wwPDB X-ray Structure Validation Summary Report (i)

Sep 24, 2023 – 10:12 PM EDT

PDB ID	:	5UM8
Title	:	Crystal structure of HIV-1 envelope trimer 16055 NFL TD CC (T569G) in complex with Fabs 35022 and PGT124
Authors	:	Garces, F.; Stanfield, R.L.; Wilson, I.A.
Deposited on	:	2017-01-26
Resolution	:	3.94 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 (1)) were used in the production of this report:

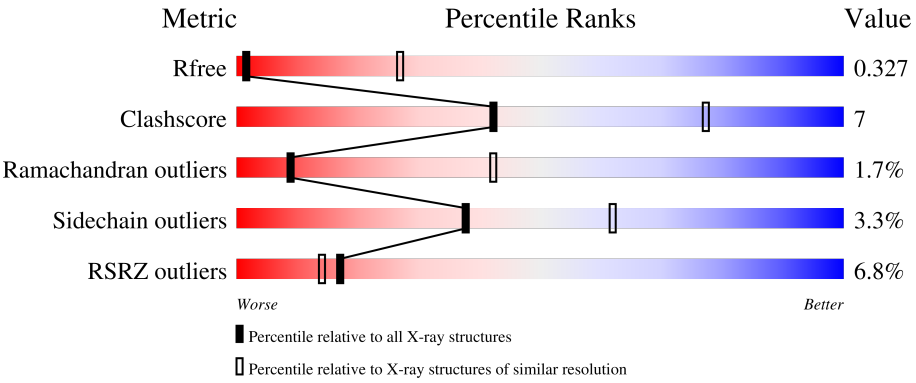
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.94 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	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)

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	G	485	3% 72% 22%
2	B	153	3% 61% 22% 16%
3	L	214	3% 78% 20%
4	H	236	4% 77% 22%
5	D	240	15% 88% 12%

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Mol	Chain	Length	Quality of chain
6	E	216	15% 88% 10%
7	A	2	100%
7	C	2	100%
7	F	2	100%
7	I	2	100%
7	J	2	50% 50%
7	M	2	50% 50%
7	O	2	50% 50%
7	S	2	100%
8	K	5	40% 40% 20%
9	N	3	100%
10	P	10	20% 80%
11	Q	7	14% 71% 14%
12	R	6	33% 67%

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
11	NAG	Q	2	-	-	-	X
11	BMA	Q	3	-	-	-	X
13	NAG	B	703	-	-	-	X
9	BMA	N	3	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 12221 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 glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	471	Total	C	N	O	S	0	0	0
			3681	2304	645	705	27			

- Molecule 2 is a protein called glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	129	Total	C	N	O	S	0	0	0
			1017	641	178	193	5			

- Molecule 3 is a protein called Fab PGT124 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1599	1007	271	316	5			

- Molecule 4 is a protein called Fab PGT124 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	234	Total	C	N	O	S	0	0	0
			1775	1123	297	349	6			

- Molecule 5 is a protein called Fab 35022 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

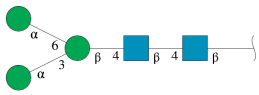
- Molecule 6 is a protein called Fab 35022 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

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

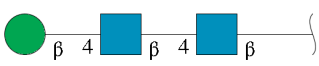
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called 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.



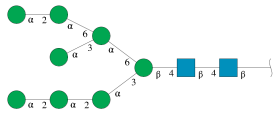
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 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.



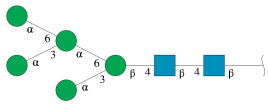
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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.



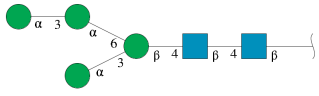
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	P	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.



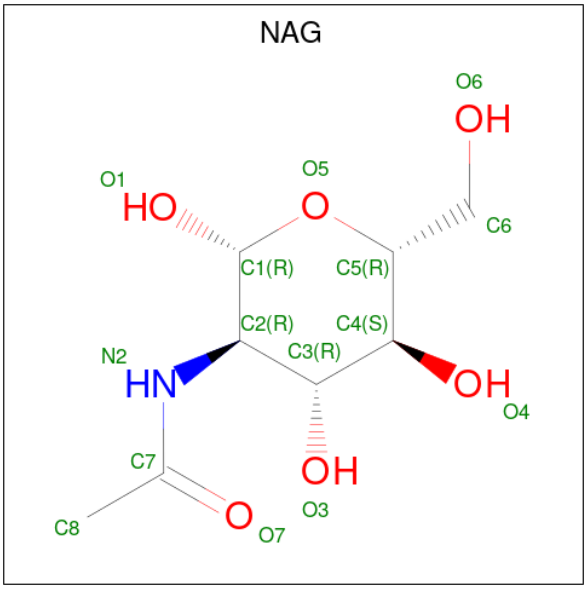
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	Q	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	R	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

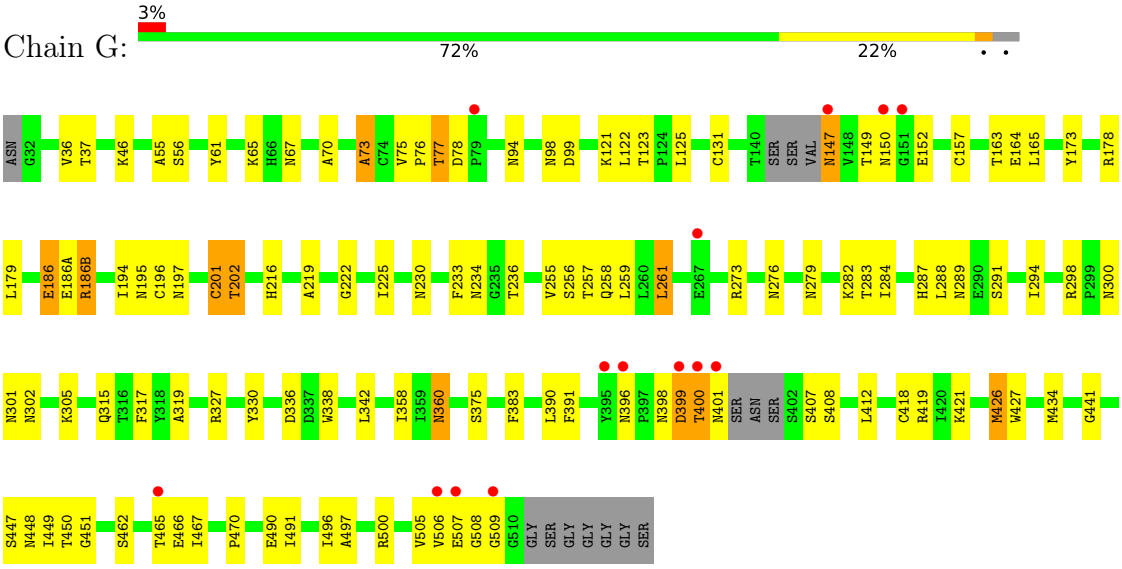


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0

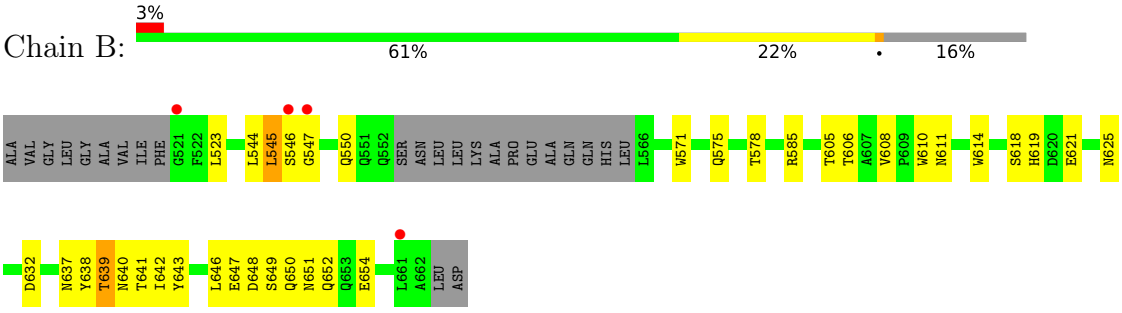
3 Residue-property plots (i)

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.

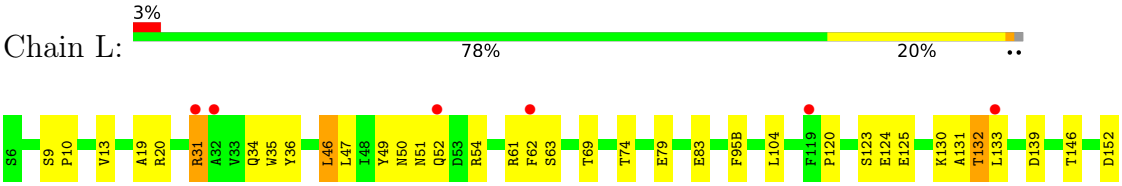
• Molecule 1: glycoprotein gp120

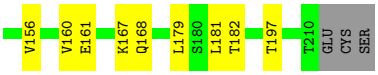


• Molecule 2: glycoprotein gp41



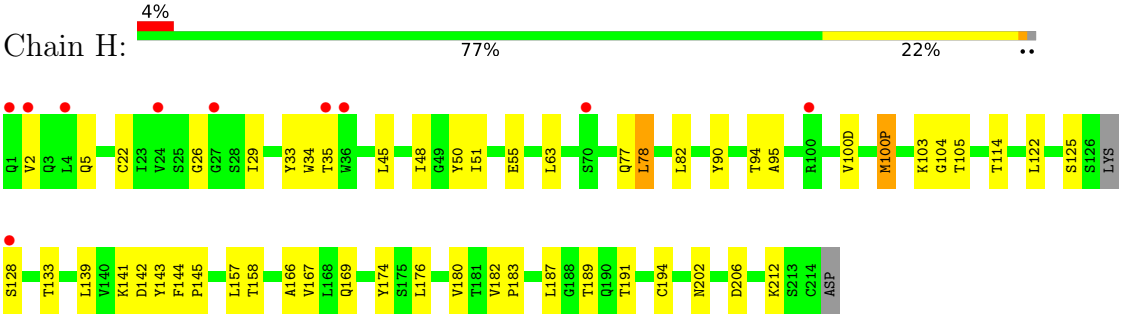
• Molecule 3: Fab PGT124 light chain





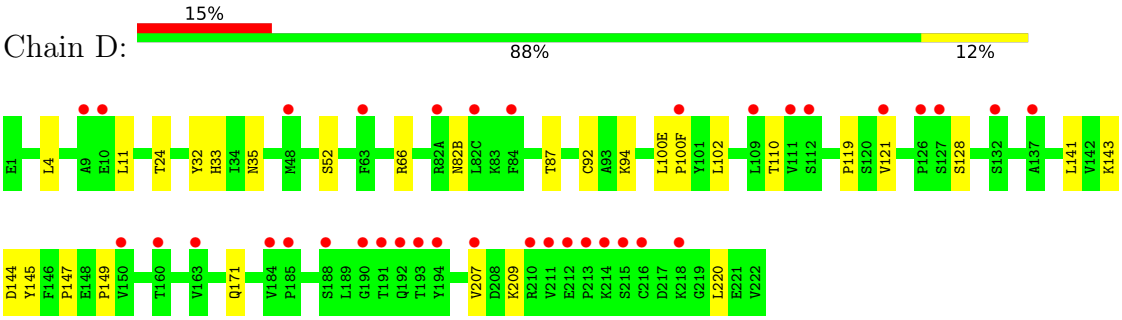
• Molecule 4: Fab PGT124 heavy chain

Chain H:



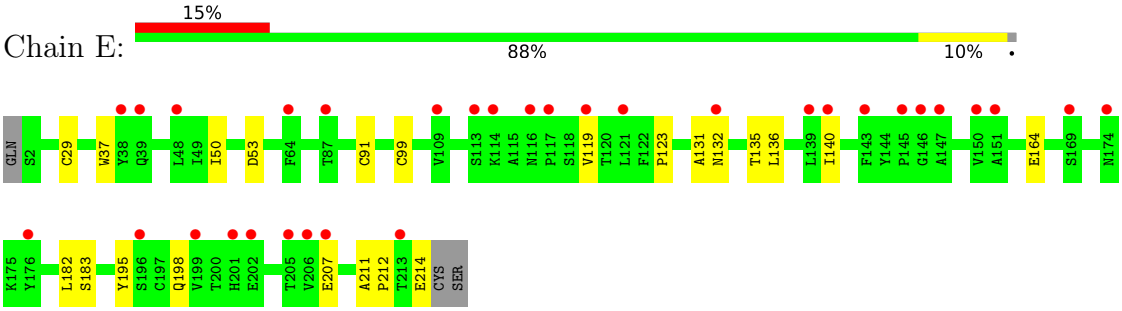
• Molecule 5: Fab 35022 heavy chain

Chain D:



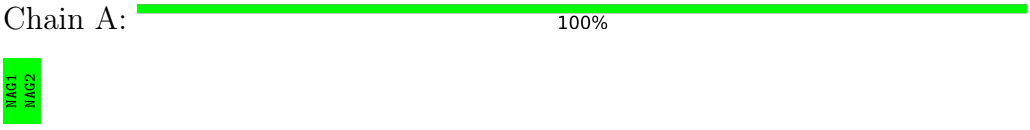
• Molecule 6: Fab 35022 light chain

Chain E:



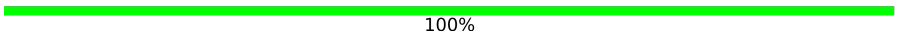
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



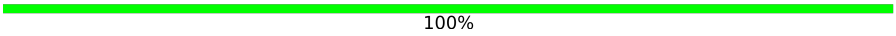
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



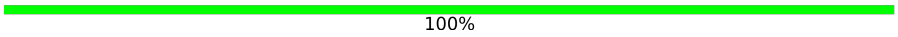
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain I:



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

Chain J:

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

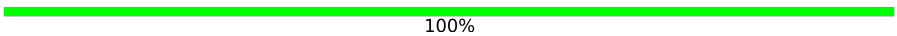
Chain M:

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

Chain O:

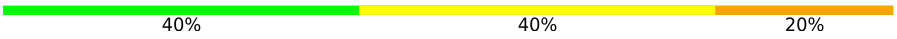
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 8: 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

Chain K:



• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

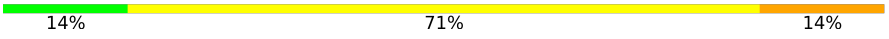
Chain N:

• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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

Chain P:

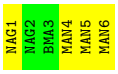
• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 12: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	126.46Å 126.46Å 314.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.25 – 3.94 49.25 – 3.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.25-3.94) 99.9 (49.25-3.94)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 3.88Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.260 , 0.329 0.261 , 0.327	Depositor DCC
R_{free} test set	1259 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	116.1	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 101.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.090 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12221	wwPDB-VP
Average B, all atoms (Å^2)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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

5.1 Standard geometry

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

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	G	0.30	1/3755 (0.0%)	0.48	0/5103
2	B	0.23	0/1035	0.40	0/1403
3	L	0.24	0/1642	0.45	0/2243
4	H	0.24	0/1818	0.45	0/2480
5	D	0.24	0/1860	0.45	0/2533
6	E	0.24	0/1659	0.44	0/2269
All	All	0.26	1/11769 (0.0%)	0.45	0/16031

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	186(B)	ARG	CA-C	-8.73	1.30	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	G	3681	0	3587	68	0
2	B	1017	0	992	26	0
3	L	1599	0	1542	26	0
4	H	1775	0	1742	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1813	0	1784	18	0
6	E	1615	0	1544	14	0
7	A	28	0	25	0	0
7	C	28	0	25	0	0
7	F	28	0	25	0	0
7	I	28	0	25	0	0
7	J	28	0	25	1	0
7	M	28	0	25	1	0
7	O	28	0	25	0	0
7	S	28	0	25	0	0
8	K	61	0	52	1	0
9	N	39	0	34	0	0
10	P	116	0	97	1	0
11	Q	83	0	70	2	0
12	R	72	0	61	1	0
13	B	42	0	39	1	0
13	G	84	0	78	3	0
All	All	12221	0	11822	166	0

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 7.

