



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:38 AM UTC

PDB ID : 7O84 / pdb_00007o84
Title : Structure of the PL6 family alginate lyase Pedsa0632 from Pseudopedobacter saltans in complex with substrate
Authors : Ballut, L.; Violot, S.; Carrique, L.; Aghajari, N.
Deposited on : 2021-04-14
Resolution : 2.18 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

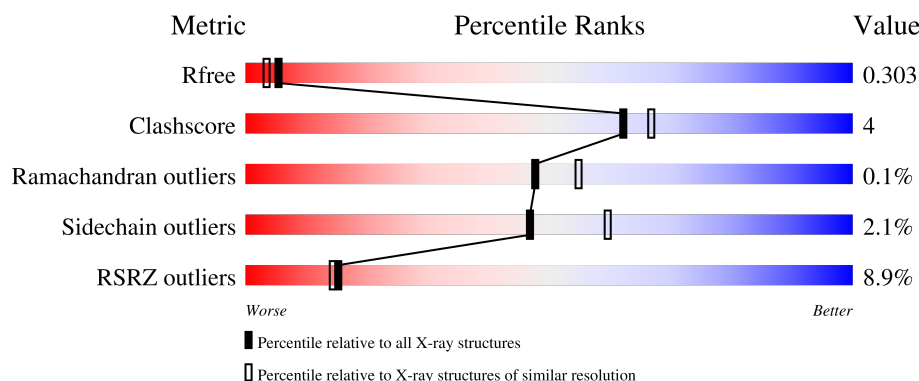
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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 $\leq 5\%$. 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	426	
1	B	426	
2	C	3	
3	D	4	

2 Entry composition [i](#)

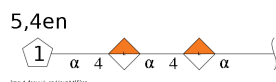
There are 4 unique types of molecules in this entry. The entry contains 6749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alginate lyase.

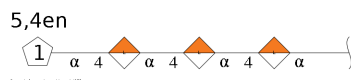
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3159	1986	547	618	8			
1	B	407	Total	C	N	O	S	0	0	0
			3134	1974	541	612	7			

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			36	18	18			

- Molecule 3 is an oligosaccharide called 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	4	Total	C	O	0	0	0
			48	24	24			

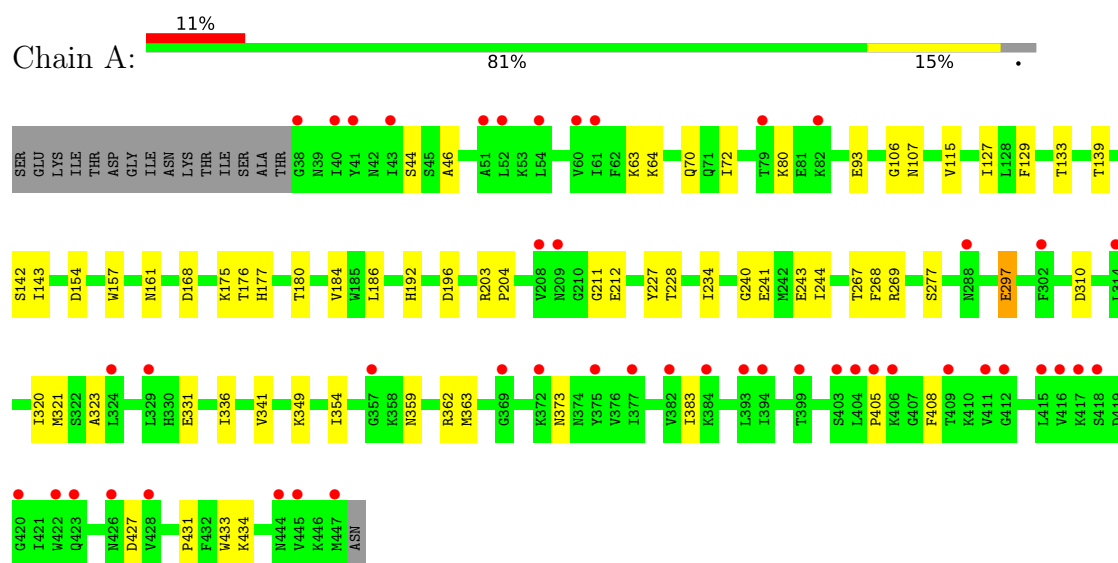
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total 178	O 178	0	0
4	B	194	Total 194	O 194	0	0

