



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 10:37 AM BST

PDB ID : 5CGM
Title : Structure of Mycobacterium thermoresistibile GlgE in complex with maltose at 1.95Å resolution
Authors : Mendes, V.; Blaszczyk, M.; Maranhã, A.; Empadinhas, N.; Blundell, T.L.
Deposited on : 2015-07-09
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

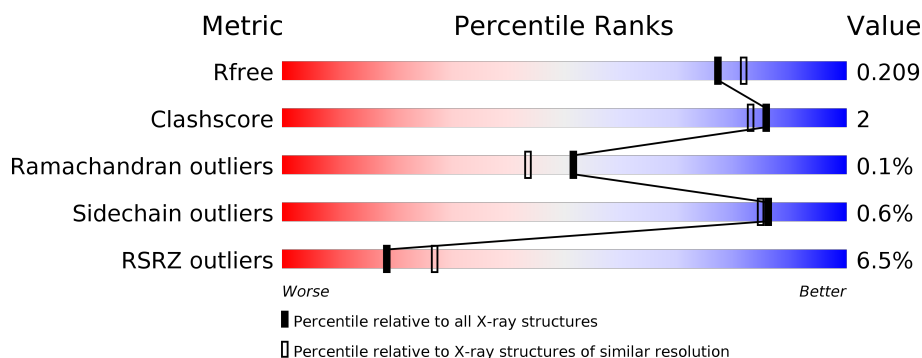
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	698	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	698	<div> <div>9%</div> <div> <div></div> <div>91%</div> <div>.</div> <div>.</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>100%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	B	712	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 11643 atoms, of which 44 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 Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	669	Total	C	N	O	S	0	6	0
			5232	3358	917	947	10			
1	B	667	Total	C	N	O	S	0	7	0
			5183	3337	898	939	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G7CL00
A	0	SER	-	expression tag	UNP G7CL00
A	1	VAL	-	cloning artifact	UNP G7CL00
B	-1	GLY	-	expression tag	UNP G7CL00
B	0	SER	-	expression tag	UNP G7CL00
B	1	VAL	-	cloning artifact	UNP G7CL00

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	O	0	0	0
			45	12	22	11			
2	D	2	Total	C	H	O	0	0	0
			45	12	22	11			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	8	Total	Na	0	0
			8	8		
4	A	11	Total	Na	0	0
			11	11		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

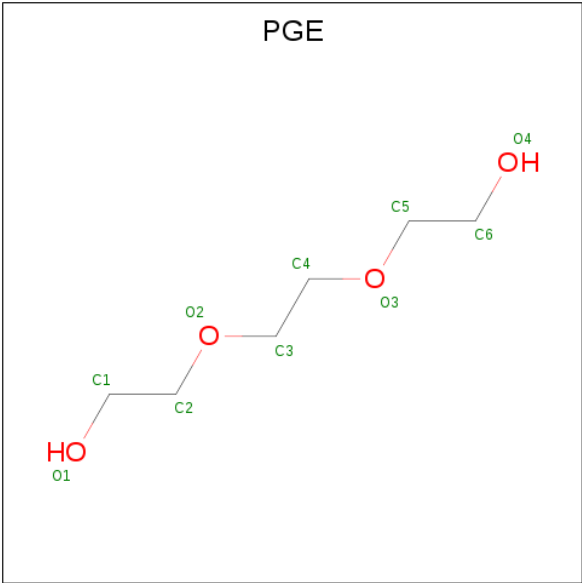
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



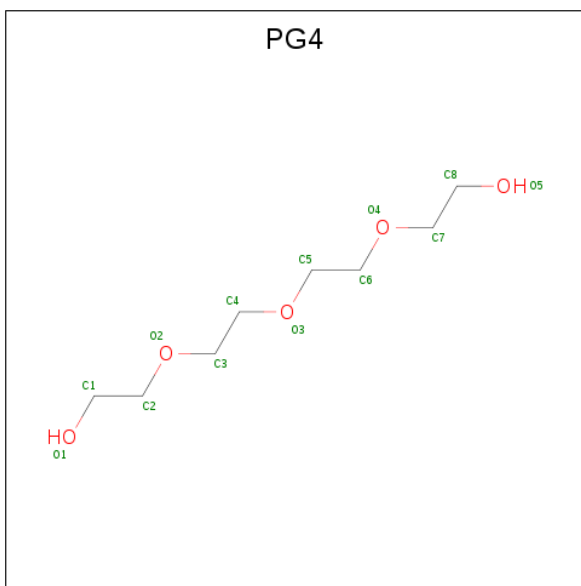
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



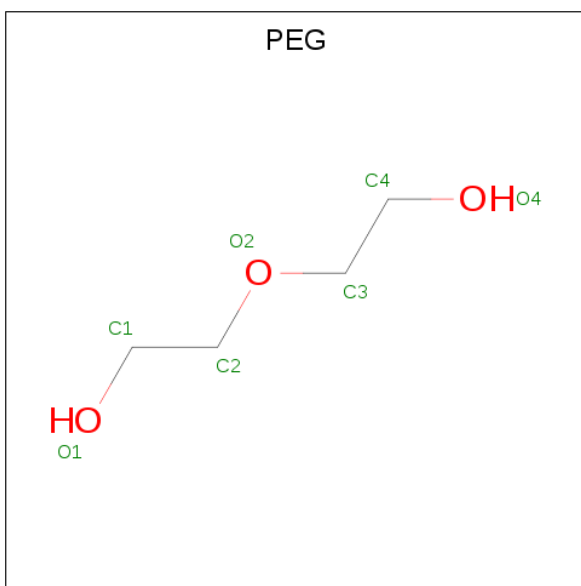
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