The worst 5 of 166 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)
1:G:149:THR:HG22	1:G:150:ASN:H	1.13	1.11
1:G:149:THR:HG22	1:G:150:ASN:N	1.77	0.93
1:G:150:ASN:HD22	1:G:419:ARG:NH2	1.66	0.93
1:G:150:ASN:ND2	1:G:419:ARG:HH22	1.66	0.92
1:G:149:THR:CG2	1:G:150:ASN:H	1.84	0.90

There are no symmetry-related clashes.

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	G	465/485 (96%)	397 (85%)	55 (12%)	13 (3%)	5 33
2	B	125/153 (82%)	108 (86%)	13 (10%)	4 (3%)	4 31
3	L	209/214 (98%)	194 (93%)	13 (6%)	2 (1%)	15 52
4	H	230/236 (98%)	211 (92%)	16 (7%)	3 (1%)	12 47
5	D	238/240 (99%)	224 (94%)	12 (5%)	2 (1%)	19 57
6	E	211/216 (98%)	201 (95%)	9 (4%)	1 (0%)	29 66
All	All	1478/1544 (96%)	1335 (90%)	118 (8%)	25 (2%)	9 42

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	186(B)	ARG
1	G	400	THR
2	B	546	SER
1	G	186	GLU
1	G	301	ASN

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	G	416/428 (97%)	395 (95%)	21 (5%)	24 52
2	B	108/128 (84%)	106 (98%)	2 (2%)	57 75
3	L	176/180 (98%)	171 (97%)	5 (3%)	43 65
4	H	202/204 (99%)	190 (94%)	12 (6%)	19 47
5	D	203/203 (100%)	203 (100%)	0	100 100
6	E	186/189 (98%)	183 (98%)	3 (2%)	62 78
All	All	1291/1332 (97%)	1248 (97%)	43 (3%)	38 62

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	45	LEU
4	H	187	LEU
4	H	78	LEU
4	H	105	THR
4	H	194	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	147	ASN
1	G	150	ASN
6	E	201	HIS

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)

47 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	$\#\|Z\| > 2$
7	NAG	A	1	1,7	14,14,15	0.50	0	17,19,21	0.57	0
7	NAG	A	2	7	14,14,15	0.28	0	17,19,21	0.65	0
7	NAG	C	1	1,7	14,14,15	0.28	0	17,19,21	0.54	0
7	NAG	C	2	7	14,14,15	0.24	0	17,19,21	0.41	0
7	NAG	F	1	1,7	14,14,15	0.32	0	17,19,21	0.42	0
7	NAG	F	2	7	14,14,15	0.24	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	I	1	1,7	14,14,15	0.20	0	17,19,21	0.43	0
7	NAG	I	2	7	14,14,15	0.25	0	17,19,21	0.41	0
7	NAG	J	1	1,7	14,14,15	0.30	0	17,19,21	0.37	0
7	NAG	J	2	7	14,14,15	0.22	0	17,19,21	0.44	0
8	NAG	K	1	1,8	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	K	2	8	14,14,15	0.21	0	17,19,21	0.40	0
8	BMA	K	3	8	11,11,12	0.58	0	15,15,17	0.77	0
8	MAN	K	4	8	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
8	MAN	K	5	8	11,11,12	0.69	0	15,15,17	1.02	2 (13%)
7	NAG	M	1	1,7	14,14,15	0.24	0	17,19,21	0.42	0
7	NAG	M	2	7	14,14,15	0.24	0	17,19,21	0.45	0
9	NAG	N	1	1,9	14,14,15	0.24	0	17,19,21	0.39	0
9	NAG	N	2	9	14,14,15	0.22	0	17,19,21	0.41	0
9	BMA	N	3	9	11,11,12	0.58	0	15,15,17	0.75	0
7	NAG	O	1	1,7	14,14,15	0.25	0	17,19,21	0.64	1 (5%)
7	NAG	O	2	7	14,14,15	0.24	0	17,19,21	0.42	0
10	NAG	P	1	10,1	14,14,15	0.21	0	17,19,21	0.40	0
10	MAN	P	10	10	11,11,12	0.66	0	15,15,17	1.00	2 (13%)
10	NAG	P	2	10	14,14,15	0.19	0	17,19,21	0.41	0
10	BMA	P	3	10	11,11,12	0.66	0	15,15,17	0.94	0
10	MAN	P	4	10	11,11,12	0.81	1 (9%)	15,15,17	1.32	2 (13%)
10	MAN	P	5	10	11,11,12	0.68	0	15,15,17	1.06	2 (13%)
10	MAN	P	6	10	11,11,12	0.66	0	15,15,17	1.03	2 (13%)
10	MAN	P	7	10	11,11,12	0.63	0	15,15,17	0.98	2 (13%)
10	MAN	P	8	10	11,11,12	0.66	0	15,15,17	1.05	2 (13%)
10	MAN	P	9	10	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
11	NAG	Q	1	1,11	14,14,15	0.26	0	17,19,21	0.47	0
11	NAG	Q	2	11	14,14,15	0.37	0	17,19,21	0.46	0
11	BMA	Q	3	11	11,11,12	0.61	0	15,15,17	0.70	0
11	MAN	Q	4	11	11,11,12	1.52	2 (18%)	15,15,17	2.10	3 (20%)
11	MAN	Q	5	11	11,11,12	0.62	0	15,15,17	0.92	2 (13%)
11	MAN	Q	6	11	11,11,12	0.63	0	15,15,17	1.03	2 (13%)
11	MAN	Q	7	11	11,11,12	0.71	0	15,15,17	0.97	2 (13%)
12	NAG	R	1	12,1	14,14,15	0.35	0	17,19,21	0.52	0
12	NAG	R	2	12	14,14,15	0.24	0	17,19,21	0.38	0
12	BMA	R	3	12	11,11,12	0.89	0	15,15,17	0.85	0
12	MAN	R	4	12	11,11,12	1.24	1 (9%)	15,15,17	1.29	2 (13%)
12	MAN	R	5	12	11,11,12	0.74	0	15,15,17	0.86	1 (6%)
12	MAN	R	6	12	11,11,12	0.63	0	15,15,17	0.94	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	S	1	1,7	14,14,15	0.50	0	17,19,21	0.51	0
7	NAG	S	2	7	14,14,15	0.26	0	17,19,21	0.52	0

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
7	NAG	A	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	3/6/23/26	0/1/1/1
7	NAG	C	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	C	2	7	-	2/6/23/26	0/1/1/1
7	NAG	F	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	F	2	7	-	2/6/23/26	0/1/1/1
7	NAG	I	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	NAG	J	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
8	NAG	K	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	K	2	8	-	2/6/23/26	0/1/1/1
8	BMA	K	3	8	-	2/2/19/22	0/1/1/1
8	MAN	K	4	8	-	1/2/19/22	0/1/1/1
8	MAN	K	5	8	-	0/2/19/22	0/1/1/1
7	NAG	M	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
9	NAG	N	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	N	2	9	-	2/6/23/26	0/1/1/1
9	BMA	N	3	9	-	0/2/19/22	0/1/1/1
7	NAG	O	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
10	NAG	P	1	10,1	-	4/6/23/26	0/1/1/1
10	MAN	P	10	10	-	0/2/19/22	0/1/1/1
10	NAG	P	2	10	-	1/6/23/26	0/1/1/1
10	BMA	P	3	10	-	0/2/19/22	0/1/1/1
10	MAN	P	4	10	-	0/2/19/22	0/1/1/1
10	MAN	P	5	10	-	1/2/19/22	0/1/1/1
10	MAN	P	6	10	-	0/2/19/22	0/1/1/1
10	MAN	P	7	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	P	8	10	-	0/2/19/22	0/1/1/1
10	MAN	P	9	10	-	0/2/19/22	0/1/1/1
11	NAG	Q	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	Q	2	11	-	0/6/23/26	0/1/1/1
11	BMA	Q	3	11	-	1/2/19/22	0/1/1/1
11	MAN	Q	4	11	-	0/2/19/22	0/1/1/1
11	MAN	Q	5	11	-	0/2/19/22	0/1/1/1
11	MAN	Q	6	11	-	2/2/19/22	0/1/1/1
11	MAN	Q	7	11	-	0/2/19/22	0/1/1/1
12	NAG	R	1	12,1	-	0/6/23/26	0/1/1/1
12	NAG	R	2	12	-	0/6/23/26	0/1/1/1
12	BMA	R	3	12	-	2/2/19/22	0/1/1/1
12	MAN	R	4	12	-	0/2/19/22	0/1/1/1
12	MAN	R	5	12	-	0/2/19/22	0/1/1/1
12	MAN	R	6	12	-	1/2/19/22	0/1/1/1
7	NAG	S	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	4	MAN	C1-C2	4.02	1.61	1.52
11	Q	4	MAN	O5-C1	2.42	1.47	1.43
10	P	4	MAN	C1-C2	2.36	1.57	1.52
12	R	4	MAN	C2-C3	2.33	1.55	1.52

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Q	4	MAN	C1-O5-C5	5.87	120.14	112.19
11	Q	4	MAN	C1-C2-C3	4.44	115.13	109.67
10	P	4	MAN	C1-O5-C5	3.14	116.45	112.19
12	R	4	MAN	C1-O5-C5	2.88	116.09	112.19
10	P	8	MAN	C1-O5-C5	2.56	115.66	112.19

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1	NAG	O5-C5-C6-O6
8	K	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	N	1	NAG	O5-C5-C6-O6
7	F	2	NAG	O5-C5-C6-O6
7	O	2	NAG	C4-C5-C6-O6

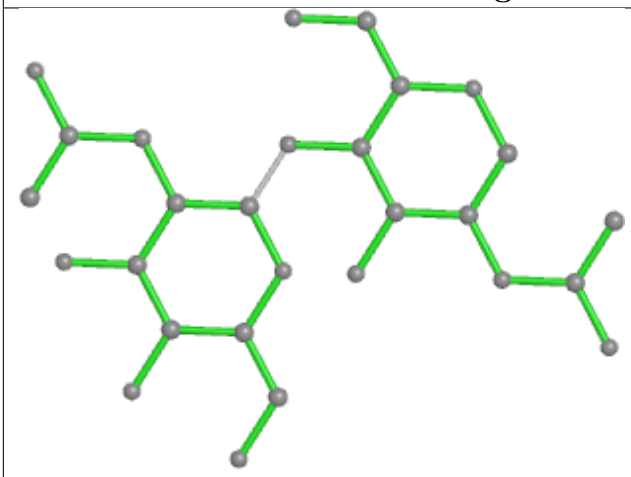
There are no ring outliers.

9 monomers are involved in 7 short contacts:

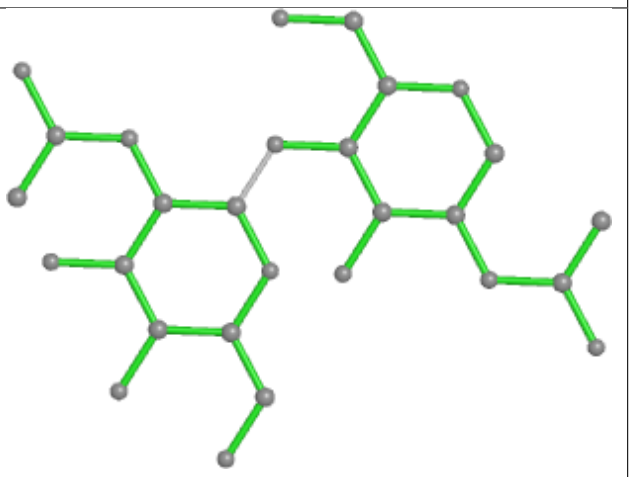
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	P	1	NAG	1	0
11	Q	3	BMA	1	0
7	J	2	NAG	1	0
8	K	5	MAN	1	0
11	Q	2	NAG	1	0
11	Q	4	MAN	1	0
12	R	1	NAG	1	0
8	K	3	BMA	1	0
7	M	1	NAG	1	0

