Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 06:07 pm GMT

PDB ID	:	6ZPW
Title	:	Structure of Unliganded MgGH51 a-L-Arabinofuranosidase Crystal Type 2
Authors	:	McGregor, N.G.S.; Davies, G.J.
Deposited on	:	2020-07-09
Resolution	:	1.33 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 (i) symbol.

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

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

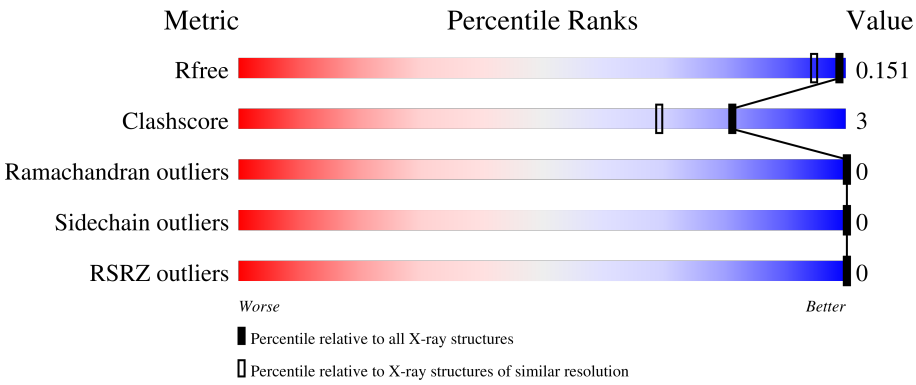
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.33 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	1611 (1.34-1.30)
Clashscore	141614	1667 (1.34-1.30)
Ramachandran outliers	138981	1615 (1.34-1.30)
Sidechain outliers	138945	1615 (1.34-1.30)
RSRZ outliers	127900	1580 (1.34-1.30)

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	AAA	627	95% 5%
2	A	4	100%
3	B	2	100%
3	C	2	100%
3	D	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	AAA	729	-	-	X	-
6	ACT	AAA	715	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10650 atoms, of which 4843 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 MgGH51.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	AAA	627	9535	3108	4678	803	939	7	313	15	0

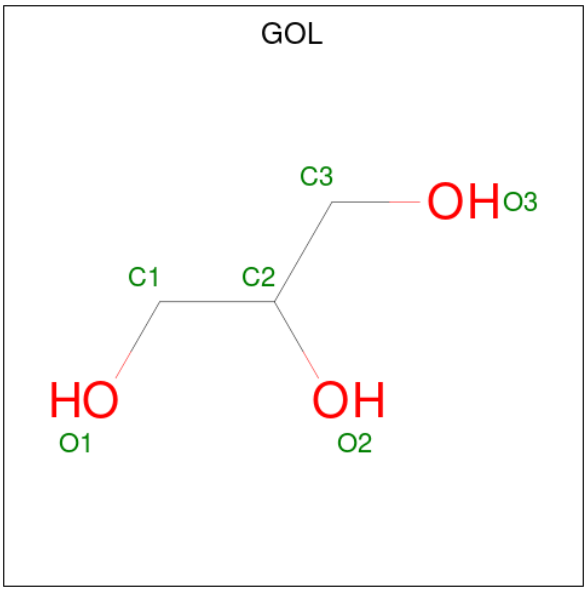
- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	A	4	98	28	48	2	20	11	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

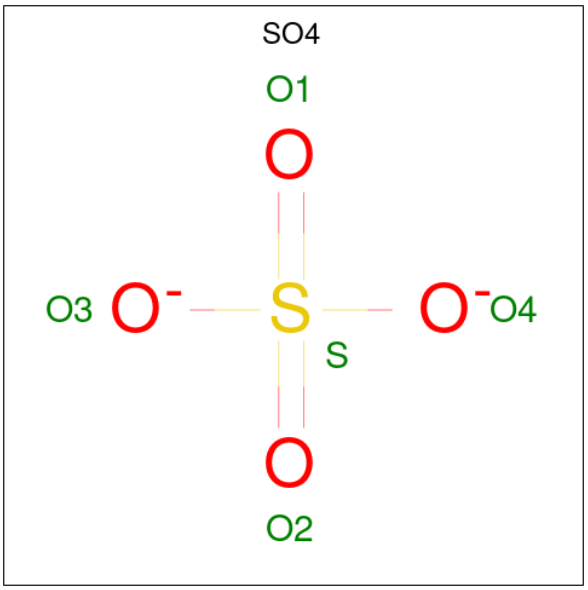
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	B	2	55	16	27	2	10	5	0	0
3	C	2	55	16	27	2	10	5	0	0
3	D	2	55	16	27	2	10	5	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	AAA	1	14	3	8	3	2	0
			Total	C	H	O		
4	AAA	1	14	3	8	3	2	0
			Total	C	H	O		
4	AAA	1	14	3	8	3	2	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



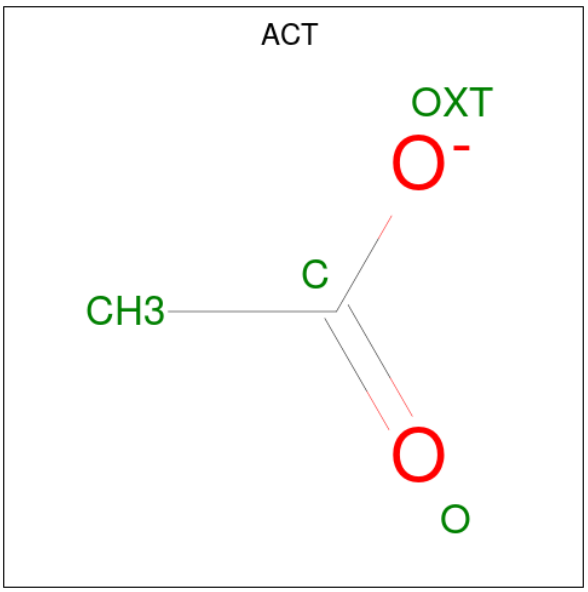
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	AAA	1	5	4	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0
5	AAA	1	Total O S 5 4 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	AAA	1	7	2	3	2	0	0
6	AAA	1	7	2	3	2	0	0
6	AAA	1	7	2	3	2	0	0
6	AAA	1	7	2	3	2	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	AAA	1	1	1	0	0

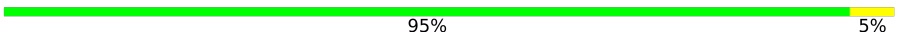
- Molecule 8 is water.

