



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 10:09 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

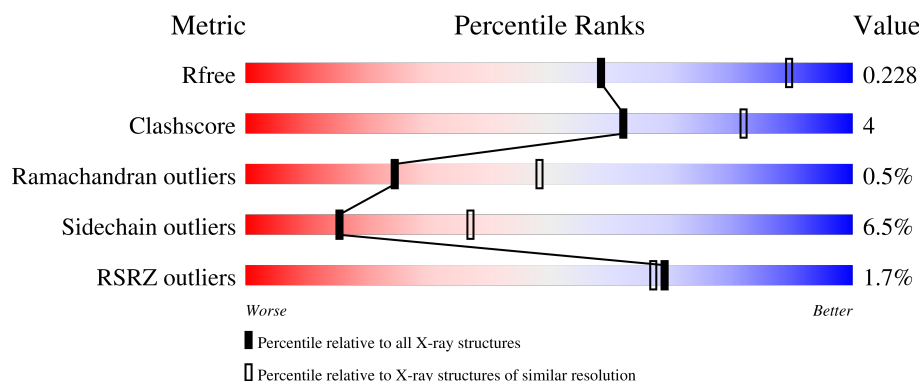
# 1 Overall quality at a glance

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  $\geq 3$ , 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>81%</div> <div>13%</div> <div>• 5%</div> </div>
1	BBB	855	<div> <div>2%</div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>
2	CCC	6	<div> <div>100%</div> </div>
3	CfC	11	<div> <div>9%</div> <div>73%</div> <div>18%</div> </div>
4	CqC	3	<div> <div>33%</div> <div>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			

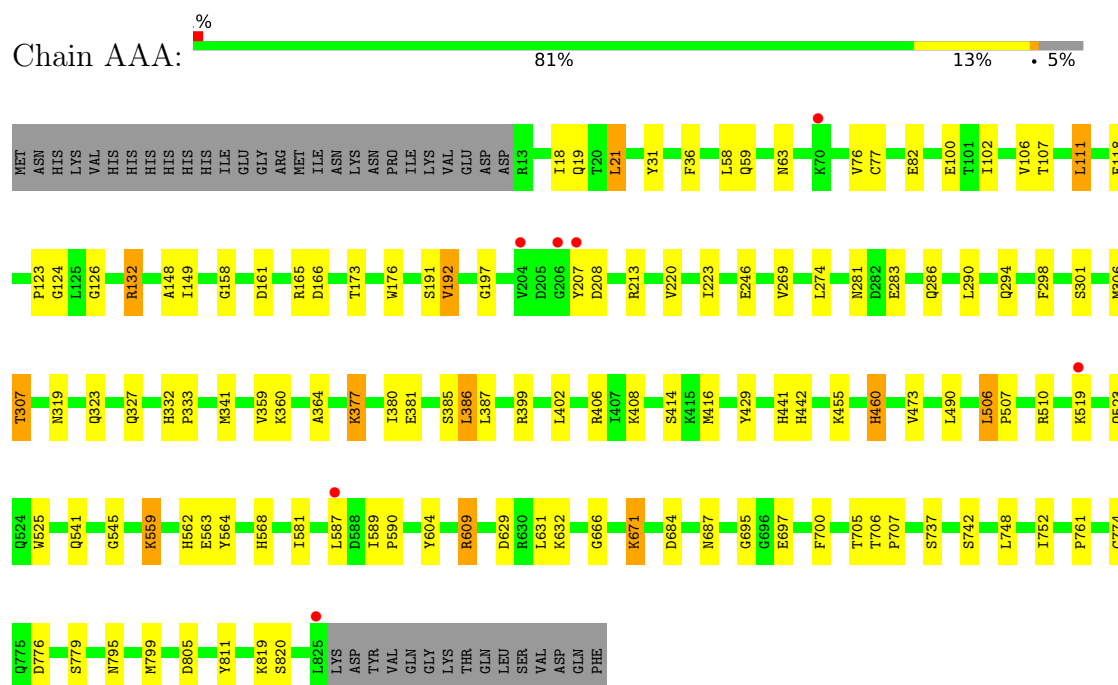
- Molecule 6 is water.

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

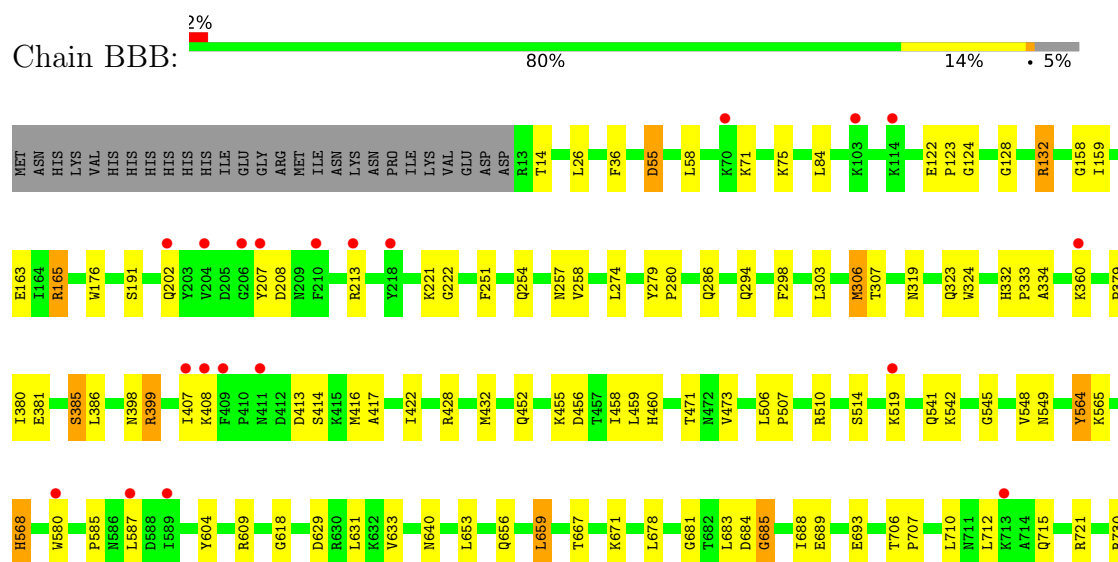
### 3 Residue-property plots [i](#)

