



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2020 – 02:47 PM GMT

PDB ID : 6ZPV
Title : Structure of Unliganded MgGH51 α -L-Arabinofuranosidase Crystal Type 3
Authors : McGregor, N.G.S.; Davies, G.J.
Deposited on : 2020-07-09
Resolution : 1.20 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 ⓘ](#)) 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 : 2.14.6
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) : 2.14.6

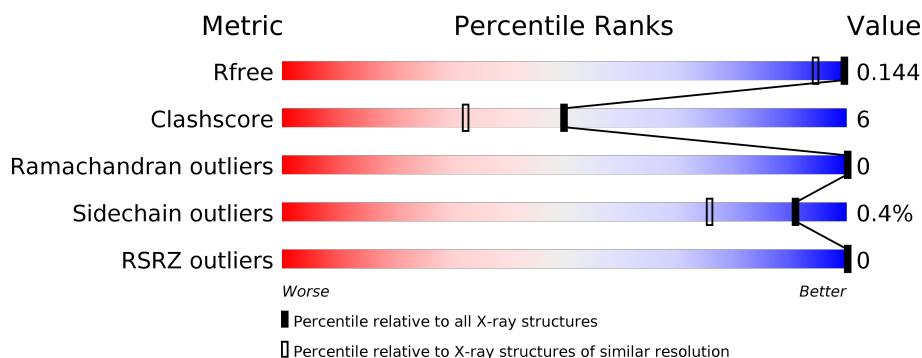
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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	1223 (1.22-1.18)
Clashscore	141614	1286 (1.22-1.18)
Ramachandran outliers	138981	1240 (1.22-1.18)
Sidechain outliers	138945	1239 (1.22-1.18)
RSRZ outliers	127900	1200 (1.22-1.18)

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 $\leq 5\%$. 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	<div> <div style="width: 93%;"></div> <div style="width: 7%;"></div> </div> <div>93% 7%</div>
2	A	6	<div> <div style="width: 83%;"></div> <div style="width: 17%;"></div> </div> <div>83% 17%</div>
3	B	2	<div> <div style="width: 100%;"></div> </div> <div>100%</div>
3	D	2	<div> <div style="width: 50%;"></div> <div style="width: 50%;"></div> </div> <div>50% 50%</div>
4	C	5	<div> <div style="width: 80%;"></div> <div style="width: 20%;"></div> </div> <div>80% 20%</div>

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
7	SO4	AAA	719	-	-	X	-
7	SO4	AAA	720	-	-	X	-
7	SO4	AAA	726	-	-	X	-

2 Entry composition [i](#)

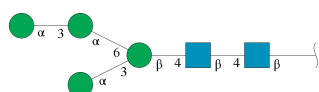
There are 8 unique types of molecules in this entry. The entry contains 11226 atoms, of which 4945 are hydrogens and 0 are deuteriums.

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
1	AAA	627	Total	C	H	N	O	S	318	22	0
			9660	3145	4745	817	946	7			

- Molecule 2 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.



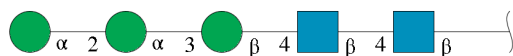
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	6	Total	C	H	N	O	17	0	0
			139	40	67	2	30			

- 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
3	B	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			
3	D	2	Total	C	H	N	O	5	0	0
			55	16	27	2	10			

- Molecule 4 is an oligosaccharide called 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
4	C	5	Total	C	H	N	O	14	0	0
			118	34	57	2	25			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



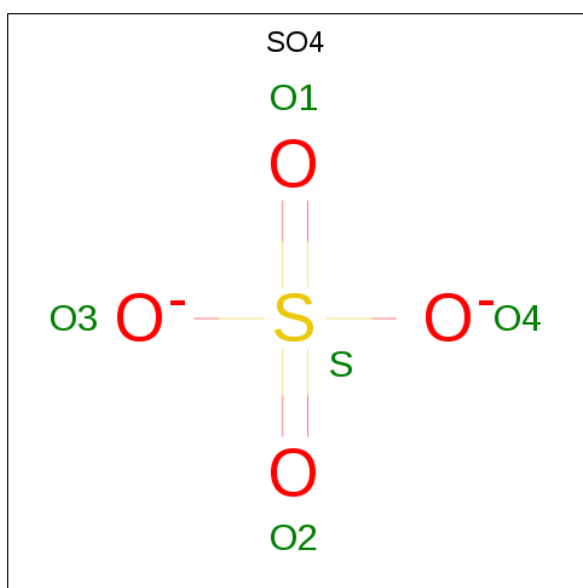
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O	2	0
			14	3	8	3		
5	AAA	1	Total	C	H	O	2	0
			14	3	8	3		

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



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	O	S	0	0
			5	4	1		
7	AAA	1	Total	O	S	0	0
			5	4	1		
7	AAA	1	Total	O	S	0	0
			5	4	1		
7	AAA	1	Total	O	S	0	0
			5	4	1		
7	AAA	1	Total	O	S	0	1
			10	8	2		
7	AAA	1	Total	O	S	0	0
			5	4	1		
7	AAA	1	Total	O	S	0	0
			5	4	1		
7	AAA	1	Total	O	S	0	0
			5	4	1		
7	AAA	1	Total	O	S	0	0
			5	4	1		

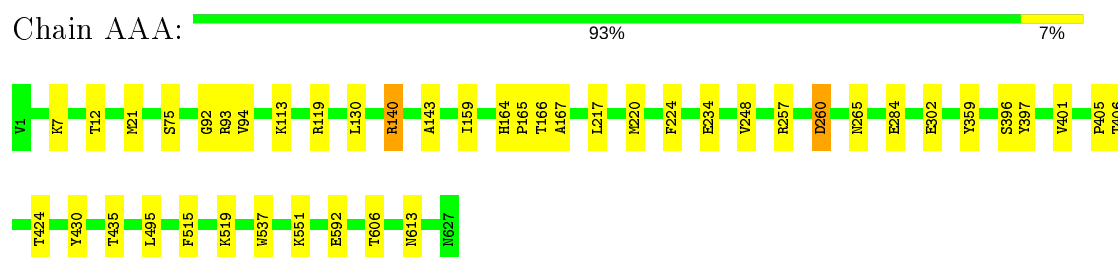
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	1082	Total	O	0	23
			1097	1097		

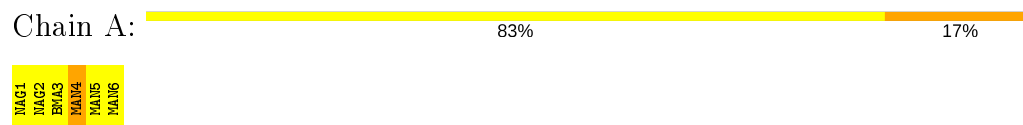
3 Residue-property plots

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.