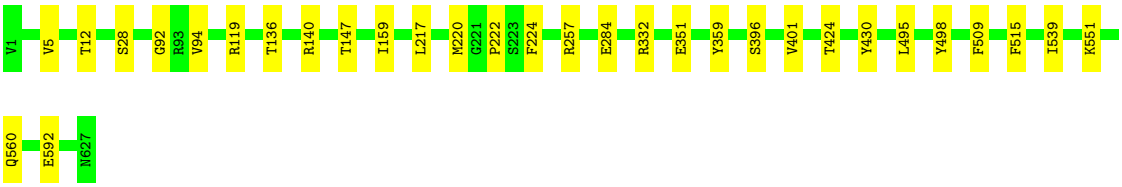
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	AAA	719	721	721	0	2

3 Residue-property plots (i)

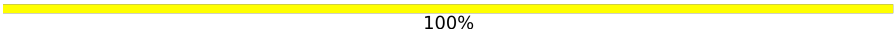
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: MgGH51

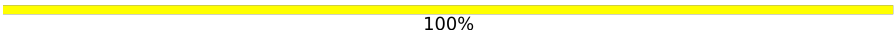
Chain AAA: 



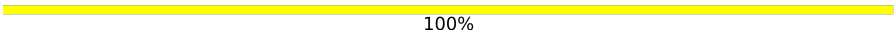
• Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 

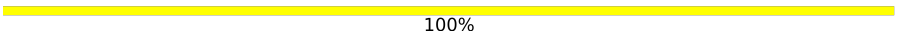
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 

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

Chain C: 

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

Chain D: 

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	114.95Å 125.84Å 161.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.74 – 1.33 80.61 – 1.33	Depositor EDS
% Data completeness (in resolution range)	99.8 (80.74-1.33) 99.9 (80.61-1.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.33Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.130 , 0.151 0.131 , 0.151	Depositor DCC
R_{free} test set	13118 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	10650	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, BMA, CL, GOL, ACT, 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	AAA	0.68	1/5030 (0.0%)	0.87	3/6887 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	592	GLU	CD-OE1	5.81	1.32	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	332	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	AAA	332	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	AAA	257	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	359	TYR	Sidechain

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	AAA	4857	4678	4672	23	1
2	A	50	48	43	0	0
3	B	28	27	25	0	0
3	C	28	27	25	0	0
3	D	28	27	25	0	0
4	AAA	18	24	24	3	0
5	AAA	60	0	0	4	0
6	AAA	16	12	12	2	0
7	AAA	1	0	0	0	0
8	AAA	721	0	0	4	0
All	All	5807	4843	4826	26	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (26) 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:AAA:560:GLN:HE22	6:AAA:715:ACT:H2	1.06	1.09
1:AAA:560:GLN:NE2	6:AAA:715:ACT:H2	1.91	0.81
1:AAA:94[A]:VAL:HG21	8:AAA:855:HOH:O	1.82	0.80
1:AAA:119:ARG:NH1	8:AAA:801:HOH:O	2.17	0.78
1:AAA:94[A]:VAL:CG2	8:AAA:855:HOH:O	2.37	0.69
1:AAA:136:THR:HG21	5:AAA:729:SO4:O1	1.94	0.68
1:AAA:220[B]:MET:HE1	1:AAA:495:LEU:HD21	1.73	0.68
1:AAA:140:ARG:NE	5:AAA:729:SO4:O1	2.39	0.56
1:AAA:220[B]:MET:HE1	1:AAA:495:LEU:CD2	2.37	0.55
1:AAA:220[A]:MET:HG2	1:AAA:509:PHE:CE1	2.44	0.52
1:AAA:515:PHE:CD2	1:AAA:551:LYS:HE3	2.47	0.49
1:AAA:220[A]:MET:HB2	1:AAA:222:PRO:HD3	1.95	0.49
1:AAA:217:LEU:O	1:AAA:220[A]:MET:HG3	2.13	0.48
1:AAA:140:ARG:HB3	5:AAA:729:SO4:O1	2.14	0.48
4:AAA:705:GOL:H12	4:AAA:720:GOL:O1	2.14	0.47
1:AAA:220[A]:MET:HE3	1:AAA:495:LEU:HD21	1.96	0.47
1:AAA:396:SER:HA	1:AAA:424:THR:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AAA:705:GOL:H12	4:AAA:720:GOL:HO1	1.81	0.46
5:AAA:729:SO4:O4	8:AAA:802:HOH:O	2.21	0.45
1:AAA:5:VAL:HG22	1:AAA:539:ILE:HD13	1.99	0.45
1:AAA:147:THR:HG21	1:AAA:159[B]:ILE:HD12	1.99	0.45
1:AAA:401:VAL:O	1:AAA:430:TYR:HA	2.17	0.44
1:AAA:220[B]:MET:HG2	1:AAA:220[B]:MET:O	2.17	0.44
1:AAA:224:PHE:HA	1:AAA:284:GLU:O	2.19	0.42
1:AAA:351:GLU:OE1	4:AAA:720:GOL:H11	2.20	0.41
1:AAA:28:SER:HA	1:AAA:498:TYR:OH	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:12:THR:HG1	1:AAA:92:GLY:H[7_544]	1.23	0.37

