



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:30 PM UTC

PDB ID : 5CGM / pdb_00005cgm
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 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

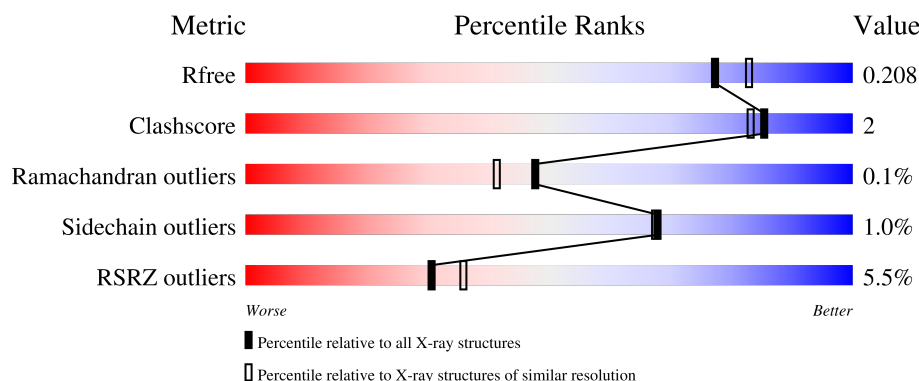
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 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	698	3% 90% 6% .
1	B	698	8% 90% 5% .
2	C	2	50% 50%
2	D	2	100%

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
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:

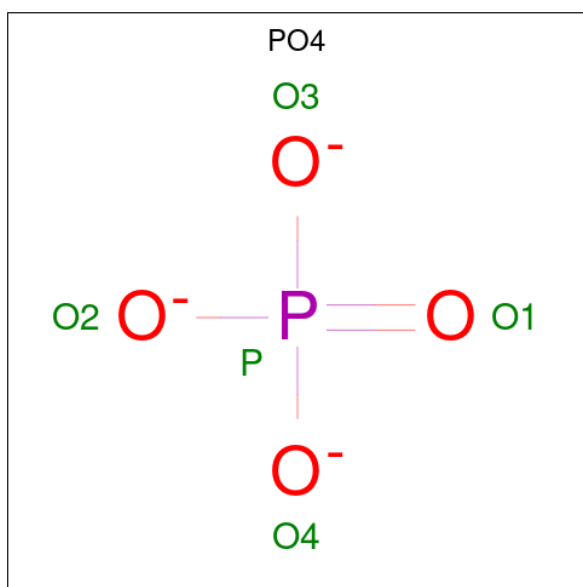
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G7CL00
A	0	SER	-	expression tag	UNP G7CL00
A	1	VAL	-	cloning artifact	UNP G7CL00
B	-1	GLY	-	expression tag	UNP G7CL00
B	0	SER	-	expression tag	UNP G7CL00
B	1	VAL	-	cloning artifact	UNP G7CL00

- 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 (CCD ID: 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		

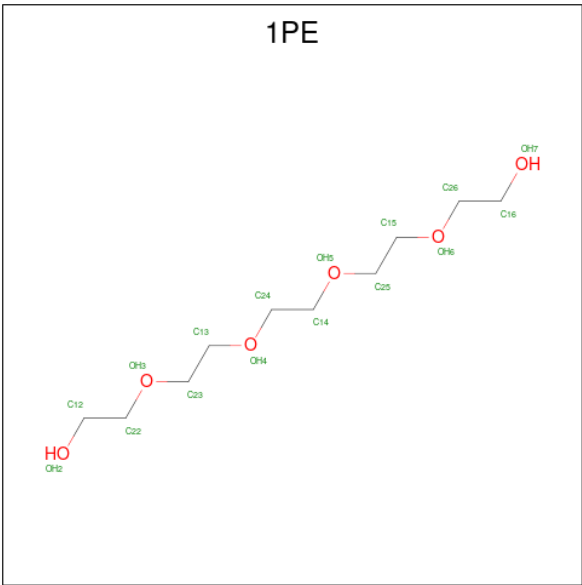
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

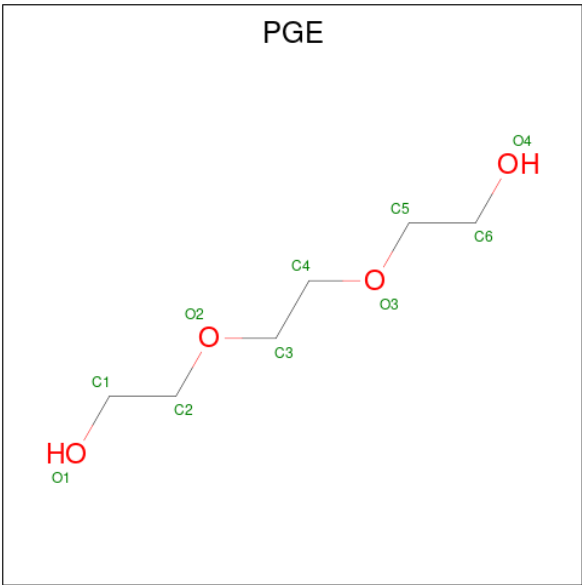
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



