Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:27 PM BST

PDB ID	:	4IIE
Title	:	Crystal structure of beta-glucosidase 1 from Aspergillus aculeatus in complex with calystegine B(2)
Authors	:	Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on	:	2012-12-20
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

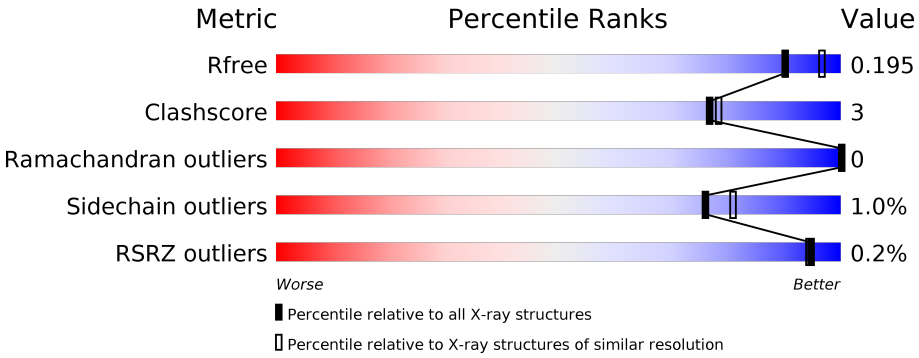
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	841	93% 6%
1	B	841	90% 8%
2	C	4	75% 25%
3	D	3	33% 67%
3	G	3	100%
3	L	3	100%

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Mol	Chain	Length	Quality of chain
3	N	3	33% 67%
4	E	2	100%
5	F	10	100%
5	M	10	100%
6	H	7	86% 14%
6	O	7	71% 29%
7	I	7	100%
8	J	7	100%
9	K	6	83% 17%
10	P	8	75% 25%

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
12	MRD	A	940	-	-	X	-
14	CGB	A	943	-	-	X	-
14	CGB	B	952	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 15193 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.

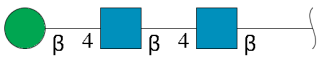
- Molecule 1 is a protein called Beta-glucosidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	834	Total	C	N	O	S	0	0	0
			6387	4031	1097	1241	18			
1	B	832	Total	C	N	O	S	0	0	0
			6375	4023	1095	1239	18			

- Molecule 2 is an oligosaccharide called 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
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

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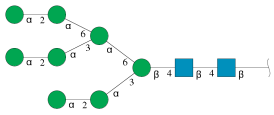
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	N	3	Total C N O 39 22 2 15	0	0	0

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

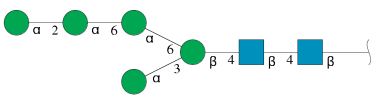
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	E	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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.



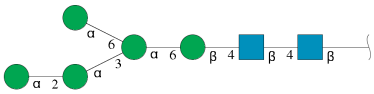
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	10	Total C N O 116 64 2 50	0	0	0
5	M	10	Total C N O 116 64 2 50	0	0	0

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



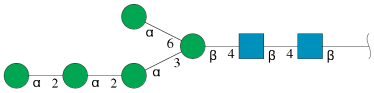
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



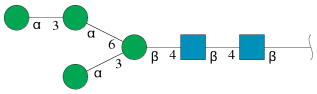
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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.



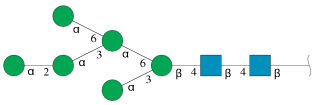
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 9 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.



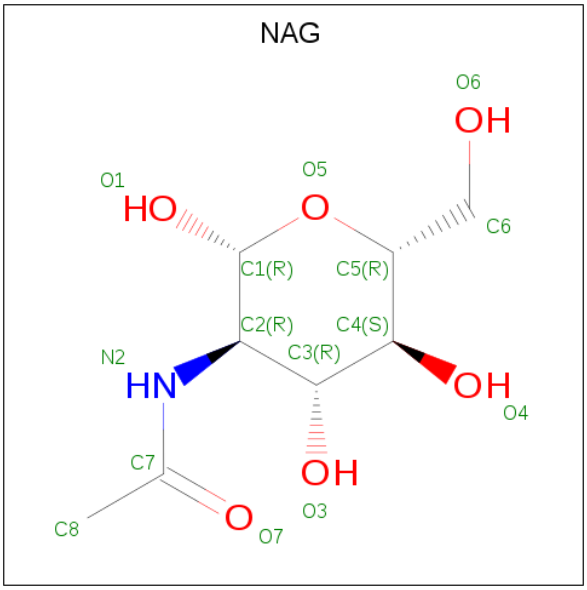
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
10	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

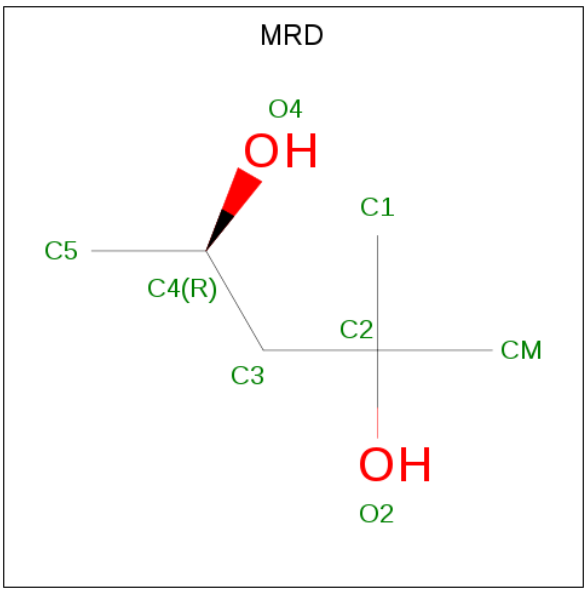
- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 12 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:

$C_6H_{14}O_2$).

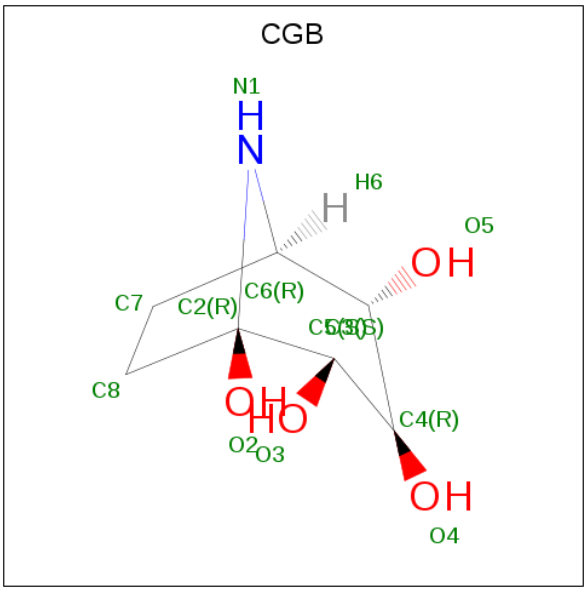


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 8 6 2	0	0
12	A	1	Total C O 8 6 2	0	0
12	A	1	Total C O 8 6 2	0	0
12	B	1	Total C O 8 6 2	0	0
12	B	1	Total C O 8 6 2	0	0
12	B	1	Total C O 8 6 2	0	0

- Molecule 13 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total Na 1 1	0	0
13	A	1	Total Na 1 1	0	0

- Molecule 14 is CALYSTEGINE B2 (three-letter code: CGB) (formula: $C_7H_{13}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C N O 12 7 1 4	0	0
14	B	1	Total C N O 12 7 1 4	0	0

- Molecule 15 is water.

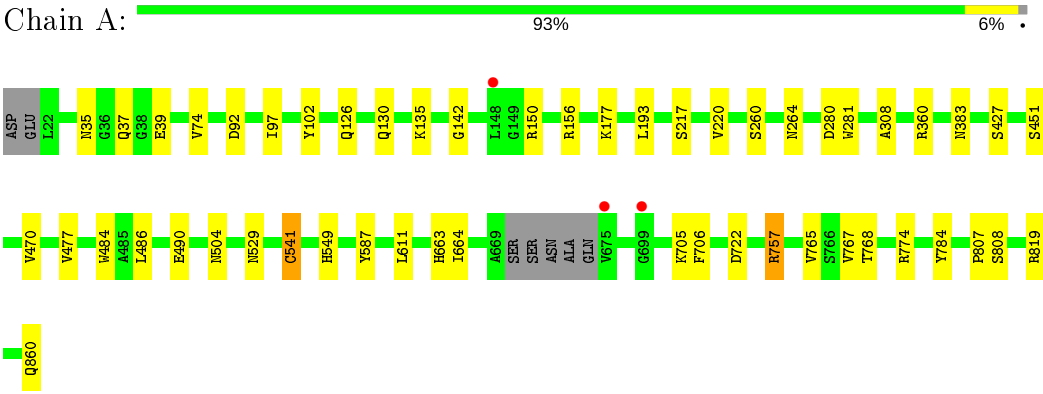
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	610	Total O 610 610	0	0
15	B	713	Total O 713 713	0	0

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.

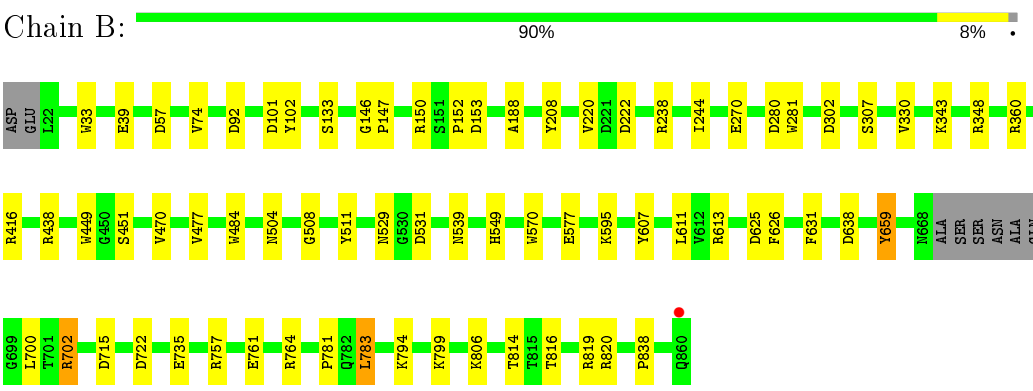
• Molecule 1: Beta-glucosidase 1

Chain A:



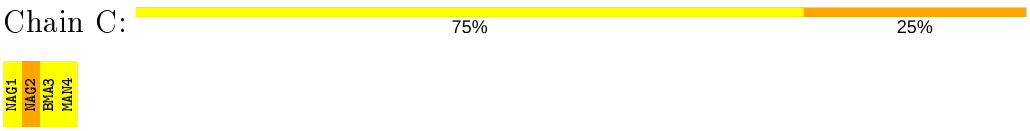
• Molecule 1: Beta-glucosidase 1

Chain B:



• Molecule 2: 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 C:



• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

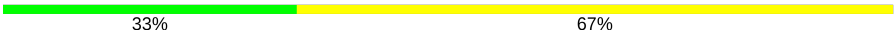
Chain G:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

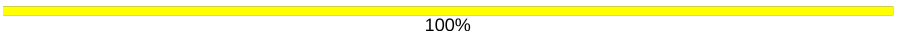


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 F:

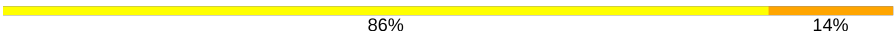


• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

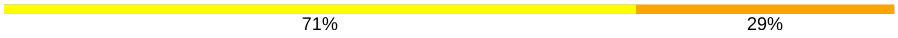
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



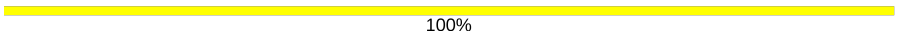
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



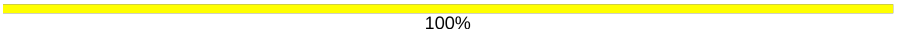
• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 J:

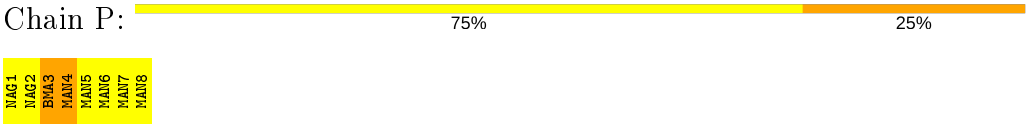


• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 10: alpha-D-mannopyranose-(1-2)-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 P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.13Å 122.15Å 222.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.07 – 2.00 39.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.07-2.00) 99.4 (39.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.149 , 0.193 0.151 , 0.195	Depositor DCC
R_{free} test set	7580 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15193	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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, NA, CGB, MRD, 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	A	1.21	6/6550 (0.1%)	1.02	10/8930 (0.1%)
1	B	1.32	9/6538 (0.1%)	1.08	25/8913 (0.3%)
All	All	1.27	15/13088 (0.1%)	1.05	35/17843 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	GLU	CD-OE2	5.76	1.31	1.25
1	B	270	GLU	CD-OE2	5.63	1.31	1.25
1	B	348	ARG	CZ-NH1	5.55	1.40	1.33
1	B	511	TYR	CG-CD2	5.45	1.46	1.39
1	B	761	GLU	CD-OE2	-5.43	1.19	1.25
1	A	217	SER	CA-CB	5.32	1.60	1.52
1	B	133	SER	CA-CB	5.28	1.60	1.52
1	B	631	PHE	CG-CD2	5.28	1.46	1.38
1	B	570	TRP	CB-CG	5.24	1.59	1.50
1	A	784	TYR	CE1-CZ	5.23	1.45	1.38
1	B	208	TYR	CE1-CZ	5.18	1.45	1.38
1	A	427	SER	CB-OG	5.10	1.48	1.42
1	A	587	TYR	CE1-CZ	5.10	1.45	1.38
1	A	463	GLU	CD-OE2	5.05	1.31	1.25
1	B	307	SER	CB-OG	5.01	1.48	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	702	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	B	348	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	B	348	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	B	702	ARG	NE-CZ-NH1	7.85	124.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	438	ARG	NE-CZ-NH1	-7.52	116.54	120.30
1	B	360	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	541	CYS	N-CA-CB	7.32	123.78	110.60
1	B	715	ASP	CB-CG-OD1	7.16	124.74	118.30
1	B	722	ASP	CB-CG-OD1	6.88	124.49	118.30
1	B	101	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	722	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	757	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	722	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	B	153	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	222	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	238	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	757	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	150	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	222	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	B	819	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	B	820	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	B	360	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	177	LYS	CD-CE-NZ	-5.53	98.98	111.70
1	A	156	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	B	150	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	531	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	722	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	330	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	B	783	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	B	659	TYR	CB-CG-CD1	-5.21	117.88	121.00
1	B	101	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	577	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	A	142	GLY	N-CA-C	-5.07	100.43	113.10
1	B	57	ASP	CB-CG-OD1	5.06	122.85	118.30
1	A	611	LEU	CB-CG-CD1	-5.00	102.49	111.00

There are no chirality outliers.

There are no planarity outliers.

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	6387	0	6097	34	0
1	B	6375	0	6082	33	0
2	C	50	0	43	1	0
3	D	39	0	34	2	0
3	G	39	0	34	0	0
3	L	39	0	34	0	0
3	N	39	0	34	0	0
4	E	28	0	24	0	0
5	F	116	0	97	0	0
5	M	116	0	97	0	0
6	H	83	0	70	2	0
6	O	83	0	69	2	0
7	I	83	0	69	0	0
8	J	83	0	70	0	0
9	K	72	0	61	2	0
10	P	94	0	78	1	0
11	A	28	0	26	0	0
11	B	42	0	39	0	0
12	A	24	0	42	8	0
12	B	24	0	42	5	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
14	A	12	0	13	7	0
14	B	12	0	12	7	0
15	A	610	0	0	4	0
15	B	713	0	0	7	0
All	All	15193	0	13167	81	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 3.

All (81) 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:A:92:ASP:OD2	14:A:943:CGB:H7C1	1.71	0.90
1:B:92:ASP:OD2	14:B:952:CGB:H7C1	1.75	0.86
1:A:280:ASP:OD1	14:A:943:CGB:H3	1.78	0.82
1:A:360:ARG:HH11	12:A:940:MRD:HMC3	1.44	0.82
1:A:819:ARG:HH12	1:A:860:GLN:C	1.82	0.82
1:B:280:ASP:OD1	14:B:952:CGB:H3	1.85	0.76
12:A:940:MRD:HMC2	15:B:1104:HOH:O	1.86	0.75
1:B:539:ASN:HB2	15:B:1702:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:764:ARG:HD2	1:B:814:THR:CG2	2.25	0.66
1:A:451:SER:OG	14:A:943:CGB:H8C2	1.94	0.66
1:A:819:ARG:NH1	1:A:860:GLN:C	2.48	0.66
10:P:3:BMA:H62	10:P:4:MAN:H5	1.78	0.66
1:B:702:ARG:HD3	15:B:1174:HOH:O	1.97	0.65
12:A:939:MRD:H5C2	15:A:1190:HOH:O	1.98	0.64
1:B:451:SER:CB	14:B:952:CGB:C8	2.77	0.62
1:A:819:ARG:NH1	1:A:860:GLN:O	2.21	0.62
1:B:451:SER:OG	14:B:952:CGB:H8C2	2.00	0.61
1:B:764:ARG:HD2	1:B:814:THR:HG21	1.82	0.60
1:B:449:TRP:CD1	1:B:508:GLY:HA3	2.37	0.60
1:A:451:SER:CB	14:A:943:CGB:C8	2.80	0.59
1:A:484:TRP:CE2	6:H:3:BMA:H62	2.38	0.59
1:B:625:ASP:HB3	12:B:950:MRD:HMC2	1.84	0.59
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.83	0.58
1:B:484:TRP:CZ2	1:B:529:ASN:HB2	2.39	0.58
12:A:940:MRD:H5C3	12:A:940:MRD:HMC1	1.84	0.58
12:A:940:MRD:C5	12:A:940:MRD:HMC1	2.36	0.55
12:A:939:MRD:O2	12:A:939:MRD:H5C3	2.08	0.54
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.90	0.53
1:B:451:SER:CB	14:B:952:CGB:H8C2	2.38	0.53
1:B:838:PRO:HD2	15:B:1586:HOH:O	2.09	0.53
1:B:416:ARG:HG3	15:B:1113:HOH:O	2.08	0.51
1:A:451:SER:CB	14:A:943:CGB:H8C2	2.41	0.51
1:B:595:LYS:HE3	15:B:1003:HOH:O	2.11	0.50
1:A:484:TRP:CZ2	1:A:529:ASN:HB2	2.48	0.48
1:B:613:ARG:NH1	15:B:1055:HOH:O	2.37	0.48
1:A:39:GLU:HG2	15:A:1223:HOH:O	2.13	0.48
1:A:484:TRP:CZ2	6:H:3:BMA:H62	2.48	0.47
1:A:35:ASN:OD1	1:A:37:GLN:HB2	2.13	0.47
1:A:757:ARG:NH1	15:A:1153:HOH:O	2.38	0.47
1:B:764:ARG:CD	1:B:814:THR:CG2	2.91	0.47
14:B:952:CGB:H7C2	14:B:952:CGB:H4	1.07	0.47
1:B:220:VAL:HG22	1:B:626:PHE:CG	2.49	0.47
1:A:767:VAL:HG22	1:A:768:THR:N	2.30	0.47
1:A:504:ASN:HA	1:A:549:HIS:O	2.14	0.47
1:B:470:VAL:HG11	1:B:477:VAL:HB	1.97	0.46
1:B:484:TRP:CE2	6:O:3:BMA:H62	2.50	0.46
1:B:659:TYR:HE1	1:B:781:PRO:HB3	1.81	0.46
1:A:360:ARG:HG2	12:A:940:MRD:HMC1	1.98	0.46
1:A:663:HIS:O	1:A:664:ILE:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:VAL:HG11	3:D:2:NAG:O3	2.15	0.45
1:B:611:LEU:HD12	1:B:613:ARG:NH2	2.32	0.45
1:A:126:GLN:O	1:A:130:GLN:HG3	2.17	0.45
1:A:308:ALA:HB2	1:A:705:LYS:HA	1.98	0.45
12:B:949:MRD:H1C2	12:B:949:MRD:H4	1.19	0.44
1:B:102:TYR:HB3	1:B:383:ASN:HA	1.99	0.44
1:A:807:PRO:O	1:A:808:SER:HB2	2.18	0.44
12:B:950:MRD:H5C1	9:K:1:NAG:H62	2.00	0.44
1:A:486:LEU:O	1:A:490:GLU:HG3	2.18	0.43
1:A:470:VAL:HG11	1:A:477:VAL:HB	2.00	0.43
1:B:152:PRO:HG3	1:B:607:TYR:CG	2.54	0.43
1:B:799:LYS:HE3	1:B:816:THR:O	2.19	0.43
1:B:806:LYS:HG3	1:B:806:LYS:HZ3	1.52	0.43
1:A:451:SER:OG	14:A:943:CGB:C8	2.65	0.42
1:B:783:LEU:HD23	1:B:783:LEU:C	2.40	0.42
1:B:451:SER:OG	14:B:952:CGB:C8	2.68	0.42
12:B:948:MRD:H1C3	12:B:948:MRD:H4	1.73	0.42
1:A:706:PHE:CZ	2:C:2:NAG:H82	2.54	0.42
1:B:146:GLY:HA2	1:B:147:PRO:C	2.40	0.42
1:A:360:ARG:HH11	12:A:940:MRD:CM	2.24	0.42
1:B:39:GLU:HG3	1:B:343:LYS:HE2	2.00	0.42
15:A:1590:HOH:O	3:D:3:BMA:H3	2.19	0.42
1:A:97:ILE:HD13	1:A:135:LYS:HG3	2.01	0.42
1:A:664:ILE:HD12	1:A:765:VAL:HG22	2.01	0.42
1:A:193:LEU:HD13	1:A:220:VAL:HG21	2.02	0.41
1:A:260:SER:O	1:A:264:ASN:HB2	2.20	0.41
14:A:943:CGB:H7C2	14:A:943:CGB:H4	1.21	0.41
12:B:950:MRD:H5C1	9:K:1:NAG:C6	2.49	0.41
1:B:504:ASN:HA	1:B:549:HIS:O	2.21	0.41
1:B:638:ASP:O	1:B:794:LYS:HE3	2.21	0.41
6:O:3:BMA:H61	6:O:4:MAN:H5	2.02	0.40
1:A:102:TYR:HB3	1:A:383:ASN:HA	2.03	0.40

