



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:41 PM UTC

PDB ID : 4CTE / pdb_00004cte
Title : Crystal structure of the catalytic domain of the modular laminarinase ZgLamC mutant E142S in complex with a thio-oligosaccharide
Authors : Labourel, A.; Jam, M.; Legentil, L.; Sylla, B.; Ficko-Blean, E.; Hehemann, J.H.; Ferrieres, V.; Czjzek, M.; Michel, G.
Deposited on : 2014-03-13
Resolution : 1.80 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

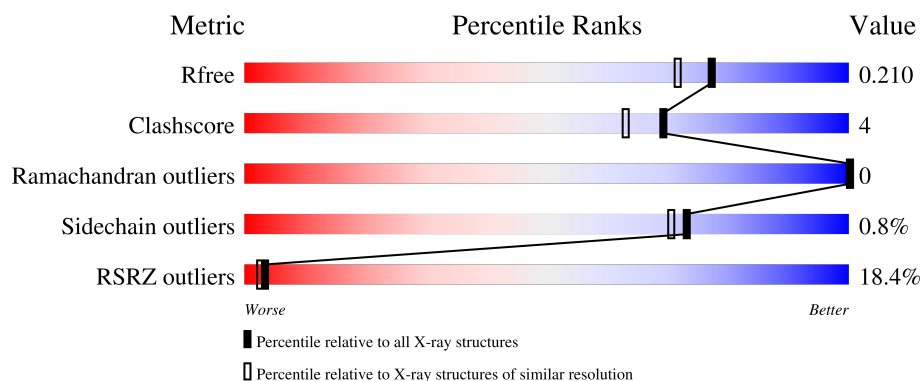
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	233	33% 93% 6%
1	B	233	3% 92% 7%
2	C	2	50% 50%
3	D	3	67% 33%

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
7	GOL	A	284	-	-	X	-
7	GOL	B	284	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4178 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 ENDO-1,3-BETA-GLUCANASE, FAMILY GH16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	7	0
			1878	1190	316	365	7			
1	B	231	Total	C	N	O	S	0	7	0
			1881	1189	319	366	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	GLU	engineered mutation	UNP G0L2L9
B	142	SER	GLU	engineered mutation	UNP G0L2L9

- Molecule 2 is an oligosaccharide called 1-thio-beta-D-glucopyranose-(1-3)-1-thio-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	S	0	0	0
			23	12	9	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	O	S	0	0	0
			34	18	14	2			

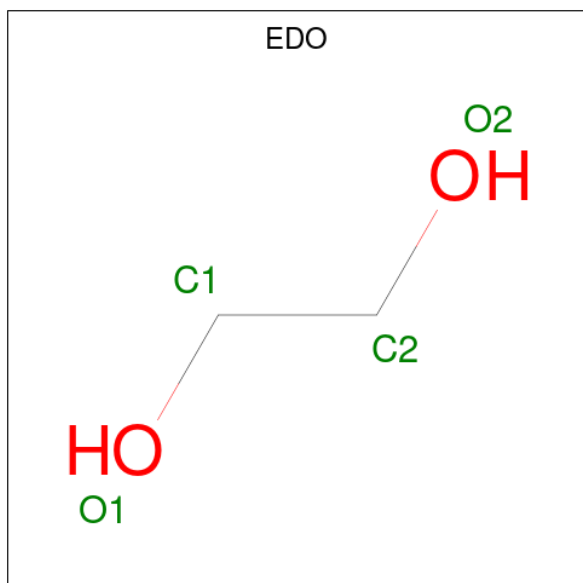
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- 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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



