



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:34 AM UTC

PDB ID : 5GR1 / pdb_00005gr1
Title : Crystal structure of branching enzyme Y500A/D501A mutant from *Cyanothoe* sp. ATCC 51142 in complex with maltoheptaose
Authors : Suzuki, R.; Suzuki, E.
Deposited on : 2016-08-08
Resolution : 2.50 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

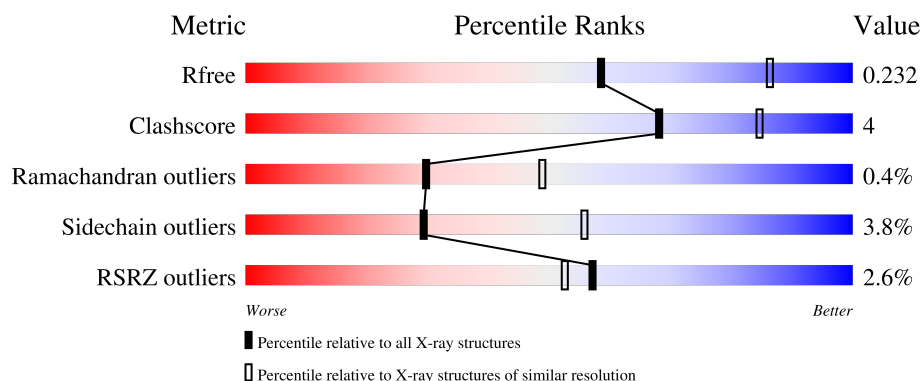
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

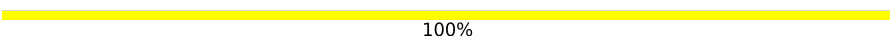
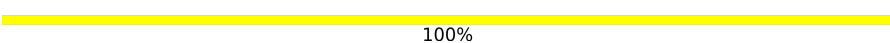
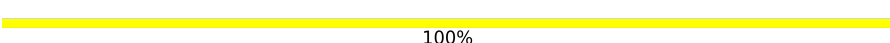
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	793	 3% 82% 12% • 5%
2	B	2	 100%
3	C	3	 67% 33%
3	G	3	 100%
4	D	4	 100%

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Mol	Chain	Length	Quality of chain
4	F	4	 25%75%
5	E	7	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6854 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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	755	Total	C	N	O	S	0	0	0
			6263	4050	1042	1147	24			

There are 22 discrepancies between the modelled and reference sequences:

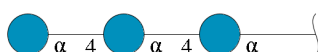
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B1WPM8
A	-18	GLY	-	expression tag	UNP B1WPM8
A	-17	SER	-	expression tag	UNP B1WPM8
A	-16	SER	-	expression tag	UNP B1WPM8
A	-15	HIS	-	expression tag	UNP B1WPM8
A	-14	HIS	-	expression tag	UNP B1WPM8
A	-13	HIS	-	expression tag	UNP B1WPM8
A	-12	HIS	-	expression tag	UNP B1WPM8
A	-11	HIS	-	expression tag	UNP B1WPM8
A	-10	HIS	-	expression tag	UNP B1WPM8
A	-9	SER	-	expression tag	UNP B1WPM8
A	-8	SER	-	expression tag	UNP B1WPM8
A	-7	GLY	-	expression tag	UNP B1WPM8
A	-6	LEU	-	expression tag	UNP B1WPM8
A	-5	VAL	-	expression tag	UNP B1WPM8
A	-4	PRO	-	expression tag	UNP B1WPM8
A	-3	ARG	-	expression tag	UNP B1WPM8
A	-2	GLY	-	expression tag	UNP B1WPM8
A	-1	SER	-	expression tag	UNP B1WPM8
A	0	HIS	-	expression tag	UNP B1WPM8
A	500	ALA	TYR	engineered mutation	UNP B1WPM8
A	501	ALA	ASP	engineered mutation	UNP B1WPM8

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	3	Total	C	O	0	0	0
			34	18	16			
3	G	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 4 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
4	D	4	Total	C	O	0	0	0
			45	24	21			
4	F	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 5 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
5	E	7	Total	C	O	0	0	0
			77	42	35			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Mg	0	0
			2	2		

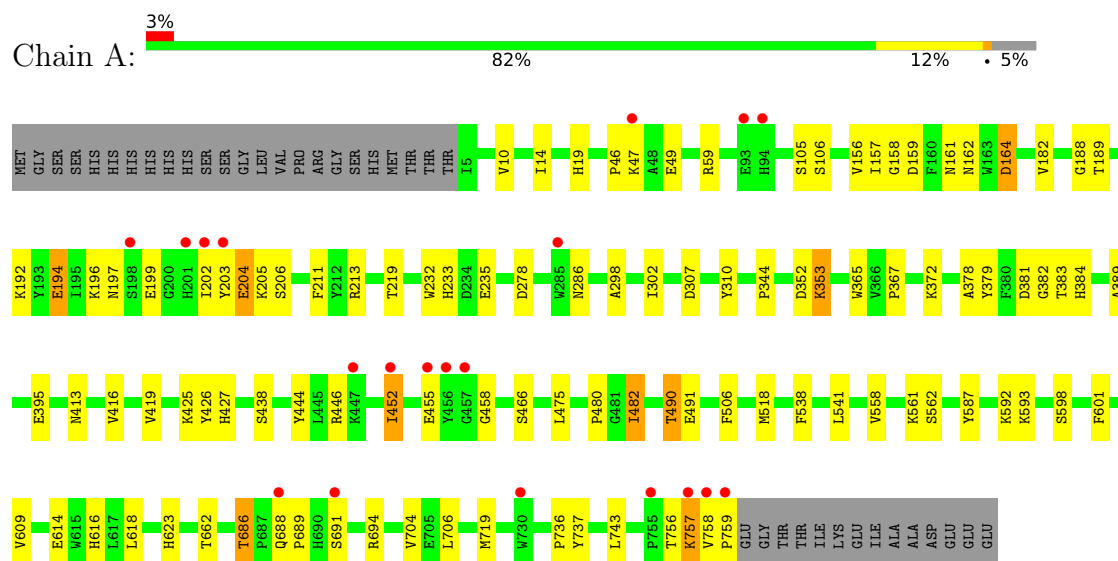
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	320	Total	O	0	0
			320	320		

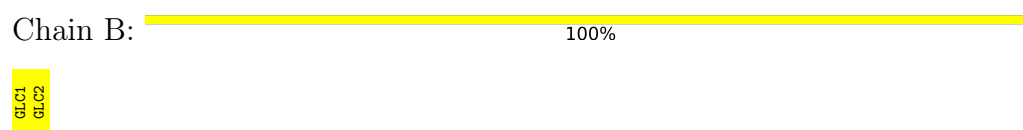
3 Residue-property plots [i](#)

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.

