



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:59 PM UTC

PDB ID : 4DOE / pdb_00004doe
Title : The liganded structure of Cbescii CelA GH9 module
Authors : Alahuhta, P.M.; Lunin, V.V.
Deposited on : 2012-02-09
Resolution : 1.56 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

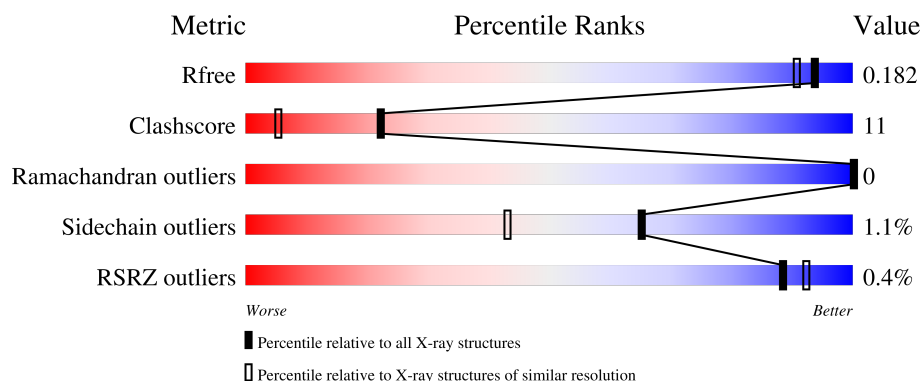
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	475	
2	B	2	
3	C	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BGC	C	1	-	-	X	-
6	GOL	A	507	-	X	-	-
7	EDO	A	511	-	X	-	-
7	EDO	A	516	-	-	X	-
7	EDO	A	517	-	-	X	-
7	EDO	A	523	-	-	X	-
7	EDO	A	536	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4866 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 1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	34	0
			3895	2485	650	749	11			

There are 25 discrepancies between the modelled and reference sequences:

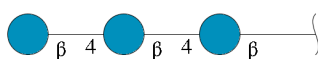
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P96311
A	2	GLY	-	expression tag	UNP P96311
A	3	SER	-	expression tag	UNP P96311
A	4	SER	-	expression tag	UNP P96311
A	5	HIS	-	expression tag	UNP P96311
A	6	HIS	-	expression tag	UNP P96311
A	7	HIS	-	expression tag	UNP P96311
A	8	HIS	-	expression tag	UNP P96311
A	9	HIS	-	expression tag	UNP P96311
A	10	HIS	-	expression tag	UNP P96311
A	11	SER	-	expression tag	UNP P96311
A	12	SER	-	expression tag	UNP P96311
A	13	GLY	-	expression tag	UNP P96311
A	14	LEU	-	expression tag	UNP P96311
A	15	VAL	-	expression tag	UNP P96311
A	16	PRO	-	expression tag	UNP P96311
A	17	ARG	-	expression tag	UNP P96311
A	18	GLY	-	expression tag	UNP P96311
A	19	SER	-	expression tag	UNP P96311
A	20	HIS	-	expression tag	UNP P96311
A	21	MET	-	expression tag	UNP P96311
A	22	ALA	-	expression tag	UNP P96311
A	23	SER	-	expression tag	UNP P96311
A	176	ALA	THR	conflict	UNP P96311
A	313	THR	ILE	conflict	UNP P96311

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



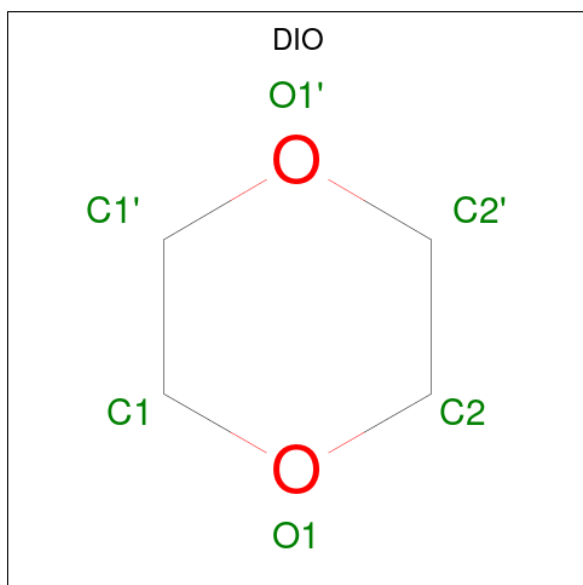
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	1	0
			25	13	12			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 4 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).

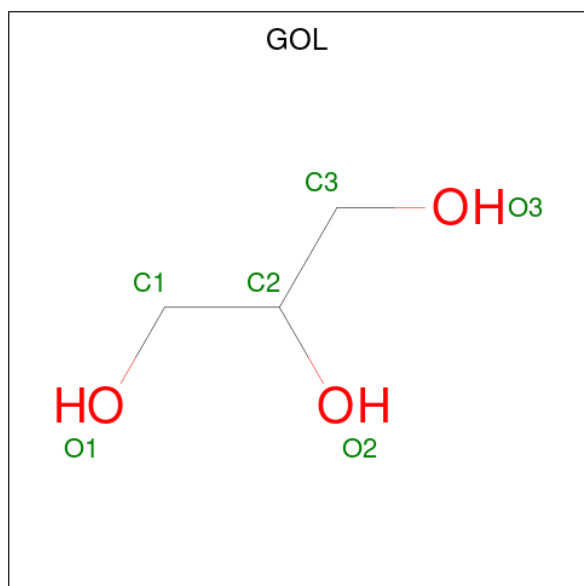


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

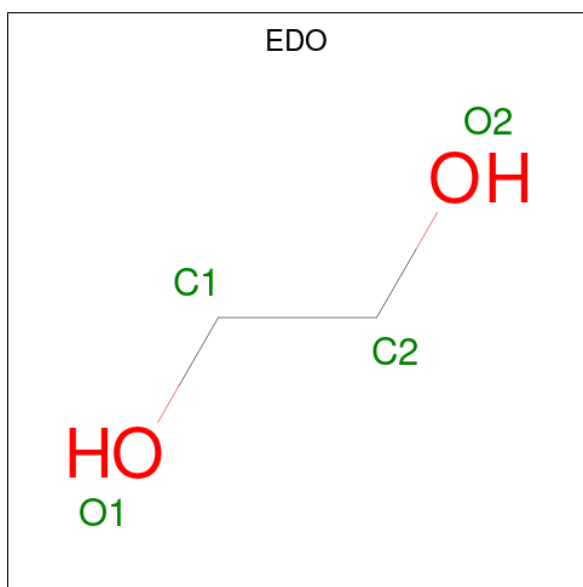
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	1
			12	6	6		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