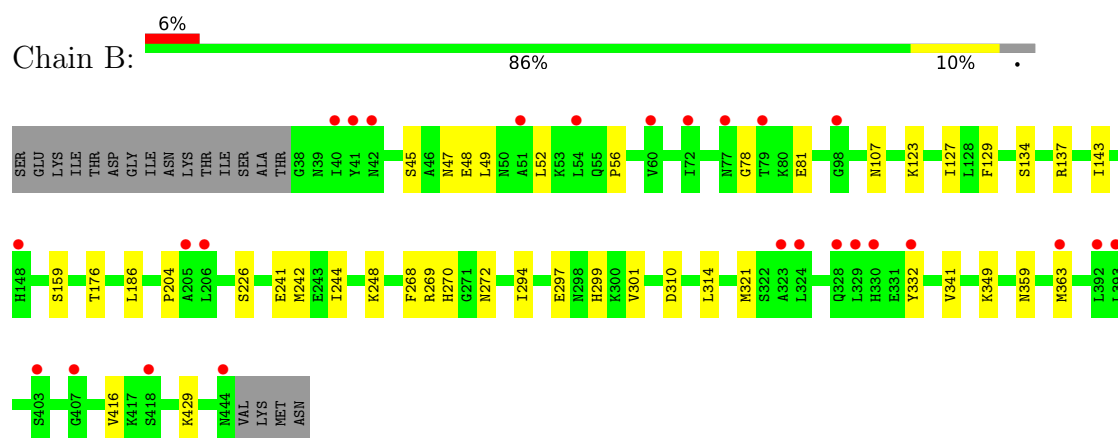
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Alginate lyase



• Molecule 1: Alginate lyase



• Molecule 2: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid





- Molecule 3: 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid-(1-4)-alpha-L-gulopyranuronic acid

Chain D:  25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.18Å 47.58Å 116.20Å 90.00° 98.25° 90.00°	Depositor
Resolution (Å)	43.97 – 2.18 43.97 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.3 (43.97-2.18) 98.3 (43.97-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.10.3 (29-NOV-2019)	Depositor
R, R_{free}	0.228 , 0.286 0.237 , 0.303	Depositor DCC
R_{free} test set	2282 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6749	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.07% 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: MAW, LGU