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



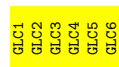
- Molecule 1: Alpha-1,4 glucan phosphorylase





- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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

All (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
1	AAA	269	VAL	CA-C-N	6.26	128.58	120.44
1	AAA	269	VAL	C-N-CA	6.26	128.58	120.44
1	BBB	306	MET	CA-C-N	6.23	128.96	120.54
1	BBB	306	MET	C-N-CA	6.23	128.96	120.54
1	BBB	159	ILE	CA-C-O	-5.76	115.80	120.70
1	BBB	737	SER	CA-C-N	5.69	128.47	120.28
1	BBB	737	SER	C-N-CA	5.69	128.47	120.28
1	BBB	36	PHE	CB-CA-C	5.54	117.08	108.61
1	AAA	307	THR	CB-CA-C	5.48	119.57	110.81
1	BBB	568	HIS	CA-CB-CG	5.47	119.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	805	ASP	CA-CB-CG	5.45	118.05	112.60
1	BBB	159	ILE	CB-CA-C	5.28	116.20	111.71
1	BBB	379	PRO	CA-C-N	5.27	127.21	120.56
1	BBB	379	PRO	C-N-CA	5.27	127.21	120.56
1	AAA	697	GLU	CB-CG-CD	5.26	121.54	112.60
1	AAA	306	MET	CA-C-N	5.22	127.59	120.54
1	AAA	306	MET	C-N-CA	5.22	127.59	120.54
1	BBB	667	THR	CB-CA-C	5.09	117.07	109.13
1	AAA	166	ASP	CB-CA-C	5.05	118.50	111.63
1	BBB	55	ASP	CA-CB-CG	5.04	117.64	112.60
1	AAA	36	PHE	CB-CA-C	5.02	116.59	108.91

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.

