



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:24 PM BST

PDB ID : 6ELY
Title : Crystal Structure of Mistletoe Lectin I (ML-I) from Viscum album in Complex with 4-N-Furfurylcytosine at 2.84 Å Resolution
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Deposited on : 2017-09-30
Resolution : 2.84 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 : 2.13.1
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

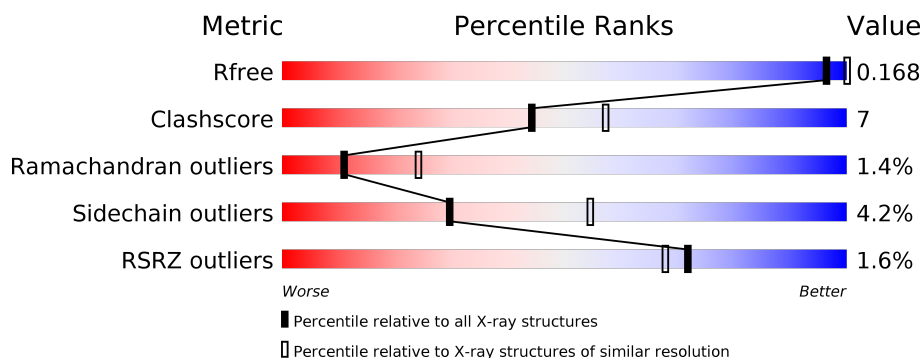
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	A	249	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
2	B	263	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>.</div> </div> </div>
3	C	2	<div> <div></div> <div>100%</div> </div>
4	D	3	<div> <div></div> <div>100%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1	X	-	-	-
5	NAG	A	301	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4324 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 Mistletoe Lectin I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1930	1220	331	375	4			

- Molecule 2 is a protein called Mistletoe Lectin I.

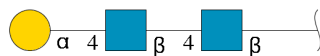
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	263	Total	C	N	O	S	0	0	0
			1995	1236	353	394	12			

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



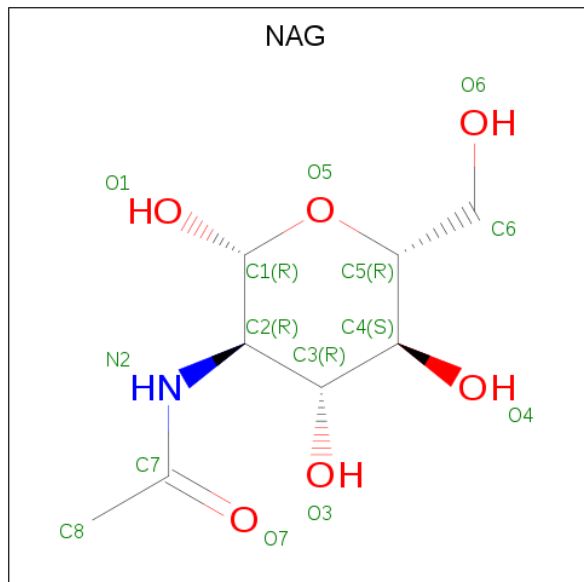
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-galactopyranose-(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	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

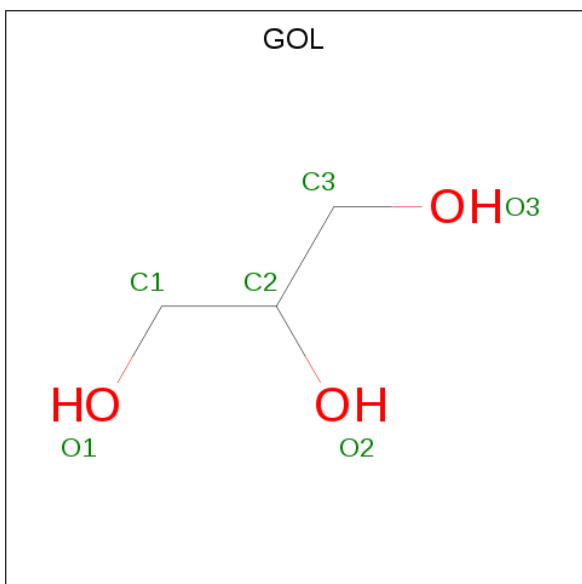
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Cl	0	0
			3	3		
6	A	5	Total	Cl	0	0
			5	5		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



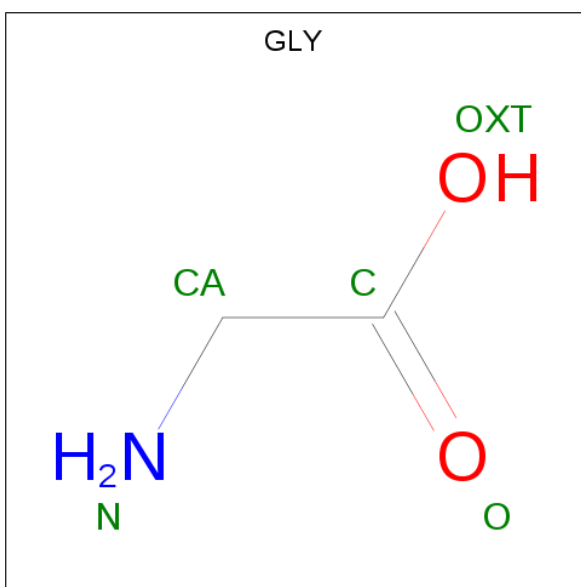
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



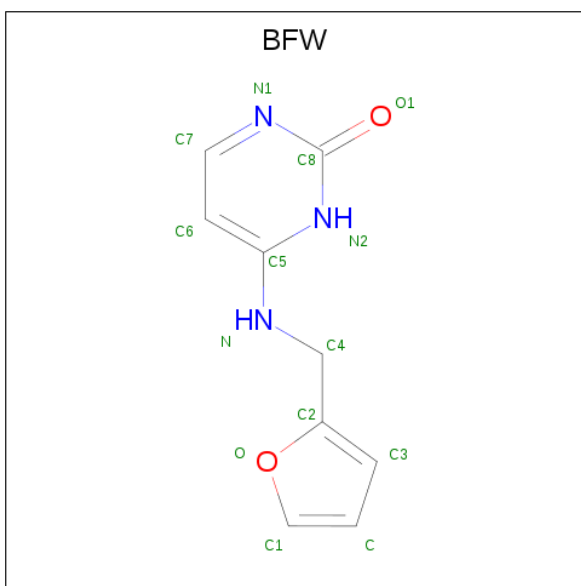
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GLYCINE (three-letter code: GLY) (formula: C₂H₅NO₂).