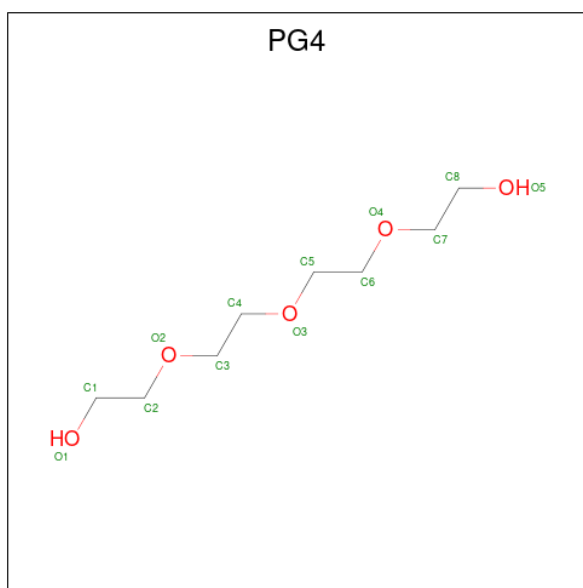
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



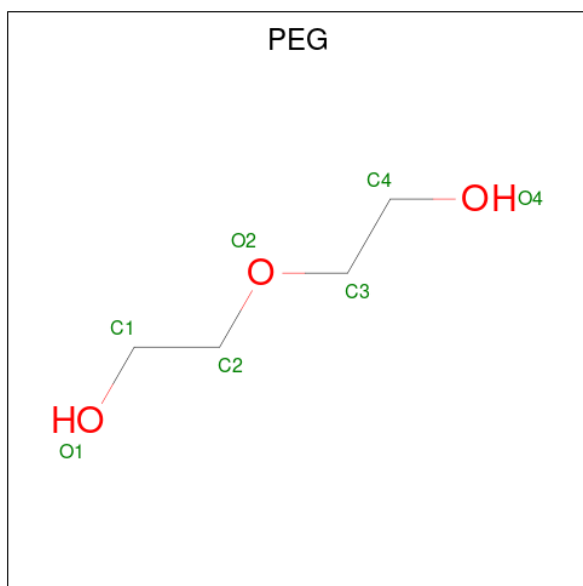
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



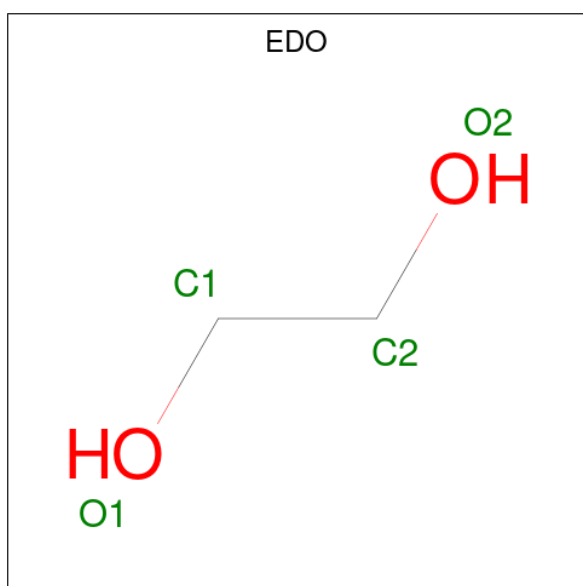
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	8	5		
8	A	1	Total	C	O	0	0
			13	8	5		
8	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: 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 (CCD ID: 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		

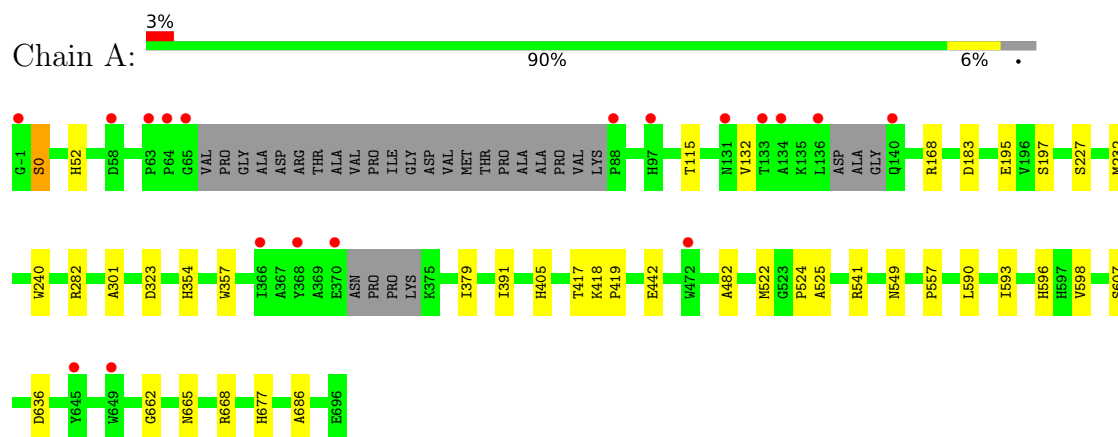
- Molecule 11 is water.

