



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2026 – 10:07 PM UTC

PDB ID : 9WVU / pdb_00009wvu
Title : Carbohydrate-bound structure of alpha-glucan phosphorylase from Crocosphaera subtropica ATCC 51142
Authors : Suzuki, R.; Ikuta, A.; Suzuki, E.
Deposited on : 2025-09-22
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

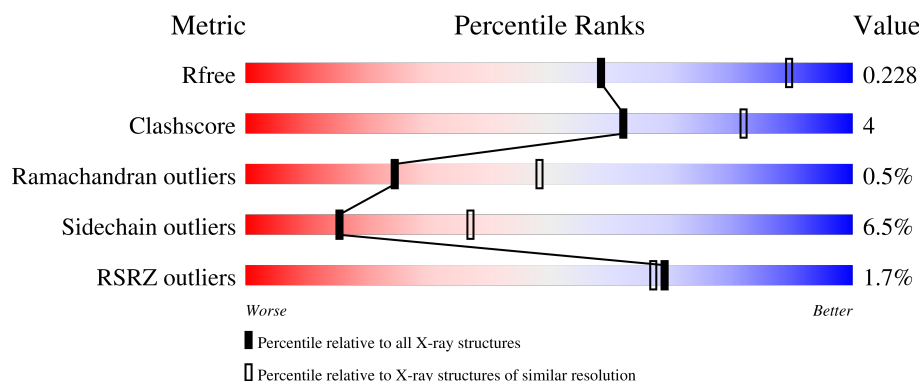
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	AAA	855	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 81% 13% • 5% </div> </div>
1	BBB	855	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 80% 14% • 5% </div> </div>
2	CCC	6	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 100% </div> </div>
3	CfC	11	<div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 9% 73% 18% </div> </div>
4	CqC	3	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> 33% 67% </div> </div>

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Mol	Chain	Length	Quality of chain
4	CxC	3	<div><div></div><div>33%</div><div>67%</div></div>
5	CtC	4	<div><div></div><div>100%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13591 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 Alpha-1,4 glucan phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	813	Total	C	N	O	P	S	0	0	0
			6601	4228	1124	1231	1	17			
1	BBB	813	Total	C	N	O	P	S	0	0	0
			6601	4228	1124	1231	1	17			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-14	MET	-	initiating methionine	UNP B1WXW6
AAA	-13	ASN	-	expression tag	UNP B1WXW6
AAA	-12	HIS	-	expression tag	UNP B1WXW6
AAA	-11	LYS	-	expression tag	UNP B1WXW6
AAA	-10	VAL	-	expression tag	UNP B1WXW6
AAA	-9	HIS	-	expression tag	UNP B1WXW6
AAA	-8	HIS	-	expression tag	UNP B1WXW6
AAA	-7	HIS	-	expression tag	UNP B1WXW6
AAA	-6	HIS	-	expression tag	UNP B1WXW6
AAA	-5	HIS	-	expression tag	UNP B1WXW6
AAA	-4	HIS	-	expression tag	UNP B1WXW6
AAA	-3	ILE	-	expression tag	UNP B1WXW6
AAA	-2	GLU	-	expression tag	UNP B1WXW6
AAA	-1	GLY	-	expression tag	UNP B1WXW6
AAA	0	ARG	-	expression tag	UNP B1WXW6
BBB	-14	MET	-	initiating methionine	UNP B1WXW6
BBB	-13	ASN	-	expression tag	UNP B1WXW6
BBB	-12	HIS	-	expression tag	UNP B1WXW6
BBB	-11	LYS	-	expression tag	UNP B1WXW6
BBB	-10	VAL	-	expression tag	UNP B1WXW6
BBB	-9	HIS	-	expression tag	UNP B1WXW6
BBB	-8	HIS	-	expression tag	UNP B1WXW6
BBB	-7	HIS	-	expression tag	UNP B1WXW6
BBB	-6	HIS	-	expression tag	UNP B1WXW6
BBB	-5	HIS	-	expression tag	UNP B1WXW6

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-4	HIS	-	expression tag	UNP B1WXW6
BBB	-3	ILE	-	expression tag	UNP B1WXW6
BBB	-2	GLU	-	expression tag	UNP B1WXW6
BBB	-1	GLY	-	expression tag	UNP B1WXW6
BBB	0	ARG	-	expression tag	UNP B1WXW6

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	CCC	6	Total	C	O	0	0	0
			66	36	30			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	CfC	11	Total	C	O	0	0	0
			122	66	56			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	CqC	3	Total	C	O	0	0	0
			33	18	15			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	CxC	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	CtC	4	Total	C	O	0	0	0
			44	24	20			

