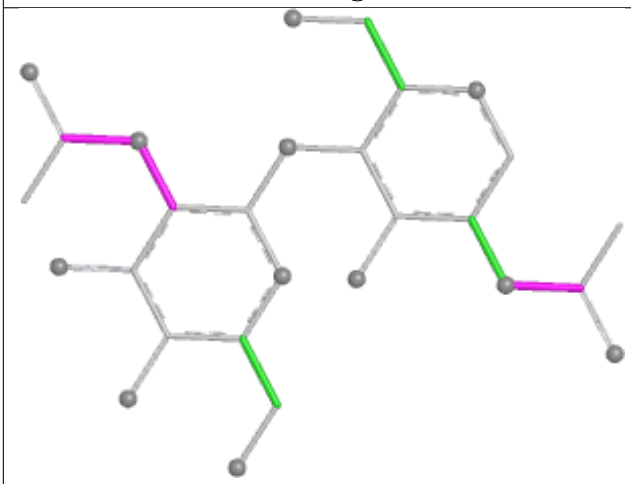
Oligosaccharide Chain Z



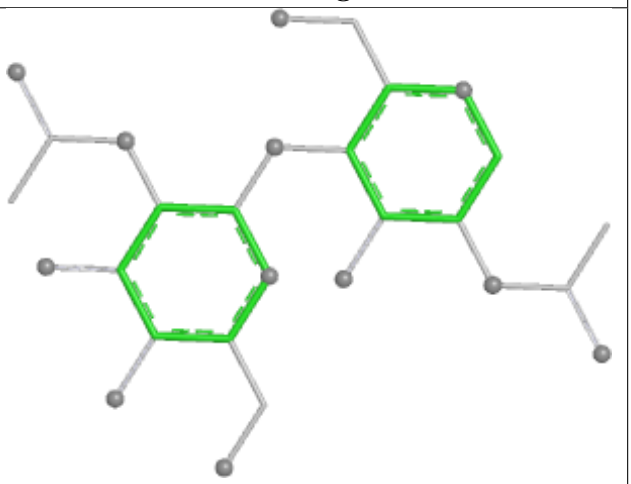
Bond lengths



Bond angles

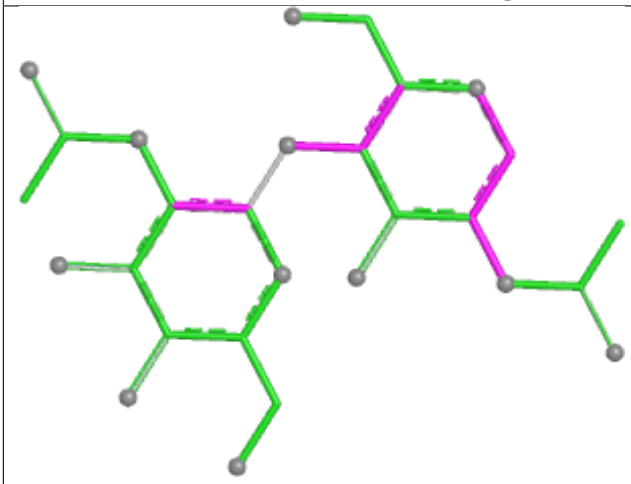


Torsions

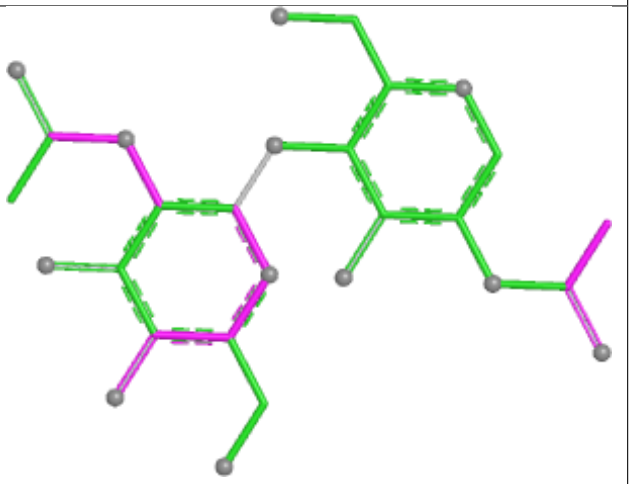


Rings

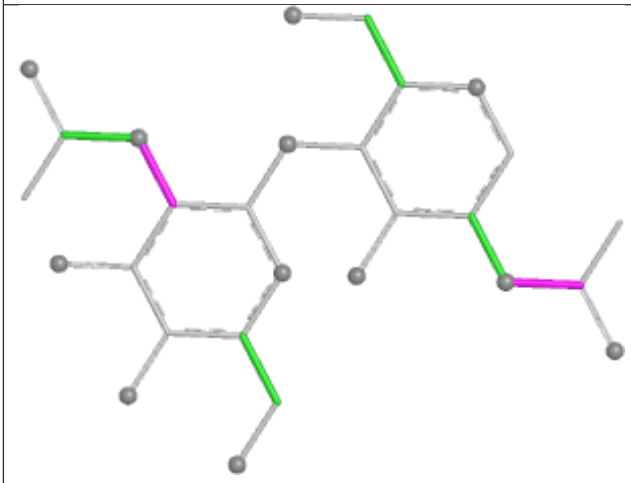
Oligosaccharide Chain a



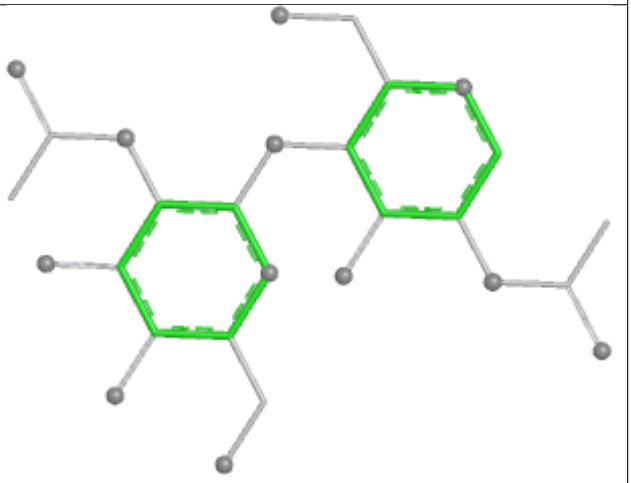
Bond lengths



Bond angles

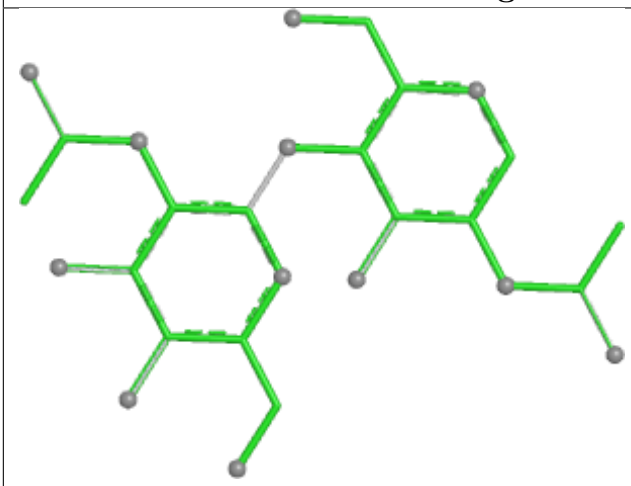


Torsions

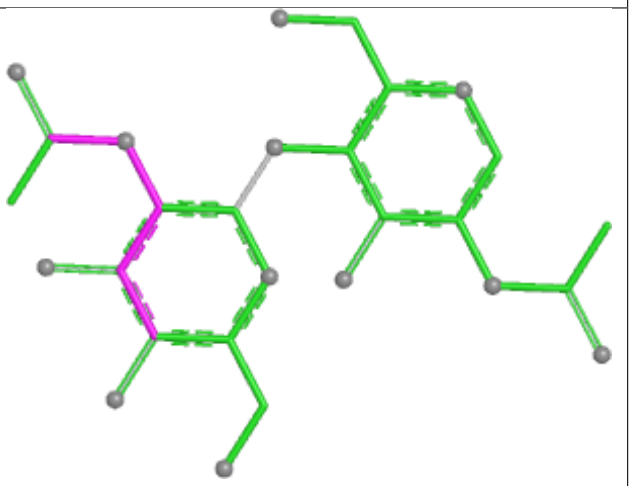


Rings

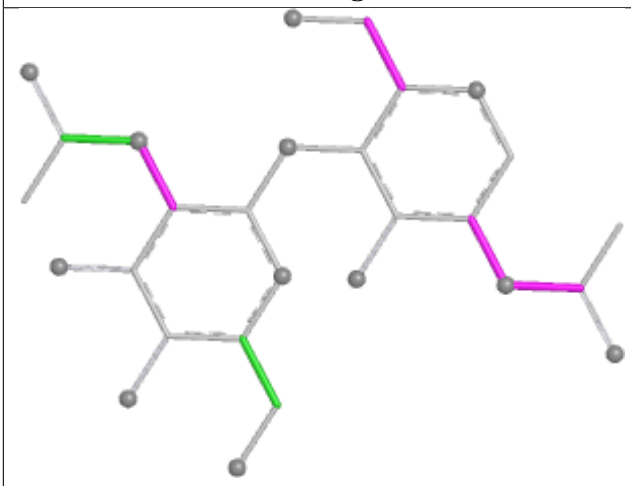
Oligosaccharide Chain b



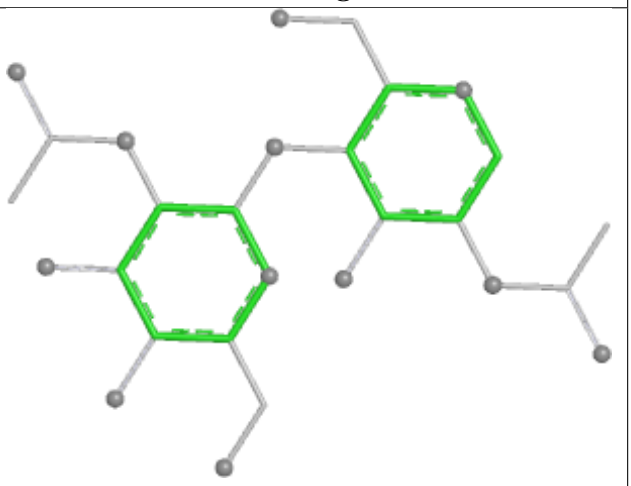
Bond lengths



Bond angles

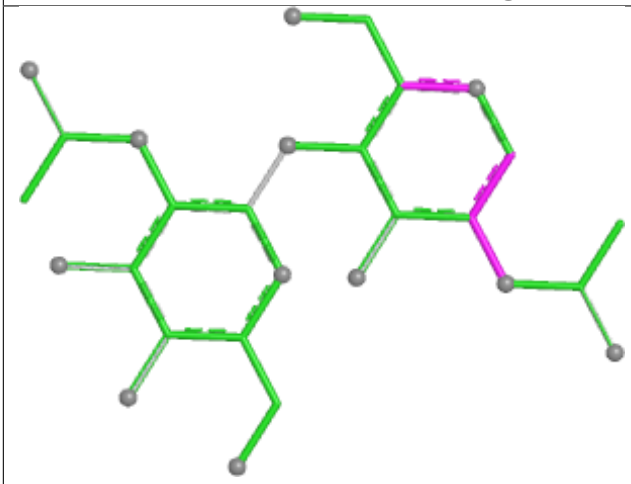


Torsions

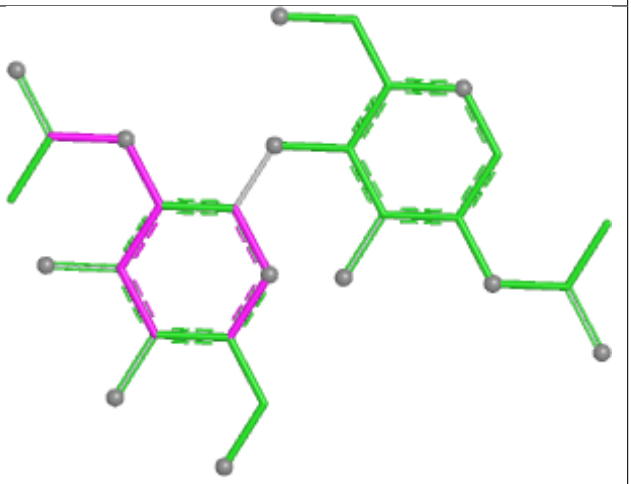


Rings

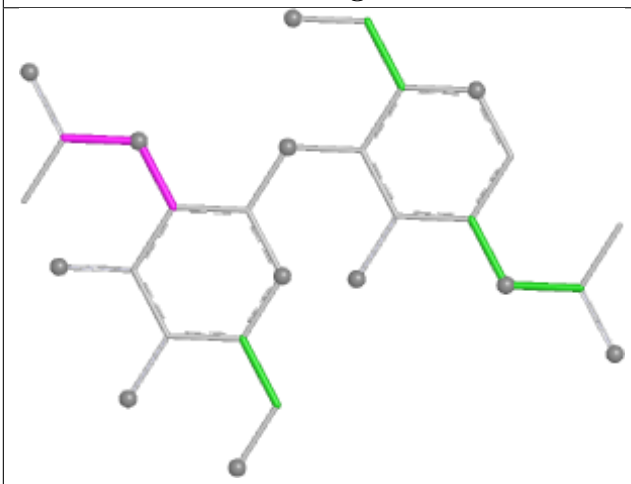
Oligosaccharide Chain c



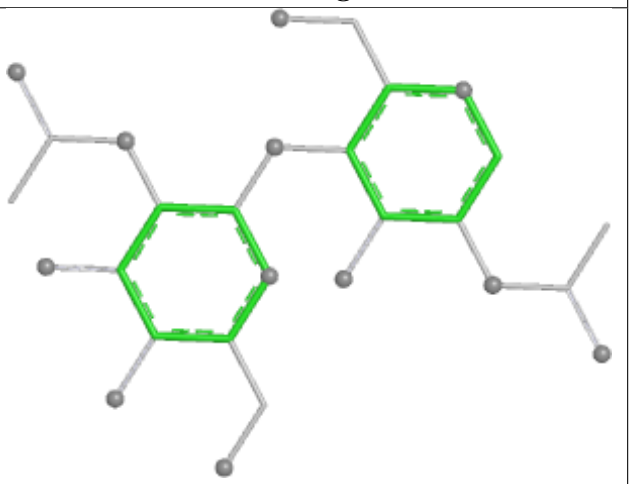
Bond lengths



Bond angles

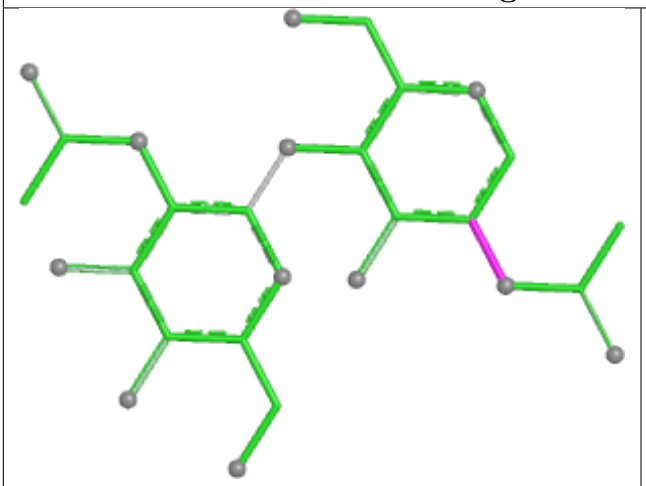


Torsions

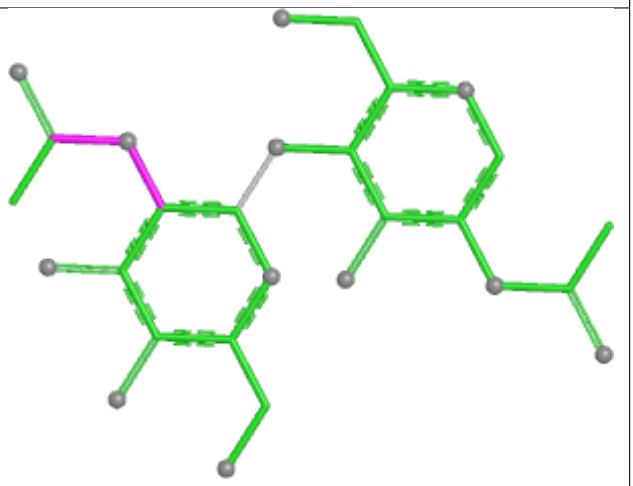


Rings

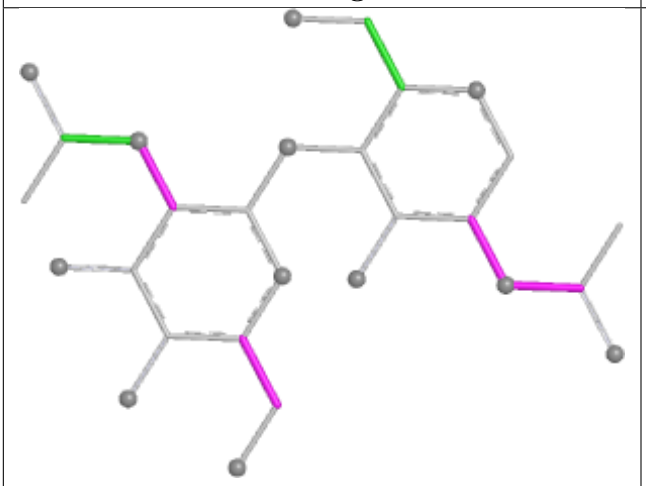
Oligosaccharide Chain e



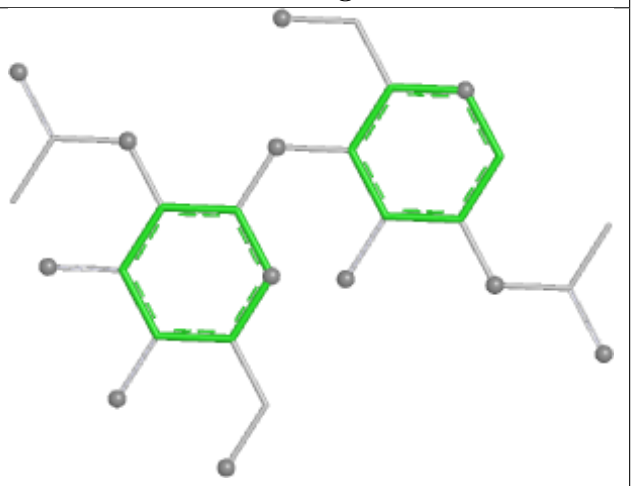
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NGT	F	26	-	13,15,15	1.31	2 (15%)	14,22,22	0.88	1 (7%)
8	NGT	C	530	-	13,15,15	1.45	2 (15%)	14,22,22	0.88	1 (7%)