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	AAA	640/627 (102%)	628 (98%)	12 (2%)	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	AAA	522/510 (102%)	522 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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)

10 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	A	1	2,1	14,14,15	0.76	0	17,19,21	1.28	2 (11%)
2	NAG	A	2	2	14,14,15	1.02	1 (7%)	17,19,21	1.21	2 (11%)
2	BMA	A	3	2	11,11,12	2.31	4 (36%)	15,15,17	4.58	11 (73%)
2	MAN	A	4	2	11,11,12	2.88	7 (63%)	15,15,17	3.84	8 (53%)
3	NAG	B	1	3,1	14,14,15	1.02	1 (7%)	17,19,21	1.00	1 (5%)
3	NAG	B	2	3	14,14,15	1.25	2 (14%)	17,19,21	1.27	2 (11%)
3	NAG	C	1	3,1	14,14,15	0.97	0	17,19,21	1.05	2 (11%)
3	NAG	C	2	3	14,14,15	0.99	1 (7%)	17,19,21	1.01	0
3	NAG	D	1	3,1	14,14,15	0.85	0	17,19,21	1.21	2 (11%)
3	NAG	D	2	3	14,14,15	0.56	0	17,19,21	0.90	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	BMA	A	3	2	-	0/2/19/22	0/1/1/1
2	MAN	A	4	2	-	2/2/19/22	0/1/1/1
3	NAG	B	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	BMA	O3-C3	5.25	1.55	1.43
2	A	4	MAN	C4-C3	4.74	1.64	1.52
2	A	4	MAN	O3-C3	4.14	1.52	1.43
2	A	4	MAN	O5-C5	3.62	1.50	1.43
2	A	4	MAN	C4-C5	3.45	1.60	1.53
2	A	4	MAN	C6-C5	3.06	1.62	1.51
2	A	3	BMA	C4-C3	2.98	1.59	1.52
2	A	3	BMA	C2-C3	2.72	1.56	1.52
3	C	2	NAG	O4-C4	2.64	1.49	1.43
2	A	4	MAN	C1-C2	2.63	1.58	1.52
2	A	4	MAN	C2-C3	-2.56	1.48	1.52
3	B	2	NAG	C2-N2	-2.56	1.41	1.46
3	B	2	NAG	O7-C7	-2.49	1.17	1.23
3	B	1	NAG	O5-C1	-2.47	1.39	1.43
2	A	2	NAG	C3-C2	-2.21	1.47	1.52
2	A	3	BMA	C4-C5	2.03	1.57	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3	BMA	C2-C3-C4	-9.41	94.60	110.89
2	A	4	MAN	O5-C1-C2	-9.40	96.25	110.77
2	A	3	BMA	O3-C3-C4	8.53	130.07	110.35
2	A	3	BMA	C1-C2-C3	5.79	116.79	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3	BMA	O6-C6-C5	5.72	130.90	111.29
2	A	4	MAN	C3-C4-C5	5.60	120.22	110.24
2	A	4	MAN	C2-C3-C4	-5.40	101.54	110.89
2	A	4	MAN	C6-C5-C4	4.81	124.28	113.00
2	A	4	MAN	O5-C5-C4	-4.13	100.78	110.83
2	A	3	BMA	C3-C4-C5	4.11	117.58	110.24
2	A	3	BMA	O4-C4-C5	-3.99	99.39	109.30
2	A	3	BMA	O2-C2-C1	-3.75	101.48	109.15
2	A	3	BMA	C1-O5-C5	-3.54	107.39	112.19
3	B	2	NAG	C2-N2-C7	3.30	127.60	122.90
2	A	1	NAG	C1-C2-N2	-3.28	104.88	110.49
2	A	4	MAN	O3-C3-C2	3.16	116.04	109.99
2	A	3	BMA	O2-C2-C3	3.05	116.24	110.14
2	A	3	BMA	C6-C5-C4	2.87	119.72	113.00
2	A	4	MAN	O2-C2-C1	2.76	114.80	109.15
3	B	1	NAG	C6-C5-C4	2.58	119.06	113.00
2	A	4	MAN	O6-C6-C5	-2.46	102.83	111.29
2	A	2	NAG	C2-N2-C7	2.45	126.39	122.90
3	C	1	NAG	O5-C1-C2	-2.43	107.45	111.29
3	C	1	NAG	C8-C7-N2	2.29	119.97	116.10
3	D	1	NAG	C1-O5-C5	2.25	115.24	112.19
2	A	1	NAG	C6-C5-C4	2.23	118.24	113.00
3	B	2	NAG	C1-O5-C5	2.17	115.13	112.19
2	A	3	BMA	O3-C3-C2	2.17	114.15	109.99
2	A	2	NAG	C3-C4-C5	2.10	113.99	110.24
3	D	2	NAG	O5-C5-C6	2.08	110.47	107.20
3	D	1	NAG	C4-C3-C2	2.02	113.97	111.02

There are no chirality outliers.

