Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 02:13 PM EDT

PDB ID	:	3WNN
Title	:	D308A mutant of Bacillus circulans T-3040 cycloisomaltooligosaccharide glucanotransferase complexed with isomaltooctaose
Authors	:	Suzuki, N.; Fujimoto, Z.; Kim, Y.M.; Momma, M.; Kishine, N.; Suzuki, R.; Suzuki, S.; Kitamura, S.; Kobayashi, M.; Kimura, A.; Funane, K.
Deposited on	:	2013-12-10
Resolution	:	2.25 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.25 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		3.8%
RSRZ outliers		1.5%

Worse .... *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
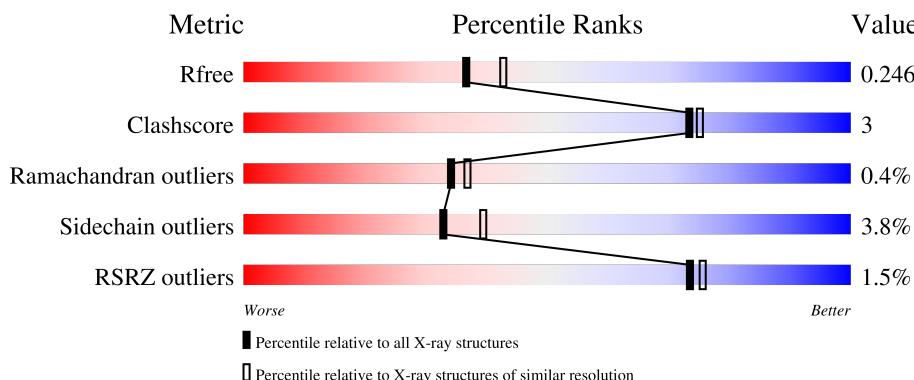
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	710	2%; 86% / 12% ••
1	B	710	%; 88% / 10% •
2	C	8	12% / 62% / 25%
2	E	8	12% / 88%
3	D	4	100%

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Mol	Chain	Length	Quality of chain
4	F	5	20% 60% 20%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 11831 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 Cycloisomaltooligosaccharide glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	699	Total	C	N	O	S	0	0	0
			5501	3457	923	1106	15			
1	B	698	Total	C	N	O	S	0	0	0
			5497	3455	922	1105	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	expression tag	UNP P94286
A	38	GLY	-	expression tag	UNP P94286
A	278	PHE	SER	SEE REMARK 999	UNP P94286
A	308	ALA	ASP	engineered mutation	UNP P94286
A	739	LEU	-	expression tag	UNP P94286
A	740	GLU	-	expression tag	UNP P94286
A	741	HIS	-	expression tag	UNP P94286
A	742	HIS	-	expression tag	UNP P94286
A	743	HIS	-	expression tag	UNP P94286
A	744	HIS	-	expression tag	UNP P94286
A	745	HIS	-	expression tag	UNP P94286
A	746	HIS	-	expression tag	UNP P94286
B	37	MET	-	expression tag	UNP P94286
B	38	GLY	-	expression tag	UNP P94286
B	278	PHE	SER	SEE REMARK 999	UNP P94286
B	308	ALA	ASP	engineered mutation	UNP P94286
B	739	LEU	-	expression tag	UNP P94286
B	740	GLU	-	expression tag	UNP P94286
B	741	HIS	-	expression tag	UNP P94286
B	742	HIS	-	expression tag	UNP P94286
B	743	HIS	-	expression tag	UNP P94286
B	744	HIS	-	expression tag	UNP P94286
B	745	HIS	-	expression tag	UNP P94286
B	746	HIS	-	expression tag	UNP P94286

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	8	Total 89	C 48	O 41	0	0	0
2	E	8	Total 89	C 48	O 41	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	4	Total 45	C 24	O 21	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.
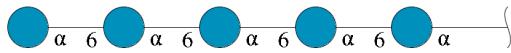
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	F	5	Total 56	C 30	O 26	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0
5	B	1	Total 1	Ca 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Na 1	0	0
6	B	1	Total 1	Na 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O$_4$S).
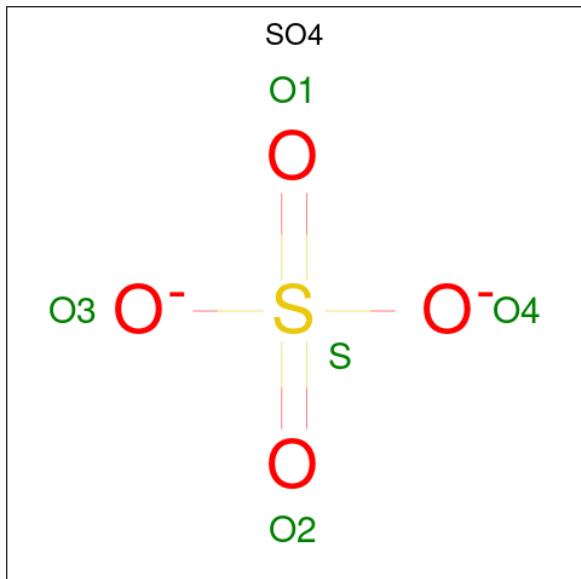
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 5	O 4	S 1	0	0
7	A	1	Total 5	O 4	S 1	0	0
7	A	1	Total 5	O 4	S 1	0	0
7	A	1	Total 5	O 4	S 1	0	0
7	A	1	Total 5	O 4	S 1	0	0
7	A	1	Total 5	O 4	S 1	0	0
7	B	1	Total 5	O 4	S 1	0	0
7	B	1	Total 5	O 4	S 1	0	0
7	B	1	Total 5	O 4	S 1	0	0