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

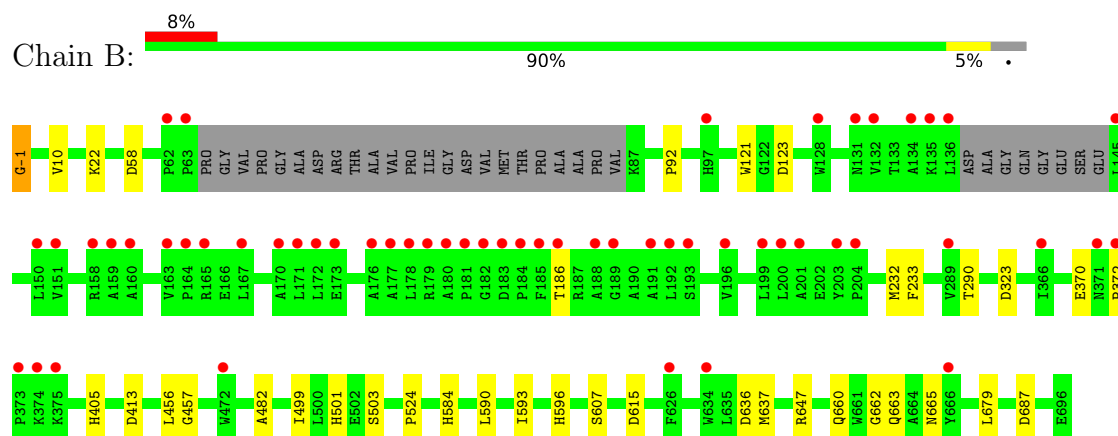
3 Residue-property plots

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



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 19.66 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.66-1.95) 99.7 (19.66-1.95)	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 , 0.208	Depositor DCC
R_{free} test set	7393 reflections (5.00%)	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)	0.39 , 62.1	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, GLC, PGE, PO4, CL, EDO, NA, 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	0.86	1/5408 (0.0%)	1.09	4/7396 (0.1%)
1	B	0.83	0/5364	1.13	12/7349 (0.2%)
All	All	0.84	1/10772 (0.0%)	1.11	16/14745 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	MET	SD-CE	-9.73	1.55	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	686	ALA	N-CA-C	6.33	118.70	111.11
1	B	123	ASP	CA-CB-CG	6.26	118.86	112.60
1	B	-1	GLY	CA-C-N	-6.03	110.02	121.54
1	B	-1	GLY	C-N-CA	-6.03	110.02	121.54
1	B	370	GLU	CA-C-N	5.98	127.94	122.37
1	B	370	GLU	C-N-CA	5.98	127.94	122.37
1	A	0	SER	N-CA-C	5.75	123.04	110.80
1	B	372	PRO	N-CA-C	5.44	117.33	110.70
1	A	168	ARG	N-CA-C	5.41	117.93	111.71
1	B	186	THR	CA-C-N	5.28	127.35	120.28
1	B	186	THR	C-N-CA	5.28	127.35	120.28
1	B	679	LEU	N-CA-C	5.25	118.17	109.46
1	A	598	VAL	CB-CA-C	5.11	117.32	110.42
1	B	233	PHE	CA-CB-CG	5.10	118.90	113.80
1	B	499	ILE	N-CA-C	5.00	115.65	107.24

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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:-1:GLY:H2	1:B:10:VAL:H	1.60	0.50
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: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:A:442:GLU:OE1	2:C:1:GLC:O1	2.36	0.43
1:B:596:HIS:HE1	1:B:607:SER:OG	2.01	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:354:HIS:CE1	10:A:728:EDO:H21	2.55	0.42
1:A:524:PRO:HG2	1:A:590:LEU:HG	2.01	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:357:TRP:HB3	1:A:391:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ARG:H	7:A:717:PGE:H5	1.85	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%)	48	41
1	B	668/698 (96%)	655 (98%)	13 (2%)	0	100	100
All	All	1335/1396 (96%)	1309 (98%)	25 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	526/566 (93%)	520 (99%)	6 (1%)	65	64
1	B	517/566 (91%)	513 (99%)	4 (1%)	73	74
All	All	1043/1132 (92%)	1033 (99%)	10 (1%)	68	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	VAL
1	A	183	ASP
1	A	195	GLU
1	A	197	SER
1	A	232	MET
1	A	541	ARG
1	B	58	ASP
1	B	232	MET
1	B	290	THR
1	B	687	ASP

Sometimes 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	414	ASN
1	A	578	ASN
1	A	596	HIS
1	A	665	ASN
1	A	677	HIS
1	B	52	HIS
1	B	405	HIS
1	B	501	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	4,2	12,12,12	1.27	1 (8%)	17,17,17	1.84	4 (23%)
2	GLC	C	2	2	11,11,12	1.43	2 (18%)	15,15,17	0.80	1 (6%)
2	GLC	D	1	2	12,12,12	1.35	1 (8%)	17,17,17	1.66	2 (11%)
2	GLC	D	2	2	11,11,12	1.46	2 (18%)	15,15,17	0.69	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	GLC	C	1	4,2	-	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	3.59	1.51	1.42
2	C	2	GLC	O5-C5	3.39	1.50	1.43
2	C	1	GLC	O5-C1	3.33	1.51	1.42
2	D	2	GLC	O5-C5	3.06	1.49	1.43
2	D	2	GLC	O5-C1	2.77	1.48	1.43
2	C	2	GLC	O5-C1	2.37	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GLC	O5-C1-C2	5.10	119.27	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	O5-C1-C2	4.82	118.78	110.30
2	D	1	GLC	C1-O5-C5	3.20	119.85	113.65
2	C	1	GLC	C1-O5-C5	2.76	119.00	113.65
2	C	1	GLC	O5-C5-C4	2.45	114.12	109.70
2	C	2	GLC	C1-C2-C3	2.11	112.72	109.64
2	C	1	GLC	C1-C2-C3	2.10	114.64	110.36

There are no chirality outliers.