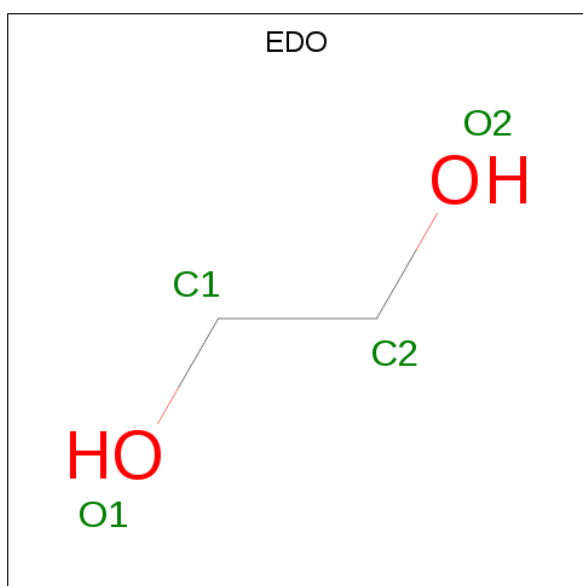
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	8	5		
8	A	1	Total	C	O	0	0
			13	8	5		
8	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	A	1	Total C O 7 4 3	0	0
9	B	1	Total C O 7 4 3	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		

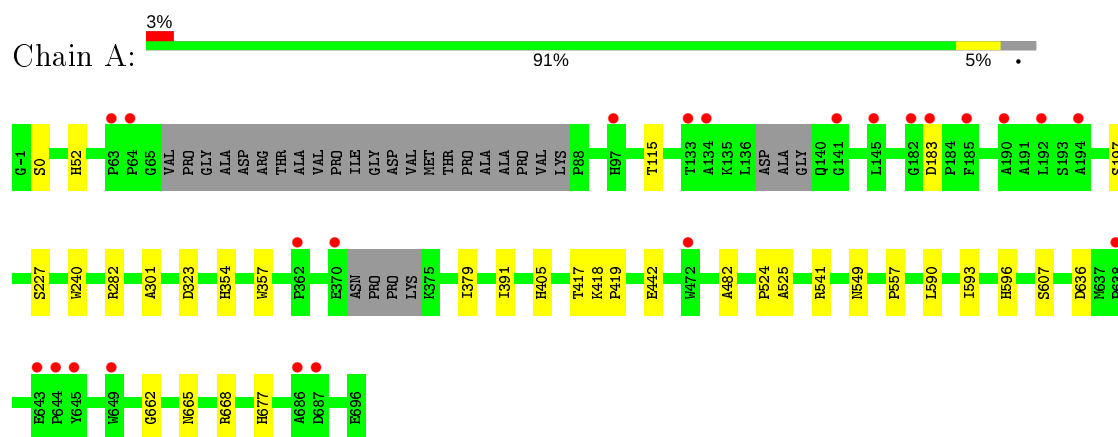
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	497	Total	O	0	0
			497	497		
11	B	437	Total	O	0	0
			437	437		

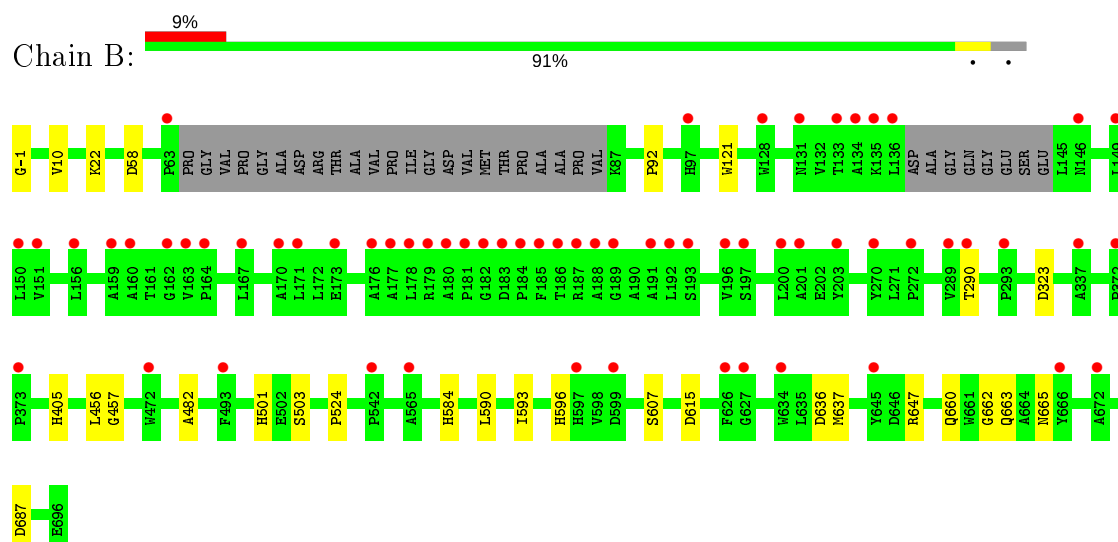
3 Residue-property plots [i](#)

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: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase



- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase



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



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

Chain D:

100%

GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.33Å 113.90Å 220.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.66 – 1.95 37.74 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.66-1.95) 99.9 (37.74-1.95)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.95Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.175 , 0.203 0.180 , 0.209	Depositor DCC
R_{free} test set	7393 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11643	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, CL, NA, PO4, GLC, EDO, 1PE, PG4, PEG

