



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:26 PM BST

PDB ID : 3SDF
Title : Crystal Structure of C-lobe of Bovine lactoferrin Complexed with Lipoteichoic acid at 2.1 Å Resolution
Authors : Shukla, P.K.; Gautam, L.; Sinha, M.; Bhushan, A.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2011-06-09
Resolution : 2.10 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
buster-report : 1.1.7 (2018)
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

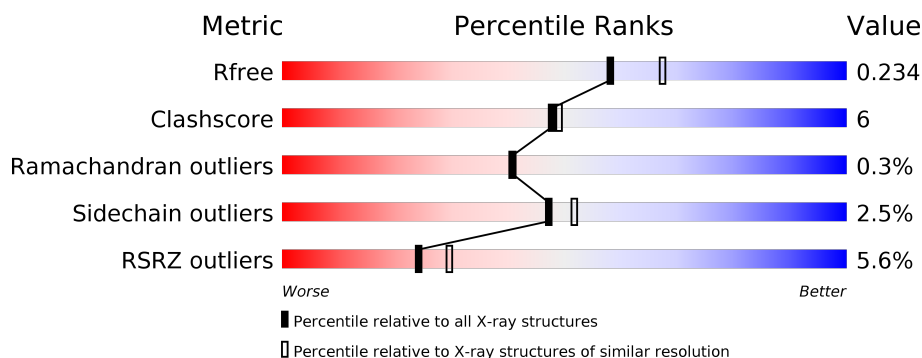
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	345	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>11% ..</div> </div> </div>
2	B	3	<div> <div>67%</div> <div>33%</div> </div>
3	C	2	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 3038 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 Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2604	1622	454	507	21	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	565	LYS	ASN	SEE REMARK 999	UNP P24627
A	608	GLU	LYS	SEE REMARK 999	UNP P24627

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	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	N	O			
3	C	2	28	16	2	10	0	0	0

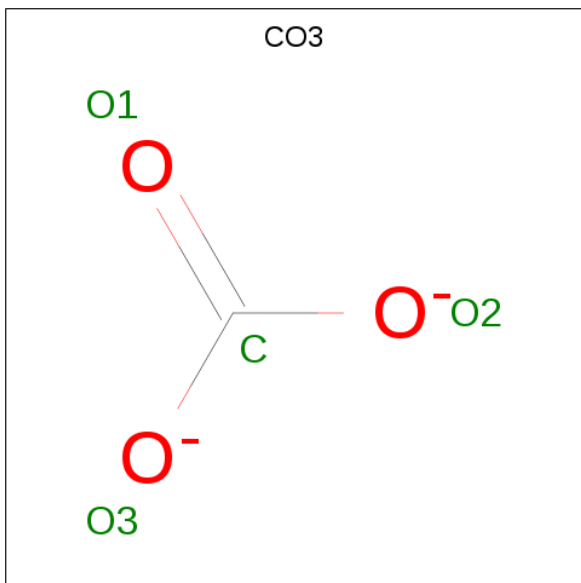
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Fe	0	0
			1	1		

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	1	3		

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



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

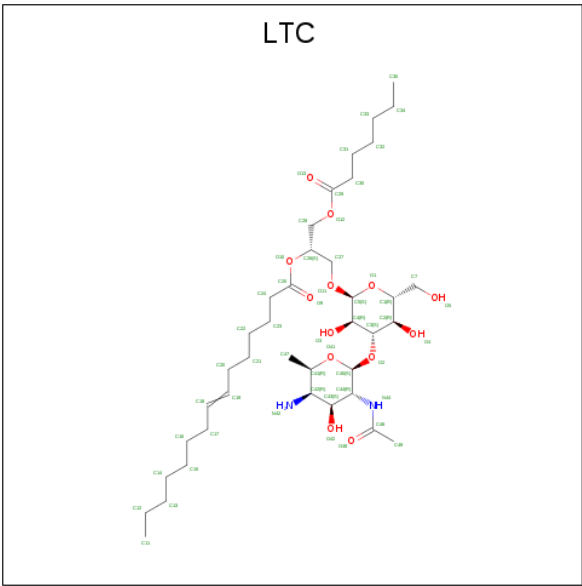
- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is (2S)-1-({3-O-[2-(acetylamino)-4-amino-2,4,6-trideoxy-beta-D-galactopyranosyl]-alpha-D-glucopyranosyl}oxy)-3-(heptanoyloxy)propan-2-yl (7Z)-pentadec-7-enoate

(three-letter code: LTC) (formula: C₃₉H₇₀N₂O₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			54	39	2	13		