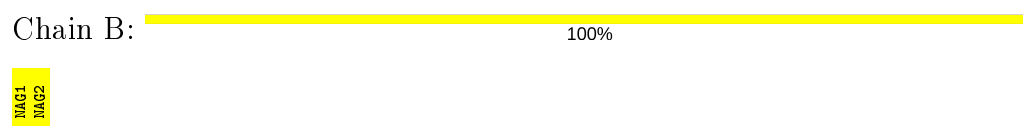
- Molecule 1: MgGH51



- Molecule 2: 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



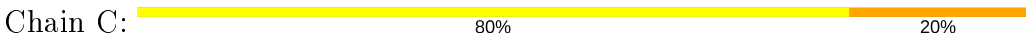
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 4: 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



HA01
HA02
HA03
HA04
HA05

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	83.95Å 83.95Å 256.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.92 – 1.20 79.79 – 1.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (79.92-1.20) 100.0 (79.79-1.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.120 , 0.144 0.121 , 0.144	Depositor DCC
R_{free} test set	14149 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	11226	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 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, BMA, NAG, SO4, 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	0.80	6/5100 (0.1%)	0.94	10/6976 (0.1%)

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	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	260	ASP	CB-CG	6.60	1.65	1.51
1	AAA	592	GLU	CD-OE2	6.41	1.32	1.25
1	AAA	260	ASP	CG-OD2	5.82	1.38	1.25
1	AAA	119	ARG	CD-NE	5.70	1.56	1.46
1	AAA	234	GLU	CD-OE1	5.61	1.31	1.25
1	AAA	260	ASP	CG-OD1	5.35	1.37	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	119	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	AAA	140[A]	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	AAA	140[B]	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	AAA	93	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	AAA	397	TYR	CB-CG-CD2	5.48	124.29	121.00
1	AAA	167[A]	ALA	CA-C-O	-5.37	108.81	120.10
1	AAA	167[B]	ALA	CA-C-O	-5.37	108.81	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	257	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	AAA	119	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	AAA	260	ASP	CB-CA-C	5.16	120.72	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	359	TYR	Sidechain
1	AAA	606[A]	THR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	4915	4745	4741	49	3
2	A	72	67	61	0	1
3	B	28	27	25	0	0
3	D	28	27	25	1	0
4	C	61	57	51	2	0
5	AAA	12	16	16	1	0
6	AAA	8	6	6	0	0
7	AAA	60	0	0	15	1
8	AAA	1097	0	0	39	0
All	All	6281	4945	4925	59	3

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 6.

All (59) 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:166[A]:THR:CB	8:AAA:811:HOH:O	1.81	1.24
1:AAA:166[A]:THR:HG23	8:AAA:810:HOH:O	1.37	1.21
1:AAA:166[A]:THR:N	8:AAA:810:HOH:O	1.71	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:519:LYS:HE3	8:AAA:1375[B]:HOH:O	0.99	1.16
1:AAA:140[A]:ARG:NE	7:AAA:726:SO4:O4	1.83	1.12
7:AAA:720:SO4:O4	8:AAA:809:HOH:O	1.66	1.11
1:AAA:140[A]:ARG:CD	7:AAA:726:SO4:O4	1.98	1.10
1:AAA:166[A]:THR:CG2	8:AAA:810:HOH:O	1.95	1.09
1:AAA:166[A]:THR:CB	8:AAA:810:HOH:O	2.02	1.07
1:AAA:260:ASP:HB3	8:AAA:837:HOH:O	1.57	1.03
1:AAA:166[A]:THR:OG1	8:AAA:811:HOH:O	1.77	0.98
1:AAA:140[A]:ARG:HD3	7:AAA:726:SO4:O4	1.61	0.97
1:AAA:166[A]:THR:HG21	8:AAA:811:HOH:O	1.67	0.94
1:AAA:166[A]:THR:CG2	8:AAA:811:HOH:O	2.09	0.93
1:AAA:94[A]:VAL:HG21	8:AAA:823:HOH:O	1.67	0.93
1:AAA:166[A]:THR:CA	8:AAA:810:HOH:O	2.06	0.93
1:AAA:140[B]:ARG:HG3	8:AAA:1138:HOH:O	1.68	0.92
1:AAA:519:LYS:CE	8:AAA:1375[B]:HOH:O	1.68	0.90
7:AAA:720:SO4:S	8:AAA:809:HOH:O	2.30	0.81
5:AAA:730:GOL:O2	8:AAA:813:HOH:O	1.93	0.79
1:AAA:613:ASN:HB2	8:AAA:836:HOH:O	1.80	0.79
7:AAA:724[B]:SO4:O1	8:AAA:815:HOH:O	2.01	0.79
7:AAA:722:SO4:O2	8:AAA:814:HOH:O	2.00	0.78
1:AAA:75[B]:SER:OG	8:AAA:816:HOH:O	2.03	0.76
1:AAA:143:ALA:HB2	1:AAA:165[A]:PRO:HA	1.68	0.75
7:AAA:720:SO4:O2	8:AAA:809:HOH:O	2.05	0.72
8:AAA:833:HOH:O	4:C:3:BMA:C6	2.38	0.70
1:AAA:94[A]:VAL:CG2	8:AAA:823:HOH:O	2.29	0.68
1:AAA:519:LYS:NZ	8:AAA:1375[B]:HOH:O	1.98	0.65
8:AAA:821:HOH:O	3:D:2:NAG:O4	2.15	0.65
1:AAA:113:LYS:NZ	8:AAA:819:HOH:O	2.14	0.65
1:AAA:166[A]:THR:N	8:AAA:808:HOH:O	2.32	0.62
7:AAA:719:SO4:O3	8:AAA:822:HOH:O	2.16	0.59
1:AAA:159[B]:ILE:HD13	8:AAA:1041:HOH:O	2.04	0.57
1:AAA:166[A]:THR:HB	8:AAA:811:HOH:O	1.73	0.56
1:AAA:435:THR:HG22	7:AAA:719:SO4:O3	2.05	0.56
1:AAA:217:LEU:O	1:AAA:220[A]:MET:HG2	2.06	0.56
1:AAA:406:THR:OG1	7:AAA:719:SO4:O4	2.19	0.54
1:AAA:220[A]:MET:HE1	1:AAA:495:LEU:HD21	1.90	0.53
8:AAA:833:HOH:O	4:C:3:BMA:H62	2.03	0.52
1:AAA:515:PHE:CD2	1:AAA:551:LYS:HE3	2.46	0.51
1:AAA:166[B]:THR:CG2	8:AAA:1528:HOH:O	0.80	0.50
1:AAA:406:THR:N	7:AAA:719:SO4:O2	2.39	0.49
1:AAA:405:PRO:HD2	7:AAA:719:SO4:O2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:396:SER:HA	1:AAA:424:THR:O	2.14	0.47
1:AAA:21:MET:HE2	8:AAA:1332:HOH:O	2.15	0.46
1:AAA:166[A]:THR:CB	8:AAA:830:HOH:O	2.64	0.46
1:AAA:166[B]:THR:HG21	8:AAA:1528:HOH:O	0.77	0.45
1:AAA:248[A]:VAL:CG2	8:AAA:1264:HOH:O	2.65	0.45
1:AAA:143:ALA:HB2	1:AAA:165[A]:PRO:CA	2.43	0.44
1:AAA:164[B]:HIS:NE2	8:AAA:820:HOH:O	2.14	0.44
1:AAA:140[B]:ARG:NH2	7:AAA:726:SO4:O4	2.52	0.42
1:AAA:220[A]:MET:H	1:AAA:220[A]:MET:HG2	1.56	0.42
1:AAA:220[A]:MET:HE1	1:AAA:495:LEU:CD2	2.49	0.42
1:AAA:140[A]:ARG:HD3	7:AAA:726:SO4:S	2.55	0.42
1:AAA:537:TRP:HA	1:AAA:551:LYS:O	2.21	0.41
1:AAA:224:PHE:HA	1:AAA:284:GLU:O	2.22	0.40
1:AAA:401:VAL:O	1:AAA:430:TYR:HA	2.21	0.40
1:AAA:140[B]:ARG:HD2	8:AAA:1136:HOH:O	2.22	0.40