All (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
1:AAA:441:HIS:CD2	1:AAA:442:HIS:HD2	2.03	0.70
1:AAA:192:VAL:HG11	1:AAA:301:SER:HA	1.75	0.68
1:AAA:705:THR:HG22	1:AAA:707:PRO:HD2	1.76	0.68
1:AAA:705:THR:CG2	1:AAA:707:PRO:HD2	2.26	0.65
1:AAA:319:ASN:HD22	1:AAA:323:GLN:NE2	1.94	0.63
1:BBB:455:LYS:O	1:BBB:460:HIS:HA	2.00	0.62
1:AAA:123:PRO:HA	1:AAA:176:TRP:CE3	2.35	0.61
1:BBB:452:GLN:NE2	1:BBB:456:ASP:OD1	2.34	0.61
1:AAA:274:LEU:O	1:AAA:294:GLN:HG3	2.01	0.61
1:AAA:197:GLY:HA2	1:AAA:385:SER:O	2.02	0.59
1:BBB:303:LEU:HD23	1:BBB:306:MET:HE1	1.85	0.58
1:BBB:165:ARG:HH11	1:BBB:165:ARG:HG2	1.68	0.57
1:BBB:303:LEU:HD23	1:BBB:306:MET:HE3	1.87	0.56
1:AAA:59:GLN:O	1:AAA:63:ASN:ND2	2.33	0.55
1:BBB:132:ARG:O	1:BBB:132:ARG:HD3	2.07	0.55
1:AAA:319:ASN:HD21	1:AAA:323:GLN:HE22	1.53	0.54
1:BBB:399:ARG:HD3	4:CqC:3:GLC:H62	1.90	0.54
1:AAA:377:LYS:HB2	1:AAA:429:TYR:HB3	1.89	0.54
1:BBB:123:PRO:HA	1:BBB:176:TRP:CE3	2.43	0.53
1:AAA:581:ILE:HD11	1:AAA:589:ILE:HD11	1.89	0.53
1:BBB:659:LEU:HG	1:BBB:762:TYR:O	2.09	0.53
1:BBB:671:LLP:O3	1:BBB:671:LLP:NZ	2.40	0.53
1:AAA:406:ARG:HE	1:AAA:416:MET:HE2	1.75	0.52
1:BBB:122:GLU:CD	1:BBB:640:ASN:HB2	2.35	0.51
1:BBB:279:TYR:N	1:BBB:280:PRO:HD3	2.26	0.51
1:BBB:712:LEU:HD12	1:BBB:712:LEU:O	2.11	0.51
1:BBB:506:LEU:N	1:BBB:507:PRO:CD	2.74	0.50
1:BBB:319:ASN:ND2	1:BBB:323:GLN:NE2	2.60	0.50
1:AAA:31:TYR:HB3	1:BBB:55:ASP:OD1	2.12	0.50
1:AAA:319:ASN:HD22	1:AAA:323:GLN:HE21	1.59	0.49
1:AAA:609:ARG:HB3	1:AAA:752:ILE:HD11	1.94	0.49
1:AAA:332:HIS:N	1:AAA:333:PRO:CD	2.75	0.49
1:BBB:165:ARG:HG2	1:BBB:165:ARG:NH1	2.27	0.48
1:AAA:706:THR:HB	1:AAA:707:PRO:HD3	1.96	0.48
3:CfC:2:GLC:H62	3:CfC:3:GLC:H5	1.96	0.48
1:AAA:281:ASN:HB2	1:BBB:257:ASN:ND2	2.29	0.47
1:BBB:565:LYS:NZ	1:BBB:671:LLP:OP1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:381:GLU:O	1:BBB:385:SER:HB2	2.15	0.47
1:AAA:684:ASP:O	1:AAA:687:ASN:HB2	2.14	0.47
1:BBB:303:LEU:HA	1:BBB:306:MET:CE	2.45	0.47
1:AAA:341:MET:HG2	1:AAA:359:VAL:HG21	1.96	0.46
1:AAA:21:LEU:HG	1:AAA:102:ILE:HD13	1.97	0.46
1:BBB:332:HIS:HB2	1:BBB:333:PRO:HD3	1.97	0.46
1:BBB:683:LEU:HG	1:BBB:688:ILE:HG12	1.98	0.46
1:BBB:380:ILE:HD11	1:BBB:422:ILE:HD12	1.98	0.46
1:AAA:506:LEU:N	1:AAA:507:PRO:CD	2.79	0.46
1:BBB:163:GLU:OE2	1:BBB:165:ARG:NE	2.44	0.46
1:BBB:458:ILE:HG23	1:BBB:459:LEU:HG	1.98	0.46
1:AAA:290:LEU:O	1:AAA:294:GLN:HB2	2.16	0.45
1:BBB:473:VAL:HG11	1:BBB:811:TYR:CE2	2.51	0.45
1:BBB:618:GLY:HA2	1:BBB:633:VAL:HB	1.98	0.45
1:AAA:124:GLY:O	1:AAA:158:GLY:HA2	2.17	0.45
1:BBB:84:LEU:HD12	1:BBB:84:LEU:HA	1.89	0.45
1:BBB:274:LEU:O	1:BBB:294:GLN:NE2	2.45	0.45
1:BBB:653:LEU:HA	1:BBB:678:LEU:O	2.17	0.45
1:BBB:506:LEU:N	1:BBB:507:PRO:HD2	2.31	0.44
1:AAA:106:VAL:HG13	1:AAA:111:LEU:HB2	2.00	0.44
1:AAA:77:CYS:HA	1:AAA:149:ILE:O	2.18	0.44
1:AAA:455:LYS:O	1:AAA:460:HIS:HA	2.18	0.44
1:BBB:689:GLU:O	1:BBB:693:GLU:HG2	2.18	0.44
1:AAA:541:GLN:O	1:AAA:545:GLY:HA2	2.18	0.44
1:BBB:191:SER:HA	1:BBB:222:GLY:O	2.18	0.44
1:AAA:705:THR:HG22	1:AAA:707:PRO:CD	2.46	0.43
1:BBB:124:GLY:O	1:BBB:158:GLY:HA2	2.18	0.43
1:BBB:706:THR:HB	1:BBB:707:PRO:HD3	2.00	0.43
1:AAA:82:GLU:HB2	1:AAA:126:GLY:HA2	1.99	0.43
1:BBB:165:ARG:HH11	1:BBB:165:ARG:CG	2.29	0.43
1:BBB:279:TYR:N	1:BBB:280:PRO:CD	2.82	0.43
1:BBB:334:ALA:HB3	1:BBB:432:MET:HE3	2.01	0.43
1:BBB:398:ASN:HB3	4:CqC:2:GLC:O6	2.19	0.43
1:AAA:402:LEU:HB3	1:AAA:416:MET:HE1	2.01	0.43
1:BBB:306:MET:HG2	1:BBB:324:TRP:CZ3	2.53	0.43
1:BBB:795:ASN:O	1:BBB:799:MET:HG2	2.19	0.43
1:AAA:386:LEU:HB3	1:AAA:387:LEU:HG	2.01	0.43
1:BBB:417:ALA:HA	4:CqC:1:GLC:O2	2.18	0.43
3:CfC:4:GLC:H61	3:CfC:5:GLC:H5	2.01	0.43
1:BBB:319:ASN:OD1	1:BBB:319:ASN:N	2.52	0.43
1:AAA:473:VAL:HG11	1:AAA:811:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:564:TYR:C	1:BBB:564:TYR:CD1	2.97	0.43
1:AAA:795:ASN:O	1:AAA:799:MET:HG2	2.18	0.42
1:AAA:18:ILE:HD12	1:AAA:18:ILE:N	2.34	0.42
1:BBB:656:GLN:O	1:BBB:681:GLY:HA2	2.18	0.42
1:AAA:776:ASP:O	1:AAA:779:SER:HB2	2.20	0.42
1:AAA:490:LEU:HD11	1:AAA:525:TRP:CZ3	2.55	0.42
1:AAA:562:HIS:O	1:AAA:563:GLU:C	2.63	0.42
1:AAA:132:ARG:HG3	1:AAA:671:LLP:NZ	2.35	0.42
1:AAA:589:ILE:HD12	1:AAA:590:PRO:O	2.20	0.42
1:AAA:506:LEU:HD23	1:AAA:506:LEU:HA	1.84	0.42
1:BBB:750:GLN:N	1:BBB:751:PRO:CD	2.83	0.42
1:BBB:319:ASN:ND2	1:BBB:323:GLN:HE22	2.18	0.41
1:BBB:811:TYR:HB3	1:BBB:816:TRP:CE3	2.56	0.41
1:BBB:811:TYR:HB3	1:BBB:816:TRP:CZ3	2.56	0.41
1:AAA:327:GLN:OE1	1:AAA:364:ALA:HB3	2.21	0.41
1:AAA:490:LEU:HD11	1:AAA:525:TRP:CH2	2.55	0.41
1:BBB:541:GLN:O	1:BBB:545:GLY:HA2	2.20	0.41
1:BBB:794:LEU:O	1:BBB:798:ARG:HG3	2.21	0.41
1:AAA:700:PHE:HB3	1:AAA:774:CYS:SG	2.61	0.41
1:BBB:473:VAL:HG11	1:BBB:811:TYR:CD2	2.55	0.41
1:AAA:76:VAL:O	1:AAA:148:ALA:HA	2.20	0.40
1:BBB:801:LYS:O	1:BBB:801:LYS:HG2	2.19	0.40
1:BBB:684:ASP:O	1:BBB:685:GLY:C	2.64	0.40
1:AAA:386:LEU:HD23	1:AAA:386:LEU:HA	1.94	0.40
1:AAA:173:THR:OG1	1:BBB:251:PHE:O	2.36	0.40
1:AAA:223:ILE:HD13	1:AAA:246:GLU:CD	2.47	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	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
All	All	1620/1710 (95%)	1551 (96%)	61 (4%)	8 (0%)	24	48

All (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
1	BBB	685	GLY
1	AAA	559	LYS
1	BBB	585	PRO

### 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

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	19	GLN
1	AAA	21	LEU
1	AAA	58	LEU
1	AAA	107	THR
1	AAA	111	LEU
1	AAA	118	GLU
1	AAA	132	ARG
1	AAA	161	ASP