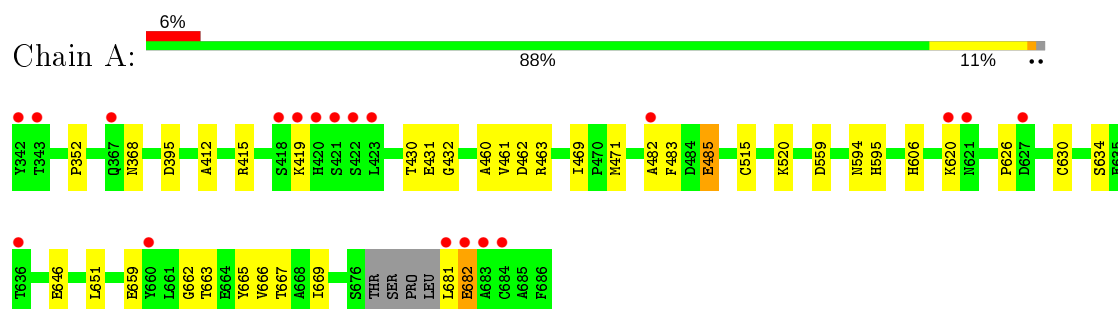
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	287	Total	O	0	0
			287	287		

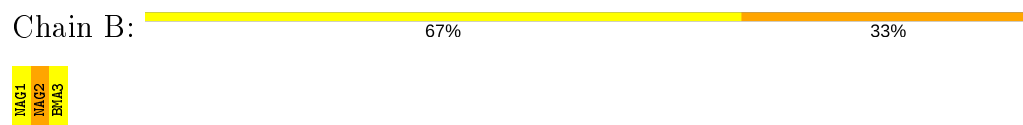
3 Residue-property plots

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.

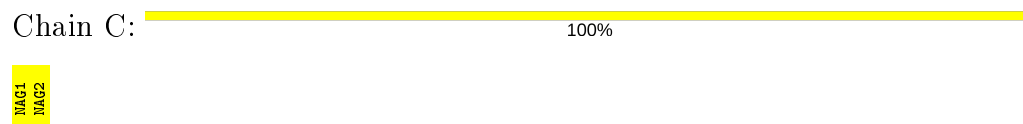
- Molecule 1: Lactotransferrin



- Molecule 2: 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.42Å 50.40Å 65.94Å 90.00° 107.72° 90.00°	Depositor
Resolution (Å)	62.00 – 2.10 39.31 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.7 (62.00-2.10) 95.8 (39.31-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.197 , 0.234 0.198 , 0.234	Depositor DCC
R_{free} test set	1168 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3038	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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: ZN, BMA, NAG, CO3, LTC, FE, 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	0.35	0/2652	0.53	0/3591

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2604	0	2519	28	0
2	B	39	0	34	1	0
3	C	28	0	25	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	4	0	0	0	0
7	A	5	0	0	0	0
8	A	14	0	13	3	0
9	A	54	0	70	12	0
10	A	287	0	0	0	0
All	All	3038	0	2661	33	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 6.

All (33) 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:368:ASN:HD21	8:A:1:NAG:C1	1.82	0.91
1:A:659:GLU:O	9:A:172:LTC:H17A	1.70	0.91
1:A:662:GLY:HA2	9:A:172:LTC:H15	1.65	0.78
1:A:663:THR:HG22	9:A:172:LTC:H14A	1.66	0.75
1:A:662:GLY:O	1:A:666:VAL:HG23	1.88	0.74
1:A:471:MET:CE	1:A:483:PHE:HB2	2.20	0.70
9:A:172:LTC:H20	9:A:172:LTC:H49B	1.76	0.66
1:A:352:PRO:HG2	1:A:520:LYS:HD3	1.78	0.66
1:A:415:ARG:NH2	1:A:432:GLY:O	2.35	0.59
1:A:431:GLU:O	9:A:172:LTC:H47A	2.04	0.58
1:A:368:ASN:HD21	8:A:1:NAG:C2	2.17	0.57
1:A:482:ALA:HB1	1:A:485:GLU:HG3	1.87	0.56
1:A:471:MET:HE3	1:A:483:PHE:HB2	1.88	0.56
9:A:172:LTC:H1	9:A:172:LTC:C26	2.39	0.53
1:A:626:PRO:HA	1:A:630:CYS:SG	2.50	0.51
1:A:430:THR:HB	1:A:594:ASN:ND2	2.26	0.51
1:A:681:LEU:HB2	1:A:682:GLU:OE2	2.12	0.49
9:A:172:LTC:H49	9:A:172:LTC:H14	1.94	0.49
9:A:172:LTC:H26	9:A:172:LTC:H1	1.95	0.48
1:A:471:MET:HE2	1:A:483:PHE:HB2	1.94	0.48
1:A:352:PRO:CG	1:A:520:LYS:HD3	2.42	0.48
1:A:461:VAL:O	1:A:462:ASP:HB2	2.13	0.48
1:A:432:GLY:HA3	9:A:172:LTC:H47	1.96	0.47
9:A:172:LTC:H24	9:A:172:LTC:H21	1.67	0.47
1:A:460:ALA:HB3	1:A:463:ARG:HD3	1.96	0.47
1:A:663:THR:H	9:A:172:LTC:H14A	1.80	0.47
1:A:368:ASN:ND2	8:A:1:NAG:C1	2.63	0.46
1:A:620:LYS:HD3	1:A:646:GLU:HG3	1.99	0.45
1:A:667:THR:HG21	2:B:2:NAG:H2	2.00	0.43
1:A:665:TYR:CE2	1:A:669:ILE:HD11	2.54	0.42
1:A:412:ALA:HB2	1:A:651:LEU:HD21	2.02	0.41
1:A:432:GLY:HA3	9:A:172:LTC:C47	2.50	0.41
1:A:395:ASP:HA	1:A:595:HIS:CD2	2.55	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	337/345 (98%)	318 (94%)	18 (5%)	1 (0%)	41	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	634	SER