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

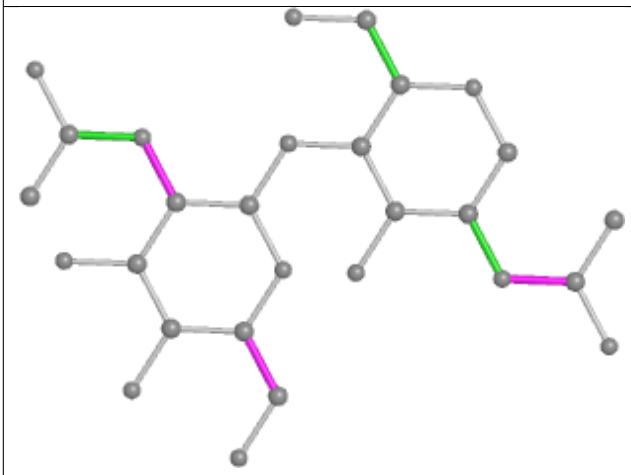
Oligosaccharide Chain A



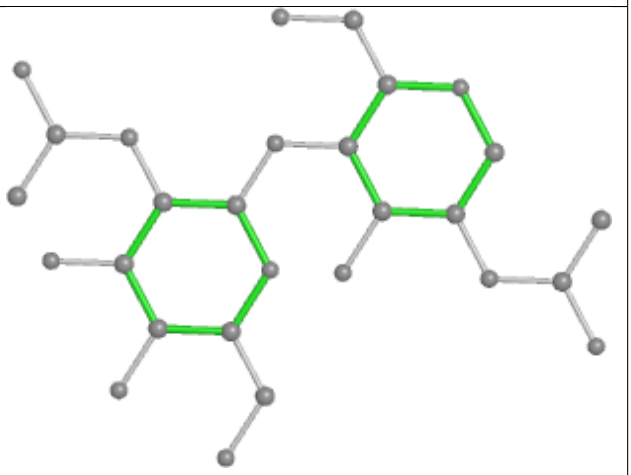
Bond lengths



Bond angles

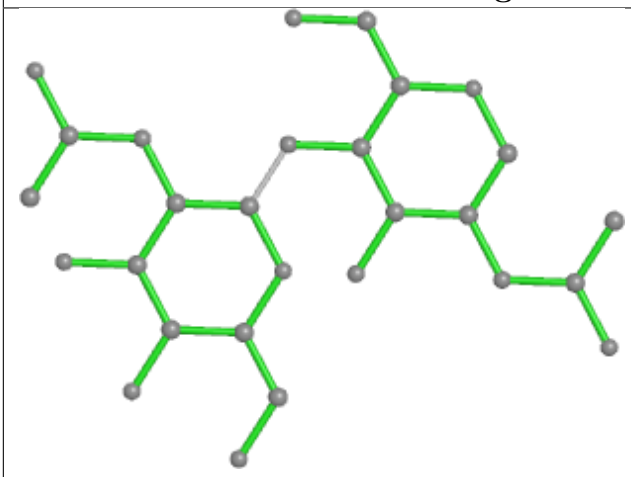


Torsions

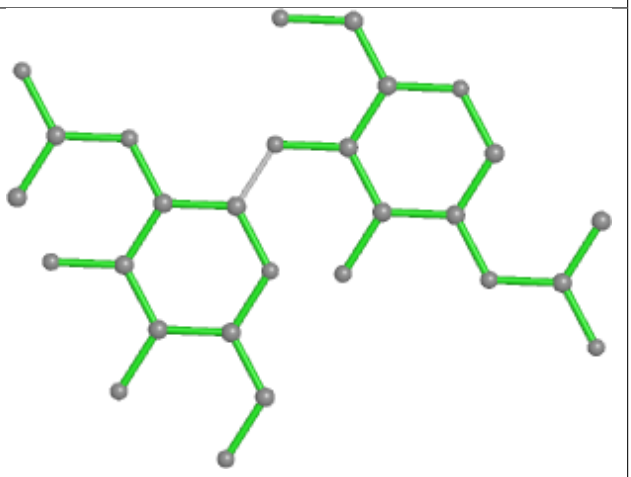


Rings

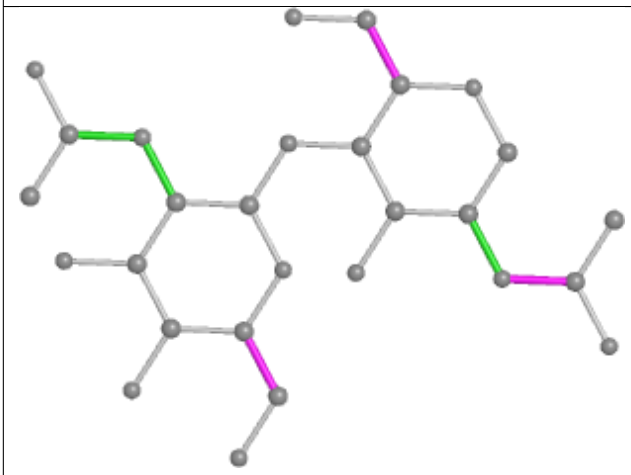
Oligosaccharide Chain C



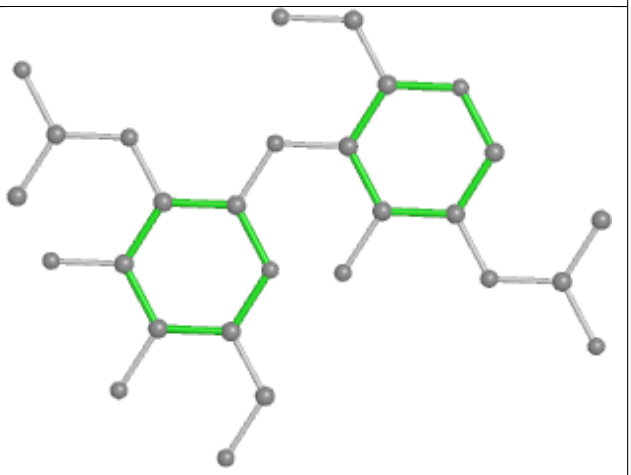
Bond lengths



Bond angles

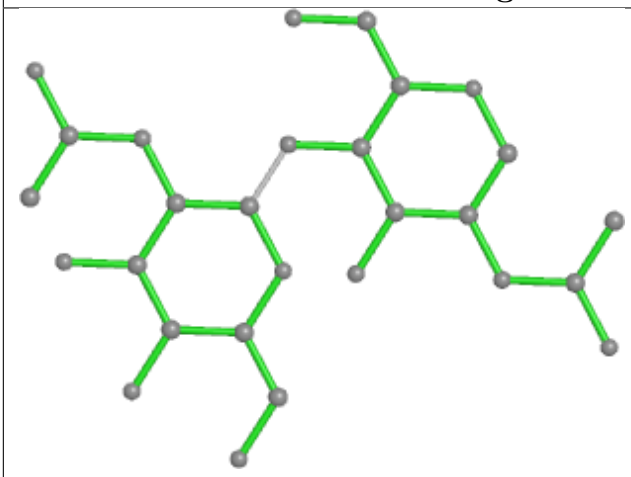


Torsions

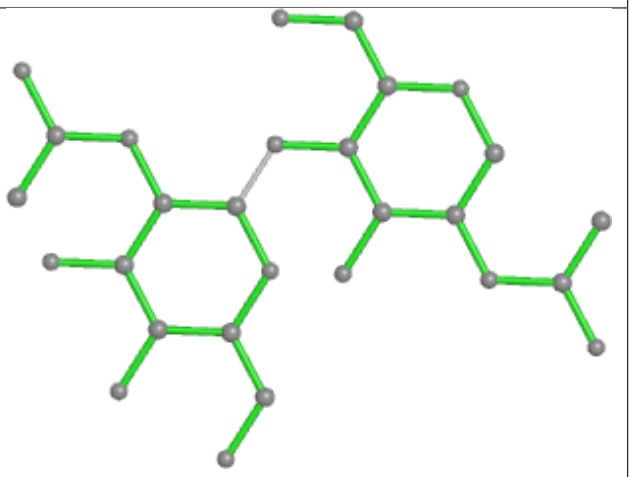


Rings

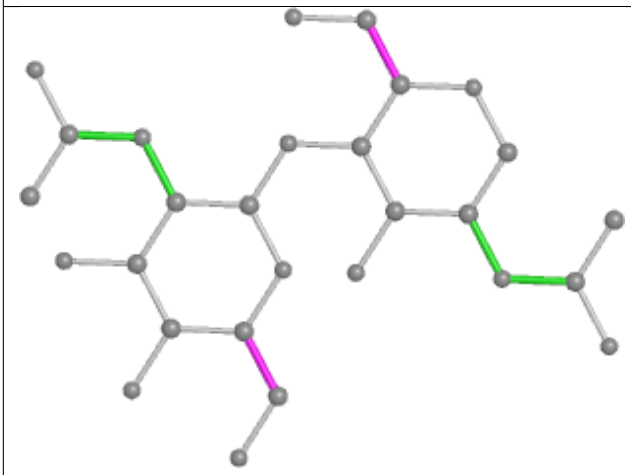
Oligosaccharide Chain F



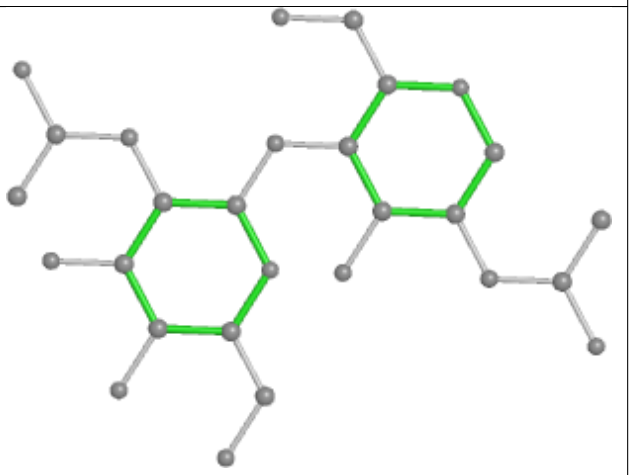
Bond lengths



Bond angles

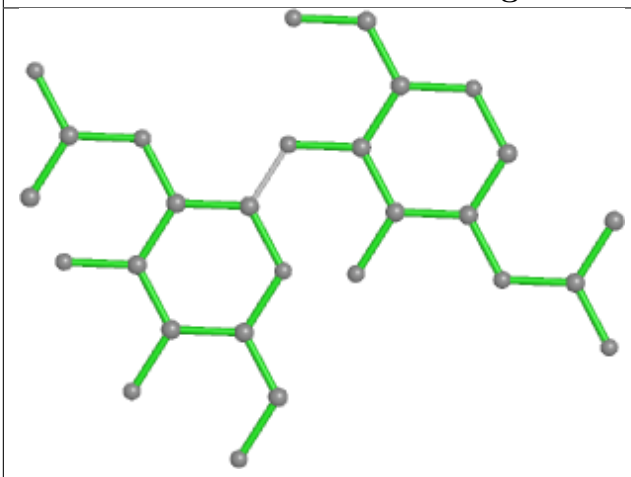


Torsions

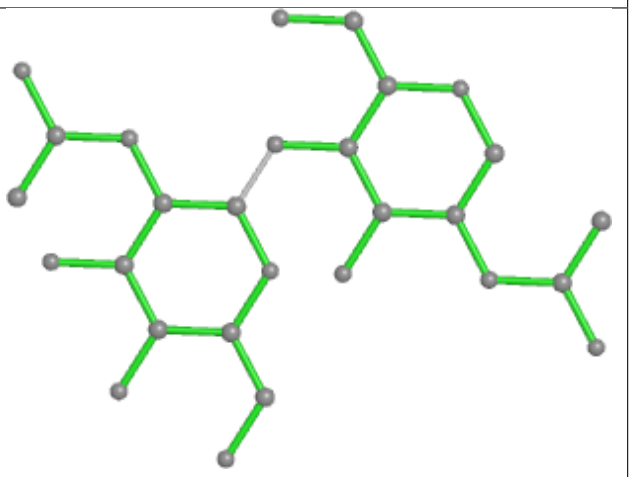


Rings

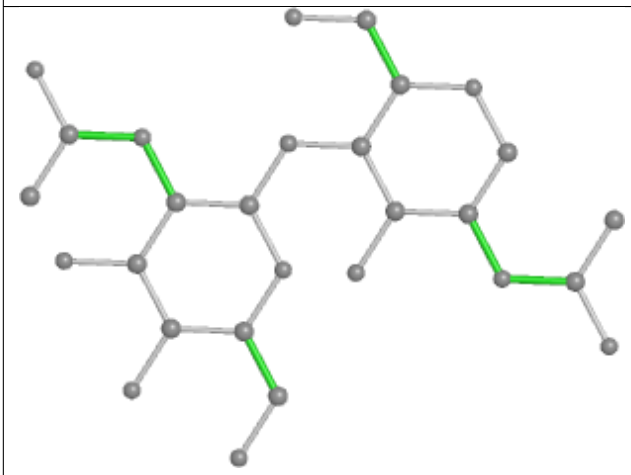
Oligosaccharide Chain I



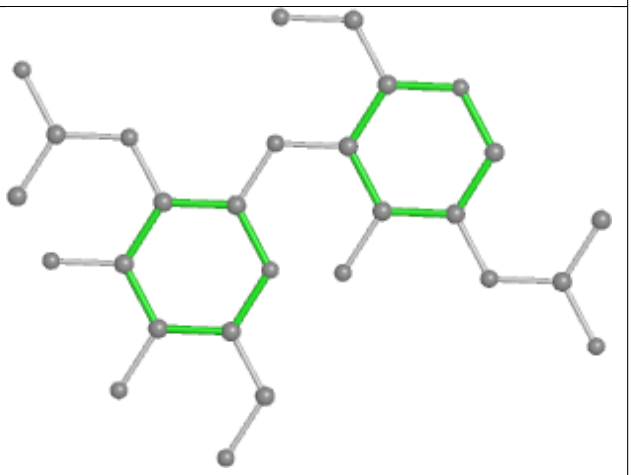
Bond lengths



Bond angles

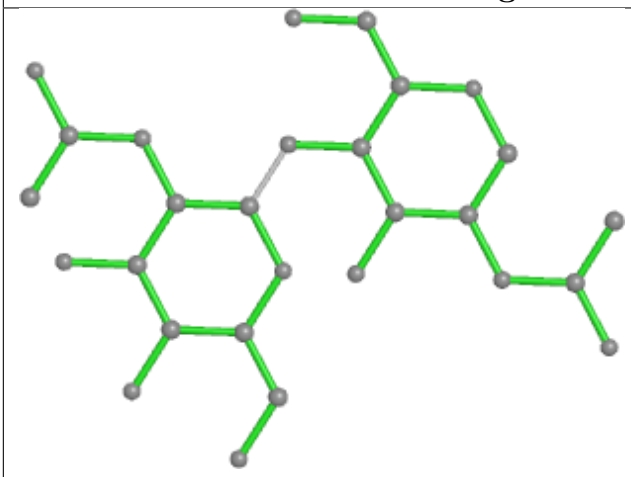


Torsions

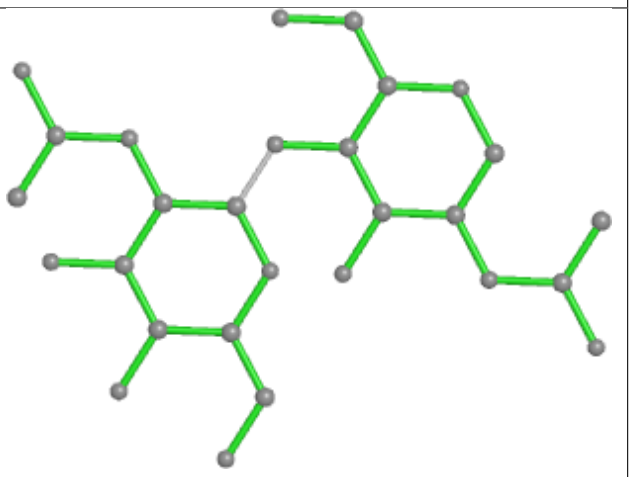


Rings

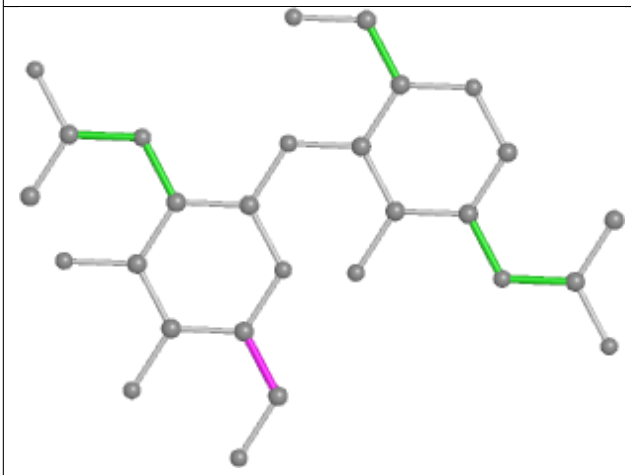
Oligosaccharide Chain J



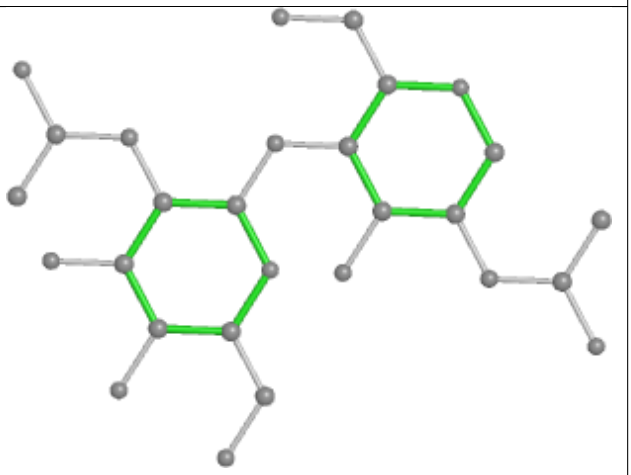
Bond lengths



Bond angles

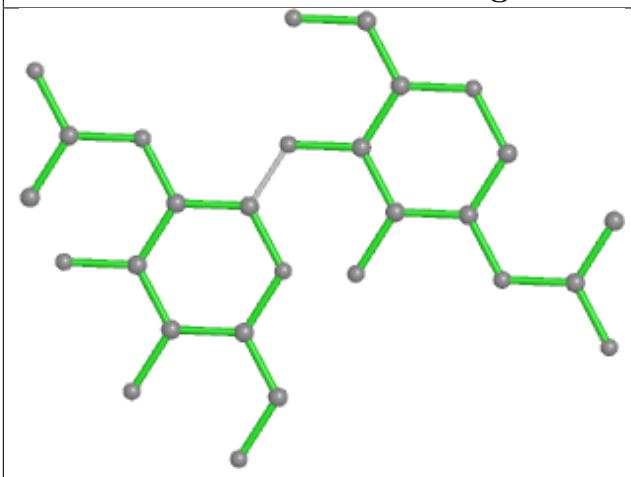


Torsions

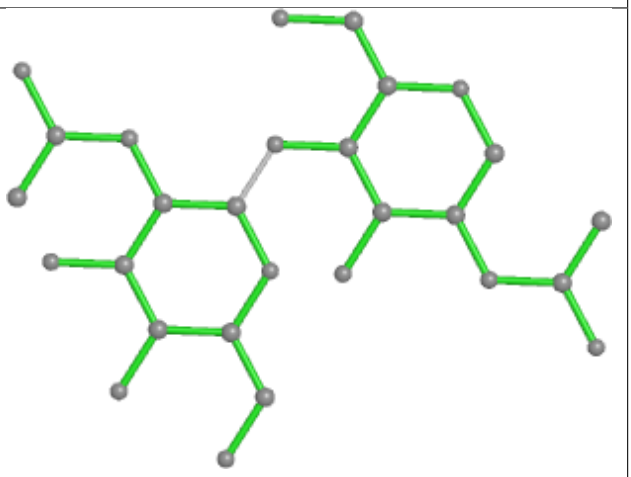


Rings

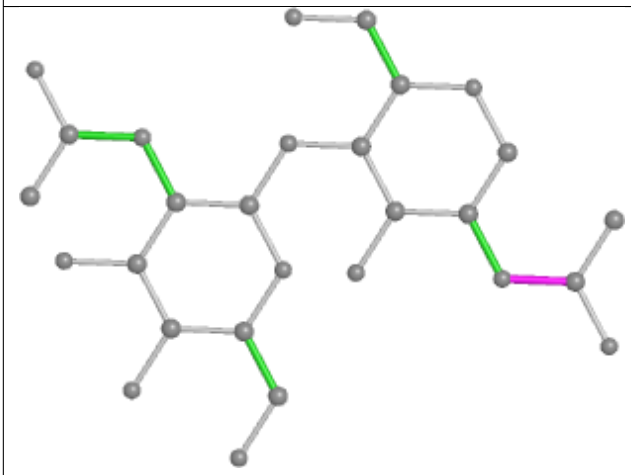
Oligosaccharide Chain M



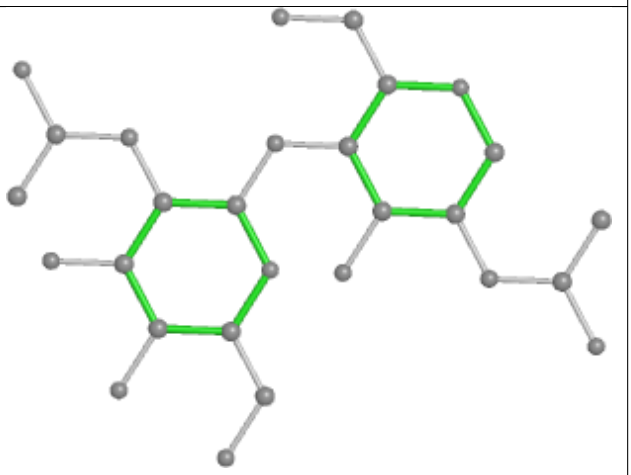
Bond lengths



Bond angles

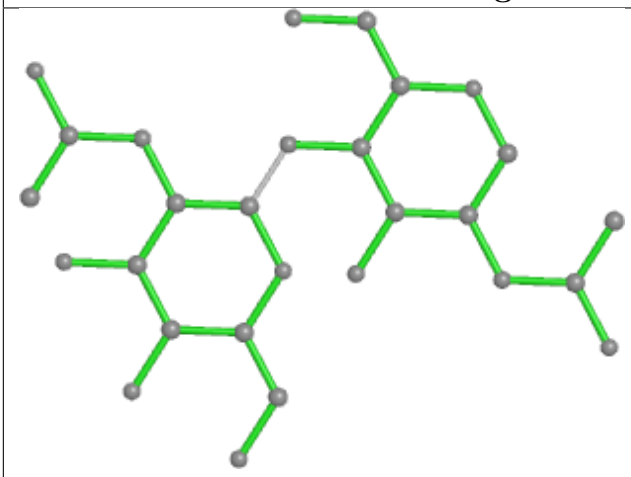


Torsions

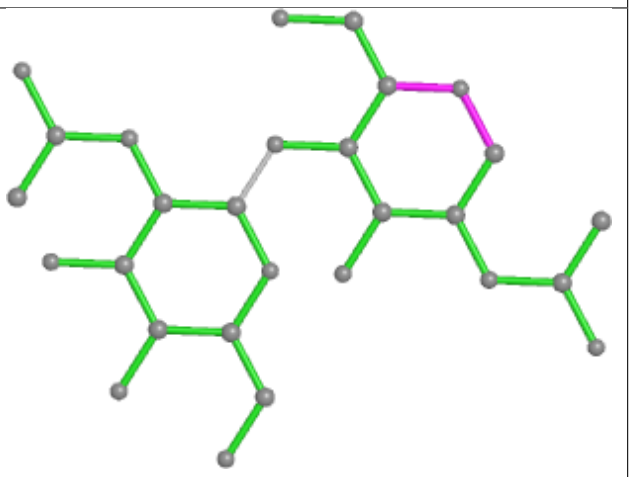


Rings

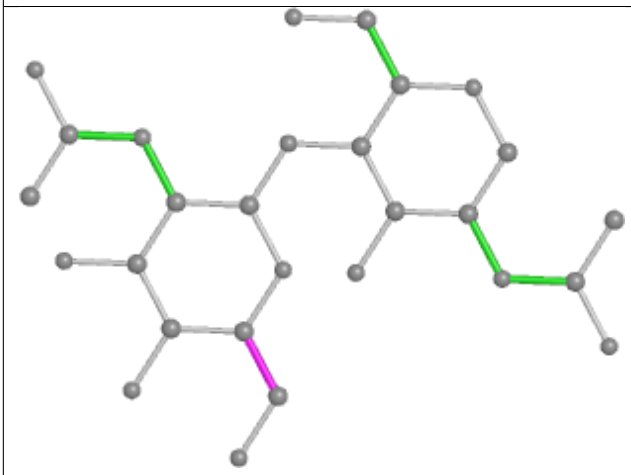
Oligosaccharide Chain O



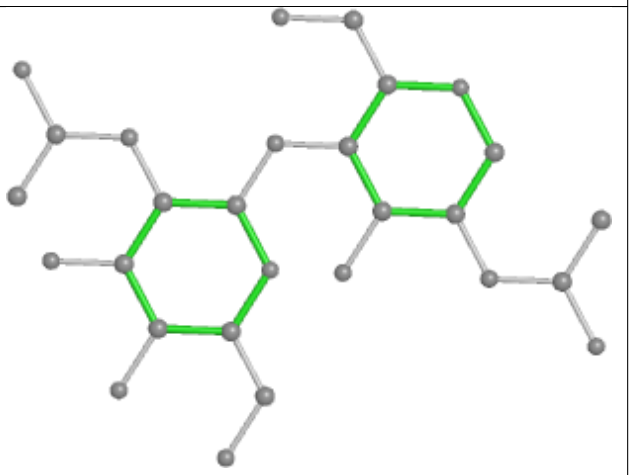
Bond lengths



Bond angles

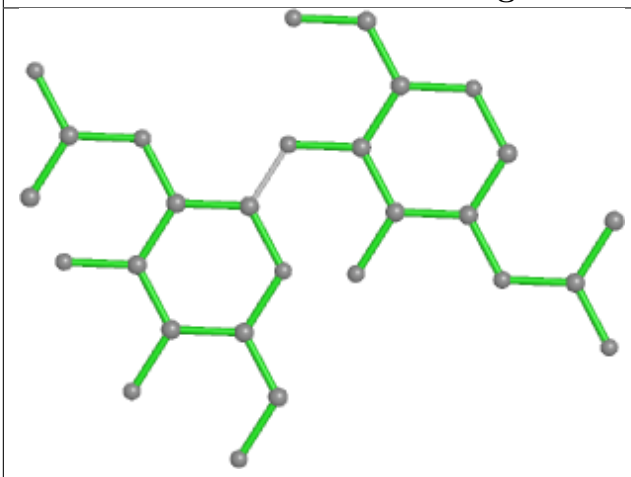


Torsions

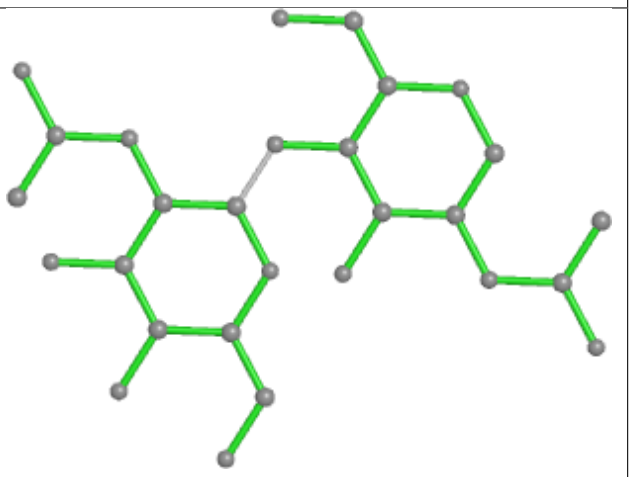


Rings

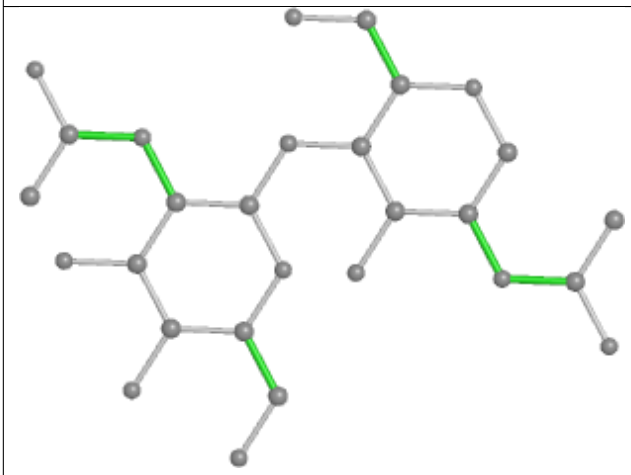
Oligosaccharide Chain S



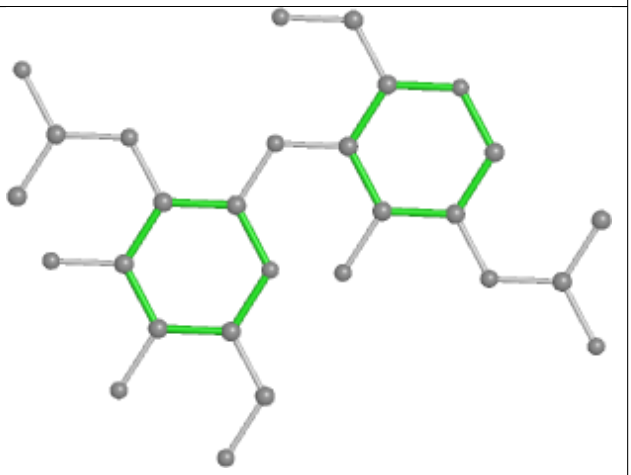