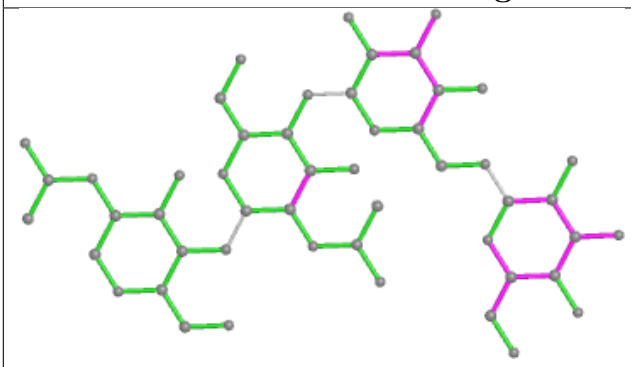
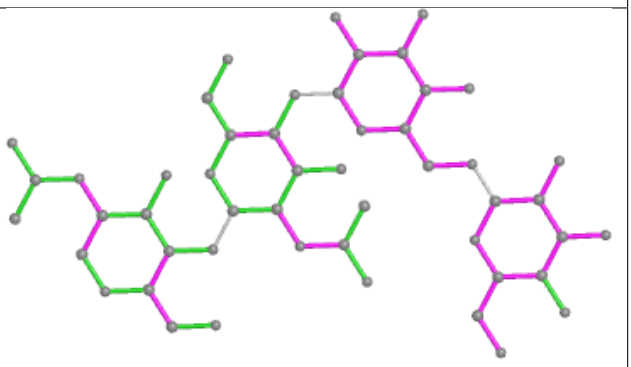
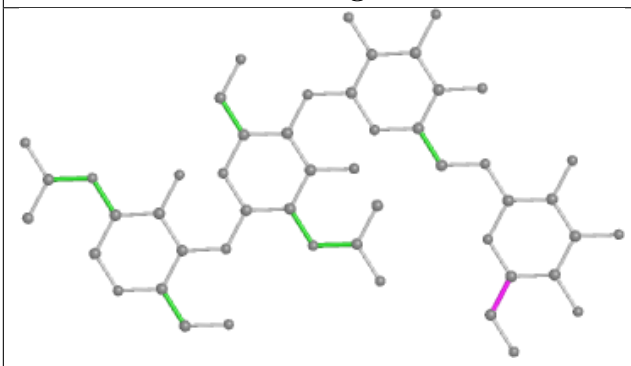
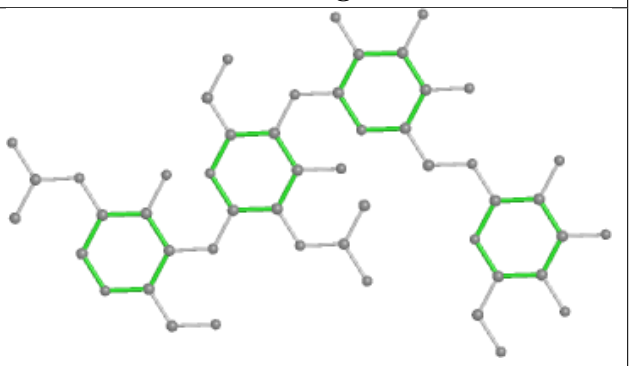
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4	MAN	O5-C5-C6-O6
2	A	4	MAN	C4-C5-C6-O6

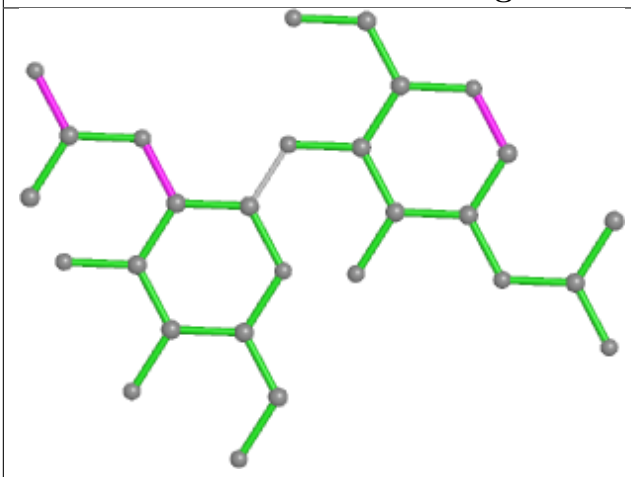
There are no ring outliers.

No monomer is involved in short contacts.

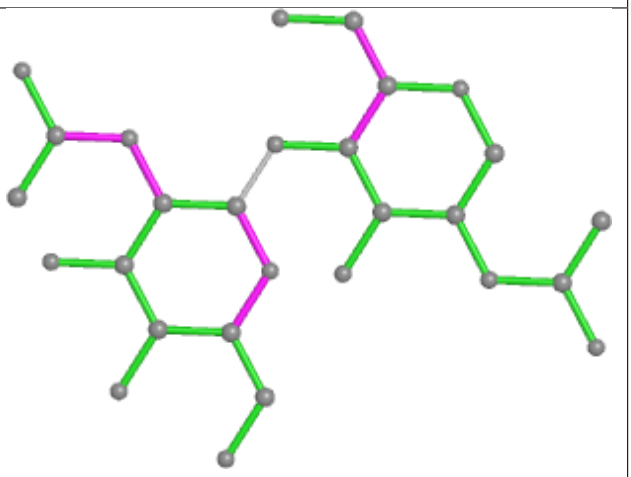
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain A	
 Bond lengths	 Bond angles
 Torsions	 Rings