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	A	830/841 (99%)	798 (96%)	32 (4%)	0	100	100
1	B	828/841 (98%)	803 (97%)	25 (3%)	0	100	100
All	All	1658/1682 (99%)	1601 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	671/677 (99%)	667 (99%)	4 (1%)	86	90
1	B	670/677 (99%)	661 (99%)	9 (1%)	69	74
All	All	1341/1354 (99%)	1328 (99%)	13 (1%)	76	81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	281	TRP
1	A	541	CYS
1	A	774	ARG
1	B	33	TRP
1	B	74	VAL
1	B	281	TRP
1	B	302	ASP
1	B	377	LYS
1	B	698	GLU
1	B	700	LEU
1	B	735	GLU
1	B	757	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

80 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	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	1.09	1 (7%)	17,19,21	1.59	3 (17%)
2	NAG	C	2	2	14,14,15	0.92	1 (7%)	17,19,21	2.04	5 (29%)
2	BMA	C	3	2	11,11,12	1.28	1 (9%)	15,15,17	2.00	6 (40%)
2	MAN	C	4	2	11,11,12	0.98	0	15,15,17	2.82	6 (40%)
3	NAG	D	1	1,3	14,14,15	1.00	1 (7%)	17,19,21	1.41	3 (17%)
3	NAG	D	2	3	14,14,15	1.16	1 (7%)	17,19,21	1.34	2 (11%)
3	BMA	D	3	3	11,11,12	1.14	0	15,15,17	2.77	9 (60%)
4	NAG	E	1	1,4	14,14,15	0.97	0	17,19,21	1.78	4 (23%)
4	NAG	E	2	4	14,14,15	1.03	1 (7%)	17,19,21	2.56	5 (29%)
5	NAG	F	1	1,5	14,14,15	1.58	3 (21%)	17,19,21	1.72	4 (23%)
5	MAN	F	10	5	11,11,12	1.52	3 (27%)	15,15,17	2.35	5 (33%)
5	NAG	F	2	5	14,14,15	0.99	1 (7%)	17,19,21	0.95	0
5	BMA	F	3	5	11,11,12	1.11	1 (9%)	15,15,17	1.25	1 (6%)
5	MAN	F	4	5	11,11,12	0.61	0	15,15,17	1.73	5 (33%)
5	MAN	F	5	5	11,11,12	1.27	1 (9%)	15,15,17	1.29	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MAN	F	6	5	11,11,12	0.84	0	15,15,17	1.79	2 (13%)
5	MAN	F	7	5	11,11,12	1.03	1 (9%)	15,15,17	1.25	1 (6%)
5	MAN	F	8	5	11,11,12	1.12	1 (9%)	15,15,17	1.81	4 (26%)
5	MAN	F	9	5	11,11,12	1.09	1 (9%)	15,15,17	1.88	3 (20%)
3	NAG	G	1	1,3	14,14,15	0.96	1 (7%)	17,19,21	1.33	1 (5%)
3	NAG	G	2	3	14,14,15	0.97	1 (7%)	17,19,21	1.47	4 (23%)
3	BMA	G	3	3	11,11,12	1.05	1 (9%)	15,15,17	2.41	4 (26%)
6	NAG	H	1	1,6	14,14,15	0.89	0	17,19,21	1.50	4 (23%)
6	NAG	H	2	6	14,14,15	0.89	0	17,19,21	2.08	5 (29%)
6	BMA	H	3	6	11,11,12	0.92	0	15,15,17	1.23	1 (6%)
6	MAN	H	4	6	11,11,12	0.70	0	15,15,17	1.60	4 (26%)
6	MAN	H	5	6	11,11,12	1.37	3 (27%)	15,15,17	2.20	5 (33%)
6	MAN	H	6	6	11,11,12	1.18	1 (9%)	15,15,17	1.50	2 (13%)
6	MAN	H	7	6	11,11,12	0.87	1 (9%)	15,15,17	2.20	6 (40%)
7	NAG	I	1	1,13,7	14,14,15	1.14	1 (7%)	17,19,21	1.65	3 (17%)
7	NAG	I	2	7	14,14,15	1.21	2 (14%)	17,19,21	1.47	3 (17%)
7	BMA	I	3	7	11,11,12	0.87	0	15,15,17	2.11	3 (20%)
7	MAN	I	4	7	11,11,12	1.16	1 (9%)	15,15,17	1.62	1 (6%)
7	MAN	I	5	7	11,11,12	1.37	2 (18%)	15,15,17	2.22	5 (33%)
7	MAN	I	6	7	11,11,12	0.85	0	15,15,17	1.87	6 (40%)
7	MAN	I	7	7	11,11,12	1.10	1 (9%)	15,15,17	2.55	7 (46%)
8	NAG	J	1	1,8	14,14,15	1.56	1 (7%)	17,19,21	1.45	4 (23%)
8	NAG	J	2	8	14,14,15	1.05	1 (7%)	17,19,21	1.52	2 (11%)
8	BMA	J	3	8	11,11,12	1.15	1 (9%)	15,15,17	2.20	6 (40%)
8	MAN	J	4	8	11,11,12	0.64	0	15,15,17	2.09	6 (40%)
8	MAN	J	5	8	11,11,12	1.09	1 (9%)	15,15,17	1.81	3 (20%)
8	MAN	J	6	8	11,11,12	0.98	0	15,15,17	1.69	4 (26%)
8	MAN	J	7	8	11,11,12	0.71	0	15,15,17	2.19	5 (33%)
9	NAG	K	1	1,9	14,14,15	1.13	1 (7%)	17,19,21	1.46	3 (17%)
9	NAG	K	2	9	14,14,15	1.22	2 (14%)	17,19,21	1.58	4 (23%)
9	BMA	K	3	9	11,11,12	0.77	0	15,15,17	1.68	4 (26%)
9	MAN	K	4	9	11,11,12	0.68	0	15,15,17	1.85	7 (46%)
9	MAN	K	5	9	11,11,12	0.71	0	15,15,17	1.51	3 (20%)
9	MAN	K	6	9	11,11,12	1.65	1 (9%)	15,15,17	2.56	5 (33%)
3	NAG	L	1	1,3	14,14,15	0.66	0	17,19,21	1.83	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	L	2	3	14,14,15	0.56	0	17,19,21	1.67	5 (29%)
3	BMA	L	3	3	11,11,12	0.85	0	15,15,17	1.92	6 (40%)
5	NAG	M	1	1,5	14,14,15	1.15	2 (14%)	17,19,21	1.89	5 (29%)
5	MAN	M	10	5	11,11,12	1.08	1 (9%)	15,15,17	1.82	5 (33%)
5	NAG	M	2	5	14,14,15	1.36	3 (21%)	17,19,21	1.34	2 (11%)
5	BMA	M	3	5	11,11,12	1.10	1 (9%)	15,15,17	1.86	4 (26%)
5	MAN	M	4	5	11,11,12	0.81	0	15,15,17	1.79	5 (33%)
5	MAN	M	5	5	11,11,12	0.76	0	15,15,17	2.51	6 (40%)
5	MAN	M	6	5	11,11,12	0.76	0	15,15,17	1.46	4 (26%)
5	MAN	M	7	5	11,11,12	1.31	1 (9%)	15,15,17	2.34	3 (20%)
5	MAN	M	8	5	11,11,12	1.36	1 (9%)	15,15,17	2.02	6 (40%)
5	MAN	M	9	5	11,11,12	0.82	0	15,15,17	1.61	3 (20%)
3	NAG	N	1	1,3	14,14,15	0.63	0	17,19,21	1.28	2 (11%)
3	NAG	N	2	3	14,14,15	0.86	0	17,19,21	1.21	0
3	BMA	N	3	3	11,11,12	0.91	0	15,15,17	1.48	2 (13%)
6	NAG	O	1	1,6	14,14,15	1.08	1 (7%)	17,19,21	2.11	6 (35%)
6	NAG	O	2	6	14,14,15	1.08	0	17,19,21	1.79	5 (29%)
6	BMA	O	3	6	11,11,12	1.08	0	15,15,17	2.00	3 (20%)
6	MAN	O	4	6	11,11,12	1.04	1 (9%)	15,15,17	1.62	5 (33%)
6	MAN	O	5	6	11,11,12	1.26	1 (9%)	15,15,17	2.21	7 (46%)
6	MAN	O	6	6	11,11,12	0.79	0	15,15,17	1.68	4 (26%)
6	MAN	O	7	6	11,11,12	0.92	0	15,15,17	2.11	7 (46%)
10	NAG	P	1	1,10,13	14,14,15	1.21	1 (7%)	17,19,21	1.60	4 (23%)
10	NAG	P	2	10	14,14,15	0.79	0	17,19,21	1.53	3 (17%)
10	BMA	P	3	10	11,11,12	1.41	2 (18%)	15,15,17	4.27	9 (60%)
10	MAN	P	4	10	11,11,12	1.05	1 (9%)	15,15,17	1.99	4 (26%)
10	MAN	P	5	10	11,11,12	1.05	0	15,15,17	1.85	4 (26%)
10	MAN	P	6	10	11,11,12	0.67	0	15,15,17	2.75	7 (46%)
10	MAN	P	7	10	11,11,12	0.94	1 (9%)	15,15,17	1.85	3 (20%)
10	MAN	P	8	10	11,11,12	0.95	0	15,15,17	2.11	7 (46%)

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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	F	10	5	-	2/2/19/22	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
5	MAN	F	7	5	-	0/2/19/22	0/1/1/1
5	MAN	F	8	5	-	0/2/19/22	0/1/1/1
5	MAN	F	9	5	-	1/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
6	NAG	H	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
6	MAN	H	5	6	-	2/2/19/22	0/1/1/1
6	MAN	H	6	6	-	2/2/19/22	0/1/1/1
6	MAN	H	7	6	-	2/2/19/22	0/1/1/1
7	NAG	I	1	1,13,7	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
7	MAN	I	4	7	-	2/2/19/22	0/1/1/1
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
7	MAN	I	6	7	-	2/2/19/22	0/1/1/1
7	MAN	I	7	7	-	1/2/19/22	0/1/1/1
8	NAG	J	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
8	BMA	J	3	8	-	0/2/19/22	0/1/1/1
8	MAN	J	4	8	-	0/2/19/22	0/1/1/1
8	MAN	J	5	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	J	6	8	-	2/2/19/22	0/1/1/1
8	MAN	J	7	8	-	0/2/19/22	0/1/1/1
9	NAG	K	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	K	2	9	-	0/6/23/26	0/1/1/1
9	BMA	K	3	9	-	0/2/19/22	0/1/1/1
9	MAN	K	4	9	-	0/2/19/22	0/1/1/1
9	MAN	K	5	9	-	1/2/19/22	0/1/1/1
9	MAN	K	6	9	-	1/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	M	10	5	-	0/2/19/22	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
5	MAN	M	6	5	-	0/2/19/22	0/1/1/1
5	MAN	M	7	5	-	0/2/19/22	0/1/1/1
5	MAN	M	8	5	-	0/2/19/22	0/1/1/1
5	MAN	M	9	5	-	0/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	BMA	N	3	3	-	1/2/19/22	0/1/1/1
6	NAG	O	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	0/2/19/22	0/1/1/1
6	MAN	O	5	6	-	0/2/19/22	0/1/1/1
6	MAN	O	6	6	-	0/2/19/22	0/1/1/1
6	MAN	O	7	6	-	2/2/19/22	0/1/1/1
10	NAG	P	1	1,10,13	-	1/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1
10	BMA	P	3	10	-	2/2/19/22	0/1/1/1
10	MAN	P	4	10	-	1/2/19/22	0/1/1/1
10	MAN	P	5	10	-	0/2/19/22	0/1/1/1
10	MAN	P	6	10	-	2/2/19/22	0/1/1/1
10	MAN	P	7	10	-	2/2/19/22	0/1/1/1
10	MAN	P	8	10	-	2/2/19/22	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	NAG	C1-C2	4.51	1.59	1.52
9	K	6	MAN	C2-C3	4.22	1.58	1.52
5	F	1	NAG	C2-N2	3.77	1.52	1.46
5	F	5	MAN	O5-C1	-3.20	1.38	1.43
7	I	2	NAG	O5-C1	-3.19	1.38	1.43
10	P	3	BMA	C2-C3	3.18	1.57	1.52
5	M	7	MAN	O5-C1	-3.12	1.38	1.43
5	M	8	MAN	C2-C3	3.07	1.57	1.52
10	P	1	NAG	C2-N2	3.00	1.51	1.46
5	F	10	MAN	O5-C1	-2.93	1.39	1.43
4	E	2	NAG	O3-C3	-2.89	1.36	1.43
6	H	5	MAN	O2-C2	-2.84	1.37	1.43
7	I	7	MAN	C2-C3	2.81	1.56	1.52
3	G	2	NAG	O5-C1	-2.77	1.39	1.43
6	O	5	MAN	O3-C3	-2.76	1.36	1.43
5	F	10	MAN	C2-C3	2.74	1.56	1.52
5	M	2	NAG	C4-C3	2.67	1.59	1.52
2	C	1	NAG	C1-C2	2.63	1.56	1.52
9	K	1	NAG	C1-C2	2.62	1.56	1.52
5	M	1	NAG	O5-C1	-2.58	1.39	1.43
5	M	2	NAG	C1-C2	2.54	1.56	1.52
5	M	3	BMA	O4-C4	-2.52	1.37	1.43
10	P	7	MAN	C2-C3	2.52	1.56	1.52
10	P	3	BMA	O5-C1	-2.46	1.39	1.43
5	F	8	MAN	O2-C2	-2.41	1.38	1.43
5	F	9	MAN	O3-C3	-2.37	1.37	1.43
9	K	2	NAG	O5-C1	-2.33	1.40	1.43
5	M	1	NAG	C1-C2	2.32	1.55	1.52
7	I	4	MAN	O5-C5	2.32	1.48	1.43
8	J	5	MAN	C1-C2	2.32	1.57	1.52
7	I	5	MAN	C2-C3	-2.28	1.49	1.52
3	D	1	NAG	C1-C2	2.28	1.55	1.52
2	C	2	NAG	O5-C1	-2.27	1.40	1.43
7	I	2	NAG	O3-C3	-2.26	1.37	1.43
3	G	3	BMA	C1-C2	2.24	1.57	1.52
8	J	3	BMA	O5-C5	-2.22	1.38	1.43
6	H	7	MAN	O3-C3	-2.19	1.37	1.43
9	K	2	NAG	C3-C2	2.19	1.57	1.52
8	J	2	NAG	C4-C3	2.19	1.57	1.52
2	C	3	BMA	C4-C5	2.19	1.57	1.53
3	D	2	NAG	C4-C5	2.15	1.57	1.53
5	F	2	NAG	O4-C4	-2.15	1.37	1.43
5	F	10	MAN	O3-C3	-2.15	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	4	MAN	O4-C4	-2.14	1.37	1.43
6	O	1	NAG	O5-C1	-2.14	1.40	1.43
5	M	2	NAG	C4-C5	2.14	1.57	1.53
5	F	1	NAG	C4-C3	2.14	1.57	1.52
6	H	5	MAN	C1-C2	2.12	1.57	1.52
7	I	5	MAN	O5-C1	-2.11	1.40	1.43
6	H	6	MAN	O5-C5	2.11	1.47	1.43
3	G	1	NAG	O4-C4	-2.09	1.38	1.43
5	F	3	BMA	C4-C5	2.07	1.57	1.53
5	F	1	NAG	O5-C1	-2.07	1.40	1.43
5	F	7	MAN	C4-C3	2.07	1.57	1.52
5	M	10	MAN	O5-C1	-2.07	1.40	1.43
6	O	4	MAN	O2-C2	-2.06	1.39	1.43
6	H	5	MAN	O3-C3	-2.02	1.38	1.43
7	I	1	NAG	O4-C4	2.02	1.47	1.43