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/286 (99%)	275 (98%)	7 (2%)	47	52

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	LYS
1	A	469	ILE
1	A	485	GLU
1	A	515	CYS
1	A	559	ASP
1	A	606	HIS
1	A	682	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	A	368	ASN
1	A	585	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 ⓘ

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$
2	NAG	B	1	1,2	14,14,15	1.37	2 (14%)	17,19,21	1.88	3 (17%)
2	NAG	B	2	2	14,14,15	0.50	0	17,19,21	1.49	3 (17%)
2	BMA	B	3	2	11,11,12	1.40	1 (9%)	15,15,17	1.66	3 (20%)
3	NAG	C	1	1,3	14,14,15	0.79	0	17,19,21	0.92	1 (5%)
3	NAG	C	2	3	14,14,15	0.51	0	17,19,21	1.37	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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C2-N2	-3.01	1.41	1.46
2	B	3	BMA	O5-C1	-2.45	1.39	1.43
2	B	1	NAG	O5-C1	-2.39	1.39	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	5.03	119.01	112.19
3	C	2	NAG	C1-O5-C5	3.87	117.43	112.19
2	B	3	BMA	O5-C5-C6	3.58	112.81	107.20
2	B	2	NAG	C4-C3-C2	3.50	116.15	111.02
2	B	3	BMA	O5-C1-C2	3.50	116.17	110.77
2	B	2	NAG	C1-O5-C5	3.20	116.52	112.19
2	B	1	NAG	C1-C2-N2	-2.47	106.27	110.49
2	B	1	NAG	C3-C4-C5	-2.35	106.06	110.24
2	B	2	NAG	O4-C4-C3	-2.27	105.09	110.35
2	B	3	BMA	O4-C4-C5	-2.23	103.75	109.30
3	C	1	NAG	O5-C5-C6	2.21	110.67	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

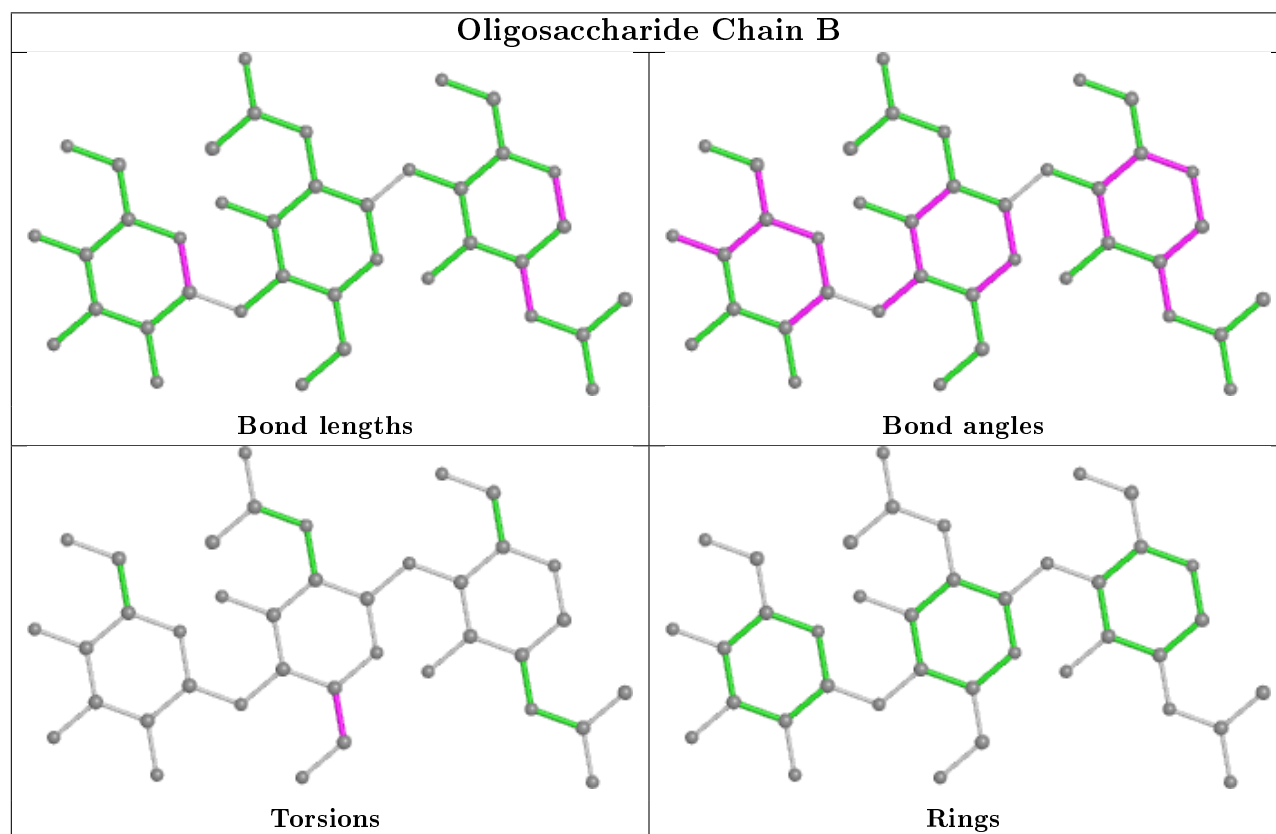
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