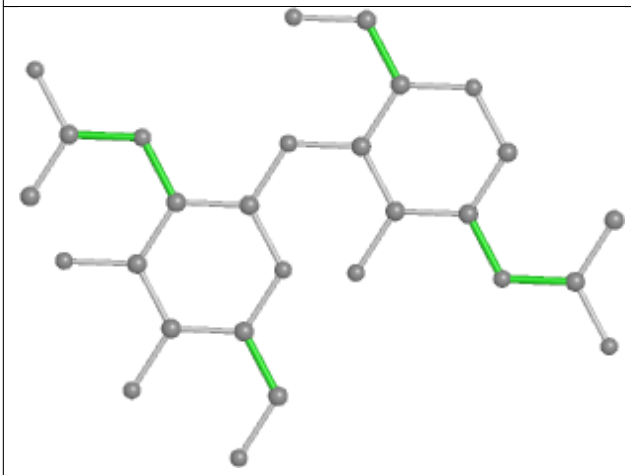
Oligosaccharide Chain B



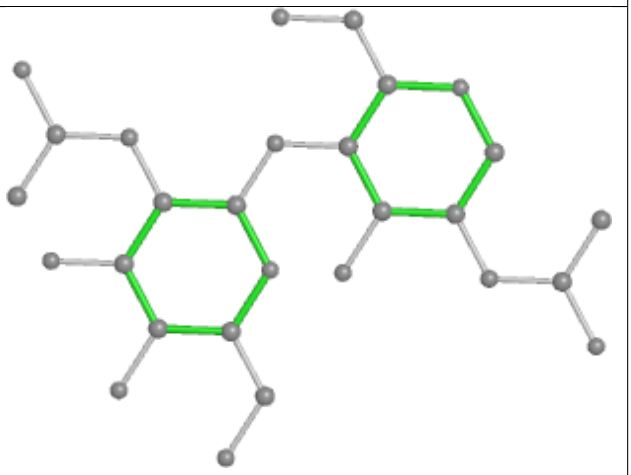
Bond lengths



Bond angles

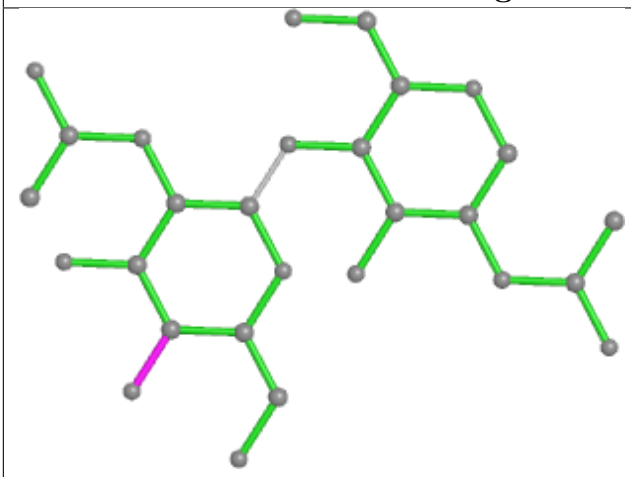


Torsions

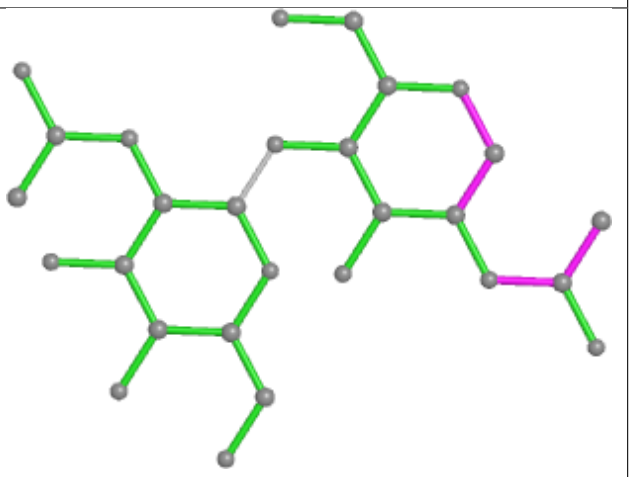


Rings

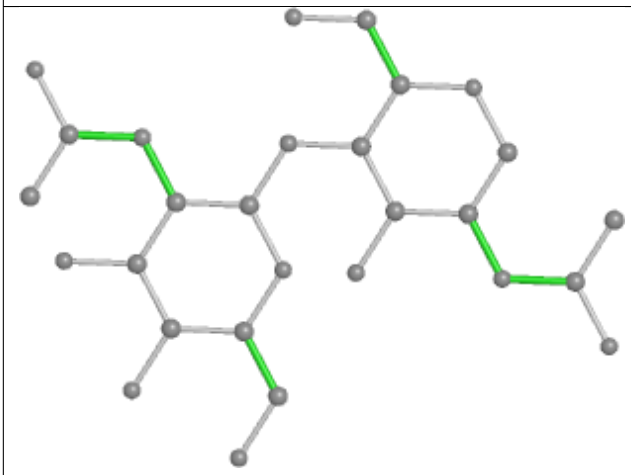
Oligosaccharide Chain C



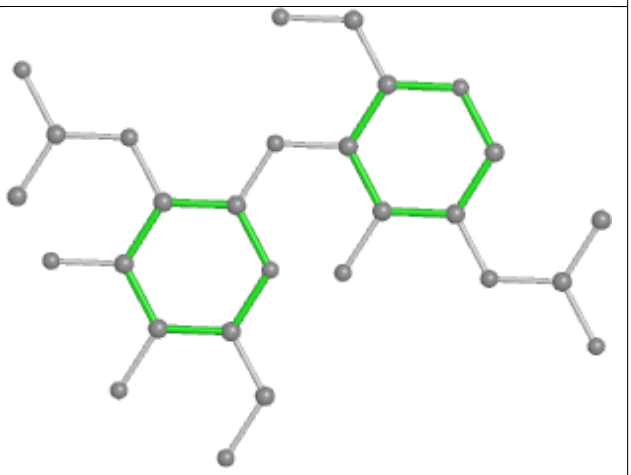
Bond lengths



Bond angles

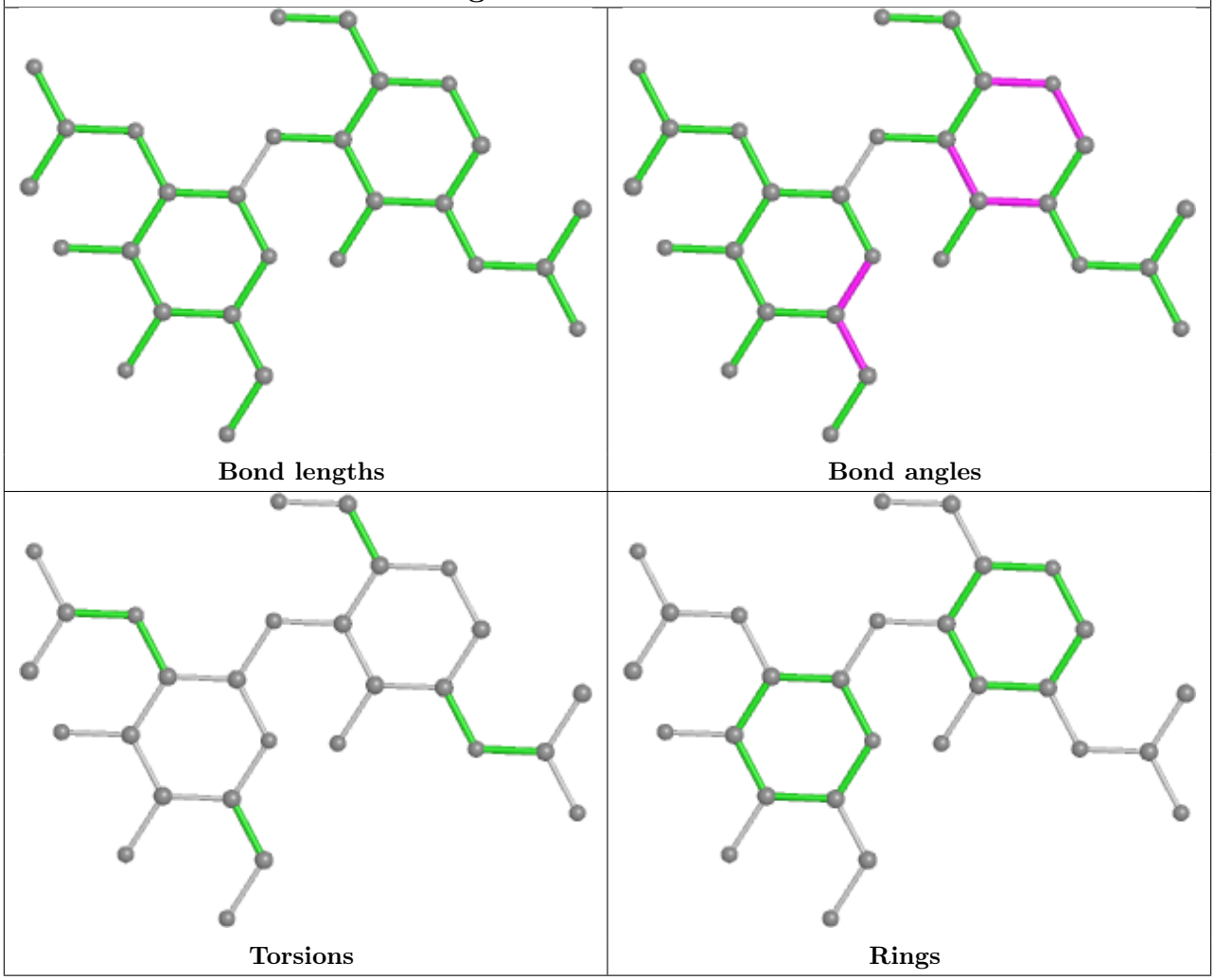


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\#\|Z\| > 2$
5	SO4	AAA	719	-	4,4,4	0.68	0	6,6,6	0.10	0
5	SO4	AAA	724	-	4,4,4	0.60	0	6,6,6	0.35	0
4	GOL	AAA	705	-	5,5,5	0.59	0	5,5,5	0.82	0
5	SO4	AAA	716	-	4,4,4	0.48	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	AAA	706	-	4,4,4	0.46	0	6,6,6	0.76	0
5	SO4	AAA	722	-	4,4,4	0.49	0	6,6,6	0.31	0
4	GOL	AAA	720	-	5,5,5	0.40	0	5,5,5	1.18	0
6	ACT	AAA	730	-	3,3,3	1.85	1 (33%)	3,3,3	0.53	0
4	GOL	AAA	721	-	5,5,5	0.17	0	5,5,5	0.48	0
6	ACT	AAA	714	-	3,3,3	0.85	0	3,3,3	1.62	1 (33%)
5	SO4	AAA	728	-	4,4,4	0.54	0	6,6,6	0.15	0
5	SO4	AAA	717	-	4,4,4	0.61	0	6,6,6	0.75	0