All (331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	3	BMA	C1-O5-C5	9.84	125.53	112.19
10	P	3	BMA	C6-C5-C4	-8.41	93.32	113.00
2	C	4	MAN	O5-C5-C6	7.52	118.99	107.20
4	E	2	NAG	C3-C4-C5	-7.07	97.63	110.24
3	G	3	BMA	C1-O5-C5	6.64	121.19	112.19
5	M	7	MAN	C1-O5-C5	6.47	120.96	112.19
7	I	3	BMA	C1-O5-C5	6.10	120.45	112.19
10	P	3	BMA	O2-C2-C3	6.08	122.31	110.14
8	J	7	MAN	O5-C5-C6	5.86	116.39	107.20
9	K	6	MAN	O5-C5-C6	5.84	116.36	107.20
5	F	10	MAN	O2-C2-C3	5.79	121.73	110.14
5	M	5	MAN	O6-C6-C5	-5.70	91.74	111.29
4	E	2	NAG	O5-C5-C6	5.57	115.94	107.20
10	P	6	MAN	O3-C3-C4	5.51	123.10	110.35
6	O	3	BMA	O5-C5-C6	5.39	115.66	107.20
5	F	6	MAN	O5-C5-C6	5.36	115.61	107.20
9	K	6	MAN	O2-C2-C3	5.32	120.80	110.14
5	F	9	MAN	O5-C5-C6	5.31	115.53	107.20
7	I	4	MAN	O5-C5-C6	5.20	115.36	107.20
6	H	2	NAG	C2-N2-C7	-5.18	115.52	122.90
8	J	3	BMA	C1-C2-C3	-5.13	103.36	109.67
8	J	4	MAN	O5-C5-C6	4.86	114.82	107.20
6	H	5	MAN	O5-C5-C6	4.85	114.81	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	4	MAN	O2-C2-C1	-4.76	99.41	109.15
3	D	3	BMA	O5-C5-C6	4.69	114.56	107.20
6	O	1	NAG	C1-O5-C5	4.64	118.48	112.19
2	C	2	NAG	C2-N2-C7	4.63	129.50	122.90
7	I	7	MAN	O2-C2-C3	4.62	119.39	110.14
10	P	3	BMA	O3-C3-C2	4.59	118.79	109.99
6	H	6	MAN	O5-C5-C6	4.54	114.33	107.20
10	P	7	MAN	O5-C5-C6	4.54	114.32	107.20
5	M	7	MAN	O2-C2-C3	-4.53	101.06	110.14
6	H	7	MAN	C1-C2-C3	-4.51	104.12	109.67
10	P	6	MAN	O4-C4-C3	4.50	120.74	110.35
6	H	7	MAN	O4-C4-C3	-4.44	100.09	110.35
10	P	6	MAN	O5-C5-C6	4.33	113.99	107.20
5	M	8	MAN	C1-O5-C5	4.32	118.05	112.19
7	I	7	MAN	O5-C5-C6	4.28	113.91	107.20
10	P	2	NAG	C1-O5-C5	4.27	117.98	112.19
7	I	7	MAN	C1-O5-C5	4.27	117.97	112.19
7	I	1	NAG	C1-O5-C5	4.24	117.94	112.19
3	D	3	BMA	O3-C3-C2	-4.24	101.88	109.99
3	G	3	BMA	O2-C2-C1	4.22	117.80	109.15
3	N	3	BMA	O5-C5-C6	4.22	113.83	107.20
2	C	4	MAN	C1-C2-C3	4.22	114.86	109.67
7	I	5	MAN	O2-C2-C3	-4.19	101.74	110.14
7	I	5	MAN	C3-C4-C5	-4.16	102.81	110.24
6	O	5	MAN	C6-C5-C4	-4.16	103.26	113.00
10	P	6	MAN	C3-C4-C5	-4.15	102.83	110.24
3	L	1	NAG	O4-C4-C5	-4.13	99.05	109.30
8	J	5	MAN	C6-C5-C4	-4.12	103.35	113.00
10	P	5	MAN	C3-C4-C5	-4.08	102.97	110.24
5	M	5	MAN	C6-C5-C4	-4.07	103.47	113.00
9	K	4	MAN	O5-C5-C6	4.05	113.55	107.20
5	M	1	NAG	O4-C4-C5	-4.04	99.26	109.30
3	D	3	BMA	C3-C4-C5	4.03	117.42	110.24
5	M	3	BMA	O5-C5-C4	-4.00	101.11	110.83
4	E	1	NAG	O5-C5-C6	3.99	113.46	107.20
8	J	5	MAN	O5-C5-C6	3.95	113.40	107.20
8	J	6	MAN	C6-C5-C4	-3.95	103.75	113.00
4	E	1	NAG	C1-O5-C5	3.91	117.49	112.19
5	M	5	MAN	C1-O5-C5	3.87	117.44	112.19
8	J	2	NAG	O6-C6-C5	-3.82	98.20	111.29
10	P	8	MAN	O5-C5-C6	3.77	113.11	107.20
3	G	1	NAG	C1-C2-N2	-3.77	104.06	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1	NAG	O5-C5-C6	-3.74	101.35	107.20
5	M	8	MAN	O3-C3-C4	-3.72	101.76	110.35
6	O	6	MAN	C1-O5-C5	3.71	117.22	112.19
6	O	7	MAN	C1-O5-C5	-3.71	107.17	112.19
5	F	10	MAN	C1-O5-C5	3.70	117.20	112.19
3	D	3	BMA	C1-C2-C3	3.69	114.20	109.67
5	F	10	MAN	O3-C3-C4	-3.69	101.82	110.35
9	K	3	BMA	C1-O5-C5	3.68	117.18	112.19
3	L	3	BMA	O5-C1-C2	-3.65	105.13	110.77
10	P	4	MAN	O5-C1-C2	3.65	116.41	110.77
7	I	7	MAN	C1-C2-C3	-3.65	105.18	109.67
8	J	3	BMA	O5-C5-C4	-3.62	102.02	110.83
5	M	9	MAN	O2-C2-C3	-3.56	103.00	110.14
6	O	5	MAN	O2-C2-C1	3.53	116.38	109.15
7	I	5	MAN	O6-C6-C5	-3.51	99.24	111.29
6	H	5	MAN	O2-C2-C3	-3.48	103.16	110.14
5	M	5	MAN	O3-C3-C4	-3.47	102.33	110.35
3	L	2	NAG	O6-C6-C5	-3.46	99.42	111.29
2	C	3	BMA	C3-C4-C5	3.45	116.39	110.24
3	D	3	BMA	O6-C6-C5	3.45	123.12	111.29
8	J	7	MAN	O3-C3-C2	3.43	116.57	109.99
2	C	4	MAN	C1-O5-C5	3.43	116.84	112.19
6	O	1	NAG	O4-C4-C5	-3.40	100.85	109.30
5	F	8	MAN	O3-C3-C4	-3.34	102.62	110.35
6	O	5	MAN	C1-C2-C3	-3.34	105.56	109.67
9	K	5	MAN	C1-O5-C5	3.34	116.71	112.19
9	K	6	MAN	O3-C3-C2	3.33	116.36	109.99
6	H	5	MAN	C6-C5-C4	-3.32	105.22	113.00
6	O	5	MAN	C1-O5-C5	3.30	116.66	112.19
5	M	1	NAG	C4-C3-C2	3.29	115.85	111.02
5	M	4	MAN	O6-C6-C5	-3.28	100.03	111.29
6	H	2	NAG	C4-C3-C2	3.28	115.83	111.02
3	L	1	NAG	O5-C5-C6	3.26	112.31	107.20
3	G	2	NAG	C4-C3-C2	3.26	115.79	111.02
9	K	6	MAN	C2-C3-C4	3.25	116.53	110.89
7	I	6	MAN	O2-C2-C1	3.25	115.80	109.15
6	H	2	NAG	O6-C6-C5	-3.25	100.14	111.29
3	N	1	NAG	C1-C2-N2	-3.24	104.95	110.49
10	P	5	MAN	O2-C2-C3	-3.24	103.65	110.14
3	D	3	BMA	O3-C3-C4	3.24	117.83	110.35
8	J	4	MAN	C2-C3-C4	-3.23	105.30	110.89
5	F	8	MAN	C3-C4-C5	3.23	116.00	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	BMA	O5-C1-C2	3.23	115.75	110.77
10	P	8	MAN	C1-C2-C3	3.22	113.62	109.67
6	O	3	BMA	O2-C2-C1	-3.20	102.61	109.15
5	F	4	MAN	O5-C5-C6	3.17	112.18	107.20
6	H	1	NAG	C1-C2-N2	-3.17	105.06	110.49
6	O	4	MAN	C1-C2-C3	3.17	113.56	109.67
5	F	6	MAN	O3-C3-C2	3.15	116.03	109.99
2	C	1	NAG	O3-C3-C2	-3.12	103.01	109.47
2	C	2	NAG	C3-C4-C5	-3.12	104.68	110.24
10	P	3	BMA	O6-C6-C5	-3.11	100.60	111.29
5	M	6	MAN	C1-C2-C3	-3.11	105.85	109.67
8	J	3	BMA	O6-C6-C5	-3.11	100.63	111.29
5	M	3	BMA	O5-C5-C6	3.11	112.08	107.20
5	F	5	MAN	O6-C6-C5	-3.10	100.65	111.29
5	M	4	MAN	C1-O5-C5	3.09	116.38	112.19
2	C	4	MAN	C6-C5-C4	-3.09	105.77	113.00
5	M	10	MAN	O6-C6-C5	-3.09	100.70	111.29
9	K	5	MAN	O5-C5-C6	3.09	112.04	107.20
6	H	2	NAG	O4-C4-C3	-3.08	103.23	110.35
6	H	7	MAN	O5-C1-C2	-3.07	106.04	110.77
2	C	3	BMA	C1-C2-C3	3.05	113.41	109.67
10	P	3	BMA	O3-C3-C4	-3.04	103.31	110.35
10	P	3	BMA	C2-C3-C4	3.04	116.16	110.89
6	O	1	NAG	C1-C2-N2	-3.04	105.30	110.49
4	E	1	NAG	O4-C4-C5	-3.02	101.79	109.30
2	C	3	BMA	C2-C3-C4	-3.02	105.67	110.89
10	P	2	NAG	O5-C5-C6	3.00	111.91	107.20
3	D	3	BMA	C1-O5-C5	2.99	116.24	112.19
3	L	2	NAG	C2-N2-C7	2.97	127.13	122.90
6	O	7	MAN	O5-C5-C6	2.96	111.85	107.20
8	J	3	BMA	O2-C2-C3	-2.96	104.21	110.14
5	F	4	MAN	C1-C2-C3	-2.96	106.03	109.67
8	J	5	MAN	O2-C2-C3	-2.96	104.22	110.14
7	I	5	MAN	C6-C5-C4	2.95	119.91	113.00
6	O	7	MAN	O2-C2-C1	2.94	115.17	109.15
2	C	4	MAN	C2-C3-C4	-2.94	105.81	110.89
3	L	3	BMA	C3-C4-C5	2.93	115.47	110.24
10	P	1	NAG	O5-C5-C6	2.93	111.80	107.20
3	L	3	BMA	C2-C3-C4	2.93	115.96	110.89
6	O	7	MAN	C3-C4-C5	2.92	115.44	110.24
8	J	7	MAN	O4-C4-C3	-2.91	103.63	110.35
6	O	1	NAG	O5-C1-C2	-2.91	106.70	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	2	NAG	C1-O5-C5	2.90	116.12	112.19
10	P	4	MAN	C1-C2-C3	2.90	113.23	109.67
3	L	1	NAG	C3-C4-C5	2.90	115.41	110.24
6	H	2	NAG	C3-C4-C5	-2.90	105.07	110.24
10	P	1	NAG	O6-C6-C5	-2.89	101.39	111.29
2	C	2	NAG	O5-C5-C6	2.87	111.70	107.20
5	M	1	NAG	O3-C3-C2	2.87	115.40	109.47
6	O	7	MAN	O5-C1-C2	-2.86	106.35	110.77
9	K	4	MAN	C3-C4-C5	-2.86	105.13	110.24
7	I	6	MAN	O3-C3-C4	2.85	116.94	110.35
10	P	1	NAG	C1-O5-C5	2.85	116.05	112.19
3	D	2	NAG	C6-C5-C4	2.85	119.67	113.00
10	P	8	MAN	C2-C3-C4	2.84	115.81	110.89
6	O	3	BMA	O3-C3-C2	2.84	115.42	109.99
8	J	6	MAN	O5-C1-C2	-2.83	106.40	110.77
5	F	4	MAN	O6-C6-C5	-2.81	101.66	111.29
3	L	2	NAG	C3-C4-C5	-2.81	105.23	110.24
5	M	10	MAN	C6-C5-C4	-2.79	106.47	113.00
7	I	7	MAN	C6-C5-C4	-2.78	106.48	113.00
6	O	2	NAG	O5-C1-C2	-2.77	106.92	111.29
3	L	2	NAG	O5-C5-C6	2.77	111.54	107.20
6	O	7	MAN	C2-C3-C4	2.76	115.67	110.89
5	M	10	MAN	O3-C3-C4	-2.76	103.97	110.35
7	I	6	MAN	O6-C6-C5	-2.75	101.85	111.29
7	I	3	BMA	O3-C3-C4	2.75	116.71	110.35
10	P	3	BMA	O5-C5-C6	-2.75	102.90	107.20
6	H	1	NAG	C3-C4-C5	2.75	115.14	110.24
6	O	2	NAG	O7-C7-N2	-2.74	116.92	121.95
7	I	3	BMA	O5-C5-C4	-2.71	104.23	110.83
7	I	5	MAN	O4-C4-C3	-2.71	104.09	110.35
5	F	1	NAG	C1-O5-C5	2.70	115.85	112.19
6	H	4	MAN	O3-C3-C4	2.70	116.59	110.35
5	F	1	NAG	C8-C7-N2	2.69	120.66	116.10
4	E	2	NAG	C1-C2-N2	2.69	115.08	110.49
5	M	4	MAN	C1-C2-C3	-2.68	106.37	109.67
6	O	6	MAN	O4-C4-C5	-2.67	102.67	109.30
5	M	9	MAN	O5-C5-C6	2.65	111.36	107.20
3	G	2	NAG	C1-O5-C5	2.65	115.78	112.19
7	I	2	NAG	O3-C3-C4	-2.65	104.23	110.35
9	K	2	NAG	O6-C6-C5	-2.65	102.22	111.29
8	J	3	BMA	O3-C3-C4	-2.63	104.27	110.35
6	H	1	NAG	O3-C3-C2	-2.63	104.02	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	8	MAN	C1-O5-C5	2.63	115.75	112.19
9	K	4	MAN	C1-C2-C3	2.63	112.90	109.67
6	O	4	MAN	O5-C1-C2	2.62	114.82	110.77
9	K	1	NAG	C4-C3-C2	-2.62	107.17	111.02
5	M	10	MAN	C1-O5-C5	2.62	115.74	112.19
10	P	6	MAN	O4-C4-C5	-2.62	102.80	109.30
7	I	1	NAG	C4-C3-C2	2.61	114.85	111.02
9	K	6	MAN	C1-C2-C3	-2.61	106.45	109.67
10	P	3	BMA	O5-C5-C4	2.61	117.18	110.83
10	P	8	MAN	O4-C4-C5	-2.61	102.81	109.30
5	M	4	MAN	O3-C3-C4	-2.60	104.33	110.35
5	F	7	MAN	O3-C3-C4	-2.60	104.33	110.35
10	P	6	MAN	C2-C3-C4	-2.60	106.40	110.89
3	L	3	BMA	O4-C4-C3	-2.59	104.35	110.35
5	M	5	MAN	O2-C2-C1	2.58	114.44	109.15
9	K	1	NAG	O6-C6-C5	-2.58	102.43	111.29
6	O	1	NAG	O7-C7-C8	2.58	126.85	122.06
5	F	10	MAN	O2-C2-C1	2.57	114.40	109.15
5	M	3	BMA	C2-C3-C4	-2.57	106.45	110.89
6	H	4	MAN	O4-C4-C5	-2.56	102.93	109.30
5	M	8	MAN	C1-C2-C3	2.56	112.82	109.67
5	F	5	MAN	C1-O5-C5	2.55	115.65	112.19
7	I	7	MAN	O4-C4-C3	2.55	116.25	110.35
6	H	3	BMA	O2-C2-C1	-2.55	103.93	109.15
3	D	1	NAG	O4-C4-C5	-2.54	102.98	109.30
5	M	10	MAN	O2-C2-C1	2.54	114.35	109.15
9	K	3	BMA	C6-C5-C4	-2.53	107.08	113.00
6	O	1	NAG	O5-C5-C6	2.52	111.16	107.20
3	D	3	BMA	O2-C2-C3	-2.52	105.08	110.14
10	P	4	MAN	O4-C4-C3	-2.52	104.52	110.35
6	H	7	MAN	C3-C4-C5	-2.52	105.75	110.24
5	M	2	NAG	C1-C2-N2	-2.52	106.19	110.49
5	F	8	MAN	C1-O5-C5	2.51	115.59	112.19
5	F	4	MAN	O2-C2-C1	2.51	114.28	109.15
8	J	7	MAN	O6-C6-C5	2.49	119.84	111.29
6	O	4	MAN	C1-O5-C5	2.48	115.56	112.19
7	I	2	NAG	O5-C1-C2	-2.47	107.38	111.29
5	F	9	MAN	O3-C3-C2	-2.47	105.26	109.99
5	F	1	NAG	C6-C5-C4	2.47	118.79	113.00
9	K	5	MAN	C3-C4-C5	2.47	114.64	110.24
5	M	7	MAN	O5-C5-C6	2.45	111.04	107.20
8	J	7	MAN	C1-C2-C3	2.44	112.67	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	10	MAN	C2-C3-C4	2.44	115.12	110.89
6	H	5	MAN	O3-C3-C2	2.43	114.65	109.99
8	J	2	NAG	O4-C4-C5	-2.43	103.26	109.30
5	M	1	NAG	C1-C2-N2	-2.42	106.35	110.49
2	C	1	NAG	O5-C5-C4	-2.41	104.95	110.83
8	J	1	NAG	O4-C4-C3	-2.41	104.77	110.35
5	M	9	MAN	C1-C2-C3	2.41	112.62	109.67
5	M	2	NAG	O4-C4-C3	-2.38	104.86	110.35
9	K	2	NAG	O5-C5-C4	-2.38	105.05	110.83
10	P	5	MAN	C6-C5-C4	2.37	118.56	113.00
8	J	4	MAN	O3-C3-C2	-2.36	105.47	109.99
3	G	2	NAG	O4-C4-C5	-2.35	103.45	109.30
5	F	9	MAN	C3-C4-C5	-2.35	106.05	110.24
6	H	4	MAN	O5-C1-C2	2.34	114.38	110.77
6	O	5	MAN	O6-C6-C5	-2.34	103.26	111.29
6	H	5	MAN	C2-C3-C4	-2.33	106.86	110.89
6	O	6	MAN	C6-C5-C4	-2.30	107.61	113.00
10	P	6	MAN	C1-C2-C3	-2.30	106.84	109.67
8	J	1	NAG	O7-C7-C8	-2.29	117.80	122.06
2	C	3	BMA	O3-C3-C4	2.29	115.64	110.35
3	N	3	BMA	O3-C3-C2	2.28	114.36	109.99
6	H	4	MAN	C1-O5-C5	2.28	115.28	112.19
3	D	3	BMA	O4-C4-C5	-2.28	103.64	109.30
8	J	6	MAN	C1-O5-C5	2.27	115.26	112.19
5	M	6	MAN	O5-C5-C6	2.27	110.76	107.20
9	K	2	NAG	O7-C7-N2	-2.27	117.79	121.95
5	M	5	MAN	O2-C2-C3	-2.25	105.62	110.14
5	M	8	MAN	O5-C1-C2	-2.25	107.30	110.77
7	I	6	MAN	C1-C2-C3	-2.25	106.91	109.67
6	H	7	MAN	O3-C3-C2	2.25	114.29	109.99
3	G	2	NAG	C1-C2-N2	-2.24	106.65	110.49
4	E	2	NAG	C4-C3-C2	2.24	114.31	111.02
9	K	2	NAG	C6-C5-C4	2.24	118.24	113.00
6	O	5	MAN	O2-C2-C3	-2.23	105.67	110.14
3	N	1	NAG	O3-C3-C2	-2.23	104.86	109.47
10	P	7	MAN	O5-C1-C2	2.22	114.20	110.77
7	I	1	NAG	O6-C6-C5	-2.21	103.69	111.29
3	G	3	BMA	C2-C3-C4	-2.21	107.06	110.89
3	L	1	NAG	C1-O5-C5	2.21	115.19	112.19
5	F	3	BMA	O6-C6-C5	-2.21	103.72	111.29
8	J	4	MAN	C6-C5-C4	-2.20	107.84	113.00
2	C	2	NAG	O3-C3-C2	-2.20	104.91	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	MAN	O3-C3-C2	2.20	114.21	109.99
5	M	4	MAN	O3-C3-C2	2.20	114.21	109.99
7	I	6	MAN	O5-C5-C6	-2.20	103.76	107.20
8	J	1	NAG	C4-C3-C2	-2.19	107.80	111.02
5	M	8	MAN	O6-C6-C5	-2.19	103.77	111.29
6	H	1	NAG	O5-C1-C2	2.19	114.74	111.29
5	F	8	MAN	O2-C2-C1	-2.18	104.69	109.15
5	F	4	MAN	O4-C4-C5	2.18	114.71	109.30
4	E	1	NAG	C2-N2-C7	2.18	126.00	122.90
2	C	2	NAG	O4-C4-C5	-2.17	103.90	109.30
6	O	7	MAN	C1-C2-C3	2.17	112.34	109.67
7	I	6	MAN	C6-C5-C4	2.17	118.09	113.00
8	J	1	NAG	O5-C1-C2	-2.16	107.88	111.29
9	K	4	MAN	C6-C5-C4	2.16	118.06	113.00
5	M	1	NAG	O6-C6-C5	-2.16	103.88	111.29
5	M	3	BMA	O2-C2-C3	2.15	114.44	110.14
6	O	5	MAN	O5-C5-C6	2.14	110.56	107.20
6	H	6	MAN	O4-C4-C3	-2.14	105.40	110.35
9	K	3	BMA	O6-C6-C5	-2.14	103.95	111.29
3	D	1	NAG	O7-C7-C8	-2.14	118.08	122.06
3	D	2	NAG	O6-C6-C5	-2.13	103.97	111.29
3	D	1	NAG	C1-C2-N2	2.13	114.13	110.49
8	J	4	MAN	O2-C2-C3	-2.13	105.87	110.14
3	L	3	BMA	O4-C4-C5	2.13	114.58	109.30
5	M	6	MAN	O2-C2-C1	-2.12	104.81	109.15
7	I	7	MAN	O5-C5-C4	-2.12	105.67	110.83
5	M	6	MAN	C1-O5-C5	2.12	115.06	112.19
3	L	3	BMA	O5-C5-C6	-2.12	103.89	107.20
6	H	7	MAN	O6-C6-C5	-2.10	104.09	111.29
10	P	2	NAG	O3-C3-C2	-2.10	105.12	109.47
8	J	6	MAN	O3-C3-C2	2.10	114.01	109.99
2	C	1	NAG	O5-C1-C2	-2.09	107.98	111.29
6	O	6	MAN	O5-C5-C6	2.09	110.48	107.20
10	P	8	MAN	C6-C5-C4	-2.09	108.12	113.00
6	O	2	NAG	O4-C4-C3	-2.08	105.53	110.35
8	J	4	MAN	O6-C6-C5	-2.08	104.16	111.29
10	P	1	NAG	C4-C3-C2	2.07	114.06	111.02
9	K	1	NAG	C1-C2-N2	2.07	114.03	110.49
3	L	2	NAG	O4-C4-C3	-2.07	105.57	110.35
9	K	3	BMA	O3-C3-C2	2.07	113.95	109.99
6	O	2	NAG	O5-C5-C4	-2.06	105.81	110.83
6	O	4	MAN	O5-C5-C6	2.06	110.44	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	O	4	MAN	O6-C6-C5	-2.06	104.22	111.29
5	F	5	MAN	C6-C5-C4	-2.05	108.19	113.00
2	C	3	BMA	O2-C2-C3	-2.04	106.05	110.14
6	O	2	NAG	O6-C6-C5	-2.04	104.31	111.29
3	G	3	BMA	O5-C1-C2	2.03	113.91	110.77
8	J	3	BMA	C1-O5-C5	2.03	114.94	112.19
10	P	8	MAN	O3-C3-C2	-2.01	106.14	109.99
9	K	4	MAN	O5-C1-C2	2.01	113.88	110.77
10	P	7	MAN	C6-C5-C4	-2.01	108.30	113.00
9	K	4	MAN	C1-O5-C5	2.01	114.91	112.19
5	M	8	MAN	O4-C4-C3	2.01	114.99	110.35
10	P	5	MAN	O2-C2-C1	2.01	113.26	109.15
9	K	4	MAN	O5-C5-C4	-2.00	105.96	110.83
4	E	2	NAG	O6-C6-C5	-2.00	104.43	111.29

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	6	MAN	C4-C5-C6-O6
7	I	4	MAN	O5-C5-C6-O6
6	H	5	MAN	O5-C5-C6-O6
6	O	7	MAN	O5-C5-C6-O6
6	H	6	MAN	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
7	I	6	MAN	O5-C5-C6-O6
7	I	4	MAN	C4-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
10	P	8	MAN	O5-C5-C6-O6
6	H	6	MAN	C4-C5-C6-O6
6	H	5	MAN	C4-C5-C6-O6
6	H	7	MAN	C4-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
10	P	7	MAN	O5-C5-C6-O6
6	O	7	MAN	C4-C5-C6-O6
10	P	7	MAN	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
9	K	6	MAN	C4-C5-C6-O6
5	F	10	MAN	C4-C5-C6-O6
10	P	8	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	P	3	BMA	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
10	P	1	NAG	C4-C5-C6-O6
10	P	3	BMA	O5-C5-C6-O6
10	P	6	MAN	C4-C5-C6-O6
5	F	10	MAN	O5-C5-C6-O6
10	P	6	MAN	O5-C5-C6-O6
6	H	7	MAN	O5-C5-C6-O6
3	N	3	BMA	C4-C5-C6-O6
8	J	6	MAN	O5-C5-C6-O6
8	J	6	MAN	C4-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
10	P	4	MAN	O5-C5-C6-O6
5	F	9	MAN	O5-C5-C6-O6
4	E	2	NAG	C3-C2-N2-C7
3	L	2	NAG	C3-C2-N2-C7
7	I	7	MAN	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
9	K	5	MAN	O5-C5-C6-O6

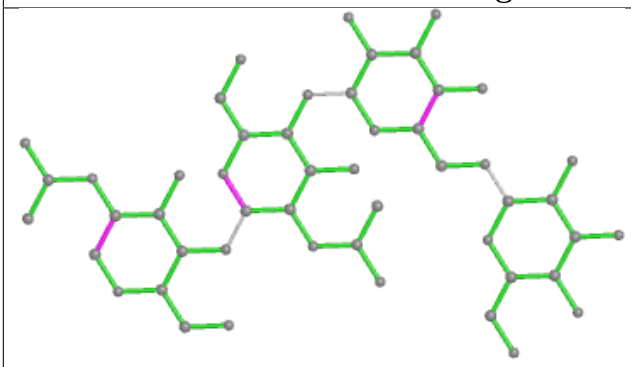
There are no ring outliers.