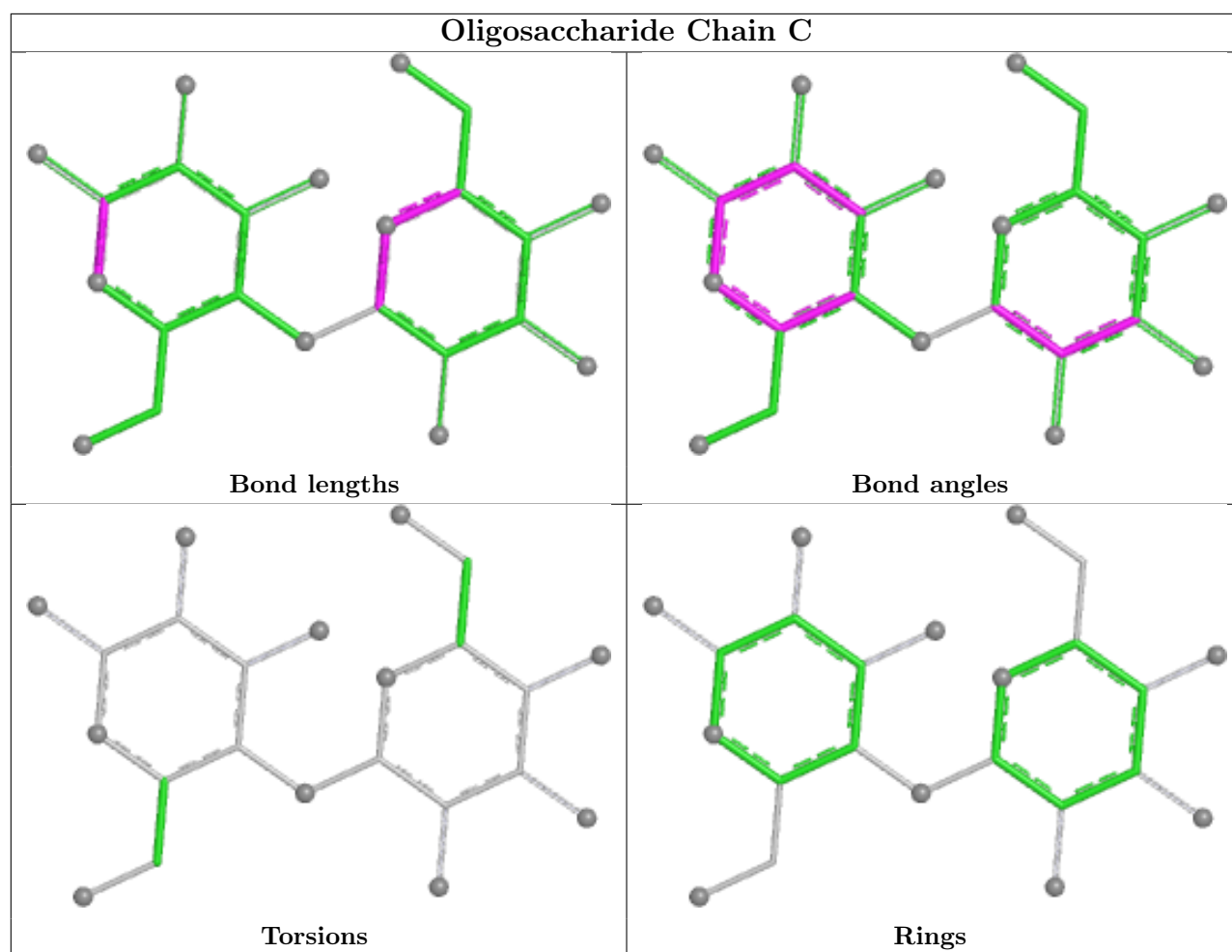
There are no torsion outliers.