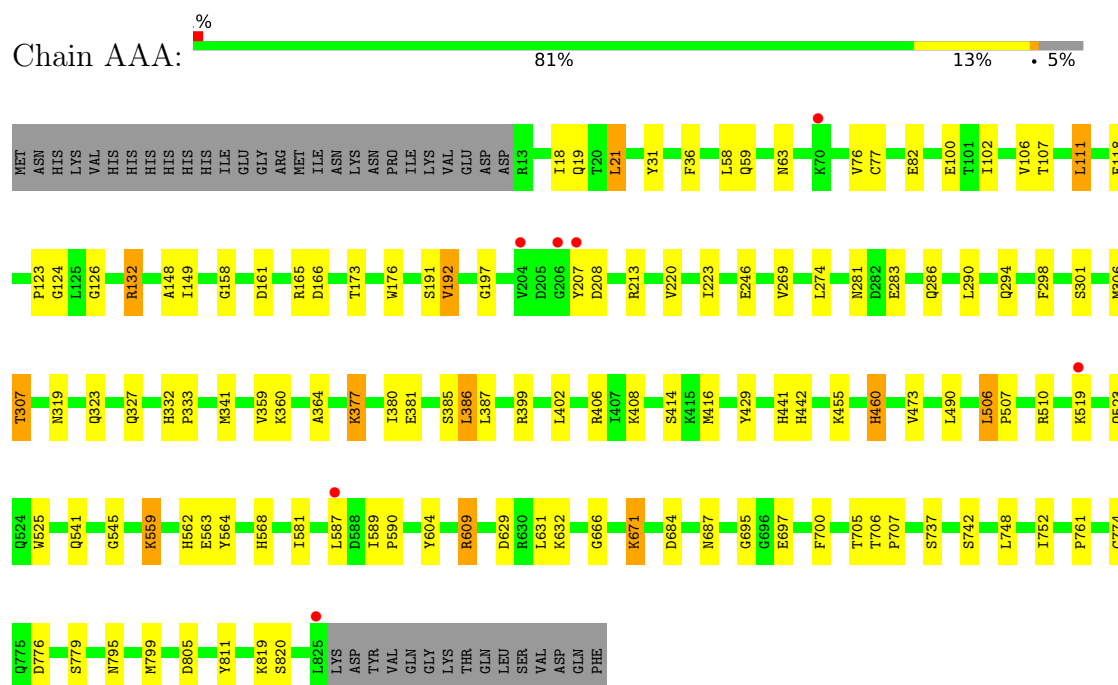
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	67	Total	O	0	0
			67	67		
6	BBB	24	Total	O	0	0
			24	24		

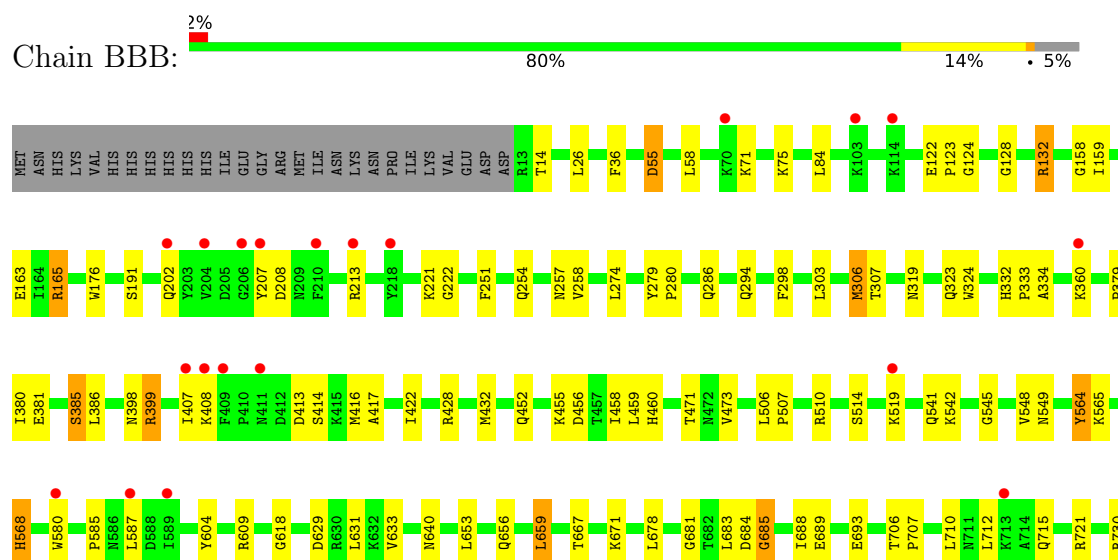
3 Residue-property plots [i](#)

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 phosphorylase



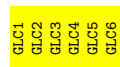
- Molecule 1: Alpha-1,4 glucan phosphorylase





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

Chain CCC: 100%



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

Chain CfC: 9% 73% 18%



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

Chain CqC: 33% 67%



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

Chain CxC: 33% 67%



- Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain CtC: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	267.24Å 267.24Å 204.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.01 – 2.70 50.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.01-2.70) 100.0 (50.01-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.91 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.174 , 0.227 0.180 , 0.228	Depositor DCC
R_{free} test set	3786 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13591	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: LLP, GLC

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	AAA	1.05	2/6732 (0.0%)	1.46	14/9140 (0.2%)
1	BBB	1.04	2/6732 (0.0%)	1.49	12/9140 (0.1%)
All	All	1.05	4/13464 (0.0%)	1.47	26/18280 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	761	PRO	C-O	-5.36	1.17	1.24
1	BBB	128	GLY	C-O	5.34	1.28	1.24
1	AAA	460	HIS	CE1-NE2	5.26	1.37	1.32
1	BBB	815	ILE	N-CA	5.18	1.50	1.46

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	100	GLU	CB-CG-CD	7.46	125.28	112.60
1	AAA	100	GLU	CB-CA-C	7.44	122.57	110.88
1	AAA	666	GLY	CA-C-O	-6.78	116.35	122.24
1	AAA	695	GLY	CA-C-N	6.36	127.16	120.03
1	AAA	695	GLY	C-N-CA	6.36	127.16	120.03

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	AAA	6601	0	6517	53	0
1	BBB	6601	0	6517	57	0
2	CCC	66	0	55	0	0
3	CfC	122	0	102	2	0
4	CqC	33	0	28	3	0
4	CxC	33	0	28	0	0
5	CtC	44	0	37	0	0
6	AAA	67	0	0	0	0
6	BBB	24	0	0	0	0
All	All	13591	0	13284	109	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.