8	NGT	E	530	-	13,15,15	1.39	3 (23%)	14,22,22	0.88	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NGT	A	21	-	13,15,15	1.25	1 (7%)	14,22,22	0.88	1 (7%)
8	NGT	B	22	-	13,15,15	1.31	2 (15%)	14,22,22	0.88	1 (7%)
8	NGT	G	533	-	13,15,15	1.34	2 (15%)	14,22,22	0.87	1 (7%)
8	NGT	H	28	-	13,15,15	1.42	4 (30%)	14,22,22	0.88	1 (7%)
8	NGT	D	24	-	13,15,15	1.38	2 (15%)	14,22,22	0.88	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NGT	F	26	-	-	0/2/30/30	0/2/2/2
8	NGT	C	530	-	-	0/2/30/30	0/2/2/2
8	NGT	E	530	-	-	0/2/30/30	0/2/2/2
8	NGT	A	21	-	-	0/2/30/30	0/2/2/2
8	NGT	B	22	-	-	2/2/30/30	0/2/2/2
8	NGT	G	533	-	-	0/2/30/30	0/2/2/2
8	NGT	H	28	-	-	0/2/30/30	0/2/2/2
8	NGT	D	24	-	-	0/2/30/30	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	530	NGT	C3-C2	3.60	1.59	1.53
8	G	533	NGT	C3-C2	3.31	1.59	1.53
8	B	22	NGT	C3-C2	3.22	1.59	1.53
8	A	21	NGT	C3-C2	3.20	1.58	1.53
8	F	26	NGT	C3-C2	3.15	1.58	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	22	NGT	C1-O5-C5	2.36	116.80	112.56
8	C	530	NGT	C1-O5-C5	2.36	116.80	112.56
8	A	21	NGT	C1-O5-C5	2.36	116.79	112.56
8	E	530	NGT	C1-O5-C5	2.35	116.77	112.56
8	F	26	NGT	C1-O5-C5	2.35	116.77	112.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	22	NGT	C4-C5-C6-O6