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

- Molecule 10 is 4-N-Furfurylcytosine (three-letter code: BFW) (formula: $C_9H_9N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	9	3	2		

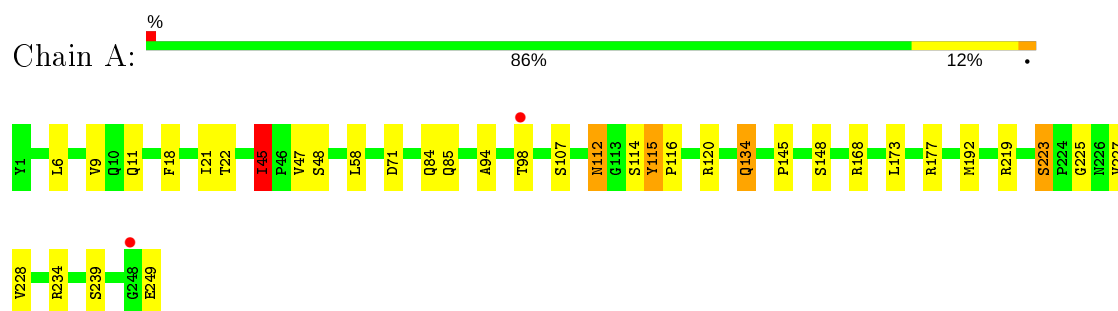
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	65	Total 65	O 65	0	0
11	B	80	Total 80	O 80	0	0

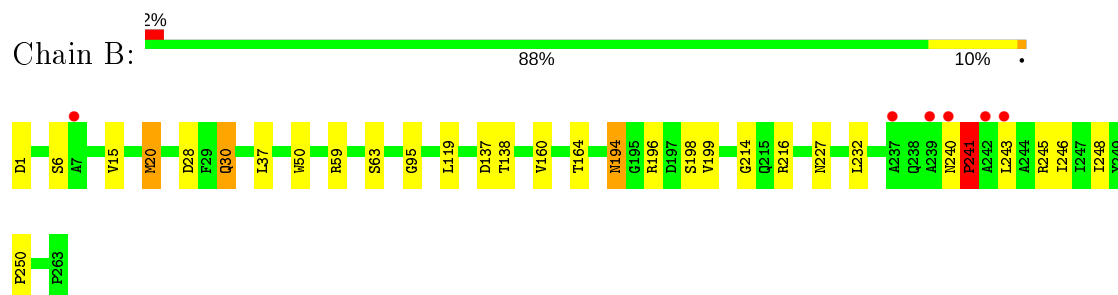
3 Residue-property plots

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.

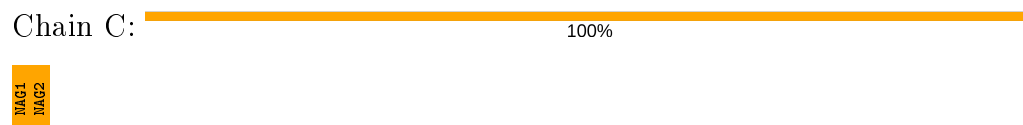
• Molecule 1: Mistletoe Lectin I



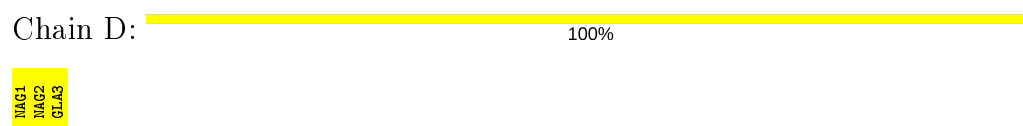
• Molecule 2: Mistletoe Lectin I



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	106.68Å 106.68Å 312.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.50 – 2.84 47.48 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.50-2.84) 99.8 (47.48-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.164 , 0.218 0.177 , 0.168	Depositor DCC
R_{free} test set	1222 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4324	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, CL, GLA, BFW, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	0/1968	0.97	1/2679 (0.0%)
2	B	0.85	0/2034	0.98	6/2776 (0.2%)
All	All	0.86	0/4002	0.97	7/5455 (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
2	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	196	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	B	216	ARG	NE-CZ-NH1	5.69	123.15	120.30
2	B	137	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	71	ASP	CB-CG-OD2	-5.18	113.63	118.30
2	B	241	PRO	N-CA-C	5.14	125.47	112.10
2	B	20	MET	CG-SD-CE	-5.05	92.12	100.20
2	B	137	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	243	LEU	Peptide

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	A	1930	0	1904	32	0
2	B	1995	0	1928	17	0
3	C	28	0	25	2	0
4	D	39	0	34	0	0
5	A	14	0	13	2	0
5	B	14	0	13	0	0
6	A	5	0	0	1	1
6	B	3	0	0	0	0
7	A	25	0	0	1	0
8	A	24	0	32	2	0
8	B	78	0	104	1	0
9	A	5	0	2	0	0
9	B	5	0	2	0	0
10	A	14	0	0	1	0
11	A	65	0	0	4	0
11	B	80	0	0	2	0
All	All	4324	0	4057	54	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 7.