All (3) 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:302:GLU:H	2:A:4:MAN:HO2[7_555]	1.20	0.40
1:AAA:12:THR:HG1	1:AAA:92:GLY:H[7_545]	1.23	0.37
1:AAA:7:LYS:HZ2	7:AAA:721:SO4:O3[7_545]	1.59	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	646/627 (103%)	634 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	529/510 (104%)	526 (99%)	3 (1%)	86	63

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	130[A]	LEU
1	AAA	130[B]	LEU
1	AAA	265	ASN

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 ⓘ

15 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	1,2	14,14,15	1.06	1 (7%)	17,19,21	1.61	3 (17%)
2	NAG	A	2	2	14,14,15	0.87	0	17,19,21	1.53	3 (17%)
2	BMA	A	3	2	11,11,12	0.86	0	15,15,17	1.03	1 (6%)
2	MAN	A	4	2	11,11,12	1.02	1 (9%)	15,15,17	1.22	2 (13%)
2	MAN	A	5	2	11,11,12	1.87	3 (27%)	15,15,17	2.90	9 (60%)
2	MAN	A	6	2	11,11,12	1.08	1 (9%)	15,15,17	1.81	3 (20%)
3	NAG	B	1	1,3	14,14,15	1.11	2 (14%)	17,19,21	1.46	4 (23%)
3	NAG	B	2	3	14,14,15	2.02	4 (28%)	17,19,21	1.21	3 (17%)
4	NAG	C	1	1,4	14,14,15	1.06	2 (14%)	17,19,21	0.79	0
4	NAG	C	2	4	14,14,15	1.11	1 (7%)	17,19,21	1.70	5 (29%)
4	BMA	C	3	4	11,11,12	1.47	2 (18%)	15,15,17	3.39	7 (46%)
4	MAN	C	4	4	11,11,12	2.10	3 (27%)	15,15,17	2.21	5 (33%)
4	MAN	C	5	4	11,11,12	1.74	3 (27%)	15,15,17	2.42	4 (26%)
3	NAG	D	1	1,3	14,14,15	1.22	2 (14%)	17,19,21	1.00	1 (5%)
3	NAG	D	2	3	14,14,15	0.61	0	17,19,21	1.00	2 (11%)