9 monomers are involved in 10 short contacts:

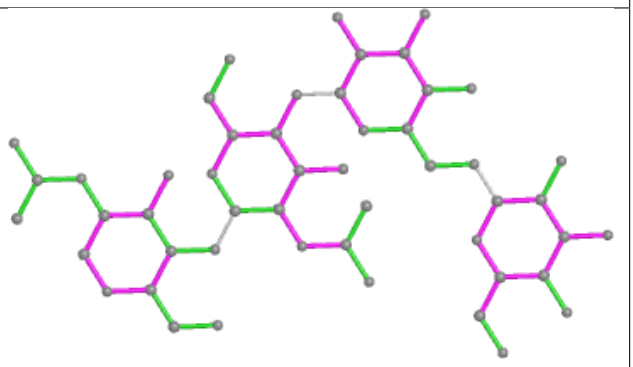
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	4	MAN	1	0
2	C	2	NAG	1	0
6	H	3	BMA	2	0
6	O	3	BMA	2	0
10	P	3	BMA	1	0
3	D	2	NAG	1	0
3	D	3	BMA	1	0
9	K	1	NAG	2	0
10	P	4	MAN	1	0

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

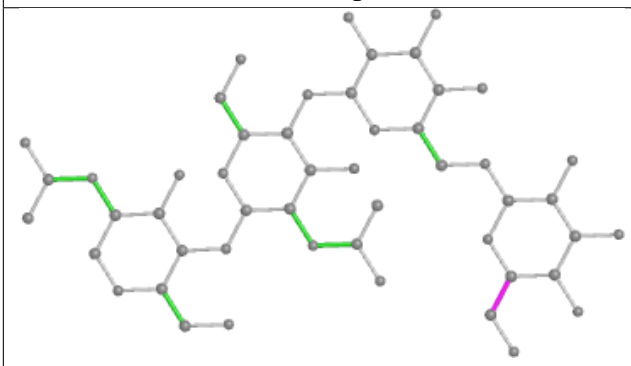
Oligosaccharide Chain C



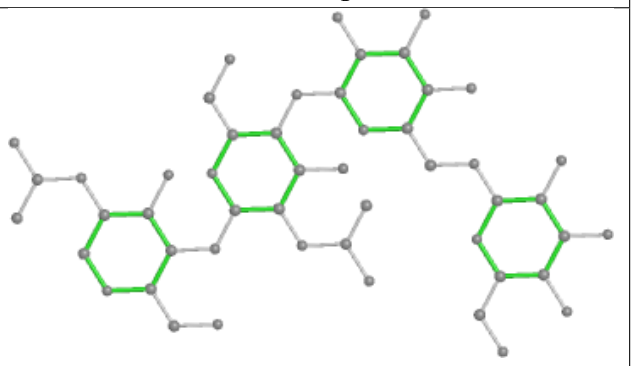
Bond lengths



Bond angles

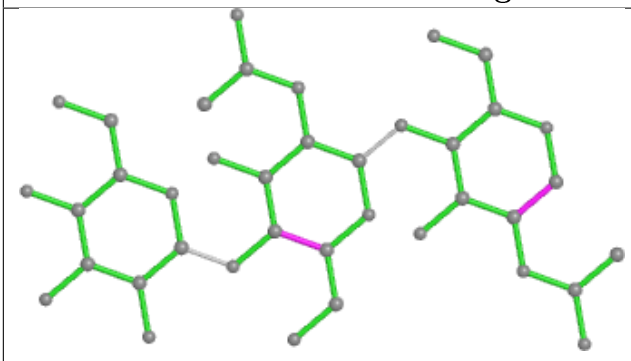


Torsions

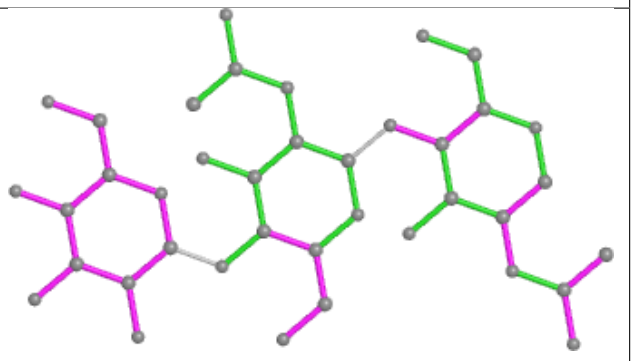


Rings

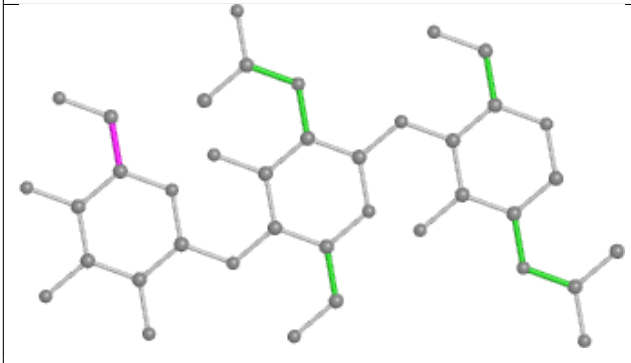
Oligosaccharide Chain D



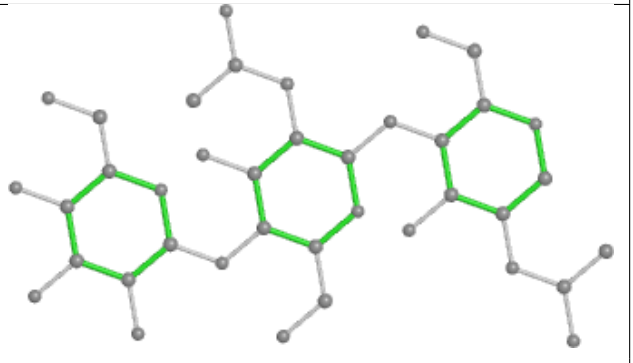
Bond lengths



Bond angles

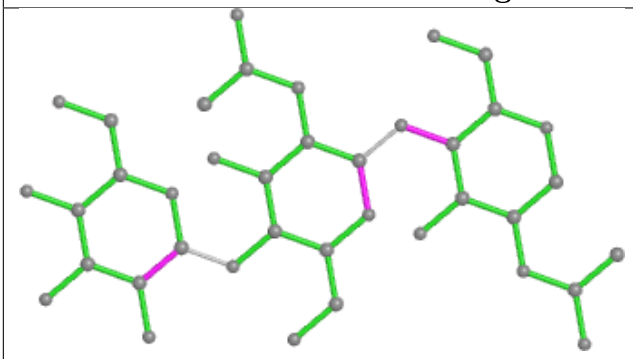


Torsions

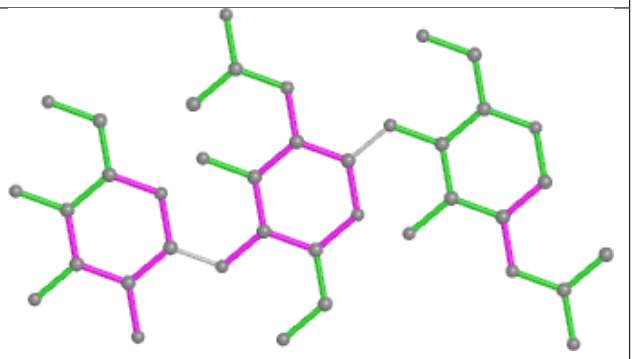


Rings

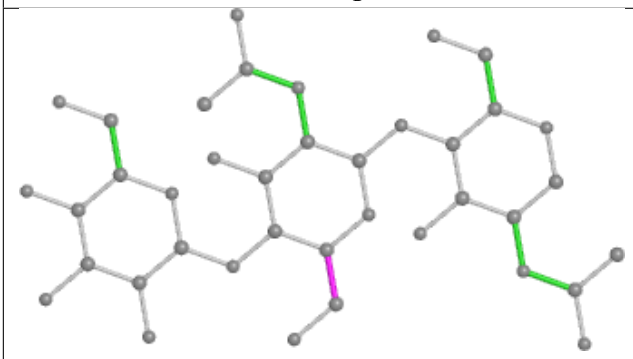
Oligosaccharide Chain G



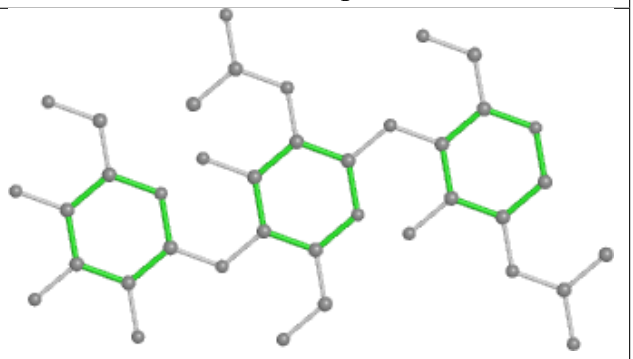
Bond lengths



Bond angles

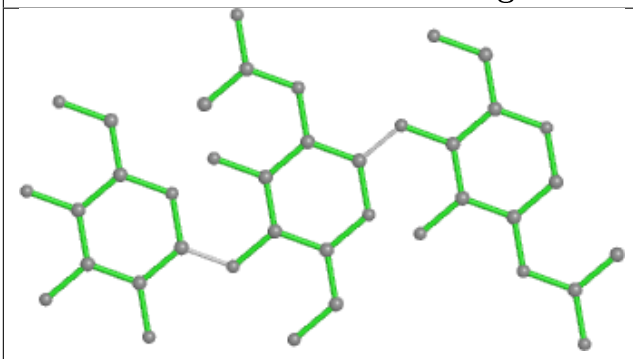


Torsions

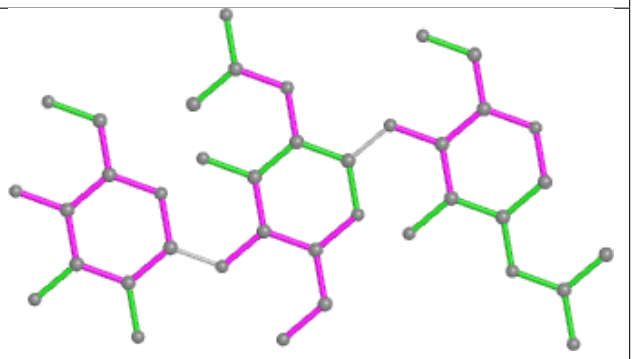


Rings

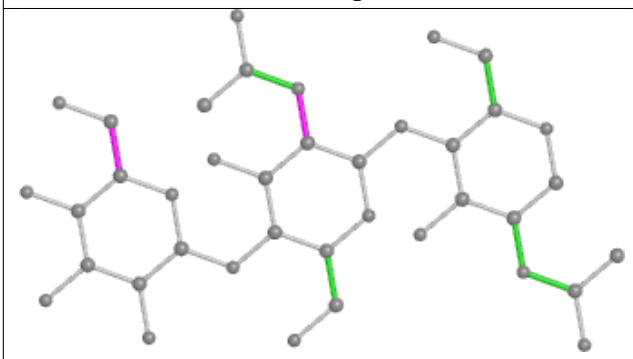
Oligosaccharide Chain L



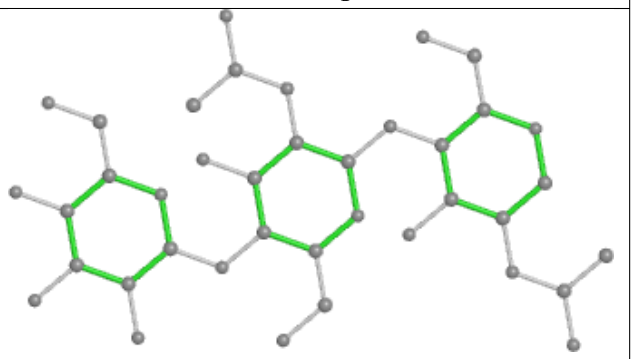
Bond lengths



Bond angles

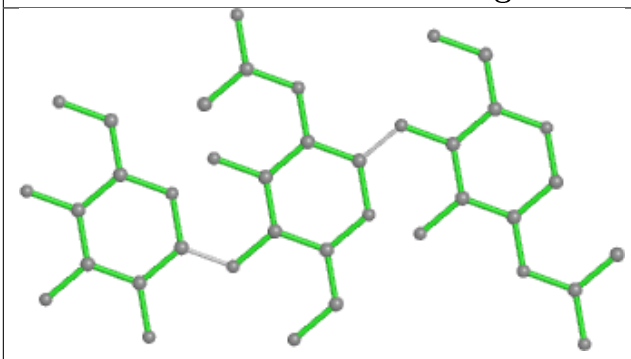


Torsions

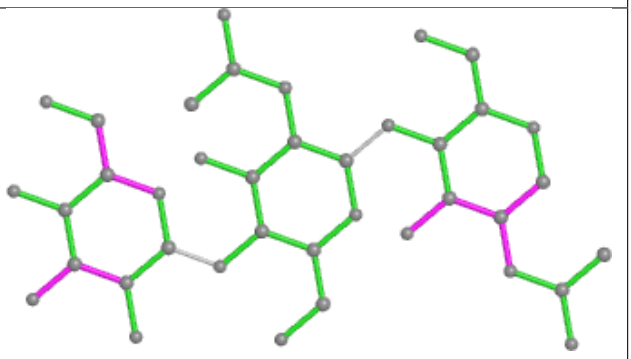


Rings