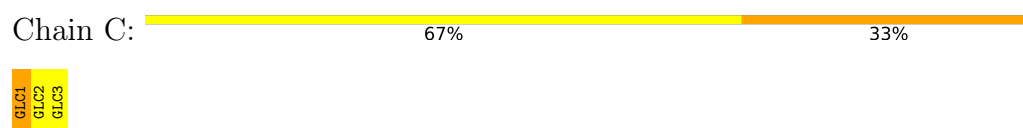
- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



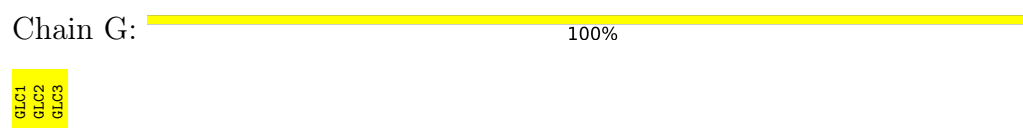
- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



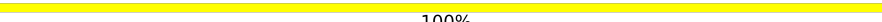
- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



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

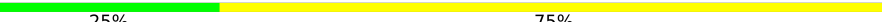


- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  100%

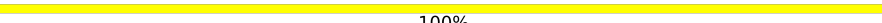
GLC1
GLC2
GLC3
GLC4

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

Chain F:  25% 75%

GLC1
GLC2
GLC3
GLC4

- Molecule 5: 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 E:  100%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.00Å 134.00Å 181.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.38 – 2.50 47.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.38-2.50) 97.3 (47.38-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.42 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.182 , 0.227 0.189 , 0.232	Depositor DCC
R_{free} test set	2873 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.4	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	6854	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GLC, MG

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	1.20	10/6482 (0.2%)	1.13	15/8821 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	758	VAL	CA-C	6.71	1.59	1.52
1	A	686	THR	N-CA	6.50	1.50	1.46
1	A	161	ASN	CA-C	6.16	1.61	1.52
1	A	286	ASN	C-O	-5.79	1.17	1.23
1	A	480	PRO	C-O	5.66	1.30	1.23
1	A	156	VAL	N-CA	-5.62	1.39	1.46
1	A	182	VAL	N-CA	-5.46	1.39	1.46
1	A	458	GLY	N-CA	5.26	1.49	1.44
1	A	182	VAL	CA-C	-5.22	1.47	1.52
1	A	310	TYR	N-CA	5.01	1.52	1.45

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	743	LEU	CA-C-N	-6.30	113.89	120.38
1	A	743	LEU	C-N-CA	-6.30	113.89	120.38
1	A	506	PHE	N-CA-C	-6.12	102.45	110.53
1	A	541	LEU	N-CA-C	5.68	117.47	111.28
1	A	278	ASP	CA-C-N	5.64	125.58	119.78
1	A	278	ASP	C-N-CA	5.64	125.58	119.78
1	A	688	GLN	CA-CB-CG	5.55	125.20	114.10
1	A	425	LYS	N-CA-C	5.51	118.21	111.82
1	A	538	PHE	N-CA-C	5.22	116.98	111.28
1	A	490	THR	CB-CA-C	-5.21	102.30	110.85
1	A	475	LEU	CB-CA-C	-5.18	102.75	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ASP	CB-CA-C	5.14	118.70	110.16
1	A	758	VAL	N-CA-C	5.14	119.98	108.88
1	A	757	LYS	N-CA-C	-5.02	101.45	109.23
1	A	211	PHE	N-CA-C	5.00	119.47	113.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6263	0	5854	46	0
2	B	23	0	21	0	0
3	C	34	0	30	1	0
3	G	33	0	28	0	0
4	D	45	0	39	0	0
4	F	45	0	39	0	0
5	E	77	0	64	0	0
6	A	12	0	16	0	0
7	A	2	0	0	0	0
8	A	320	0	0	3	0
All	All	6854	0	6091	46	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:HD13	1:A:194:GLU:HG3	1.62	0.80
1:A:202:ILE:HG22	1:A:202:ILE:O	1.88	0.71
1:A:452:ILE:H	1:A:452:ILE:HD13	1.58	0.68
1:A:490:THR:O	1:A:491:GLU:HB2	1.99	0.62
1:A:19:HIS:HD2	8:A:1075:HOH:O	1.85	0.59
1:A:46:PRO:O	1:A:47:LYS:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:TYR:HA	1:A:383:THR:O	2.04	0.57
1:A:206:SER:OG	1:A:219:THR:O	2.20	0.56
1:A:298:ALA:HA	1:A:302:ILE:HD12	1.91	0.53
1:A:558:VAL:O	1:A:561:LYS:HG3	2.09	0.53
1:A:614:GLU:OE1	1:A:616:HIS:HE1	1.92	0.53
1:A:192:LYS:HB3	1:A:205:LYS:O	2.11	0.51
1:A:372:LYS:NZ	1:A:395:GLU:OE1	2.39	0.51
1:A:592:LYS:C	1:A:593:LYS:HD3	2.36	0.50
1:A:482:ILE:C	1:A:482:ILE:HD12	2.38	0.48
1:A:756:THR:O	1:A:756:THR:OG1	2.24	0.48
1:A:378:ALA:O	1:A:379:TYR:C	2.56	0.48
1:A:490:THR:O	1:A:491:GLU:CB	2.57	0.48
1:A:601:PHE:O	1:A:623:HIS:HD2	1.98	0.47
1:A:202:ILE:O	1:A:202:ILE:CG2	2.59	0.46
1:A:395:GLU:O	1:A:446:ARG:NH2	2.42	0.46
1:A:203:TYR:OH	1:A:382:GLY:N	2.47	0.46
1:A:344:PRO:HB3	1:A:426:TYR:OH	2.15	0.46
1:A:365:TRP:CZ2	1:A:419:VAL:HB	2.51	0.46
1:A:158:GLY:O	1:A:159:ASP:C	2.58	0.46
1:A:736:PRO:HB2	1:A:737:TYR:CD1	2.51	0.46
1:A:381:ASP:OD1	1:A:383:THR:OG1	2.23	0.45
1:A:233:HIS:HD2	1:A:352:ASP:OD2	1.99	0.45
1:A:587:TYR:HA	1:A:593:LYS:HE3	1.98	0.45
1:A:561:LYS:O	1:A:562:SER:HB2	2.18	0.44
1:A:10:VAL:O	1:A:14:ILE:HG12	2.17	0.44
1:A:188:GLY:O	1:A:189:THR:C	2.60	0.44
1:A:197:ASN:HB2	1:A:382:GLY:HA3	1.99	0.43
1:A:353:LYS:HD2	8:A:1115:HOH:O	2.17	0.43
1:A:757:LYS:O	1:A:759:PRO:HD3	2.19	0.43
1:A:438:SER:HA	1:A:444:TYR:CG	2.54	0.42
1:A:353:LYS:CD	8:A:1115:HOH:O	2.67	0.42
1:A:204:GLU:HG3	3:C:1:GLC:O2	2.20	0.41
1:A:609:VAL:O	1:A:609:VAL:HG22	2.19	0.41
1:A:384:HIS:CD2	1:A:389:ALA:HA	2.56	0.41
1:A:601:PHE:O	1:A:623:HIS:CD2	2.73	0.41
1:A:736:PRO:HB2	1:A:737:TYR:CE1	2.56	0.41
1:A:416:VAL:O	1:A:419:VAL:HG12	2.21	0.41
1:A:689:PRO:CB	1:A:719:MET:HE1	2.50	0.41
1:A:618:LEU:HD23	1:A:618:LEU:HA	1.93	0.40
1:A:232:TRP:CD2	1:A:427:HIS:CE1	3.10	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	753/793 (95%)	715 (95%)	35 (5%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	455	GLU
1	A	162	ASN
1	A	598	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	666/698 (95%)	641 (96%)	25 (4%)	29	56