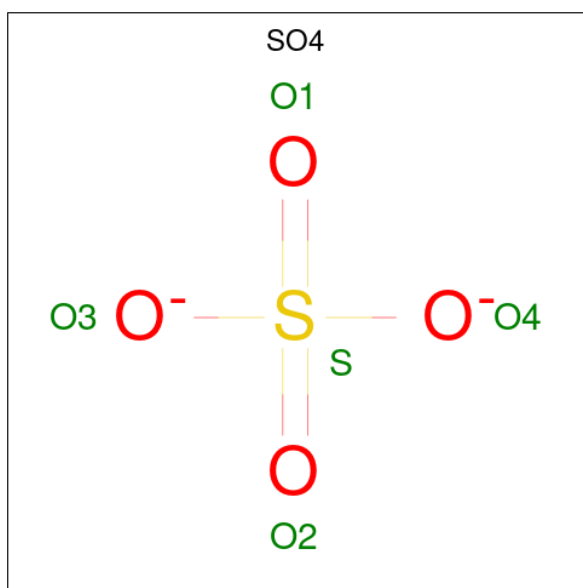
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	1
			8	4	4		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	1
			8	4	4		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

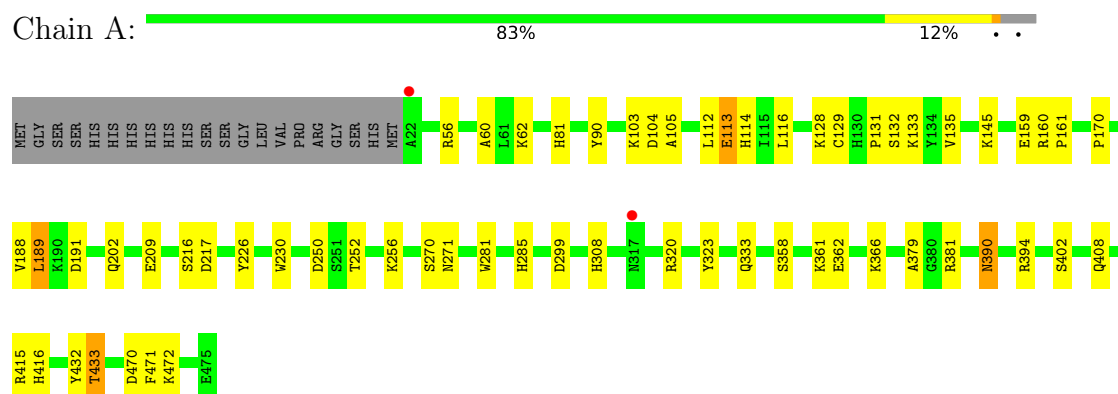
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	704	Total	O	0	33
			736	736		

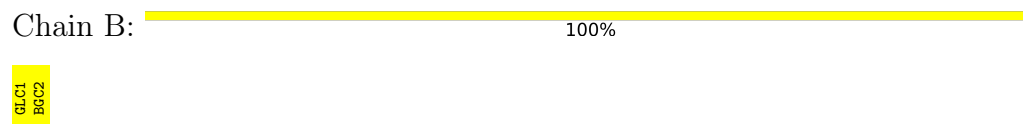
3 Residue-property plots [i](#)

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: 1,4-beta-glucanase



- Molecule 2: beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.93Å 147.93Å 59.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.62 – 1.56 25.62 – 1.56	Depositor EDS
% Data completeness (in resolution range)	97.3 (25.62-1.56) 97.3 (25.62-1.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.148 , 0.175 0.158 , 0.182	Depositor DCC
R_{free} test set	5118 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4866	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: EDO, DIO, SO4, CA, GOL, GLC, BGC

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	1.15	7/4017 (0.2%)	1.06	0/5463

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	HIS	ND1-CE1	7.08	1.39	1.32
1	A	308	HIS	ND1-CE1	6.22	1.38	1.32
1	A	81	HIS	ND1-CE1	6.22	1.38	1.32
1	A	323	TYR	N-CA	-5.56	1.39	1.46
1	A	285	HIS	ND1-CE1	5.53	1.38	1.32
1	A	128	LYS	C-O	5.48	1.30	1.24
1	A	416	HIS	CA-C	-5.27	1.46	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	390	ASN	Mainchain
1	A	394	ARG	Sidechain
1	A	56	ARG	Sidechain

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	3895	0	3631	75	0
2	B	25	0	18	0	0
3	C	34	0	30	9	0
4	A	6	0	8	0	0
5	A	1	0	0	0	0
6	A	42	0	56	6	0
7	A	112	0	168	43	0
8	A	15	0	0	0	0
9	A	736	0	0	8	0
All	All	4866	0	3911	86	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 11.