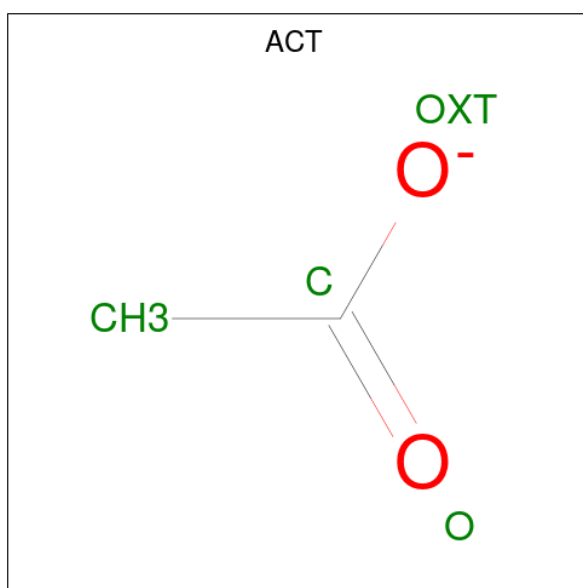
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Na 1	0	0

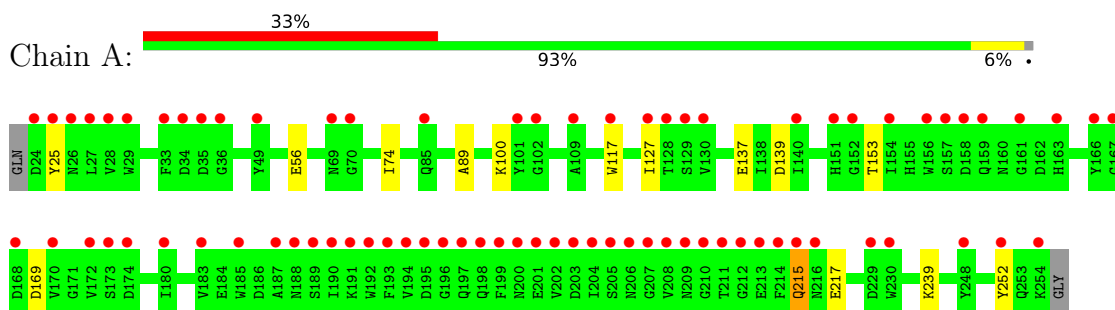
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	140	Total 140	O 140	0	0
10	B	193	Total 193	O 193	0	0

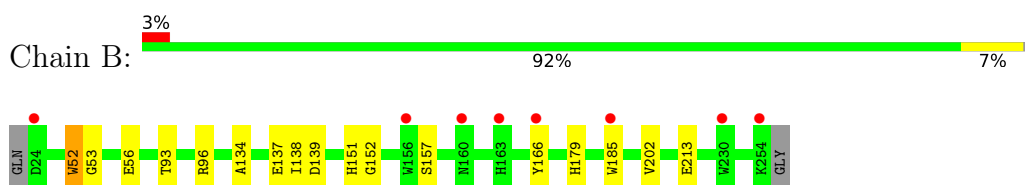
3 Residue-property plots [i](#)

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: ENDO-1,3-BETA-GLUCANASE, FAMILY GH16



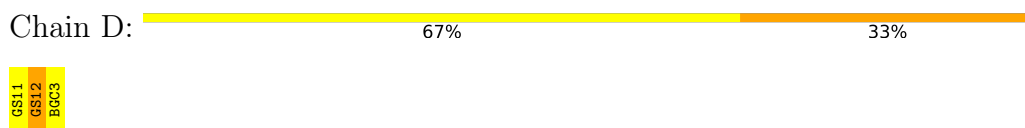
- Molecule 1: ENDO-1,3-BETA-GLUCANASE, FAMILY GH16



- Molecule 2: 1-thio-beta-D-glucopyranose-(1-3)-1-thio-beta-D-glucopyranose



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.01Å 93.93Å 142.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 1.80 48.11 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.11-1.80) 99.9 (48.11-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.177 , 0.222 (Not available) , 0.210	Depositor DCC
R_{free} test set	3536 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4178	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: CA, GS1, GOL, ACT, CL, EDO, BGC, NA