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	0.53	0/5408	0.62	0/7396
1	B	0.50	0/5364	0.62	0/7349
All	All	0.52	0/10772	0.62	0/14745

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

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	5232	0	5020	23	0
1	B	5183	0	4947	20	0
2	C	23	22	20	1	0
2	D	23	22	20	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	11	0	0	0	0
4	B	8	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	2	0
6	A	16	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	16	0	22	0	0
7	A	10	0	14	2	0
7	B	10	0	14	0	0
8	A	39	0	54	3	0
9	A	21	0	30	0	0
9	B	7	0	10	0	0
10	A	32	0	48	4	0
10	B	12	0	18	6	0
11	A	497	0	0	3	0
11	B	437	0	0	1	0
All	All	11599	44	10238	46	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 2.

All (46) 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:662:GLY:H	1:A:665:ASN:HD21	1.18	0.91
1:B:662:GLY:H	1:B:665:ASN:HD21	1.19	0.87
1:B:22:LYS:O	10:B:717:EDO:H21	1.88	0.73
1:B:596:HIS:HD2	1:B:636:ASP:H	1.38	0.70
1:B:647:ARG:HE	1:B:660:GLN:HE21	1.38	0.70
1:A:596:HIS:HD2	1:A:636:ASP:H	1.38	0.68
1:B:456:LEU:O	5:B:712:CL:CL	2.49	0.68
1:A:323:ASP:OD1	1:A:405:HIS:HD2	1.85	0.59
1:A:282:ARG:HH12	8:A:720:PG4:H31	1.67	0.59
1:B:662:GLY:H	1:B:665:ASN:ND2	1.96	0.58
1:B:482:ALA:HB2	1:B:593[A]:ILE:HG22	1.86	0.58
1:A:596:HIS:CD2	1:A:636:ASP:H	2.19	0.57
1:A:482:ALA:HB2	1:A:593:ILE:HG22	1.89	0.55
1:B:596:HIS:CD2	1:B:636:ASP:H	2.22	0.54
1:B:92:PRO:HA	10:B:718:EDO:H21	1.89	0.54
1:A:549:ASN:HD22	8:A:719:PG4:H41	1.73	0.54
1:B:323:ASP:OD1	1:B:405:HIS:HD2	1.92	0.53
5:A:715:CL:CL	11:A:832:HOH:O	2.56	0.52
1:B:457:GLY:HA3	5:B:712:CL:CL	2.49	0.50
1:A:52:HIS:HE1	1:A:115:THR:OG1	1.97	0.47
1:A:677:HIS:HD2	11:A:822:HOH:O	1.95	0.47
1:A:662:GLY:H	1:A:665:ASN:ND2	2.00	0.46
1:B:-1:GLY:H2	1:B:10:VAL:H	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:HH22	8:A:720:PG4:H21	1.81	0.45
7:A:717:PGE:H22	11:A:1200:HOH:O	2.15	0.45
1:B:121:TRP:HZ2	10:B:718:EDO:H11	1.81	0.45
1:B:92:PRO:HA	10:B:718:EDO:C2	2.46	0.45
1:B:524:PRO:HG2	1:B:590:LEU:HG	1.98	0.44
1:B:596:HIS:HE1	1:B:607:SER:OG	2.01	0.43
1:A:442:GLU:OE1	2:C:1:GLC:O1	2.36	0.43
1:B:637:MET:HG3	1:B:663:GLN:HG3	2.01	0.43
1:B:501:HIS:CD2	1:B:503:SER:H	2.36	0.43
1:A:301:ALA:HA	1:A:379:ILE:CG2	2.49	0.43
1:A:417:THR:O	10:A:729:EDO:H12	2.18	0.43
10:B:717:EDO:H12	11:B:878:HOH:O	2.19	0.43
1:B:584:HIS:HD2	1:B:615:ASP:OD1	2.01	0.43
1:A:596:HIS:HE1	1:A:607:SER:OG	2.03	0.42
1:A:418:LYS:HA	10:A:729:EDO:H21	2.00	0.42
1:A:524:PRO:HG2	1:A:590:LEU:HG	2.01	0.42
1:A:354:HIS:CE1	10:A:728:EDO:H21	2.55	0.42
1:A:419:PRO:HD3	10:A:729:EDO:H21	2.02	0.42
1:B:22:LYS:O	10:B:717:EDO:C2	2.62	0.41
1:A:240:TRP:CE2	1:A:557:PRO:HG2	2.56	0.41
1:A:668:ARG:H	7:A:717:PGE:H5	1.85	0.41
1:A:357:TRP:HB3	1:A:391:ILE:HD12	2.03	0.41
1:A:227:SER:O	1:A:525:ALA:HA	2.21	0.40

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	667/698 (96%)	654 (98%)	12 (2%)	1 (0%)	51 43
1	B	668/698 (96%)	655 (98%)	13 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1335/1396 (96%)	1309 (98%)	25 (2%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	526/566 (93%)	523 (99%)	3 (1%)	86 85
1	B	517/566 (91%)	514 (99%)	3 (1%)	86 85
All	All	1043/1132 (92%)	1037 (99%)	6 (1%)	86 85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	ASP
1	A	197	SER
1	A	541	ARG
1	B	58	ASP
1	B	290	THR
1	B	687	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	147	ASN
1	A	405	HIS
1	A	578	ASN
1	A	596	HIS
1	A	665	ASN