All (86) 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:381[A]:ARG:NH1	1:A:432[A]:TYR:HE2	1.30	1.28
1:A:381[A]:ARG:NH2	1:A:432[A]:TYR:CE2	2.01	1.28
1:A:381[A]:ARG:NH1	1:A:432[A]:TYR:CE2	2.13	1.17
1:A:381[A]:ARG:CZ	1:A:432[A]:TYR:CE2	2.28	1.16
1:A:113:GLU:HB2	6:A:507:GOL:H31	1.24	1.08
1:A:381[A]:ARG:NH2	1:A:432[A]:TYR:CD2	2.22	1.08
1:A:202[B]:GLN:OE1	6:A:510[B]:GOL:O2	1.77	1.02
1:A:299:ASP:H	7:A:524:EDO:H12	1.36	0.91
1:A:113:GLU:CB	6:A:507:GOL:H31	2.00	0.91
1:A:381[B]:ARG:NH2	1:A:390:ASN:O	2.03	0.91
1:A:381[A]:ARG:HH12	1:A:432[A]:TYR:HE2	0.98	0.89
1:A:113:GLU:HB2	6:A:507:GOL:C3	2.04	0.87
1:A:415[A]:ARG:NH1	9:A:637[A]:HOH:O	1.98	0.86
7:A:536:EDO:O1	3:C:1:BGC:O6	1.95	0.83
1:A:230:TRP:HE1	7:A:536:EDO:H22	1.44	0.82
1:A:362[B]:GLU:CG	1:A:366[B]:LYS:HE3	2.09	0.81
1:A:333:GLN:HB2	9:A:1270:HOH:O	1.83	0.77
1:A:471:PHE:HA	7:A:516:EDO:H21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381[B]:ARG:CZ	1:A:390:ASN:O	2.36	0.72
1:A:432[A]:TYR:CE2	1:A:433[A]:THR:O	2.43	0.71
7:A:536:EDO:O1	3:C:1:BGC:H4	1.90	0.71
1:A:362[B]:GLU:HG3	1:A:366[B]:LYS:HE3	1.72	0.70
7:A:536:EDO:H11	3:C:2:BGC:C1	2.21	0.70
1:A:230:TRP:HE1	7:A:536:EDO:C2	2.05	0.68
1:A:112:LEU:HD21	7:A:517:EDO:H11	1.77	0.67
1:A:104[A]:ASP:C	7:A:523:EDO:H12	2.21	0.65
1:A:60:ALA:HA	7:A:529:EDO:H12	1.78	0.64
1:A:381[A]:ARG:CZ	1:A:432[A]:TYR:CD2	2.71	0.64
1:A:299:ASP:N	7:A:524:EDO:H12	2.11	0.64
1:A:145:LYS:HE3	9:A:1116:HOH:O	1.98	0.64
7:A:536:EDO:C1	3:C:1:BGC:H6	2.12	0.62
1:A:160:ARG:HD3	7:A:529:EDO:H21	1.79	0.62
7:A:536:EDO:C1	3:C:1:BGC:O6	2.47	0.62
1:A:113:GLU:HB3	9:A:1162:HOH:O	1.98	0.62
1:A:362[B]:GLU:HG2	1:A:366[B]:LYS:HE3	1.82	0.62
1:A:112:LEU:HD21	7:A:517:EDO:C1	2.30	0.61
1:A:159:GLU:HB3	7:A:532:EDO:H11	1.84	0.59
1:A:381[B]:ARG:NE	1:A:390:ASN:O	2.34	0.59
1:A:116:LEU:HD11	7:A:517:EDO:H22	1.85	0.58
1:A:188:VAL:HG12	7:A:535:EDO:H21	1.85	0.58
1:A:408:GLN:N	7:A:520:EDO:H11	2.18	0.58
1:A:381[B]:ARG:HD3	1:A:381[B]:ARG:C	2.29	0.58
1:A:362[B]:GLU:HG2	1:A:366[B]:LYS:CE	2.35	0.57
1:A:133:LYS:NZ	1:A:209:GLU:OE1	2.30	0.57
7:A:536:EDO:C1	3:C:1:BGC:H4	2.35	0.56
1:A:432[A]:TYR:CD2	1:A:433[A]:THR:O	2.61	0.54
1:A:217:ASP:H	7:A:513[B]:EDO:H11	1.74	0.52
1:A:432[A]:TYR:CZ	1:A:433[A]:THR:O	2.61	0.52
1:A:470[B]:ASP:OD2	7:A:521:EDO:O1	2.24	0.52
1:A:472:LYS:O	7:A:516:EDO:H12	2.08	0.51
1:A:226:TYR:O	7:A:536:EDO:H21	2.09	0.51
7:A:536:EDO:O1	3:C:1:BGC:C4	2.59	0.50
1:A:358[A]:SER:O	1:A:361[A]:LYS:HB2	2.12	0.49
1:A:116:LEU:CD1	7:A:517:EDO:H22	2.41	0.49
1:A:381[B]:ARG:NH1	1:A:432[B]:TYR:CE1	2.80	0.49
1:A:116:LEU:HD22	1:A:189[A]:LEU:HD13	1.95	0.49
7:A:523:EDO:H22	9:A:1222:HOH:O	2.14	0.47
1:A:252[B]:THR:O	1:A:256[B]:LYS:HG3	2.15	0.46
1:A:104[A]:ASP:HB3	7:A:523:EDO:H11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:OD1	1:A:252[B]:THR:HG23	2.16	0.45
1:A:132[A]:SER:HB2	1:A:135:VAL:CG2	2.46	0.45
1:A:402:SER:HB3	1:A:415[A]:ARG:HD3	1.99	0.45
1:A:230:TRP:NE1	7:A:536:EDO:H22	2.23	0.44
1:A:188:VAL:HA	7:A:535:EDO:H22	2.00	0.44
1:A:471:PHE:CD1	7:A:516:EDO:H21	2.52	0.44
7:A:523:EDO:H21	9:A:905:HOH:O	2.17	0.44
1:A:129:CYS:C	1:A:131[A]:PRO:HD3	2.43	0.44
1:A:161:PRO:HB3	7:A:532:EDO:H22	2.00	0.44
1:A:270[B]:SER:OG	1:A:271:ASN:N	2.52	0.43
1:A:170:PRO:HG2	1:A:216:SER:HB3	2.01	0.42
1:A:104[A]:ASP:HB3	7:A:523:EDO:C1	2.49	0.42
1:A:415[A]:ARG:CZ	9:A:637[A]:HOH:O	2.57	0.42
1:A:379:ALA:HB3	9:A:944:HOH:O	2.19	0.42
1:A:202[A]:GLN:CB	6:A:510[A]:GOL:H2	2.50	0.42
1:A:381[B]:ARG:HD3	1:A:381[B]:ARG:O	2.20	0.41
1:A:103:LYS:HE3	7:A:517:EDO:O1	2.20	0.41
1:A:408:GLN:H	7:A:520:EDO:H11	1.84	0.41
1:A:62:LYS:H	7:A:529:EDO:H11	1.84	0.41
1:A:112:LEU:HD21	7:A:517:EDO:H12	2.03	0.41
1:A:202[A]:GLN:HB2	6:A:510[A]:GOL:H2	2.02	0.41
7:A:536:EDO:H11	3:C:1:BGC:H4	2.00	0.41
7:A:536:EDO:H12	3:C:1:BGC:O6	2.20	0.41
1:A:90:TYR:CG	1:A:281:TRP:HA	2.56	0.41
1:A:191:ASP:HB2	7:A:517:EDO:H21	2.03	0.41
1:A:471:PHE:HD1	7:A:516:EDO:H21	1.86	0.41
1:A:105:ALA:N	7:A:523:EDO:H12	2.36	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	487/475 (102%)	470 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/389 (104%)	399 (98%)	7 (2%)	53	25