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	1,2	-	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	-	0/2/19/22	0/1/1/1
2	MAN	A	5	2	-	1/2/19/22	0/1/1/1
2	MAN	A	6	2	-	0/2/19/22	0/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	1/6/23/26	0/1/1/1
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	MAN	C	4	4	-	0/2/19/22	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5	MAN	O5-C5	5.12	1.53	1.43
4	C	4	MAN	C2-C3	5.08	1.60	1.52
3	B	2	NAG	C2-N2	-4.63	1.38	1.46
3	B	2	NAG	O5-C1	-3.70	1.37	1.43
4	C	3	BMA	O5-C5	3.36	1.50	1.43
4	C	5	MAN	C4-C3	3.26	1.60	1.52
3	B	2	NAG	O5-C5	2.98	1.49	1.43
4	C	5	MAN	O3-C3	-2.88	1.36	1.43
4	C	4	MAN	C6-C5	2.80	1.61	1.51
2	A	4	MAN	O5-C1	-2.79	1.39	1.43
3	D	1	NAG	O5-C1	-2.61	1.39	1.43
2	A	6	MAN	C2-C3	2.55	1.56	1.52
4	C	5	MAN	C4-C5	-2.54	1.47	1.53
2	A	5	MAN	O4-C4	2.47	1.48	1.43
3	D	1	NAG	C2-N2	-2.43	1.42	1.46
3	B	1	NAG	C4-C5	-2.33	1.48	1.53
3	B	2	NAG	O4-C4	2.15	1.48	1.43
4	C	4	MAN	O5-C5	2.12	1.47	1.43
3	B	1	NAG	C1-C2	2.09	1.55	1.52
2	A	5	MAN	O6-C6	2.07	1.51	1.42
4	C	2	NAG	C3-C2	2.06	1.56	1.52
4	C	1	NAG	O5-C1	2.06	1.47	1.43
4	C	3	BMA	O5-C1	-2.06	1.40	1.43
4	C	1	NAG	O7-C7	-2.03	1.18	1.23
2	A	1	NAG	C1-C2	2.02	1.55	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	BMA	C1-O5-C5	-10.10	98.51	112.19
4	C	4	MAN	O4-C4-C3	5.48	123.01	110.35
4	C	5	MAN	O5-C5-C6	5.45	115.75	107.20
4	C	5	MAN	C1-O5-C5	5.44	119.56	112.19
2	A	5	MAN	C1-O5-C5	-5.18	105.17	112.19
2	A	5	MAN	O5-C5-C4	5.09	123.22	110.83
2	A	6	MAN	C1-O5-C5	4.78	118.67	112.19
2	A	5	MAN	O6-C6-C5	-4.62	95.44	111.29
4	C	3	BMA	O6-C6-C5	-4.37	96.30	111.29
4	C	4	MAN	C1-O5-C5	4.10	117.75	112.19
4	C	3	BMA	O5-C1-C2	4.06	117.04	110.77
4	C	2	NAG	O7-C7-C8	-3.74	115.12	122.06
2	A	1	NAG	C4-C3-C2	3.49	116.14	111.02
2	A	6	MAN	O5-C5-C6	3.49	112.67	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5	MAN	C6-C5-C4	-3.48	104.85	113.00
2	A	2	NAG	C4-C3-C2	-3.43	105.99	111.02
2	A	5	MAN	O3-C3-C4	-3.13	103.12	110.35
4	C	3	BMA	C2-C3-C4	3.08	116.22	110.89
4	C	2	NAG	C3-C4-C5	3.06	115.70	110.24
2	A	4	MAN	O6-C6-C5	-3.05	100.82	111.29
3	B	1	NAG	C8-C7-N2	-3.02	110.98	116.10
2	A	1	NAG	O5-C1-C2	-2.88	106.74	111.29
3	B	1	NAG	O7-C7-N2	2.74	126.99	121.95
4	C	3	BMA	O5-C5-C6	2.74	111.49	107.20
2	A	6	MAN	C1-C2-C3	2.71	113.00	109.67
2	A	3	BMA	O5-C1-C2	-2.71	106.59	110.77
4	C	5	MAN	O5-C1-C2	-2.64	106.69	110.77
2	A	5	MAN	C1-C2-C3	2.58	112.83	109.67
2	A	2	NAG	C1-O5-C5	-2.57	108.71	112.19
3	B	2	NAG	C2-N2-C7	2.48	126.44	122.90
4	C	4	MAN	O3-C3-C4	-2.47	104.64	110.35
4	C	3	BMA	C3-C4-C5	-2.44	105.88	110.24
4	C	4	MAN	O2-C2-C3	-2.42	105.28	110.14
3	D	2	NAG	O6-C6-C5	-2.37	103.17	111.29
3	D	2	NAG	C2-N2-C7	2.34	126.24	122.90
4	C	5	MAN	O2-C2-C1	2.33	113.92	109.15
4	C	4	MAN	O6-C6-C5	-2.32	103.33	111.29
2	A	1	NAG	O4-C4-C3	2.32	115.71	110.35
2	A	2	NAG	O4-C4-C5	-2.27	103.66	109.30
2	A	5	MAN	O3-C3-C2	-2.27	105.65	109.99
2	A	5	MAN	O4-C4-C3	2.24	115.52	110.35
3	B	2	NAG	O4-C4-C5	2.22	114.81	109.30
3	D	1	NAG	C1-O5-C5	2.20	115.17	112.19
3	B	1	NAG	O4-C4-C3	-2.18	105.30	110.35
2	A	4	MAN	C6-C5-C4	-2.12	108.04	113.00
4	C	2	NAG	O3-C3-C4	2.07	115.14	110.35
2	A	5	MAN	C2-C3-C4	-2.07	107.32	110.89
4	C	3	BMA	C1-C2-C3	-2.06	107.13	109.67
3	B	1	NAG	O5-C1-C2	-2.06	108.03	111.29
4	C	2	NAG	O6-C6-C5	-2.04	104.30	111.29
3	B	2	NAG	O3-C3-C2	2.03	113.67	109.47
4	C	2	NAG	O7-C7-N2	2.02	125.66	121.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