The worst 5 of 109 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:AAA:441:HIS:HD2	1:AAA:442:HIS:HD2	1.11	0.91
1:AAA:319:ASN:ND2	1:AAA:323:GLN:NE2	2.22	0.88
1:AAA:441:HIS:HD2	1:AAA:442:HIS:CD2	2.00	0.76
1:BBB:303:LEU:HD23	1:BBB:306:MET:CE	2.16	0.75
1:AAA:319:ASN:ND2	1:AAA:323:GLN:HE22	1.83	0.74

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	AAA	810/855 (95%)	782 (96%)	25 (3%)	3 (0%)	30 54
1	BBB	810/855 (95%)	769 (95%)	36 (4%)	5 (1%)	21 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1620/1710 (95%)	1551 (96%)	61 (4%)	8 (0%)	24	48

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	207	TYR
1	BBB	414	SER
1	BBB	407	ILE
1	AAA	208	ASP
1	BBB	428	ARG

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	AAA	716/756 (95%)	673 (94%)	43 (6%)	17	41
1	BBB	716/756 (95%)	666 (93%)	50 (7%)	14	34
All	All	1432/1512 (95%)	1339 (94%)	93 (6%)	15	37

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	286	GLN
1	BBB	542	LYS
1	BBB	307	THR
1	BBB	413	ASP
1	BBB	568	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	LLP	AAA	671	1	23,24,25	0.66	0	25,32,34	0.83	1 (4%)
1	LLP	BBB	671	1	23,24,25	0.63	0	25,32,34	0.76	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
1	LLP	AAA	671	1	-	2/16/17/19	0/1/1/1
1	LLP	BBB	671	1	-	3/16/17/19	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	671	LLP	CE-NZ-C4'	2.60	127.06	118.72

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BBB	671	LLP	C5'-OP4-P-OP1
1	AAA	671	LLP	C5'-OP4-P-OP1
1	BBB	671	LLP	C5'-OP4-P-OP3
1	BBB	671	LLP	CE-CD-CG-CB
1	AAA	671	LLP	C5'-OP4-P-OP3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AAA	671	LLP	1	0
1	BBB	671	LLP	2	0

5.5 Carbohydrates

27 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	CCC	1	2	11,11,12	1.05	1 (9%)	15,15,17	2.06	4 (26%)
2	GLC	CCC	2	2	11,11,12	0.55	0	15,15,17	1.55	2 (13%)
2	GLC	CCC	3	2	11,11,12	0.46	0	15,15,17	1.03	1 (6%)
2	GLC	CCC	4	2	11,11,12	0.59	0	15,15,17	1.35	1 (6%)
2	GLC	CCC	5	2	11,11,12	0.75	0	15,15,17	1.59	2 (13%)
2	GLC	CCC	6	2	11,11,12	0.68	0	15,15,17	2.18	2 (13%)
3	GLC	CfC	1	3	12,12,12	1.04	1 (8%)	17,17,17	2.50	9 (52%)
3	GLC	CfC	10	3	11,11,12	0.80	0	15,15,17	1.23	3 (20%)
3	GLC	CfC	11	3	11,11,12	0.97	0	15,15,17	2.38	5 (33%)