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

Mol	Chain	Res	Type
1	A	113	GLU
1	A	189[A]	LEU
1	A	189[B]	LEU
1	A	320[A]	ARG
1	A	320[B]	ARG
1	A	433[A]	THR
1	A	433[B]	THR

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

Mol	Chain	Res	Type
1	A	67	ASN
1	A	123	ASN
1	A	408	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 ⓘ

6 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	GLC	B	1[A]	-	12,12,12	0.67	0	17,17,17	1.38	2 (11%)
2	GLC	B	1[B]	-	12,12,12	0.69	0	17,17,17	1.48	3 (17%)
2	BGC	B	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.47	3 (20%)
3	BGC	C	1	3	12,12,12	0.98	1 (8%)	17,17,17	1.71	5 (29%)
3	BGC	C	2	3	11,11,12	1.04	2 (18%)	15,15,17	1.87	3 (20%)
3	BGC	C	3	3	11,11,12	0.75	0	15,15,17	1.30	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
2	GLC	B	1[A]	-	-	0/2/22/22	0/1/1/1
2	GLC	B	1[B]	-	-	0/2/22/22	0/1/1/1
2	BGC	B	2	2	-	0/2/19/22	0/1/1/1
3	BGC	C	1	3	-	1/2/22/22	0/1/1/1
3	BGC	C	2	3	-	0/2/19/22	0/1/1/1
3	BGC	C	3	3	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	BGC	C4-C5	-2.47	1.47	1.53
3	C	2	BGC	O5-C5	-2.08	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	BGC	O5-C1	-2.02	1.40	1.43
3	C	1	BGC	O4-C4	2.01	1.47	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	BGC	C1-O5-C5	4.47	118.18	112.19
3	C	2	BGC	C1-C2-C3	3.77	115.14	109.64
3	C	1	BGC	O1-C1-C2	3.28	118.49	108.98
3	C	1	BGC	O5-C1-C2	3.19	115.91	110.30
2	B	1[A]	GLC	O3-C3-C2	-3.17	102.91	110.38
2	B	1[B]	GLC	O3-C3-C2	-3.17	102.91	110.38
2	B	2	BGC	O5-C5-C4	-3.07	103.37	110.83
3	C	2	BGC	C3-C4-C5	-2.91	104.96	110.23
2	B	1[A]	GLC	O4-C4-C3	-2.84	103.68	110.38
2	B	1[B]	GLC	O4-C4-C3	-2.84	103.68	110.38
2	B	2	BGC	O5-C1-C2	-2.52	104.78	110.79
2	B	1[B]	GLC	C6-C5-C4	-2.28	107.42	113.02
3	C	1	BGC	C3-C4-C5	-2.21	106.22	110.23
2	B	2	BGC	O5-C5-C6	2.18	111.92	107.66
3	C	1	BGC	C6-C5-C4	2.18	118.38	113.02
3	C	3	BGC	O4-C4-C5	2.11	114.52	109.32
3	C	3	BGC	C1-C2-C3	2.02	112.59	109.64
3	C	1	BGC	O4-C4-C3	2.01	115.12	110.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