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

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).
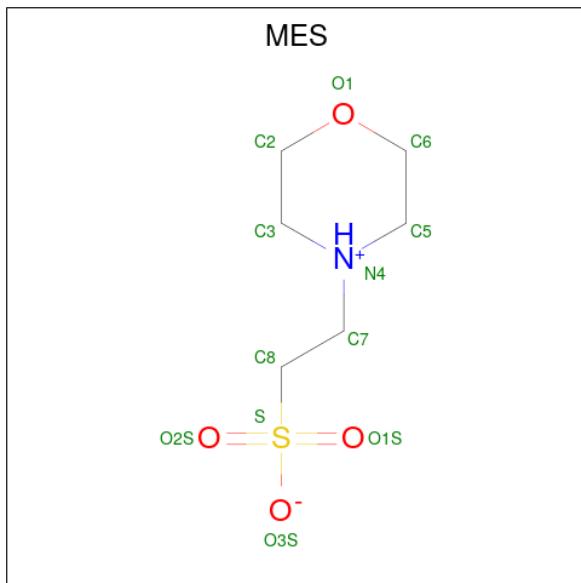
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total C N O S 12 6 1 4 1					0	0
8	B	1	Total C N O S 12 6 1 4 1					0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	204	Total O 204 204		0	0
9	B	267	Total O 267 267		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: Cycloisomaltooligosaccharide glucanotransferase
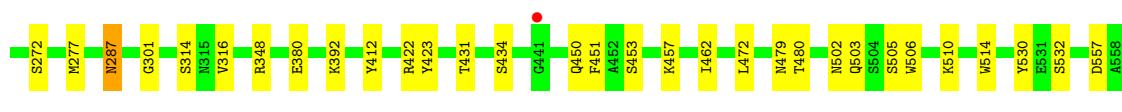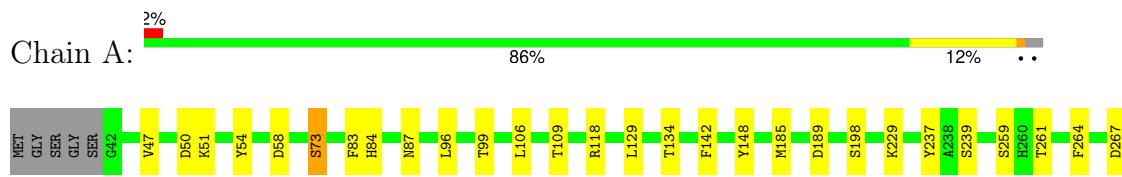
Chain A:

• Molecule 1: Cycloisomaltooligosaccharide glucanotransferase

Chain B:

• Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain C:

BGC1 GLC2 GLC3 GLC4 GLC5 GLC6 GLC7 GLC8

• Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(
1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alph
a-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain E: 12%   88%

BGC1 GLC2 GLC3 GLC4 GLC5 GLC6 GLC7 GLC8
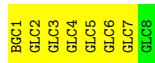
• Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(
1-6)-alpha-D-glucopyranose

Chain D: 100%

GLC1 GLC2 GLC3 GLC4

• Molecule 4: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(
1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain F: 20%   60%   20%

GLC1 GLC2 GLC3 GLC4 GLC5

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.03Å 171.26Å 173.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.35 – 2.25 35.32 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.35-2.25) 95.8 (35.32-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.202 , 0.244 0.206 , 0.246	Depositor DCC
R_{free} test set	4321 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 21.9	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.166 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11831	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MES, GLC, BGC, CA, NA, 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	0.67	1/5641 (0.0%)	0.78	4/7683 (0.1%)
1	B	0.69	1/5637 (0.0%)	0.79	1/7678 (0.0%)
All	All	0.68	2/11278 (0.0%)	0.78	5/15361 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	ASP	CB-CG	6.81	1.66	1.51
1	A	50	ASP	CB-CG	5.19	1.62	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	267	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	58	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	50	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	277	MET	CG-SD-CE	-5.38	91.60	100.20

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	5501	0	5106	35	0
1	B	5497	0	5103	35	0
2	C	89	0	75	2	0
2	E	89	0	75	0	0
3	D	45	0	39	1	0
4	F	56	0	48	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	30	0	0	0	0
7	B	25	0	0	0	0
8	A	12	0	13	0	0
8	B	12	0	13	1	0
9	A	204	0	0	3	0
9	B	267	0	0	3	0
All	All	11831	0	10472	73	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 3.