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	1.14	0/1950	1.08	2/2650 (0.1%)
1	B	1.35	6/1950 (0.3%)	1.10	1/2650 (0.0%)
All	All	1.25	6/3900 (0.2%)	1.09	3/5300 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	52	TRP	NE1-CE2	-6.75	1.30	1.37
1	B	151	HIS	CG-CD2	6.33	1.42	1.35
1	B	179	HIS	ND1-CE1	5.55	1.38	1.32
1	B	93	THR	N-CA	5.47	1.52	1.46
1	B	138	ILE	C-O	-5.15	1.18	1.24
1	B	96	ARG	C-O	-5.05	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ILE	CA-C-N	5.51	127.92	120.38
1	A	127	ILE	C-N-CA	5.51	127.92	120.38
1	B	152	GLY	N-CA-C	-5.04	101.23	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1878	0	1726	12	0
1	B	1881	0	1722	8	0
2	C	23	0	21	2	0
3	D	34	0	30	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0
7	A	6	0	8	5	0
7	B	6	0	8	4	0
8	B	4	0	3	0	0
9	B	1	0	0	0	0
10	A	140	0	0	5	0
10	B	193	0	0	4	0
All	All	4178	0	3530	26	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 4.

All (26) 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:B:157:SER:O	10:B:2127:HOH:O	2.11	0.68
1:B:134:ALA:O	1:B:213:GLU:HG3	1.96	0.65
1:A:239:LYS:NZ	10:A:2133:HOH:O	2.33	0.61
7:A:284:GOL:H2	2:C:1:GS1:H61	1.82	0.61
1:B:56:GLU:OE2	7:B:284:GOL:H11	2.01	0.61
1:A:100:LYS:HE3	1:A:215:GLN:O	2.03	0.59
7:B:284:GOL:H12	10:B:2041:HOH:O	2.03	0.57
7:B:284:GOL:C1	10:B:2041:HOH:O	2.52	0.57
1:A:239:LYS:NZ	10:A:2127:HOH:O	2.39	0.55
1:B:185:TRP:CD1	1:B:185:TRP:C	2.86	0.54
1:B:166:TYR:CD2	1:B:202:VAL:HG12	2.44	0.53
1:A:117:TRP:HZ2	2:C:1:GS1:O5	1.92	0.52
1:A:56:GLU:OE2	7:A:284:GOL:H11	2.12	0.49
1:A:100:LYS:NZ	10:A:2070:HOH:O	2.45	0.49
1:B:137:GLU:OE2	1:B:139[A]:ASP:OD1	2.32	0.47
1:A:117:TRP:CE2	7:A:284:GOL:H31	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TRP:C	1:A:117:TRP:CD1	2.94	0.45
1:B:52:TRP:HA	5:B:281:CL:CL	2.54	0.45
1:A:137:GLU:OE2	1:A:139:ASP:OD1	2.35	0.45
7:A:284:GOL:H12	10:A:2032:HOH:O	2.15	0.44
1:A:100:LYS:HB2	1:A:217:GLU:HG2	2.01	0.43
7:A:284:GOL:C1	10:A:2032:HOH:O	2.67	0.42
7:B:284:GOL:H11	10:B:2041:HOH:O	2.18	0.42
1:A:74:ILE:HG23	1:A:89:ALA:HB3	2.02	0.42
1:A:25:TYR:HB3	1:A:252:TYR:HB3	2.04	0.40
1:B:53:GLY:HA3	3:D:2:GS1:O3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/233 (101%)	228 (97%)	8 (3%)	0	100	100
1	B	236/233 (101%)	226 (96%)	10 (4%)	0	100	100
All	All	472/466 (101%)	454 (96%)	18 (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	197/191 (103%)	194 (98%)	3 (2%)	57	49
1	B	197/191 (103%)	197 (100%)	0	100	100
All	All	394/382 (103%)	391 (99%)	3 (1%)	73	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	THR
1	A	169	ASP
1	A	215	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	54	ASN
1	A	55	ASN
1	A	114	GLN
1	A	215	GLN
1	B	54	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