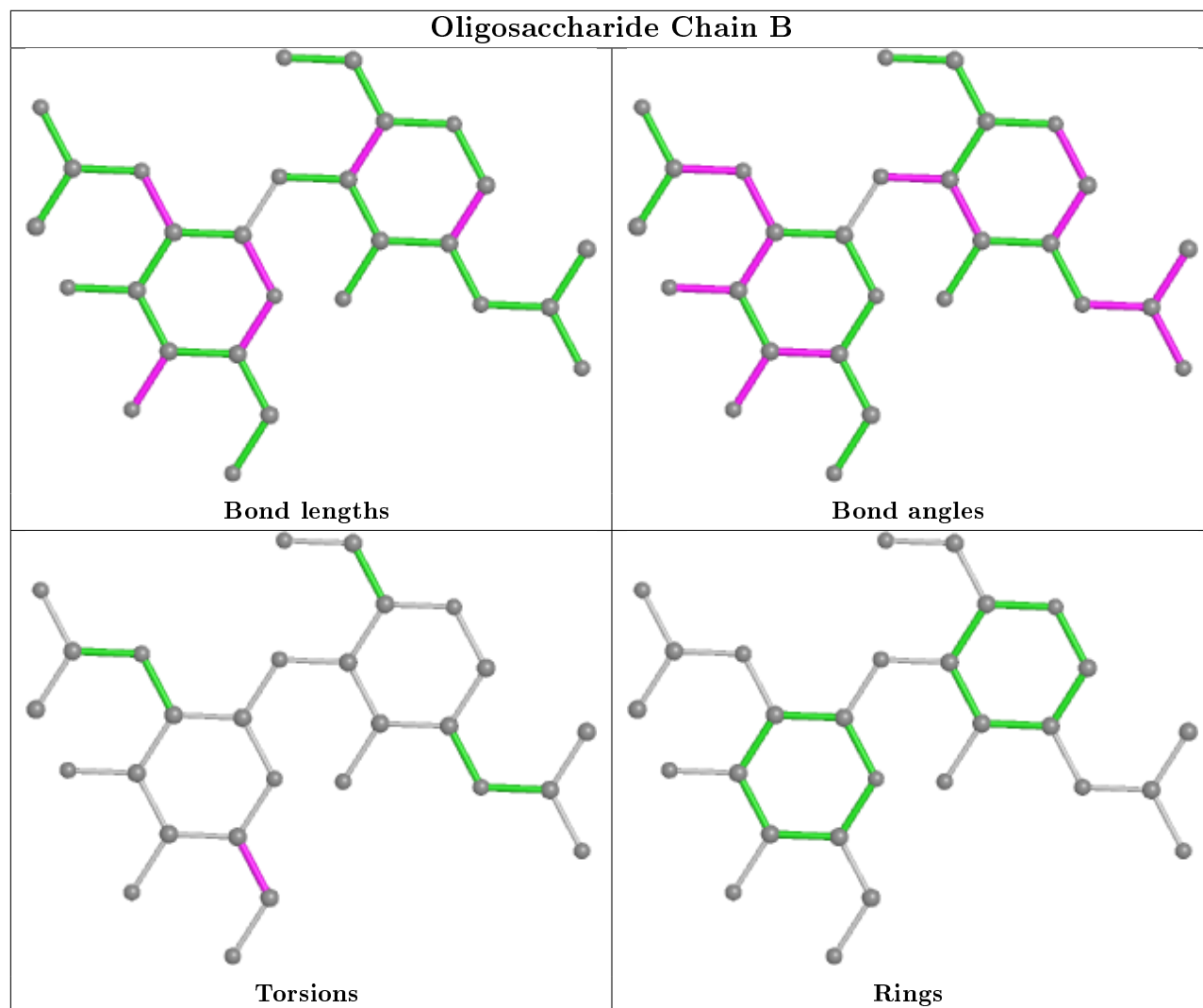
Mol	Chain	Res	Type	Atoms
2	A	5	MAN	O5-C5-C6-O6
3	B	2	NAG	C4-C5-C6-O6

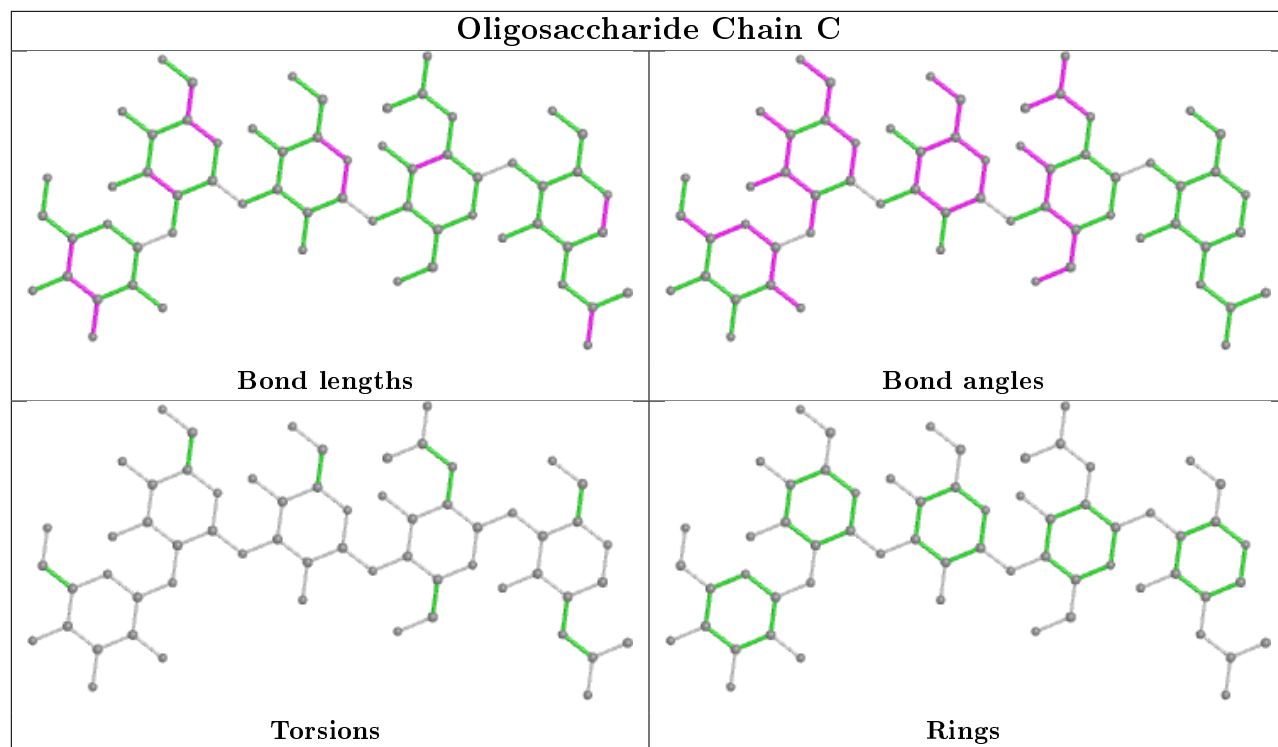
There are no ring outliers.