3	GLC	CfC	2	3	11,11,12	0.80	0	15,15,17	1.23	0
3	GLC	CfC	3	3	11,11,12	0.34	0	15,15,17	1.12	0
3	GLC	CfC	4	3	11,11,12	1.32	1 (9%)	15,15,17	1.21	1 (6%)
3	GLC	CfC	5	3	11,11,12	0.90	1 (9%)	15,15,17	1.67	3 (20%)
3	GLC	CfC	6	3	11,11,12	0.82	0	15,15,17	1.19	2 (13%)
3	GLC	CfC	7	3	11,11,12	0.94	1 (9%)	15,15,17	1.45	2 (13%)
3	GLC	CfC	8	3	11,11,12	0.55	0	15,15,17	1.21	1 (6%)
3	GLC	CfC	9	3	11,11,12	0.81	0	15,15,17	1.09	0
4	GLC	CqC	1	4	11,11,12	0.96	0	15,15,17	1.59	4 (26%)
4	GLC	CqC	2	4	11,11,12	0.55	0	15,15,17	1.27	1 (6%)
4	GLC	CqC	3	4	11,11,12	0.53	0	15,15,17	0.80	0
5	GLC	CtC	1	5	11,11,12	0.79	0	15,15,17	1.75	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GLC	CtC	2	5	11,11,12	0.47	0	15,15,17	1.30	1 (6%)
5	GLC	CtC	3	5	11,11,12	0.42	0	15,15,17	1.12	1 (6%)
5	GLC	CtC	4	5	11,11,12	0.66	0	15,15,17	2.14	3 (20%)
4	GLC	CxC	1	4	11,11,12	0.89	0	15,15,17	1.42	2 (13%)
4	GLC	CxC	2	4	11,11,12	0.78	0	15,15,17	1.61	2 (13%)
4	GLC	CxC	3	4	11,11,12	0.78	0	15,15,17	1.02	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	CCC	1	2	-	0/2/19/22	0/1/1/1
2	GLC	CCC	2	2	-	0/2/19/22	0/1/1/1
2	GLC	CCC	3	2	-	0/2/19/22	0/1/1/1
2	GLC	CCC	4	2	-	0/2/19/22	0/1/1/1
2	GLC	CCC	5	2	-	2/2/19/22	0/1/1/1
2	GLC	CCC	6	2	-	0/2/19/22	0/1/1/1
3	GLC	CfC	1	3	-	0/2/22/22	0/1/1/1
3	GLC	CfC	10	3	-	0/2/19/22	0/1/1/1
3	GLC	CfC	11	3	-	0/2/19/22	0/1/1/1
3	GLC	CfC	2	3	-	0/2/19/22	0/1/1/1
3	GLC	CfC	3	3	-	0/2/19/22	0/1/1/1
3	GLC	CfC	4	3	-	0/2/19/22	0/1/1/1
3	GLC	CfC	5	3	-	0/2/19/22	0/1/1/1
3	GLC	CfC	6	3	-	2/2/19/22	0/1/1/1
3	GLC	CfC	7	3	-	0/2/19/22	0/1/1/1
3	GLC	CfC	8	3	-	0/2/19/22	0/1/1/1
3	GLC	CfC	9	3	-	0/2/19/22	0/1/1/1
4	GLC	CqC	1	4	-	1/2/19/22	0/1/1/1
4	GLC	CqC	2	4	-	0/2/19/22	0/1/1/1
4	GLC	CqC	3	4	-	2/2/19/22	0/1/1/1
5	GLC	CtC	1	5	-	0/2/19/22	0/1/1/1
5	GLC	CtC	2	5	-	0/2/19/22	0/1/1/1
5	GLC	CtC	3	5	-	0/2/19/22	0/1/1/1
5	GLC	CtC	4	5	-	1/2/19/22	0/1/1/1
4	GLC	CxC	1	4	-	2/2/19/22	0/1/1/1
4	GLC	CxC	2	4	-	2/2/19/22	0/1/1/1
4	GLC	CxC	3	4	-	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)
3	CfC	4	GLC	C2-C3	-3.05	1.47	1.52
2	CCC	1	GLC	C2-C3	2.90	1.56	1.52
3	CfC	7	GLC	C2-C3	2.30	1.56	1.52
3	CfC	1	GLC	C1-C2	2.13	1.57	1.52
3	CfC	5	GLC	O2-C2	-2.03	1.39	1.43