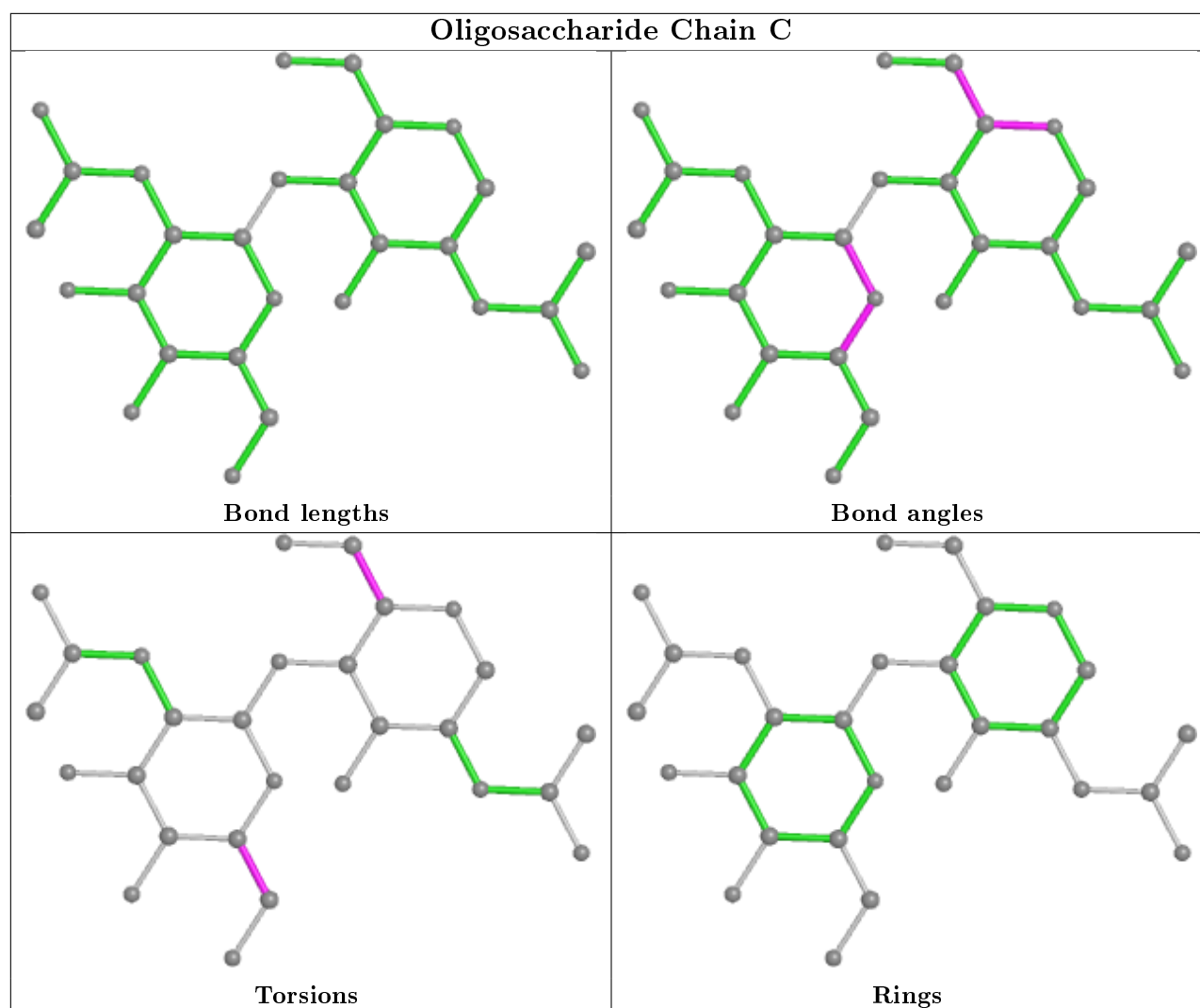
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	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 ⓘ