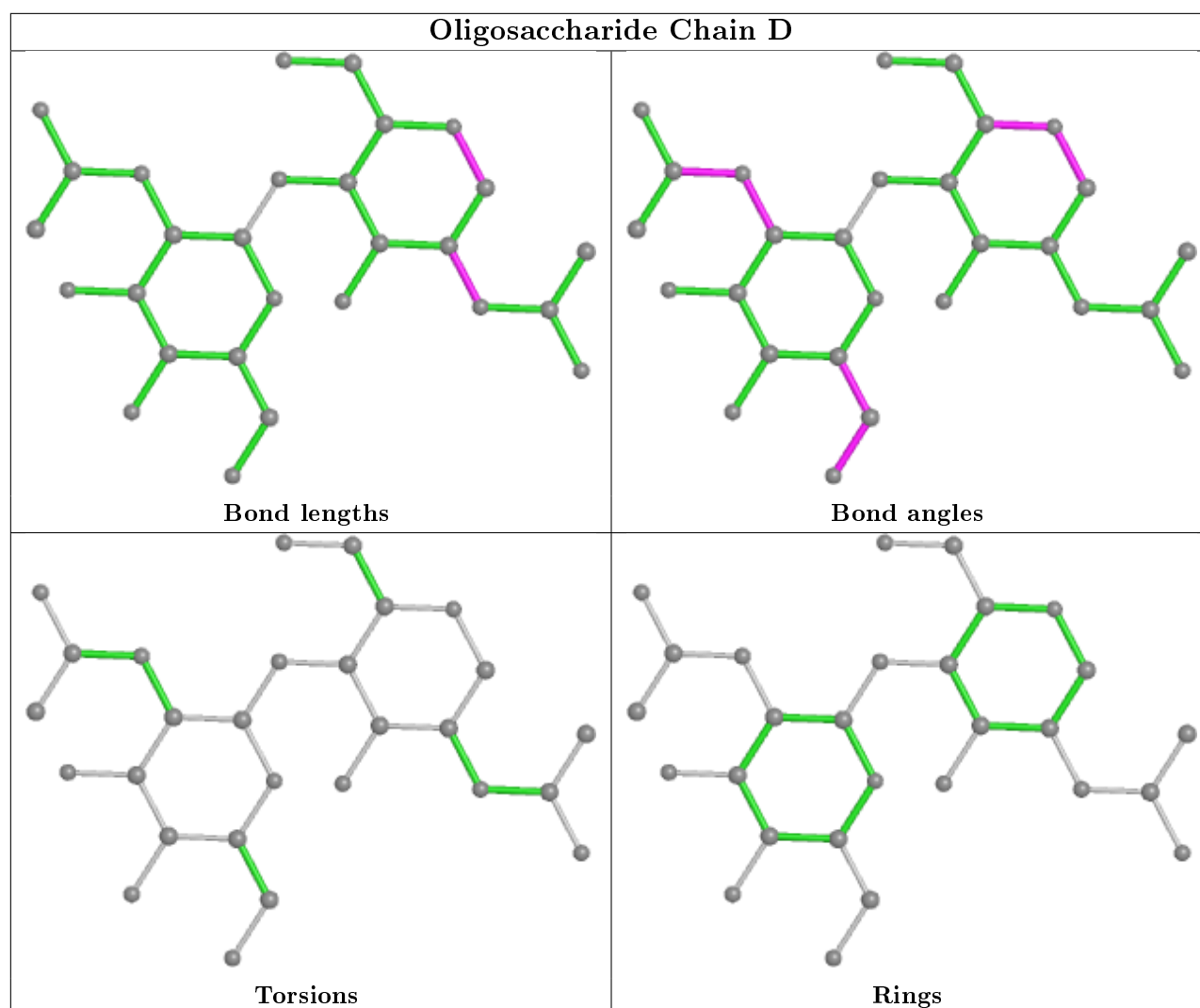
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3	BMA	2	0
2	A	4	MAN	0	1
3	D	2	NAG	1	0

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







5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	ACT	AAA	729	-	1,3,3	6.82	1 (100%)	0,3,3	0.00	-
7	SO4	AAA	720	-	4,4,4	0.24	0	6,6,6	0.32	0
7	SO4	AAA	727	-	4,4,4	0.97	0	6,6,6	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	AAA	718	-	4,4,4	0.64	0	6,6,6	1.13	1 (16%)
7	SO4	AAA	723	-	4,4,4	1.21	1 (25%)	6,6,6	0.31	0
7	SO4	AAA	722	-	4,4,4	0.73	0	6,6,6	0.22	0
6	ACT	AAA	708	-	1,3,3	9.14	1 (100%)	0,3,3	0.00	-
5	GOL	AAA	707	-	5,5,5	0.22	0	5,5,5	0.73	0
7	SO4	AAA	719	-	4,4,4	0.44	0	6,6,6	0.15	0
7	SO4	AAA	725	-	4,4,4	0.33	0	6,6,6	0.37	0
7	SO4	AAA	724[A]	-	4,4,4	0.20	0	6,6,6	0.28	0
7	SO4	AAA	721	-	4,4,4	0.48	0	6,6,6	0.39	0
7	SO4	AAA	726	-	4,4,4	0.86	0	6,6,6	0.55	0
5	GOL	AAA	730	-	5,5,5	0.16	0	5,5,5	0.68	0
7	SO4	AAA	728	-	4,4,4	0.40	0	6,6,6	0.71	0
7	SO4	AAA	724[B]	-	4,4,4	2.58	1 (25%)	6,6,6	1.23	1 (16%)

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
5	GOL	AAA	707	-	-	0/4/4/4	-
5	GOL	AAA	730	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AAA	708	ACT	CH3-C	9.14	1.60	1.48
6	AAA	729	ACT	CH3-C	6.82	1.57	1.48
7	AAA	724[B]	SO4	O1-S	4.72	1.71	1.46
7	AAA	723	SO4	O2-S	-2.35	1.33	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AAA	718	SO4	O4-S-O2	2.31	121.35	109.31
7	AAA	724[B]	SO4	O3-S-O1	-2.12	98.26	109.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	730	GOL	C1-C2-C3-O3
5	AAA	730	GOL	O2-C2-C3-O3
5	AAA	730	GOL	O1-C1-C2-C3
5	AAA	730	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	AAA	720	SO4	3	0
7	AAA	722	SO4	1	0
7	AAA	719	SO4	5	0
7	AAA	721	SO4	0	1
7	AAA	726	SO4	5	0
5	AAA	730	GOL	1	0
7	AAA	724[B]	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.82	0 100 100	10, 14, 21, 33	0

There are no RSRZ outliers to report.