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	6	GLC	C1-O5-C5	7.17	121.79	112.19
5	CtC	4	GLC	C1-O5-C5	6.90	121.44	112.19
3	CfC	11	GLC	O2-C2-C3	-5.40	98.97	110.15
3	CfC	11	GLC	C1-O5-C5	4.88	118.73	112.19
3	CfC	1	GLC	O5-C5-C4	4.52	117.85	109.70

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

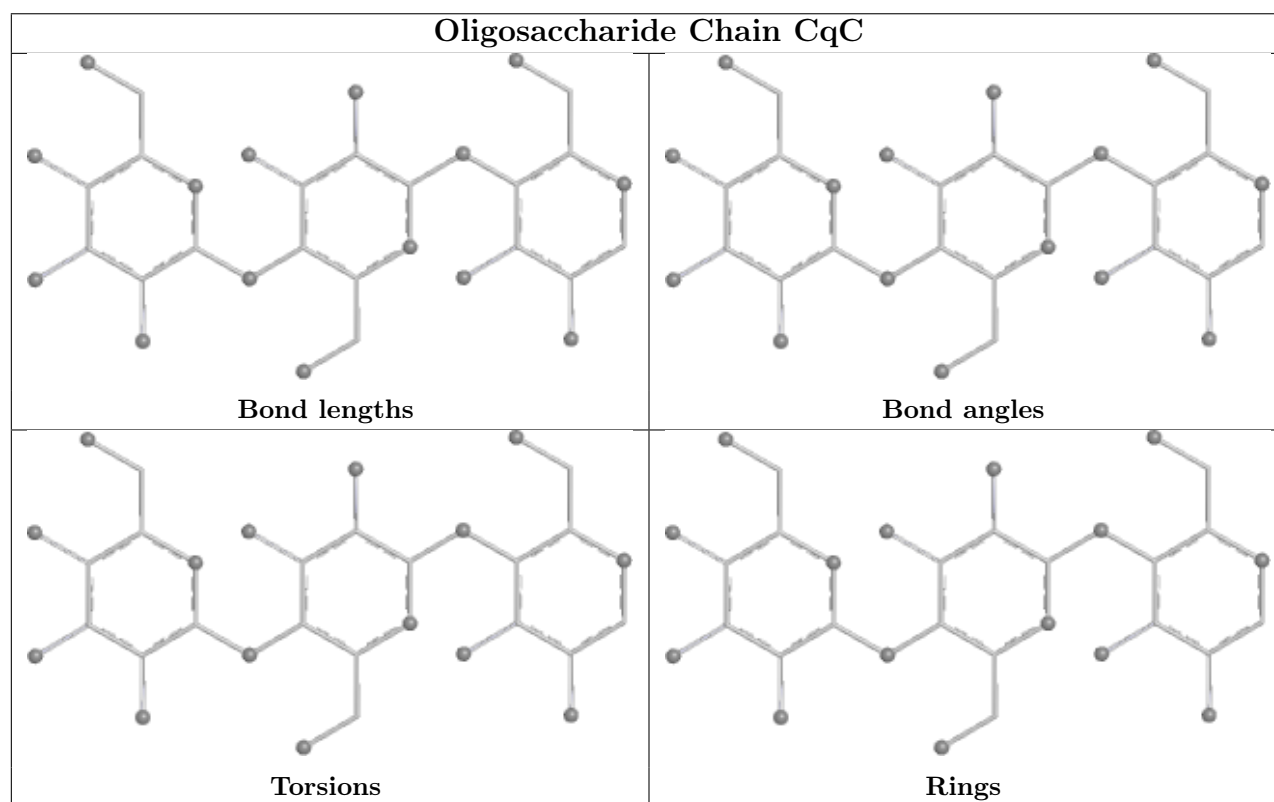
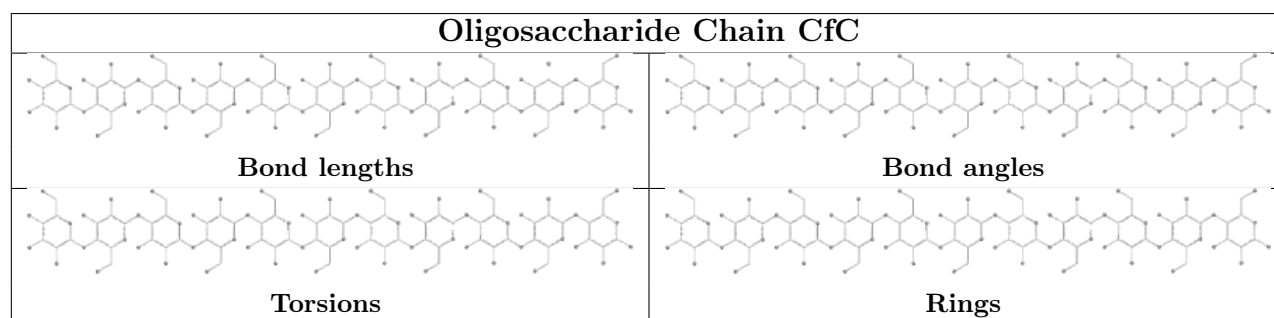
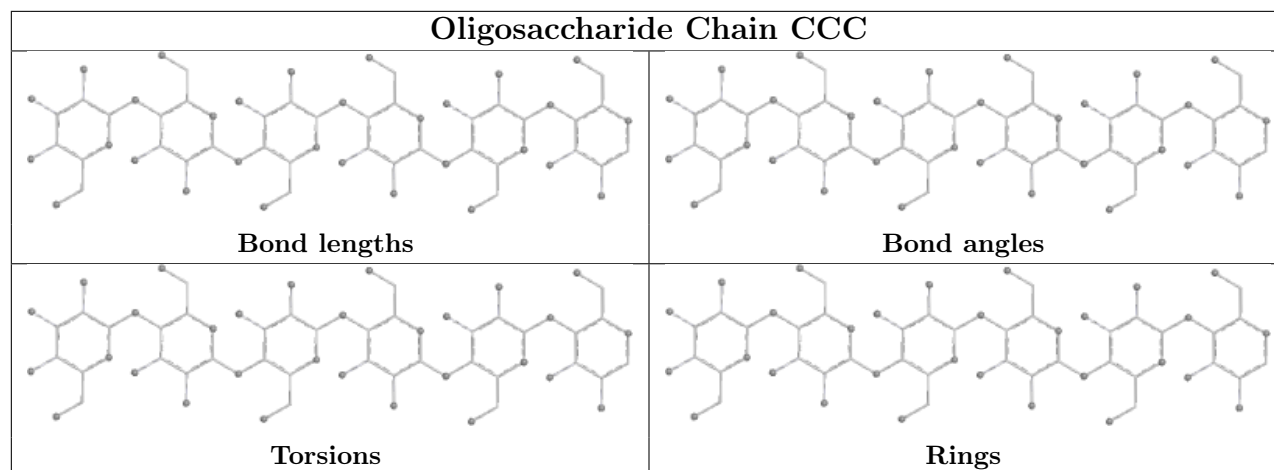
Mol	Chain	Res	Type	Atoms
4	CxC	2	GLC	O5-C5-C6-O6
4	CxC	1	GLC	C4-C5-C6-O6
2	CCC	5	GLC	O5-C5-C6-O6
3	CfC	6	GLC	O5-C5-C6-O6
4	CxC	2	GLC	C4-C5-C6-O6