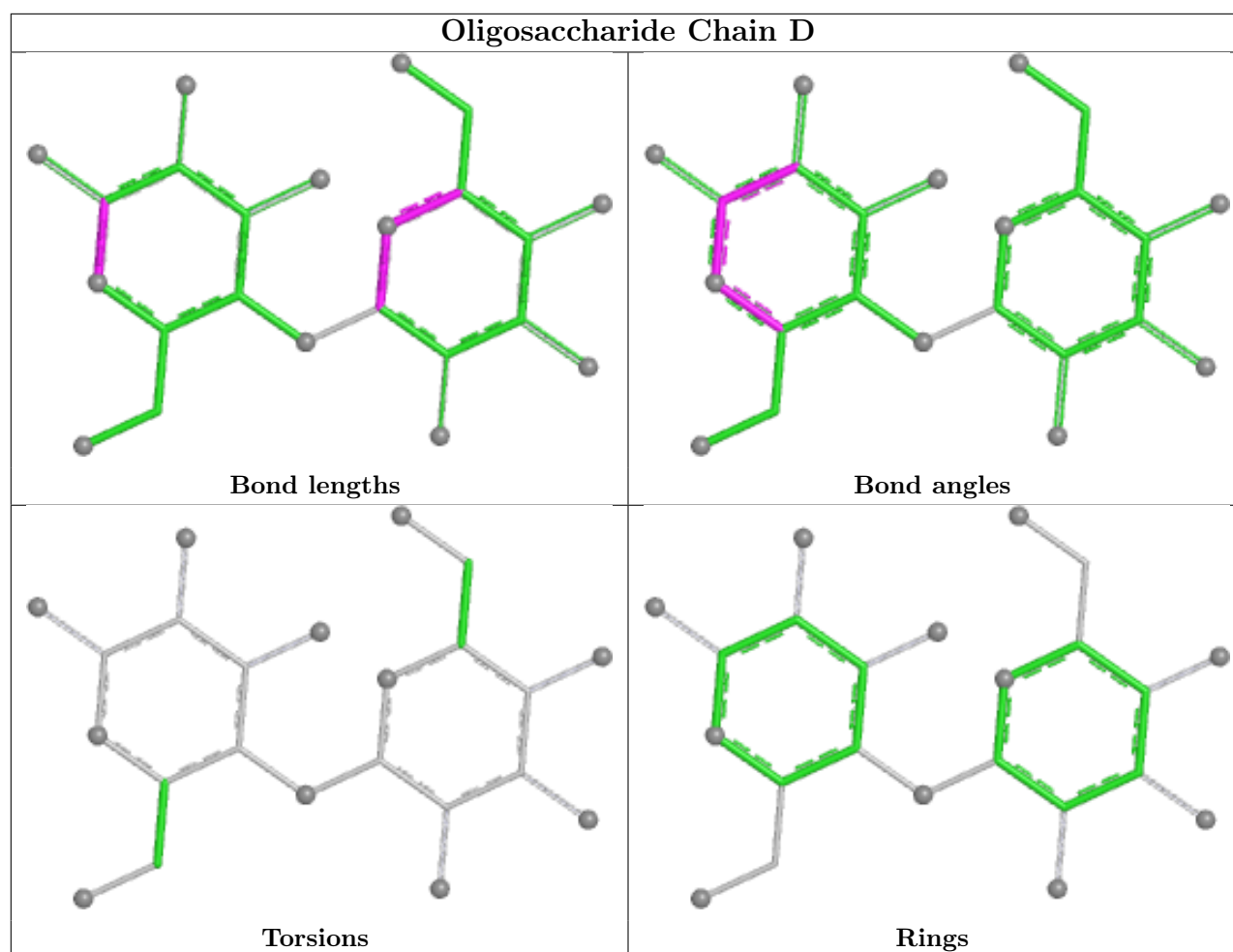
There are no ring outliers.