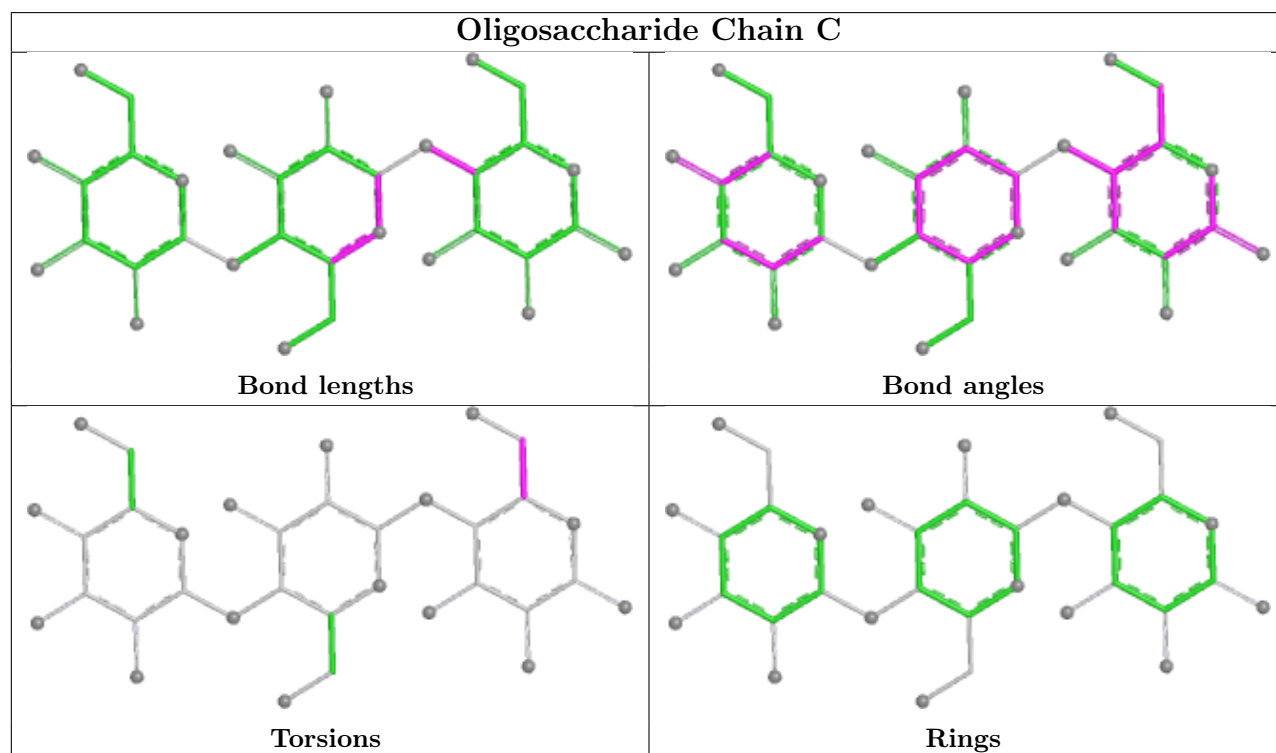
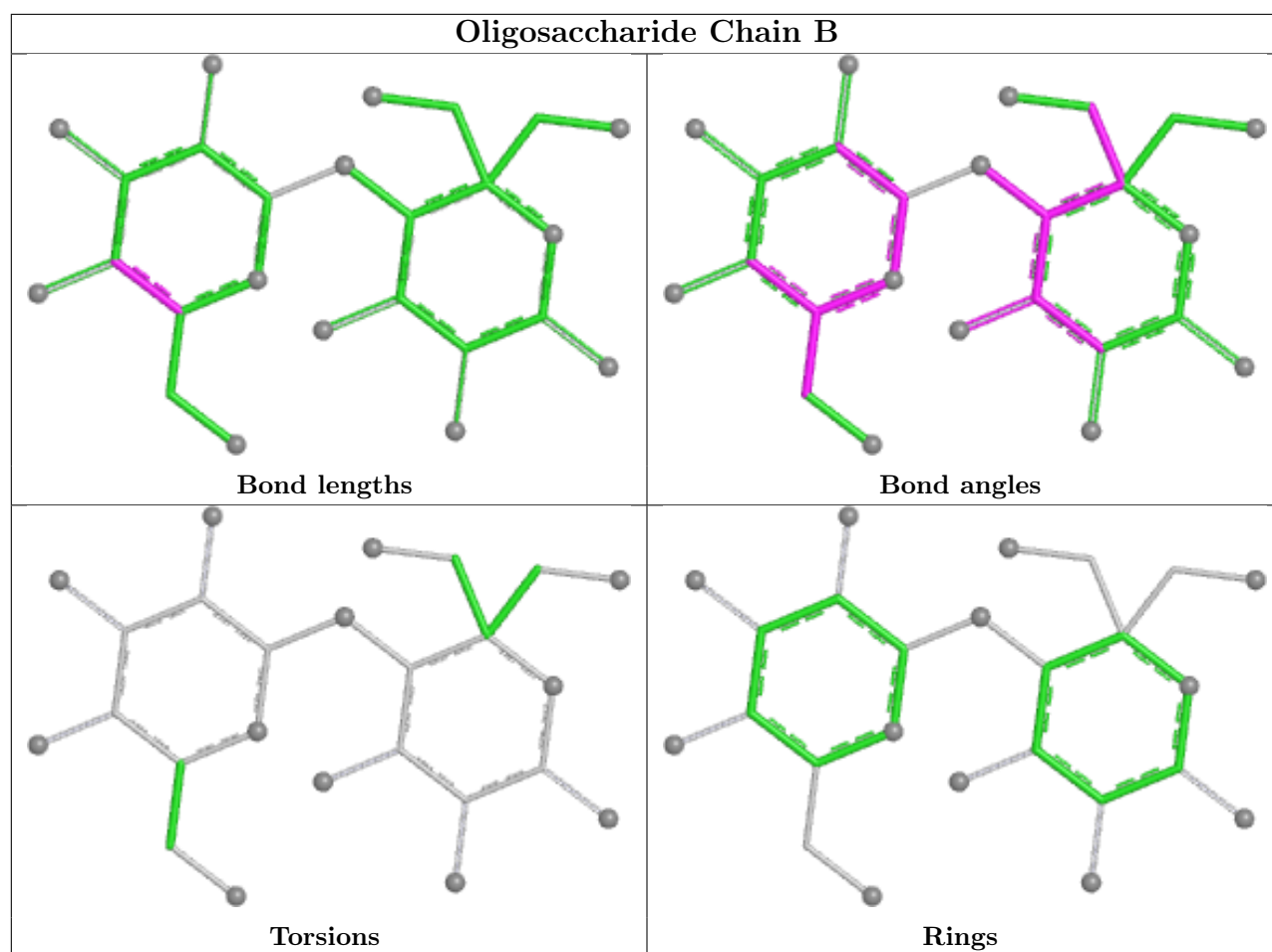
Mol	Chain	Res	Type	Atoms
3	C	1	BGC	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	BGC	8	0
3	C	2	BGC	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 40 ligands modelled in this entry, 1 is monoatomic - leaving 39 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	EDO	A	524	-	3,3,3	0.36	0	2,2,2	0.19	0
6	GOL	A	510[A]	-	5,5,5	0.38	0	5,5,5	0.65	0
6	GOL	A	505	-	5,5,5	0.44	0	5,5,5	1.20	0
7	EDO	A	527	-	3,3,3	0.48	0	2,2,2	0.34	0
7	EDO	A	517	-	3,3,3	0.27	0	2,2,2	0.72	0
7	EDO	A	522	-	3,3,3	0.32	0	2,2,2	0.20	0
7	EDO	A	528	-	3,3,3	0.37	0	2,2,2	0.26	0
8	SO4	A	537	-	4,4,4	0.41	0	6,6,6	1.25	0
7	EDO	A	518[B]	-	3,3,3	0.45	0	2,2,2	0.40	0
7	EDO	A	536	-	3,3,3	0.32	0	2,2,2	0.60	0
8	SO4	A	538	-	4,4,4	0.66	0	6,6,6	0.36	0
8	SO4	A	539	-	4,4,4	0.54	0	6,6,6	0.43	0
7	EDO	A	515	-	3,3,3	0.32	0	2,2,2	0.56	0
7	EDO	A	519	-	3,3,3	0.41	0	2,2,2	0.66	0
7	EDO	A	511	-	3,3,3	0.30	0	2,2,2	2.34	2 (100%)
7	EDO	A	518[A]	-	3,3,3	0.39	0	2,2,2	0.63	0
7	EDO	A	512	-	3,3,3	0.28	0	2,2,2	0.52	0
7	EDO	A	520	-	3,3,3	0.44	0	2,2,2	0.86	0
6	GOL	A	506	-	5,5,5	0.30	0	5,5,5	0.34	0
7	EDO	A	513[B]	-	3,3,3	0.29	0	2,2,2	0.61	0
7	EDO	A	530	-	3,3,3	0.53	0	2,2,2	0.24	0
7	EDO	A	533	-	3,3,3	0.41	0	2,2,2	0.25	0
7	EDO	A	521	-	3,3,3	0.53	0	2,2,2	0.80	0
7	EDO	A	526	-	3,3,3	0.11	0	2,2,2	0.65	0
7	EDO	A	531	-	3,3,3	0.27	0	2,2,2	0.33	0
6	GOL	A	508	-	5,5,5	0.42	0	5,5,5	0.84	0
6	GOL	A	510[B]	-	5,5,5	0.41	0	5,5,5	0.61	0
7	EDO	A	523	-	3,3,3	0.32	0	2,2,2	0.28	0
7	EDO	A	532	-	3,3,3	0.55	0	2,2,2	0.18	0
7	EDO	A	535	-	3,3,3	0.62	0	2,2,2	0.37	0
7	EDO	A	513[A]	-	3,3,3	0.46	0	2,2,2	0.23	0
7	EDO	A	514	-	3,3,3	0.32	0	2,2,2	1.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	529	-	3,3,3	0.62	0	2,2,2	0.25	0
7	EDO	A	525	-	3,3,3	0.45	0	2,2,2	0.21	0
7	EDO	A	516	-	3,3,3	0.42	0	2,2,2	0.24	0
4	DIO	A	501	-	6,6,6	0.62	0	6,6,6	1.76	1 (16%)
7	EDO	A	534	-	3,3,3	0.38	0	2,2,2	0.48	0
6	GOL	A	509	-	5,5,5	0.73	0	5,5,5	0.64	0
6	GOL	A	507	-	5,5,5	0.58	0	5,5,5	1.62	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
7	EDO	A	524	-	-	1/1/1/1	-
6	GOL	A	510[A]	-	-	2/4/4/4	-
6	GOL	A	505	-	-	4/4/4/4	-
7	EDO	A	527	-	-	1/1/1/1	-
7	EDO	A	517	-	-	1/1/1/1	-
7	EDO	A	522	-	-	1/1/1/1	-
7	EDO	A	528	-	-	1/1/1/1	-
7	EDO	A	518[B]	-	-	1/1/1/1	-
7	EDO	A	536	-	-	1/1/1/1	-
7	EDO	A	515	-	-	0/1/1/1	-
7	EDO	A	519	-	-	1/1/1/1	-
7	EDO	A	511	-	-	1/1/1/1	-
7	EDO	A	518[A]	-	-	1/1/1/1	-
7	EDO	A	512	-	-	0/1/1/1	-
7	EDO	A	520	-	-	0/1/1/1	-
6	GOL	A	506	-	-	2/4/4/4	-
7	EDO	A	513[B]	-	-	1/1/1/1	-
7	EDO	A	530	-	-	0/1/1/1	-
7	EDO	A	533	-	-	0/1/1/1	-
7	EDO	A	521	-	-	0/1/1/1	-
7	EDO	A	526	-	-	0/1/1/1	-
7	EDO	A	531	-	-	0/1/1/1	-
6	GOL	A	508	-	-	4/4/4/4	-
6	GOL	A	510[B]	-	-	0/4/4/4	-
7	EDO	A	523	-	-	1/1/1/1	-
7	EDO	A	532	-	-	1/1/1/1	-
7	EDO	A	535	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	513[A]	-	-	1/1/1/1	-
7	EDO	A	514	-	-	1/1/1/1	-
7	EDO	A	529	-	-	1/1/1/1	-
7	EDO	A	525	-	-	0/1/1/1	-
7	EDO	A	516	-	-	1/1/1/1	-
7	EDO	A	534	-	-	0/1/1/1	-
4	DIO	A	501	-	-	-	0/1/1/1
6	GOL	A	509	-	-	1/4/4/4	-
6	GOL	A	507	-	-	4/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	DIO	C2'-O1'-C1'	-3.83	97.50	109.88
7	A	511	EDO	O2-C2-C1	-2.55	92.96	112.39
6	A	507	GOL	O2-C2-C1	2.53	119.66	109.18
6	A	507	GOL	O1-C1-C2	2.28	120.66	110.38
7	A	511	EDO	O1-C1-C2	-2.11	96.30	112.39