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Mol	Chain	Res	Type
1	AAA	165	ARG
1	AAA	191	SER
1	AAA	192	VAL
1	AAA	213	ARG
1	AAA	220	VAL
1	AAA	283	GLU
1	AAA	286	GLN
1	AAA	298	PHE
1	AAA	307	THR
1	AAA	360	LYS
1	AAA	377	LYS
1	AAA	380	ILE
1	AAA	381	GLU
1	AAA	386	LEU
1	AAA	399	ARG
1	AAA	408	LYS
1	AAA	414	SER
1	AAA	506	LEU
1	AAA	510	ARG
1	AAA	519	LYS
1	AAA	523	GLN
1	AAA	559	LYS
1	AAA	564	TYR
1	AAA	568	HIS
1	AAA	587	LEU
1	AAA	604	TYR
1	AAA	609	ARG
1	AAA	629	ASP
1	AAA	631	LEU
1	AAA	632	LYS
1	AAA	737	SER
1	AAA	742	SER
1	AAA	748	LEU
1	AAA	819	LYS
1	AAA	820	SER
1	BBB	14	THR
1	BBB	26	LEU
1	BBB	58	LEU
1	BBB	71	LYS
1	BBB	75	LYS
1	BBB	132	ARG
1	BBB	165	ARG

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Mol	Chain	Res	Type
1	BBB	202	GLN
1	BBB	207	TYR
1	BBB	208	ASP
1	BBB	213	ARG
1	BBB	221	LYS
1	BBB	254	GLN
1	BBB	258	VAL
1	BBB	286	GLN
1	BBB	298	PHE
1	BBB	307	THR
1	BBB	360	LYS
1	BBB	385	SER
1	BBB	386	LEU
1	BBB	399	ARG
1	BBB	408	LYS
1	BBB	413	ASP
1	BBB	416	MET
1	BBB	471	THR
1	BBB	510	ARG
1	BBB	514	SER
1	BBB	519	LYS
1	BBB	542	LYS
1	BBB	548	VAL
1	BBB	549	ASN
1	BBB	564	TYR
1	BBB	568	HIS
1	BBB	580	TRP
1	BBB	587	LEU
1	BBB	604	TYR
1	BBB	609	ARG
1	BBB	629	ASP
1	BBB	631	LEU
1	BBB	659	LEU
1	BBB	710	LEU
1	BBB	715	GLN
1	BBB	721	ARG
1	BBB	730	ARG
1	BBB	737	SER
1	BBB	742	SER
1	BBB	769	LYS
1	BBB	794	LEU
1	BBB	819	LYS

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Mol	Chain	Res	Type
1	BBB	820	SER

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 [i](#)

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
2	CCC	2	GLC	C1-O5-C5	4.45	118.15	112.19
2	CCC	1	GLC	C1-C2-C3	4.36	115.99	109.64
4	CxC	2	GLC	O5-C5-C6	4.21	115.86	107.66
4	CxC	1	GLC	C1-O5-C5	4.14	117.73	112.19
3	CfC	1	GLC	C1-O5-C5	4.09	121.57	113.65
3	CfC	5	GLC	O2-C2-C1	-3.93	100.24	109.22
2	CCC	5	GLC	C1-O5-C5	3.82	117.31	112.19
3	CfC	1	GLC	O5-C1-C2	3.82	117.01	110.30
3	CfC	1	GLC	O2-C2-C1	3.64	117.64	109.25
3	CfC	5	GLC	C1-C2-C3	3.56	114.83	109.64
3	CfC	11	GLC	C1-C2-C3	3.45	114.67	109.64
5	CtC	2	GLC	C1-O5-C5	3.43	116.79	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	1	GLC	O2-C2-C1	-3.37	101.50	109.22
5	CtC	1	GLC	O5-C1-C2	-3.31	102.88	110.79
3	CfC	7	GLC	C1-O5-C5	3.20	116.47	112.19
5	CtC	3	GLC	O3-C3-C2	-3.12	103.70	110.05
2	CCC	1	GLC	O3-C3-C4	-3.11	103.04	110.38
5	CtC	1	GLC	O3-C3-C2	3.04	116.26	110.05
3	CfC	10	GLC	O5-C5-C6	-3.00	101.82	107.66
3	CfC	1	GLC	O3-C3-C2	-3.00	103.31	110.38
2	CCC	6	GLC	C1-C2-C3	2.96	113.96	109.64
3	CfC	7	GLC	O5-C1-C2	-2.96	103.73	110.79
4	CqC	1	GLC	O5-C1-C2	-2.89	103.89	110.79
4	CqC	1	GLC	C1-O5-C5	2.87	116.03	112.19
3	CfC	11	GLC	C2-C3-C4	2.84	115.86	110.86
5	CtC	1	GLC	C1-O5-C5	2.80	115.94	112.19
4	CqC	2	GLC	C1-O5-C5	2.77	115.89	112.19
3	CfC	1	GLC	O1-C1-C2	2.72	116.86	108.98
2	CCC	1	GLC	C2-C3-C4	2.69	115.59	110.86
3	CfC	1	GLC	O4-C4-C5	-2.67	102.74	109.32
3	CfC	8	GLC	C3-C4-C5	-2.60	105.52	110.23
2	CCC	4	GLC	C2-C3-C4	-2.56	106.36	110.86
5	CtC	1	GLC	O5-C5-C6	2.55	112.62	107.66
4	CqC	1	GLC	O5-C5-C4	2.54	117.01	110.83
3	CfC	4	GLC	C1-O5-C5	-2.53	108.79	112.19
4	CqC	1	GLC	O3-C3-C2	2.50	115.16	110.05
2	CCC	5	GLC	O5-C5-C6	-2.45	102.89	107.66
2	CCC	2	GLC	O5-C1-C2	-2.43	105.00	110.79
5	CtC	4	GLC	O5-C5-C4	2.42	116.71	110.83
3	CfC	1	GLC	C1-C2-C3	2.34	115.13	110.36
3	CfC	6	GLC	C1-C2-C3	2.33	113.04	109.64
5	CtC	4	GLC	C2-C3-C4	-2.25	106.91	110.86
3	CfC	1	GLC	C3-C4-C5	-2.20	106.23	110.23
3	CfC	11	GLC	O5-C1-C2	2.17	115.96	110.79
3	CfC	10	GLC	C3-C4-C5	-2.16	106.31	110.23
4	CxC	1	GLC	O5-C5-C4	2.13	116.01	110.83
3	CfC	5	GLC	O6-C6-C5	-2.12	104.10	111.33
2	CCC	3	GLC	C6-C5-C4	2.10	118.17	113.02
3	CfC	6	GLC	O5-C5-C6	2.05	111.65	107.66
4	CxC	2	GLC	O3-C3-C2	2.03	114.20	110.05
3	CfC	10	GLC	O2-C2-C3	2.03	114.35	110.15

There are no chirality outliers.