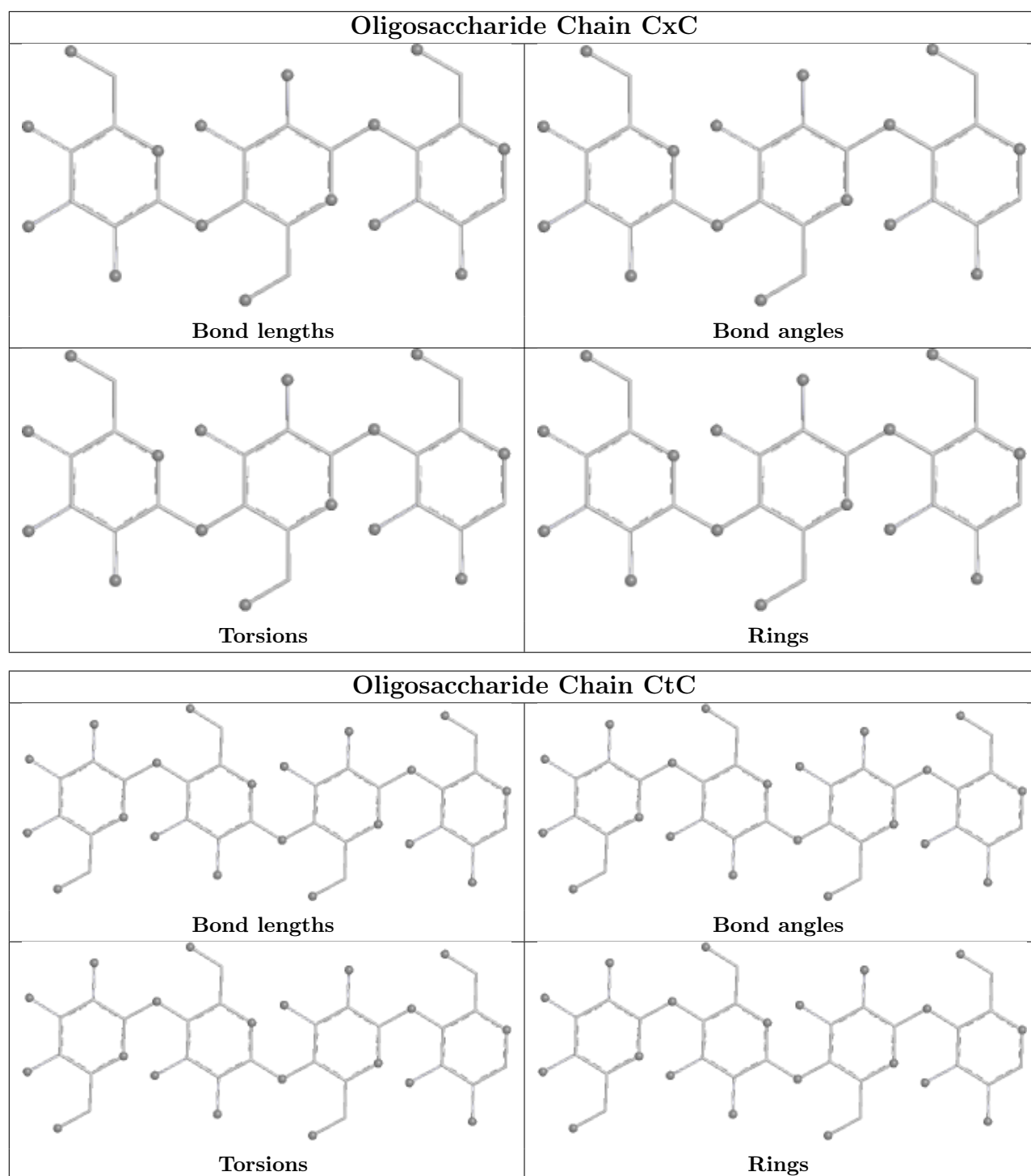
There are no ring outliers.

7 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CqC	3	GLC	1	0
3	CfC	5	GLC	1	0
3	CfC	3	GLC	1	0
3	CfC	2	GLC	1	0
4	CqC	1	GLC	1	0
4	CqC	2	GLC	1	0
3	CfC	4	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 ⓘ

There are no ligands in this entry.

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 [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	AAA	812/855 (94%)	-0.41	7 (0%) 81 80	29, 43, 69, 116	0
1	BBB	812/855 (94%)	-0.03	21 (2%) 57 54	36, 58, 91, 133	0
All	All	1624/1710 (94%)	-0.22	28 (1%) 69 67	29, 51, 82, 133	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	204	VAL	3.9
1	AAA	587	LEU	3.4
1	BBB	409	PHE	3.4
1	BBB	360	LYS	3.3
1	BBB	589	ILE	3.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	BBB	671	24/25	0.96	0.10	45,52,57,59	0
1	LLP	AAA	671	24/25	0.98	0.06	36,41,46,47	0