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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$
9	LTC	A	172	-	54,55,55	1.32	5 (9%)	69,70,70	1.88	19 (27%)
8	NAG	A	1	-	14,14,15	0.53	0	17,19,21	1.37	2 (11%)
6	CO3	A	85	5	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	A	692	-	4,4,4	0.14	0	6,6,6	0.06	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
8	NAG	A	1	-	-	0/6/23/26	0/1/1/1
9	LTC	A	172	-	-	26/44/84/84	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	172	LTC	O10-C25	5.01	1.48	1.34
9	A	172	LTC	O12-C29	4.05	1.45	1.33
9	A	172	LTC	C19-C18	3.77	1.53	1.31
9	A	172	LTC	O11-C5	2.45	1.44	1.40
9	A	172	LTC	C45-C44	2.10	1.56	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	172	LTC	C45-C44-N44	-4.88	102.60	111.00
9	A	172	LTC	O41-C41-C42	4.82	119.15	110.09
9	A	172	LTC	O10-C25-C24	4.77	121.78	111.50
9	A	172	LTC	C45-O41-C41	4.55	121.48	113.67
9	A	172	LTC	O2-C3-C2	3.56	116.76	107.28
8	A	1	NAG	O5-C1-C2	-3.52	105.73	111.29
9	A	172	LTC	C47-C41-C42	-3.40	106.96	114.10
9	A	172	LTC	C41-C42-N42	-3.20	104.29	110.92
8	A	1	NAG	C3-C4-C5	3.04	115.66	110.24
9	A	172	LTC	C28-O12-C29	2.84	127.64	117.12
9	A	172	LTC	C43-C42-C41	2.82	116.54	110.67
9	A	172	LTC	O42-C43-C44	2.78	115.27	109.66
9	A	172	LTC	O10-C25-O9	-2.70	117.17	123.70
9	A	172	LTC	O12-C28-C26	-2.64	100.75	108.43
9	A	172	LTC	C32-C31-C30	-2.37	104.67	113.19
9	A	172	LTC	O12-C29-O13	-2.36	117.63	123.59
9	A	172	LTC	O1-C1-C2	2.32	113.91	109.69
9	A	172	LTC	O4-C2-C3	-2.30	103.85	109.94
9	A	172	LTC	O12-C29-C30	2.25	118.97	111.91

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	172	LTC	O2-C45-C44	2.13	111.92	108.24
9	A	172	LTC	C27-O11-C5	2.13	117.89	113.74

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	172	LTC	C24-C25-O10-C26
9	A	172	LTC	C45-C44-N44-C48
9	A	172	LTC	C30-C29-O12-C28
9	A	172	LTC	O13-C29-O12-C28
9	A	172	LTC	O9-C25-O10-C26
9	A	172	LTC	O1-C1-C7-O5
9	A	172	LTC	C2-C1-C7-O5
9	A	172	LTC	C21-C22-C23-C24
9	A	172	LTC	C22-C23-C24-C25
9	A	172	LTC	C4-C3-O2-C45
9	A	172	LTC	C2-C3-O2-C45
9	A	172	LTC	C28-C26-O10-C25
9	A	172	LTC	C17-C18-C19-C20
9	A	172	LTC	C20-C21-C22-C23
9	A	172	LTC	C12-C13-C14-C15
9	A	172	LTC	O10-C26-C27-O11
9	A	172	LTC	C27-C26-C28-O12
9	A	172	LTC	C13-C14-C15-C16
9	A	172	LTC	C28-C26-C27-O11
9	A	172	LTC	C32-C33-C34-C35
9	A	172	LTC	O1-C5-O11-C27
9	A	172	LTC	O10-C26-C28-O12
9	A	172	LTC	C16-C17-C18-C19
9	A	172	LTC	C43-C44-N44-C48
9	A	172	LTC	C31-C32-C33-C34
9	A	172	LTC	C30-C31-C32-C33

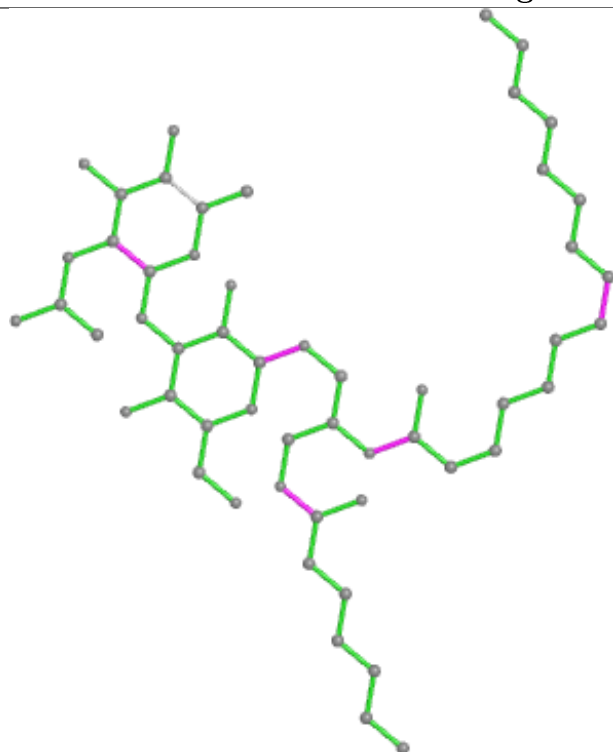
There are no ring outliers.