All (12) torsion outliers are listed below:

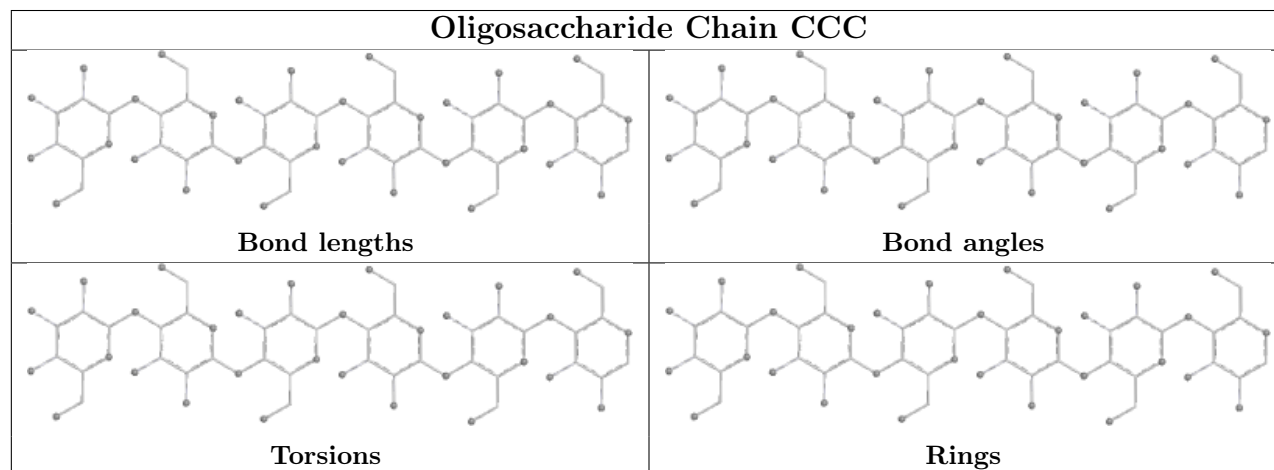
Mol	Chain	Res	Type	Atoms
4	CxC	2	GLC	O5-C5-C6-O6
4	CxC	1	GLC	C4-C5-C6-O6
2	CCC	5	GLC	O5-C5-C6-O6
3	CfC	6	GLC	O5-C5-C6-O6
4	CxC	2	GLC	C4-C5-C6-O6
5	CtC	4	GLC	O5-C5-C6-O6
2	CCC	5	GLC	C4-C5-C6-O6
4	CxC	1	GLC	O5-C5-C6-O6
4	CqC	3	GLC	C4-C5-C6-O6
4	CqC	3	GLC	O5-C5-C6-O6
4	CqC	1	GLC	O5-C5-C6-O6
3	CfC	6	GLC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

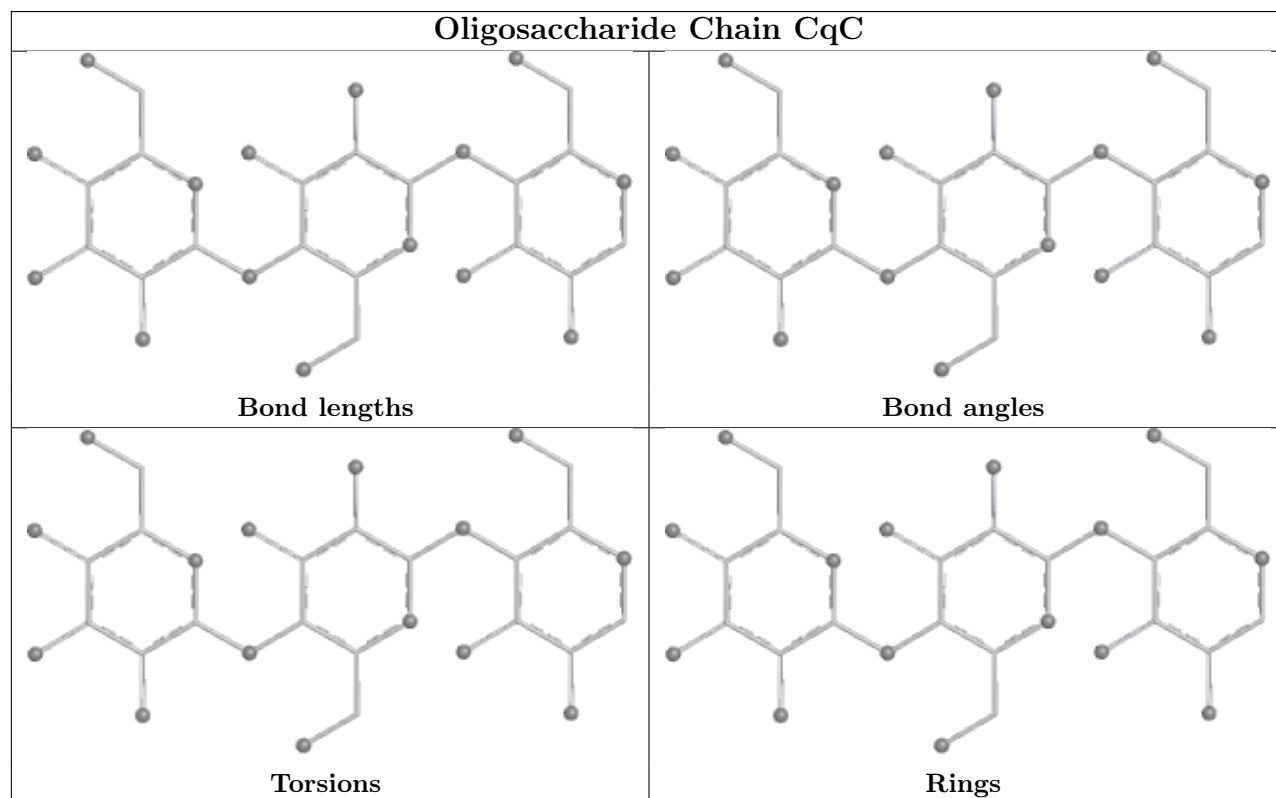
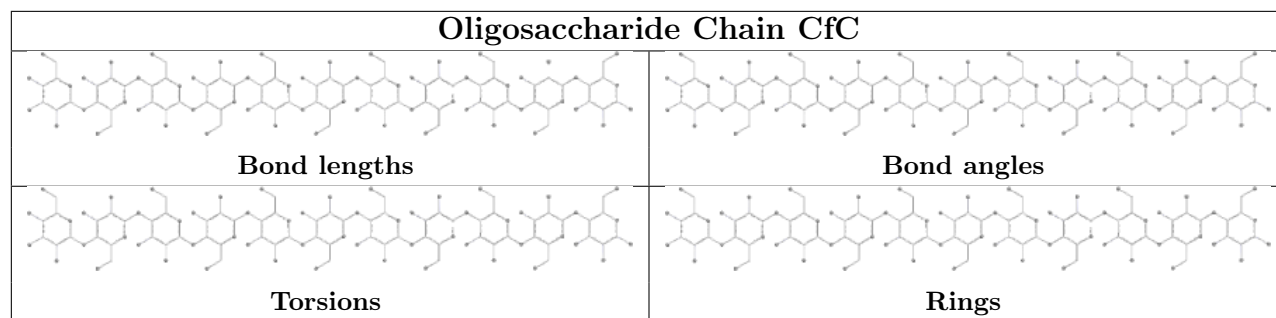
There are no ring outliers.