All (54) 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:115:TYR:CG	1:A:116:PRO:HD3	2.02	0.94
1:A:115:TYR:CD2	1:A:116:PRO:HD3	2.09	0.88
1:A:115:TYR:CB	1:A:116:PRO:CD	2.62	0.77
11:B:401:HOH:O	3:C:2:NAG:O4	2.01	0.76
2:B:194:ASN:H	2:B:194:ASN:HD22	1.34	0.76
1:A:115:TYR:CB	1:A:116:PRO:HD3	2.16	0.75
1:A:115:TYR:HB3	1:A:116:PRO:CD	2.17	0.74
1:A:116:PRO:O	1:A:120:ARG:HG3	1.94	0.67
1:A:134:GLN:H	1:A:134:GLN:HE21	1.46	0.64
1:A:192:MET:HB2	6:A:304:CL:CL	2.36	0.63
1:A:219:ARG:NH2	1:A:227:VAL:HG21	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:HB3	1:A:116:PRO:HD3	1.82	0.61
1:A:9:VAL:HG23	1:A:11:GLN:H	1.66	0.60
1:A:115:TYR:HB3	1:A:116:PRO:HD2	1.83	0.60
2:B:232:LEU:HD12	2:B:248:ILE:HD12	1.83	0.59
1:A:84:GLN:HG2	1:A:85:GLN:HE21	1.66	0.58
1:A:115:TYR:CG	1:A:116:PRO:CD	2.84	0.58
2:B:194:ASN:HD21	2:B:227:ASN:ND2	2.02	0.57
5:A:301:NAG:H62	11:A:428:HOH:O	2.04	0.56
1:A:219:ARG:CZ	1:A:227:VAL:HG21	2.36	0.55
5:A:301:NAG:O3	11:A:401:HOH:O	2.17	0.55
1:A:134:GLN:NE2	1:A:134:GLN:H	2.06	0.54
8:A:314:GOL:O3	8:A:314:GOL:O1	2.26	0.53
2:B:30:GLN:HE21	8:B:313:GOL:H31	1.76	0.51
8:A:312:GOL:H12	11:A:442:HOH:O	2.10	0.51
1:A:45:ILE:O	1:A:45:ILE:HG23	2.10	0.51
1:A:47:VAL:HG21	1:A:94:ALA:O	2.12	0.50
1:A:112:ASN:HB2	1:A:114:SER:H	1.78	0.49
1:A:84:GLN:HG2	1:A:85:GLN:NE2	2.27	0.49
1:A:9:VAL:HG23	1:A:11:GLN:N	2.27	0.48
2:B:240:ASN:HB3	2:B:241:PRO:HD2	1.95	0.48
1:A:115:TYR:CD1	1:A:115:TYR:C	2.85	0.48
1:A:21:ILE:HG21	1:A:173:LEU:HD13	1.96	0.48
1:A:6:LEU:HB3	1:A:58:LEU:HD23	1.96	0.47
2:B:37:LEU:HD13	2:B:119:LEU:HD21	1.96	0.47
1:A:134:GLN:NE2	1:A:134:GLN:N	2.64	0.46
2:B:194:ASN:N	2:B:194:ASN:HD22	2.08	0.45
2:B:199:VAL:HG22	2:B:250:PRO:HD3	1.98	0.45
1:A:84:GLN:CG	1:A:85:GLN:HE21	2.30	0.44
2:B:50:TRP:HA	2:B:59:ARG:O	2.17	0.44
1:A:234:ARG:HD2	2:B:95:GLY:O	2.17	0.44
2:B:194:ASN:ND2	2:B:214:GLY:HA2	2.33	0.43
1:A:115:TYR:HA	10:A:317:BFW:O	2.19	0.43
1:A:98:THR:HG23	7:A:308:SO4:O2	2.18	0.42
2:B:194:ASN:HD21	2:B:214:GLY:HA2	1.84	0.42
1:A:18:PHE:CD2	1:A:177:ARG:NH1	2.87	0.42
1:A:168:ARG:NH1	11:A:409:HOH:O	2.51	0.42
1:A:45:ILE:O	1:A:45:ILE:CG2	2.67	0.42
2:B:240:ASN:CB	2:B:241:PRO:HD2	2.48	0.42
2:B:160:VAL:HG22	2:B:246:ILE:HD12	2.02	0.42
2:B:28:ASP:OD1	2:B:30:GLN:HB2	2.18	0.42
2:B:15:VAL:CG2	2:B:138:THR:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:MET:HB2	2:B:37:LEU:HG	2.03	0.41
11:B:471:HOH:O	3:C:1:NAG:H83	2.21	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)
6:A:303:CL:CL	6:A:303:CL:CL[11_555]	1.18	1.02

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	247/249 (99%)	230 (93%)	12 (5%)	5 (2%)	7	16
2	B	261/263 (99%)	251 (96%)	8 (3%)	2 (1%)	19	38
All	All	508/512 (99%)	481 (95%)	20 (4%)	7 (1%)	11	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	241	PRO
2	B	245	ARG
1	A	145	PRO
1	A	45	ILE
1	A	115	TYR
1	A	225	GLY
1	A	223	SER

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	A	212/212 (100%)	201 (95%)	11 (5%)	23	44
2	B	217/217 (100%)	210 (97%)	7 (3%)	39	63
All	All	429/429 (100%)	411 (96%)	18 (4%)	30	54