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Mol	Chain	Res	Type
1	A	677	HIS
1	B	52	HIS
1	B	405	HIS
1	B	501	HIS
1	B	584	HIS
1	B	596	HIS
1	B	660	GLN
1	B	665	ASN
1	B	677	HIS

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 ⓘ

4 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	C	1	2,4	12,12,12	1.26	1 (8%)	17,17,17	1.83	4 (23%)
2	GLC	C	2	2	11,11,12	1.43	2 (18%)	15,15,17	0.90	1 (6%)
2	GLC	D	1	2	12,12,12	1.34	1 (8%)	17,17,17	1.66	2 (11%)
2	GLC	D	2	2	11,11,12	1.48	2 (18%)	15,15,17	0.77	1 (6%)

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	C	1	2,4	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GLC	O5-C1	3.51	1.51	1.42
2	C	2	GLC	O5-C5	3.25	1.50	1.43
2	C	1	GLC	O5-C1	3.25	1.51	1.42
2	D	2	GLC	O5-C5	2.94	1.49	1.43
2	D	2	GLC	O5-C1	2.90	1.48	1.43
2	C	2	GLC	O5-C1	2.48	1.47	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	O5-C1-C2	5.03	119.27	110.28
2	D	1	GLC	O5-C1-C2	4.76	118.78	110.28
2	D	1	GLC	C1-O5-C5	3.28	119.85	113.66
2	C	1	GLC	C1-O5-C5	2.83	119.00	113.66
2	C	2	GLC	C1-C2-C3	2.49	112.72	109.67
2	C	1	GLC	O5-C5-C4	2.44	114.12	109.69
2	C	1	GLC	C1-C2-C3	2.08	114.64	110.31
2	D	2	GLC	C1-C2-C3	2.07	112.21	109.67

There are no chirality outliers.

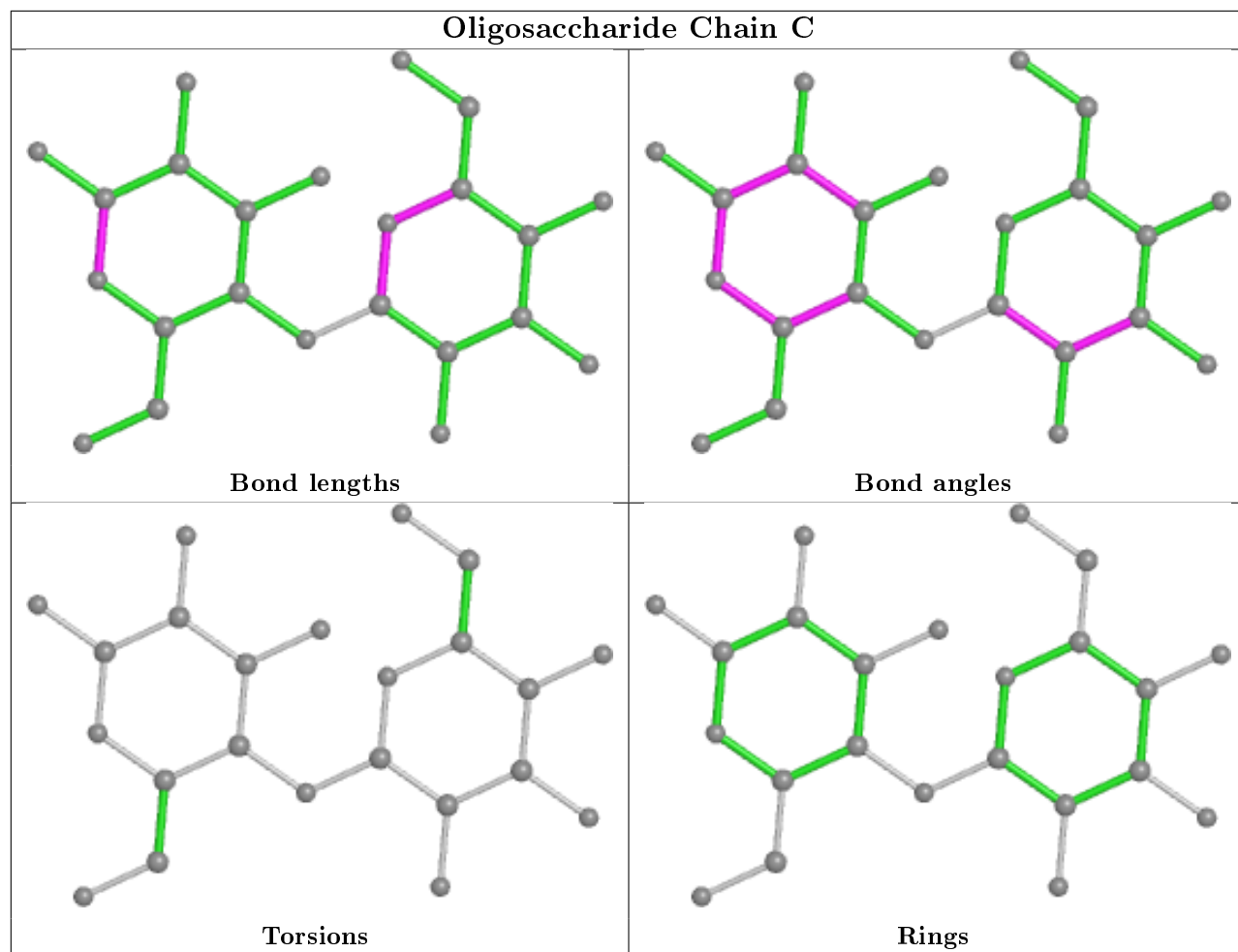
There are no torsion outliers.