8	B	22	NGT	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	26	NGT	2	0
8	C	530	NGT	12	0
8	E	530	NGT	6	0
8	A	21	NGT	6	0
8	B	22	NGT	3	0
8	G	533	NGT	8	0
8	H	28	NGT	6	0
8	D	24	NGT	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	52/52 (100%)	0.19	0 100 100	31, 56, 60, 63	0
1	C	52/52 (100%)	0.11	1 (1%) 66 64	31, 55, 62, 62	0
1	E	52/52 (100%)	0.43	5 (9%) 8 8	32, 54, 57, 59	0
1	G	52/52 (100%)	0.30	2 (3%) 40 37	31, 54, 59, 60	0
2	I	440/440 (100%)	0.34	9 (2%) 65 63	41, 53, 60, 66	0
2	J	440/440 (100%)	0.35	20 (4%) 33 31	42, 57, 62, 66	0
2	K	440/440 (100%)	0.68	49 (11%) 5 5	43, 57, 62, 64	0
2	L	440/440 (100%)	0.80	62 (14%) 2 2	42, 56, 60, 61	0
3	B	54/58 (93%)	0.18	1 (1%) 66 64	50, 58, 60, 60	0
3	D	54/58 (93%)	0.31	1 (1%) 66 64	51, 57, 59, 60	0
3	F	54/58 (93%)	1.02	12 (22%) 0 1	57, 60, 62, 63	0
3	H	54/58 (93%)	1.74	16 (29%) 0 0	56, 58, 60, 61	0
4	M	190/190 (100%)	0.54	11 (5%) 23 22	48, 55, 59, 63	0
4	O	189/190 (99%)	0.43	8 (4%) 36 33	28, 54, 57, 60	0
4	Q	190/190 (100%)	0.88	28 (14%) 2 2	54, 57, 61, 63	0
4	S	190/190 (100%)	1.00	31 (16%) 1 2	50, 56, 59, 61	0
5	N	236/237 (99%)	0.36	9 (3%) 40 37	21, 56, 60, 62	0
5	P	236/237 (99%)	0.44	9 (3%) 40 37	21, 57, 61, 62	0
5	R	236/237 (99%)	0.80	27 (11%) 5 5	21, 59, 63, 64	0
5	T	236/237 (99%)	1.59	75 (31%) 0 0	21, 57, 58, 59	0