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	45	ILE
1	A	48	SER
1	A	107	SER
1	A	112	ASN
1	A	134	GLN
1	A	148	SER
1	A	223	SER
1	A	228	VAL
1	A	239	SER
1	A	249	GLU
2	B	1	ASP
2	B	6	SER
2	B	30	GLN
2	B	63	SER
2	B	164	THR
2	B	194	ASN
2	B	198	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	42	GLN
1	A	85	GLN
1	A	134	GLN

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Mol	Chain	Res	Type
1	A	161	GLN
2	B	30	GLN
2	B	122	GLN
2	B	227	ASN
2	B	238	GLN
2	B	240	ASN

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 ⓘ

5 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$
3	NAG	C	1	3,2	14,14,15	0.71	0	17,19,21	2.17	7 (41%)
3	NAG	C	2	3	14,14,15	0.55	0	17,19,21	1.56	3 (17%)
4	NAG	D	1	2,4	14,14,15	0.94	0	17,19,21	2.06	8 (47%)
4	NAG	D	2	4	14,14,15	1.01	1 (7%)	17,19,21	1.74	3 (17%)
4	GLA	D	3	4	11,11,12	1.30	1 (9%)	15,15,17	2.28	2 (13%)

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
3	NAG	C	1	3,2	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	GLA	D	3	4	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2	NAG	O4-C4	2.40	1.48	1.43
4	D	3	GLA	C2-C3	2.08	1.55	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	GLA	C1-O5-C5	7.82	122.79	112.19
4	D	2	NAG	C4-C3-C2	4.57	117.72	111.02
3	C	1	NAG	C2-N2-C7	4.15	128.82	122.90
4	D	1	NAG	C3-C4-C5	-3.83	103.41	110.24
3	C	1	NAG	C8-C7-N2	3.72	122.41	116.10
3	C	2	NAG	O5-C1-C2	-3.69	105.46	111.29
4	D	1	NAG	O3-C3-C2	-3.31	102.61	109.47
4	D	2	NAG	O5-C1-C2	-3.25	106.15	111.29
3	C	2	NAG	C1-C2-N2	3.11	115.80	110.49
3	C	2	NAG	C1-O5-C5	3.03	116.30	112.19
3	C	1	NAG	O7-C7-N2	-3.01	116.43	121.95
4	D	1	NAG	C8-C7-N2	2.97	121.12	116.10
4	D	2	NAG	O3-C3-C2	-2.94	103.38	109.47
4	D	1	NAG	O7-C7-C8	-2.94	116.60	122.06
3	C	1	NAG	O3-C3-C4	-2.86	103.74	110.35
4	D	1	NAG	C4-C3-C2	2.81	115.14	111.02
3	C	1	NAG	C1-O5-C5	2.66	115.80	112.19
4	D	1	NAG	O5-C1-C2	-2.65	107.10	111.29
4	D	1	NAG	C1-O5-C5	2.63	115.76	112.19
3	C	1	NAG	C4-C3-C2	2.59	114.82	111.02
4	D	1	NAG	O5-C5-C6	2.24	110.71	107.20
3	C	1	NAG	C1-C2-N2	-2.23	106.68	110.49
4	D	3	GLA	O5-C5-C6	2.17	110.60	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1	NAG	C1

All (11) torsion outliers are listed below:

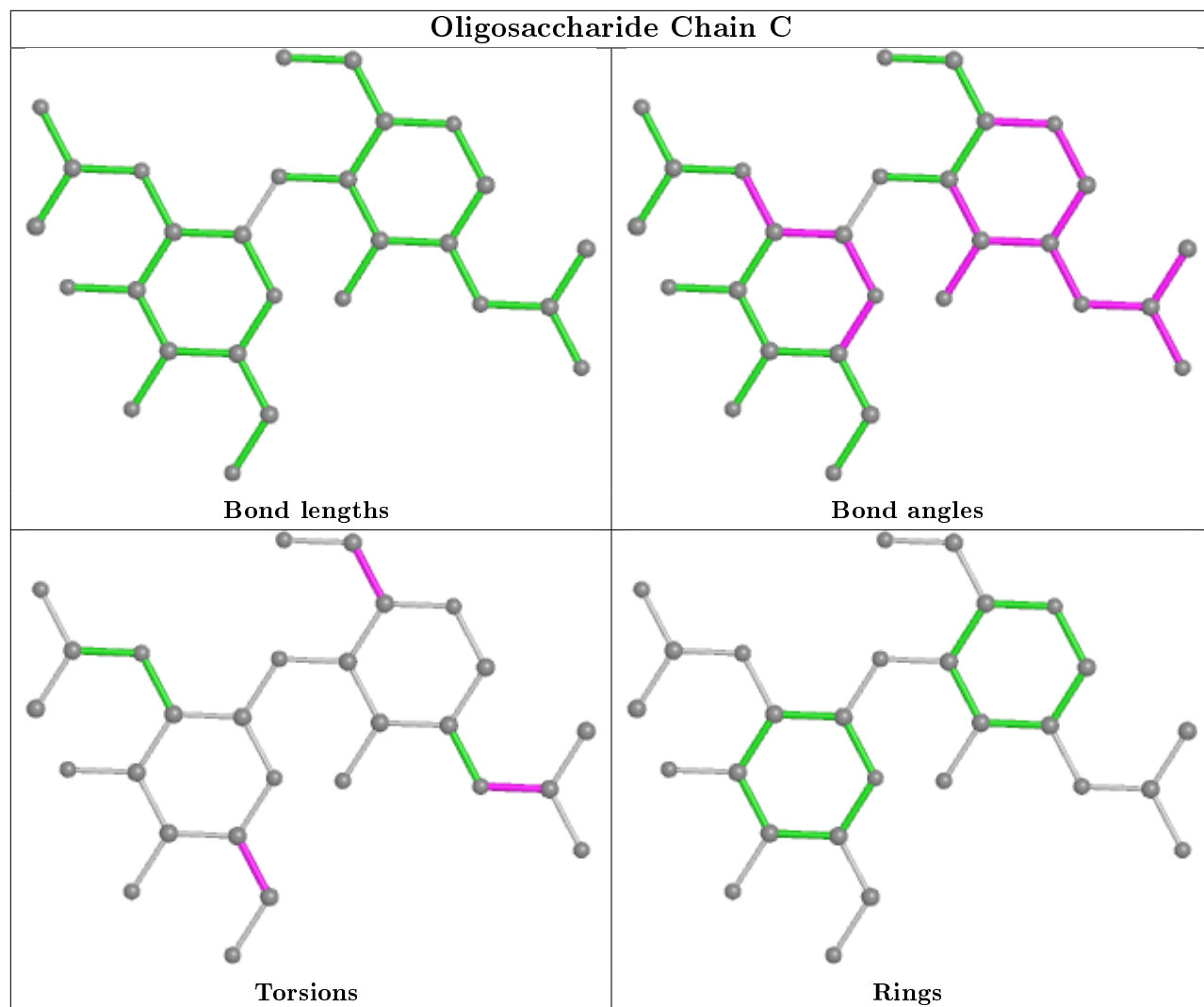
Mol	Chain	Res	Type	Atoms
4	D	3	GLA	O5-C5-C6-O6
4	D	3	GLA	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