All (73) 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)
9:B:1071:HOH:O	4:F:3:GLC:H61	1.88	0.74
1:A:84:HIS:CE1	1:A:118:ARG:HD3	2.31	0.65
1:A:502:ASN:ND2	1:A:503:GLN:O	2.31	0.64
1:A:51:LYS:HB2	1:A:54:TYR:CZ	2.34	0.63
1:A:287:ASN:C	1:A:287:ASN:HD22	2.03	0.62
1:A:301:GLY:O	1:A:348:ARG:NH1	2.34	0.61
1:B:495:VAL:CG1	1:B:515:TYR:CE2	2.84	0.60
1:A:557:ASP:HB3	1:A:600:HIS:CE1	2.38	0.59
1:B:260:HIS:O	1:B:260:HIS:ND1	2.36	0.58
1:A:557:ASP:OD2	1:A:569:GLU:OE2	2.23	0.57
1:A:96:LEU:HD13	1:A:106:LEU:HD21	1.90	0.54
1:B:72:SER:HA	1:B:100:ASN:HB2	1.90	0.53
1:B:313:ARG:NH2	9:B:962:HOH:O	2.41	0.53
1:A:503:GLN:NE2	1:A:510:LYS:HG3	2.24	0.52
1:A:628:LEU:HD12	1:A:633:ALA:HB2	1.91	0.52
2:C:5:GLC:H61	2:C:6:GLC:O2	2.10	0.51
1:B:495:VAL:CG1	1:B:515:TYR:CD2	2.93	0.51
1:B:495:VAL:HG13	1:B:515:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG12	1:A:134:THR:CG2	2.41	0.51
1:B:644:TYR:HA	1:B:656:HIS:O	2.11	0.50
1:B:338:LYS:NZ	1:B:375:ASP:OD2	2.45	0.50
1:B:599:ASP:OD1	8:B:808:MES:N4	2.43	0.49
1:B:696:TYR:O	1:B:736:ILE:HA	2.13	0.48
1:B:72:SER:O	1:B:73:SER:C	2.52	0.47
1:A:422:ARG:HD3	9:A:1109:HOH:O	2.14	0.47
1:A:47:VAL:HG12	1:A:134:THR:HG22	1.97	0.46
1:B:639:ALA:O	1:B:641:THR:HG23	2.15	0.46
1:B:695:VAL:HG22	1:B:738:MET:HG2	1.97	0.46
1:A:609:ASN:O	1:A:613:ASP:HB2	2.16	0.46
1:B:244:SER:HB2	1:B:245:PRO:HD3	1.96	0.46
1:B:699:SER:O	1:B:705:GLY:HA2	2.15	0.46
1:B:98:LEU:HB3	1:B:102:GLN:HB3	1.96	0.45
1:A:380:GLU:OE2	1:A:412:TYR:OH	2.16	0.45
1:A:627:ASN:HB2	1:A:683:LYS:HB3	1.98	0.45
1:B:386:ASP:HB3	1:B:666:GLN:OE1	2.16	0.45
1:A:287:ASN:C	1:A:287:ASN:ND2	2.68	0.45
1:A:264:PHE:CE2	1:A:316:VAL:HG22	2.52	0.44
1:A:589:MET:HG2	1:A:593:LEU:HD23	1.99	0.44
1:A:450:GLN:OE1	3:D:3:GLC:O2	2.36	0.44
1:B:605:THR:O	1:B:608:GLU:HG2	2.17	0.44
1:A:83:PHE:HA	1:A:87:ASN:O	2.17	0.44
1:A:431:THR:HB	1:A:457:LYS:HB2	2.00	0.44
1:A:73:SER:HB3	1:A:99:THR:HA	1.99	0.44
1:A:472:LEU:O	1:A:514:TRP:HA	2.18	0.43
1:A:503:GLN:CD	1:A:510:LYS:HG3	2.39	0.43
1:A:571:GLY:O	1:A:572:ASP:C	2.56	0.43
1:A:676:PHE:CD1	1:A:731:LYS:HA	2.53	0.43
1:A:51:LYS:HB2	1:A:54:TYR:CE1	2.53	0.43
1:B:244:SER:N	1:B:245:PRO:CD	2.81	0.43
1:B:641:THR:CA	1:B:661:LEU:HD23	2.48	0.43
1:B:153:GLU:OE1	1:B:585:ARG:NH2	2.52	0.43
1:B:217:GLN:NE2	1:B:217:GLN:HA	2.34	0.43
1:B:721:LYS:HE2	1:B:721:LYS:HA	2.00	0.43
1:A:480:THR:OG1	9:A:1137:HOH:O	2.21	0.42
1:B:252:TRP:CE2	1:B:284:ASN:HB3	2.55	0.42
2:C:5:GLC:C6	2:C:6:GLC:O2	2.68	0.42
1:A:189:ASP:OD2	1:A:239:SER:HB2	2.19	0.42
1:A:423:TYR:CE1	1:A:462:ILE:HG22	2.55	0.42
1:B:422:ARG:HD3	9:B:983:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:679:ASN:O	1:B:681:PRO:HD3	2.19	0.41
1:A:573:ASP:OD1	1:A:575:GLN:NE2	2.44	0.41
1:B:577:LEU:HA	1:B:578:PRO:HD3	1.90	0.41
1:A:142:PHE:CD2	1:A:229:LYS:HG3	2.54	0.41
1:B:557:ASP:HB3	1:B:600:HIS:CE1	2.55	0.41
1:B:678:THR:O	1:B:679:ASN:C	2.59	0.41
1:B:694:ASP:HB2	1:B:739:LEU:HB3	2.02	0.41
1:B:713:THR:HG22	1:B:714:SER:N	2.35	0.41
1:B:538:VAL:HG12	1:B:539:ASN:N	2.36	0.41
1:A:109:THR:O	9:A:1142:HOH:O	2.21	0.41
1:B:495:VAL:HG11	1:B:515:TYR:CD2	2.56	0.41
1:B:80:LEU:HD13	1:B:124:ILE:CD1	2.51	0.40
1:A:479:ASN:HB3	1:A:506:TRP:CE2	2.55	0.40
1:B:469:ASP:O	1:B:588:THR:HG21	2.21	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	697/710 (98%)	662 (95%)	32 (5%)	3 (0%)	34	37
1	B	696/710 (98%)	657 (94%)	36 (5%)	3 (0%)	34	37
All	All	1393/1420 (98%)	1319 (95%)	68 (5%)	6 (0%)	34	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	SER
1	B	686	ILE
1	A	572	ASP
1	A	718	ALA

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Mol	Chain	Res	Type
1	A	272	SER
1	B	578	PRO

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	587/596 (98%)	557 (95%)	30 (5%)	24	25
1	B	587/596 (98%)	572 (97%)	15 (3%)	46	55
All	All	1174/1192 (98%)	1129 (96%)	45 (4%)	33	39

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	SER
1	A	129	LEU
1	A	148	TYR
1	A	185	MET
1	A	198	SER
1	A	237	TYR
1	A	259	SER
1	A	261	THR
1	A	287	ASN
1	A	314	SER
1	A	392	LYS
1	A	434	SER
1	A	451	PHE
1	A	453	SER
1	A	505	SER
1	A	530	TYR
1	A	532	SER
1	A	559	MET
1	A	578	PRO
1	A	613	ASP
1	A	621	THR

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Mol	Chain	Res	Type
1	A	646	ASN
1	A	647	LYS
1	A	650	SER
1	A	672	SER
1	A	701	ASP
1	A	714	SER
1	A	716	THR
1	A	717	ASP
1	A	721	LYS
1	B	99	THR
1	B	148	TYR
1	B	185	MET
1	B	198	SER
1	B	237	TYR
1	B	451	PHE
1	B	505	SER
1	B	614	SER
1	B	621	THR
1	B	624	GLN
1	B	625	PHE
1	B	632	SER
1	B	650	SER
1	B	691	THR
1	B	737	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	287	ASN
1	A	315	ASN
1	A	320	ASN
1	A	371	ASN
1	A	479	ASN
1	A	483	ASN
1	A	521	GLN
1	A	600	HIS
1	A	619	ASN
1	B	242	ASN
1	B	320	ASN
1	B	450	GLN
1	B	496	GLN

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Mol	Chain	Res	Type
1	B	511	HIS
1	B	521	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 ⓘ