All	All	3887/3908 (99%)	0.64	376 (9%) 7 8	21, 56, 61, 66	0

The worst 5 of 376 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	107	GLY	10.3
2	L	279	SER	9.2
3	H	54	PRO	7.3
5	T	480	LEU	6.7
5	T	483	GLY	6.5

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	a	2	14/15	0.50	0.46	73,76,78,79	0
7	NAG	c	2	14/15	0.64	0.46	72,75,76,76	0
6	BMA	Y	3	11/12	0.65	0.41	46,49,51,51	0
7	NAG	X	2	14/15	0.67	0.48	65,68,69,69	0
6	NAG	Y	2	14/15	0.71	0.32	55,59,63,63	0
7	NAG	X	1	14/15	0.72	0.43	51,56,60,62	0
7	NAG	Z	1	14/15	0.74	0.33	60,62,67,67	0
7	NAG	b	2	14/15	0.75	0.38	73,76,77,77	0
7	NAG	b	1	14/15	0.77	0.32	61,62,62,66	0
7	NAG	c	1	14/15	0.80	0.55	59,60,63,65	0
7	NAG	a	1	14/15	0.80	0.31	58,59,62,64	0
6	NAG	V	2	14/15	0.81	0.45	61,66,71,71	0
7	NAG	e	1	14/15	0.81	0.26	61,62,63,66	0
6	BMA	V	3	11/12	0.82	0.26	52,53,55,56	0
6	NAG	W	2	14/15	0.82	0.34	61,66,68,68	0
6	BMA	W	3	11/12	0.82	0.18	48,54,56,57	0
7	NAG	e	2	14/15	0.82	0.27	73,76,76,76	0
6	NAG	Y	1	14/15	0.83	0.21	45,47,48,51	0
6	NAG	W	1	14/15	0.83	0.30	47,50,53,56	0
6	NAG	d	2	14/15	0.84	0.35	57,63,64,65	0
6	BMA	d	3	11/12	0.85	0.20	48,48,50,52	0
6	NAG	U	1	14/15	0.86	0.21	45,47,50,51	0
7	NAG	Z	2	14/15	0.86	0.46	74,76,78,78	0
6	NAG	V	1	14/15	0.87	0.24	54,55,58,60	0