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	505	GOL	O1-C1-C2-C3
6	A	505	GOL	C1-C2-C3-O3
6	A	508	GOL	C1-C2-C3-O3
6	A	510[A]	GOL	O1-C1-C2-C3
6	A	505	GOL	O1-C1-C2-O2
6	A	505	GOL	O2-C2-C3-O3
6	A	506	GOL	C1-C2-C3-O3
6	A	507	GOL	O1-C1-C2-C3
6	A	507	GOL	C1-C2-C3-O3
6	A	508	GOL	O1-C1-C2-C3
6	A	508	GOL	O2-C2-C3-O3
6	A	510[A]	GOL	O1-C1-C2-O2
7	A	516	EDO	O1-C1-C2-O2
7	A	517	EDO	O1-C1-C2-O2
7	A	518[A]	EDO	O1-C1-C2-O2
7	A	535	EDO	O1-C1-C2-O2
7	A	536	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	507	GOL	O1-C1-C2-O2
6	A	508	GOL	O1-C1-C2-O2
7	A	511	EDO	O1-C1-C2-O2
7	A	513[A]	EDO	O1-C1-C2-O2
7	A	518[B]	EDO	O1-C1-C2-O2
7	A	527	EDO	O1-C1-C2-O2
6	A	506	GOL	O2-C2-C3-O3
6	A	509	GOL	O2-C2-C3-O3
7	A	529	EDO	O1-C1-C2-O2
7	A	532	EDO	O1-C1-C2-O2
7	A	523	EDO	O1-C1-C2-O2
7	A	513[B]	EDO	O1-C1-C2-O2
7	A	519	EDO	O1-C1-C2-O2
6	A	507	GOL	O2-C2-C3-O3
7	A	522	EDO	O1-C1-C2-O2
7	A	524	EDO	O1-C1-C2-O2
7	A	528	EDO	O1-C1-C2-O2
7	A	514	EDO	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	524	EDO	2	0
6	A	510[A]	GOL	2	0
7	A	517	EDO	7	0
7	A	536	EDO	13	0
7	A	520	EDO	2	0
7	A	513[B]	EDO	1	0
7	A	521	EDO	1	0
6	A	510[B]	GOL	1	0
7	A	523	EDO	6	0
7	A	532	EDO	2	0
7	A	535	EDO	2	0
7	A	529	EDO	3	0
7	A	516	EDO	4	0
6	A	507	GOL	3	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 [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	454/475 (95%)	-0.62	2 (0%) 88 92	4, 10, 20, 44	34 (7%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	ALA	2.6
1	A	317[A]	ASN	2.2