25 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	BGC	C	1	2	12,12,12	0.68	0	17,17,17	1.48	5 (29%)
2	GLC	C	2	2	11,11,12	0.83	0	15,15,17	1.24	0
2	GLC	C	3	2	11,11,12	0.89	0	15,15,17	1.66	5 (33%)
2	GLC	C	4	2	11,11,12	0.61	0	15,15,17	1.32	1 (6%)
2	GLC	C	5	2	11,11,12	0.65	0	15,15,17	2.57	4 (26%)
2	GLC	C	6	2	11,11,12	0.82	0	15,15,17	1.27	1 (6%)
2	GLC	C	7	2	11,11,12	0.63	0	15,15,17	1.11	2 (13%)
2	GLC	C	8	2	11,11,12	0.76	0	15,15,17	1.37	2 (13%)
3	GLC	D	1	3	12,12,12	0.65	0	17,17,17	2.33	3 (17%)
3	GLC	D	2	3	11,11,12	0.64	0	15,15,17	1.58	4 (26%)
3	GLC	D	3	3	11,11,12	0.76	0	15,15,17	0.82	0
3	GLC	D	4	3	11,11,12	0.57	0	15,15,17	1.66	1 (6%)
2	BGC	E	1	2	12,12,12	0.82	0	17,17,17	1.24	1 (5%)
2	GLC	E	2	2	11,11,12	0.79	0	15,15,17	1.30	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	GLC	E	3	2	11,11,12	0.86	0	15,15,17	1.37	1 (6%)
2	GLC	E	4	2	11,11,12	0.63	0	15,15,17	1.24	2 (13%)
2	GLC	E	5	2	11,11,12	1.05	0	15,15,17	2.59	8 (53%)
2	GLC	E	6	2	11,11,12	0.95	1 (9%)	15,15,17	1.75	4 (26%)
2	GLC	E	7	2	11,11,12	0.83	0	15,15,17	1.07	1 (6%)
2	GLC	E	8	2	11,11,12	0.82	0	15,15,17	1.14	0
4	GLC	F	1	4	12,12,12	0.69	0	17,17,17	1.24	2 (11%)
4	GLC	F	2	4	11,11,12	0.72	0	15,15,17	1.28	2 (13%)
4	GLC	F	3	4	11,11,12	0.56	0	15,15,17	2.78	3 (20%)
4	GLC	F	4	4	11,11,12	0.54	0	15,15,17	2.63	2 (13%)
4	GLC	F	5	4	11,11,12	0.60	0	15,15,17	0.96	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
2	BGC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	2/2/19/22	0/1/1/1
2	GLC	C	5	2	-	1/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	C	7	2	-	0/2/19/22	0/1/1/1
2	GLC	C	8	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	2/2/22/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1
3	GLC	D	3	3	-	0/2/19/22	0/1/1/1
3	GLC	D	4	3	-	2/2/19/22	0/1/1/1
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	4	2	-	2/2/19/22	0/1/1/1
2	GLC	E	5	2	-	1/2/19/22	0/1/1/1
2	GLC	E	6	2	-	0/2/19/22	0/1/1/1
2	GLC	E	7	2	-	0/2/19/22	0/1/1/1
2	GLC	E	8	2	-	2/2/19/22	0/1/1/1
4	GLC	F	1	4	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	F	2	4	-	1/2/19/22	0/1/1/1
4	GLC	F	3	4	-	2/2/19/22	0/1/1/1
4	GLC	F	4	4	-	0/2/19/22	0/1/1/1
4	GLC	F	5	4	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	6	GLC	O5-C5	-2.28	1.39	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	4	GLC	C1-O5-C5	9.36	124.73	112.19
4	F	3	GLC	C1-O5-C5	9.13	124.42	112.19
2	C	5	GLC	C1-O5-C5	6.82	121.32	112.19
2	E	5	GLC	C6-C5-C4	-6.27	97.62	113.02
3	D	1	GLC	C1-O5-C5	5.99	125.24	113.65
3	D	4	GLC	C1-O5-C5	5.69	119.81	112.19
3	D	1	GLC	O5-C5-C4	4.66	118.09	109.70
2	C	5	GLC	C6-C5-C4	-4.46	102.06	113.02
2	E	6	GLC	O2-C2-C1	4.16	118.74	109.22
2	C	5	GLC	O5-C5-C4	3.96	120.46	110.83
3	D	1	GLC	C3-C4-C5	3.71	116.96	110.23
2	E	3	GLC	O2-C2-C3	3.50	117.40	110.15
4	F	3	GLC	C3-C4-C5	3.47	116.53	110.23
2	E	5	GLC	O4-C4-C5	-3.35	101.06	109.32
3	D	2	GLC	C2-C3-C4	-3.30	105.06	110.86
2	C	6	GLC	O2-C2-C1	3.20	116.56	109.22
2	C	8	GLC	O3-C3-C2	-3.19	103.55	110.05
4	F	3	GLC	O5-C5-C4	3.02	118.17	110.83
2	C	8	GLC	C1-O5-C5	2.98	116.18	112.19
2	E	5	GLC	C3-C4-C5	2.95	115.57	110.23
2	C	3	GLC	O3-C3-C4	-2.91	103.52	110.38
2	E	5	GLC	C2-C3-C4	-2.85	105.84	110.86
3	D	2	GLC	O3-C3-C2	2.73	115.63	110.05
2	E	2	GLC	C1-O5-C5	2.72	115.83	112.19
2	C	3	GLC	O5-C5-C4	-2.64	104.42	110.83
2	E	5	GLC	O6-C6-C5	-2.60	102.47	111.33
2	C	1	BGC	O2-C2-C3	-2.60	104.24	110.38
2	E	1	BGC	C4-C3-C2	2.59	115.38	110.83
2	C	1	BGC	C1-O5-C5	-2.59	108.64	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	GLC	O5-C5-C6	2.58	112.68	107.66
2	C	1	BGC	C3-C4-C5	-2.49	105.71	110.23
2	C	4	GLC	C1-C2-C3	2.49	113.26	109.64
2	C	7	GLC	C1-C2-C3	2.46	113.23	109.64
2	C	3	GLC	C2-C3-C4	-2.44	106.57	110.86
2	E	4	GLC	O2-C2-C3	-2.41	105.16	110.15
4	F	2	GLC	C2-C3-C4	-2.41	106.63	110.86
2	E	6	GLC	C1-C2-C3	2.37	113.09	109.64
2	E	5	GLC	O5-C5-C6	2.31	112.16	107.66
2	C	7	GLC	C1-O5-C5	2.31	115.28	112.19
2	E	4	GLC	O2-C2-C1	2.30	114.50	109.22
2	C	1	BGC	C4-C3-C2	2.28	114.83	110.83
4	F	4	GLC	O5-C1-C2	2.27	116.21	110.79
2	E	5	GLC	O3-C3-C4	-2.26	105.05	110.38
2	E	7	GLC	O4-C4-C3	-2.24	105.10	110.38
4	F	1	GLC	O2-C2-C1	2.21	114.36	109.25
2	C	1	BGC	O5-C1-C2	-2.20	106.44	110.30
2	E	6	GLC	O5-C5-C4	-2.19	105.50	110.83
4	F	2	GLC	C3-C4-C5	-2.18	106.28	110.23
2	E	5	GLC	C1-O5-C5	2.17	115.10	112.19
2	E	6	GLC	C3-C4-C5	-2.13	106.36	110.23
2	C	5	GLC	O5-C5-C6	-2.09	103.60	107.66
3	D	2	GLC	O4-C4-C5	2.04	114.35	109.32
2	C	3	GLC	O5-C1-C2	-2.03	105.94	110.79
4	F	1	GLC	C4-C3-C2	-2.03	107.26	110.83
3	D	2	GLC	O6-C6-C5	-2.01	104.50	111.33