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	0.73	1/3228 (0.0%)	1.13	9/4380 (0.2%)
1	B	0.74	0/3203	1.09	5/4350 (0.1%)
All	All	0.74	1/6431 (0.0%)	1.11	14/8730 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	GLU	CA-C	6.61	1.57	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ILE	N-CA-C	-6.48	104.44	110.53
1	A	321	MET	N-CA-C	6.37	118.94	110.53
1	B	244	ILE	N-CA-C	-6.15	104.75	110.53
1	B	321	MET	N-CA-C	6.12	118.61	110.53
1	A	359	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	297	GLU	N-CA-C	5.35	118.46	109.95
1	A	277	SER	N-CA-C	5.27	117.40	109.23
1	A	268	PHE	CA-CB-CG	5.12	118.92	113.80
1	B	129	PHE	N-CA-C	-5.08	100.88	109.07
1	A	154	ASP	N-CA-C	5.08	117.01	108.73
1	B	268	PHE	CA-CB-CG	5.06	118.86	113.80
1	B	297	GLU	N-CA-C	5.04	117.97	109.95
1	A	177	HIS	CA-C-N	5.02	128.79	121.31
1	A	177	HIS	C-N-CA	5.02	128.79	121.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3159	0	2988	31	0
1	B	3134	0	2961	15	0
2	C	36	0	19	1	0
3	D	48	0	25	5	0
4	A	178	0	0	1	0
4	B	194	0	0	0	0
All	All	6749	0	5993	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (51) 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:433:TRP:NE1	1:A:434:LYS:HE3	1.92	0.85
1:A:433:TRP:HE1	1:A:434:LYS:HE3	1.54	0.71
1:B:242:MET:HE1	1:B:314:LEU:HB3	1.73	0.71
1:A:297:GLU:HG2	1:A:336:ILE:HB	1.79	0.64
1:A:46:ALA:HB2	1:A:72:ILE:HD13	1.82	0.60
1:A:176:THR:HG22	1:A:204:PRO:HG3	1.85	0.58
1:B:107:ASN:OD1	1:B:134:SER:OG	2.22	0.55
1:A:234:ILE:HD11	1:A:433:TRP:HB2	1.89	0.55
1:A:44:SER:HB3	1:A:63:LYS:HD2	1.88	0.55
1:A:323:ALA:HA	1:A:362:ARG:HG2	1.91	0.52
1:A:139:THR:HA	1:A:168:ASP:O	2.10	0.52
3:D:1:LGU:H3	3:D:2:LGU:H5	1.93	0.51
1:A:405:PRO:HD2	1:A:408:PHE:HB2	1.94	0.49
1:A:433:TRP:CD1	1:A:434:LYS:HE3	2.46	0.49
1:B:56:PRO:HG3	1:B:78:GLY:HA2	1.95	0.49
1:B:248:LYS:HE3	1:B:269:ARG:HG2	1.95	0.49
1:A:211:GLY:C	1:A:241:GLU:HG2	2.37	0.49
1:A:431:PRO:HD2	1:A:434:LYS:HG3	1.94	0.48
1:A:127:ILE:HD12	1:A:143:ILE:HD11	1.95	0.48
1:B:49:LEU:HA	1:B:52:LEU:HD12	1.96	0.48
1:A:184:VAL:HG21	1:A:228:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:HG23	1:A:212:GLU:HB2	1.96	0.47
1:B:45:SER:HB3	1:B:48:GLU:HG3	1.96	0.47
1:A:157:TRP:CD1	1:A:175:LYS:HE2	2.50	0.47
1:B:332:TYR:OH	3:D:4:MAW:C4	2.62	0.47
1:B:294:ILE:HD11	1:B:301:VAL:HG21	1.97	0.46
3:D:1:LGU:H2	3:D:2:LGU:H5	1.98	0.46
1:A:168:ASP:HA	1:A:196:ASP:O	2.16	0.46
1:A:310:ASP:O	1:A:349:LYS:HD3	2.16	0.45
1:A:341:VAL:HG23	1:A:373:ASN:HB2	1.98	0.45
1:B:176:THR:HG22	1:B:204:PRO:HG3	1.98	0.45
4:A:562:HOH:O	2:C:3:MAW:H4	2.16	0.45
1:A:192:HIS:HA	1:A:227:TYR:O	2.17	0.45
1:B:186:LEU:HD21	1:B:226:SER:HB2	1.98	0.45
1:B:272:ASN:HA	1:B:299:HIS:CE1	2.51	0.45
1:A:106:GLY:O	1:A:133:THR:HA	2.17	0.44
1:A:115:VAL:HG13	1:A:142:SER:HB2	1.99	0.44
1:A:354:ILE:HD11	1:A:383:ILE:HD11	2.00	0.44
3:D:1:LGU:H3	3:D:2:LGU:C5	2.48	0.43
1:A:431:PRO:HB3	1:A:433:TRP:CZ3	2.55	0.42
1:A:70:GLN:HB3	1:A:72:ILE:HD11	2.00	0.42
1:B:310:ASP:O	1:B:349:LYS:HD2	2.20	0.41
1:A:243:GLU:HG2	1:A:267:THR:HB	2.01	0.41
1:B:248:LYS:HE2	1:B:270:HIS:CD2	2.56	0.41
1:A:269:ARG:HD2	1:A:269:ARG:HA	1.90	0.41
1:A:64:LYS:HG3	1:A:93:GLU:HB3	2.03	0.41
1:B:127:ILE:HD12	1:B:143:ILE:HD11	2.03	0.41
1:A:203:ARG:HD3	1:A:240:GLY:HA3	2.02	0.41
1:B:359:ASN:O	1:B:363:MET:SD	2.79	0.41
3:D:1:LGU:C2	3:D:2:LGU:H5	2.50	0.40
1:A:129:PHE:O	1:A:161:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