2 monomers are involved in 15 short contacts:

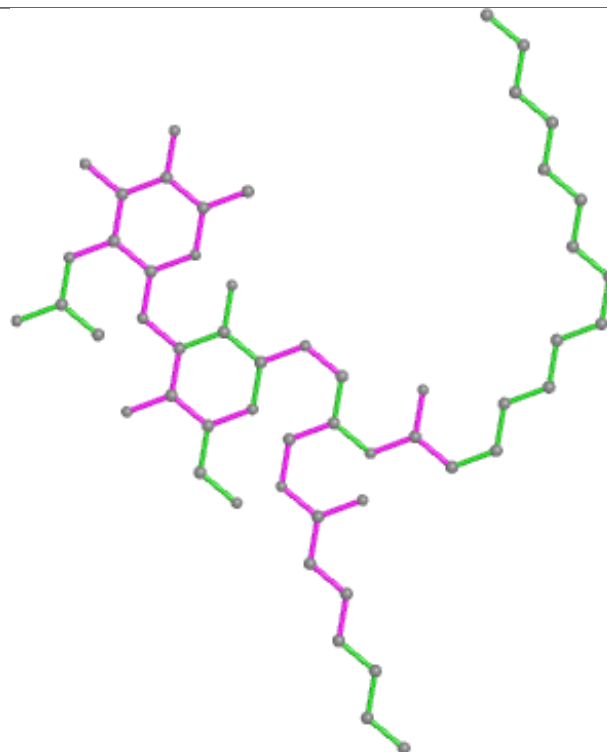
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	172	LTC	12	0
8	A	1	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

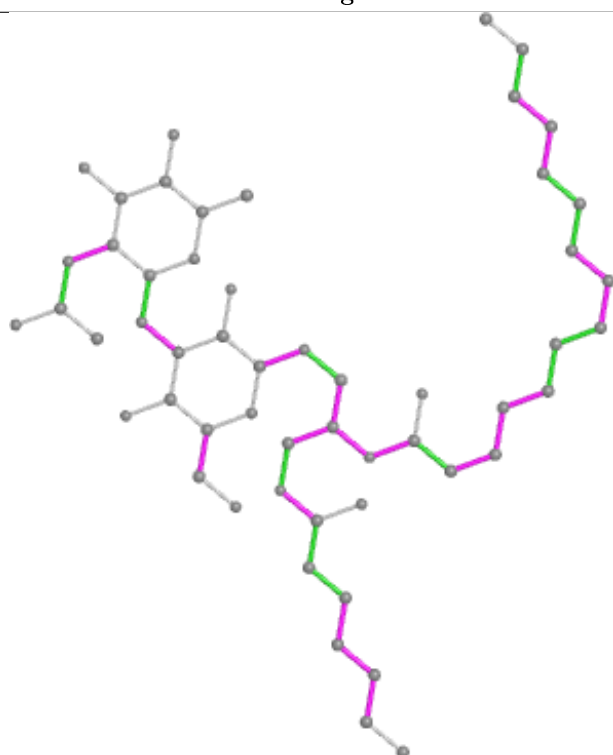
Ligand LTC A 172



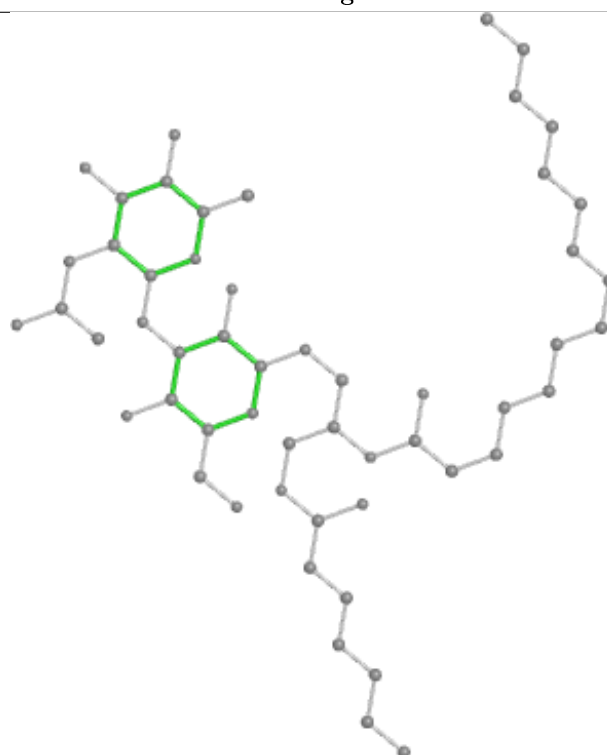
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	341/345 (98%)	0.38	19 (5%) 24 29	19, 31, 53, 77	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	TYR	9.4
1	A	681	LEU	8.1
1	A	419	LYS	5.1
1	A	683	ALA	5.0
1	A	420	HIS	4.4
1	A	422	SER	4.2
1	A	682	GLU	3.8
1	A	621	ASN	3.8
1	A	421	SER	3.3
1	A	343	THR	3.1
1	A	418	SER	3.0
1	A	367	GLN	2.9
1	A	482	ALA	2.9
1	A	627	ASP	2.6
1	A	684	CYS	2.3
1	A	620	LYS	2.2
1	A	423	LEU	2.2
1	A	660	TYR	2.2
1	A	636	THR	2.2