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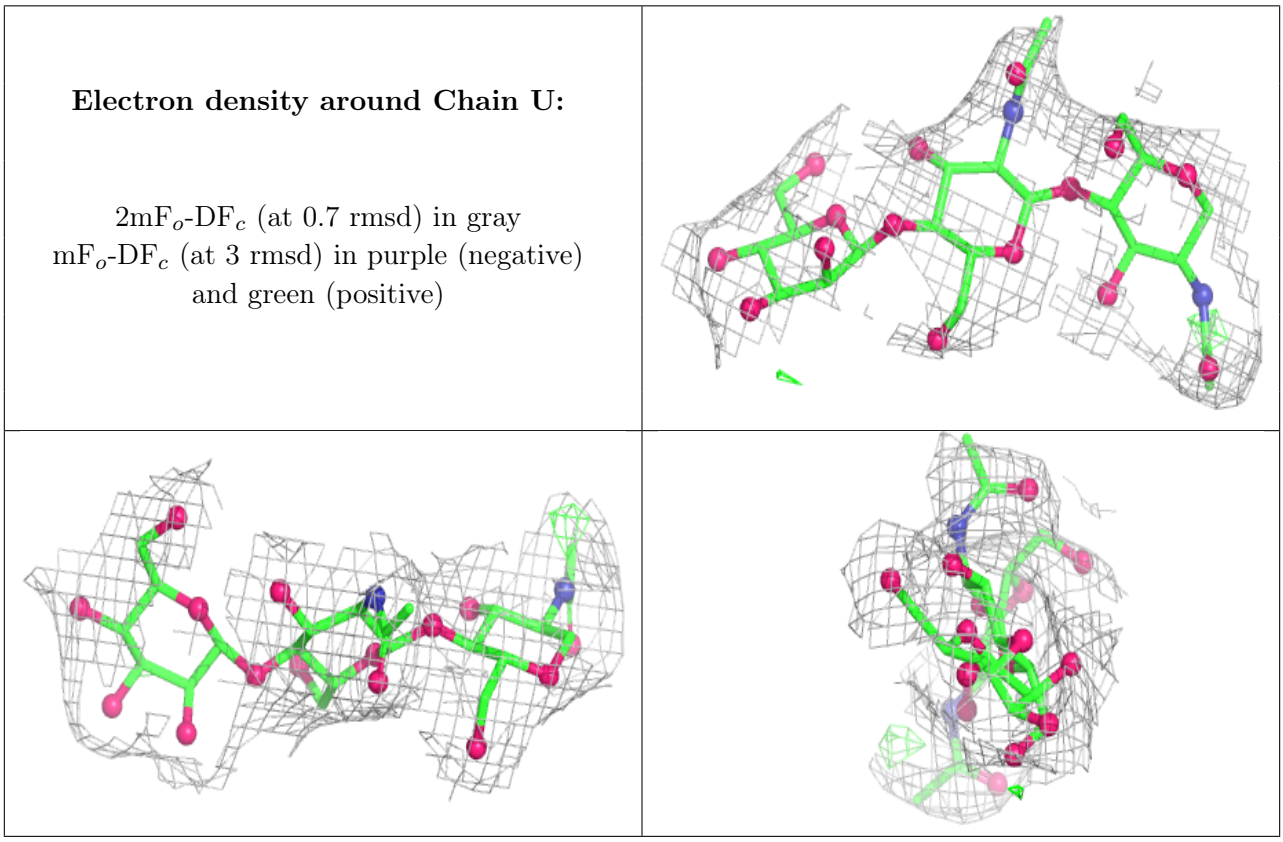
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	U	3	11/12	0.88	0.29	50,52,54,55	0
6	NAG	U	2	14/15	0.91	0.31	58,61,63,63	0
6	NAG	d	1	14/15	0.91	0.16	52,54,57,58	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

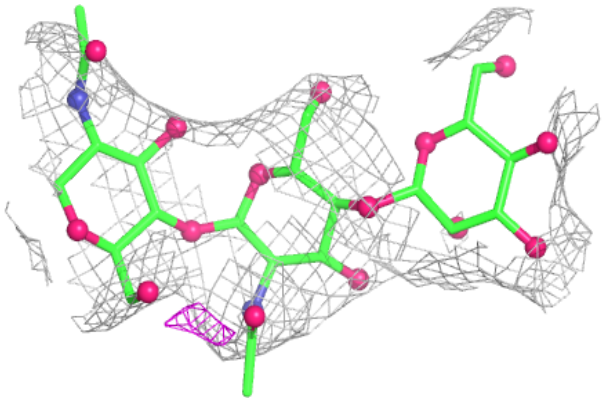
Electron density around Chain U:

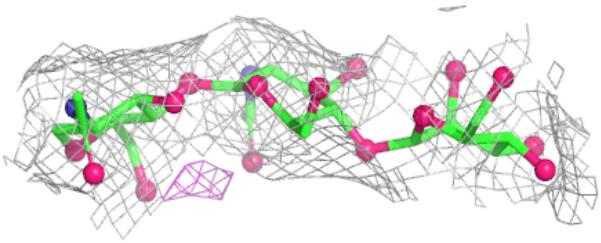
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

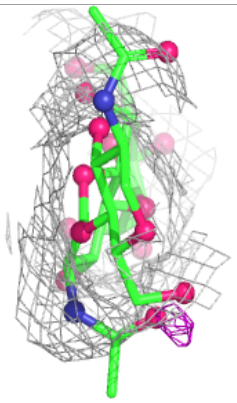


Electron density around Chain V:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