Bond lengths



Bond angles

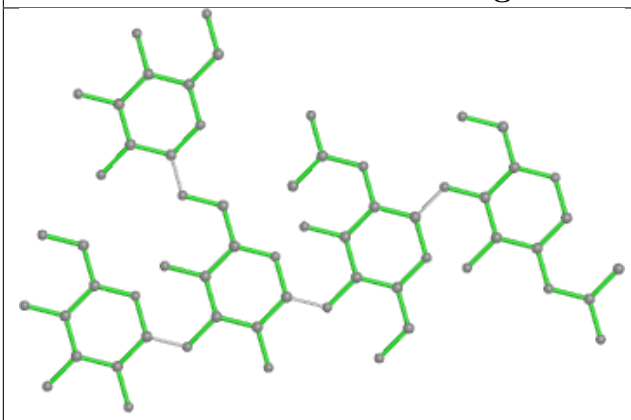


Torsions

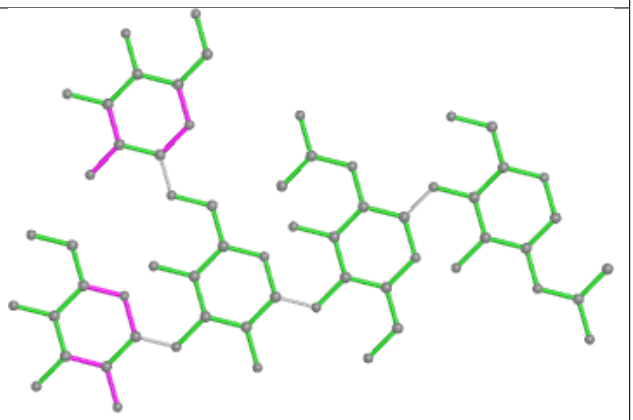


Rings

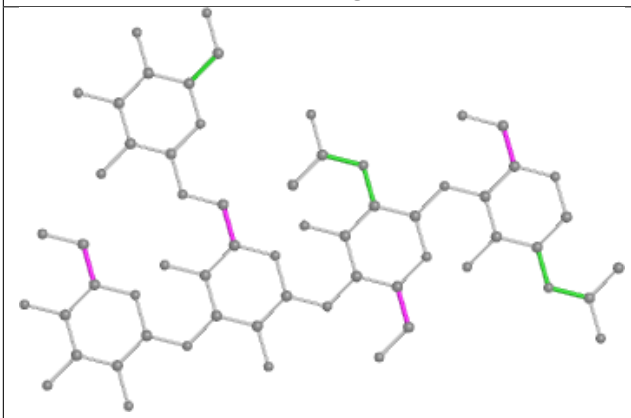
Oligosaccharide Chain K



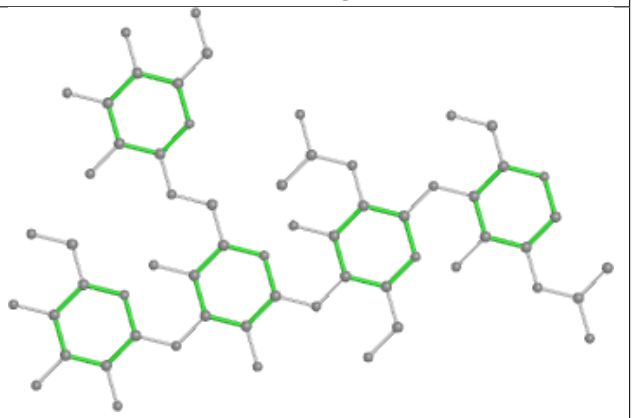
Bond lengths



Bond angles

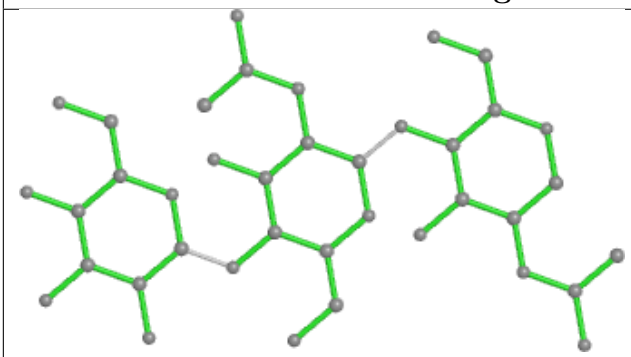


Torsions

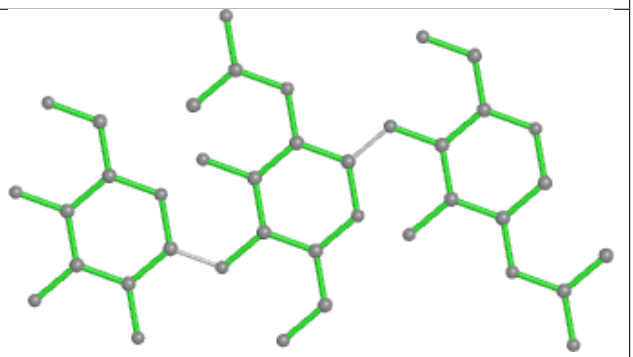


Rings

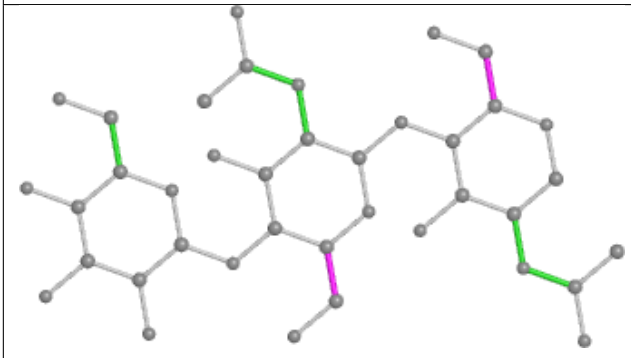
Oligosaccharide Chain N



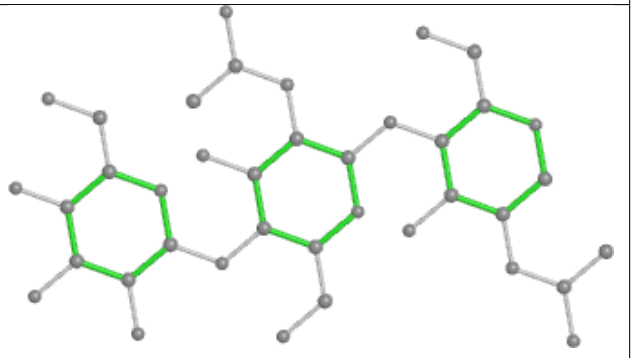
Bond lengths



Bond angles

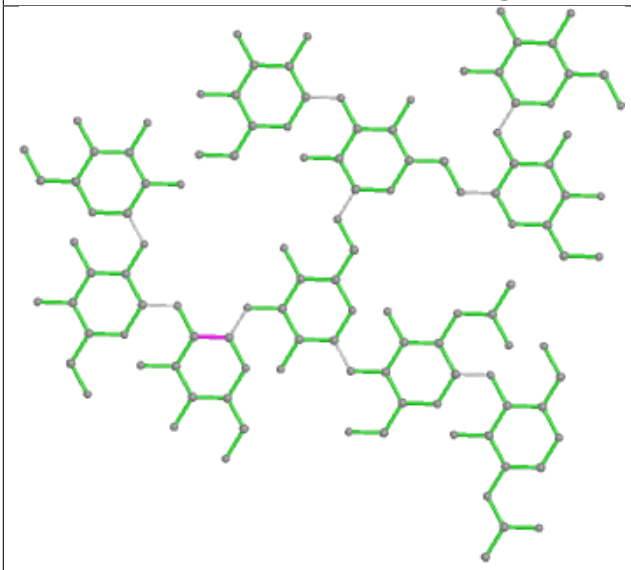


Torsions

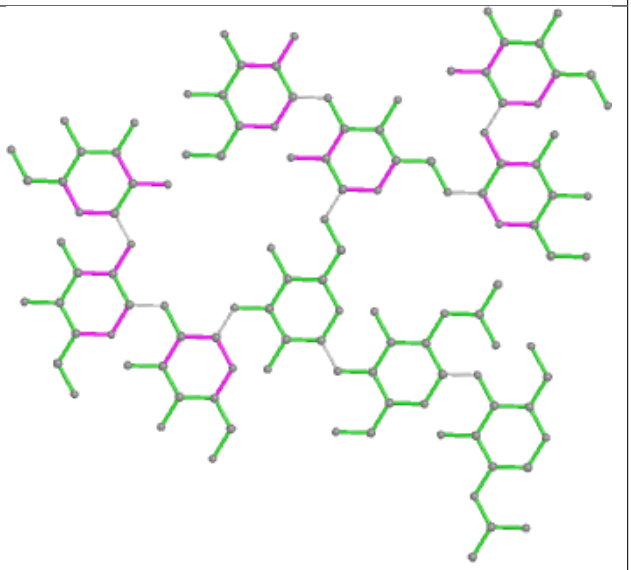


Rings

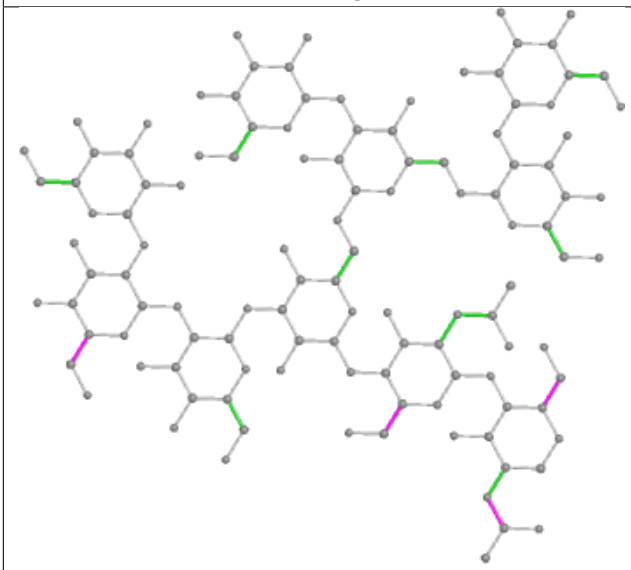
Oligosaccharide Chain P



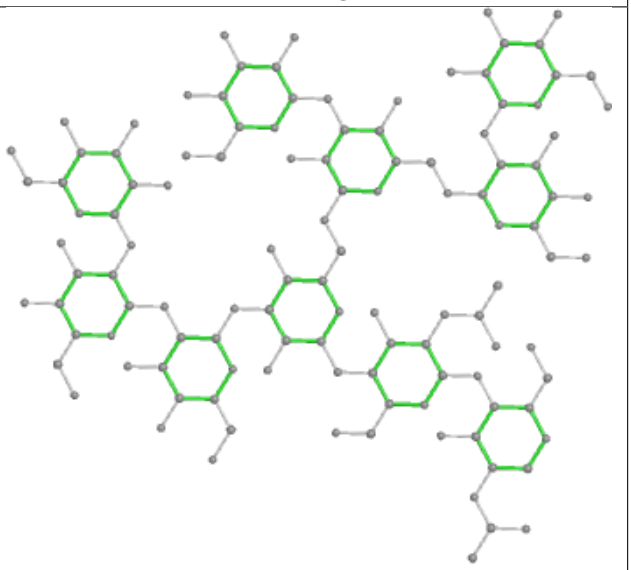
Bond lengths



Bond angles

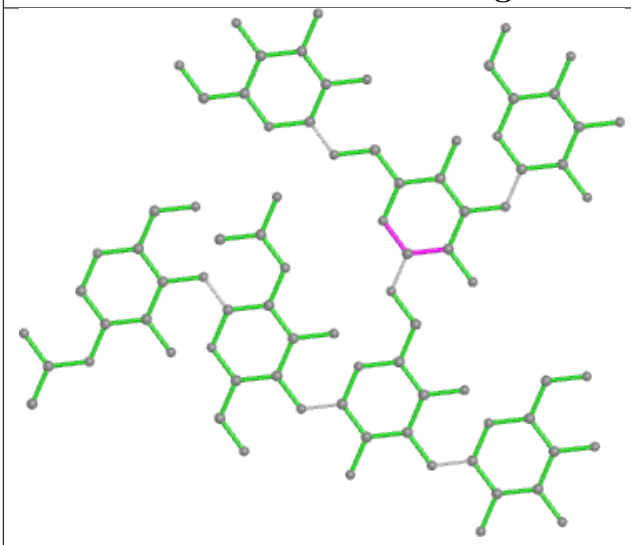


Torsions

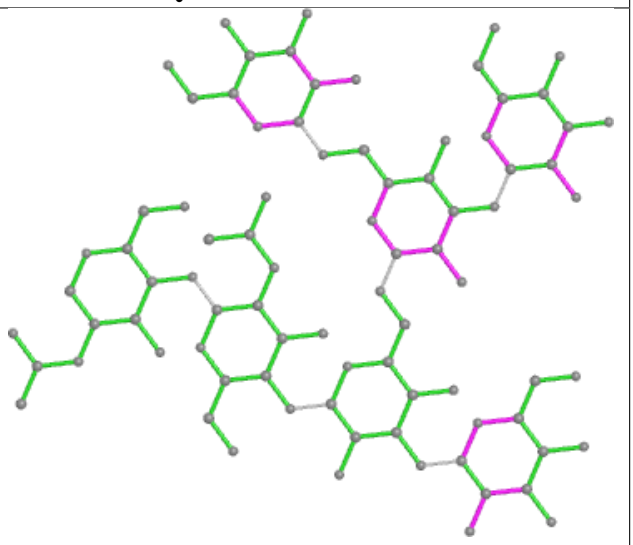


Rings

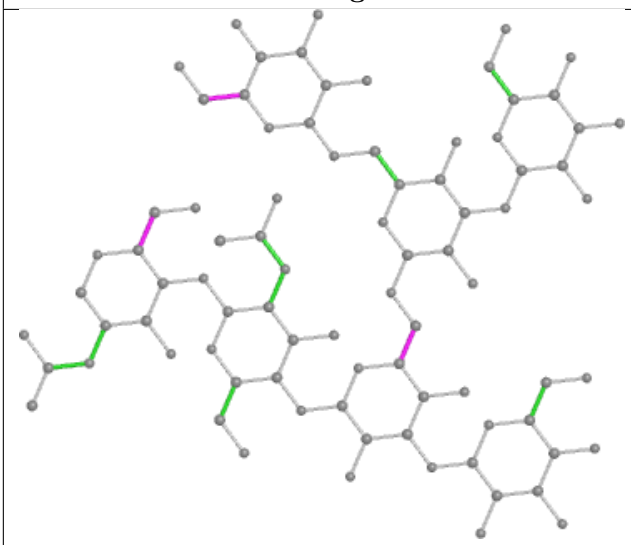
Oligosaccharide Chain Q



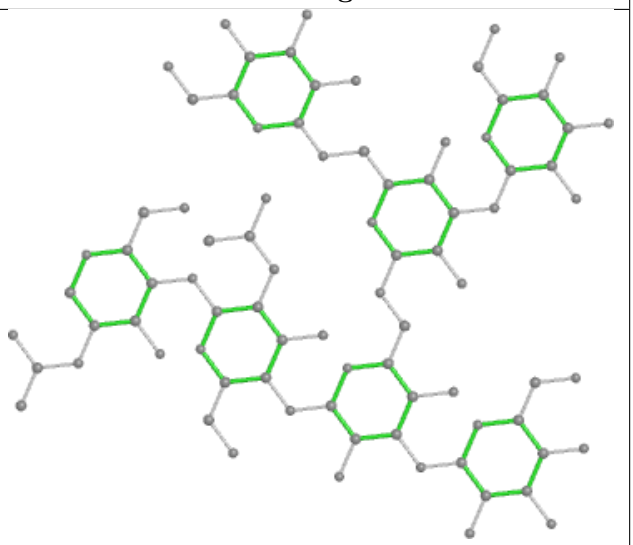
Bond lengths



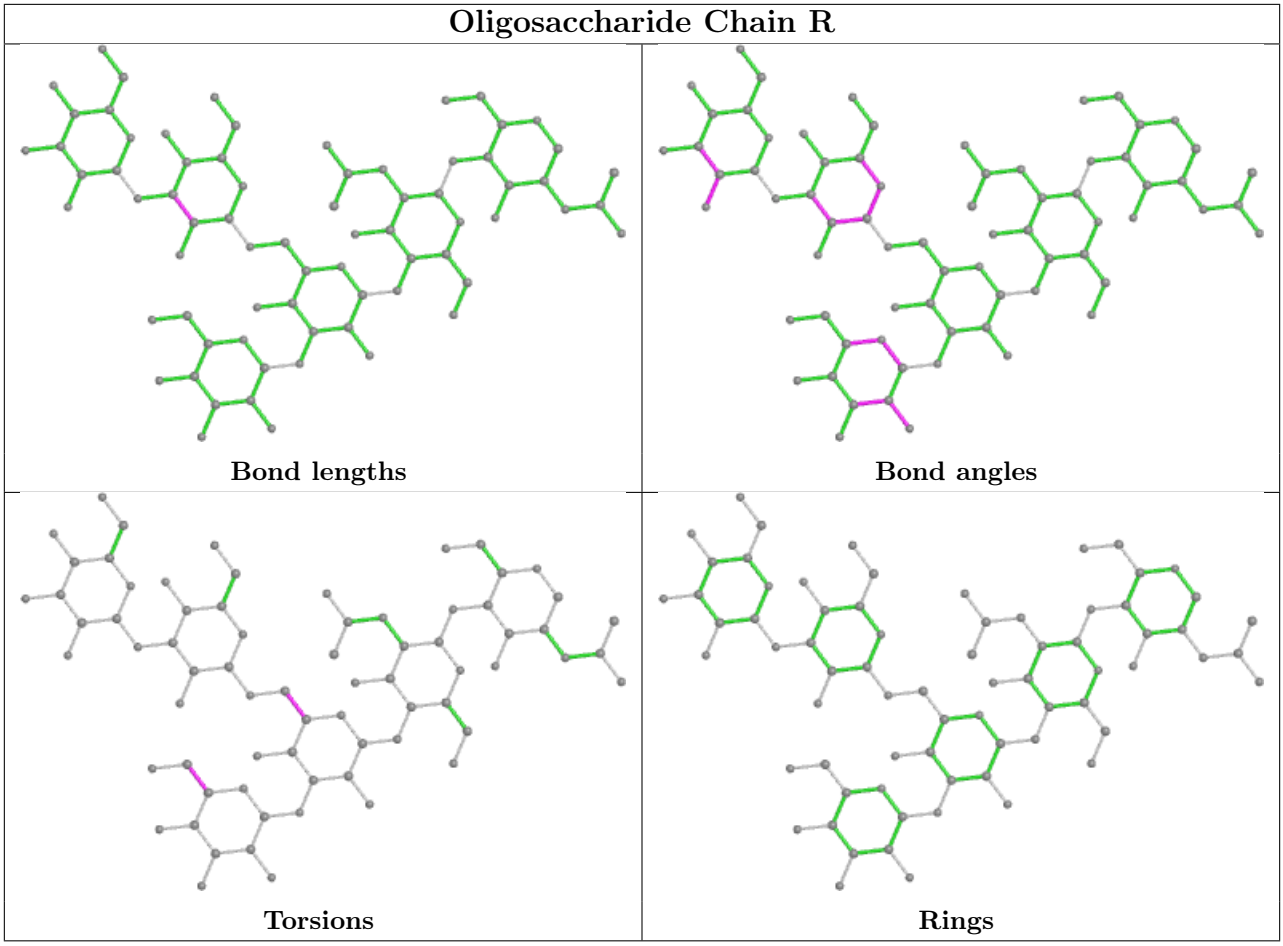
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
13	NAG	B	701	2	14,14,15	0.17	0	17,19,21	0.35	0
13	NAG	B	703	2	14,14,15	0.40	0	17,19,21	1.25	2 (11%)
13	NAG	G	703	1	14,14,15	0.18	0	17,19,21	0.36	0
13	NAG	G	707	1	14,14,15	0.20	0	17,19,21	0.42	0
13	NAG	G	700	1	14,14,15	0.44	0	17,19,21	0.40	0
13	NAG	G	704	1	14,14,15	0.49	0	17,19,21	1.27	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	G	708	1	14,14,15	0.19	0	17,19,21	0.42	0
13	NAG	G	727	1	14,14,15	0.22	0	17,19,21	0.42	0
13	NAG	B	702	2	14,14,15	0.22	0	17,19,21	0.39	0

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
13	NAG	B	701	2	-	0/6/23/26	0/1/1/1
13	NAG	B	703	2	-	3/6/23/26	0/1/1/1
13	NAG	G	703	1	-	0/6/23/26	0/1/1/1
13	NAG	G	707	1	-	2/6/23/26	0/1/1/1
13	NAG	G	700	1	-	2/6/23/26	0/1/1/1
13	NAG	G	704	1	-	5/6/23/26	0/1/1/1
13	NAG	G	708	1	-	2/6/23/26	0/1/1/1