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLU
1	A	59	ARG
1	A	105	SER
1	A	106	SER
1	A	164	ASP
1	A	194	GLU
1	A	196	LYS
1	A	199	GLU

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Mol	Chain	Res	Type
1	A	204	GLU
1	A	213	ARG
1	A	235	GLU
1	A	307	ASP
1	A	353	LYS
1	A	367	PRO
1	A	413	ASN
1	A	452	ILE
1	A	466	SER
1	A	482	ILE
1	A	518	MET
1	A	662	THR
1	A	686	THR
1	A	691	SER
1	A	694	ARG
1	A	704	VAL
1	A	706	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	86	GLN
1	A	233	HIS
1	A	286	ASN
1	A	616	HIS
1	A	623	HIS
1	A	634	ASN
1	A	639	GLN
1	A	734	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 ⓘ

23 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	B	1	2	12,12,12	0.70	0	17,17,17	1.89	6 (35%)
2	GLC	B	2	2	11,11,12	1.32	2 (18%)	15,15,17	3.37	6 (40%)
3	GLC	C	1	3	12,12,12	1.06	1 (8%)	17,17,17	1.69	5 (29%)
3	GLC	C	2	3	11,11,12	0.90	1 (9%)	15,15,17	1.33	1 (6%)
3	GLC	C	3	3	11,11,12	0.69	0	15,15,17	1.18	2 (13%)
4	GLC	D	1	4	12,12,12	0.81	0	17,17,17	1.32	3 (17%)
4	GLC	D	2	4	11,11,12	0.84	0	15,15,17	1.65	2 (13%)
4	GLC	D	3	4	11,11,12	0.75	0	15,15,17	1.02	1 (6%)
4	GLC	D	4	4	11,11,12	0.74	0	15,15,17	1.67	2 (13%)
5	GLC	E	1	5	11,11,12	1.59	2 (18%)	15,15,17	2.41	8 (53%)
5	GLC	E	2	5	11,11,12	0.77	0	15,15,17	2.15	6 (40%)
5	GLC	E	3	5	11,11,12	0.74	0	15,15,17	1.74	3 (20%)
5	GLC	E	4	5	11,11,12	0.74	0	15,15,17	1.83	7 (46%)
5	GLC	E	5	5	11,11,12	0.89	0	15,15,17	1.44	3 (20%)
5	GLC	E	6	5	11,11,12	0.47	0	15,15,17	1.29	2 (13%)
5	GLC	E	7	5	11,11,12	0.66	0	15,15,17	1.82	2 (13%)
4	GLC	F	1	4	12,12,12	0.70	0	17,17,17	1.98	5 (29%)
4	GLC	F	2	4	11,11,12	1.10	0	15,15,17	1.40	2 (13%)
4	GLC	F	3	4	11,11,12	0.66	0	15,15,17	1.14	1 (6%)
4	GLC	F	4	4	11,11,12	0.76	0	15,15,17	1.15	0
3	GLC	G	1	3	11,11,12	1.27	2 (18%)	15,15,17	2.68	6 (40%)
3	GLC	G	2	3	11,11,12	0.74	0	15,15,17	2.27	6 (40%)
3	GLC	G	3	3	11,11,12	1.26	1 (9%)	15,15,17	1.85	3 (20%)

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	B	1	2	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	1/2/19/22	0/1/1/1
3	GLC	C	1	3	-	0/2/22/22	0/1/1/1
3	GLC	C	2	3	-	2/2/19/22	0/1/1/1
3	GLC	C	3	3	-	0/2/19/22	0/1/1/1
4	GLC	D	1	4	-	1/2/22/22	0/1/1/1
4	GLC	D	2	4	-	1/2/19/22	0/1/1/1
4	GLC	D	3	4	-	0/2/19/22	0/1/1/1
4	GLC	D	4	4	-	2/2/19/22	0/1/1/1
5	GLC	E	1	5	-	1/2/19/22	0/1/1/1
5	GLC	E	2	5	-	2/2/19/22	0/1/1/1
5	GLC	E	3	5	-	2/2/19/22	0/1/1/1
5	GLC	E	4	5	-	0/2/19/22	0/1/1/1
5	GLC	E	5	5	-	0/2/19/22	0/1/1/1
5	GLC	E	6	5	-	2/2/19/22	0/1/1/1
5	GLC	E	7	5	-	0/2/19/22	0/1/1/1
4	GLC	F	1	4	-	2/2/22/22	0/1/1/1
4	GLC	F	2	4	-	0/2/19/22	0/1/1/1
4	GLC	F	3	4	-	0/2/19/22	0/1/1/1
4	GLC	F	4	4	-	2/2/19/22	0/1/1/1
3	GLC	G	1	3	-	1/2/19/22	0/1/1/1
3	GLC	G	2	3	-	2/2/19/22	0/1/1/1
3	GLC	G	3	3	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	GLC	C2-C3	3.67	1.58	1.52
3	G	3	GLC	C2-C3	3.64	1.58	1.52
2	B	2	GLC	C2-C3	2.57	1.56	1.52
3	G	1	GLC	C2-C3	2.49	1.56	1.52
3	C	1	GLC	C1-C2	2.33	1.57	1.52
3	C	2	GLC	O5-C5	-2.33	1.38	1.43
5	E	1	GLC	C4-C5	2.18	1.57	1.53
3	G	1	GLC	O5-C1	-2.18	1.40	1.43
2	B	2	GLC	O4-C4	2.04	1.48	1.43