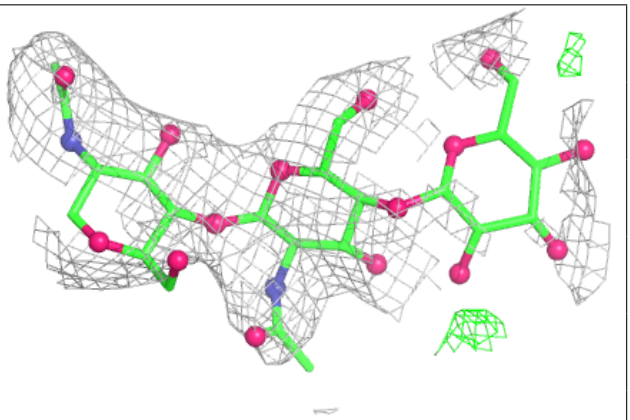


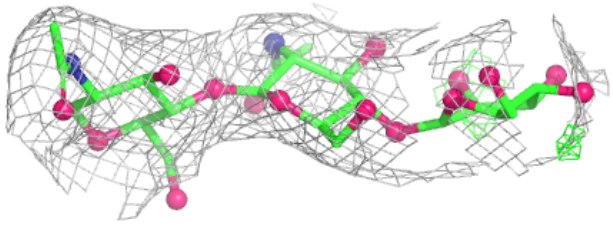


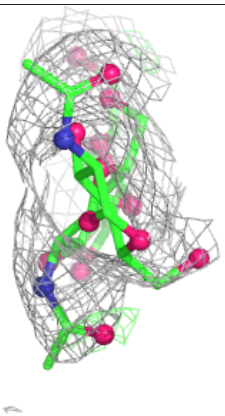


Electron density around Chain W:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

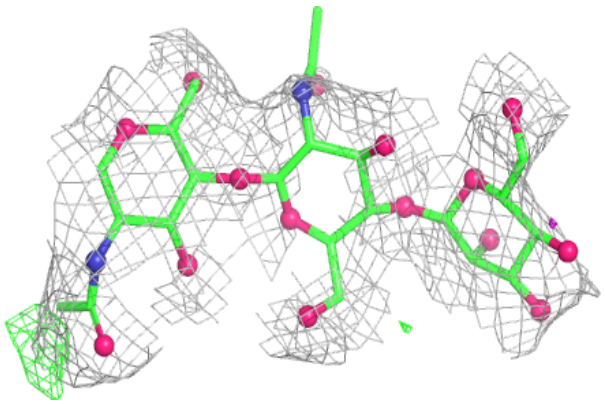


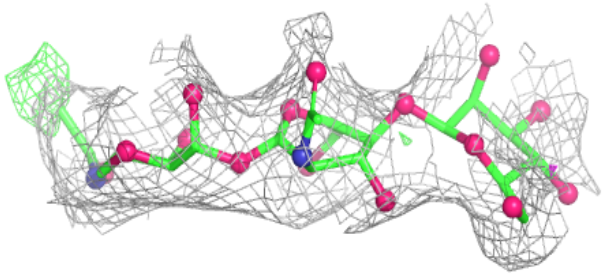


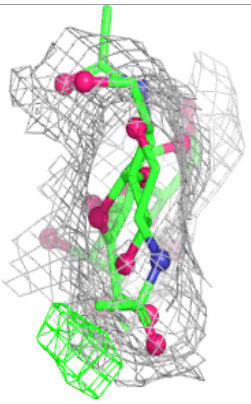


Electron density around Chain Y:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

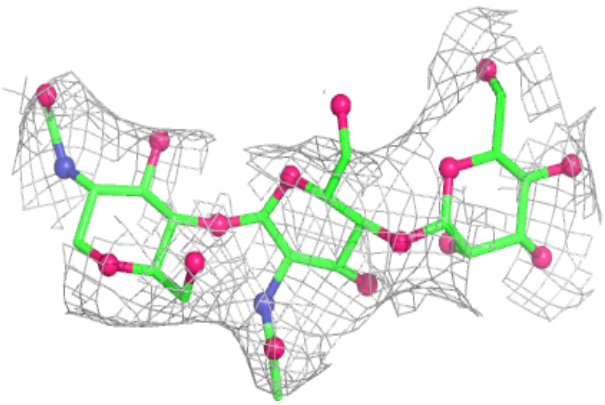


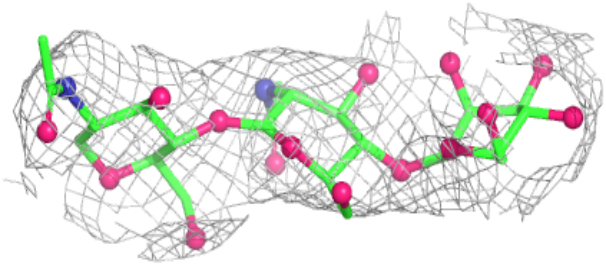


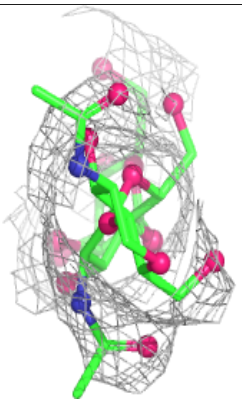


Electron density around Chain d:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

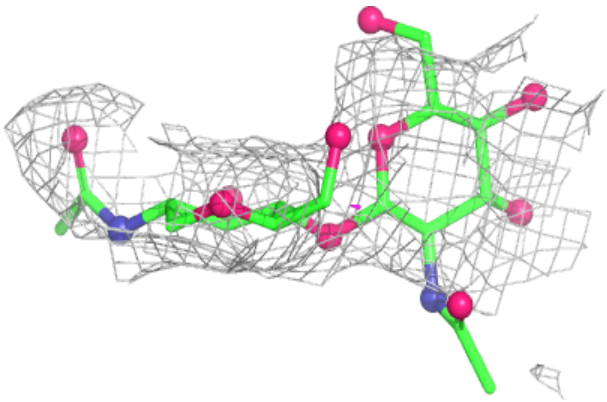


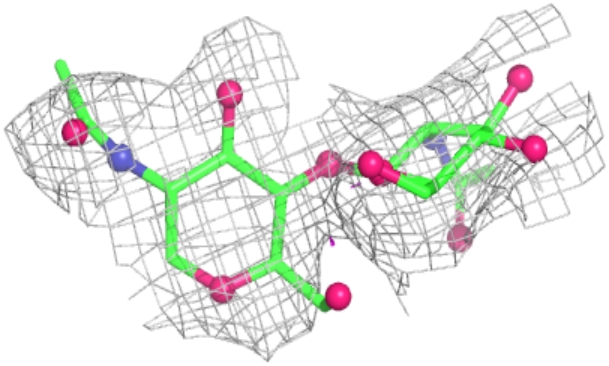


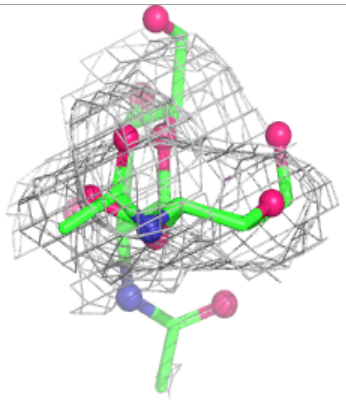


Electron density around Chain X:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