5 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GS1	C	1	2	10,11,12	1.22	2 (20%)	13,15,17	3.79	8 (61%)
2	GS1	C	2	2	11,12,12	1.62	3 (27%)	15,17,17	1.31	3 (20%)
3	GS1	D	1	3	10,11,12	0.42	0	13,15,17	1.03	2 (15%)
3	GS1	D	2	3	11,12,12	0.58	0	15,17,17	1.60	3 (20%)
3	BGC	D	3	3	11,11,12	0.66	0	15,15,17	1.20	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	GS1	C	1	2	-	2/2/18/22	0/1/1/1
2	GS1	C	2	2	-	0/2/22/22	0/1/1/1
3	GS1	D	1	3	-	1/2/18/22	0/1/1/1
3	GS1	D	2	3	-	0/2/22/22	0/1/1/1
3	BGC	D	3	3	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	GS1	O5-C1	2.73	1.46	1.42
2	C	2	GS1	C4-C3	2.69	1.59	1.52
2	C	1	GS1	C3-C2	-2.54	1.47	1.52
2	C	1	GS1	C3-C4	-2.13	1.48	1.52
2	C	2	GS1	O3-C3	2.08	1.48	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GS1	C4-C3-C2	-8.88	101.17	111.50
2	C	1	GS1	C3-C4-C5	-5.70	103.49	110.76
2	C	1	GS1	O5-C5-C4	-5.14	103.09	110.10
2	C	1	GS1	O5-C5-C6	3.71	115.63	106.44
3	D	2	GS1	C1-C2-C3	-3.54	103.63	110.55
3	D	3	BGC	C1-C2-C3	2.94	113.92	109.64
3	D	2	GS1	O5-C5-C4	-2.91	104.46	109.70
2	C	1	GS1	O2-C2-C1	2.78	115.41	110.26
2	C	1	GS1	O4-C4-C3	-2.64	103.28	109.86
3	D	2	GS1	O5-C5-C6	2.41	112.42	106.44
2	C	1	GS1	C3-C2-C1	-2.40	101.39	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	GS1	O3-C3-C4	2.38	115.98	110.38
2	C	2	GS1	O5-C1-C2	2.29	113.47	110.32
2	C	1	GS1	C1-O5-C5	-2.24	108.55	112.55
2	C	2	GS1	C1-C2-C3	-2.10	106.45	110.55
3	D	1	GS1	C6-C5-C4	-2.06	110.72	113.53
3	D	1	GS1	C4-C3-C2	-2.01	109.16	111.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