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GLC	C1-O5-C5	8.11	123.06	112.19
2	B	2	GLC	C1-C2-C3	6.45	119.04	109.64
3	G	2	GLC	C1-O5-C5	5.48	119.53	112.19
3	G	1	GLC	O5-C1-C2	-5.05	98.75	110.79
5	E	2	GLC	C1-O5-C5	5.02	118.91	112.19
4	F	1	GLC	O5-C1-C2	-4.95	101.60	110.30
5	E	7	GLC	C1-O5-C5	4.88	118.72	112.19
2	B	2	GLC	O4-C4-C5	4.75	121.02	109.32
3	G	1	GLC	C3-C4-C5	-4.70	101.71	110.23
4	D	2	GLC	C1-O5-C5	4.50	118.22	112.19
2	B	2	GLC	C3-C4-C5	-4.29	102.46	110.23
2	B	1	GLC	C1-O5-C5	4.26	121.89	113.65
3	G	1	GLC	O5-C5-C4	4.14	120.90	110.83
3	G	3	GLC	O5-C5-C6	4.13	115.69	107.66
3	G	1	GLC	C1-O5-C5	4.01	117.56	112.19
5	E	3	GLC	C3-C4-C5	-3.99	102.99	110.23
5	E	1	GLC	O2-C2-C1	-3.98	100.10	109.22
5	E	1	GLC	O5-C1-C2	-3.98	101.29	110.79
4	D	4	GLC	C2-C3-C4	-3.84	104.10	110.86
5	E	6	GLC	C1-O5-C5	3.83	117.31	112.19
3	C	1	GLC	C1-O5-C5	3.68	120.76	113.65
4	F	1	GLC	C3-C4-C5	3.60	116.77	110.23
5	E	1	GLC	C1-C2-C3	3.44	114.65	109.64
2	B	1	GLC	O5-C5-C4	3.42	115.87	109.70
3	G	1	GLC	C1-C2-C3	3.39	114.58	109.64
3	G	2	GLC	O5-C5-C4	3.38	119.06	110.83
3	G	2	GLC	C1-C2-C3	3.31	114.47	109.64
5	E	7	GLC	O3-C3-C2	-3.28	103.35	110.05
5	E	2	GLC	O3-C3-C2	3.23	116.65	110.05
3	C	2	GLC	C1-O5-C5	3.21	116.48	112.19
2	B	2	GLC	O4-C4-C3	3.19	117.89	110.38
5	E	1	GLC	O2-C2-C3	3.15	116.67	110.15
5	E	1	GLC	O5-C5-C4	3.03	118.19	110.83
4	D	4	GLC	C1-C2-C3	-3.01	105.26	109.64
5	E	3	GLC	O2-C2-C3	-2.99	103.95	110.15
5	E	4	GLC	C1-O5-C5	2.98	116.17	112.19
5	E	1	GLC	C1-O5-C5	2.88	116.05	112.19
3	G	1	GLC	O6-C6-C5	-2.85	101.62	111.33
4	F	3	GLC	O5-C5-C6	2.84	113.20	107.66
4	F	2	GLC	C1-O5-C5	2.80	115.94	112.19
5	E	4	GLC	O5-C1-C2	-2.78	104.15	110.79
5	E	2	GLC	O5-C1-C2	-2.74	104.26	110.79
4	D	1	GLC	C3-C4-C5	-2.72	105.29	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	GLC	O5-C5-C4	2.72	114.60	109.70
3	G	3	GLC	C1-C2-C3	2.71	113.58	109.64
4	D	2	GLC	O5-C5-C6	2.71	112.93	107.66
5	E	5	GLC	C3-C4-C5	-2.68	105.38	110.23
2	B	1	GLC	C1-C2-C3	2.65	115.76	110.36
4	D	1	GLC	O3-C3-C2	2.59	116.48	110.38
2	B	1	GLC	O4-C4-C3	-2.58	104.30	110.38
5	E	5	GLC	O2-C2-C1	-2.57	103.33	109.22
3	C	3	GLC	C1-O5-C5	2.57	115.63	112.19
4	D	1	GLC	O4-C4-C3	-2.52	104.43	110.38
4	F	1	GLC	O1-C1-C2	2.52	116.30	108.98
5	E	2	GLC	O5-C5-C6	2.51	112.55	107.66
5	E	4	GLC	C1-C2-C3	2.50	113.29	109.64
5	E	4	GLC	O4-C4-C3	-2.49	104.50	110.38
5	E	4	GLC	C3-C4-C5	-2.49	105.72	110.23
5	E	1	GLC	O4-C4-C3	2.45	116.16	110.38
4	F	1	GLC	O2-C2-C1	2.43	114.85	109.25
4	F	2	GLC	C1-C2-C3	2.40	113.13	109.64
5	E	5	GLC	O2-C2-C3	-2.35	105.29	110.15
3	C	1	GLC	O4-C4-C5	-2.25	103.78	109.32
5	E	6	GLC	C2-C3-C4	2.23	114.78	110.86
3	G	2	GLC	O3-C3-C4	-2.22	105.14	110.38
5	E	4	GLC	O2-C2-C3	-2.22	105.56	110.15
2	B	1	GLC	O4-C4-C5	2.20	114.74	109.32
3	C	1	GLC	C4-C3-C2	-2.15	107.06	110.83
3	C	1	GLC	C1-C2-C3	2.14	114.73	110.36
5	E	1	GLC	O3-C3-C2	2.13	114.41	110.05
3	C	1	GLC	O2-C2-C1	2.13	114.16	109.25
3	G	2	GLC	O5-C1-C2	-2.12	105.72	110.79
3	C	3	GLC	C1-C2-C3	2.11	112.72	109.64
2	B	2	GLC	O5-C5-C4	2.10	115.94	110.83
5	E	3	GLC	O6-C6-C5	-2.09	104.21	111.33
5	E	2	GLC	O5-C5-C4	2.09	115.91	110.83
5	E	2	GLC	O4-C4-C3	-2.06	105.51	110.38
5	E	4	GLC	C2-C3-C4	2.05	114.46	110.86
4	D	3	GLC	O2-C2-C1	2.02	113.84	109.22
2	B	1	GLC	C3-C4-C5	-2.02	106.58	110.23
3	G	2	GLC	O3-C3-C2	2.00	114.14	110.05
3	G	3	GLC	O4-C4-C3	2.00	115.09	110.38

There are no chirality outliers.