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	A	408/426 (96%)	397 (97%)	11 (3%)	0	100	100
1	B	405/426 (95%)	394 (97%)	10 (2%)	1 (0%)	43	49
All	All	813/852 (95%)	791 (97%)	21 (3%)	1 (0%)	48	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	LYS

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	337/370 (91%)	331 (98%)	6 (2%)	51	65
1	B	333/370 (90%)	325 (98%)	8 (2%)	43	55
All	All	670/740 (90%)	656 (98%)	14 (2%)	47	59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	107	ASN
1	A	186	LEU
1	A	320	ILE
1	A	363	MET
1	A	427	ASP
1	B	47	ASN
1	B	81	GLU
1	B	137	ARG
1	B	159	SER
1	B	241	GLU
1	B	341	VAL

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Mol	Chain	Res	Type
1	B	416	VAL
1	B	429	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	251	HIS
1	A	255	ASN
1	A	256	ASN
1	A	278	ASN
1	B	47	ASN
1	B	99	ASN
1	B	278	ASN
1	B	328	GLN

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 ⓘ

7 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	LGU	C	1	2	13,13,13	0.92	0	18,19,19	1.10	2 (11%)
2	LGU	C	2	2	12,12,13	0.82	0	14,17,19	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAW	C	3	2	10,11,12	2.40	1 (10%)	12,15,17	2.05	4 (33%)
3	LGU	D	1	3	13,13,13	0.88	0	18,19,19	1.51	2 (11%)
3	LGU	D	2	3	12,12,13	0.84	0	14,17,19	1.12	1 (7%)
3	LGU	D	3	3	12,12,13	0.83	0	14,17,19	1.51	2 (14%)
3	MAW	D	4	3	10,11,12	2.36	1 (10%)	12,15,17	2.42	2 (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
2	LGU	C	1	2	-	0/4/24/24	0/1/1/1
2	LGU	C	2	2	-	0/4/21/24	0/1/1/1
2	MAW	C	3	2	-	4/4/17/20	0/1/1/1
3	LGU	D	1	3	-	0/4/24/24	0/1/1/1
3	LGU	D	2	3	-	0/4/21/24	0/1/1/1
3	LGU	D	3	3	-	0/4/21/24	0/1/1/1
3	MAW	D	4	3	-	0/4/17/20	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	MAW	O5-C5	6.92	1.46	1.37
3	D	4	MAW	O5-C5	6.62	1.46	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAW	O5-C5-C4	-6.59	118.89	124.94
3	D	1	LGU	C1-O5-C5	4.70	119.14	112.22
2	C	3	MAW	O5-C5-C6	4.38	119.89	111.85
3	D	4	MAW	O5-C5-C6	4.16	119.50	111.85
2	C	3	MAW	O5-C5-C4	-4.16	121.12	124.94
3	D	3	LGU	C3-C4-C5	3.44	115.22	109.30
2	C	1	LGU	C3-C4-C5	2.52	113.63	109.30
3	D	1	LGU	O5-C1-C2	2.43	114.57	110.30
2	C	3	MAW	O6B-C6-C5	2.42	119.54	114.06
2	C	1	LGU	C4-C3-C2	2.19	114.67	110.83
3	D	2	LGU	C3-C4-C5	2.12	112.95	109.30
2	C	3	MAW	C4-C5-C6	-2.11	118.98	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	LGU	O2-C2-C3	2.11	114.52	110.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