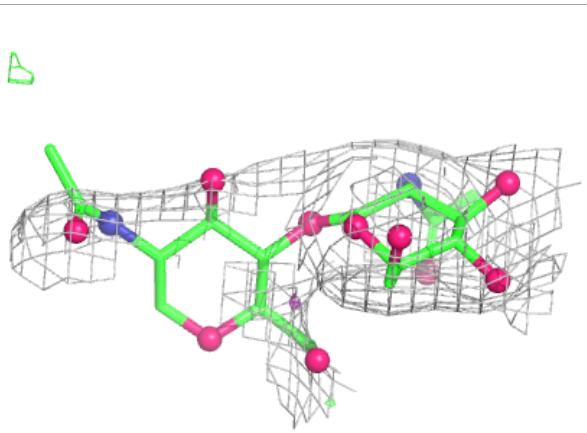


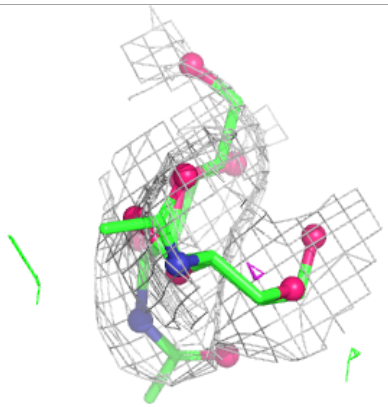




Electron density around Chain Z:

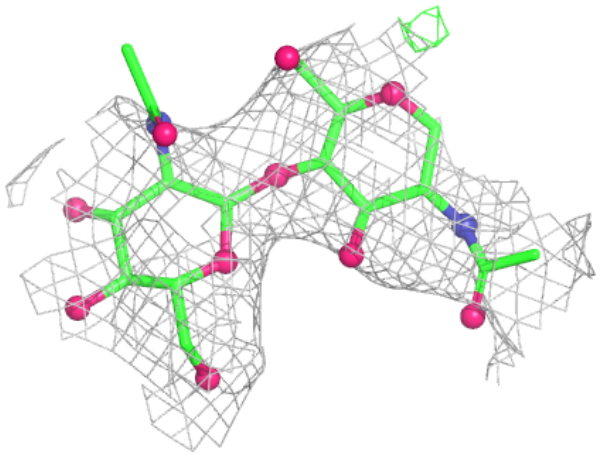
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

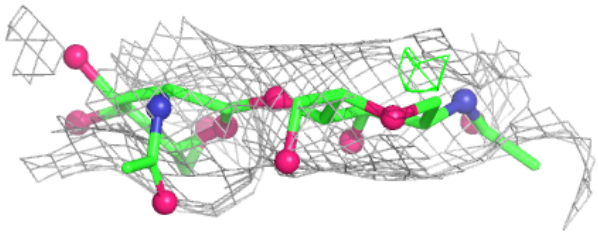


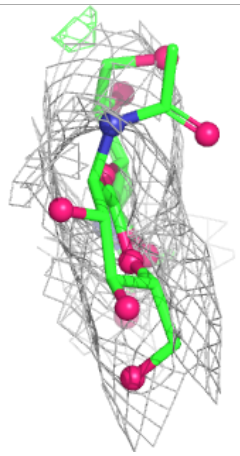


Electron density around Chain a:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

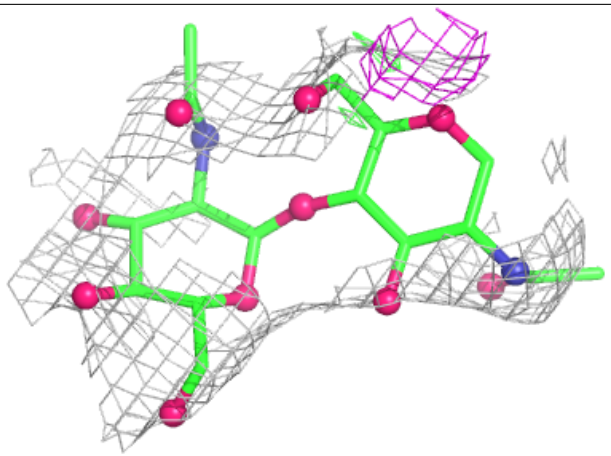


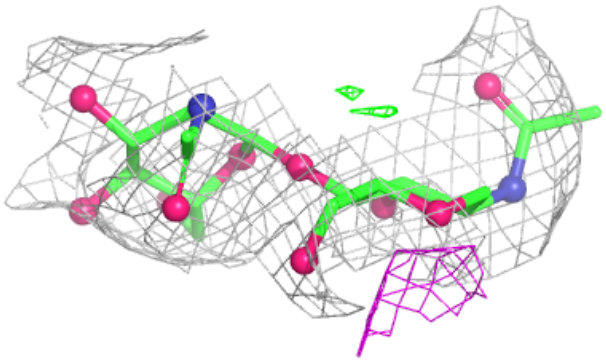


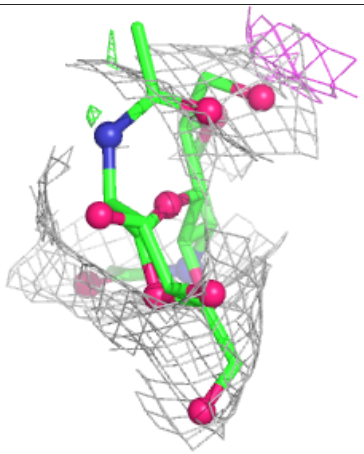


Electron density around Chain b:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