All (21) torsion outliers are listed below:

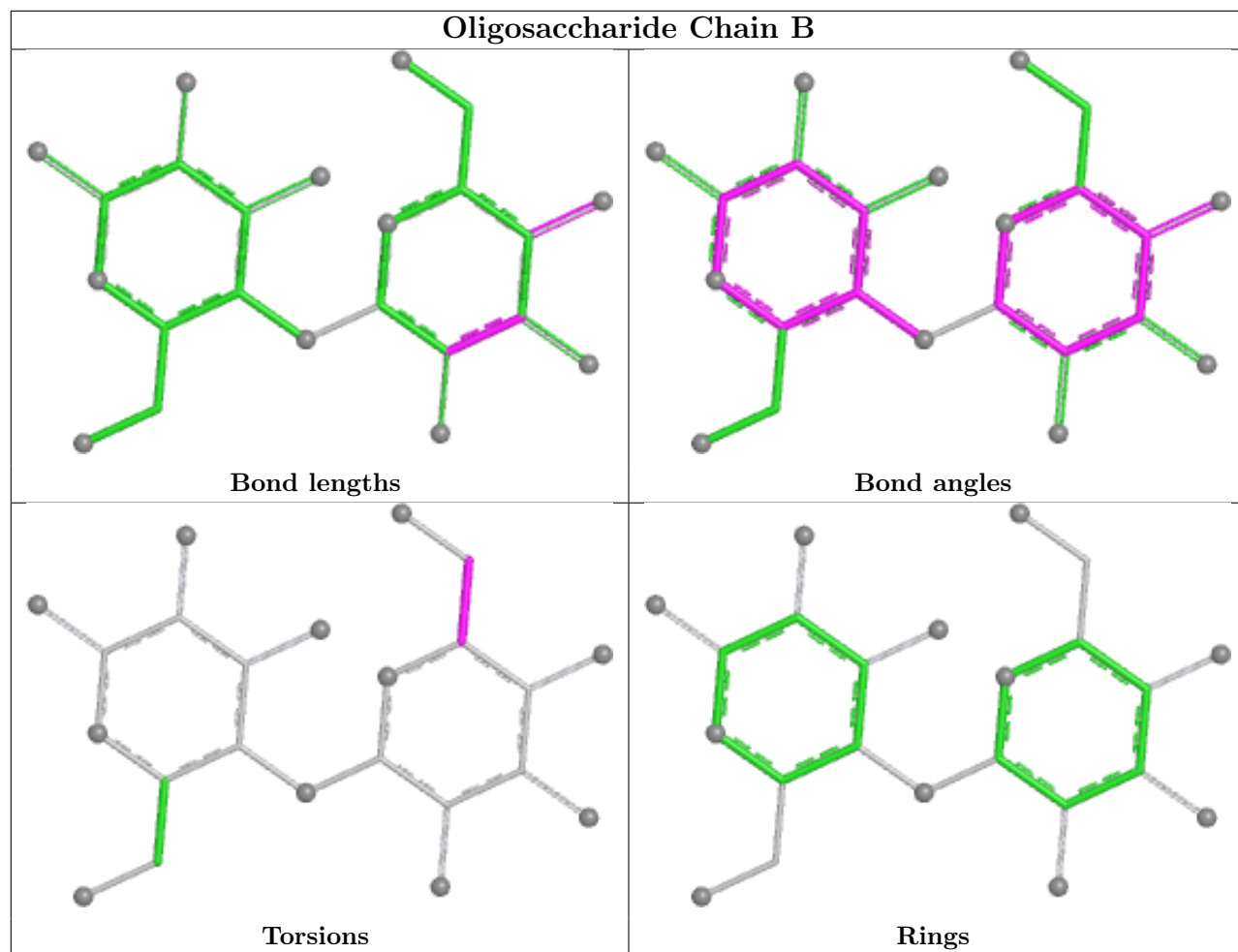
Mol	Chain	Res	Type	Atoms
5	E	3	GLC	C4-C5-C6-O6
4	F	1	GLC	O5-C5-C6-O6
4	D	4	GLC	O5-C5-C6-O6
4	F	1	GLC	C4-C5-C6-O6
5	E	3	GLC	O5-C5-C6-O6
3	G	2	GLC	O5-C5-C6-O6
5	E	2	GLC	C4-C5-C6-O6
4	D	4	GLC	C4-C5-C6-O6
4	F	4	GLC	O5-C5-C6-O6
5	E	6	GLC	C4-C5-C6-O6
3	G	2	GLC	C4-C5-C6-O6
5	E	6	GLC	O5-C5-C6-O6
2	B	2	GLC	C4-C5-C6-O6
5	E	1	GLC	O5-C5-C6-O6
3	G	1	GLC	O5-C5-C6-O6
5	E	2	GLC	O5-C5-C6-O6
4	D	1	GLC	O5-C5-C6-O6
3	C	2	GLC	O5-C5-C6-O6
3	C	2	GLC	C4-C5-C6-O6
4	D	2	GLC	O5-C5-C6-O6
4	F	4	GLC	C4-C5-C6-O6