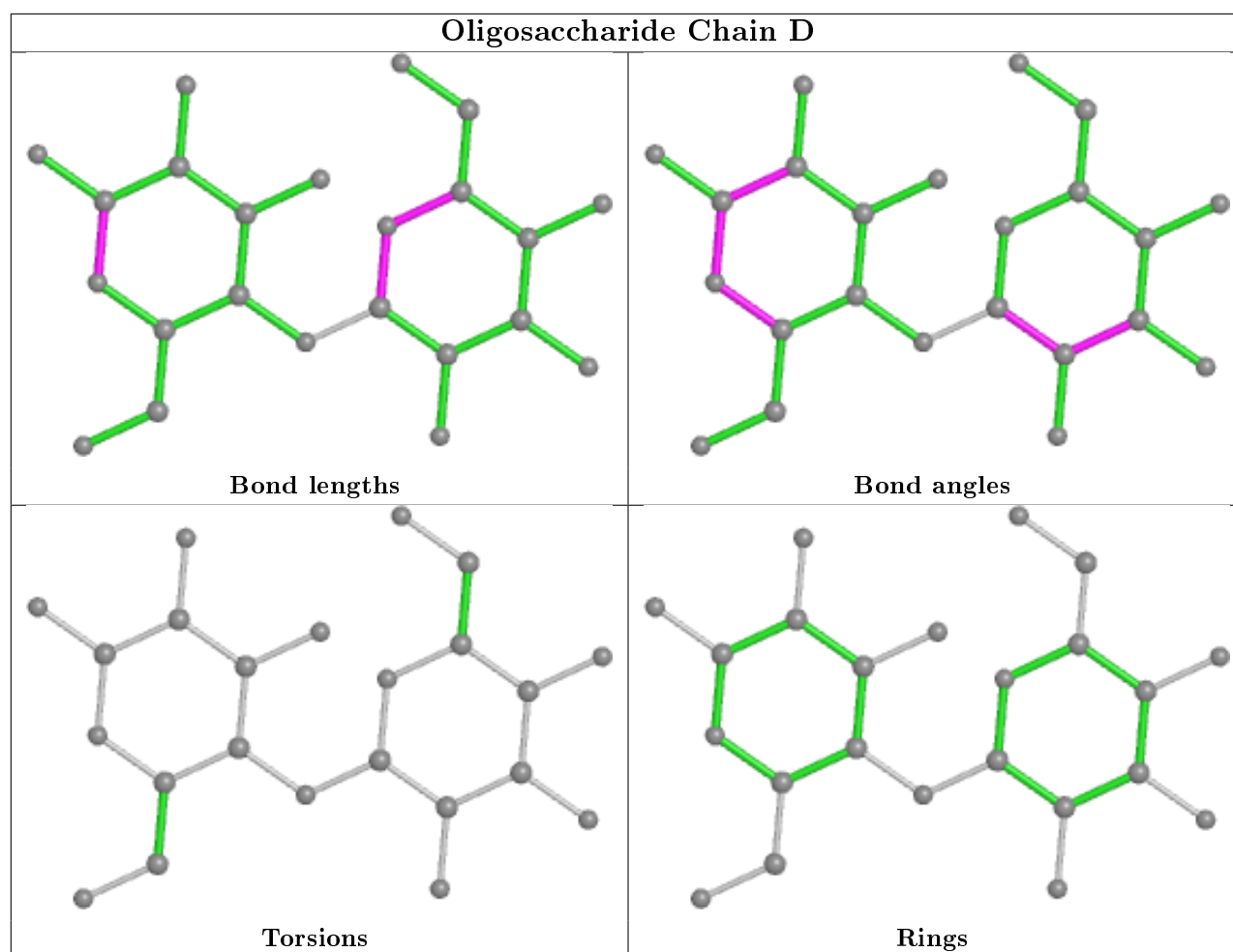
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	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.