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	GLC	O5-C5-C6-O6
4	F	3	GLC	O5-C5-C6-O6
4	F	5	GLC	O5-C5-C6-O6
3	D	4	GLC	O5-C5-C6-O6
3	D	1	GLC	C4-C5-C6-O6
4	F	3	GLC	C4-C5-C6-O6
4	F	5	GLC	C4-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
3	D	4	GLC	C4-C5-C6-O6
3	D	2	GLC	O5-C5-C6-O6
2	E	8	GLC	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	4	GLC	C4-C5-C6-O6
2	C	5	GLC	C4-C5-C6-O6
2	E	8	GLC	C4-C5-C6-O6
2	E	5	GLC	O5-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
4	F	2	GLC	C4-C5-C6-O6
2	E	4	GLC	O5-C5-C6-O6
2	C	4	GLC	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	GLC	1	0
2	C	6	GLC	2	0
2	C	5	GLC	2	0
4	F	3	GLC	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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
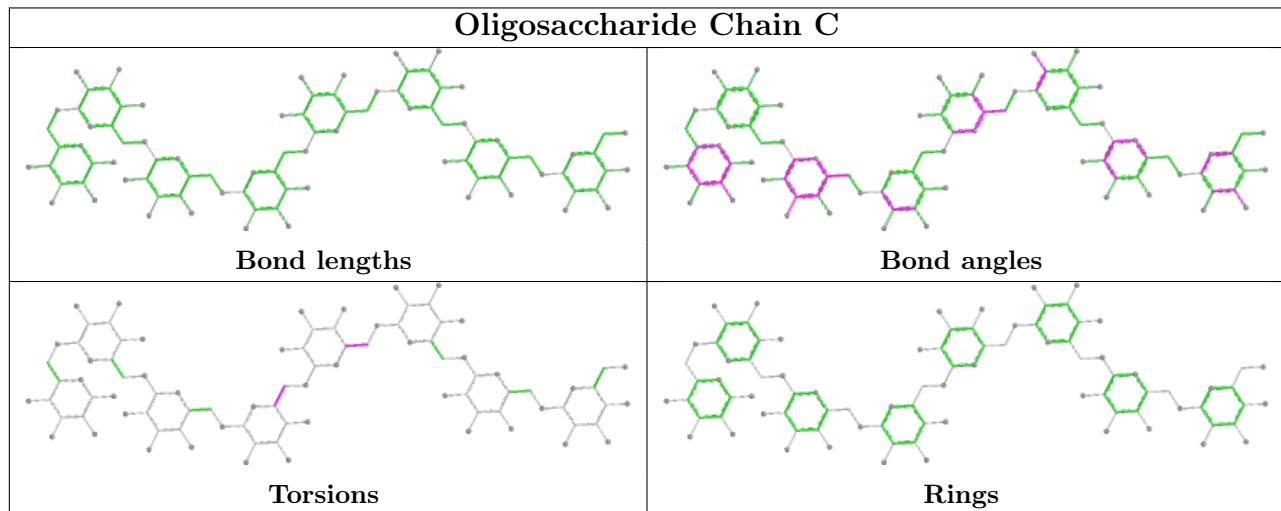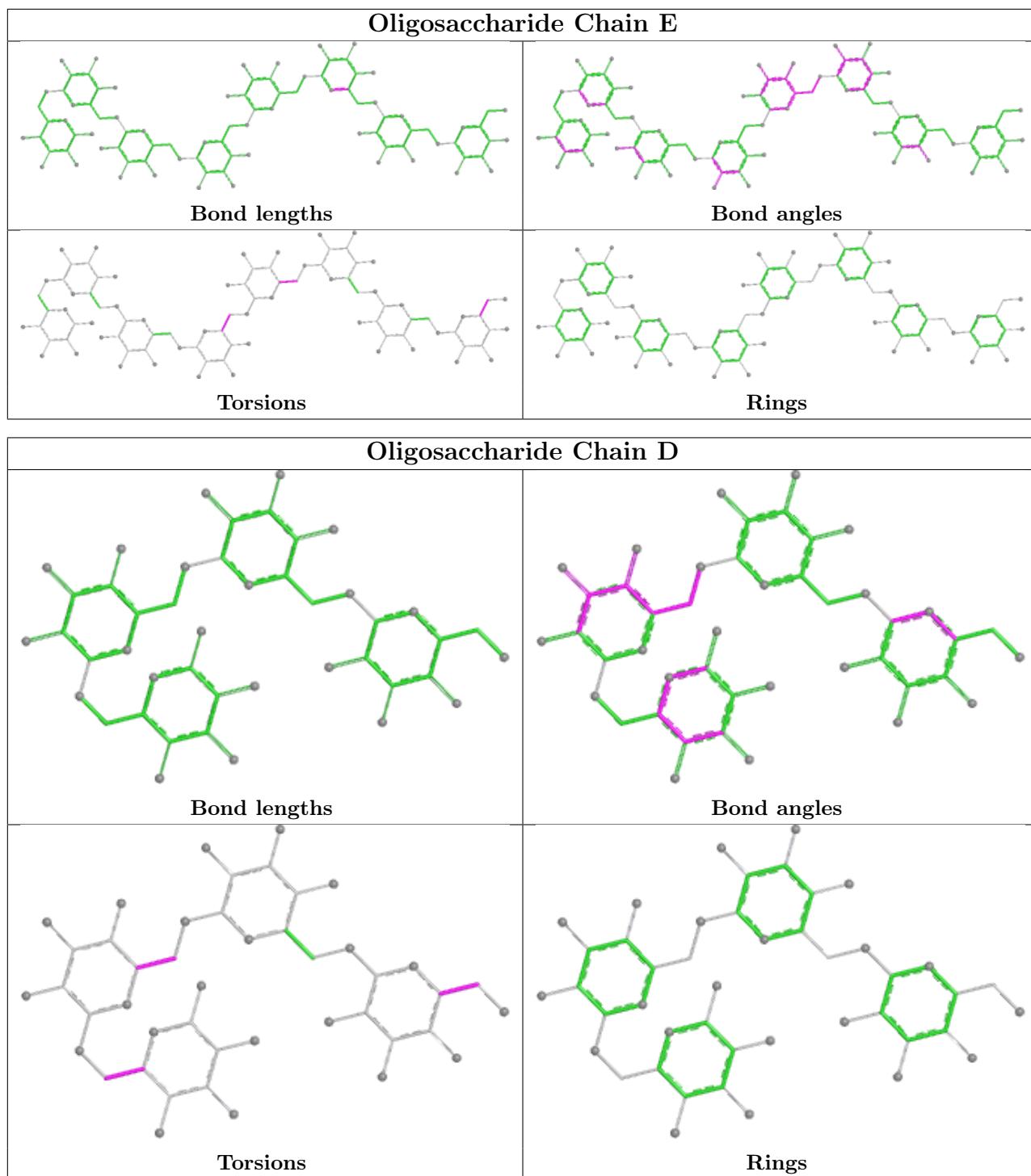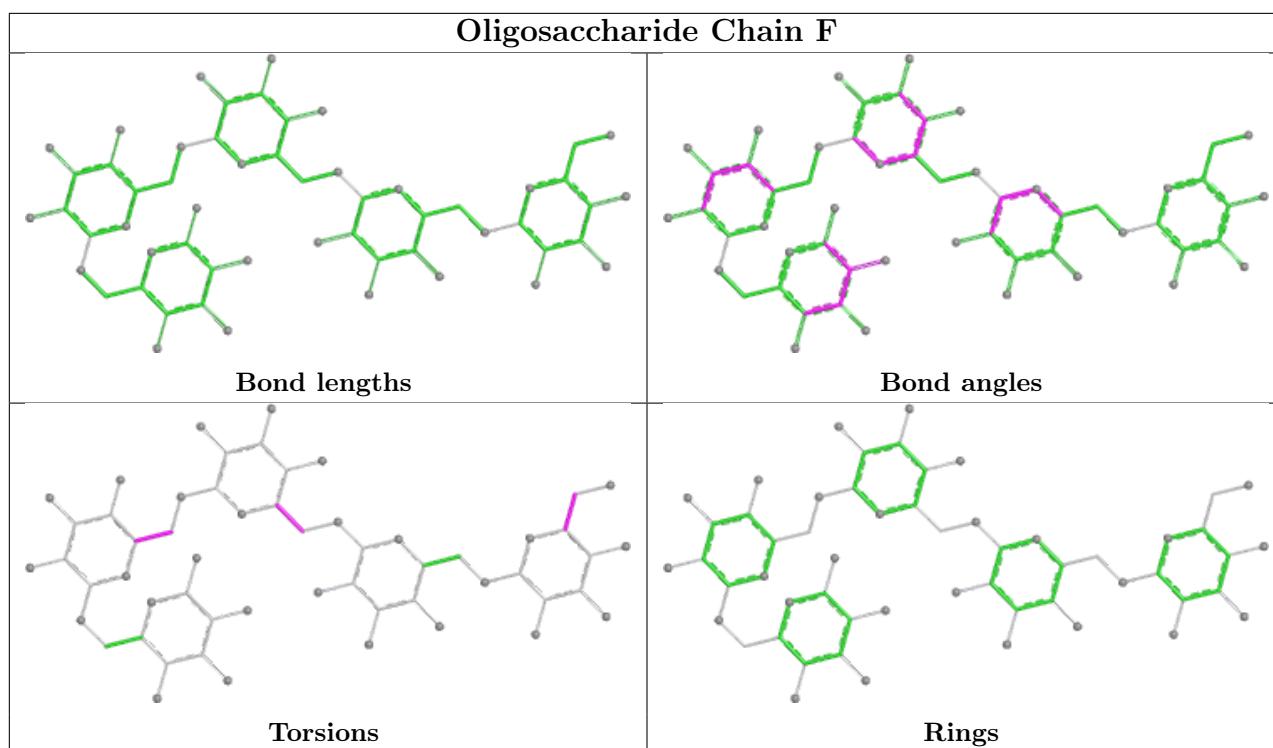
5.6   Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
7	SO4	B	803	-	4,4,4	0.39	0	6,6,6	0.43	0
7	SO4	B	807	-	4,4,4	0.54	0	6,6,6	0.37	0
8	MES	B	808	-	12,12,12	1.66	1 (8%)	15,16,16	1.88	3 (20%)
7	SO4	A	808	-	4,4,4	0.48	0	6,6,6	0.39	0