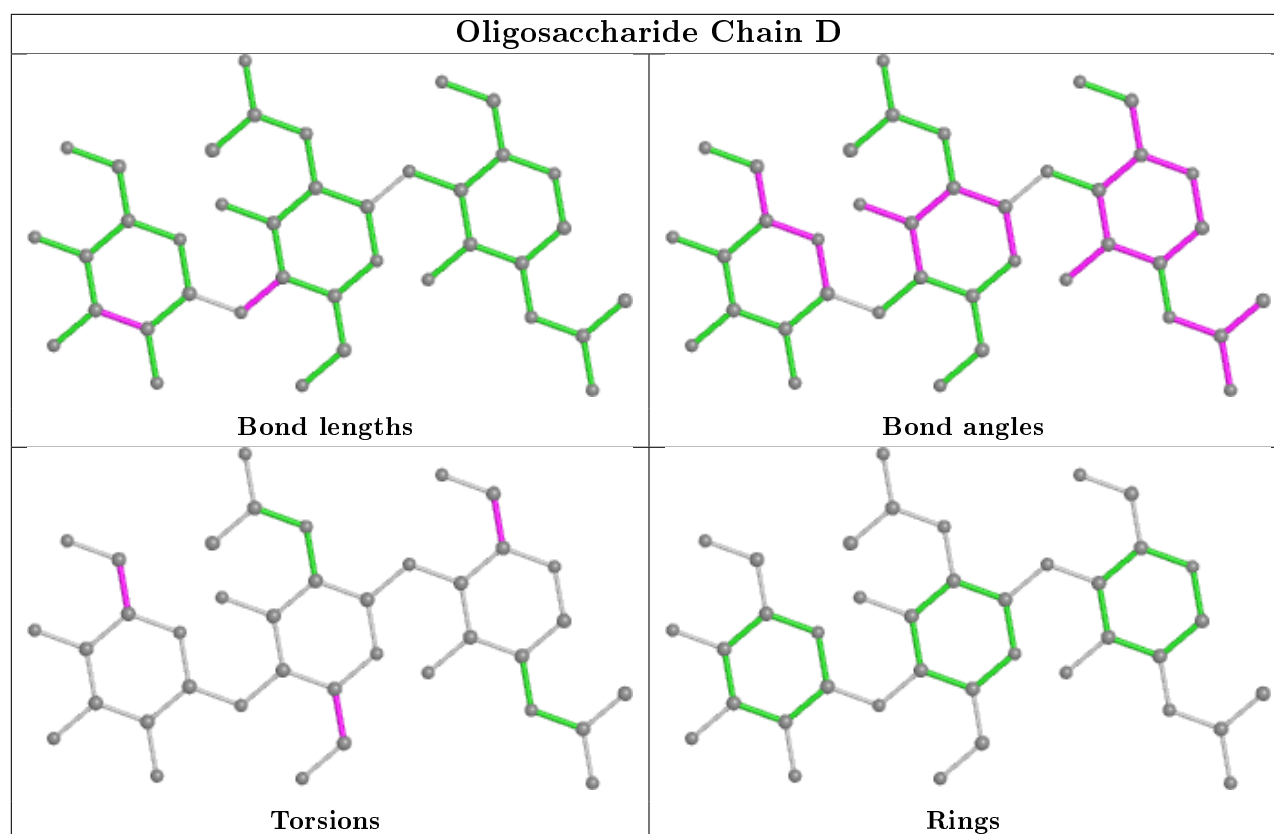
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	1	0
3	C	1	NAG	1	0