5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 21 are monoatomic - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	PG4	A	719	-	12,12,12	0.54	0	11,11,11	0.39	0
9	PEG	B	715	-	6,6,6	0.49	0	5,5,5	0.38	0
10	EDO	A	729	-	3,3,3	0.44	0	2,2,2	0.54	0
10	EDO	A	728	-	3,3,3	0.47	0	2,2,2	0.30	0
10	EDO	B	716	-	3,3,3	0.43	0	2,2,2	0.42	0
3	PO4	B	702	-	4,4,4	1.68	1 (25%)	6,6,6	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PGE	B	713	-	9,9,9	0.49	0	8,8,8	0.78	0
10	EDO	A	730	-	3,3,3	0.46	0	2,2,2	0.45	0
10	EDO	A	727	-	3,3,3	0.47	0	2,2,2	0.53	0
9	PEG	A	723	-	6,6,6	0.49	0	5,5,5	0.50	0
7	PGE	A	717	-	9,9,9	0.52	0	8,8,8	0.52	0
9	PEG	A	722	-	6,6,6	0.46	0	5,5,5	0.49	0
10	EDO	A	731	-	3,3,3	0.46	0	2,2,2	0.50	0
3	PO4	A	702	-	4,4,4	1.49	1 (25%)	6,6,6	0.56	0
9	PEG	A	721	-	6,6,6	0.51	0	5,5,5	0.32	0
8	PG4	A	720	-	12,12,12	0.53	0	11,11,11	0.32	0
3	PO4	A	703	-	4,4,4	1.35	1 (25%)	6,6,6	0.40	0
10	EDO	B	717	-	3,3,3	0.41	0	2,2,2	0.31	0
6	1PE	B	714	-	15,15,15	0.53	0	14,14,14	0.35	0
8	PG4	A	718	-	12,12,12	0.51	0	11,11,11	0.37	0
10	EDO	A	725	-	3,3,3	0.46	0	2,2,2	0.33	0
10	EDO	A	724	-	3,3,3	0.47	0	2,2,2	0.38	0
10	EDO	B	718	-	3,3,3	0.46	0	2,2,2	0.34	0
3	PO4	B	703	-	4,4,4	1.31	1 (25%)	6,6,6	0.47	0
6	1PE	A	716	4	15,15,15	0.51	0	14,14,14	0.37	0
10	EDO	A	726	-	3,3,3	0.44	0	2,2,2	0.40	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	PG4	A	719	-	-	3/10/10/10	-
9	PEG	B	715	-	-	3/4/4/4	-
10	EDO	A	729	-	-	0/1/1/1	-
10	EDO	A	728	-	-	1/1/1/1	-
10	EDO	B	716	-	-	0/1/1/1	-
7	PGE	B	713	-	-	6/7/7/7	-
10	EDO	A	727	-	-	1/1/1/1	-
9	PEG	A	723	-	-	4/4/4/4	-
7	PGE	A	717	-	-	4/7/7/7	-
9	PEG	A	722	-	-	0/4/4/4	-
10	EDO	A	731	-	-	1/1/1/1	-
9	PEG	A	721	-	-	1/4/4/4	-
8	PG4	A	720	-	-	6/10/10/10	-
10	EDO	B	717	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	B	714	-	-	2/13/13/13	-
8	PG4	A	718	-	-	8/10/10/10	-
10	EDO	A	725	-	-	1/1/1/1	-
10	EDO	A	724	-	-	0/1/1/1	-
10	EDO	B	718	-	-	1/1/1/1	-
10	EDO	A	730	-	-	1/1/1/1	-
6	1PE	A	716	4	-	4/13/13/13	-
10	EDO	A	726	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	PO4	P-O1	2.87	1.57	1.50
3	A	702	PO4	P-O1	2.74	1.57	1.50
3	A	703	PO4	P-O1	2.63	1.57	1.50
3	B	703	PO4	P-O1	2.14	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	713	PGE	O2-C3-C4-O3
7	A	717	PGE	O2-C3-C4-O3
8	A	718	PG4	O2-C3-C4-O3
8	A	720	PG4	O2-C3-C4-O3
9	A	723	PEG	O2-C3-C4-O4
8	A	718	PG4	O1-C1-C2-O2
7	B	713	PGE	O1-C1-C2-O2
7	A	717	PGE	O1-C1-C2-O2
8	A	718	PG4	O3-C5-C6-O4
8	A	720	PG4	O1-C1-C2-O2
10	A	728	EDO	O1-C1-C2-O2
10	A	730	EDO	O1-C1-C2-O2
9	A	723	PEG	O1-C1-C2-O2
7	B	713	PGE	O3-C5-C6-O4
10	A	727	EDO	O1-C1-C2-O2
10	B	717	EDO	O1-C1-C2-O2
10	A	725	EDO	O1-C1-C2-O2
10	A	726	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	B	715	PEG	O1-C1-C2-O2
6	B	714	1PE	OH5-C14-C24-OH4
6	A	716	1PE	OH7-C16-C26-OH6
8	A	719	PG4	C8-C7-O4-C6
7	A	717	PGE	C4-C3-O2-C2
8	A	719	PG4	C4-C3-O2-C2
8	A	720	PG4	C1-C2-O2-C3
8	A	718	PG4	C4-C3-O2-C2
6	A	716	1PE	C16-C26-OH6-C15
9	B	715	PEG	C4-C3-O2-C2
7	B	713	PGE	C6-C5-O3-C4
6	B	714	1PE	C25-C15-OH6-C26
8	A	720	PG4	C6-C5-O3-C4
8	A	718	PG4	C6-C5-O3-C4
8	A	718	PG4	C5-C6-O4-C7
7	A	717	PGE	C1-C2-O2-C3
10	A	731	EDO	O1-C1-C2-O2
6	A	716	1PE	C25-C15-OH6-C26
9	A	721	PEG	O1-C1-C2-O2
8	A	718	PG4	O4-C7-C8-O5
7	B	713	PGE	C1-C2-O2-C3
6	A	716	1PE	OH6-C15-C25-OH5
8	A	719	PG4	C5-C6-O4-C7
9	B	715	PEG	C1-C2-O2-C3
7	B	713	PGE	C3-C4-O3-C5
10	B	718	EDO	O1-C1-C2-O2
8	A	718	PG4	C3-C4-O3-C5
8	A	720	PG4	C3-C4-O3-C5
9	A	723	PEG	C1-C2-O2-C3
9	A	723	PEG	C4-C3-O2-C2
8	A	720	PG4	O3-C5-C6-O4