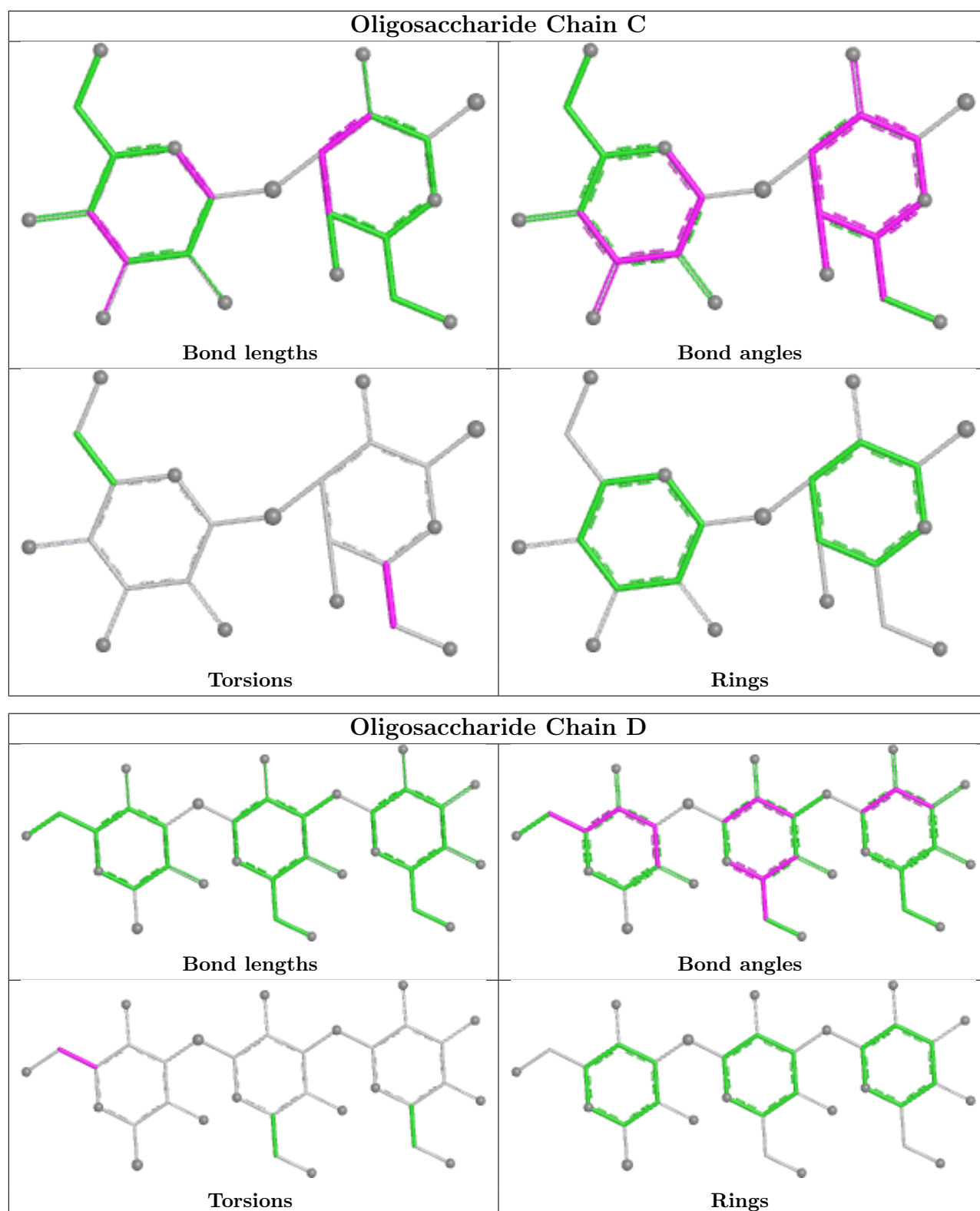
Mol	Chain	Res	Type	Atoms
2	C	1	GS1	O5-C5-C6-O6
2	C	1	GS1	C4-C5-C6-O6
3	D	1	GS1	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	GS1	1	0
2	C	1	GS1	2	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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	ACT	B	282	4	3,3,3	1.72	1 (33%)	3,3,3	1.94	1 (33%)
6	EDO	B	283	-	3,3,3	0.56	0	2,2,2	1.08	0
6	EDO	A	263	-	3,3,3	0.53	0	2,2,2	0.77	0
7	GOL	B	284	-	5,5,5	0.53	0	5,5,5	1.27	1 (20%)
7	GOL	A	284	-	5,5,5	0.46	0	5,5,5	0.97	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
7	GOL	B	284	-	-	4/4/4/4	-
6	EDO	B	283	-	-	1/1/1/1	-
6	EDO	A	263	-	-	0/1/1/1	-
7	GOL	A	284	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	282	ACT	O-C	2.60	1.33	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	282	ACT	OXT-C-O	2.84	132.58	122.03
7	B	284	GOL	O2-C2-C1	-2.13	100.36	109.18