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





5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 8 are monoatomic - leaving 27 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	$\# Z > 2$
8	GOL	B	320	-	5,5,5	0.58	0	5,5,5	0.84	0
8	GOL	B	315	-	5,5,5	0.40	0	5,5,5	0.55	0
8	GOL	B	311	-	5,5,5	0.25	0	5,5,5	0.85	0
10	BFW	A	317	-	11,15,15	1.05	1 (9%)	12,19,19	7.20	6 (50%)
8	GOL	A	315	-	5,5,5	0.42	0	5,5,5	0.53	0
8	GOL	B	313	-	5,5,5	0.97	0	5,5,5	1.16	0
8	GOL	B	316	-	5,5,5	0.45	0	5,5,5	0.86	0
8	GOL	A	313	-	5,5,5	1.02	1 (20%)	5,5,5	1.46	1 (20%)
8	GOL	B	314	-	5,5,5	0.62	0	5,5,5	1.16	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	A	308	-	4,4,4	0.50	0	6,6,6	0.62	0
7	SO4	A	310	-	4,4,4	0.45	0	6,6,6	0.52	0
8	GOL	B	318	-	5,5,5	0.64	0	5,5,5	0.87	0
7	SO4	A	307	-	4,4,4	0.53	0	6,6,6	0.81	0
8	GOL	B	321	-	5,5,5	0.47	0	5,5,5	0.68	0
8	GOL	A	314	-	5,5,5	0.62	0	5,5,5	0.49	0
8	GOL	B	322	-	5,5,5	0.68	0	5,5,5	1.20	0
5	NAG	A	301	1	14,14,15	1.19	2 (14%)	17,19,21	2.70	7 (41%)
8	GOL	A	312	-	5,5,5	1.14	1 (20%)	5,5,5	1.12	0
8	GOL	B	312	-	5,5,5	1.18	0	5,5,5	0.97	0
7	SO4	A	309	-	4,4,4	0.48	0	6,6,6	0.68	0
7	SO4	A	311	-	4,4,4	0.57	0	6,6,6	0.74	0
5	NAG	B	301	2	14,14,15	0.75	0	17,19,21	2.37	7 (41%)
8	GOL	B	319	-	5,5,5	0.81	0	5,5,5	0.80	0
8	GOL	B	317	-	5,5,5	0.68	0	5,5,5	0.96	0
8	GOL	B	310	-	5,5,5	1.20	0	5,5,5	1.96	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	315	-	-	2/4/4/4	-
8	GOL	B	313	-	-	2/4/4/4	-
10	BFW	A	317	-	-	2/3/5/5	0/2/2/2
8	GOL	B	320	-	-	0/4/4/4	-
8	GOL	B	318	-	-	2/4/4/4	-
5	NAG	A	301	1	1/1/5/7	2/6/23/26	0/1/1/1
8	GOL	B	316	-	-	1/4/4/4	-
8	GOL	A	313	-	-	0/4/4/4	-
8	GOL	A	312	-	-	1/4/4/4	-
8	GOL	B	312	-	-	3/4/4/4	-
8	GOL	B	315	-	-	3/4/4/4	-
8	GOL	B	311	-	-	2/4/4/4	-
8	GOL	A	314	-	-	2/4/4/4	-
8	GOL	B	321	-	-	2/4/4/4	-
5	NAG	B	301	2	-	3/6/23/26	0/1/1/1
8	GOL	B	322	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	314	-	-	2/4/4/4	-
8	GOL	B	319	-	-	3/4/4/4	-
8	GOL	B	317	-	-	2/4/4/4	-
8	GOL	B	310	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	317	BFW	C8-N2	-2.59	1.33	1.38
5	A	301	NAG	C1-C2	2.44	1.56	1.52
5	A	301	NAG	C2-N2	2.24	1.50	1.46
8	A	313	GOL	O2-C2	-2.07	1.37	1.43
8	A	312	GOL	O3-C3	2.04	1.51	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	317	BFW	C7-N1-C8	18.35	123.47	114.42
10	A	317	BFW	N1-C8-N2	-13.93	117.36	128.43
10	A	317	BFW	C2-C4-N	-7.51	96.44	112.71
5	A	301	NAG	O5-C1-C2	6.94	122.24	111.29
5	A	301	NAG	C2-N2-C7	5.81	131.17	122.90
5	B	301	NAG	C8-C7-N2	4.88	124.36	116.10
5	B	301	NAG	O7-C7-N2	-4.23	114.18	121.95
10	A	317	BFW	C6-C7-N1	-4.14	118.81	123.96
5	B	301	NAG	O5-C1-C2	-3.84	105.22	111.29
5	A	301	NAG	C1-O5-C5	3.02	116.28	112.19
8	B	310	GOL	O3-C3-C2	2.95	124.36	110.20
5	A	301	NAG	O4-C4-C5	2.85	116.38	109.30
5	B	301	NAG	C2-N2-C7	2.80	126.88	122.90
5	B	301	NAG	O3-C3-C2	2.67	114.99	109.47
5	B	301	NAG	C3-C4-C5	-2.65	105.52	110.24
8	B	310	GOL	O2-C2-C3	2.48	120.05	109.12
8	A	313	GOL	O2-C2-C3	-2.38	98.63	109.12
8	B	314	GOL	O1-C1-C2	2.37	121.56	110.20
10	A	317	BFW	N-C5-N2	-2.36	112.46	116.43
5	A	301	NAG	O3-C3-C2	2.34	114.31	109.47
10	A	317	BFW	C4-C2-C3	-2.31	125.18	129.01
5	B	301	NAG	O5-C5-C6	2.29	110.79	107.20
5	A	301	NAG	O7-C7-C8	-2.12	118.12	122.06
5	A	301	NAG	O7-C7-N2	2.10	125.81	121.95