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

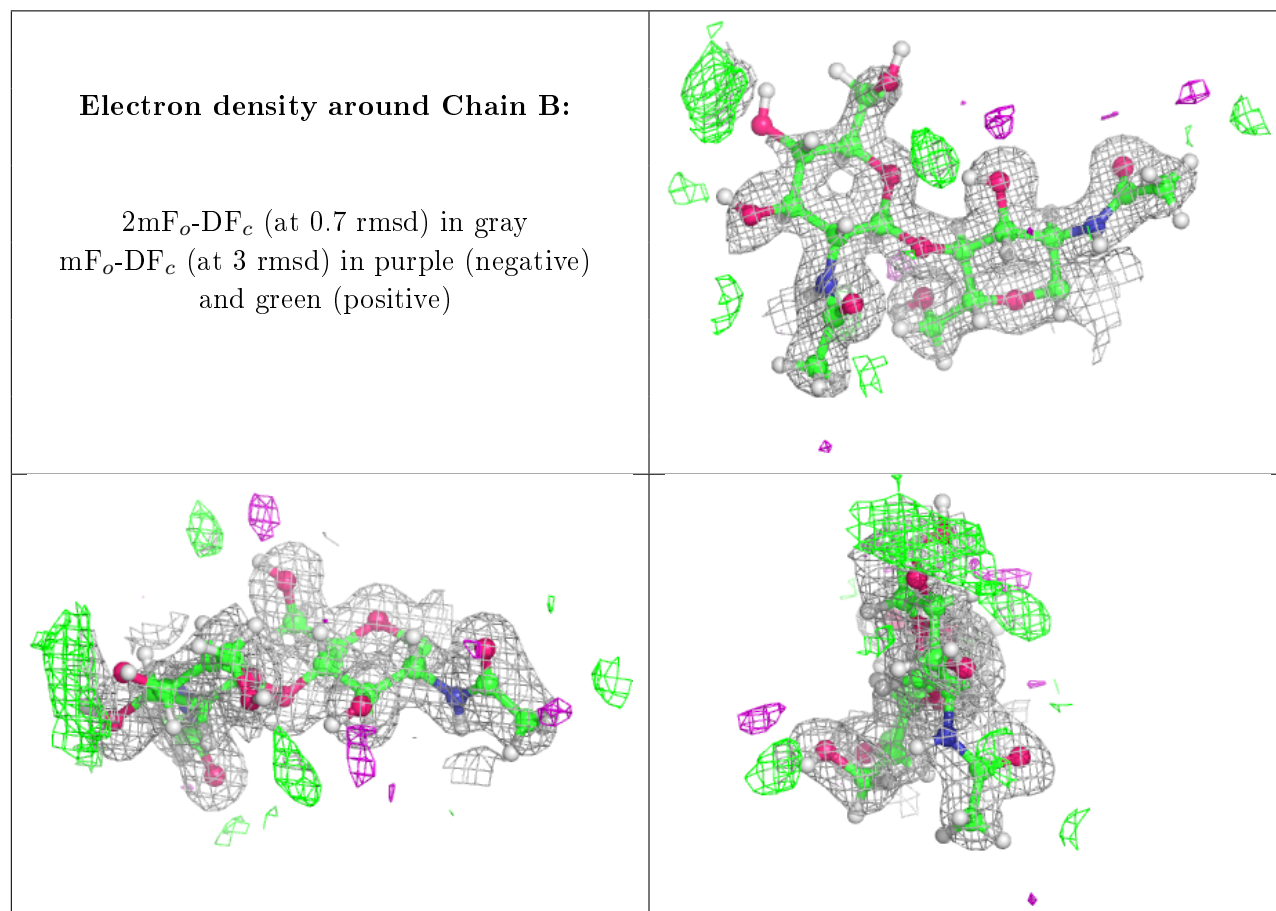
There are no non-standard protein/DNA/RNA residues in this entry.

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.

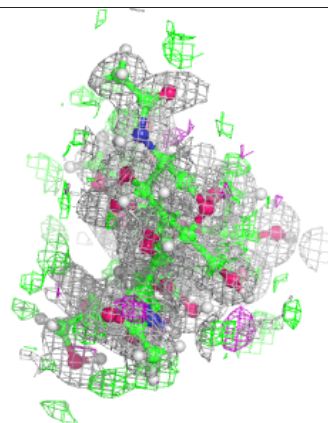
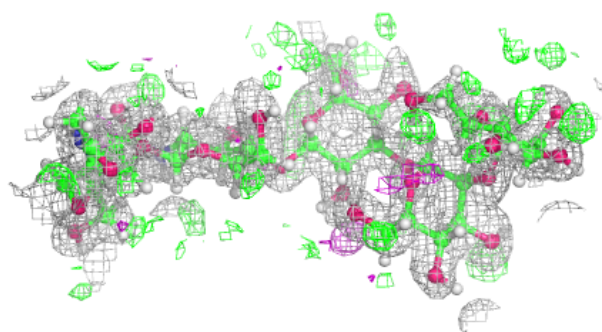
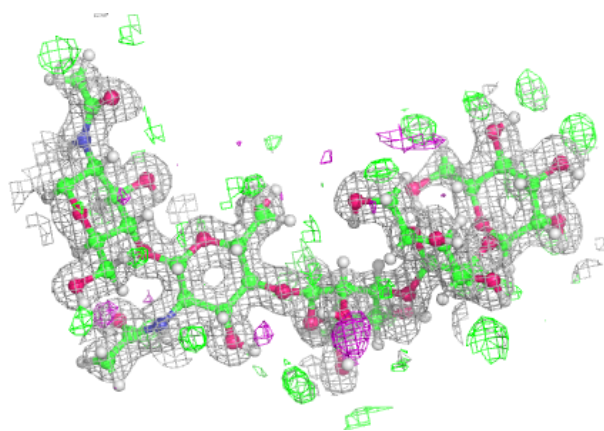
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	A	5	11/12	0.91	0.14	24,40,51,69	4
2	MAN	A	6	11/12	0.93	0.17	30,41,47,47	4
4	BMA	C	3	11/12	0.96	0.15	26,42,62,65	3
4	MAN	C	4	11/12	0.96	0.09	20,26,29,34	3
3	NAG	B	2	14/15	0.96	0.14	28,41,62,80	3
2	BMA	A	3	11/12	0.96	0.09	20,22,28,31	2
3	NAG	B	1	14/15	0.97	0.06	17,22,28,30	2
2	NAG	A	2	14/15	0.97	0.06	17,21,27,28	2
3	NAG	D	2	14/15	0.97	0.07	28,41,48,49	3
4	MAN	C	5	11/12	0.97	0.11	21,33,50,58	4
4	NAG	C	2	14/15	0.98	0.07	14,18,25,30	2
2	NAG	A	1	14/15	0.98	0.04	17,18,22,23	2
2	MAN	A	4	11/12	0.98	0.06	17,21,28,37	3
4	NAG	C	1	14/15	0.99	0.04	13,15,23,39	2
3	NAG	D	1	14/15	0.99	0.04	16,19,26,26	2