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	719	PG4	1	0
10	A	729	EDO	3	0
10	A	728	EDO	1	0
7	A	717	PGE	2	0
8	A	720	PG4	2	0
10	B	717	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	718	EDO	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	669/698 (95%)	0.07	23 (3%) 45 55	14, 26, 52, 88	0
1	B	667/698 (95%)	0.38	64 (9%) 8 13	18, 30, 59, 88	0
All	All	1336/1396 (95%)	0.22	87 (6%) 18 27	14, 28, 56, 88	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	LEU	7.5
1	B	180	ALA	6.7
1	B	134	ALA	6.4
1	B	185	PHE	6.4
1	A	645	TYR	6.1
1	B	188	ALA	6.1
1	B	178	LEU	5.9
1	B	200	LEU	5.4
1	B	183	ASP	5.4
1	B	184	PRO	5.3
1	B	171	LEU	5.0
1	B	181	PRO	4.8
1	A	194	ALA	4.8
1	B	150	LEU	4.8
1	B	189	GLY	4.6
1	B	170	ALA	4.5
1	B	626	PHE	4.4
1	B	634	TRP	4.3
1	B	182	GLY	4.3
1	B	472	TRP	4.3
1	B	128	TRP	4.2
1	B	97	HIS	4.2
1	B	160	ALA	4.2
1	B	191	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	134	ALA	4.1
1	B	203	TYR	4.1
1	B	136	LEU	4.0
1	B	186	THR	3.9
1	B	164	PRO	3.9
1	B	133	THR	3.9
1	B	187	ARG	3.6
1	B	63	PRO	3.5
1	B	179	ARG	3.5
1	B	167	LEU	3.4
1	B	177	ALA	3.3
1	A	183	ASP	3.3
1	B	193	SER	3.2
1	B	159	ALA	3.2
1	B	149	LEU	3.2
1	B	666	TYR	3.2
1	A	133	THR	3.2
1	B	293	PRO	3.1
1	B	289	VAL	3.1
1	A	649	TRP	3.0
1	B	135	LYS	3.0
1	B	197	SER	3.0
1	B	196	VAL	3.0
1	A	192	LEU	3.0
1	B	131	ASN	3.0
1	A	472	TRP	3.0
1	B	373	PRO	3.0
1	B	201	ALA	2.9
1	B	372	PRO	2.9
1	B	627	GLY	2.9
1	A	687	ASP	2.7
1	A	185	PHE	2.6
1	B	156	LEU	2.6
1	B	565	ALA	2.6
1	A	141	GLY	2.6
1	A	638	PRO	2.6
1	B	645	TYR	2.6
1	A	190	ALA	2.6
1	B	146	ASN	2.6
1	B	151	VAL	2.5
1	A	63	PRO	2.5
1	A	182	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	290	THR	2.4
1	B	173	GLU	2.4
1	A	64	PRO	2.4
1	A	97	HIS	2.4
1	B	542	PRO	2.3
1	B	270	TYR	2.3
1	B	162	GLY	2.3
1	A	362	PRO	2.2
1	A	644	PRO	2.2
1	A	686	ALA	2.1
1	B	337	ALA	2.1
1	A	643	GLU	2.1
1	B	493	PHE	2.1
1	B	599	ASP	2.1
1	A	145	LEU	2.1
1	B	176	ALA	2.1
1	B	597	HIS	2.1
1	A	370	GLU	2.1
1	B	672	ALA	2.1
1	B	163	VAL	2.0
1	B	272	PRO	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 ⓘ

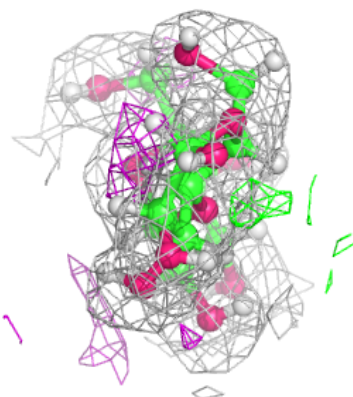
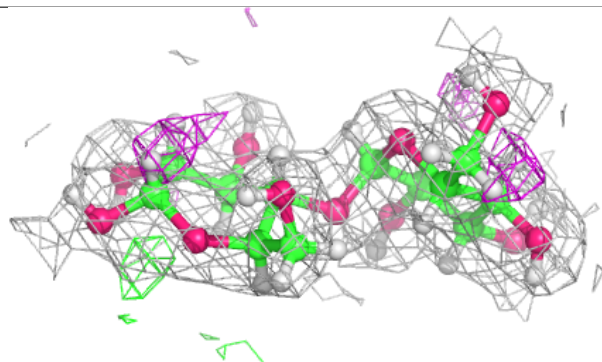
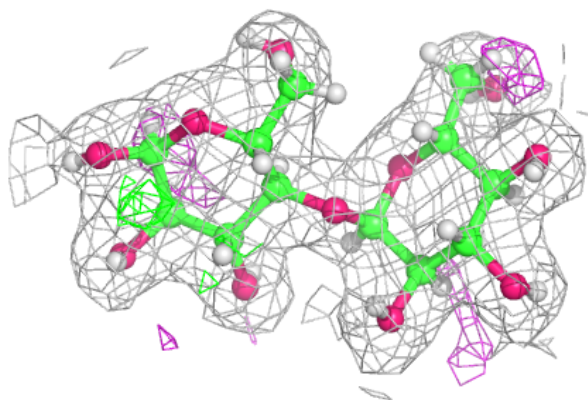
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	D	1	12/12	0.94	0.10	24,32,40,42	0
2	GLC	C	1	12/12	0.95	0.09	20,32,39,42	0
2	GLC	D	2	11/12	0.96	0.08	24,27,29,29	0
2	GLC	C	2	11/12	0.98	0.07	21,22,23,24	0