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](#)

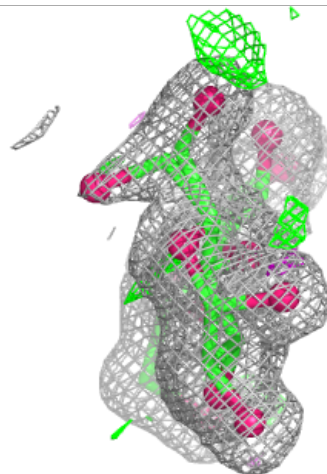
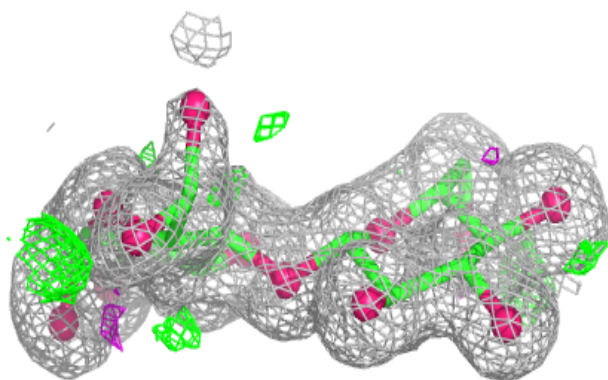
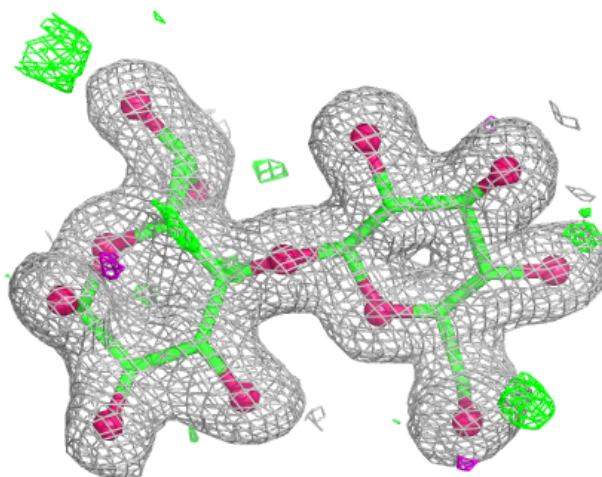
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