7 monomers are involved in 5 short contacts:

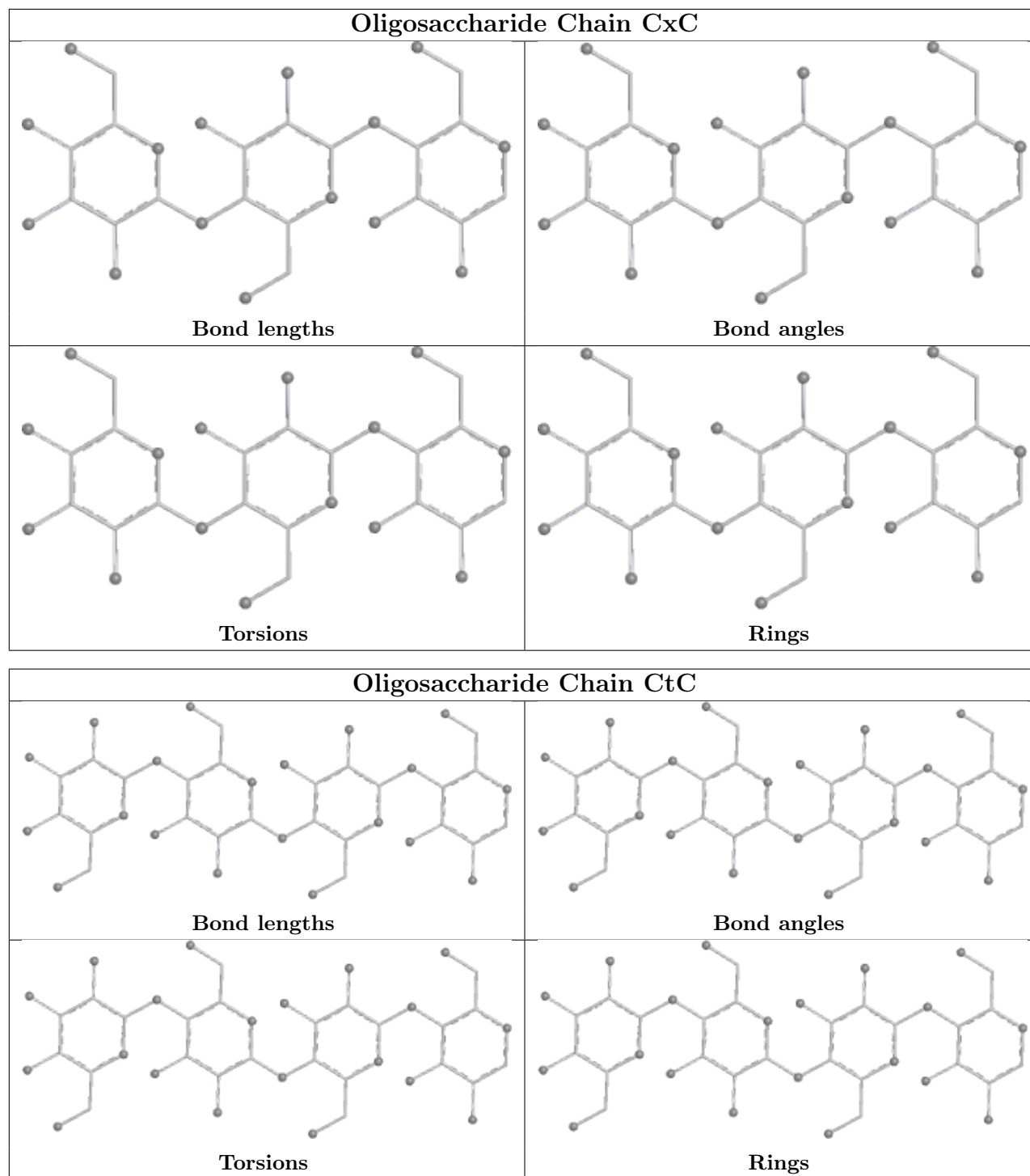
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CqC	3	GLC	1	0
3	CfC	5	GLC	1	0
3	CfC	3	GLC	1	0
3	CfC	2	GLC	1	0
4	CqC	1	GLC	1	0
4	CqC	2	GLC	1	0
3	CfC	4	GLC	1	0

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 [i](#)

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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	AAA	206	GLY	3.2
1	BBB	519	LYS	3.1
1	BBB	587	LEU	3.1
1	BBB	580	TRP	3.0
1	BBB	202	GLN	3.0
1	BBB	207	TYR	2.9
1	BBB	825	LEU	2.9
1	BBB	204	VAL	2.8
1	BBB	103	LYS	2.8
1	BBB	114	LYS	2.8
1	AAA	825	LEU	2.8
1	BBB	218	TYR	2.7
1	BBB	713	LYS	2.6
1	AAA	519	LYS	2.6
1	AAA	70	LYS	2.5
1	BBB	210	PHE	2.4
1	BBB	206	GLY	2.3
1	BBB	213	ARG	2.3
1	BBB	411	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	70	LYS	2.2
1	BBB	407	ILE	2.2
1	AAA	207	TYR	2.1
1	BBB	408	LYS	2.1

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	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, 95<sup>th</sup> 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.