5	SO4	AAA	727	-	4,4,4	0.51	0	6,6,6	0.23	0
5	SO4	AAA	726	-	4,4,4	0.57	0	6,6,6	0.10	0
5	SO4	AAA	718	-	4,4,4	0.92	0	6,6,6	0.14	0
6	ACT	AAA	725	-	3,3,3	1.39	0	3,3,3	0.57	0
6	ACT	AAA	715	-	3,3,3	1.11	0	3,3,3	1.01	0
5	SO4	AAA	729	-	4,4,4	0.75	0	6,6,6	0.43	0
5	SO4	AAA	713	-	4,4,4	0.58	0	6,6,6	0.19	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
4	GOL	AAA	720	-	-	2/4/4/4	-
4	GOL	AAA	705	-	-	0/4/4/4	-
4	GOL	AAA	721	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AAA	730	ACT	O-C	2.23	1.32	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	AAA	714	ACT	O-C-CH3	-2.29	113.41	122.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	720	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	AAA	720	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	705	GOL	2	0
4	AAA	720	GOL	3	0
6	AAA	715	ACT	2	0
5	AAA	729	SO4	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	AAA	627/627 (100%)	-0.38	0	100	100	11, 14, 23, 33	1 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

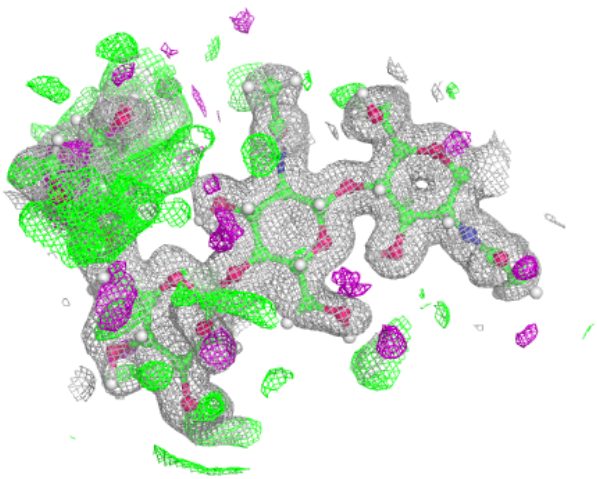
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