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

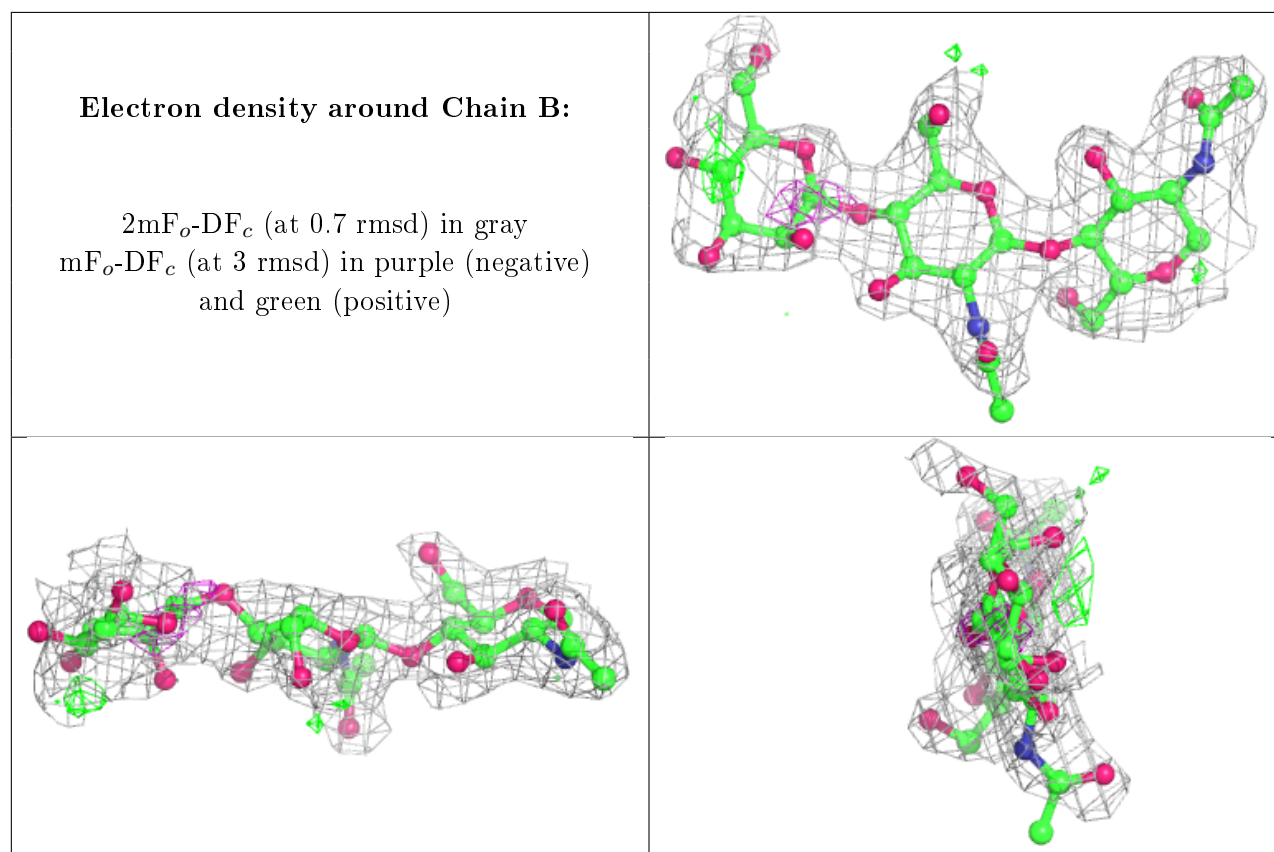
There are no non-standard protein/DNA/RNA residues in this entry.