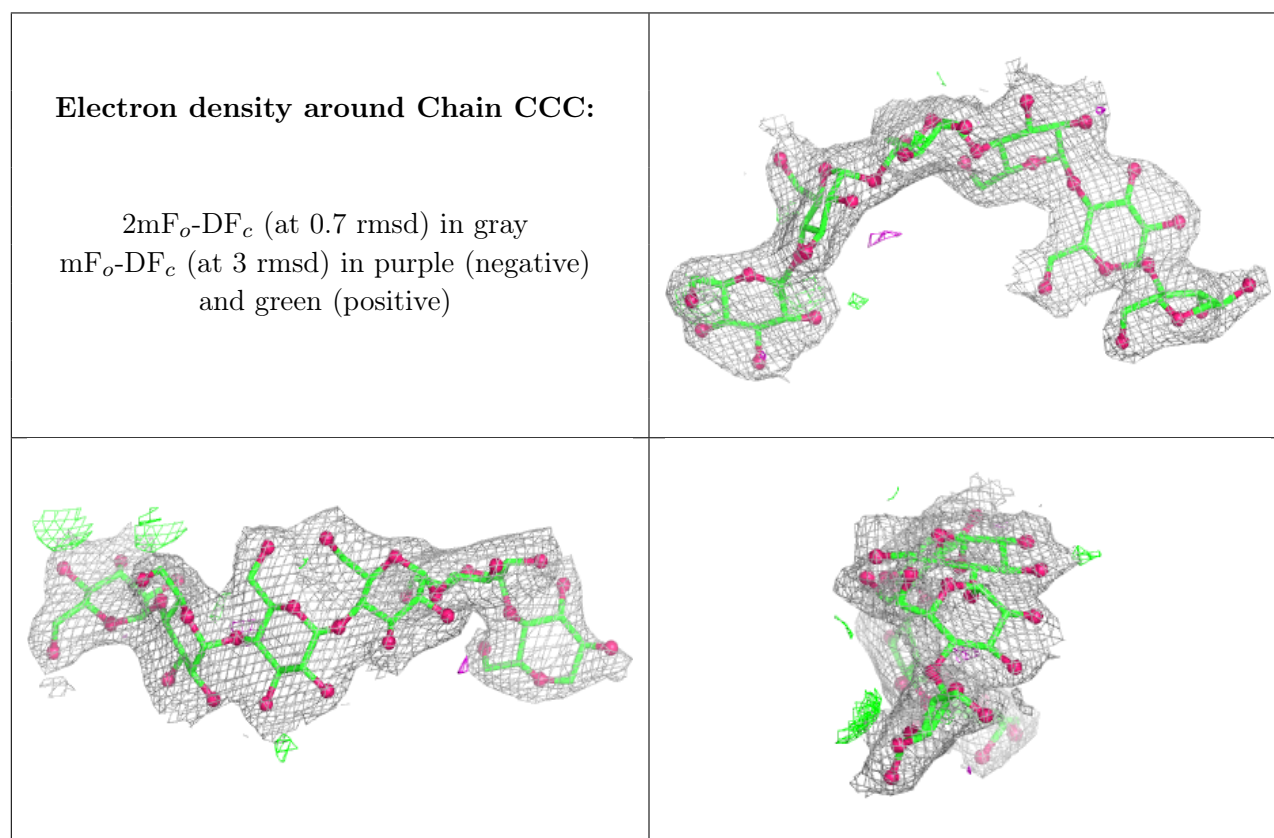
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	CCC	1	11/12	-	-	67,74,83,85	0
2	GLC	CCC	2	11/12	-	-	46,54,59,61	0
2	GLC	CCC	3	11/12	-	-	33,43,50,51	0
2	GLC	CCC	4	11/12	-	-	41,48,51,52	0
2	GLC	CCC	5	11/12	-	-	41,48,49,51	0
2	GLC	CCC	6	11/12	-	-	44,48,55,61	0
3	GLC	CfC	1	12/12	-	-	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

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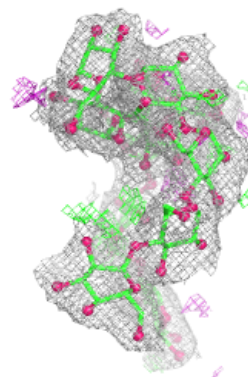
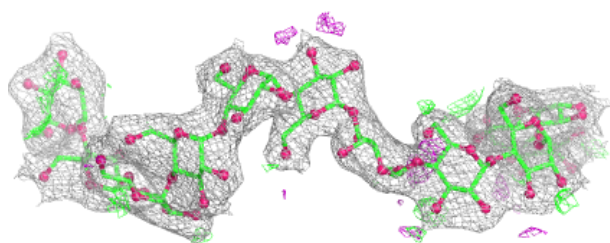
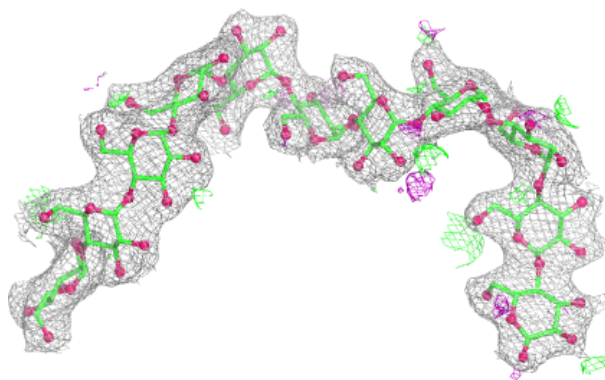
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GLC	CqC	1	11/12	-	-	81,93,101,102	0
4	GLC	CqC	2	11/12	-	-	59,68,77,79	0
4	GLC	CqC	3	11/12	-	-	79,91,97,99	0
4	GLC	CxC	1	11/12	-	-	57,79,90,90	0
4	GLC	CxC	2	11/12	-	-	53,65,70,73	0
4	GLC	CxC	3	11/12	-	-	58,66,72,72	0
5	GLC	CtC	1	11/12	-	-	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.