7	SO4	B	806	-	4,4,4	0.58	0	6,6,6	0.31	0
8	MES	A	809	-	12,12,12	1.94	1 (8%)	15,16,16	1.38	3 (20%)
7	SO4	B	805	-	4,4,4	0.54	0	6,6,6	0.33	0
7	SO4	A	805	-	4,4,4	0.50	0	6,6,6	0.27	0
7	SO4	B	804	-	4,4,4	0.49	0	6,6,6	0.20	0
7	SO4	A	807	-	4,4,4	0.56	0	6,6,6	0.39	0
7	SO4	A	806	-	4,4,4	0.77	0	6,6,6	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
7	SO4	A	804	-	4,4,4	0.57	0	6,6,6	0.27	0
7	SO4	A	803	-	4,4,4	0.26	0	6,6,6	0.75	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	MES	A	809	-	-	0/6/14/14	0/1/1/1
8	MES	B	808	-	-	3/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	809	MES	C8-S	-6.26	1.68	1.77
8	B	808	MES	C8-S	-5.16	1.70	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	808	MES	O1S-S-C8	5.07	114.38	106.73
8	A	809	MES	O3S-S-C8	2.94	111.75	106.00
8	B	808	MES	O3S-S-O1S	-2.54	105.04	111.40
8	A	809	MES	C6-C5-N4	2.40	113.76	110.12
8	B	808	MES	C6-C5-N4	2.05	113.24	110.12
8	A	809	MES	O1-C6-C5	-2.00	107.46	111.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	808	MES	C7-C8-S-O3S
8	B	808	MES	C7-C8-S-O1S
8	B	808	MES	C7-C8-S-O2S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	808	MES	1	0