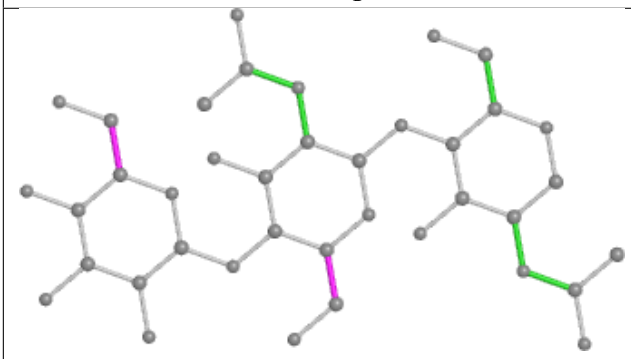
Oligosaccharide Chain N



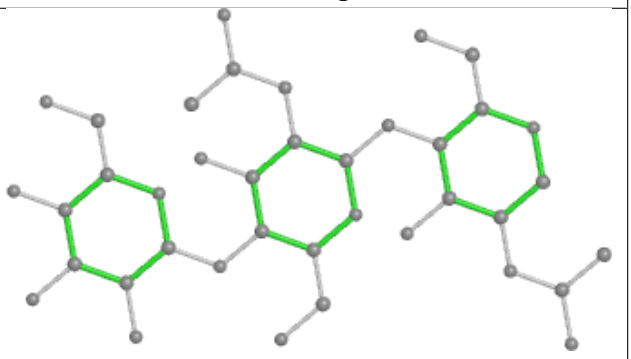
Bond lengths



Bond angles

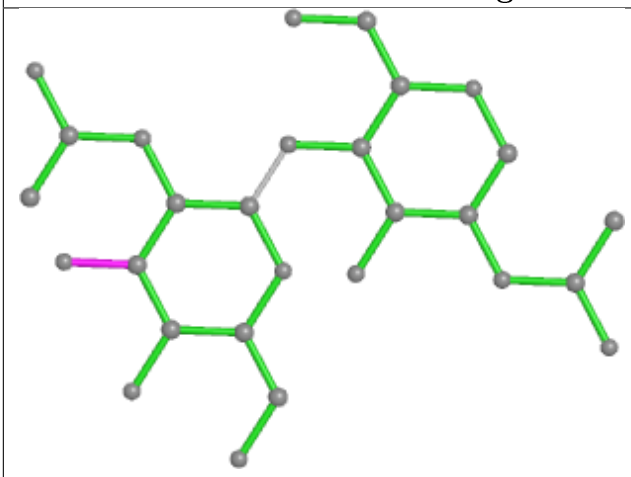


Torsions

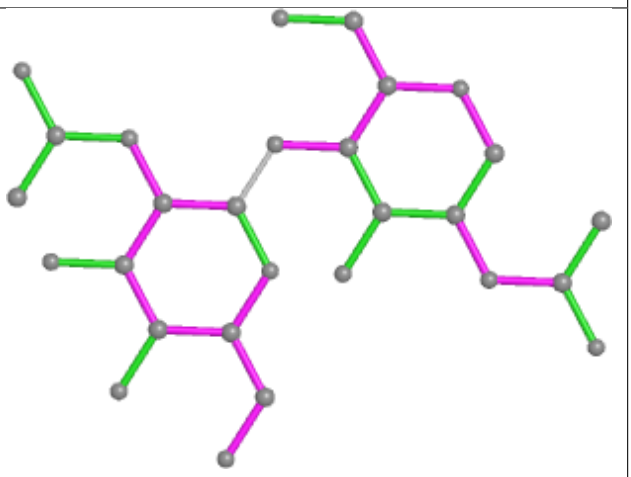


Rings

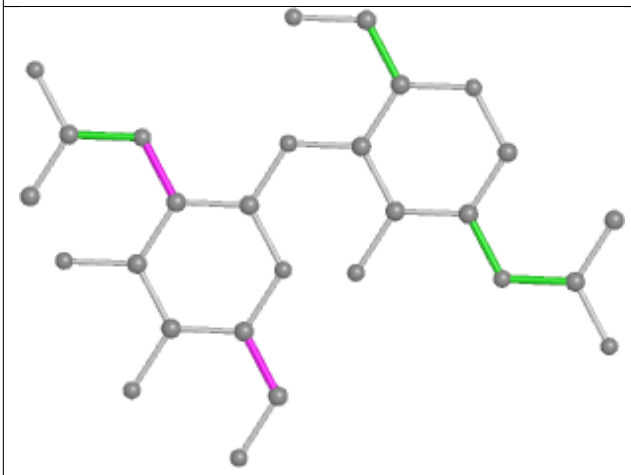
Oligosaccharide Chain E



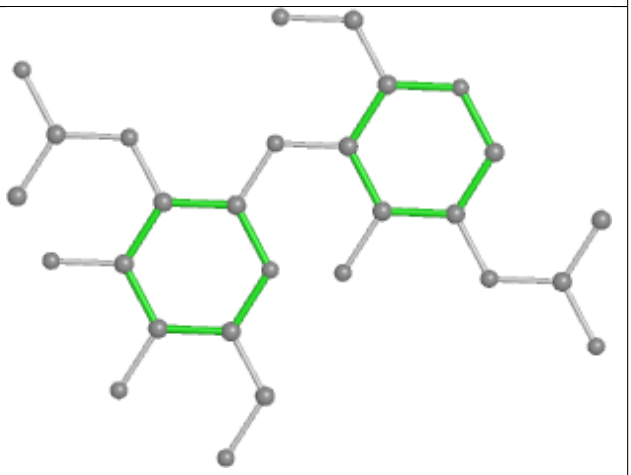
Bond lengths



Bond angles

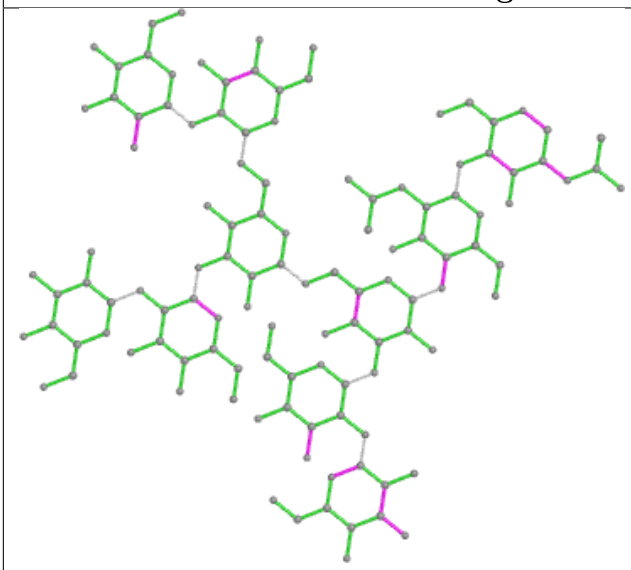


Torsions

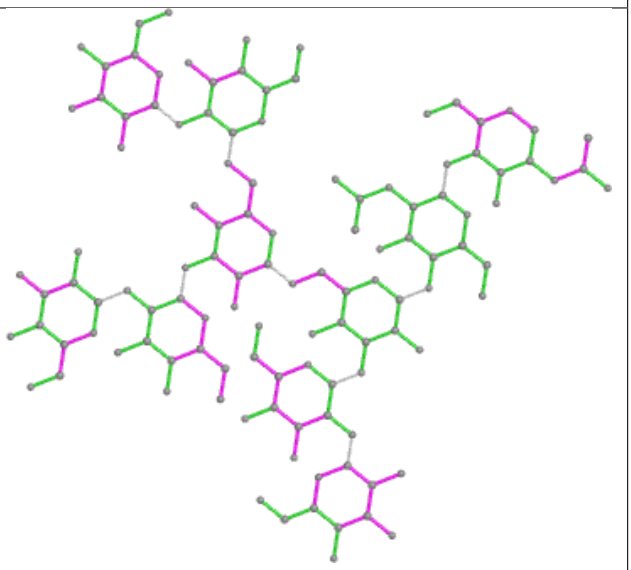


Rings

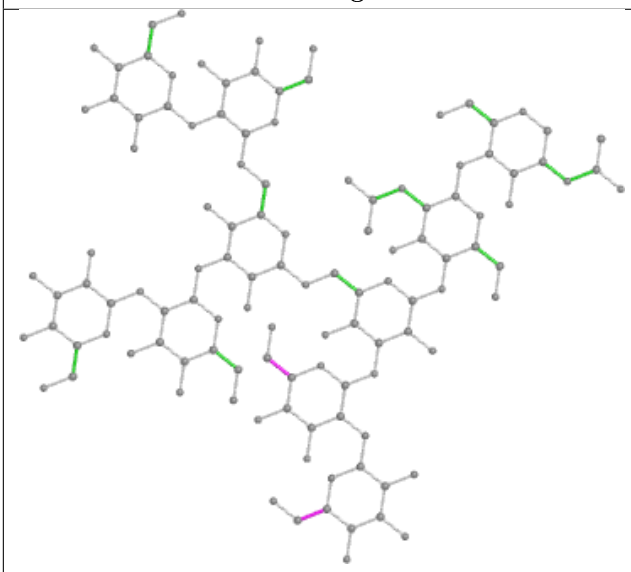
Oligosaccharide Chain F



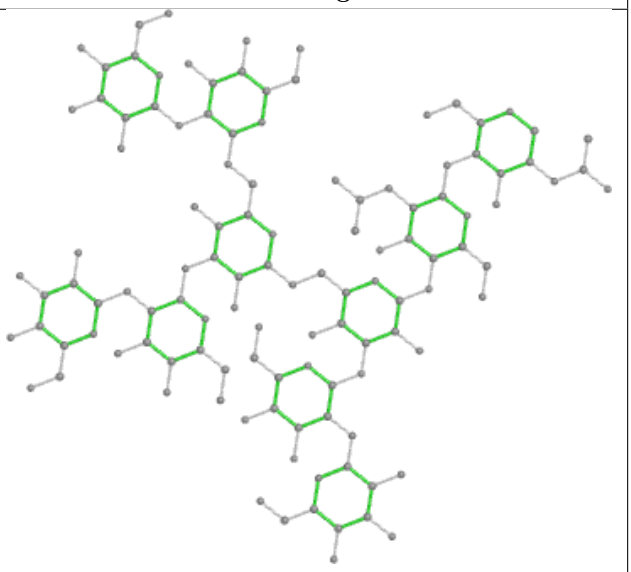
Bond lengths



Bond angles

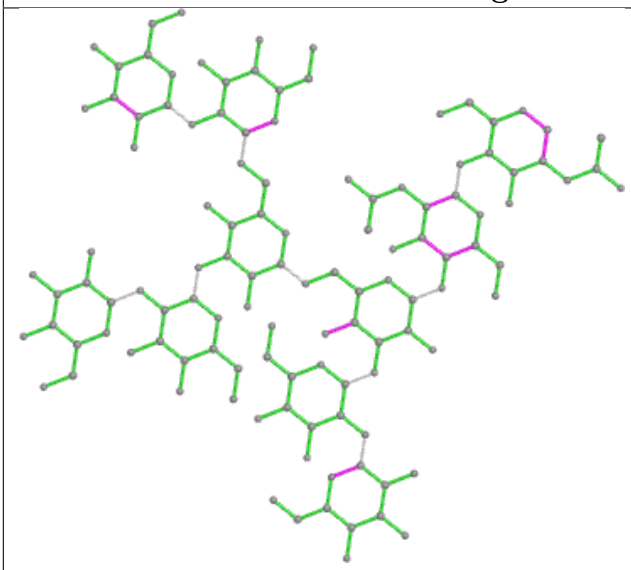


Torsions

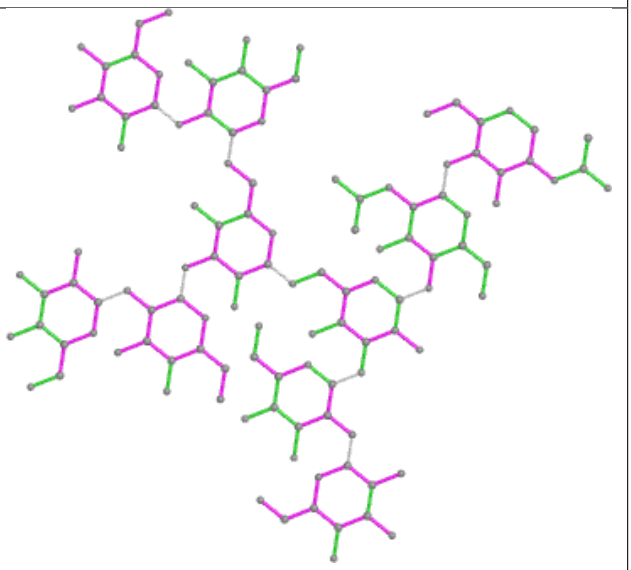


Rings

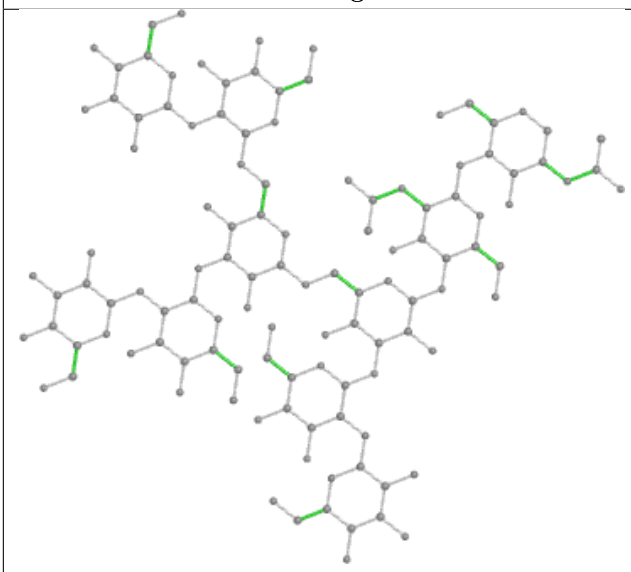
Oligosaccharide Chain M



Bond lengths



Bond angles



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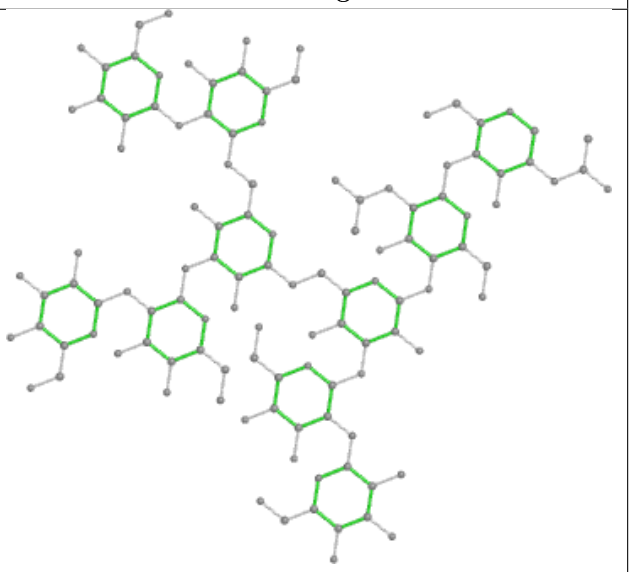
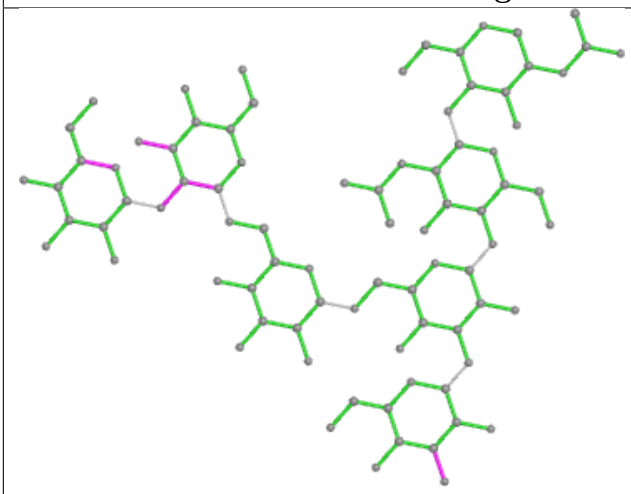
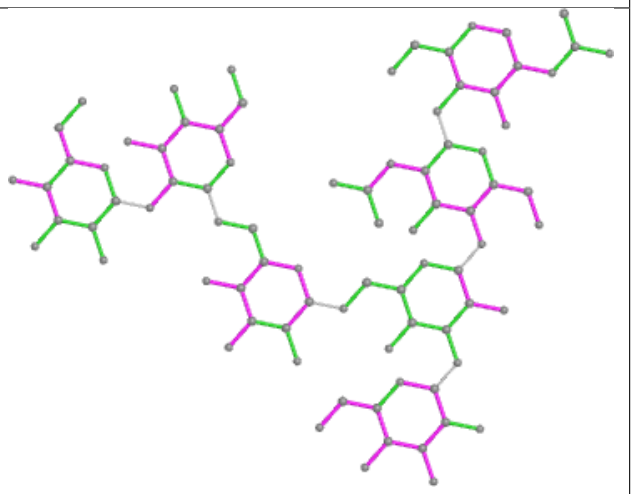


Rings

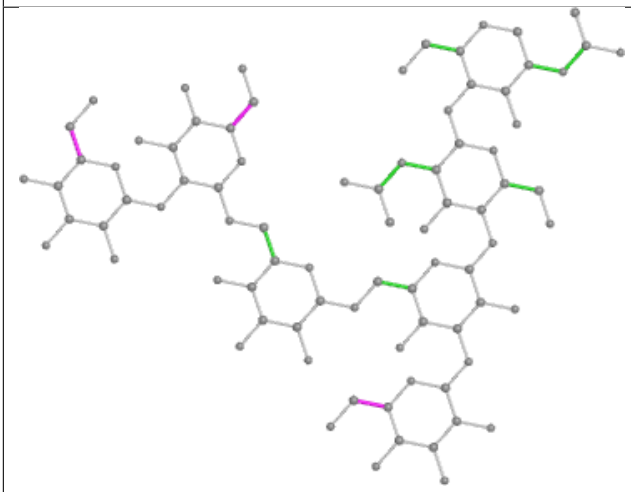
Oligosaccharide Chain H



Bond lengths



Bond angles



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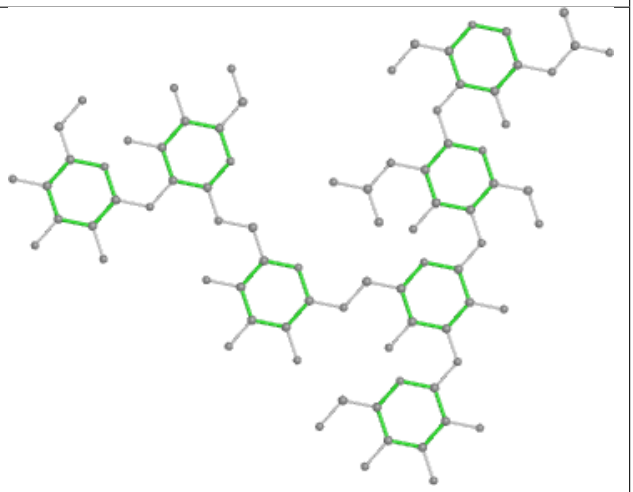
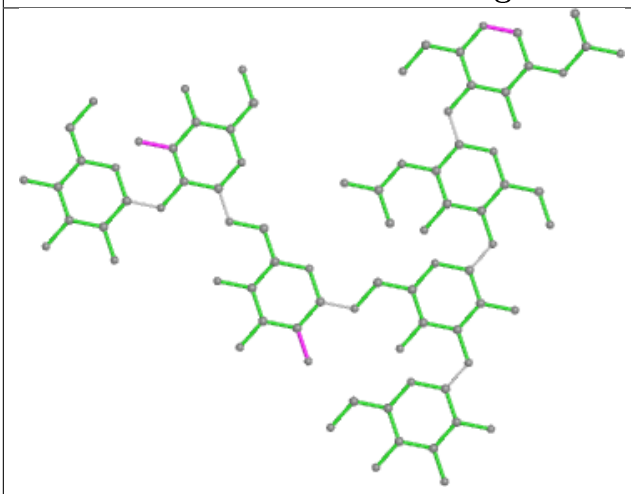
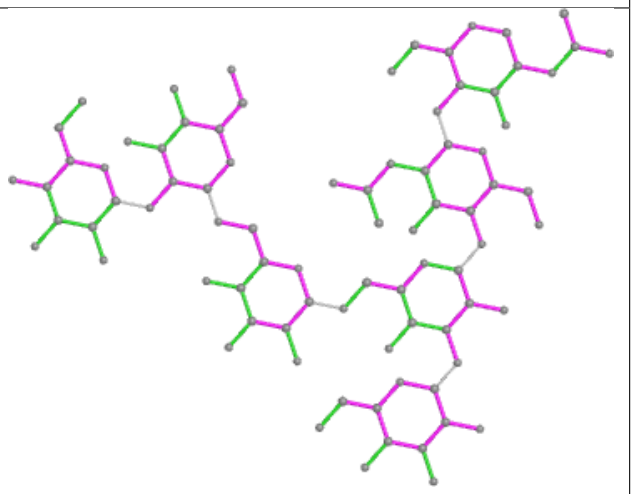