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	284	GOL	O1-C1-C2-C3
7	A	284	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	B	284	GOL	O1-C1-C2-C3
7	B	284	GOL	C1-C2-C3-O3
7	A	284	GOL	O1-C1-C2-O2
7	B	284	GOL	O1-C1-C2-O2
7	A	284	GOL	O2-C2-C3-O3
7	B	284	GOL	O2-C2-C3-O3
6	B	283	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	284	GOL	4	0
7	A	284	GOL	5	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	231/233 (99%)	1.51	77 (33%) 1 1	18, 36, 65, 91	9 (3%)
1	B	231/233 (99%)	-0.05	8 (3%) 47 47	12, 23, 36, 63	8 (3%)
All	All	462/466 (99%)	0.73	85 (18%) 3 2	12, 29, 57, 91	17 (3%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	TYR	6.2
1	A	203	ASP	6.1
1	A	202	VAL	5.6
1	A	208	VAL	5.6
1	A	163[A]	HIS	5.2
1	A	254	LYS	4.8
1	A	201	GLU	4.8
1	A	230	TRP	4.6
1	A	117	TRP	4.4
1	A	166	TYR	4.3
1	A	215	GLN	4.3
1	A	212	GLY	4.1
1	A	24	ASP	4.0
1	A	35[A]	ASP	4.0
1	A	210	GLY	3.9
1	B	163[A]	HIS	3.9
1	A	196	GLY	3.8
1	A	207	GLY	3.8
1	A	209	ASN	3.7
1	A	205	SER	3.7
1	A	193	PHE	3.7
1	A	159	GLN	3.7
1	A	188	ASN	3.5
1	A	197	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	185	TRP	3.4
1	A	200	ASN	3.4
1	A	194	VAL	3.3
1	A	173[A]	SER	3.3
1	A	204	ILE	3.2
1	A	199	PHE	3.2
1	A	214	PHE	3.2
1	A	211	THR	3.2
1	B	230	TRP	3.1
1	A	25	TYR	3.0
1	A	216	ASN	3.0
1	B	166	TYR	2.9
1	A	187	ALA	2.9
1	A	180[A]	ILE	2.9
1	A	154	ILE	2.9
1	B	254	LYS	2.7
1	A	36	GLY	2.7
1	A	168	ASP	2.7
1	B	185	TRP	2.6
1	A	69	ASN	2.6
1	A	190	ILE	2.6
1	A	195	ASP	2.6
1	A	140	ILE	2.6
1	A	170	VAL	2.6
1	A	102	GLY	2.5
1	A	128	THR	2.5
1	B	160	ASN	2.5
1	A	213[A]	GLU	2.5
1	A	192	TRP	2.5
1	A	34	ASP	2.4
1	B	24	ASP	2.4
1	A	172	VAL	2.4
1	A	183	VAL	2.4
1	A	152	GLY	2.4
1	A	158	ASP	2.4
1	A	26	ASN	2.4
1	A	206	ASN	2.4
1	A	156	TRP	2.4
1	A	27	LEU	2.3
1	A	85	GLN	2.3
1	A	229[A]	ASP	2.3
1	B	156	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	167	GLY	2.3
1	A	130	VAL	2.3
1	A	248	TYR	2.2
1	A	189	SER	2.2
1	A	252	TYR	2.2
1	A	109	ALA	2.2
1	A	191	LYS	2.2
1	A	198	GLN	2.1
1	A	70	GLY	2.1
1	A	174	ASP	2.1
1	A	29	TRP	2.1
1	A	151	HIS	2.1
1	A	33	PHE	2.1
1	A	28	VAL	2.1
1	A	157	SER	2.0
1	A	101	TYR	2.0
1	A	129	SER	2.0
1	A	127	ILE	2.0
1	A	161	GLY	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](#)