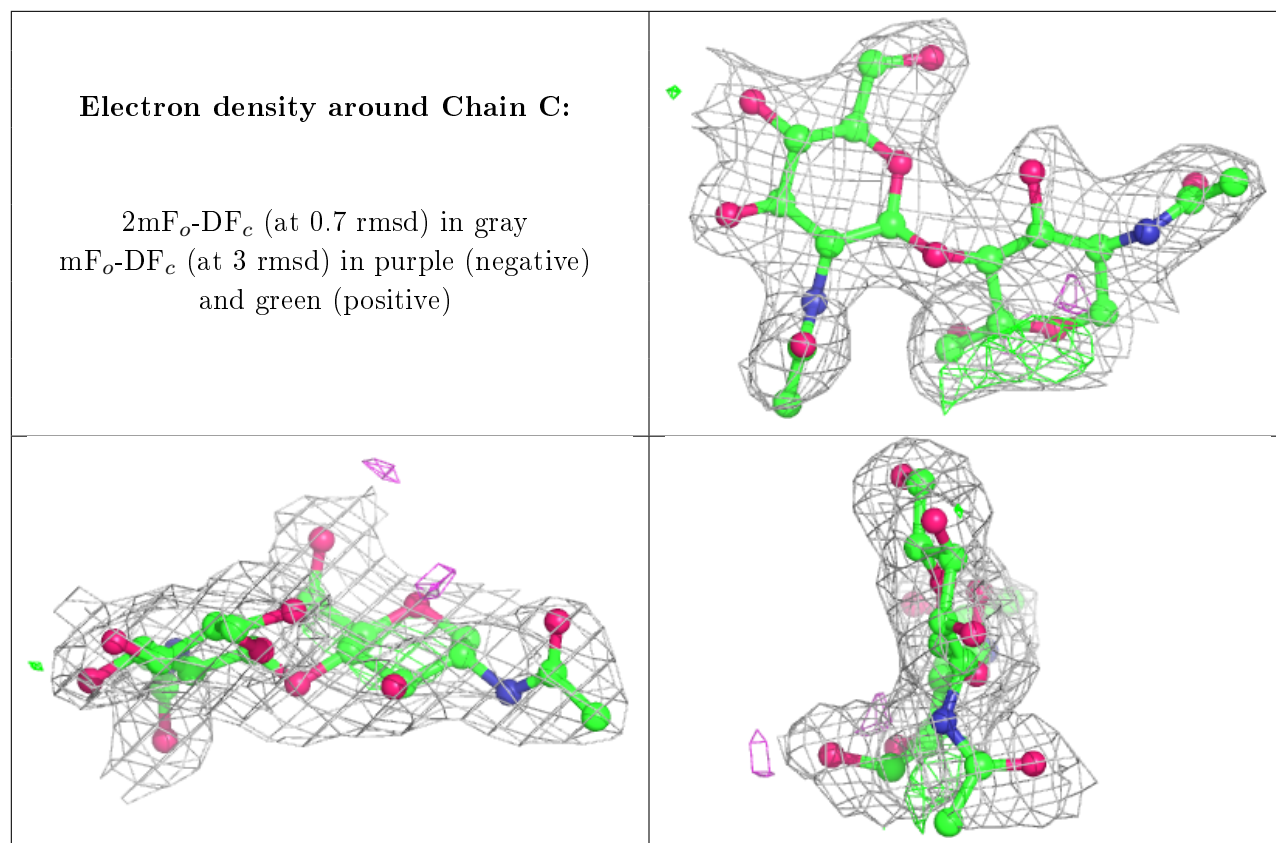
6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	BMA	B	3	11/12	0.56	0.34	71,73,73,73	0
2	NAG	B	2	14/15	0.84	0.31	61,63,65,68	0
3	NAG	C	1	14/15	0.84	0.14	39,39,42,45	0
2	NAG	B	1	14/15	0.84	0.15	49,53,55,58	0
3	NAG	C	2	14/15	0.86	0.15	47,50,50,50	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.





6.4 Ligands [i](#)

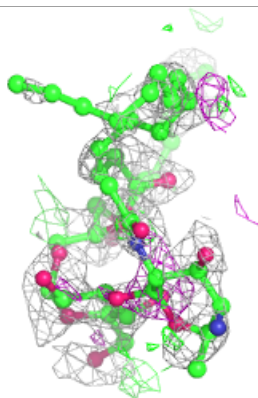
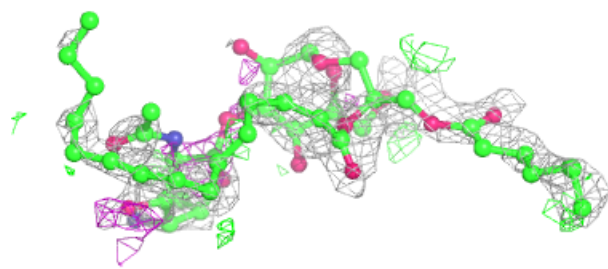
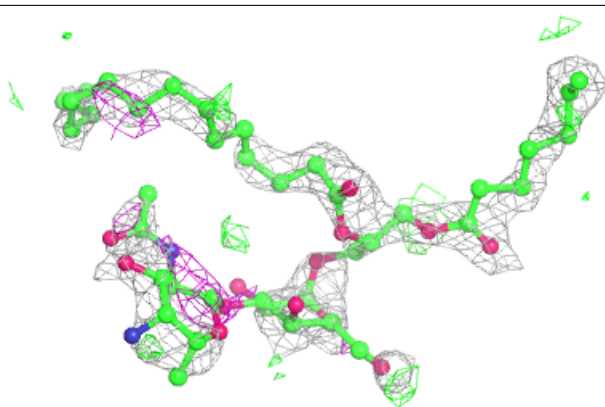
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	LTC	A	172	54/54	0.60	0.32	33,51,54,54	54
8	NAG	A	1	14/15	0.80	0.29	55,58,58,58	0
6	CO3	A	85	4/4	0.97	0.11	19,19,20,20	0
7	SO4	A	692	5/5	0.98	0.23	56,56,57,57	0
4	ZN	A	82	1/1	0.98	0.11	37,37,37,37	0
4	ZN	A	81	1/1	0.99	0.12	32,32,32,32	0
5	FE	A	84	1/1	1.00	0.09	21,21,21,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LTC A 172:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.