6.3 Carbohydrates [i](#)

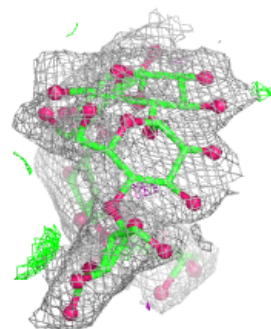
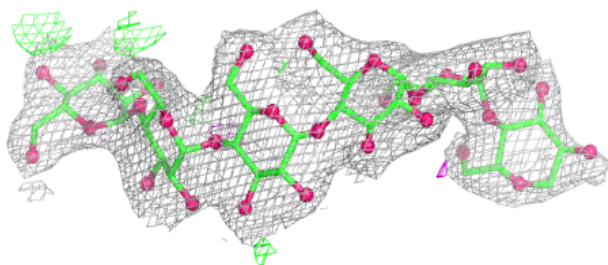
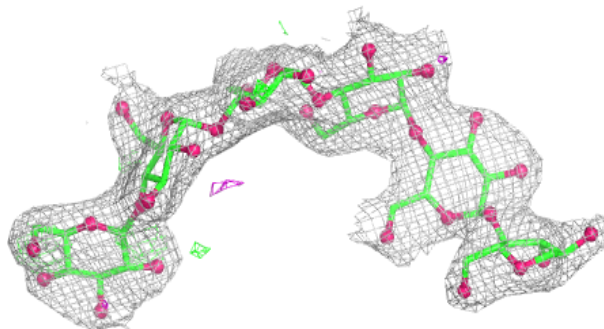
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	CCC	1	11/12	-	-	67,74,83,85	0
2	GLC	CCC	2	11/12	-	-	46,54,59,61	0
2	GLC	CCC	3	11/12	-	-	33,43,50,51	0
2	GLC	CCC	4	11/12	-	-	41,48,51,52	0
2	GLC	CCC	5	11/12	-	-	41,48,49,51	0
2	GLC	CCC	6	11/12	-	-	44,48,55,61	0
3	GLC	CfC	1	12/12	-	-	38,42,45,45	0
3	GLC	CfC	2	11/12	-	-	31,36,39,46	0
3	GLC	CfC	3	11/12	-	-	26,31,36,37	0
3	GLC	CfC	4	11/12	-	-	29,32,36,37	0
3	GLC	CfC	5	11/12	-	-	30,31,35,41	0
3	GLC	CfC	6	11/12	-	-	30,35,38,38	0
3	GLC	CfC	7	11/12	-	-	26,31,34,38	0
3	GLC	CfC	8	11/12	-	-	28,31,33,35	0
3	GLC	CfC	9	11/12	-	-	27,31,32,32	0
3	GLC	CfC	10	11/12	-	-	30,31,33,36	0
3	GLC	CfC	11	11/12	-	-	28,30,35,36	0
4	GLC	CqC	1	11/12	-	-	81,93,101,102	0
4	GLC	CqC	2	11/12	-	-	59,68,77,79	0
4	GLC	CqC	3	11/12	-	-	79,91,97,99	0
4	GLC	CxC	1	11/12	-	-	57,79,90,90	0
4	GLC	CxC	2	11/12	-	-	53,65,70,73	0
4	GLC	CxC	3	11/12	-	-	58,66,72,72	0
5	GLC	CtC	1	11/12	-	-	76,86,92,94	0
5	GLC	CtC	2	11/12	-	-	66,72,74,76	0
5	GLC	CtC	3	11/12	-	-	74,78,83,90	0
5	GLC	CtC	4	11/12	-	-	82,95,103,104	0

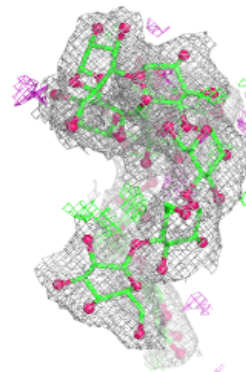
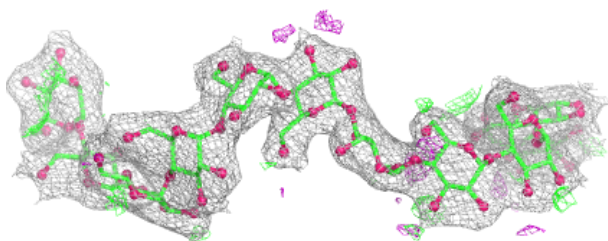
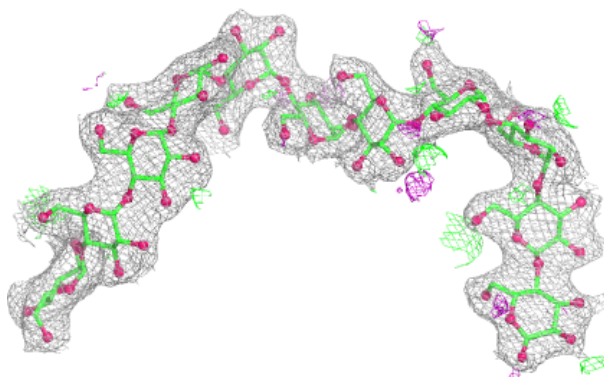
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain CCC:

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

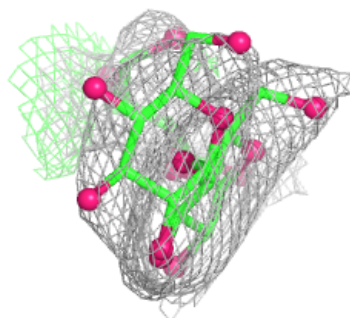
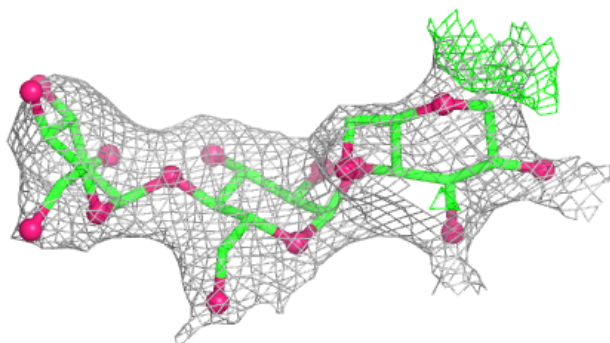
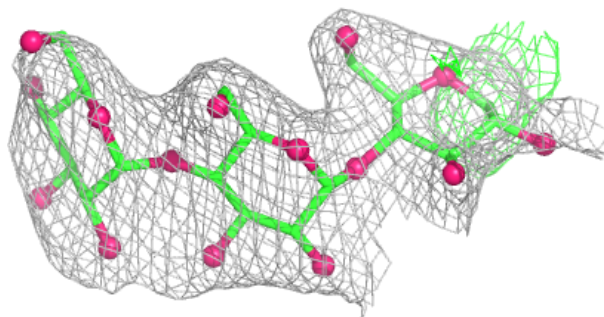
**Electron density around Chain CfC:**