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	699/710 (98%)	-0.34	11 (1%)	72	74	31, 47, 77, 124	0
1	B	698/710 (98%)	-0.34	10 (1%)	75	77	29, 45, 84, 135	0
All	All	1397/1420 (98%)	-0.34	21 (1%)	73	75	29, 46, 80, 135	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	624	GLN	6.4
1	A	688	ALA	4.4
1	A	718	ALA	4.0
1	A	622	GLY	3.9
1	B	722	TYR	3.6
1	B	688	ALA	3.6
1	A	624	GLN	3.6
1	B	625	PHE	3.5
1	A	625	PHE	3.5
1	A	623	SER	3.2
1	A	621	THR	3.1
1	B	689	ASP	3.1
1	A	691	THR	2.9
1	A	689	ASP	2.7
1	B	623	SER	2.6
1	A	441	GLY	2.6
1	A	719	GLY	2.2
1	B	95	SER	2.2
1	B	686	ILE	2.1
1	B	718	ALA	2.0
1	B	721	LYS	2.0

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(Å^2)	Q<0.9
3	GLC	D	1	12/12	0.75	0.19	69,83,93,94	0
4	GLC	F	5	11/12	0.86	0.26	78,90,94,96	0
2	GLC	C	5	11/12	0.89	0.17	47,51,63,64	0
4	GLC	F	3	11/12	0.90	0.11	50,58,63,67	0
2	GLC	C	7	11/12	0.91	0.12	55,62,65,73	0
4	GLC	F	4	11/12	0.91	0.11	64,70,76,84	0
2	GLC	C	6	11/12	0.91	0.11	56,65,69,75	0
4	GLC	F	1	12/12	0.92	0.14	59,78,83,83	0
3	GLC	D	4	11/12	0.93	0.12	57,72,84,85	0
4	GLC	F	2	11/12	0.94	0.10	49,53,55,55	0
2	GLC	C	4	11/12	0.94	0.09	41,48,52,52	0
2	GLC	E	6	11/12	0.95	0.11	40,43,47,48	0
2	GLC	E	5	11/12	0.95	0.12	35,42,45,52	0
2	GLC	C	3	11/12	0.96	0.09	40,44,51,53	0
2	GLC	E	7	11/12	0.96	0.10	41,43,53,55	0
2	GLC	E	3	11/12	0.96	0.09	39,41,43,43	0
3	GLC	D	3	11/12	0.96	0.17	66,73,81,87	0
2	BGC	C	1	12/12	0.96	0.12	31,35,37,39	0
2	GLC	E	8	11/12	0.97	0.08	32,36,40,41	0
2	GLC	C	8	11/12	0.97	0.09	44,47,53,58	0
3	GLC	D	2	11/12	0.97	0.09	58,62,65,66	0
2	GLC	E	2	11/12	0.97	0.10	30,35,37,42	0
2	GLC	C	2	11/12	0.97	0.10	31,34,35,42	0
2	GLC	E	4	11/12	0.98	0.09	35,39,42,44	0
2	BGC	E	1	12/12	0.98	0.10	28,30,34,35	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)
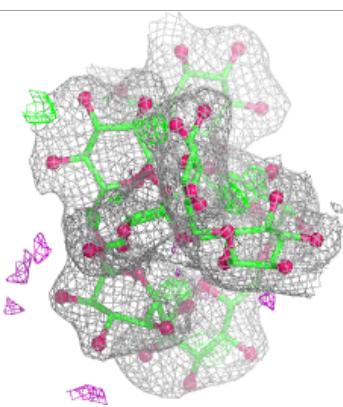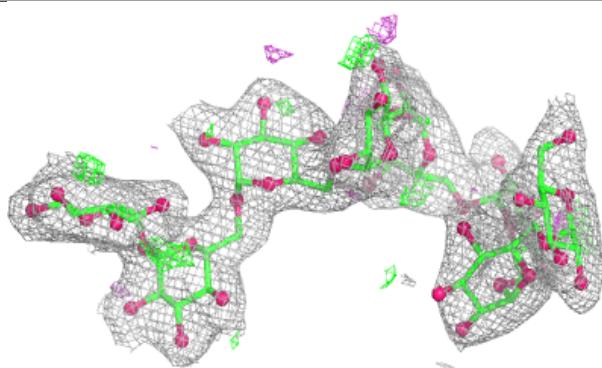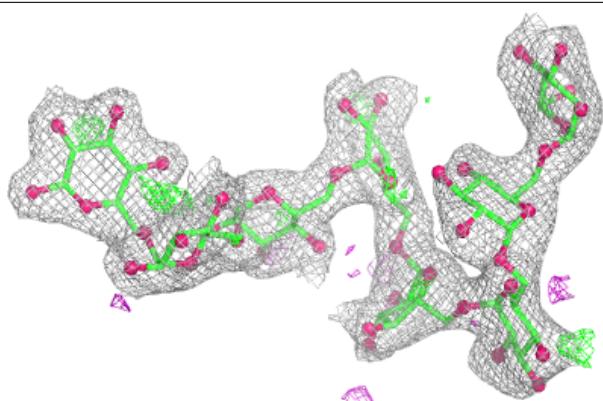
Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
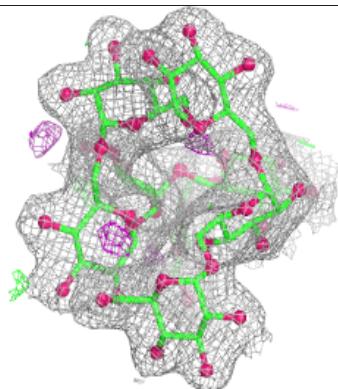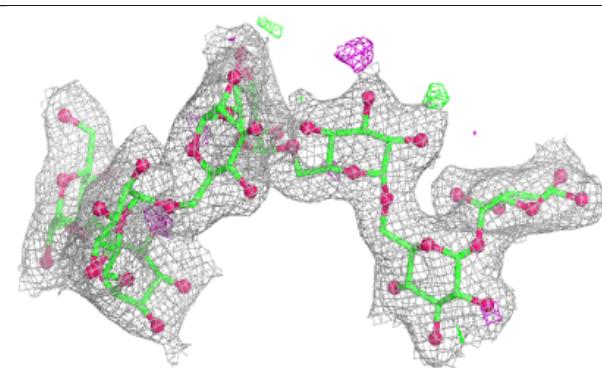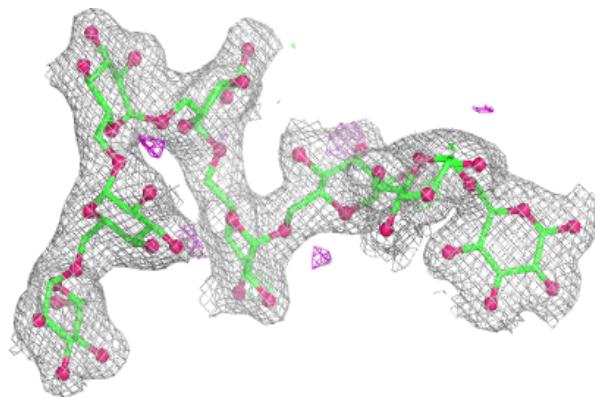
Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
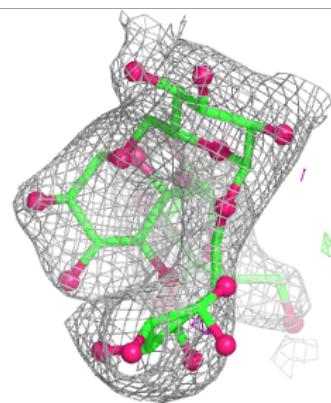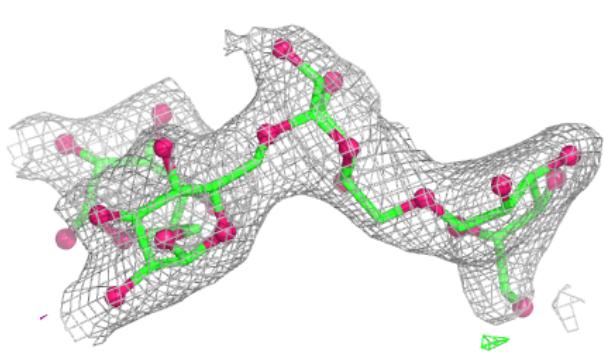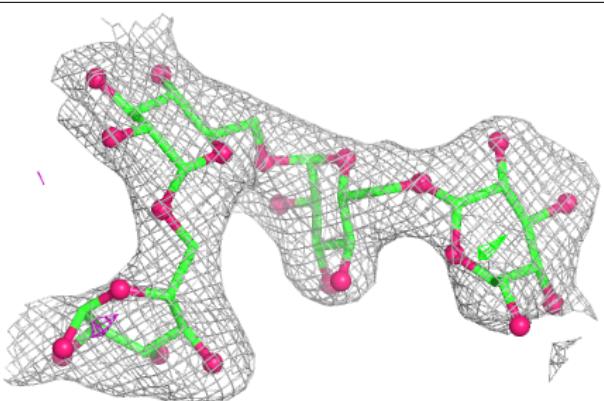
Electron density around Chain F:

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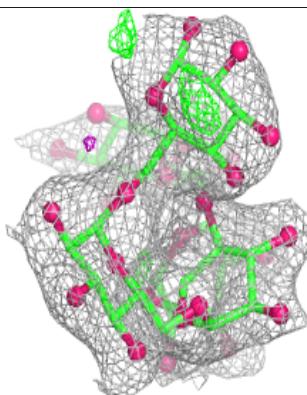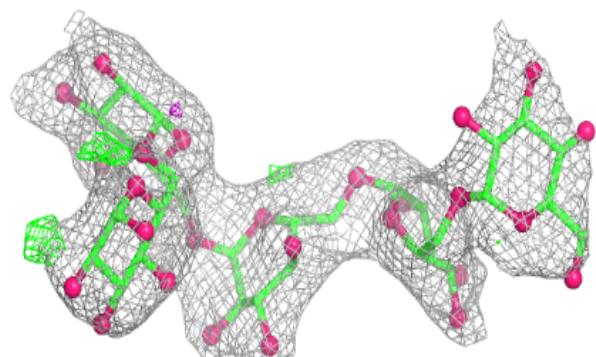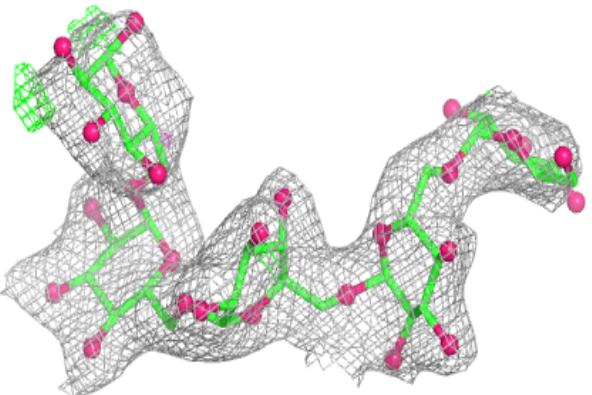
6.4 Ligands ⓘ

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	A	804	5/5	0.85	0.20	68,77,91,96	0
7	SO4	B	805	5/5	0.88	0.17	83,84,98,101	0
7	SO4	A	806	5/5	0.89	0.16	56,57,81,83	0
7	SO4	A	807	5/5	0.90	0.22	84,90,94,94	0
7	SO4	A	805	5/5	0.90	0.23	93,97,102,106	0
7	SO4	B	804	5/5	0.92	0.19	85,88,98,103	0
7	SO4	B	806	5/5	0.92	0.20	79,91,97,99	0
7	SO4	A	808	5/5	0.94	0.14	88,90,93,95	0
6	NA	B	802	1/1	0.96	0.06	49,49,49,49	0
7	SO4	B	807	5/5	0.96	0.14	74,75,80,86	0
5	CA	A	801	1/1	0.97	0.09	49,49,49,49	0
7	SO4	B	803	5/5	0.97	0.14	47,48,55,64	0
8	MES	B	808	12/12	0.97	0.09	43,50,52,53	0
7	SO4	A	803	5/5	0.98	0.09	42,50,52,60	0
6	NA	A	802	1/1	0.99	0.11	44,44,44,44	0
8	MES	A	809	12/12	0.99	0.10	44,47,50,51	0
5	CA	B	801	1/1	0.99	0.11	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.