Rings

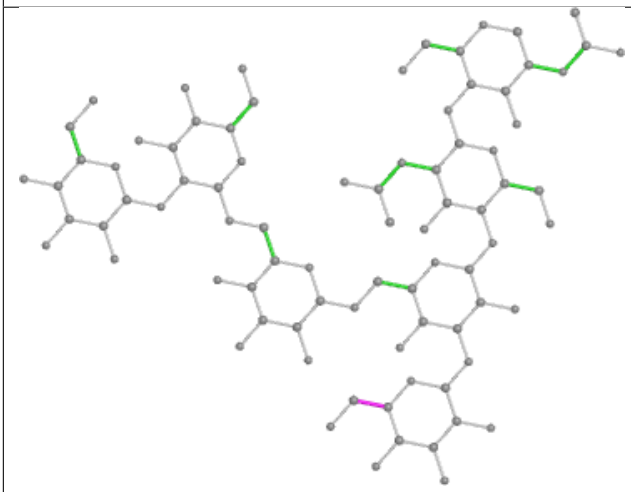
Oligosaccharide Chain O



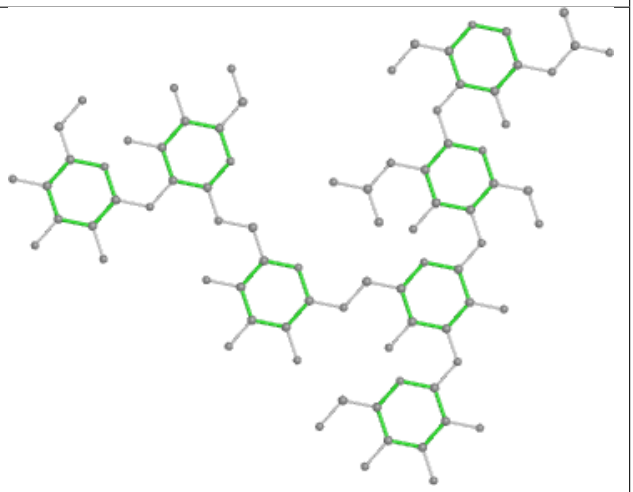
Bond lengths



Bond angles

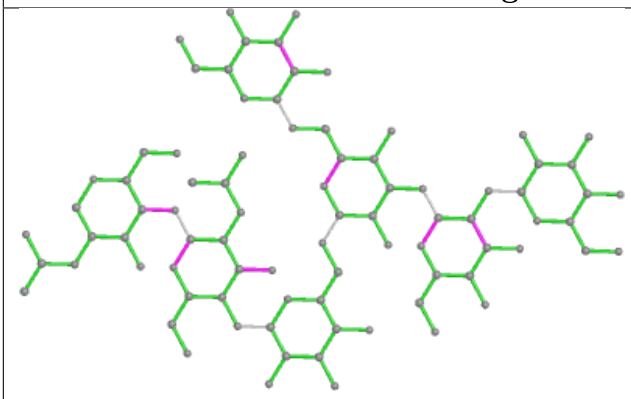


Torsions

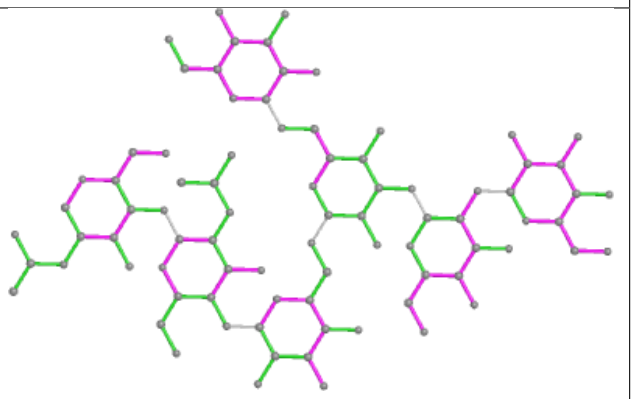


Rings

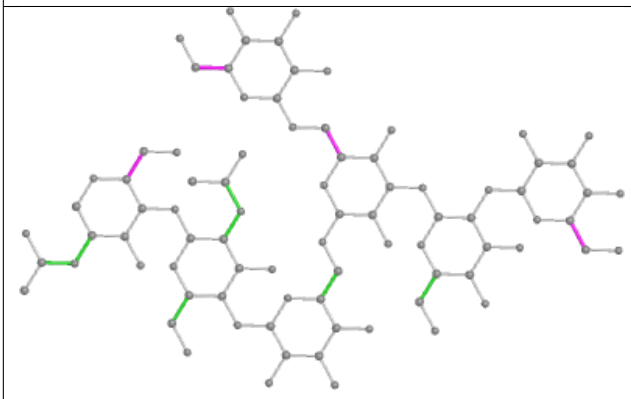
Oligosaccharide Chain I



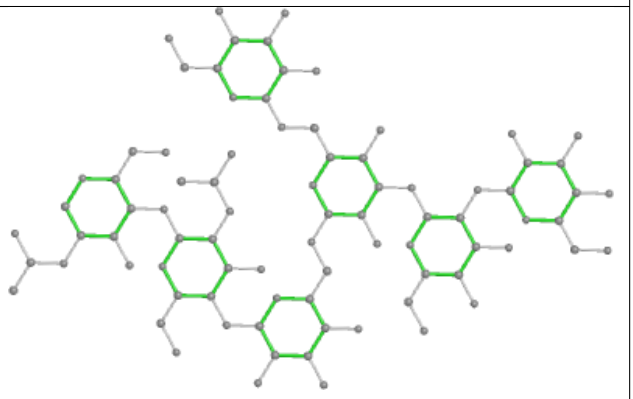
Bond lengths



Bond angles

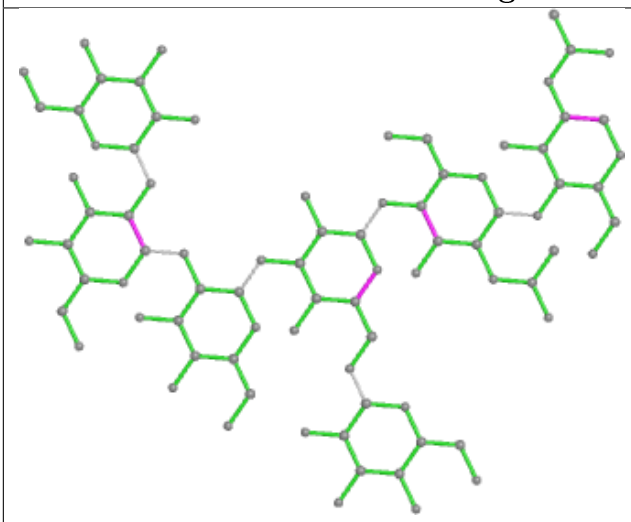


Torsions

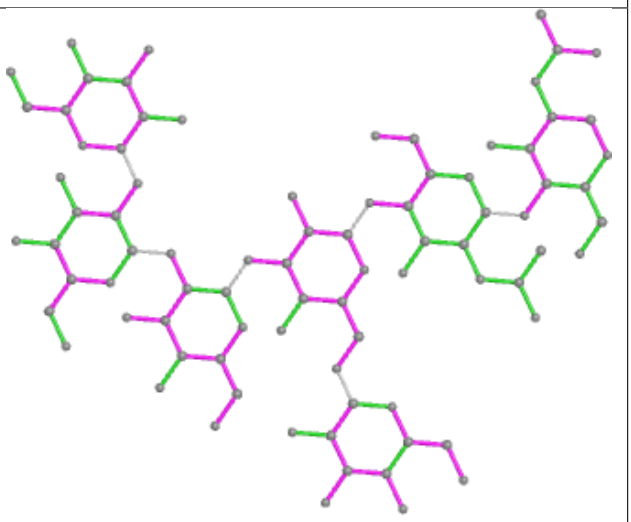


Rings

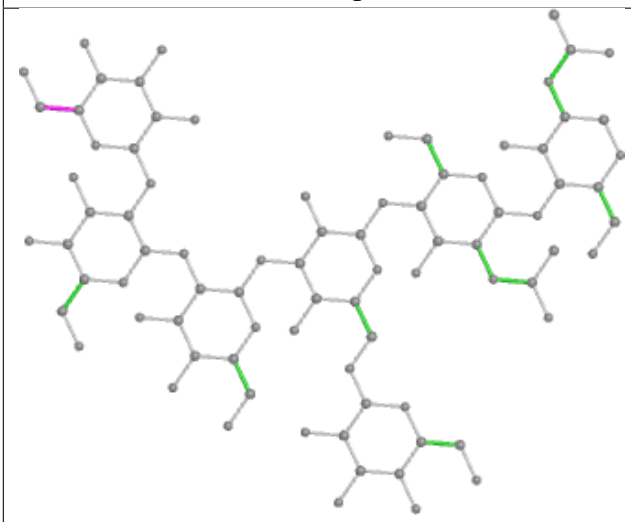
Oligosaccharide Chain J



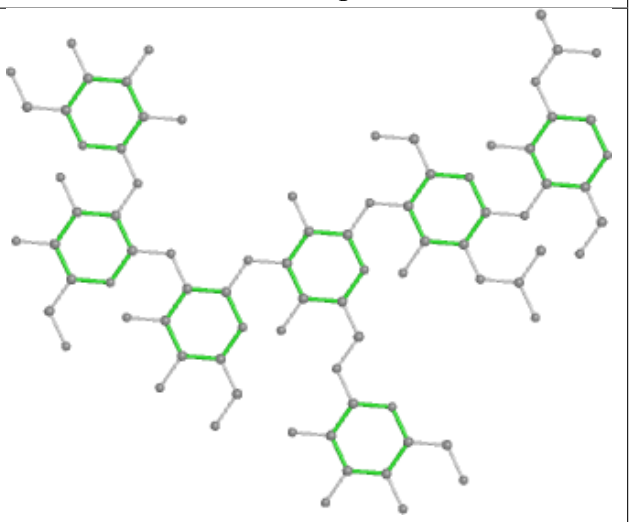
Bond lengths



Bond angles

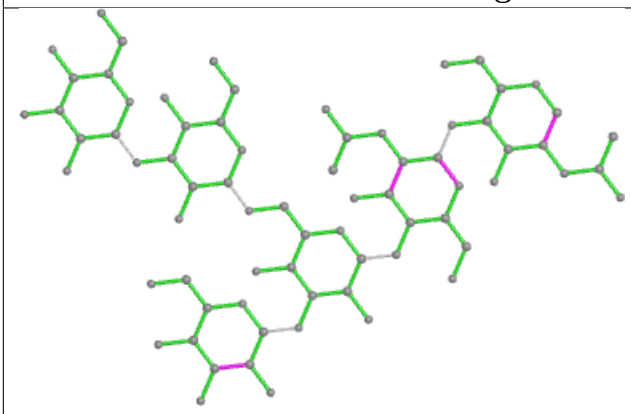


Torsions

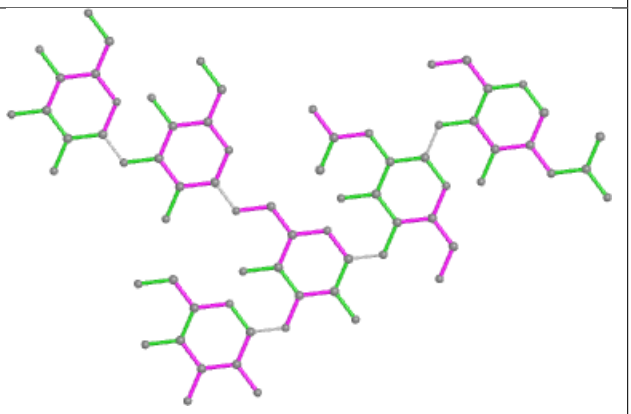


Rings

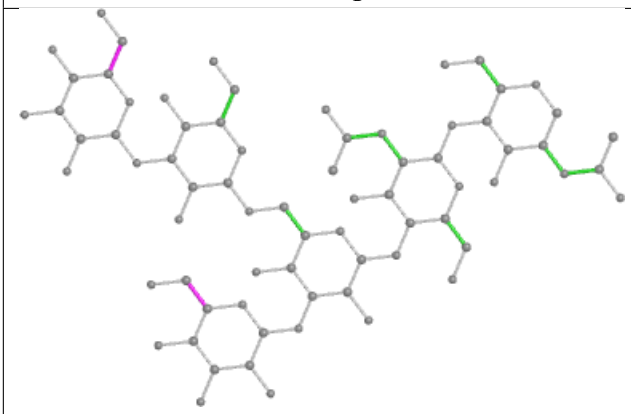
Oligosaccharide Chain K



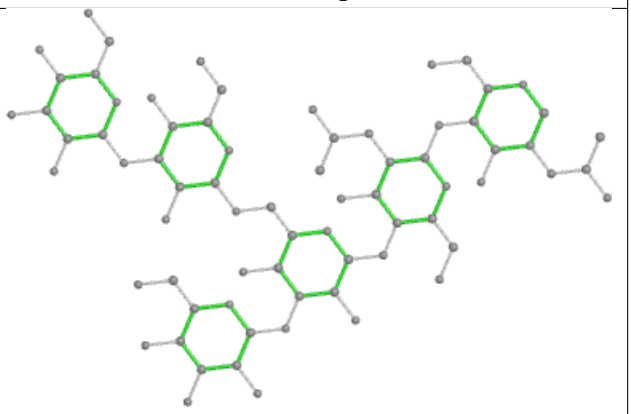
Bond lengths



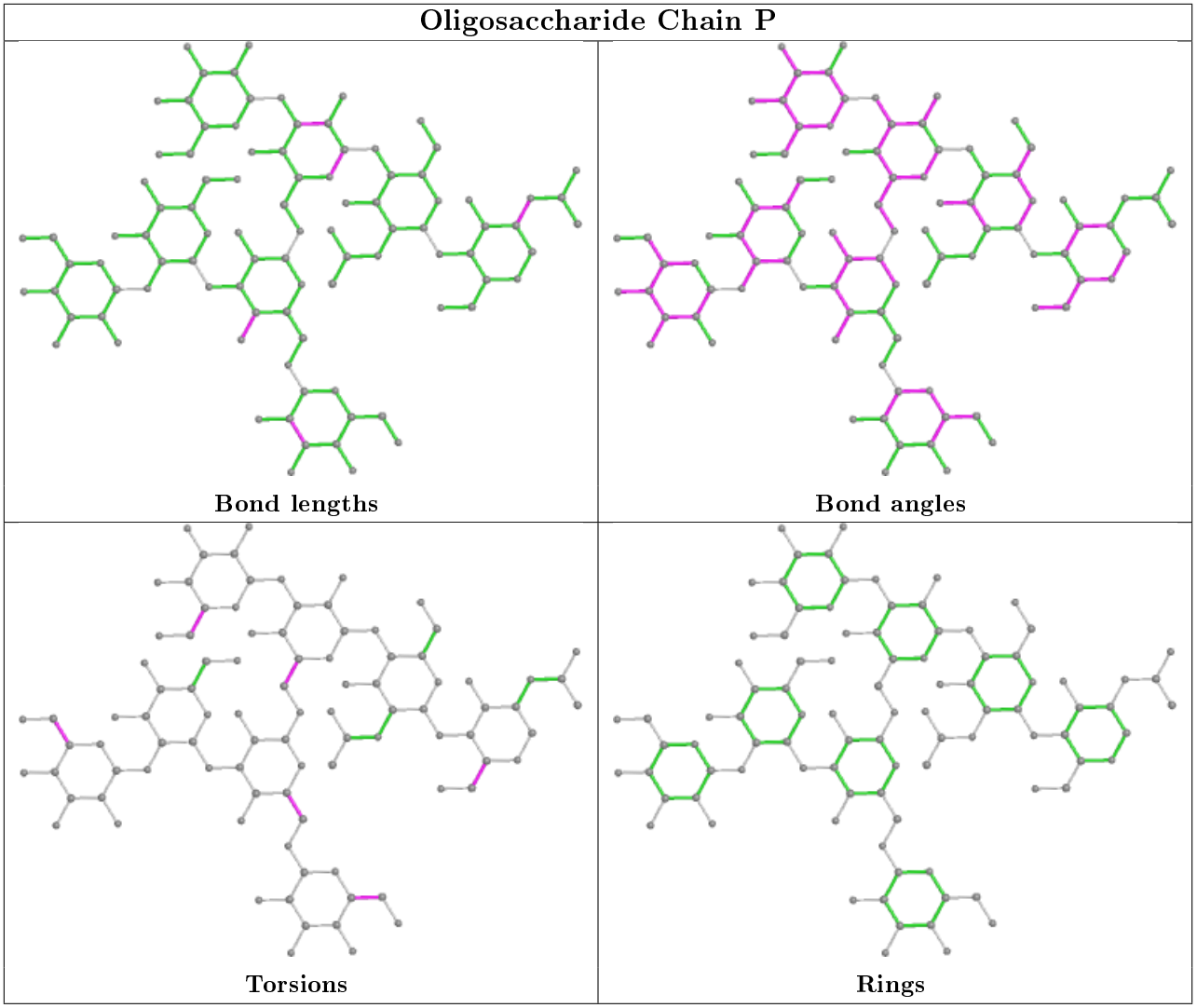
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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	$\#\|Z\| > 2$
12	MRD	B	949	-	7,7,7	0.96	0	9,10,10	1.54	2 (22%)
12	MRD	B	950	-	7,7,7	0.97	1 (14%)	9,10,10	0.96	1 (11%)
11	NAG	A	938	1	14,14,15	0.83	1 (7%)	17,19,21	2.09	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	MRD	A	939	-	7,7,7	1.28	0	9,10,10	0.59	0
14	CGB	B	952	-	12,13,13	3.47	5 (41%)	11,21,21	3.57	8 (72%)
11	NAG	B	946	1	14,14,15	1.04	0	17,19,21	1.99	4 (23%)
11	NAG	A	905	1	14,14,15	0.98	1 (7%)	17,19,21	1.29	2 (11%)
11	NAG	B	947	1	14,14,15	1.06	0	17,19,21	2.06	5 (29%)
14	CGB	A	943	-	12,13,13	3.10	5 (41%)	11,21,21	3.90	9 (81%)
12	MRD	A	941	-	7,7,7	1.22	1 (14%)	9,10,10	1.16	2 (22%)
12	MRD	B	948	-	7,7,7	1.68	1 (14%)	9,10,10	3.14	7 (77%)
11	NAG	B	908	1	14,14,15	0.95	1 (7%)	17,19,21	2.46	7 (41%)
12	MRD	A	940	-	7,7,7	1.40	1 (14%)	9,10,10	1.38	2 (22%)

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
12	MRD	B	949	-	-	3/5/5/5	-
12	MRD	B	950	-	-	1/5/5/5	-
11	NAG	A	938	1	-	0/6/23/26	0/1/1/1
12	MRD	A	939	-	-	1/5/5/5	-
14	CGB	B	952	-	-	-	0/3/2/2
11	NAG	B	946	1	-	0/6/23/26	0/1/1/1
11	NAG	A	905	1	-	0/6/23/26	0/1/1/1
11	NAG	B	947	1	-	2/6/23/26	0/1/1/1
14	CGB	A	943	-	-	-	0/3/2/2
12	MRD	A	941	-	-	0/5/5/5	-
12	MRD	B	948	-	-	0/5/5/5	-
11	NAG	B	908	1	-	6/6/23/26	0/1/1/1
12	MRD	A	940	-	-	1/5/5/5	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	943	CGB	C2-N1	7.42	1.57	1.46
14	B	952	CGB	C2-N1	7.36	1.57	1.46
14	B	952	CGB	C8-C2	-5.92	1.45	1.53
14	A	943	CGB	C8-C2	-5.90	1.45	1.53
14	B	952	CGB	C6-N1	5.20	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	948	MRD	C3-C2	3.41	1.62	1.53
14	B	952	CGB	O4-C4	-3.15	1.35	1.43
14	B	952	CGB	O3-C3	2.84	1.48	1.42
14	A	943	CGB	C4-C3	-2.83	1.48	1.53
14	A	943	CGB	O3-C3	2.71	1.48	1.42
11	A	905	NAG	O5-C1	-2.19	1.40	1.43
12	A	940	MRD	CM-C2	-2.15	1.45	1.52
11	A	938	NAG	O3-C3	-2.14	1.37	1.43
12	B	950	MRD	O2-C2	-2.12	1.39	1.44
11	B	908	NAG	O5-C1	-2.10	1.40	1.43
14	A	943	CGB	C6-N1	2.02	1.49	1.47
12	A	941	MRD	CM-C2	2.02	1.58	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	943	CGB	O4-C4-C5	7.31	127.25	110.35
14	B	952	CGB	O4-C4-C5	5.55	123.18	110.35
14	A	943	CGB	O3-C3-C2	5.12	123.14	109.90
11	B	947	NAG	C1-O5-C5	-5.11	105.27	112.19
11	B	908	NAG	C8-C7-N2	5.07	124.68	116.10
14	A	943	CGB	C8-C2-C3	4.97	118.31	111.11
14	B	952	CGB	C4-C5-C6	-4.91	103.81	111.02
14	B	952	CGB	O3-C3-C2	4.76	122.21	109.90
11	B	946	NAG	O5-C5-C6	4.74	114.64	107.20
11	B	908	NAG	C2-N2-C7	4.55	129.38	122.90
14	B	952	CGB	C8-C2-C3	4.43	117.53	111.11
12	B	948	MRD	O2-C2-C3	-4.39	93.32	109.80
14	B	952	CGB	O4-C4-C3	4.37	118.62	109.73
12	B	948	MRD	O2-C2-C1	4.37	122.11	108.08
14	A	943	CGB	O4-C4-C3	4.07	118.00	109.73
11	A	938	NAG	C2-N2-C7	-3.97	117.24	122.90
11	B	946	NAG	O7-C7-C8	-3.68	115.22	122.06
12	B	948	MRD	O2-C2-CM	3.67	119.85	108.08
12	B	948	MRD	C1-C2-C3	-3.48	93.73	109.96
11	A	938	NAG	C8-C7-N2	3.46	121.95	116.10
11	A	938	NAG	O5-C1-C2	3.41	116.68	111.29
14	A	943	CGB	O5-C5-C6	-3.41	102.42	109.47
11	B	908	NAG	C4-C3-C2	-3.39	106.05	111.02
14	A	943	CGB	C4-C5-C6	-3.36	106.10	111.02
14	B	952	CGB	O3-C3-C4	3.16	117.05	110.03
11	B	908	NAG	O7-C7-N2	-3.13	116.20	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B	908	NAG	O5-C5-C6	3.12	112.10	107.20
11	B	908	NAG	O5-C1-C2	-3.11	106.38	111.29
12	B	949	MRD	O4-C4-C3	-3.06	99.01	111.36
12	B	948	MRD	CM-C2-C3	-2.98	96.10	109.96
11	A	938	NAG	C1-O5-C5	2.93	116.16	112.19
11	B	947	NAG	O5-C5-C6	2.91	111.76	107.20
11	B	946	NAG	O3-C3-C4	-2.83	103.82	110.35
12	B	948	MRD	CM-C2-C1	2.76	116.33	110.57
11	A	905	NAG	C1-C2-N2	2.75	115.19	110.49
12	B	948	MRD	O4-C4-C5	-2.65	97.90	109.38
12	A	940	MRD	O2-C2-C3	-2.65	99.86	109.80
14	A	943	CGB	O3-C3-C4	2.61	115.83	110.03
14	B	952	CGB	C5-C4-C3	2.61	114.89	111.30
11	B	947	NAG	C3-C4-C5	-2.57	105.65	110.24
11	B	947	NAG	O4-C4-C3	-2.57	104.42	110.35
14	A	943	CGB	C7-C6-N1	-2.51	98.60	103.19
12	A	941	MRD	O2-C2-CM	2.49	116.08	108.08
12	B	949	MRD	O2-C2-C1	2.42	115.86	108.08
11	A	938	NAG	O3-C3-C4	-2.31	105.02	110.35
14	A	943	CGB	O5-C5-C4	-2.26	105.13	110.35
12	B	950	MRD	O4-C4-C3	-2.26	102.24	111.36
11	A	938	NAG	O7-C7-N2	-2.22	117.87	121.95
11	A	938	NAG	O6-C6-C5	-2.22	103.68	111.29
14	B	952	CGB	C7-C6-N1	-2.19	99.19	103.19
11	B	947	NAG	O3-C3-C4	-2.14	105.39	110.35
12	A	940	MRD	O4-C4-C3	-2.14	102.72	111.36
11	A	905	NAG	O7-C7-C8	-2.10	118.17	122.06
11	B	946	NAG	C4-C3-C2	2.08	114.07	111.02
12	A	941	MRD	CM-C2-C1	-2.08	106.24	110.57
11	B	908	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	949	MRD	C2-C3-C4-O4
11	B	908	NAG	C8-C7-N2-C2
11	B	908	NAG	O7-C7-N2-C2
11	B	947	NAG	O5-C5-C6-O6
11	B	947	NAG	C4-C5-C6-O6
11	B	908	NAG	C4-C5-C6-O6
11	B	908	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	A	940	MRD	C2-C3-C4-C5
12	B	949	MRD	C1-C2-C3-C4
11	B	908	NAG	C1-C2-N2-C7
11	B	908	NAG	C3-C2-N2-C7
12	B	950	MRD	C2-C3-C4-C5
12	B	949	MRD	C2-C3-C4-C5
12	A	939	MRD	C2-C3-C4-C5

There are no ring outliers.

7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	949	MRD	1	0
12	B	950	MRD	3	0
12	A	939	MRD	2	0
14	B	952	CGB	7	0
14	A	943	CGB	7	0
12	B	948	MRD	1	0
12	A	940	MRD	6	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	834/841 (99%)	-0.53	3 (0%)	92	92	11, 20, 34, 63	0
1	B	832/841 (98%)	-0.70	1 (0%)	95	95	9, 16, 28, 53	0
All	All	1666/1682 (99%)	-0.62	4 (0%)	95	94	9, 17, 31, 63	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	VAL	2.4
1	A	148	LEU	2.4
1	B	860	GLN	2.2
1	A	699	GLY	2.0

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
9	MAN	K	6	11/12	0.47	0.30	57,62,68,68	0
3	BMA	G	3	11/12	0.64	0.32	46,60,73,77	0
6	MAN	O	7	11/12	0.71	0.29	62,71,74,79	0
10	MAN	P	8	11/12	0.79	0.25	58,71,82,84	0
7	MAN	I	7	11/12	0.79	0.21	50,54,60,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	MAN	P	6	11/12	0.80	0.26	49,52,56,61	0
10	MAN	P	7	11/12	0.81	0.22	47,56,66,68	0
3	BMA	L	3	11/12	0.82	0.28	55,65,76,80	0
3	BMA	D	3	11/12	0.84	0.23	42,48,57,62	0
6	MAN	H	7	11/12	0.84	0.34	54,60,65,69	0
3	BMA	N	3	11/12	0.86	0.19	43,52,60,62	0
9	MAN	K	5	11/12	0.86	0.31	68,74,76,85	0
10	BMA	P	3	11/12	0.86	0.19	37,41,54,60	0
2	BMA	C	3	11/12	0.86	0.12	36,44,48,53	0
9	MAN	K	4	11/12	0.86	0.25	56,66,70,70	0
7	MAN	I	6	11/12	0.86	0.26	54,58,62,66	0
7	BMA	I	3	11/12	0.86	0.13	30,41,52,63	0
3	NAG	G	2	14/15	0.88	0.20	42,50,61,69	0
2	MAN	C	4	11/12	0.90	0.18	45,52,65,71	0
5	MAN	M	10	11/12	0.90	0.10	30,37,41,42	0
10	MAN	P	4	11/12	0.91	0.17	31,34,43,48	0
8	MAN	J	7	11/12	0.92	0.09	27,31,36,38	0
6	NAG	H	2	14/15	0.93	0.15	20,26,32,40	0
3	NAG	D	2	14/15	0.93	0.12	25,29,34,37	0
6	BMA	H	3	11/12	0.93	0.19	23,27,34,43	0
5	MAN	F	6	11/12	0.93	0.14	33,38,43,44	0
9	BMA	K	3	11/12	0.93	0.16	40,44,54,60	0
6	BMA	O	3	11/12	0.93	0.14	23,27,34,46	0
6	MAN	H	4	11/12	0.93	0.14	27,30,40,43	0
7	MAN	I	4	11/12	0.94	0.09	24,30,38,45	0
5	MAN	F	10	11/12	0.94	0.13	39,40,50,51	0
5	MAN	M	6	11/12	0.94	0.09	24,29,33,36	0
10	MAN	P	5	11/12	0.95	0.13	28,35,42,47	0
6	NAG	O	2	14/15	0.95	0.10	19,24,32,33	0
5	MAN	F	5	11/12	0.95	0.07	23,30,33,42	0
8	MAN	J	6	11/12	0.95	0.11	26,30,35,42	0
6	NAG	O	1	14/15	0.95	0.10	16,21,36,38	0
8	MAN	J	5	11/12	0.95	0.13	28,34,42,49	0
7	MAN	I	5	11/12	0.95	0.11	28,34,44,44	0
6	MAN	H	5	11/12	0.95	0.12	21,24,34,41	0
6	NAG	H	1	14/15	0.95	0.13	20,22,41,47	0
7	NAG	I	2	14/15	0.95	0.10	23,27,36,42	0
3	NAG	N	2	14/15	0.95	0.15	31,33,46,48	0
10	NAG	P	2	14/15	0.95	0.12	26,30,37,39	0
3	NAG	L	2	14/15	0.95	0.10	19,26,41,45	0
5	MAN	F	7	11/12	0.96	0.06	20,22,25,26	0
9	NAG	K	2	14/15	0.96	0.07	20,27,31,35	0