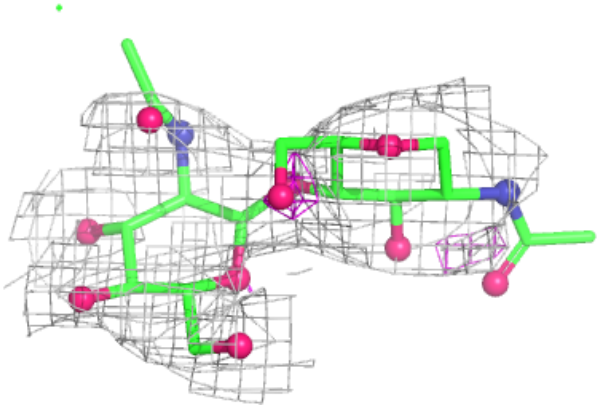


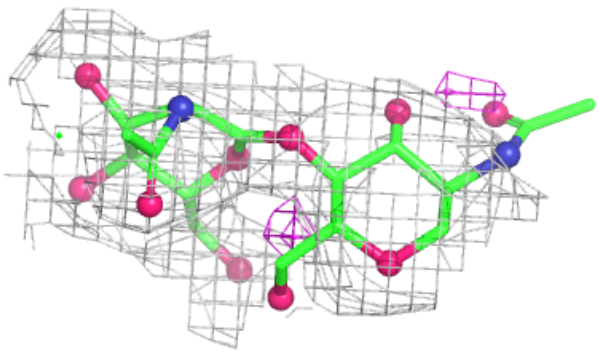


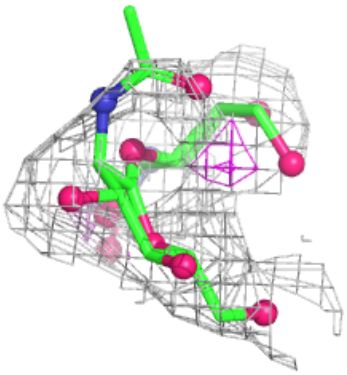


Electron density around Chain c:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

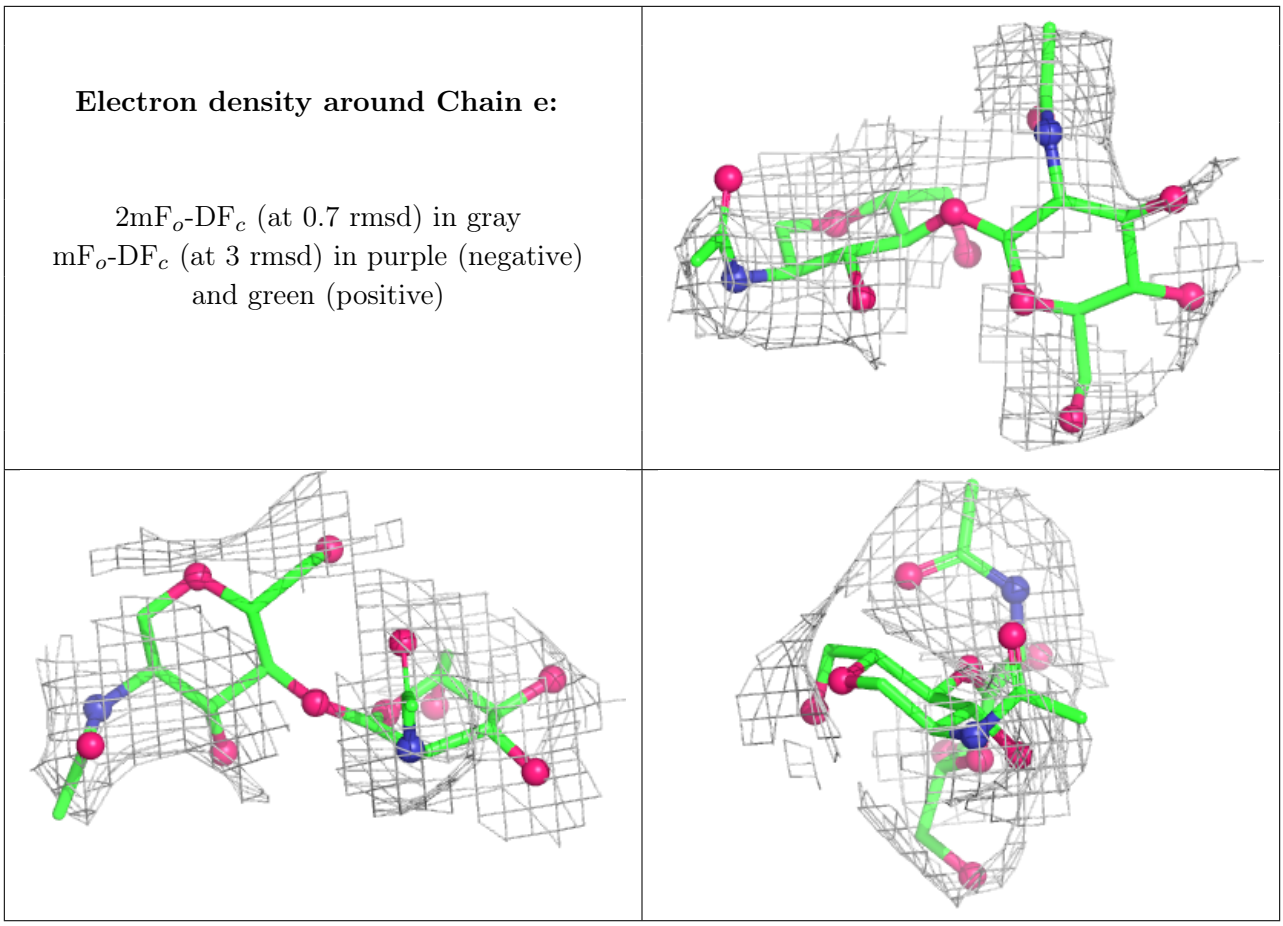






Electron density around Chain e:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NGT	H	28	14/14	0.73	0.33	48,50,53,54	0
8	NGT	G	533	14/14	0.75	0.35	47,47,49,50	0
8	NGT	E	530	14/14	0.77	0.25	47,49,52,53	0
8	NGT	C	530	14/14	0.81	0.25	44,46,49,50	0
8	NGT	F	26	14/14	0.85	0.23	40,41,42,43	0
8	NGT	B	22	14/14	0.90	0.23	38,39,41,44	0
8	NGT	D	24	14/14	0.93	0.18	39,41,43,43	0
8	NGT	A	21	14/14	0.94	0.17	33,35,37,37	0

6.5 Other polymers

There are no such residues in this entry.