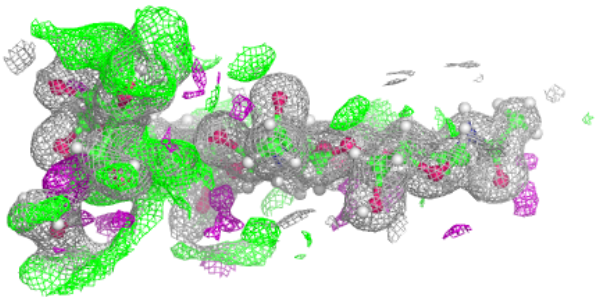
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	A	4	11/12	0.85	0.14	20,26,29,35	4
2	BMA	A	3	11/12	0.91	0.08	20,30,39,42	3
3	NAG	C	2	14/15	0.96	0.07	17,20,28,34	3
3	NAG	D	2	14/15	0.96	0.14	20,45,56,65	3
3	NAG	B	2	14/15	0.97	0.21	20,30,49,56	3
2	NAG	A	1	14/15	0.98	0.06	15,17,27,28	2
3	NAG	C	1	14/15	0.98	0.06	14,17,22,32	2
2	NAG	A	2	14/15	0.98	0.05	16,20,25,29	2
3	NAG	D	1	14/15	0.98	0.06	17,21,29,33	2
3	NAG	B	1	14/15	0.98	0.07	16,20,24,29	2

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:

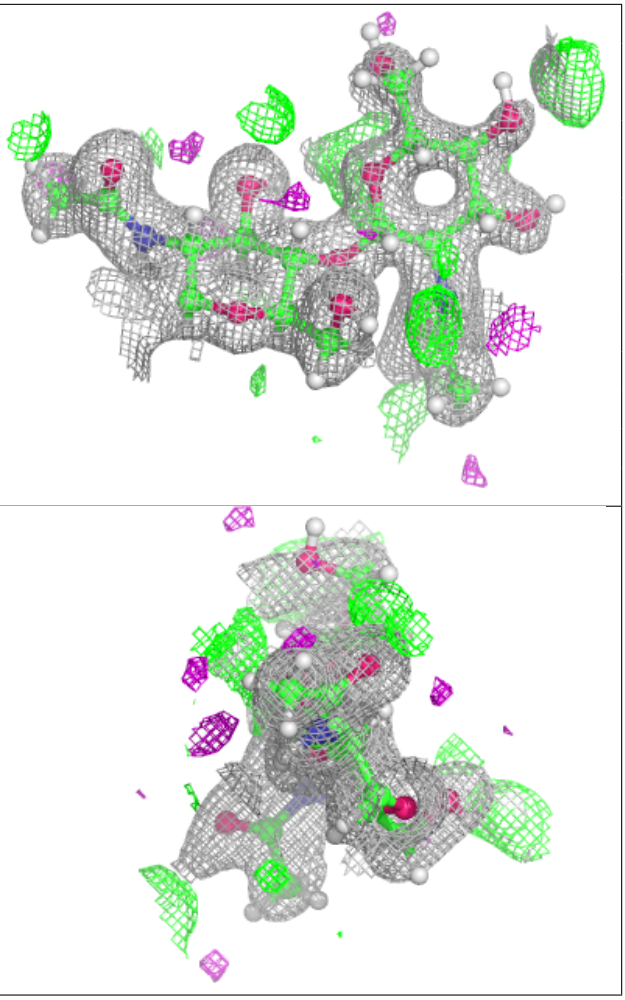
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





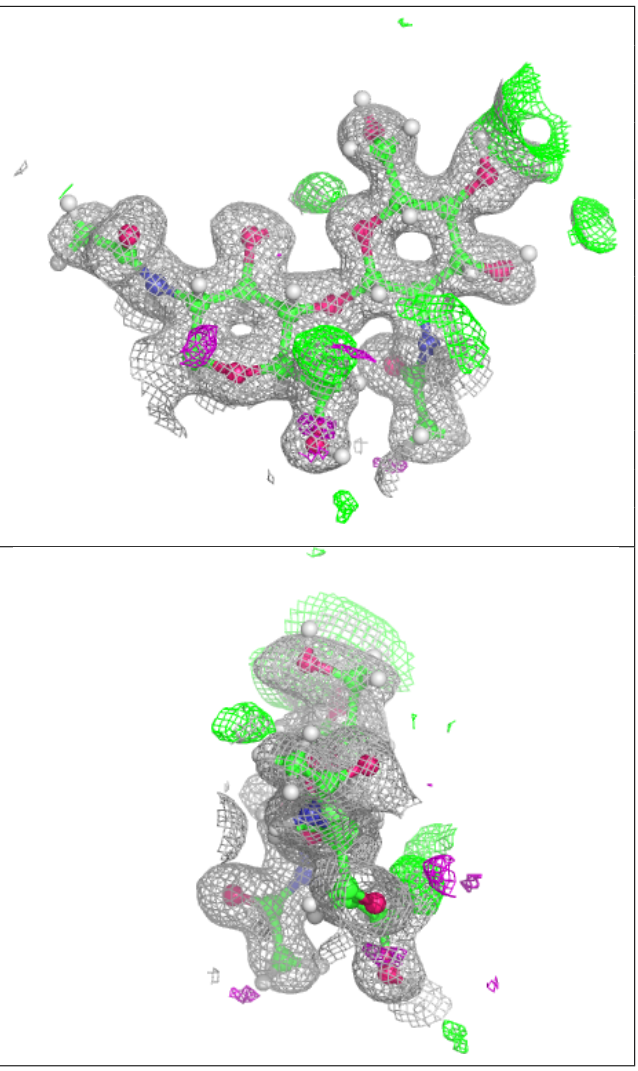
Electron density around Chain B:

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



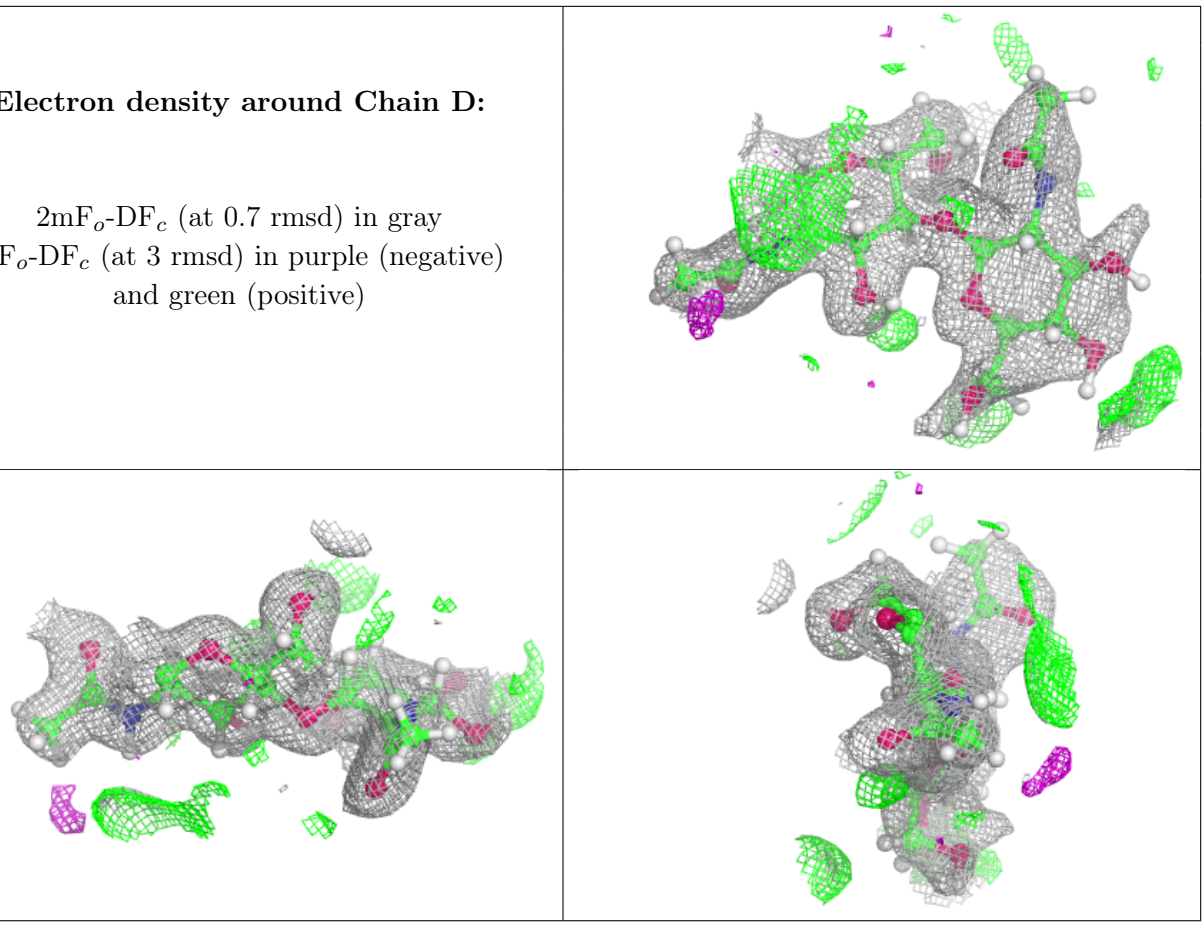
Electron density around Chain C:

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



Electron density around Chain D:

$2mF_o$-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, 95th 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
6	ACT	AAA	725	4/4	0.79	0.24	34,43,47,53	0
4	GOL	AAA	721	6/6	0.83	0.20	11,20,27,27	14
5	SO4	AAA	729	5/5	0.88	0.22	25,29,32,35	4
6	ACT	AAA	715	4/4	0.91	0.13	24,36,45,48	0
5	SO4	AAA	718	5/5	0.91	0.22	22,36,44,48	5
5	SO4	AAA	713	5/5	0.92	0.16	29,31,35,45	5
5	SO4	AAA	728	5/5	0.93	0.27	16,21,27,29	4
6	ACT	AAA	714	4/4	0.93	0.12	32,42,44,48	0
4	GOL	AAA	705	6/6	0.94	0.16	13,20,25,26	2
4	GOL	AAA	720	6/6	0.94	0.22	10,19,27,35	14
6	ACT	AAA	730	4/4	0.94	0.12	30,43,48,53	0
5	SO4	AAA	716	5/5	0.95	0.10	27,35,44,47	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	AAA	722	5/5	0.96	0.14	30,33,40,49	5
5	SO4	AAA	727	5/5	0.96	0.15	20,21,23,27	4
5	SO4	AAA	724	5/5	0.97	0.08	23,24,34,36	5
5	SO4	AAA	726	5/5	0.97	0.10	27,29,32,35	5
5	SO4	AAA	719	5/5	0.97	0.12	30,30,38,40	5
5	SO4	AAA	706	5/5	0.98	0.11	23,28,35,36	0
5	SO4	AAA	717	5/5	0.99	0.07	17,19,23,27	0
7	CL	AAA	723	1/1	1.00	0.13	15,15,15,15	1

6.5 Other polymers (i)

There are no such residues in this entry.