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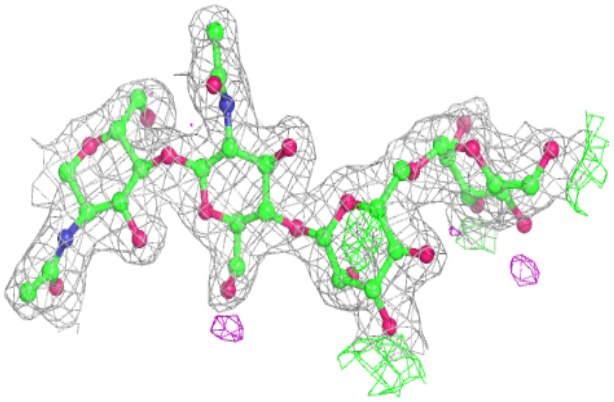
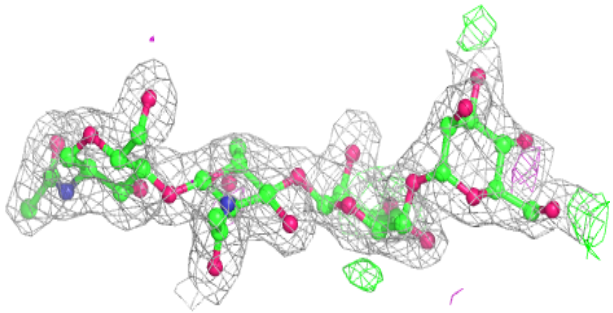
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	O	4	11/12	0.96	0.10	25,27,37,39	0
3	NAG	D	1	14/15	0.96	0.07	22,25,27,27	0
8	BMA	J	3	11/12	0.96	0.06	20,24,26,27	0
2	NAG	C	2	14/15	0.96	0.08	24,32,43,48	0
5	BMA	F	3	11/12	0.96	0.08	24,26,29,32	0
7	NAG	I	1	14/15	0.96	0.06	21,23,25,26	0
5	NAG	F	1	14/15	0.96	0.09	26,28,33,35	0
5	MAN	F	9	11/12	0.96	0.11	27,31,34,36	0
4	NAG	E	2	14/15	0.96	0.09	30,33,48,53	0
9	NAG	K	1	14/15	0.96	0.06	17,20,22,24	0
2	NAG	C	1	14/15	0.97	0.07	17,23,26,27	0
6	MAN	O	6	11/12	0.97	0.09	20,24,30,34	0
5	MAN	F	4	11/12	0.97	0.06	20,24,26,28	0
6	MAN	H	6	11/12	0.97	0.13	21,24,37,43	0
10	NAG	P	1	14/15	0.97	0.07	19,21,23,24	0
8	MAN	J	4	11/12	0.97	0.11	27,32,39,43	0
5	NAG	M	1	14/15	0.97	0.06	16,17,24,24	0
3	NAG	G	1	14/15	0.97	0.07	25,29,36,38	0
5	MAN	M	5	11/12	0.97	0.06	18,22,25,33	0
5	NAG	F	2	14/15	0.97	0.07	21,23,27,27	0
5	NAG	M	2	14/15	0.97	0.07	12,16,18,18	0
3	NAG	N	1	14/15	0.97	0.05	22,28,32,33	0
8	NAG	J	1	14/15	0.98	0.06	14,16,18,19	0
3	NAG	L	1	14/15	0.98	0.06	13,17,21,21	0
8	NAG	J	2	14/15	0.98	0.05	15,18,23,29	0
5	BMA	M	3	11/12	0.98	0.05	17,18,19,20	0
5	MAN	M	7	11/12	0.98	0.07	16,18,18,19	0
5	MAN	F	8	11/12	0.98	0.06	23,24,26,26	0
6	MAN	O	5	11/12	0.98	0.09	21,22,29,34	0
5	MAN	M	8	11/12	0.98	0.06	17,19,20,24	0
5	MAN	M	9	11/12	0.98	0.06	19,21,25,29	0
4	NAG	E	1	14/15	0.98	0.06	19,23,27,28	0
5	MAN	M	4	11/12	0.99	0.07	16,18,19,19	0

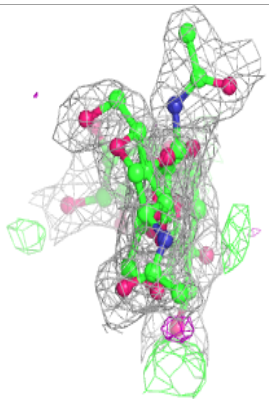
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

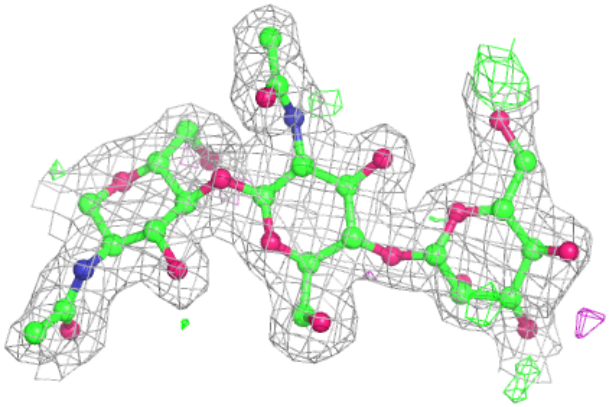


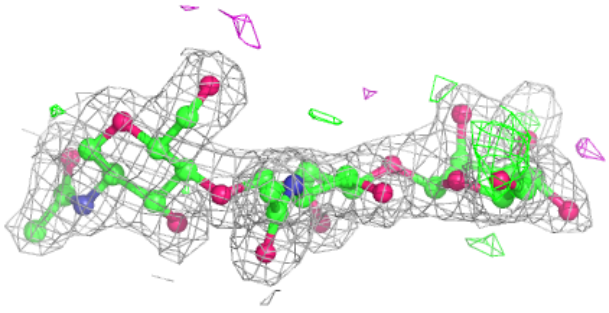


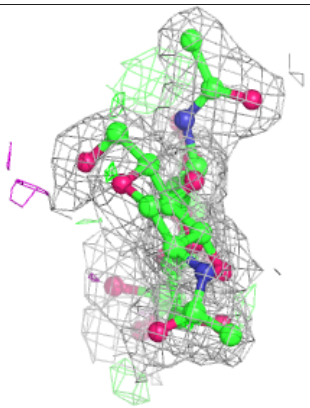


Electron density around Chain D:

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

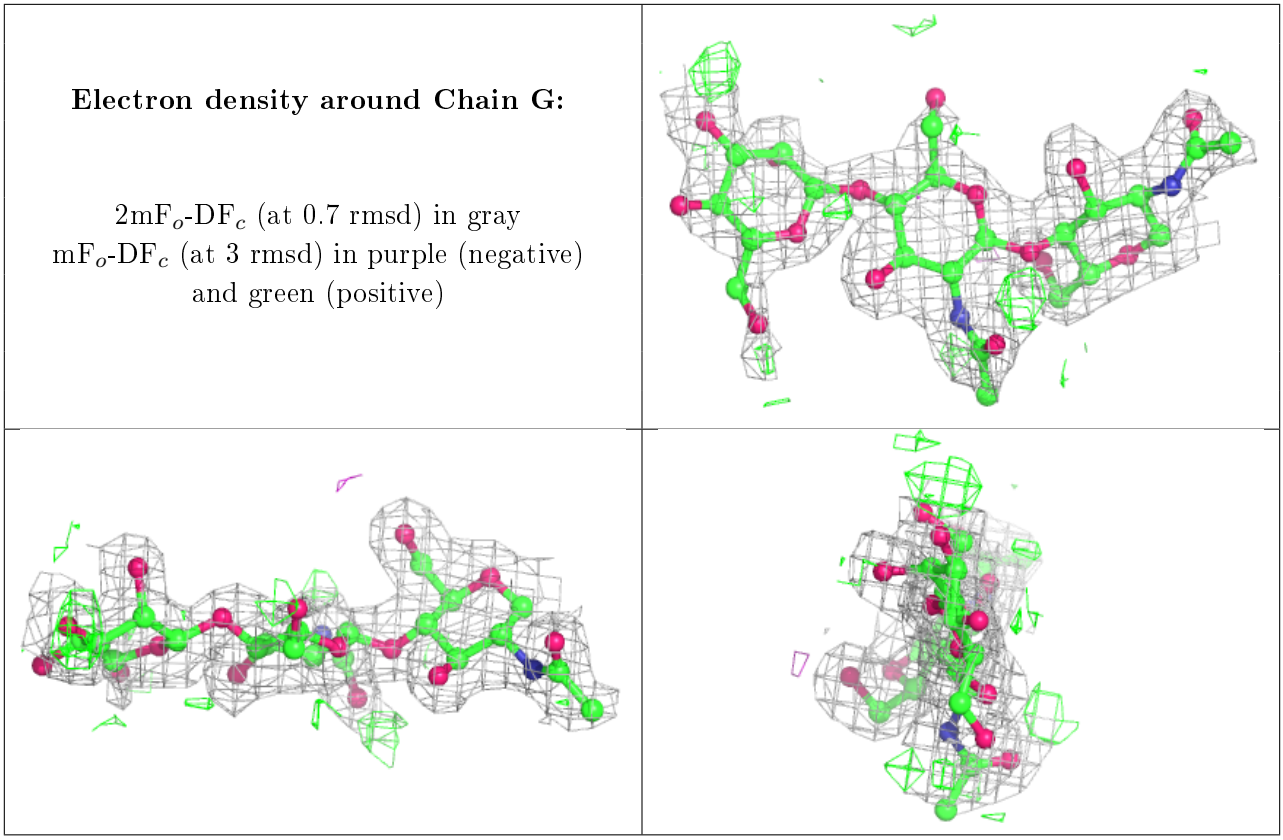






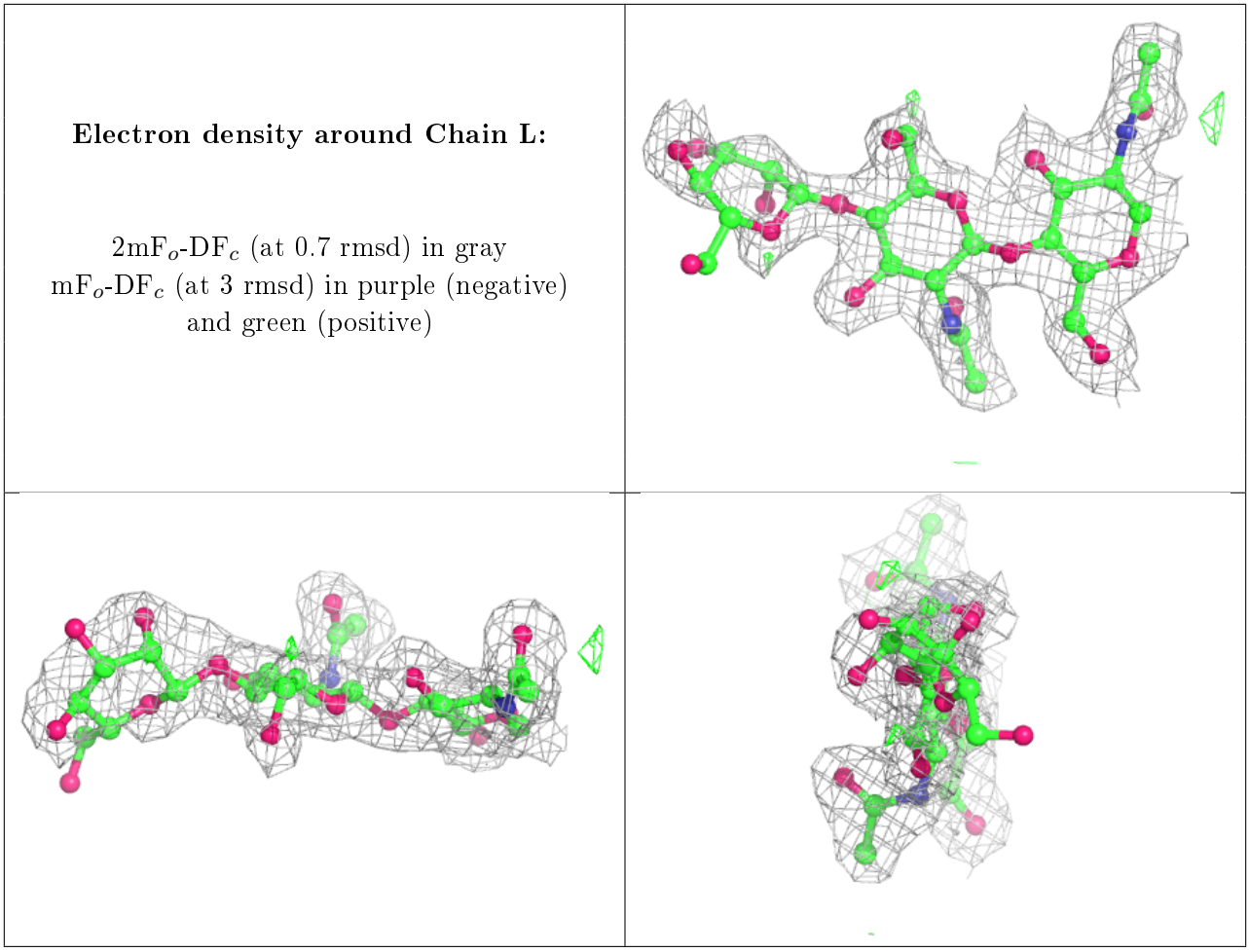
Electron density around Chain G:

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



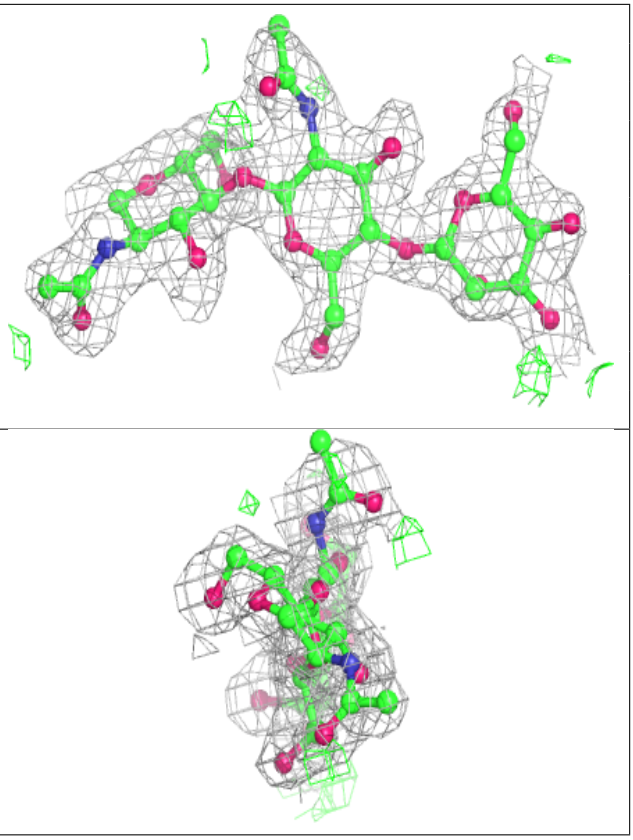
Electron density around Chain L:

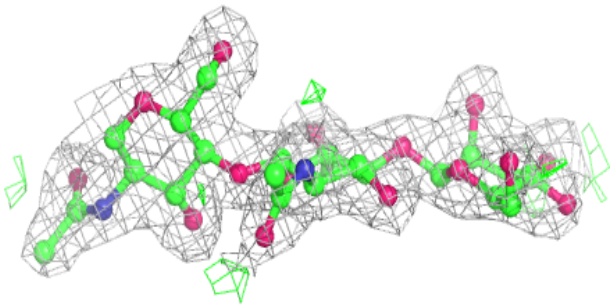
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain N:

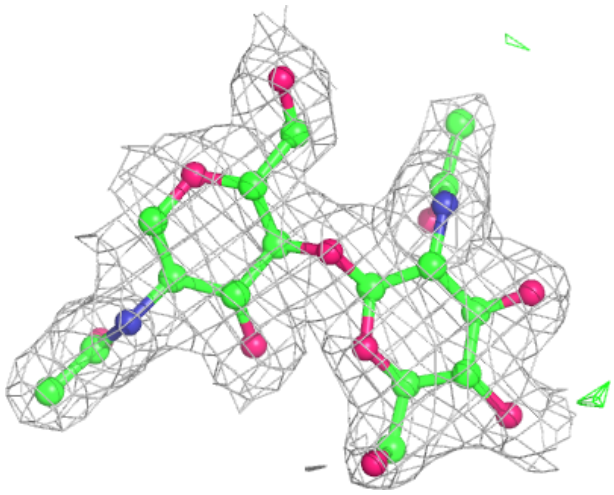
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

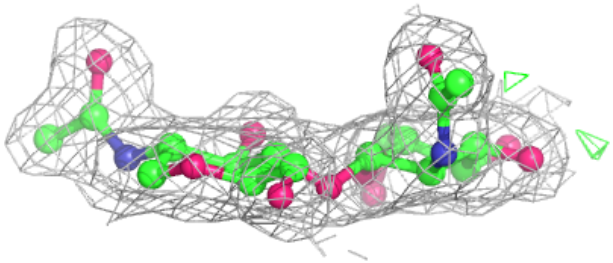


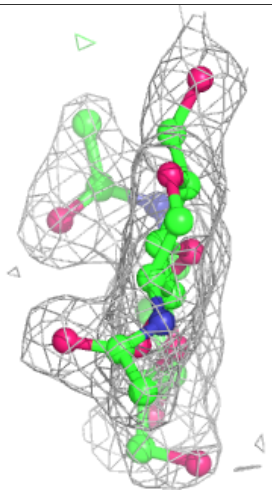


Electron density around Chain E:

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

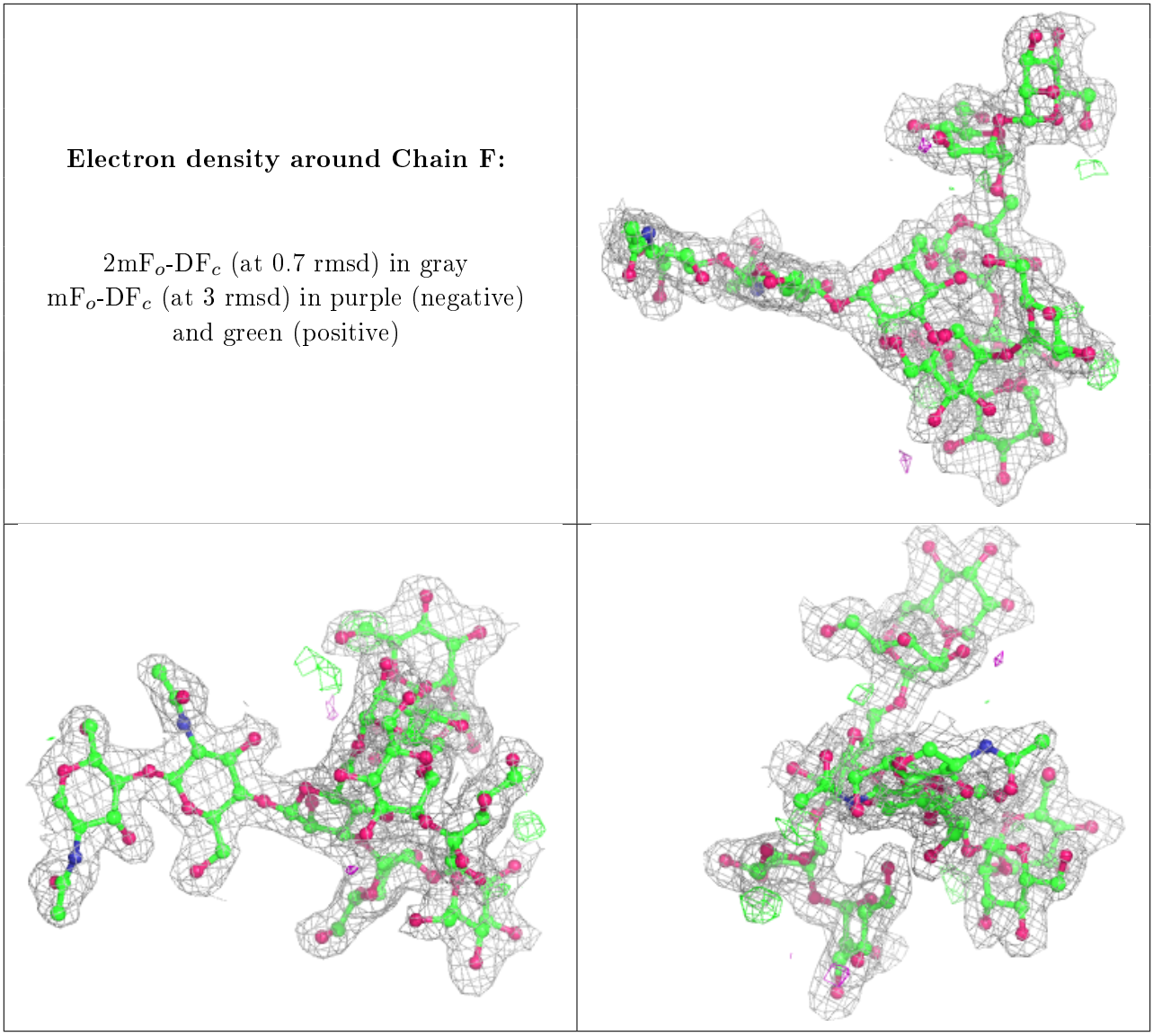






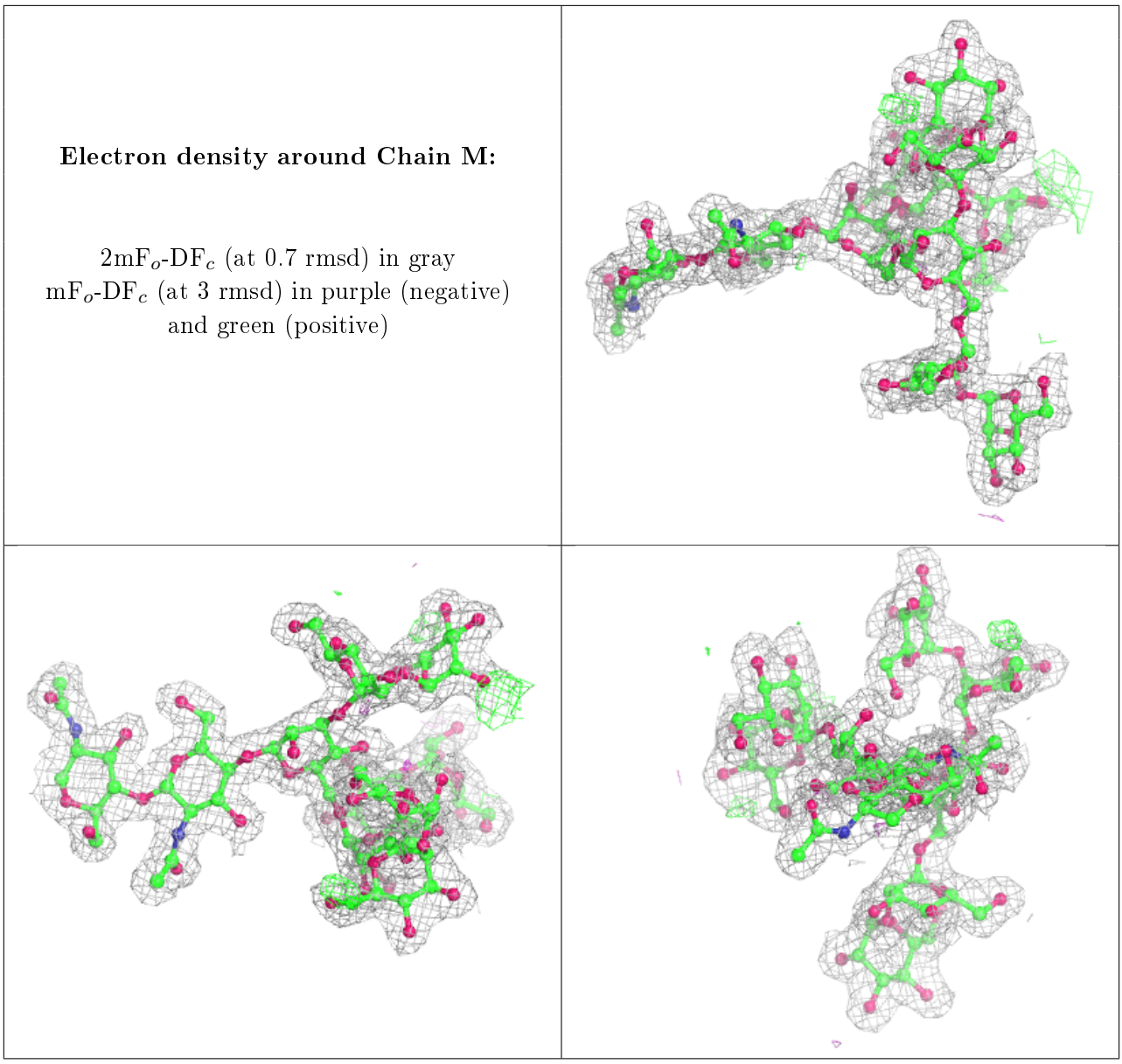
Electron density around Chain F:

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



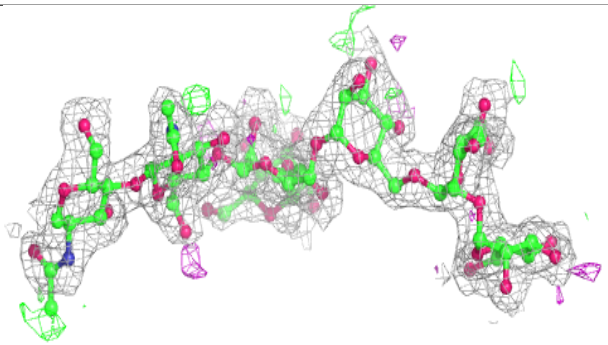
Electron density around Chain M:

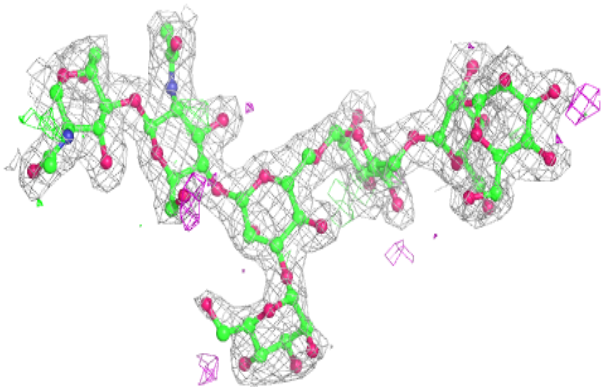
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

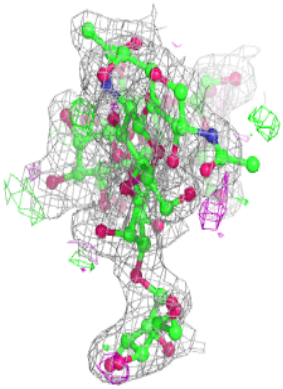


Electron density around Chain H:

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

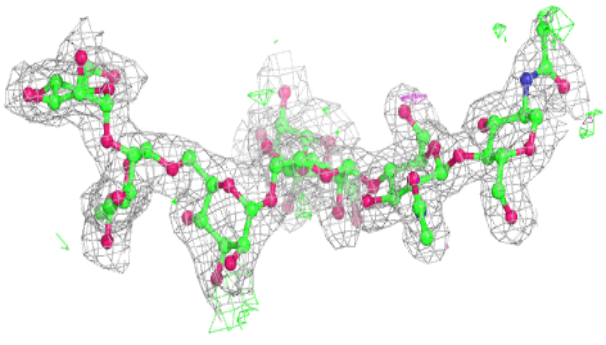


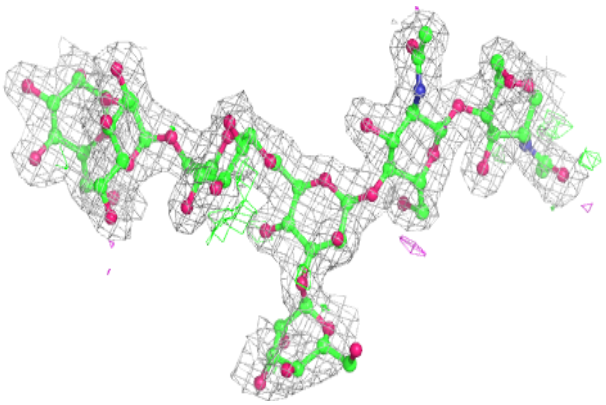


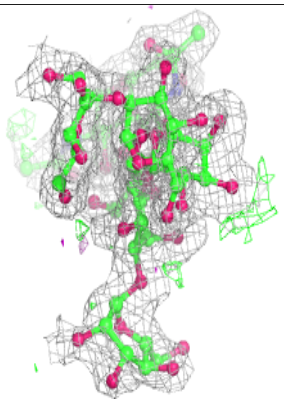


Electron density around Chain O:

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

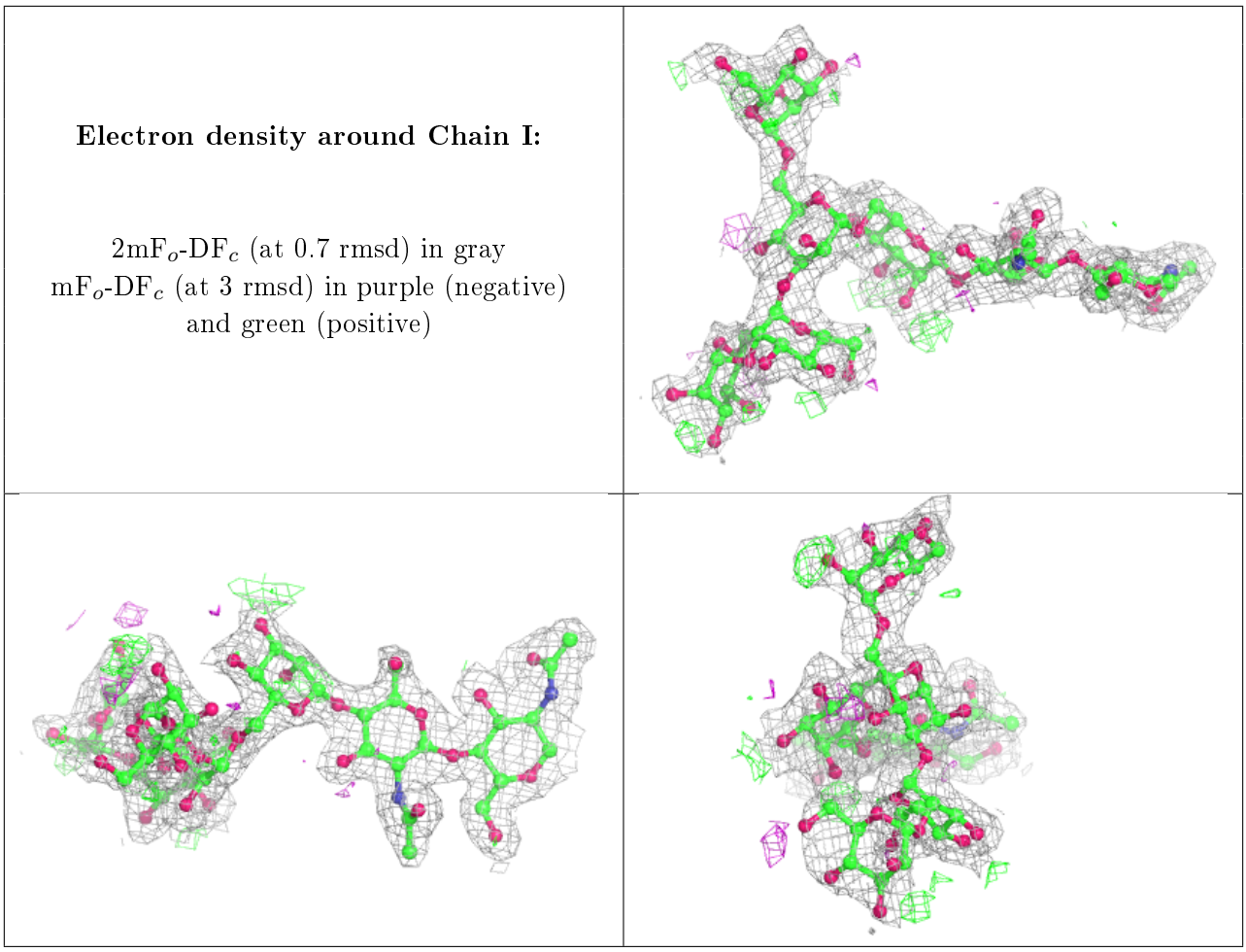






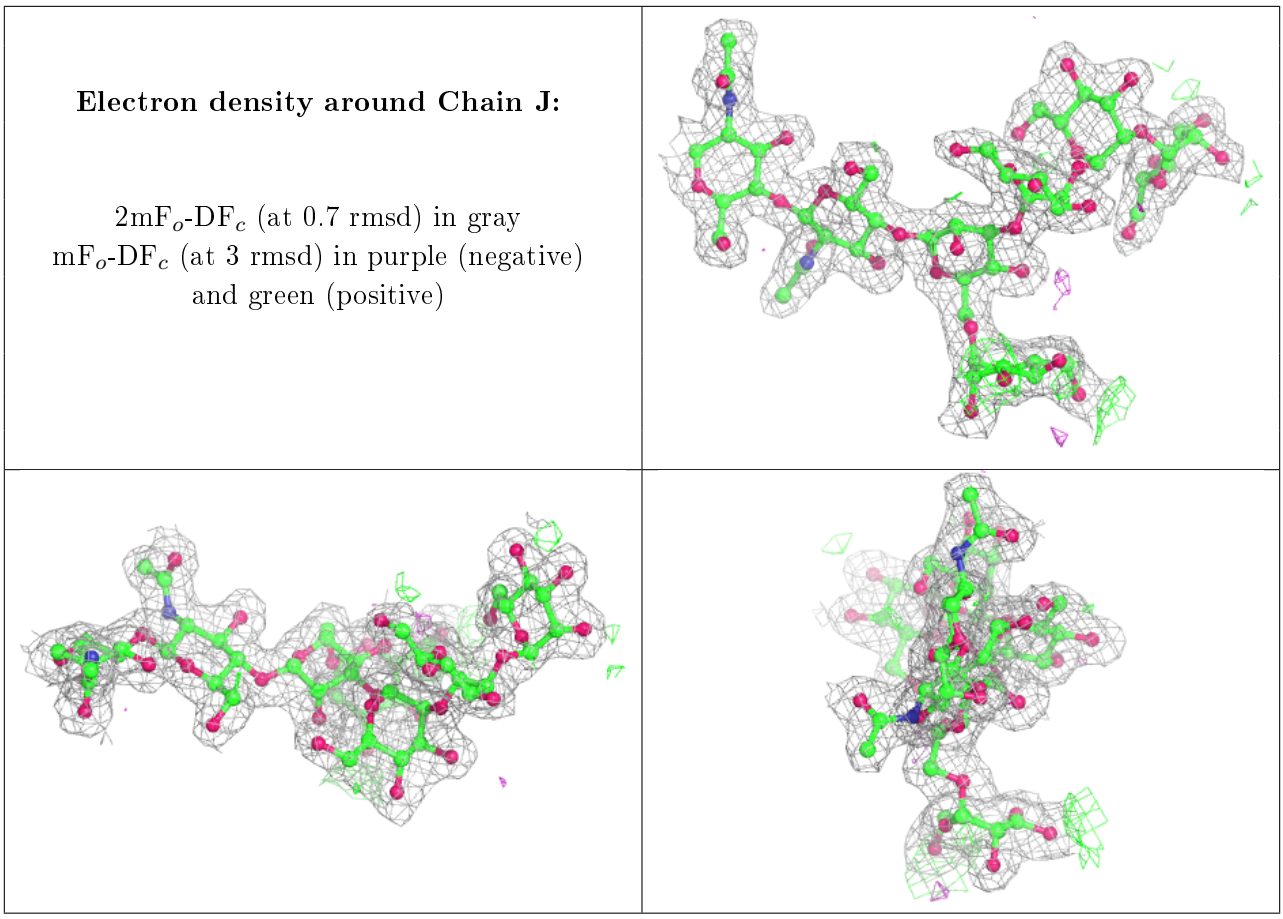
Electron density around Chain I:

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



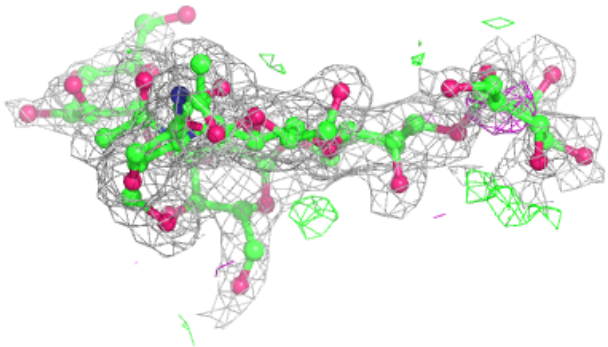
Electron density around Chain J:

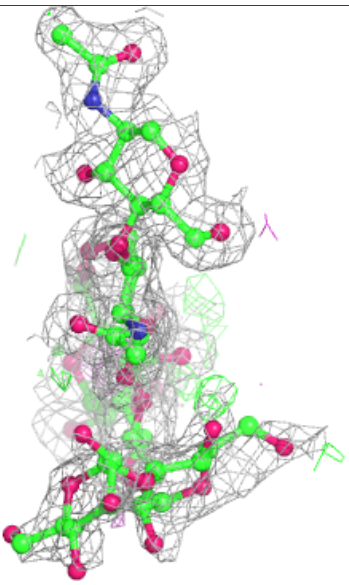
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain K:

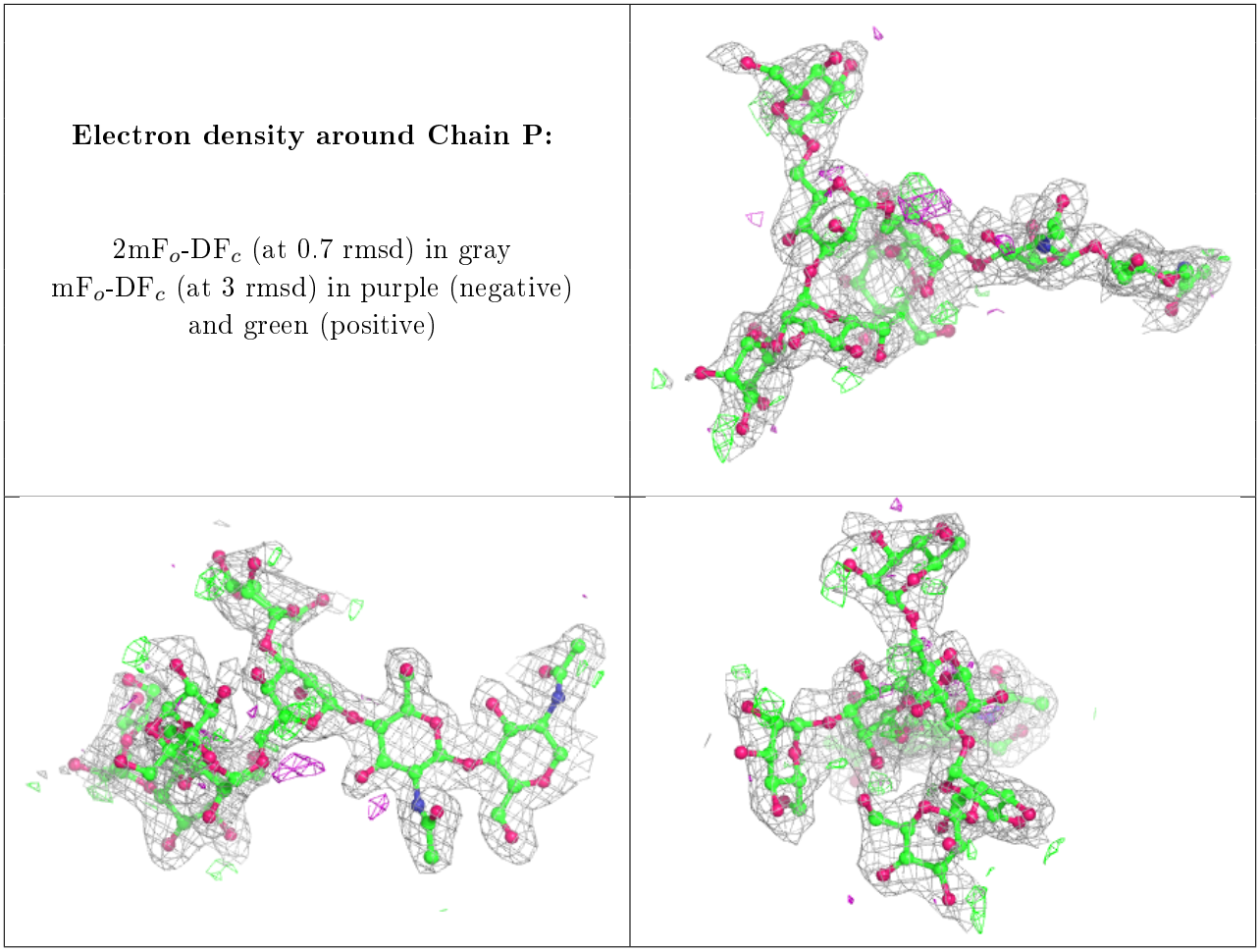
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around Chain P:

$2mF_o$-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
12	MRD	A	941	8/8	0.76	0.24	34,40,45,47	0
11	NAG	A	905	14/15	0.83	0.33	51,58,69,75	0
12	MRD	B	948	8/8	0.83	0.19	31,44,52,53	0
11	NAG	B	908	14/15	0.84	0.31	43,53,59,63	0
12	MRD	A	940	8/8	0.85	0.20	21,29,41,43	0
13	NA	B	951	1/1	0.90	0.11	32,32,32,32	0
14	CGB	A	943	12/12	0.91	0.21	21,28,33,34	0
11	NAG	B	946	14/15	0.91	0.24	38,50,53,55	0
12	MRD	B	949	8/8	0.94	0.10	21,28,35,39	0
12	MRD	B	950	8/8	0.94	0.13	33,43,45,48	0
14	CGB	B	952	12/12	0.95	0.16	15,23,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	A	938	14/15	0.95	0.13	33,42,49,50	0
12	MRD	A	939	8/8	0.96	0.07	20,25,29,31	0
13	NA	A	942	1/1	0.96	0.13	29,29,29,29	0
11	NAG	B	947	14/15	0.96	0.17	25,31,36,38	0

6.5 Other polymers

There are no such residues in this entry.