13	NAG	G	727	1	-	4/6/23/26	0/1/1/1
13	NAG	B	702	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	703	NAG	C2-N2-C7	4.35	129.09	122.90
13	G	704	NAG	C2-N2-C7	4.29	129.01	122.90
13	B	703	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	727	NAG	O5-C5-C6-O6
13	G	707	NAG	O5-C5-C6-O6
13	G	708	NAG	O5-C5-C6-O6
13	G	727	NAG	C4-C5-C6-O6
13	G	704	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	703	NAG	1	0
13	G	700	NAG	1	0
13	G	704	NAG	1	0
13	G	727	NAG	1	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	G	471/485 (97%)	0.28	14 (2%) 50 39	86, 136, 248, 325	0
2	B	129/153 (84%)	0.18	4 (3%) 49 38	93, 165, 267, 311	0
3	L	211/214 (98%)	0.13	6 (2%) 53 42	97, 150, 215, 274	0
4	H	234/236 (99%)	0.27	10 (4%) 35 29	91, 174, 255, 308	0
5	D	240/240 (100%)	0.89	36 (15%) 2 2	112, 202, 342, 382	0
6	E	213/216 (98%)	0.79	32 (15%) 2 2	124, 219, 333, 413	0
All	All	1498/1544 (97%)	0.42	102 (6%) 17 14	86, 165, 294, 413	0

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	213	PRO	11.7
5	D	191	THR	7.7
6	E	146	GLY	6.4
5	D	211	VAL	6.2
5	D	215	SER	6.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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
12	MAN	R	5	11/12	0.56	0.20	211,219,221,221	0
11	MAN	Q	4	11/12	0.71	0.39	148,166,174,175	0
7	NAG	M	2	14/15	0.73	0.32	161,187,210,240	0
9	BMA	N	3	11/12	0.75	0.64	190,202,208,209	0
8	BMA	K	3	11/12	0.76	0.19	172,190,202,220	0
7	NAG	A	2	14/15	0.76	0.24	180,181,183,184	0
11	NAG	Q	2	14/15	0.76	0.40	132,133,134,134	0
7	NAG	F	2	14/15	0.76	0.29	140,168,176,184	0
7	NAG	A	1	14/15	0.76	0.29	168,171,172,174	0
10	MAN	P	10	11/12	0.77	0.27	166,176,184,191	0
11	BMA	Q	3	11/12	0.79	0.43	139,141,153,157	0
7	NAG	C	2	14/15	0.81	0.42	152,173,190,207	0
8	MAN	K	4	11/12	0.81	0.25	161,190,203,205	0
7	NAG	I	1	14/15	0.82	0.26	145,159,192,208	0
7	NAG	I	2	14/15	0.82	0.24	146,183,218,219	0
7	NAG	F	1	14/15	0.82	0.28	137,142,155,156	0