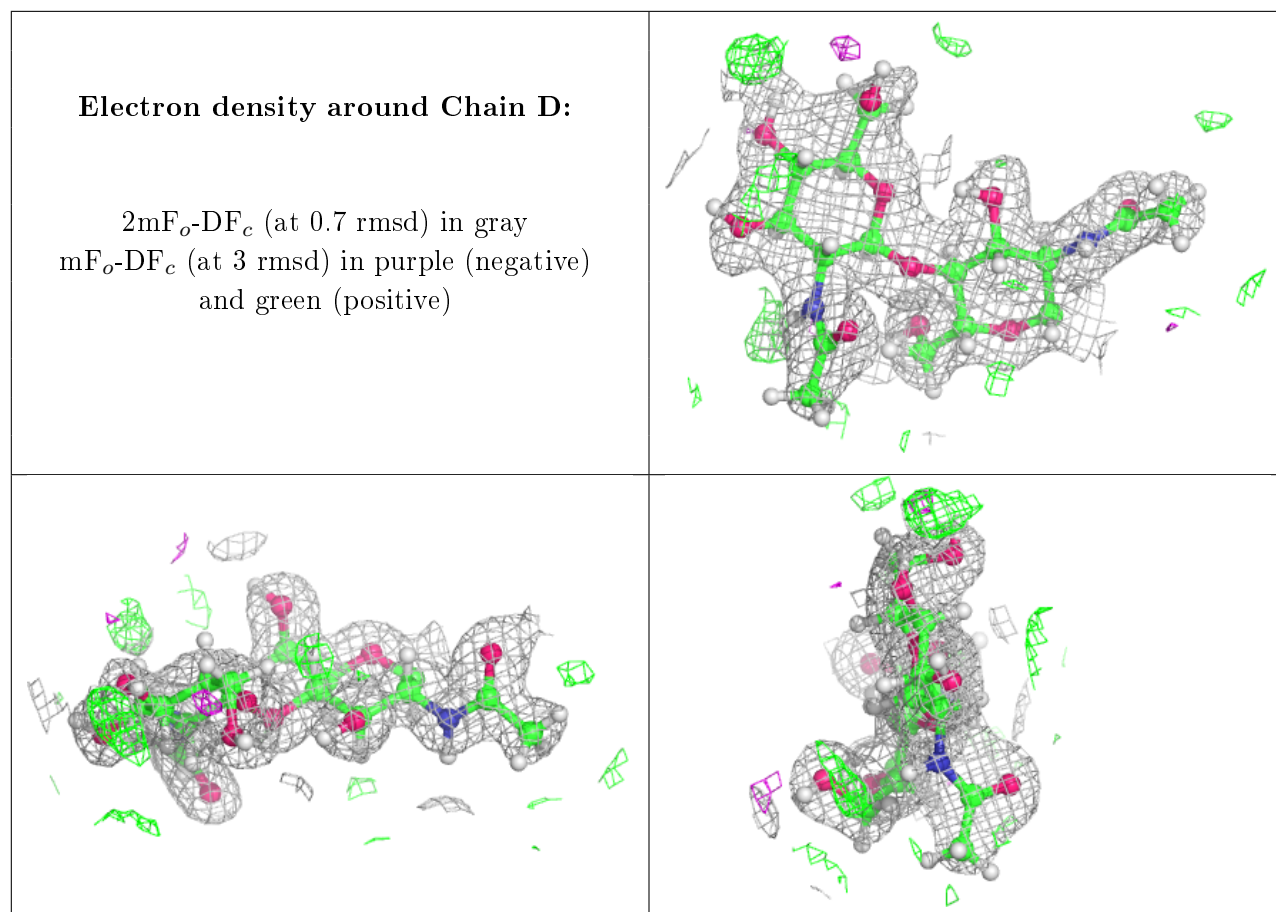
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain C:

$2mF_o-DF_c$ (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, 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
7	SO4	AAA	725	5/5	0.85	0.15	22,37,49,50	5
6	ACT	AAA	729	4/4	0.86	0.16	30,46,59,61	0
7	SO4	AAA	723	5/5	0.87	0.21	15,39,53,54	5
7	SO4	AAA	722	5/5	0.91	0.19	35,40,44,44	5
7	SO4	AAA	727	5/5	0.92	0.12	16,17,22,25	5
7	SO4	AAA	726	5/5	0.92	0.18	25,27,40,46	5
7	SO4	AAA	724[A]	5/5	0.94	0.17	26,30,39,44	5
5	GOL	AAA	730	6/6	0.94	0.16	16,25,40,41	14
7	SO4	AAA	724[B]	5/5	0.94	0.17	52,57,73,86	5
7	SO4	AAA	721	5/5	0.95	0.24	34,39,43,47	5
6	ACT	AAA	708	4/4	0.97	0.06	20,22,23,25	0
7	SO4	AAA	720	5/5	0.97	0.09	12,14,20,22	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	SO4	AAA	718	5/5	0.98	0.07	22,23,48,51	1
7	SO4	AAA	719	5/5	0.99	0.30	22,25,29,34	5
7	SO4	AAA	728	5/5	0.99	0.05	18,20,25,27	5
5	GOL	AAA	707	6/6	0.99	0.10	12,17,19,19	2

6.5 Other polymers [i](#)

There are no such residues in this entry.