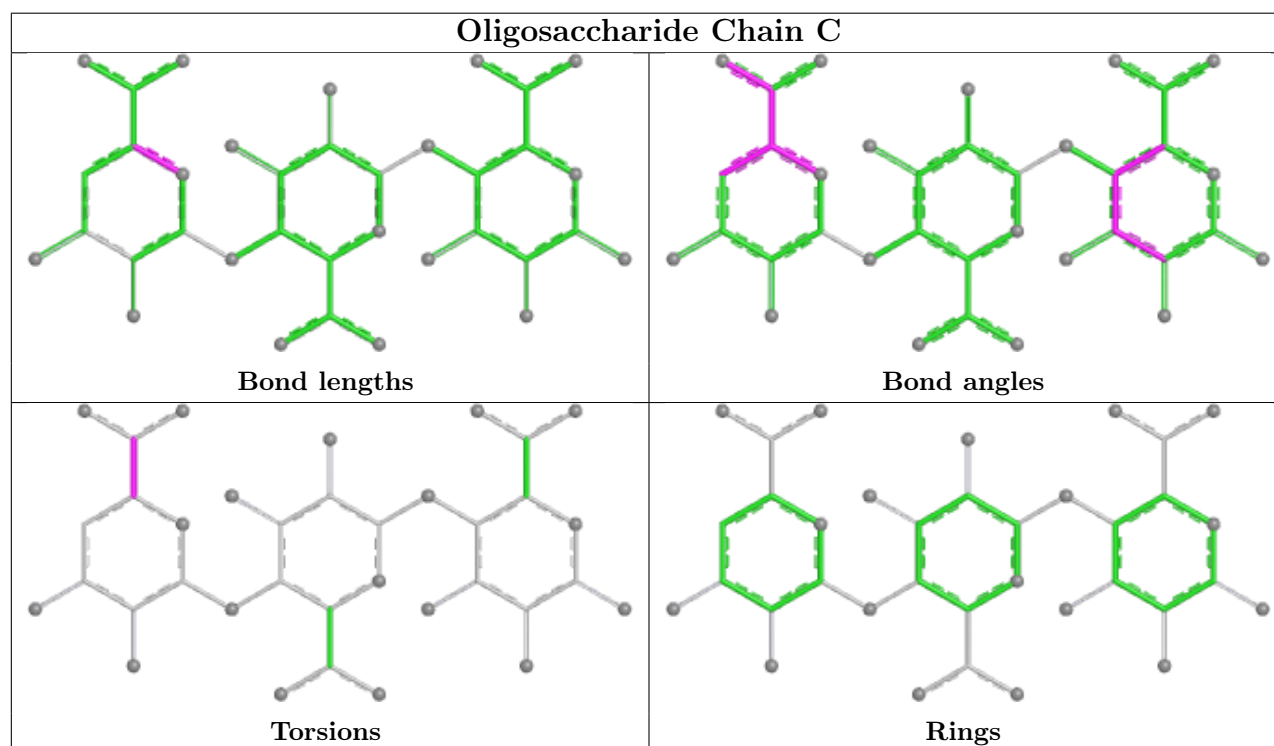
Mol	Chain	Res	Type	Atoms
2	C	3	MAW	C4-C5-C6-O6A
2	C	3	MAW	C4-C5-C6-O6B
2	C	3	MAW	O5-C5-C6-O6A
2	C	3	MAW	O5-C5-C6-O6B