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

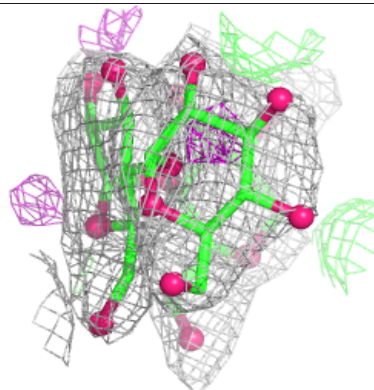
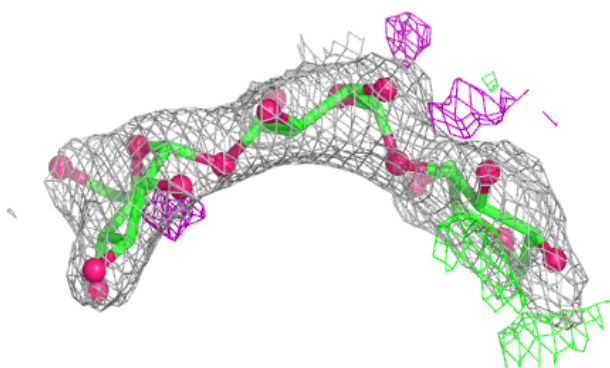
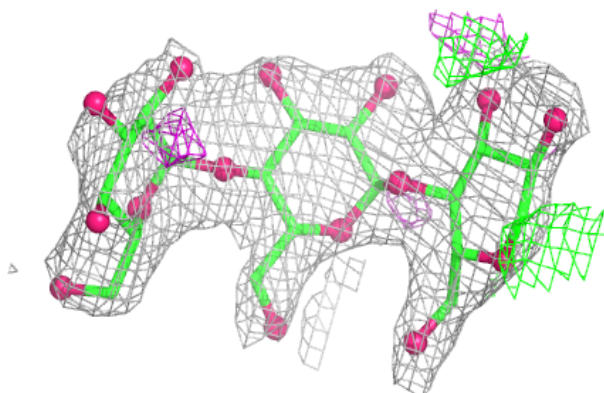


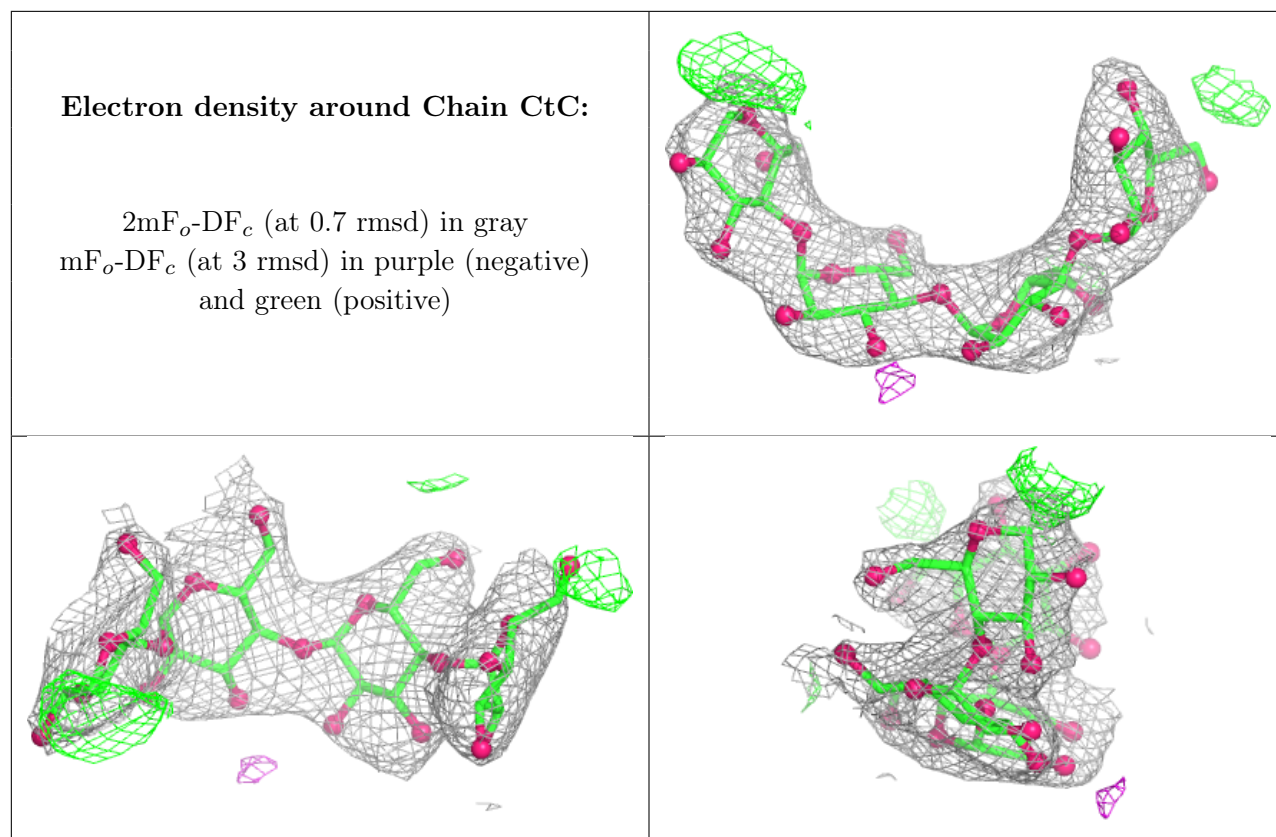
Electron density around Chain CqC:

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

**Electron density around Chain CxC:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.