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	$\# Z > 2$
6	1PE	B	714	-	15,15,15	0.55	0	14,14,14	0.34	0
7	PGE	A	717	-	9,9,9	0.54	0	8,8,8	0.51	0
10	EDO	A	729	-	3,3,3	0.42	0	2,2,2	0.57	0
10	EDO	A	724	-	3,3,3	0.43	0	2,2,2	0.42	0
8	PG4	A	720	-	12,12,12	0.54	0	11,11,11	0.32	0
10	EDO	B	716	-	3,3,3	0.40	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	EDO	B	717	-	3,3,3	0.39	0	2,2,2	0.35	0
9	PEG	B	715	-	6,6,6	0.50	0	5,5,5	0.37	0
10	EDO	A	726	-	3,3,3	0.40	0	2,2,2	0.44	0
9	PEG	A	721	-	6,6,6	0.52	0	5,5,5	0.33	0
3	PO4	A	702	-	4,4,4	1.55	1 (25%)	6,6,6	0.59	0
10	EDO	A	727	-	3,3,3	0.44	0	2,2,2	0.56	0
9	PEG	A	722	-	6,6,6	0.47	0	5,5,5	0.49	0
10	EDO	A	728	-	3,3,3	0.43	0	2,2,2	0.34	0
6	1PE	A	716	4	15,15,15	0.52	0	14,14,14	0.37	0
7	PGE	B	713	-	9,9,9	0.51	0	8,8,8	0.78	0
10	EDO	A	725	-	3,3,3	0.42	0	2,2,2	0.37	0
8	PG4	A	718	-	12,12,12	0.52	0	11,11,11	0.37	0
3	PO4	B	702	-	4,4,4	1.74	1 (25%)	6,6,6	0.72	0
8	PG4	A	719	-	12,12,12	0.56	0	11,11,11	0.39	0
3	PO4	B	703	-	4,4,4	1.37	1 (25%)	6,6,6	0.50	0
3	PO4	A	703	-	4,4,4	1.41	1 (25%)	6,6,6	0.43	0
9	PEG	A	723	-	6,6,6	0.50	0	5,5,5	0.50	0
10	EDO	A	731	-	3,3,3	0.42	0	2,2,2	0.53	0
10	EDO	B	718	-	3,3,3	0.43	0	2,2,2	0.37	0
10	EDO	A	730	-	3,3,3	0.43	0	2,2,2	0.48	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
6	1PE	B	714	-	-	2/13/13/13	-
7	PGE	A	717	-	-	5/7/7/7	-
10	EDO	A	729	-	-	0/1/1/1	-
10	EDO	A	724	-	-	0/1/1/1	-
8	PG4	A	720	-	-	5/10/10/10	-
10	EDO	B	716	-	-	0/1/1/1	-
10	EDO	B	717	-	-	1/1/1/1	-
9	PEG	B	715	-	-	3/4/4/4	-
10	EDO	A	726	-	-	1/1/1/1	-
9	PEG	A	721	-	-	1/4/4/4	-
10	EDO	A	727	-	-	1/1/1/1	-
9	PEG	A	722	-	-	0/4/4/4	-
10	EDO	A	728	-	-	1/1/1/1	-
6	1PE	A	716	4	-	4/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGE	B	713	-	-	6/7/7/7	-
10	EDO	A	725	-	-	1/1/1/1	-
8	PG4	A	718	-	-	8/10/10/10	-
8	PG4	A	719	-	-	3/10/10/10	-
9	PEG	A	723	-	-	4/4/4/4	-
10	EDO	A	731	-	-	1/1/1/1	-
10	EDO	B	718	-	-	1/1/1/1	-
10	EDO	A	730	-	-	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	3.00	1.57	1.50
3	A	702	PO4	P-O1	2.86	1.57	1.50
3	A	703	PO4	P-O1	2.75	1.57	1.50
3	B	703	PO4	P-O1	2.26	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
7	A	717	PGE	O1-C1-C2-O2
8	A	718	PG4	O1-C1-C2-O2
9	A	723	PEG	O2-C3-C4-O4
7	B	713	PGE	O1-C1-C2-O2
10	A	728	EDO	O1-C1-C2-O2
8	A	718	PG4	O3-C5-C6-O4
8	A	720	PG4	O1-C1-C2-O2
9	A	723	PEG	O1-C1-C2-O2
10	A	725	EDO	O1-C1-C2-O2
10	A	727	EDO	O1-C1-C2-O2
10	A	730	EDO	O1-C1-C2-O2
10	B	717	EDO	O1-C1-C2-O2
7	B	713	PGE	O3-C5-C6-O4
9	B	715	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
10	A	726	EDO	O1-C1-C2-O2
6	B	714	1PE	OH5-C14-C24-OH4
8	A	719	PG4	C8-C7-O4-C6
8	A	719	PG4	C4-C3-O2-C2
7	A	717	PGE	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
6	A	716	1PE	OH7-C16-C26-OH6
9	B	715	PEG	C4-C3-O2-C2
6	B	714	1PE	C25-C15-OH6-C26
7	B	713	PGE	C6-C5-O3-C4
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
8	A	718	PG4	O4-C7-C8-O5
10	A	731	EDO	O1-C1-C2-O2
6	A	716	1PE	C25-C15-OH6-C26
9	A	721	PEG	O1-C1-C2-O2
7	B	713	PGE	C1-C2-O2-C3
6	A	716	1PE	OH6-C15-C25-OH5
8	A	719	PG4	C5-C6-O4-C7
10	B	718	EDO	O1-C1-C2-O2
9	B	715	PEG	C1-C2-O2-C3
7	B	713	PGE	C3-C4-O3-C5
8	A	720	PG4	C3-C4-O3-C5
8	A	718	PG4	C3-C4-O3-C5
9	A	723	PEG	C1-C2-O2-C3
9	A	723	PEG	C4-C3-O2-C2
7	A	717	PGE	C6-C5-O3-C4

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	717	PGE	2	0
10	A	729	EDO	3	0
8	A	720	PG4	2	0
10	B	717	EDO	3	0
10	A	728	EDO	1	0
8	A	719	PG4	1	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%)	-0.13	18 (2%) 56 62	11, 26, 52, 88	6 (0%)
1	B	667/698 (95%)	0.18	56 (8%) 17 19	13, 30, 59, 88	7 (1%)
All	All	1336/1396 (95%)	0.02	74 (5%) 30 36	11, 28, 56, 88	13 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	LEU	7.1
1	A	65	GLY	6.5
1	A	136	LEU	5.5
1	B	184	PRO	4.3
1	B	134	ALA	4.2
1	B	200	LEU	4.1
1	B	63	PRO	4.0
1	B	183	ASP	4.0
1	B	199	LEU	3.7
1	A	370	GLU	3.6
1	B	170	ALA	3.5
1	B	176	ALA	3.5
1	B	185	PHE	3.5
1	B	192	LEU	3.4
1	B	178	LEU	3.4
1	B	131	ASN	3.4
1	B	196	VAL	3.4
1	B	472	TRP	3.4
1	A	134	ALA	3.3
1	B	177	ALA	3.3
1	B	128	TRP	3.2
1	B	145	LEU	3.1
1	A	133	THR	3.1
1	B	180	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	167	LEU	3.1
1	A	472	TRP	3.0
1	B	171	LEU	3.0
1	B	132	VAL	3.0
1	B	135	LYS	3.0
1	A	63	PRO	2.9
1	B	188	ALA	2.9
1	B	371	ASN	2.9
1	B	179	ARG	2.9
1	B	181	PRO	2.9
1	A	366	ILE	2.8
1	B	186	THR	2.8
1	B	372	PRO	2.8
1	B	97	HIS	2.7
1	B	173	GLU	2.6
1	A	140	GLN	2.6
1	B	203	TYR	2.6
1	B	159	ALA	2.5
1	B	164	PRO	2.5
1	A	645	TYR	2.5
1	B	165	ARG	2.4
1	B	634	TRP	2.4
1	A	88	PRO	2.3
1	B	160	ALA	2.3
1	A	64	PRO	2.3
1	B	182	GLY	2.3
1	A	368	TYR	2.3
1	B	201	ALA	2.3
1	B	366	ILE	2.3
1	A	58	ASP	2.3
1	B	150	LEU	2.3
1	B	189	GLY	2.2
1	B	163	VAL	2.2
1	B	375	LYS	2.2
1	B	191	ALA	2.2
1	A	649	TRP	2.2
1	B	626	PHE	2.2
1	B	172	LEU	2.2
1	B	666	TYR	2.2
1	A	131	ASN	2.2
1	B	374	LYS	2.2
1	B	151	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	-1	GLY	2.1
1	B	204	PRO	2.1
1	B	373	PRO	2.1
1	A	97	HIS	2.0
1	B	62	PRO	2.0
1	B	289	VAL	2.0
1	B	193	SER	2.0
1	B	158	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