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	301	NAG	C1

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	317	BFW	N2-C5-N-C4
10	A	317	BFW	C6-C5-N-C4
8	B	313	GOL	C1-C2-C3-O3
8	B	318	GOL	C1-C2-C3-O3
8	B	314	GOL	C1-C2-C3-O3
8	A	315	GOL	C1-C2-C3-O3
8	B	321	GOL	C1-C2-C3-O3
8	A	314	GOL	C1-C2-C3-O3
5	A	301	NAG	C3-C2-N2-C7
8	B	312	GOL	O1-C1-C2-C3
8	B	319	GOL	C1-C2-C3-O3
8	B	319	GOL	O2-C2-C3-O3
5	B	301	NAG	C8-C7-N2-C2
5	B	301	NAG	O7-C7-N2-C2
5	A	301	NAG	O5-C5-C6-O6
8	B	316	GOL	C1-C2-C3-O3
8	A	312	GOL	O1-C1-C2-C3
8	B	317	GOL	C1-C2-C3-O3
8	A	315	GOL	O2-C2-C3-O3
8	B	321	GOL	O2-C2-C3-O3
8	A	314	GOL	O2-C2-C3-O3
8	B	317	GOL	O2-C2-C3-O3
8	B	313	GOL	O2-C2-C3-O3
8	B	318	GOL	O2-C2-C3-O3
8	B	314	GOL	O2-C2-C3-O3
8	B	312	GOL	O1-C1-C2-O2
8	B	312	GOL	O2-C2-C3-O3
8	B	315	GOL	O1-C1-C2-O2
8	B	311	GOL	O1-C1-C2-O2
8	B	310	GOL	O2-C2-C3-O3
8	B	311	GOL	O1-C1-C2-C3
8	B	319	GOL	O1-C1-C2-C3
8	B	315	GOL	O1-C1-C2-C3
8	B	315	GOL	C1-C2-C3-O3
5	B	301	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	317	BFW	1	0
8	B	313	GOL	1	0
7	A	308	SO4	1	0
8	A	314	GOL	1	0
5	A	301	NAG	2	0
8	A	312	GOL	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	A	249/249 (100%)	-0.37	2 (0%) 86 85	25, 41, 74, 115	0
2	B	263/263 (100%)	-0.40	6 (2%) 60 55	23, 34, 70, 117	0
All	All	512/512 (100%)	-0.39	8 (1%) 72 68	23, 37, 73, 117	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	239	ALA	9.5
1	A	248	GLY	5.1
2	B	242	ALA	3.9
2	B	240	ASN	3.8
1	A	98	THR	3.0
2	B	243	LEU	3.0
2	B	7	ALA	2.6
2	B	237	ALA	2.5

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	GLA	D	3	11/12	0.65	0.39	97,109,123,129	0

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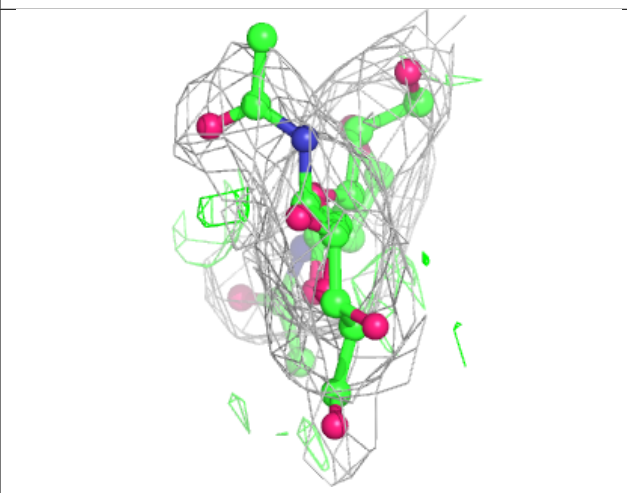
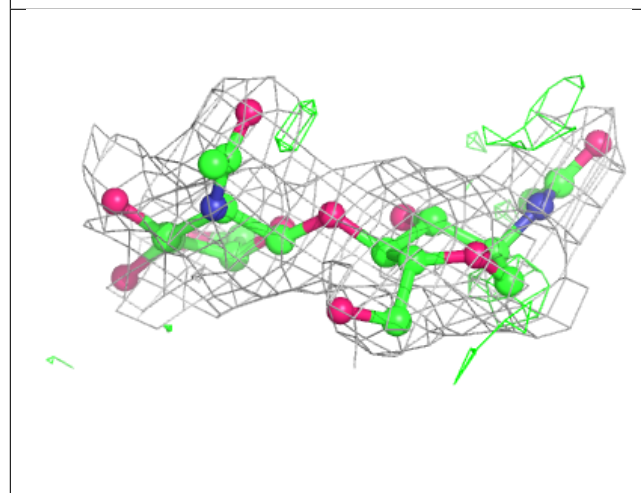
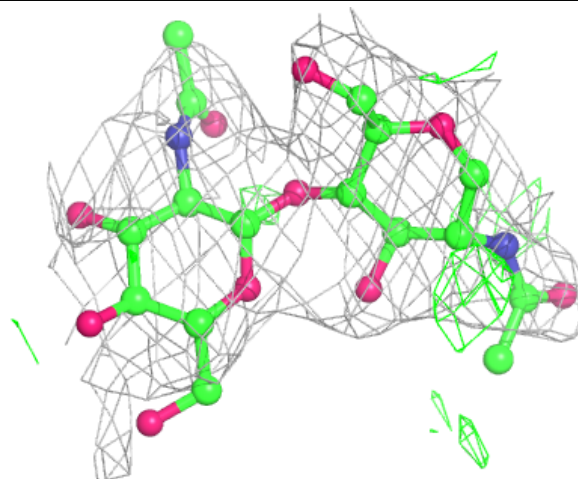
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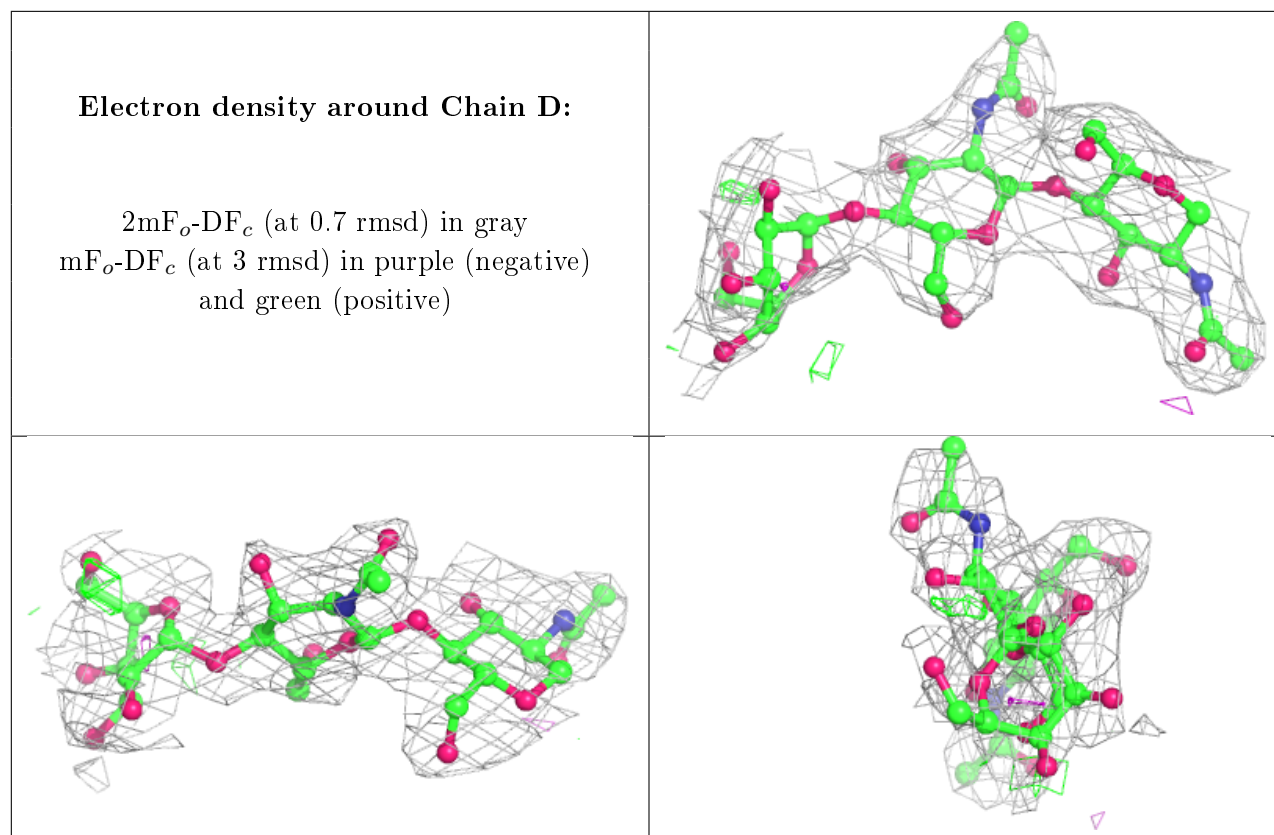
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	C	2	14/15	0.88	0.16	65,87,95,96	0
4	NAG	D	2	14/15	0.93	0.33	53,78,99,114	0
3	NAG	C	1	14/15	0.96	0.14	48,57,82,86	0
4	NAG	D	1	14/15	0.98	0.16	31,34,41,48	0