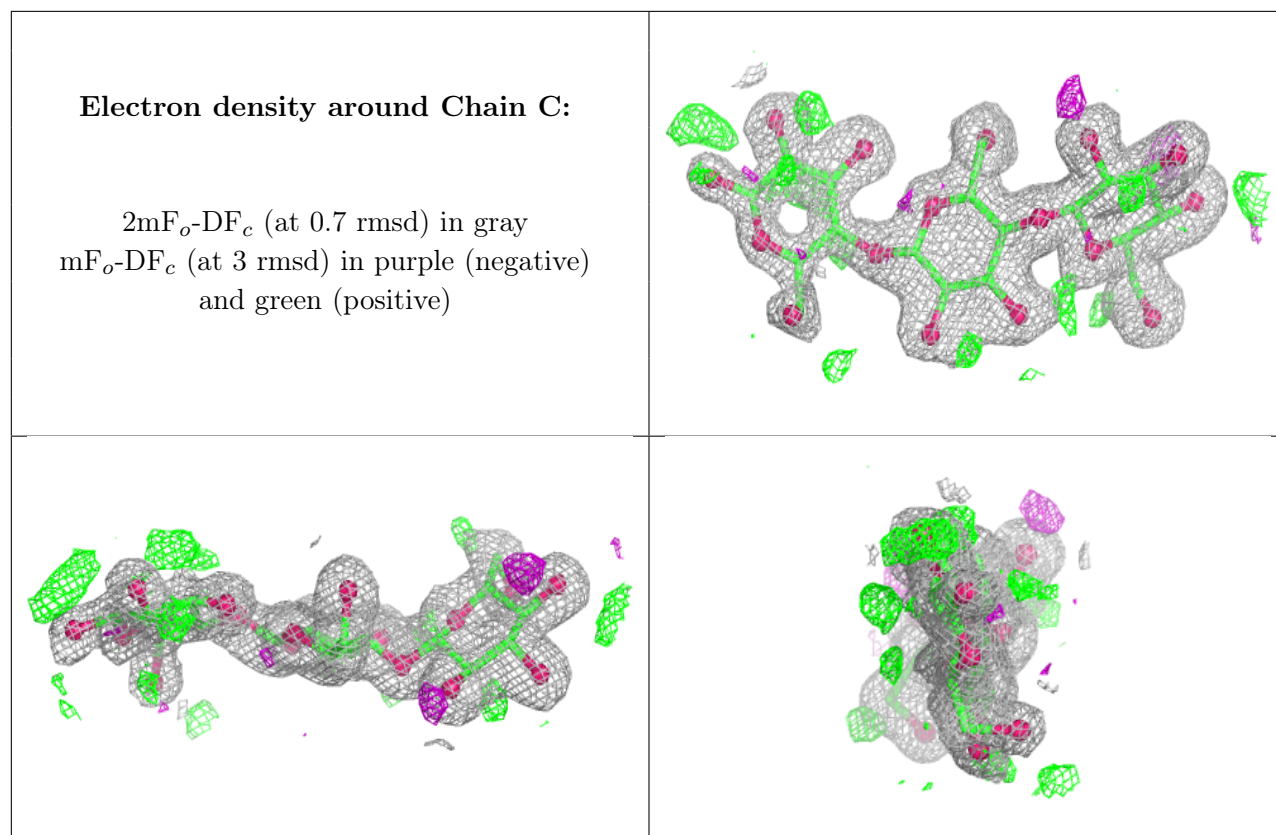
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	C	1	12/12	0.87	0.13	16,23,29,29	11
3	BGC	C	2	11/12	0.95	0.07	13,16,25,29	0
3	BGC	C	3	11/12	0.96	0.06	15,17,20,23	0
2	GLC	B	1[A]	12/12	0.97	0.06	12,16,25,26	2
2	GLC	B	1[B]	12/12	0.97	0.06	12,16,25,26	2
2	BGC	B	2	11/12	0.97	0.05	10,13,20,20	0

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 B:

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





6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
6	GOL	A	505	6/6	0.72	0.24	20,23,25,29	6
7	EDO	A	519	4/4	0.77	0.21	45,46,47,57	0
6	GOL	A	508	6/6	0.81	0.17	19,19,21,29	6
7	EDO	A	534	4/4	0.81	0.20	39,45,48,56	0
7	EDO	A	526	4/4	0.82	0.23	22,24,25,32	4
7	EDO	A	514	4/4	0.82	0.21	21,22,22,22	4
7	EDO	A	530	4/4	0.83	0.24	21,22,23,26	4
6	GOL	A	506	6/6	0.83	0.16	32,34,35,37	6
7	EDO	A	533	4/4	0.84	0.14	23,23,24,25	4
7	EDO	A	523	4/4	0.85	0.18	20,20,23,24	4
7	EDO	A	527	4/4	0.87	0.13	21,24,27,32	4
7	EDO	A	513[B]	4/4	0.87	0.15	17,19,20,21	4
7	EDO	A	532	4/4	0.87	0.16	26,26,29,30	4
7	EDO	A	513[A]	4/4	0.87	0.15	14,17,19,22	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	515	4/4	0.87	0.16	29,34,34,35	4
8	SO4	A	539	5/5	0.87	0.12	25,42,48,53	5
7	EDO	A	535	4/4	0.88	0.13	37,39,42,50	0
7	EDO	A	520	4/4	0.88	0.13	12,14,15,20	4
7	EDO	A	528	4/4	0.89	0.14	20,21,22,28	4
7	EDO	A	536	4/4	0.90	0.18	13,14,18,25	4
7	EDO	A	529	4/4	0.90	0.16	12,14,20,21	4
7	EDO	A	511	4/4	0.91	0.15	15,15,16,17	4
7	EDO	A	525	4/4	0.92	0.16	15,19,22,29	4
7	EDO	A	516	4/4	0.92	0.12	14,15,16,18	4
7	EDO	A	522	4/4	0.92	0.13	13,15,18,23	4
6	GOL	A	507	6/6	0.92	0.13	11,18,22,22	6
7	EDO	A	518[A]	4/4	0.93	0.08	18,19,20,22	4
7	EDO	A	521	4/4	0.93	0.12	10,14,14,17	4
7	EDO	A	518[B]	4/4	0.93	0.08	19,26,27,31	4
6	GOL	A	509	6/6	0.93	0.10	19,20,25,26	0
7	EDO	A	512	4/4	0.94	0.10	17,18,19,19	4
7	EDO	A	524	4/4	0.94	0.15	12,16,17,22	4
7	EDO	A	517	4/4	0.95	0.14	18,18,20,21	4
7	EDO	A	531	4/4	0.95	0.08	17,18,18,19	4
8	SO4	A	537	5/5	0.97	0.09	14,20,23,26	5
4	DIO	A	501	6/6	0.97	0.06	15,17,19,20	0
6	GOL	A	510[A]	6/6	0.98	0.08	8,8,8,9	6
8	SO4	A	538	5/5	0.98	0.06	11,11,17,20	5
6	GOL	A	510[B]	6/6	0.98	0.08	7,8,9,9	6
5	CA	A	502	1/1	1.00	0.02	9,9,9,9	0

6.5 Other polymers ⓘ

There are no such residues in this entry.