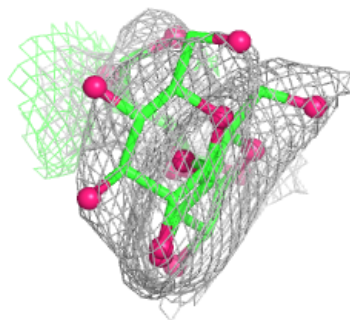
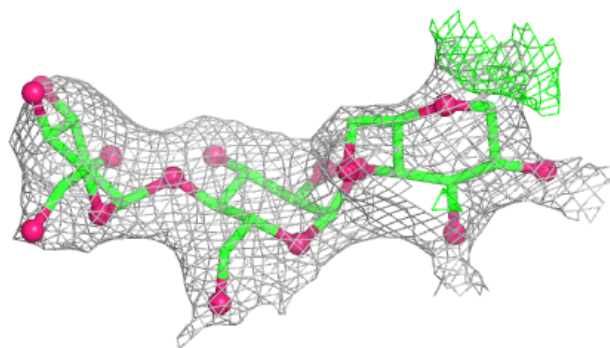
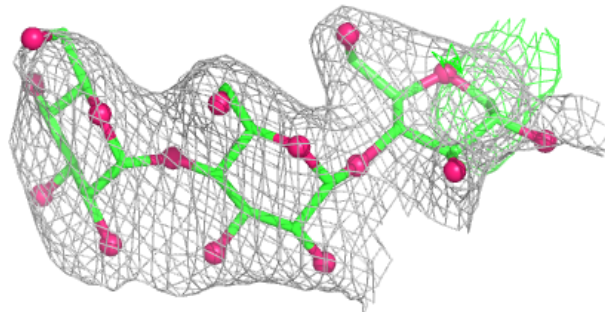


**Electron density around Chain CfC:**

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

**Electron density around Chain CqC:**

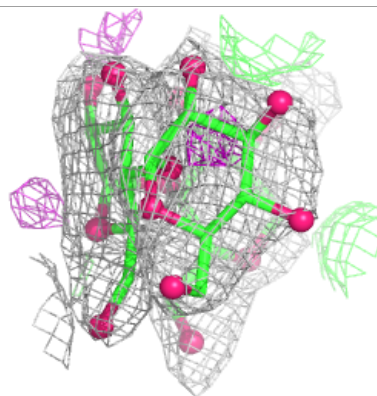
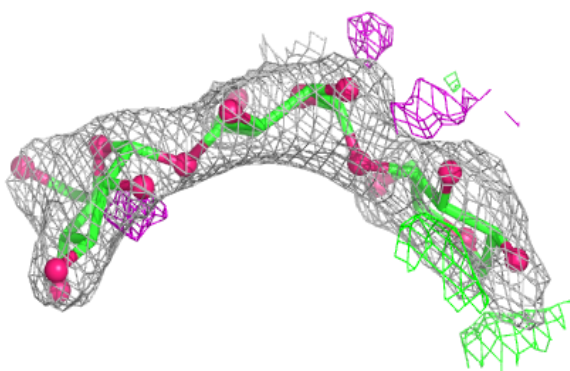
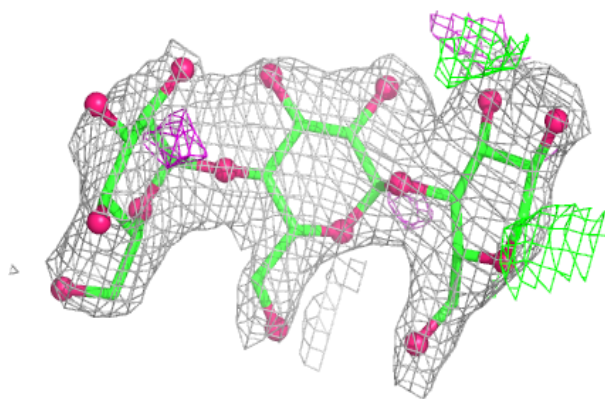
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



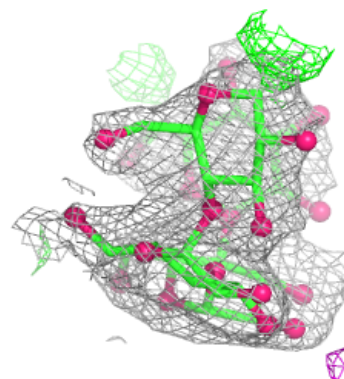
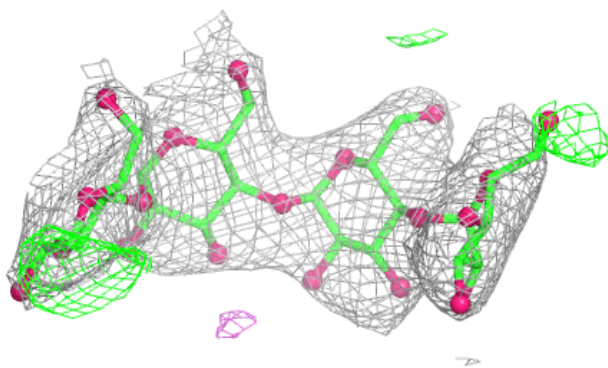
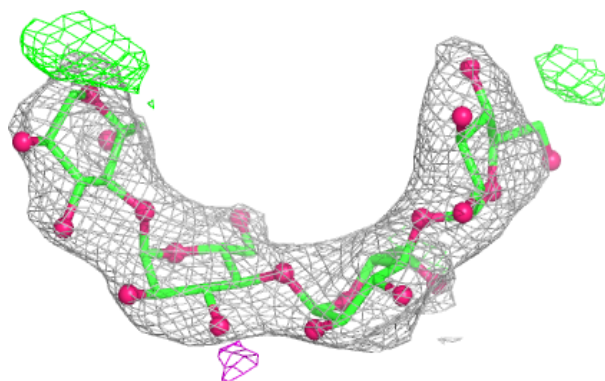


**Electron density around Chain CxC:**

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

**Electron density around Chain CtC:**

$2mF_o-DF_c$  (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.