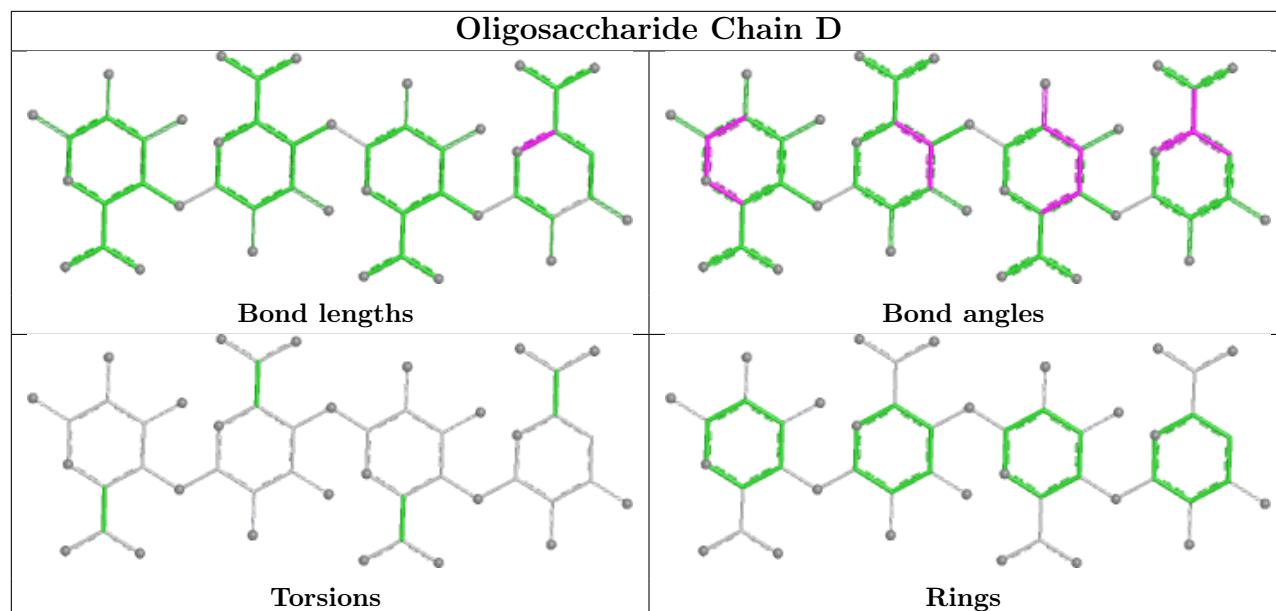
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	MAW	1	0
3	D	2	LGU	4	0
3	D	1	LGU	4	0
3	D	4	MAW	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	410/426 (96%)	0.96	47 (11%) 9 8	28, 40, 61, 69	0
1	B	407/426 (95%)	0.71	26 (6%) 25 24	27, 38, 53, 66	0
All	All	817/852 (95%)	0.84	73 (8%) 15 14	27, 39, 58, 69	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	VAL	6.6
1	A	445	VAL	4.9
1	A	54	LEU	4.8
1	A	411	VAL	3.9
1	B	329	LEU	3.9
1	A	420	GLY	3.8
1	A	422	TRP	3.5
1	B	41	TYR	3.4
1	B	332	TYR	3.4
1	B	444	ASN	3.3
1	B	330	HIS	3.2
1	A	415	LEU	3.1
1	A	405	PRO	3.0
1	B	42	ASN	3.0
1	A	417	LYS	3.0
1	A	423	GLN	2.9
1	A	412	GLY	2.9
1	A	404	LEU	2.8
1	B	40	ILE	2.8
1	A	426	ASN	2.8
1	A	375	TYR	2.8
1	A	329	LEU	2.8
1	A	38	GLY	2.7
1	B	54	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	382	VAL	2.7
1	B	323	ALA	2.5
1	A	41	TYR	2.5
1	A	40	ILE	2.4
1	A	394	ILE	2.4
1	A	377	ILE	2.4
1	B	60	VAL	2.4
1	A	447	MET	2.4
1	B	418	SER	2.4
1	A	372	LYS	2.3
1	A	444	ASN	2.3
1	A	357	GLY	2.3
1	B	392	LEU	2.3
1	B	393	LEU	2.3
1	A	60	VAL	2.3
1	A	406	LYS	2.3
1	A	51	ALA	2.2
1	A	52	LEU	2.2
1	A	393	LEU	2.2
1	A	418	SER	2.2
1	A	79	THR	2.2
1	A	384	LYS	2.2
1	A	399	THR	2.2
1	B	205	ALA	2.2
1	A	314	LEU	2.2
1	A	43	ILE	2.2
1	A	82	LYS	2.2
1	B	77	ASN	2.2
1	A	324	LEU	2.1
1	B	206	LEU	2.1
1	A	209	ASN	2.1
1	B	363	MET	2.1
1	B	79	THR	2.1
1	A	428	VAL	2.1
1	B	51	ALA	2.1
1	A	403	SER	2.1
1	A	409	THR	2.1
1	B	328	GLN	2.1
1	B	72	ILE	2.1
1	B	324	LEU	2.1
1	B	148	HIS	2.1
1	A	61	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	302	PHE	2.1
1	B	403	SER	2.1
1	B	407	GLY	2.0
1	A	208	VAL	2.0
1	A	288	ASN	2.0
1	A	369	GLY	2.0
1	B	98	GLY	2.0