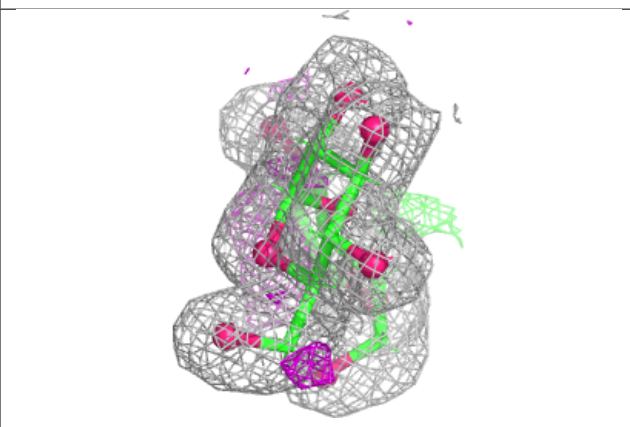
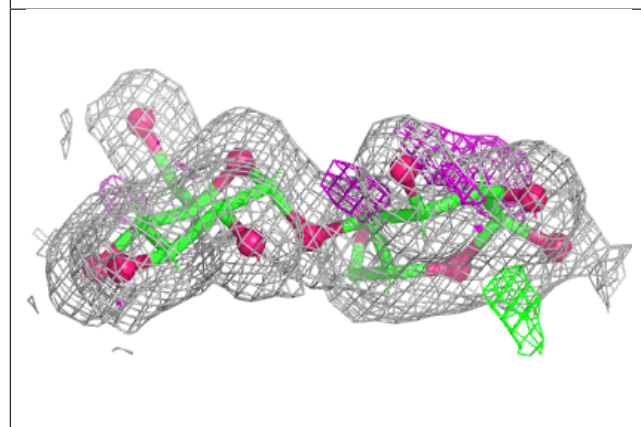
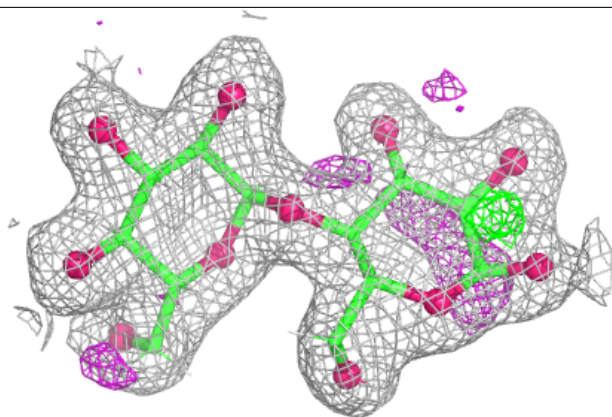
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	C	1	12/12	0.94	0.07	20,32,39,42	0
2	GLC	D	1	12/12	0.94	0.07	24,32,40,42	0
2	GLC	D	2	11/12	0.95	0.06	24,27,29,29	0
2	GLC	C	2	11/12	0.97	0.05	21,22,23,24	0