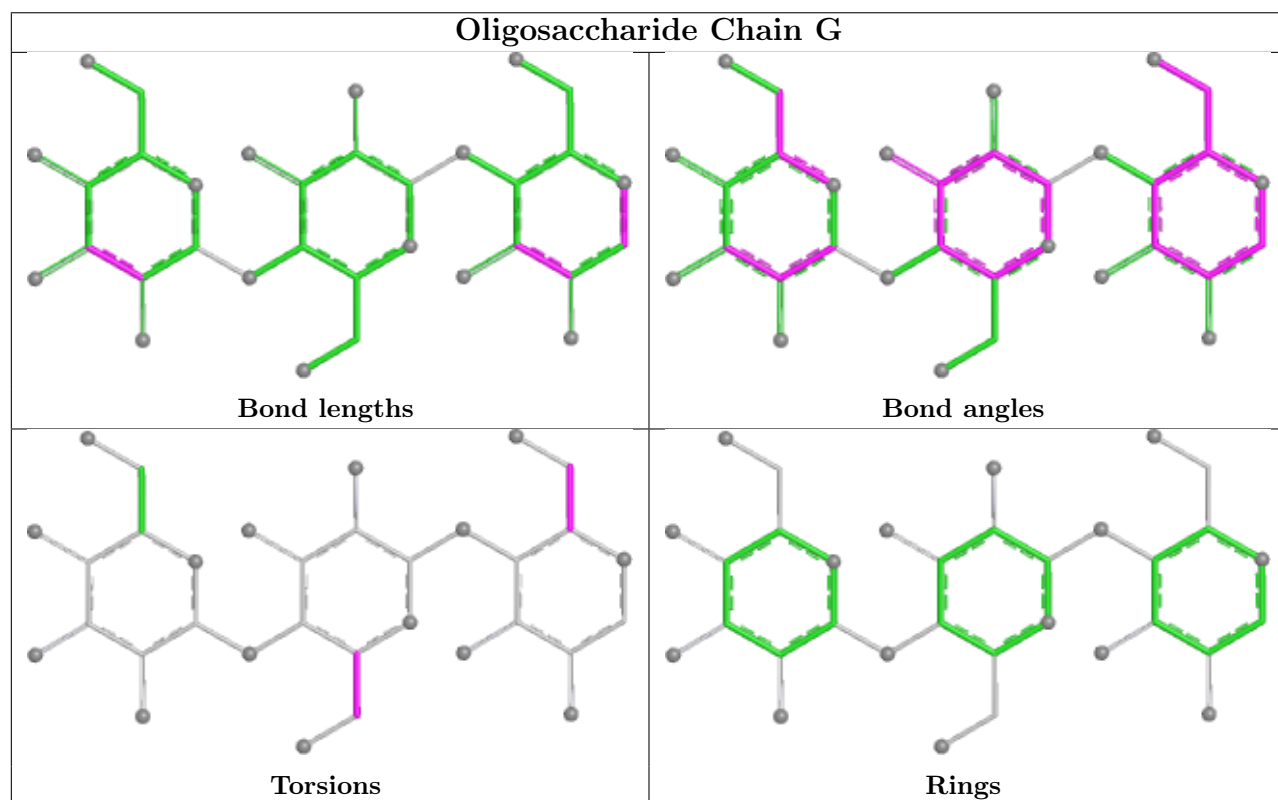
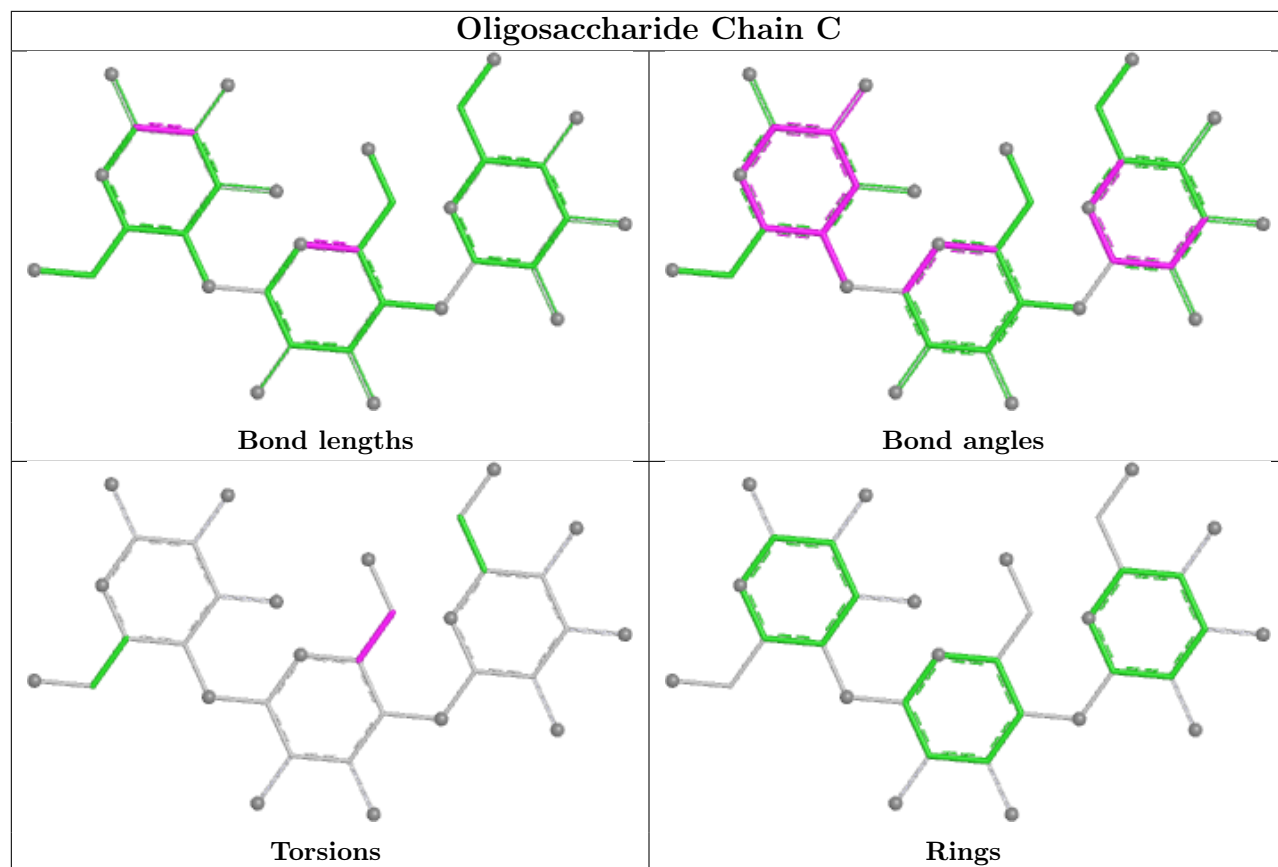
There are no ring outliers.

1 monomer is involved in 1 short contact:

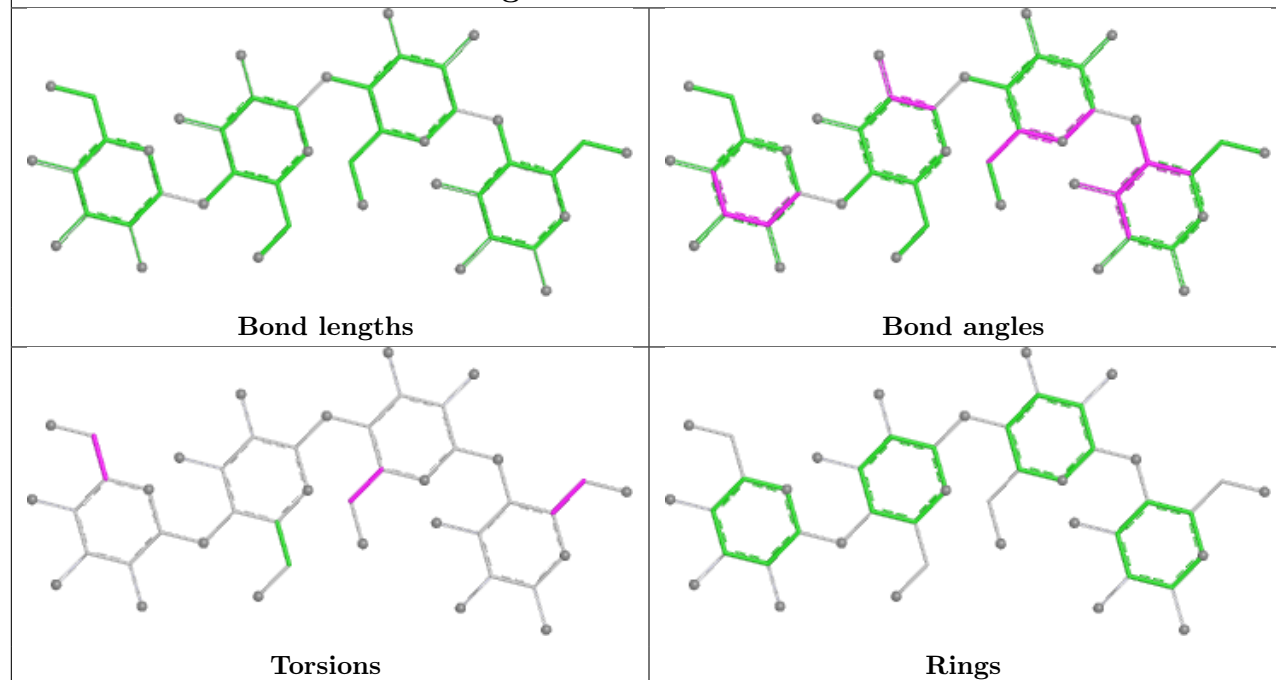
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