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](#)

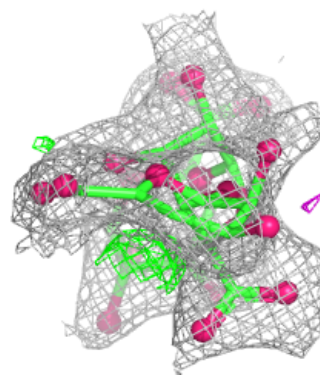
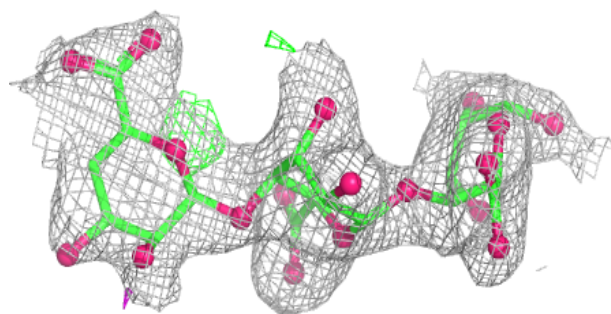
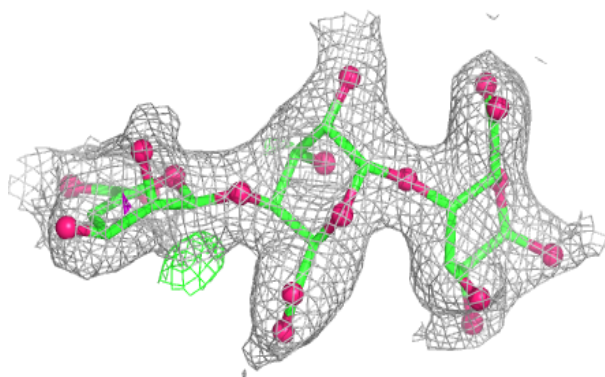
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAW	D	4	11/12	0.55	0.27	70,71,71,71	0
2	MAW	C	3	11/12	0.73	0.16	60,60,61,61	0
3	LGU	D	3	12/13	0.74	0.14	67,68,69,69	0
3	LGU	D	1	13/13	0.79	0.19	68,68,69,70	0
3	LGU	D	2	12/13	0.82	0.16	66,67,67,67	0
2	LGU	C	2	12/13	0.84	0.12	56,57,58,59	0
2	LGU	C	1	13/13	0.84	0.12	54,56,57,57	0

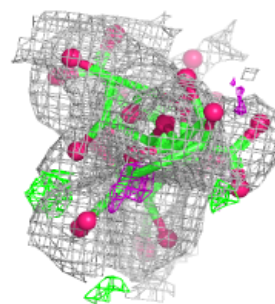
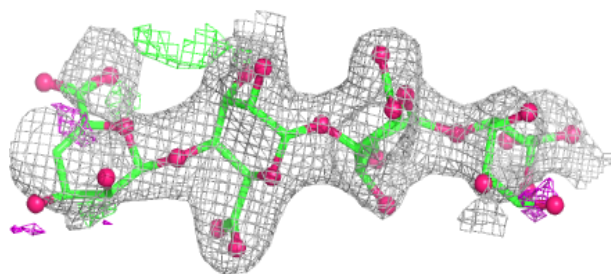
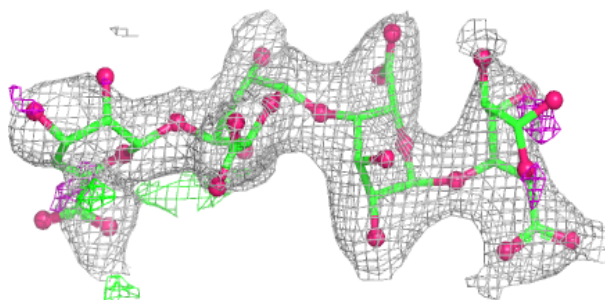
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.