11	MAN	Q	6	11/12	0.82	0.32	159,169,189,200	0
7	NAG	S	1	14/15	0.82	0.28	129,144,154,159	0
8	MAN	K	5	11/12	0.83	0.22	172,190,210,211	0
11	MAN	Q	5	11/12	0.83	0.31	171,175,184,187	0
7	NAG	C	1	14/15	0.84	0.26	134,150,160,162	0
7	NAG	O	2	14/15	0.84	0.38	172,215,223,231	0
12	MAN	R	4	11/12	0.85	0.13	196,200,216,218	0
7	NAG	M	1	14/15	0.85	0.28	143,155,164,187	0
12	MAN	R	6	11/12	0.85	0.17	170,181,196,202	0
9	NAG	N	2	14/15	0.86	0.39	147,165,202,209	0
10	BMA	P	3	11/12	0.86	0.23	137,137,140,153	0
10	MAN	P	8	11/12	0.86	0.21	185,189,202,203	0
7	NAG	S	2	14/15	0.87	0.30	150,167,176,177	0
10	MAN	P	7	11/12	0.87	0.18	160,167,182,184	0
7	NAG	J	2	14/15	0.87	0.23	129,151,181,185	0
12	BMA	R	3	11/12	0.88	0.14	160,171,187,194	0
8	NAG	K	2	14/15	0.88	0.25	147,169,195,195	0
10	MAN	P	9	11/12	0.89	0.37	181,189,200,206	0
12	NAG	R	2	14/15	0.89	0.20	125,134,158,174	0
11	NAG	Q	1	14/15	0.89	0.32	120,123,125,125	0
11	MAN	Q	7	11/12	0.90	0.49	143,147,153,153	0
7	NAG	O	1	14/15	0.90	0.36	168,191,208,215	0
10	NAG	P	1	14/15	0.91	0.33	126,128,134,139	0
7	NAG	J	1	14/15	0.91	0.18	131,134,144,148	0
9	NAG	N	1	14/15	0.91	0.22	137,140,162,165	0
10	MAN	P	6	11/12	0.92	0.23	143,144,151,152	0
10	NAG	P	2	14/15	0.92	0.24	130,135,145,146	0

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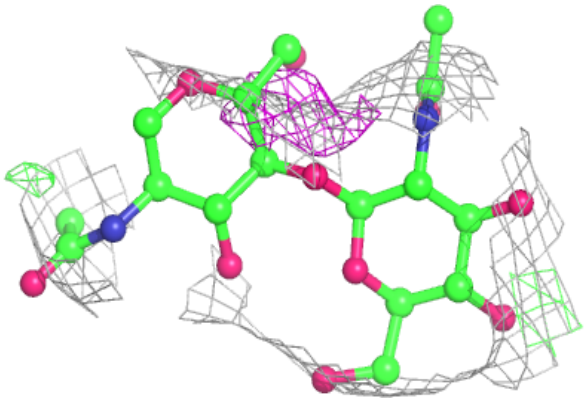
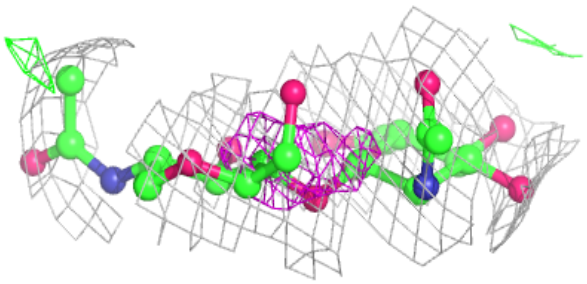
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	K	1	14/15	0.92	0.24	127,130,154,155	0
10	MAN	P	5	11/12	0.92	0.26	138,139,141,160	0
12	NAG	R	1	14/15	0.92	0.23	118,119,133,134	0
10	MAN	P	4	11/12	0.95	0.17	136,137,140,153	0

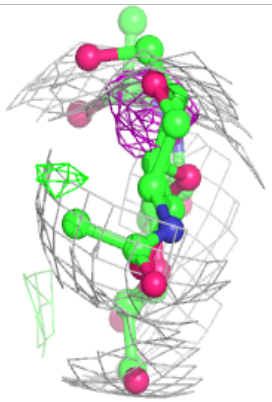
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

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

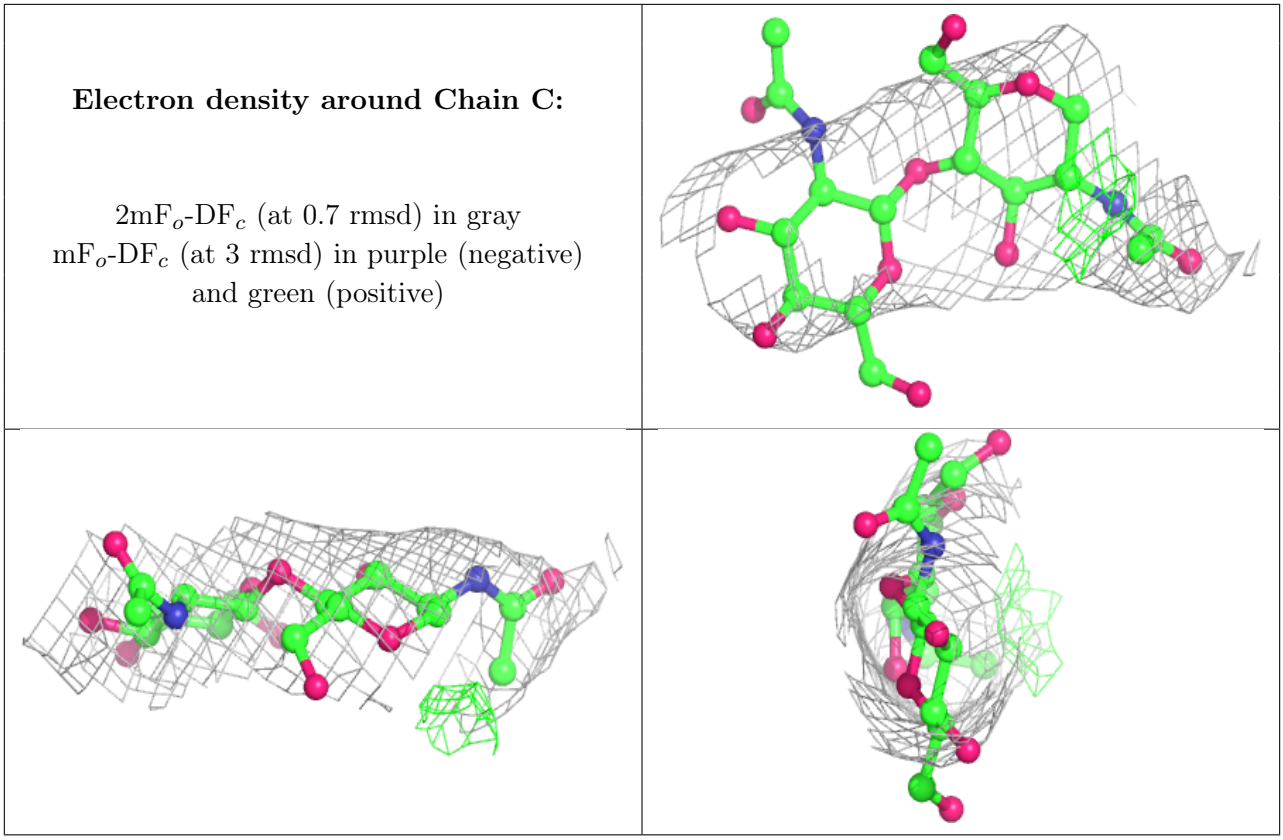






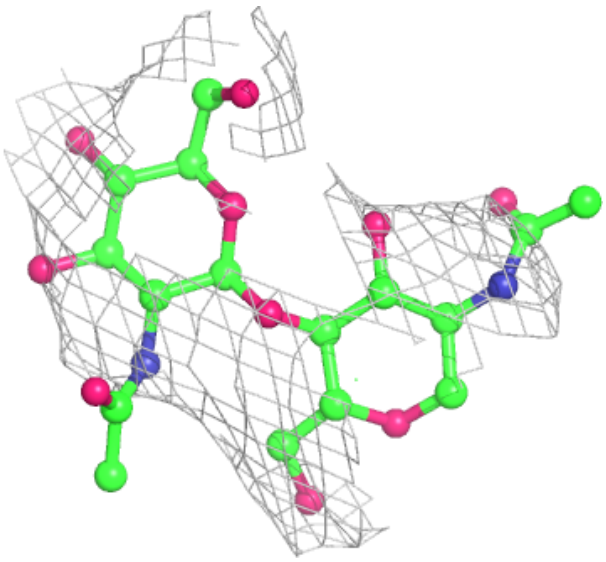
Electron density around Chain C:

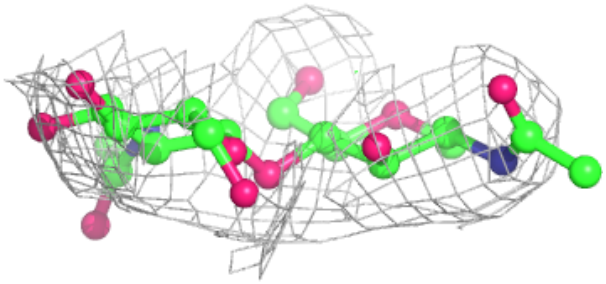
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

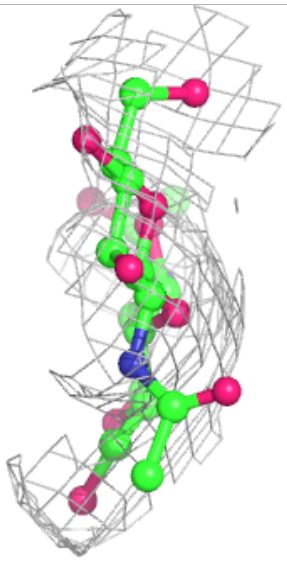


Electron density around Chain F:

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

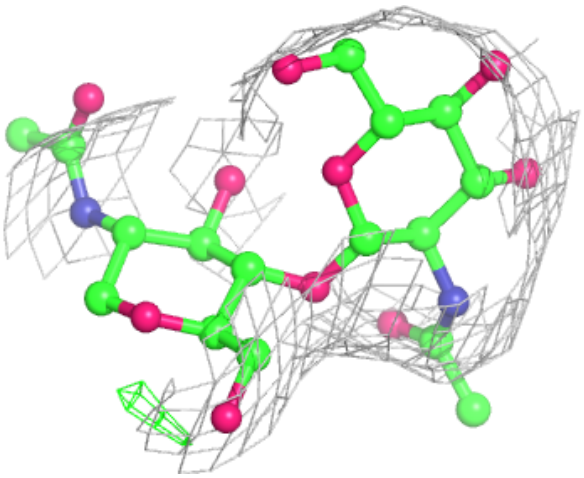


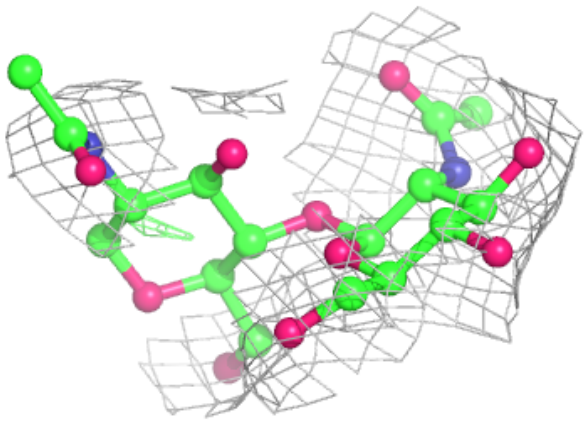


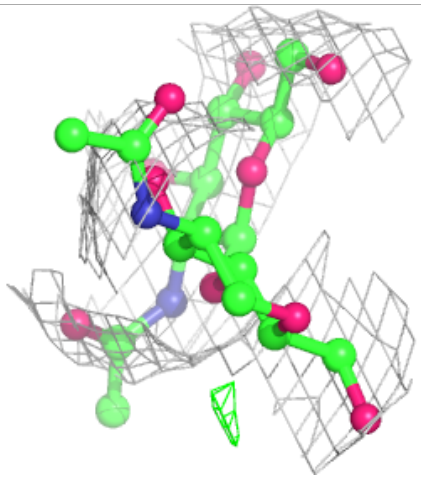


Electron density around Chain I:

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

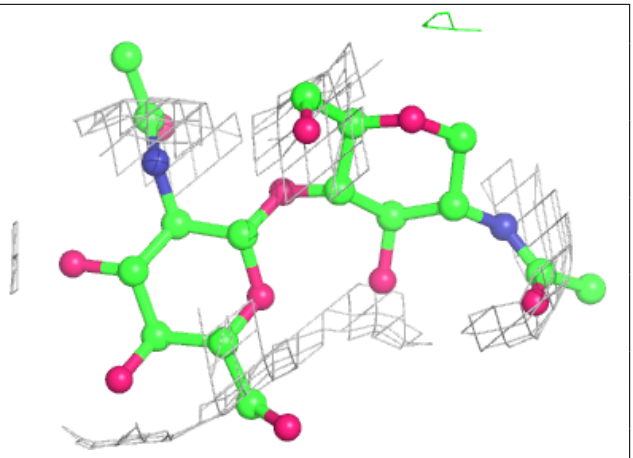


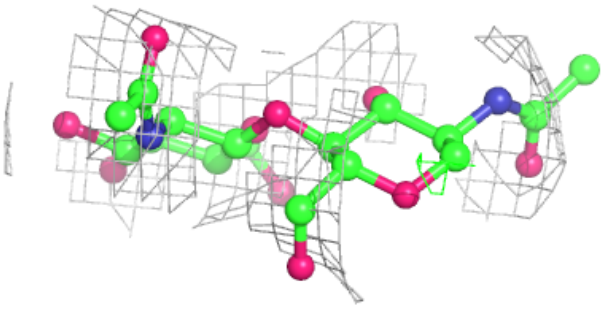


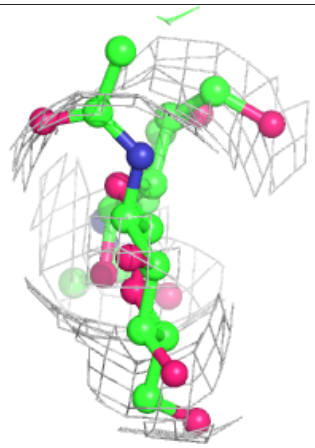


Electron density around Chain J:

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

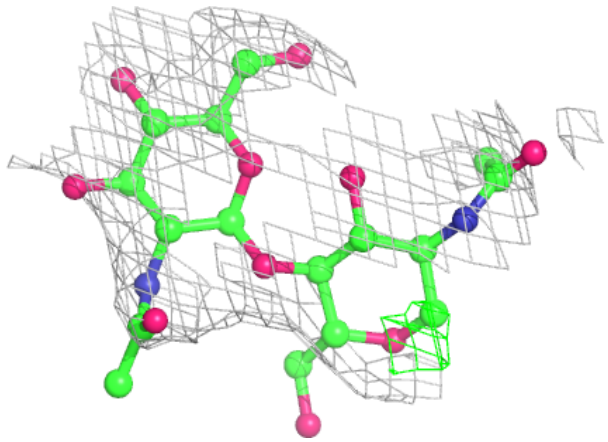


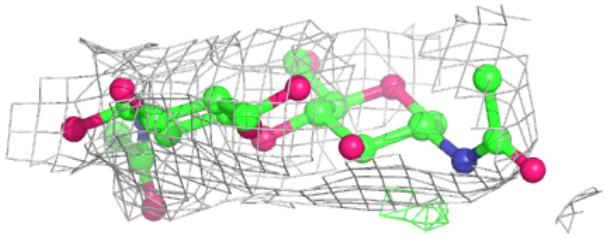


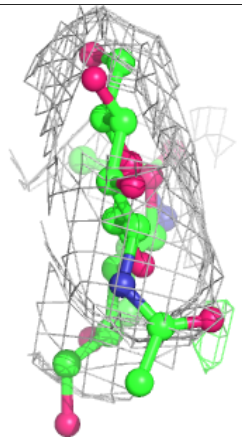


Electron density around Chain M:

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

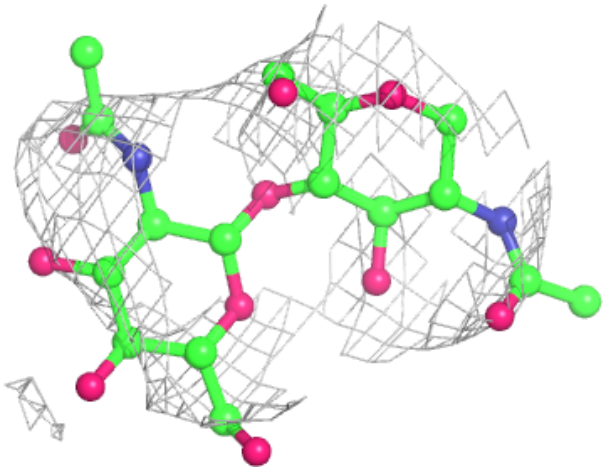


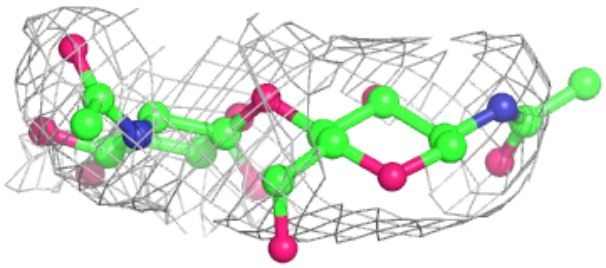


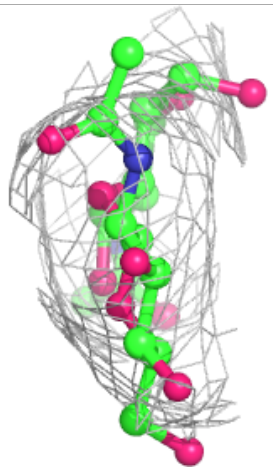


Electron density around Chain O:

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

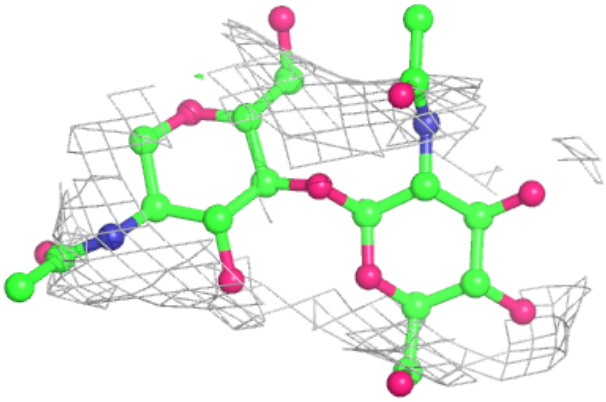


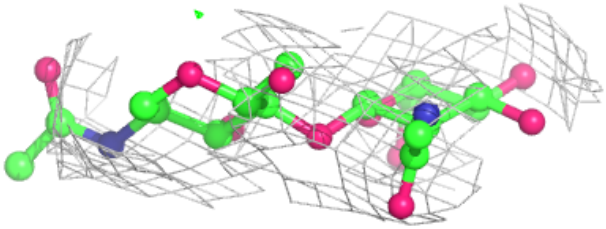


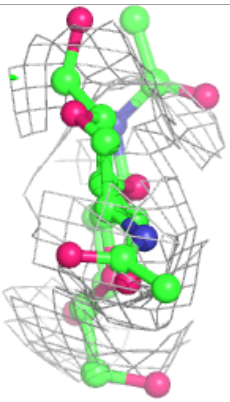


Electron density around Chain S:

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

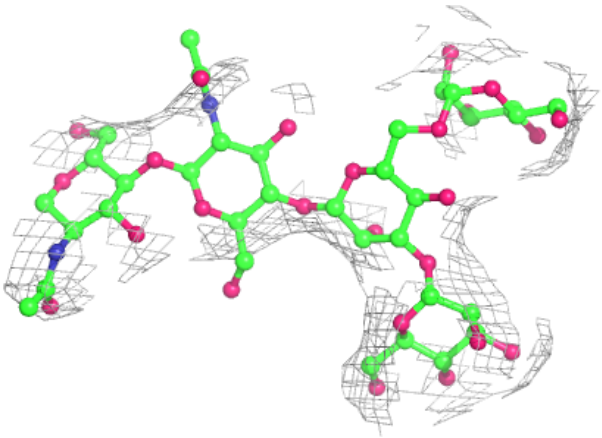


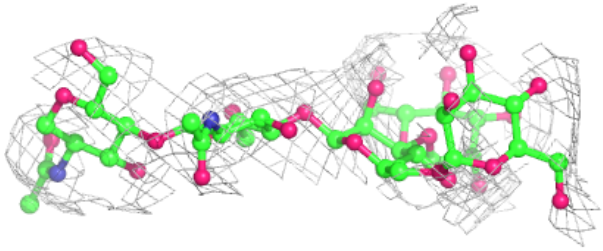


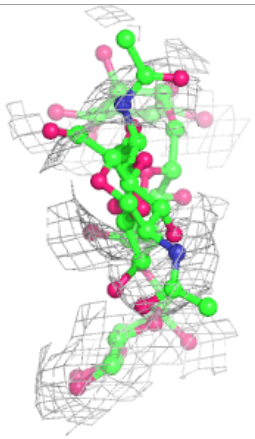


Electron density around Chain K:

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

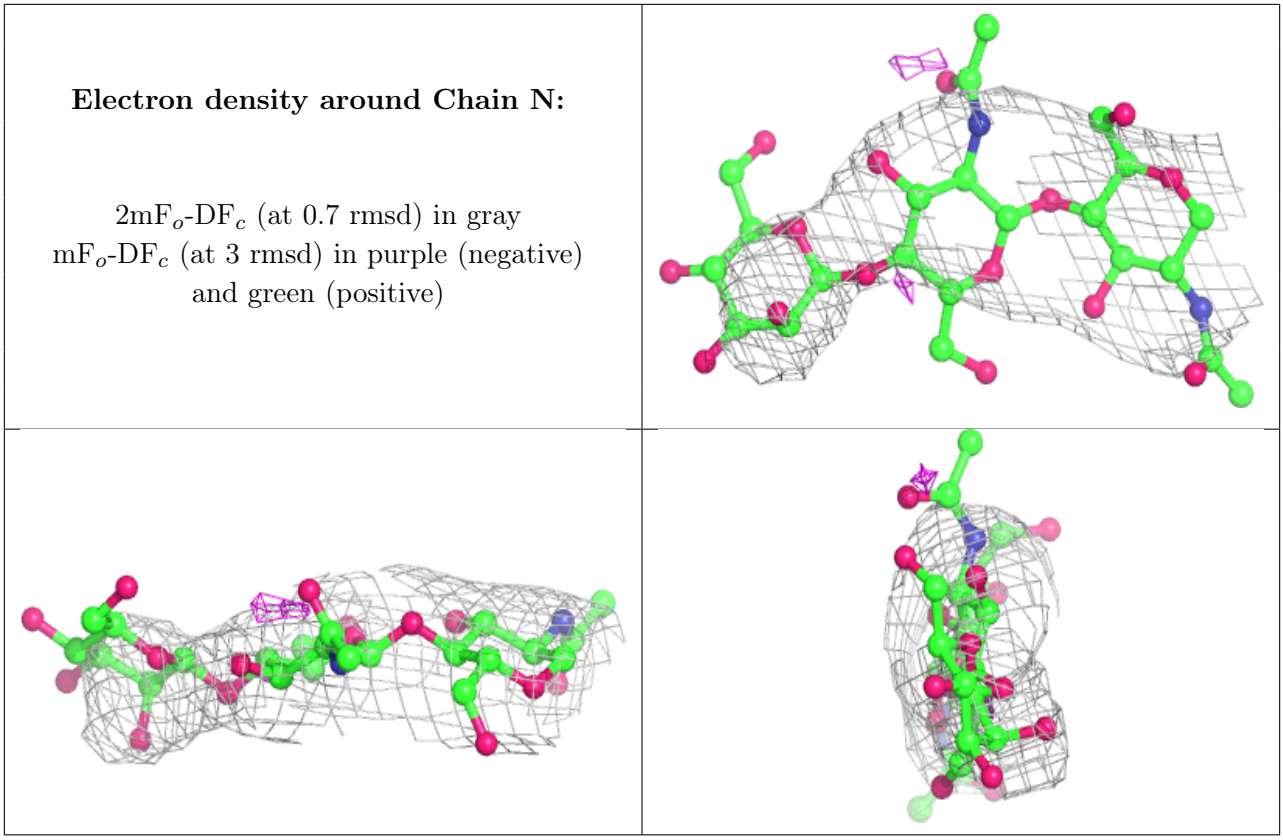






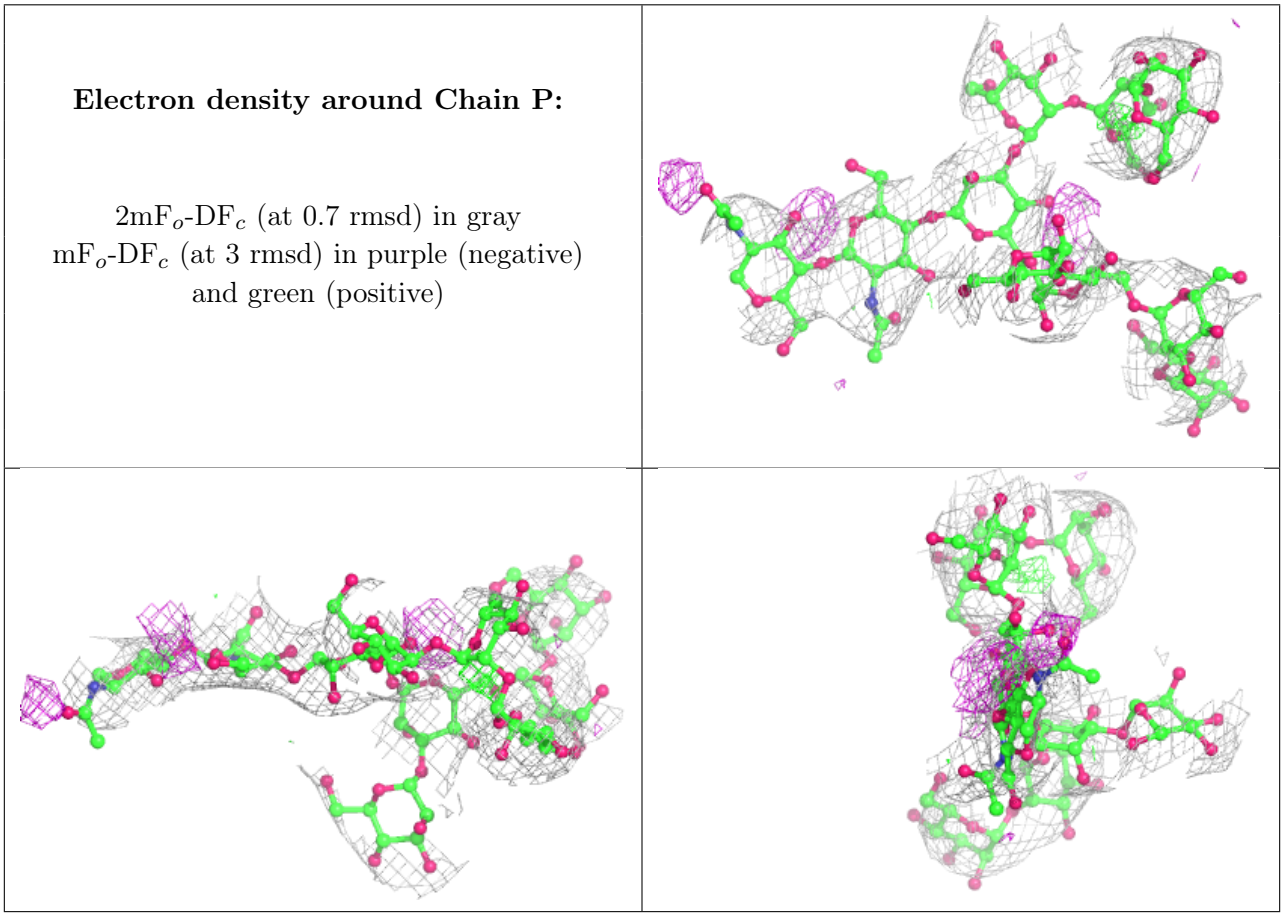
Electron density around Chain N:

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



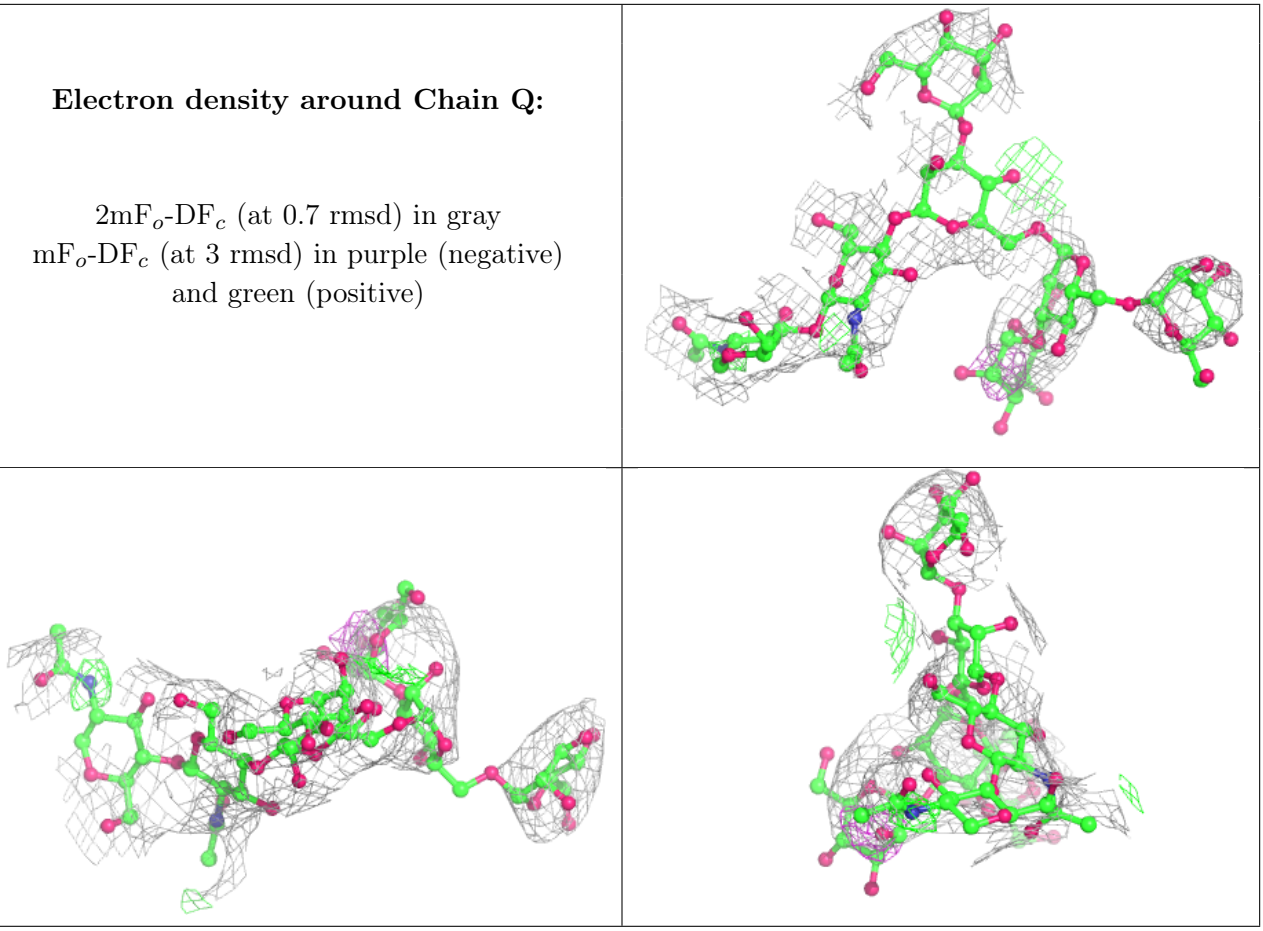
Electron density around Chain P:

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



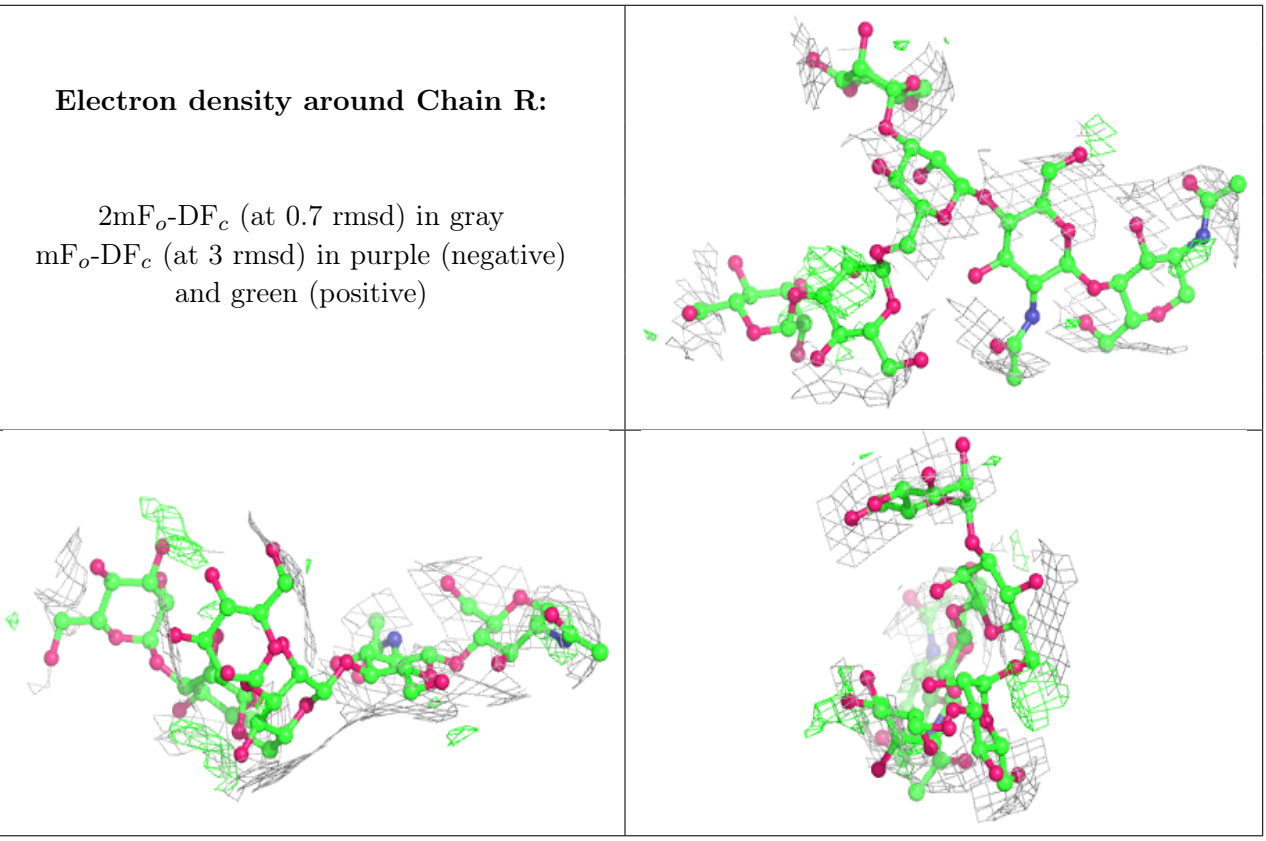
Electron density around Chain Q:

$2mF_o$-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 R:

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



6.4 Ligands (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
13	NAG	B	702	14/15	0.57	0.33	190,222,235,237	0
13	NAG	G	700	14/15	0.78	0.28	142,143,144,145	0
13	NAG	B	703	14/15	0.78	0.43	139,143,173,175	0
13	NAG	B	701	14/15	0.79	0.31	181,190,203,206	0
13	NAG	G	704	14/15	0.79	0.29	197,215,223,230	0
13	NAG	G	727	14/15	0.79	0.18	164,201,239,247	0
13	NAG	G	708	14/15	0.80	0.33	155,162,169,182	0
13	NAG	G	707	14/15	0.82	0.25	127,149,181,198	0
13	NAG	G	703	14/15	0.83	0.31	136,138,138,139	0

6.5 Other polymers (i)

There are no such residues in this entry.