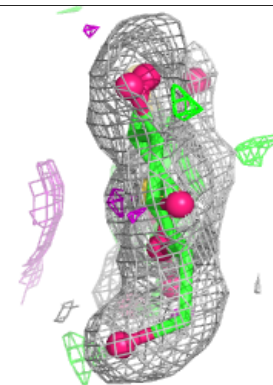
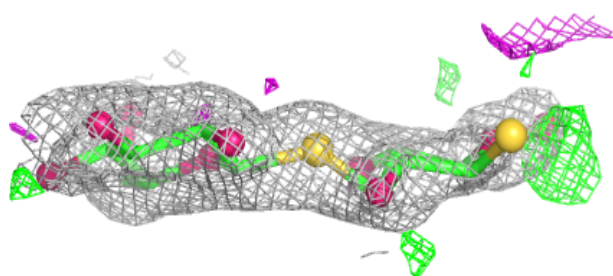
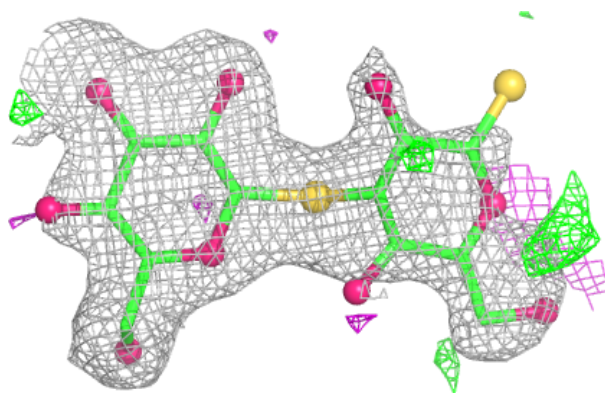
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	GS1	D	1	11/12	0.51	0.36	29,32,38,53	11
2	GS1	C	1	11/12	0.71	0.28	29,31,39,57	11
3	BGC	D	3	11/12	0.73	0.20	34,39,41,47	11
2	GS1	C	2	12/12	0.87	0.15	38,45,52,57	1
3	GS1	D	2	12/12	0.90	0.13	26,28,36,38	12

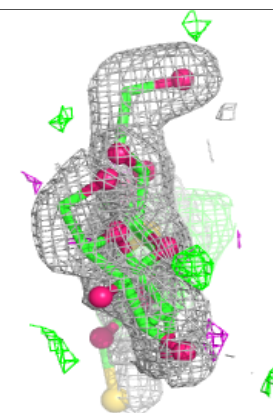
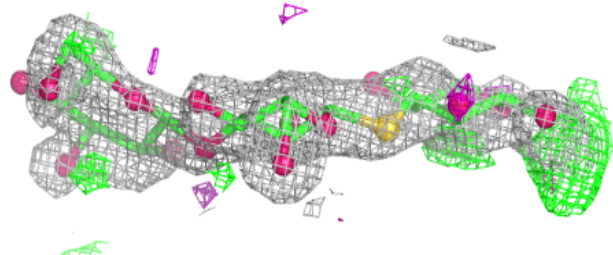
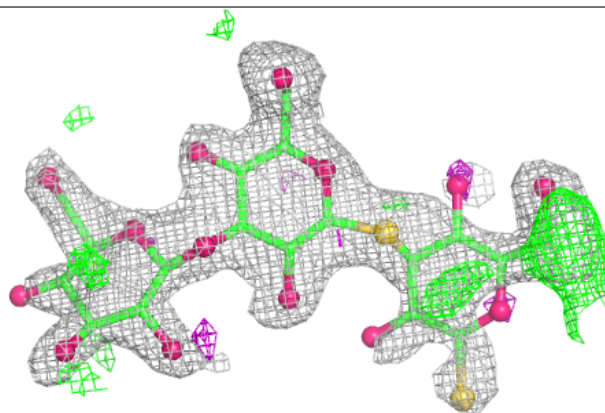
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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 [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
7	GOL	B	284	6/6	0.88	0.17	21,27,33,41	6
7	GOL	A	284	6/6	0.89	0.14	25,30,35,42	6
6	EDO	B	283	4/4	0.89	0.14	30,31,32,37	0
6	EDO	A	263	4/4	0.92	0.13	35,36,39,43	0
5	CL	B	281	1/1	0.93	0.15	43,43,43,43	0
8	ACT	B	282	4/4	0.93	0.15	25,25,31,41	0
5	CL	A	261	1/1	0.94	0.13	43,43,43,43	0
4	CA	A	260	1/1	0.98	0.05	39,39,39,39	0
9	NA	B	285	1/1	0.99	0.09	31,31,31,31	0
4	CA	B	280	1/1	1.00	0.02	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.