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)





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(\AA^2)	Q<0.9
6	CL	B	307	1/1	0.57	0.31	69,69,69,69	0
8	GOL	B	322	6/6	0.81	0.34	70,81,88,89	0
6	CL	A	305	1/1	0.82	0.13	61,61,61,61	0
8	GOL	B	321	6/6	0.84	0.27	64,78,89,98	0
5	NAG	A	301	14/15	0.84	0.16	68,81,94,98	0
9	GLY	B	323	5/5	0.84	0.26	64,71,80,86	0
8	GOL	B	313	6/6	0.85	0.26	48,54,62,63	0
8	GOL	B	318	6/6	0.86	0.36	60,69,73,74	0
8	GOL	B	316	6/6	0.86	0.20	61,72,75,78	0
6	CL	B	309	1/1	0.86	0.12	68,68,68,68	0
8	GOL	B	320	6/6	0.87	0.31	60,63,68,72	0
8	GOL	B	319	6/6	0.88	0.24	60,66,76,76	0
10	BFW	A	317	14/14	0.90	0.24	81,87,110,124	0
8	GOL	B	315	6/6	0.90	0.27	57,69,73,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	CL	A	302	1/1	0.91	0.14	66,66,66,66	0
8	GOL	B	317	6/6	0.91	0.22	50,62,63,64	0
8	GOL	A	314	6/6	0.92	0.25	48,70,77,78	0
7	SO4	A	308	5/5	0.92	0.28	86,89,104,114	0
5	NAG	B	301	14/15	0.92	0.20	45,72,81,81	0
6	CL	A	304	1/1	0.92	0.16	63,63,63,63	0
7	SO4	A	307	5/5	0.93	0.16	69,73,88,90	0
6	CL	A	306	1/1	0.93	0.28	47,47,47,47	0
8	GOL	B	311	6/6	0.93	0.26	54,57,59,66	0
8	GOL	A	312	6/6	0.93	0.25	30,37,38,40	0
8	GOL	B	312	6/6	0.93	0.21	44,48,54,59	0
9	GLY	A	316	5/5	0.94	0.26	58,66,73,75	0
8	GOL	A	315	6/6	0.94	0.20	48,59,65,74	0
6	CL	B	308	1/1	0.94	0.10	58,58,58,58	0
8	GOL	A	313	6/6	0.95	0.17	30,43,48,48	0
7	SO4	A	311	5/5	0.95	0.23	72,82,86,93	0
8	GOL	B	310	6/6	0.95	0.17	37,40,43,47	0
7	SO4	A	310	5/5	0.96	0.28	74,75,82,83	0
8	GOL	B	314	6/6	0.98	0.17	29,32,39,44	0
6	CL	A	303	1/1	0.99	0.12	52,52,52,52	0
7	SO4	A	309	5/5	0.99	0.12	35,40,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.