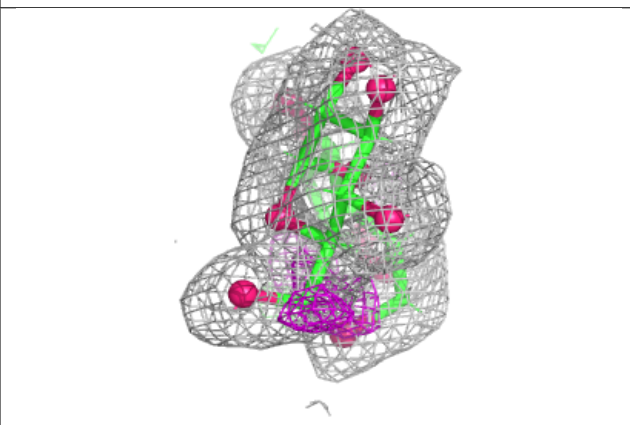
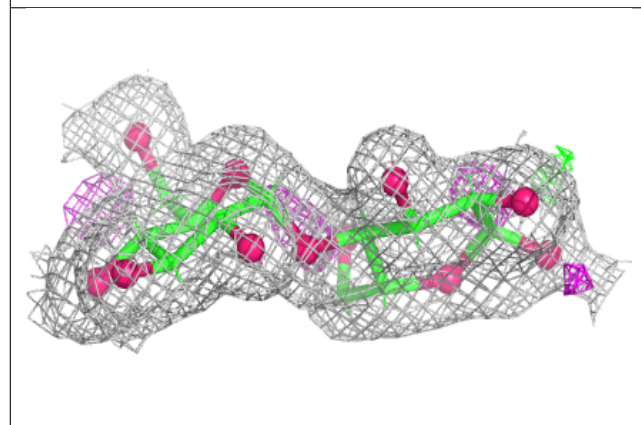
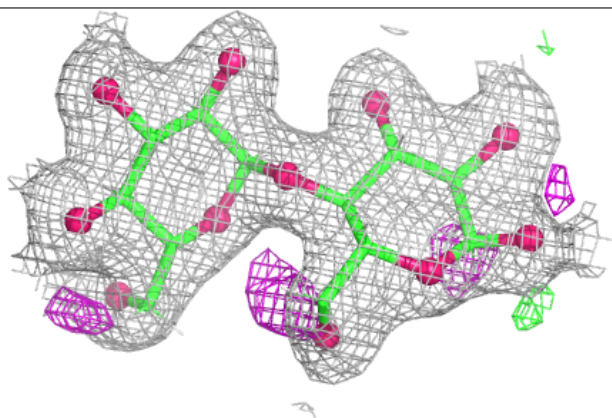
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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
10	EDO	B	716	4/4	0.65	0.20	45,49,52,55	0
8	PG4	A	718	13/13	0.66	0.23	59,65,69,69	0
7	PGE	A	717	10/10	0.66	0.21	54,62,64,66	0
9	PEG	B	715	7/7	0.67	0.23	51,57,59,59	0
10	EDO	A	731	4/4	0.69	0.20	53,56,58,61	0
8	PG4	A	720	13/13	0.69	0.24	42,61,67,68	0
10	EDO	A	724	4/4	0.77	0.23	62,63,63,64	0
9	PEG	A	723	7/7	0.78	0.18	59,62,65,66	0
10	EDO	A	725	4/4	0.78	0.21	52,53,53,54	0
10	EDO	A	728	4/4	0.80	0.20	50,54,56,57	0
10	EDO	A	727	4/4	0.82	0.18	59,61,62,63	0
3	PO4	B	703	5/5	0.84	0.17	54,59,61,63	0
3	PO4	A	703	5/5	0.86	0.11	66,68,69,70	0
10	EDO	A	726	4/4	0.86	0.14	42,44,47,49	0
10	EDO	B	717	4/4	0.86	0.23	56,58,59,59	0
6	1PE	B	714	16/16	0.87	0.13	43,52,58,61	0
10	EDO	A	729	4/4	0.89	0.19	59,59,59,59	0
4	NA	A	704	1/1	0.89	0.12	40,40,40,40	0
8	PG4	A	719	13/13	0.90	0.13	43,50,59,60	0
7	PGE	B	713	10/10	0.90	0.12	40,42,49,53	0
10	EDO	A	730	4/4	0.90	0.12	53,54,55,57	0
3	PO4	B	702	5/5	0.91	0.16	47,49,50,50	0
4	NA	B	710	1/1	0.91	0.09	45,45,45,45	0
4	NA	B	706	1/1	0.92	0.12	47,47,47,47	0
4	NA	A	709	1/1	0.92	0.17	39,39,39,39	0
9	PEG	A	721	7/7	0.92	0.11	54,55,57,60	0
9	PEG	A	722	7/7	0.92	0.10	42,45,46,47	0
10	EDO	B	718	4/4	0.92	0.19	42,43,45,46	0
4	NA	A	712	1/1	0.93	0.09	47,47,47,47	0
3	PO4	A	702	5/5	0.93	0.12	45,51,51,52	0
4	NA	B	707	1/1	0.94	0.10	39,39,39,39	0
4	NA	B	709	1/1	0.94	0.14	37,37,37,37	0
4	NA	A	714	1/1	0.95	0.12	50,50,50,50	0
4	NA	A	706	1/1	0.95	0.13	33,33,33,33	0
6	1PE	A	716	16/16	0.95	0.09	20,27,49,54	0
4	NA	A	708	1/1	0.95	0.08	42,42,42,42	0
4	NA	A	710	1/1	0.96	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	B	705	1/1	0.96	0.06	40,40,40,40	0
4	NA	A	711	1/1	0.97	0.12	38,38,38,38	0
5	CL	A	715	1/1	0.97	0.27	51,51,51,51	0
4	NA	B	704	1/1	0.97	0.10	21,21,21,21	0
4	NA	A	705	1/1	0.98	0.08	19,19,19,19	0
5	CL	B	712	1/1	0.98	0.28	53,53,53,53	0
4	NA	B	708	1/1	0.98	0.07	31,31,31,31	0
4	NA	A	713	1/1	0.98	0.04	22,22,22,22	0
4	NA	A	707	1/1	0.98	0.04	41,41,41,41	0
4	NA	B	711	1/1	0.98	0.06	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.