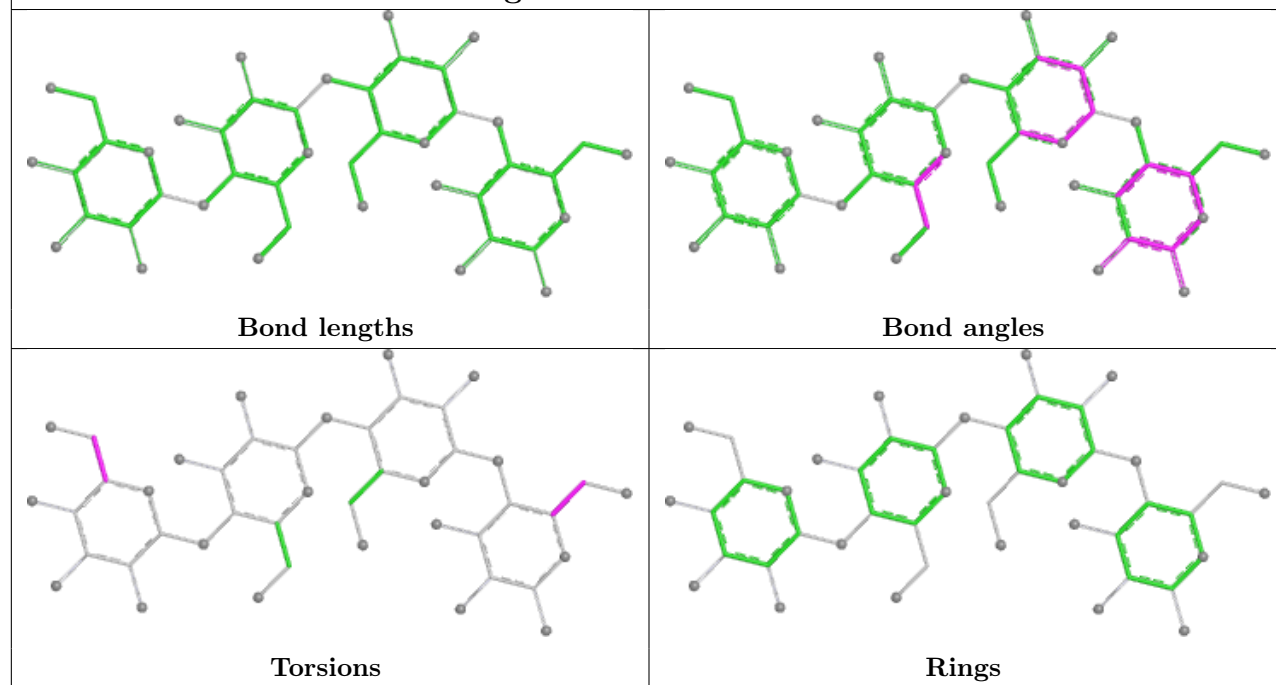


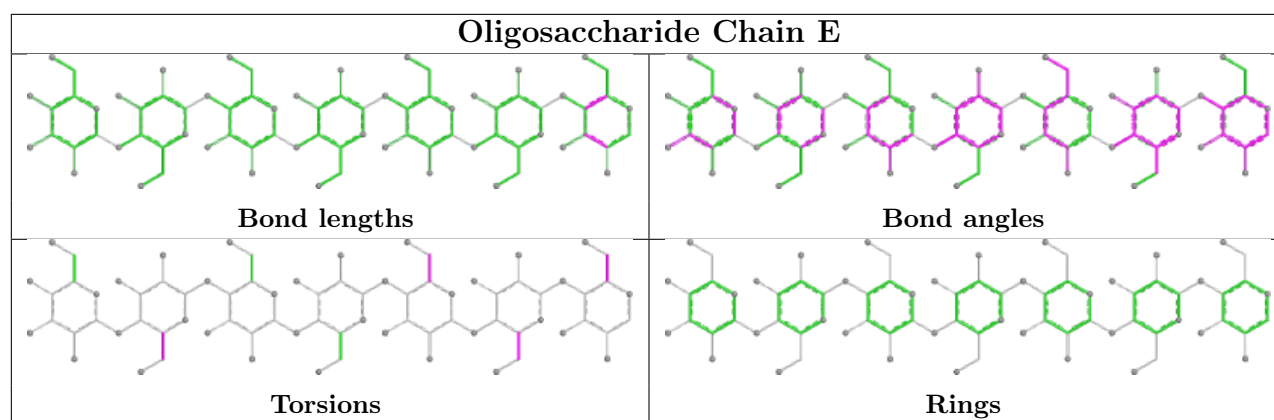


Oligosaccharide Chain D



Oligosaccharide Chain F





5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	A	824	-	5,5,5	0.97	0	5,5,5	1.52	2 (40%)
6	GOL	A	825	-	5,5,5	0.78	0	5,5,5	1.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	824	-	-	2/4/4/4	-
6	GOL	A	825	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	824	GOL	O2-C2-C1	2.01	117.52	109.18
6	A	824	GOL	O1-C1-C2	2.01	119.41	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	824	GOL	O1-C1-C2-O2
6	A	824	GOL	O1-C1-C2-C3
6	A	825	GOL	O1-C1-C2-C3
6	A	825	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	755/793 (95%)	-0.18	20 (2%) 57 52	22, 38, 67, 106	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	758	VAL	7.5
1	A	759	PRO	6.0
1	A	203	TYR	3.7
1	A	201	HIS	3.7
1	A	285	TRP	3.5
1	A	688	GLN	3.2
1	A	730	TRP	3.1
1	A	457	GLY	2.9
1	A	94	HIS	2.8
1	A	198	SER	2.6
1	A	757	LYS	2.6
1	A	202	ILE	2.3
1	A	447	LYS	2.2
1	A	456	TYR	2.2
1	A	93	GLU	2.2
1	A	691	SER	2.1
1	A	455	GLU	2.1
1	A	47	LYS	2.1
1	A	452	ILE	2.0
1	A	755	PRO	2.0