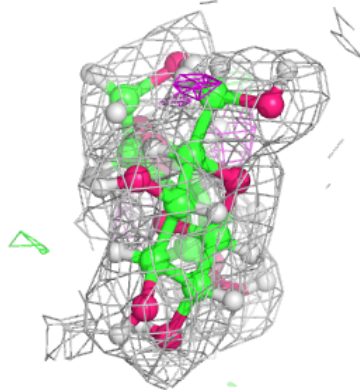
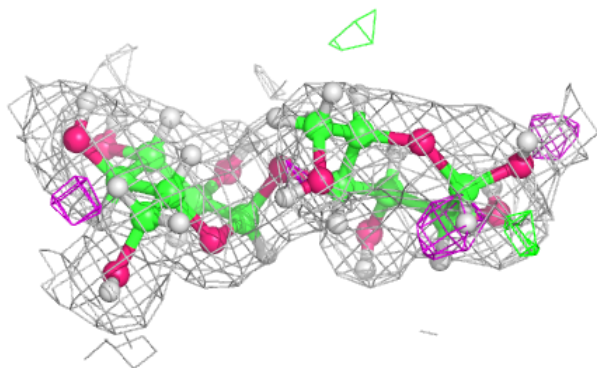
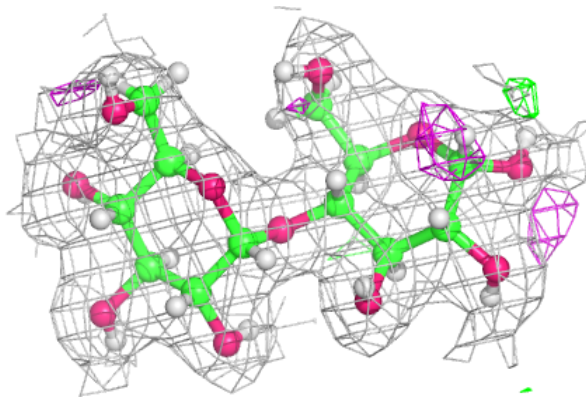
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

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



6.4 Ligands ⓘ

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	PGE	A	717	10/10	0.52	0.30	54,62,64,66	0
8	PG4	A	718	13/13	0.61	0.38	59,65,69,69	0
10	EDO	A	728	4/4	0.66	0.33	50,54,56,57	0
9	PEG	B	715	7/7	0.68	0.33	51,57,59,59	0
10	EDO	A	731	4/4	0.70	0.20	53,56,58,61	0
10	EDO	A	725	4/4	0.71	0.20	52,53,53,54	0
8	PG4	A	720	13/13	0.71	0.33	42,61,67,68	0
10	EDO	A	724	4/4	0.78	0.15	62,63,63,64	0
10	EDO	B	716	4/4	0.81	0.20	45,49,52,55	0
10	EDO	B	718	4/4	0.82	0.34	42,43,45,46	0
9	PEG	A	723	7/7	0.83	0.14	59,62,65,66	0
10	EDO	A	726	4/4	0.83	0.13	42,44,47,49	0
6	1PE	B	714	16/16	0.87	0.15	43,52,58,61	0
4	NA	A	704	1/1	0.87	0.14	40,40,40,40	0
8	PG4	A	719	13/13	0.89	0.17	43,50,59,60	0
10	EDO	A	727	4/4	0.90	0.27	59,61,62,63	0
3	PO4	A	703	5/5	0.91	0.20	66,68,69,70	0
7	PGE	B	713	10/10	0.91	0.16	40,42,49,53	0
3	PO4	B	703	5/5	0.91	0.16	54,59,61,63	0
9	PEG	A	721	7/7	0.91	0.14	54,55,57,60	0
10	EDO	A	730	4/4	0.92	0.10	53,54,55,57	0
4	NA	B	705	1/1	0.92	0.08	40,40,40,40	0
4	NA	B	706	1/1	0.92	0.11	47,47,47,47	0
10	EDO	A	729	4/4	0.92	0.24	59,59,59,59	0
9	PEG	A	722	7/7	0.92	0.21	42,45,46,47	0
4	NA	B	707	1/1	0.93	0.16	39,39,39,39	0
4	NA	A	712	1/1	0.93	0.12	47,47,47,47	0
10	EDO	B	717	4/4	0.93	0.20	56,58,59,59	0
4	NA	B	709	1/1	0.95	0.12	37,37,37,37	0
4	NA	A	709	1/1	0.95	0.15	39,39,39,39	0
4	NA	B	710	1/1	0.95	0.11	45,45,45,45	0
3	PO4	A	702	5/5	0.96	0.20	45,51,51,52	0
6	1PE	A	716	16/16	0.96	0.10	20,27,49,54	0
3	PO4	B	702	5/5	0.96	0.24	47,49,50,50	0
4	NA	A	706	1/1	0.97	0.12	33,33,33,33	0
4	NA	A	714	1/1	0.97	0.12	50,50,50,50	0
4	NA	A	708	1/1	0.97	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CL	A	715	1/1	0.98	0.17	51,51,51,51	0
5	CL	B	712	1/1	0.98	0.17	53,53,53,53	0
4	NA	B	704	1/1	0.98	0.14	21,21,21,21	0
4	NA	A	707	1/1	0.98	0.08	41,41,41,41	0
4	NA	A	713	1/1	0.98	0.05	22,22,22,22	0
4	NA	A	711	1/1	0.98	0.08	38,38,38,38	0
4	NA	A	710	1/1	0.98	0.21	37,37,37,37	0
4	NA	B	708	1/1	0.98	0.15	31,31,31,31	0
4	NA	A	705	1/1	0.99	0.14	19,19,19,19	0
4	NA	B	711	1/1	0.99	0.13	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.