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

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

6.3 Carbohydrates

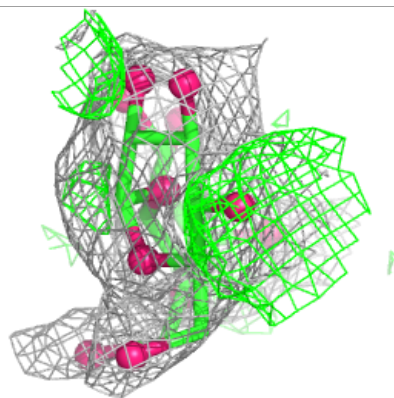
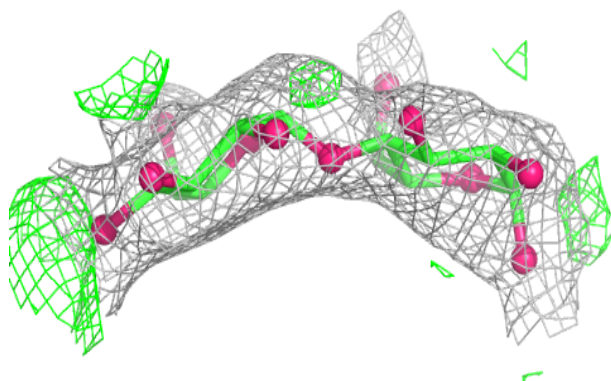
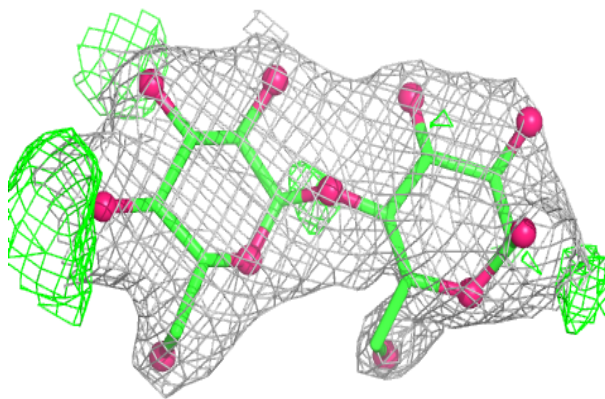
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	C	3	11/12	0.68	0.19	82,96,104,107	0
3	GLC	G	1	11/12	0.74	0.18	71,83,88,89	0
4	GLC	D	4	11/12	0.76	0.16	72,87,90,96	0
5	GLC	E	2	11/12	0.78	0.17	83,87,93,96	0
3	GLC	G	3	11/12	0.81	0.16	61,76,83,85	0
5	GLC	E	1	11/12	0.83	0.18	64,81,86,89	0
2	GLC	B	1	12/12	0.84	0.16	65,81,87,88	0
3	GLC	G	2	11/12	0.84	0.17	81,92,105,107	0
4	GLC	D	1	12/12	0.85	0.13	64,75,82,88	0
4	GLC	F	1	12/12	0.86	0.13	61,85,91,94	0
5	GLC	E	3	11/12	0.86	0.11	65,74,82,84	0
2	GLC	B	2	11/12	0.89	0.11	44,53,66,72	0
4	GLC	F	4	11/12	0.92	0.10	56,68,78,79	0
5	GLC	E	4	11/12	0.92	0.10	69,71,75,76	0
5	GLC	E	5	11/12	0.92	0.11	52,55,61,62	0
3	GLC	C	2	11/12	0.93	0.09	49,58,70,78	0
3	GLC	C	1	12/12	0.93	0.08	50,52,62,66	0
4	GLC	D	2	11/12	0.94	0.08	44,53,55,57	0
5	GLC	E	7	11/12	0.94	0.10	48,54,61,64	0
4	GLC	F	3	11/12	0.96	0.07	40,50,54,56	0
5	GLC	E	6	11/12	0.96	0.07	41,49,55,57	0
4	GLC	D	3	11/12	0.96	0.08	51,57,68,72	0
4	GLC	F	2	11/12	0.98	0.05	35,42,50,51	0

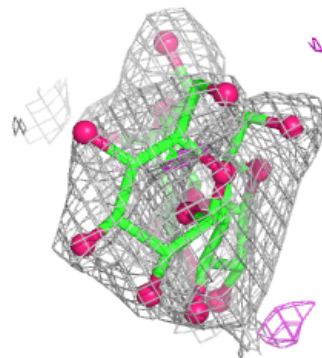
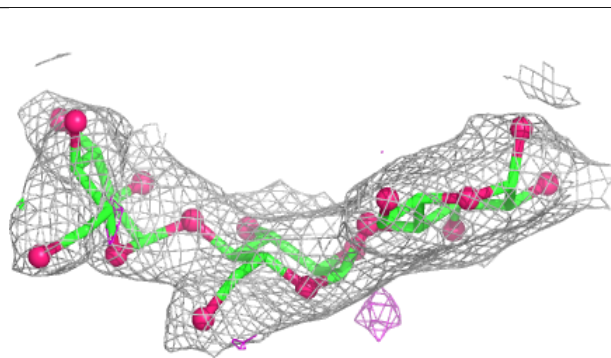
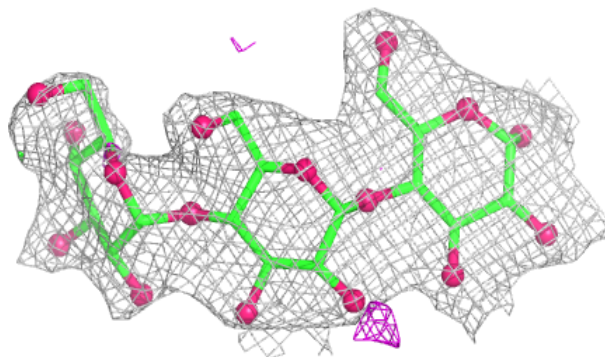
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

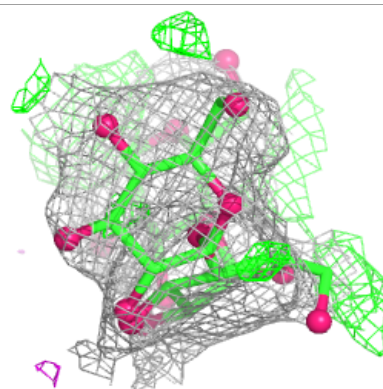
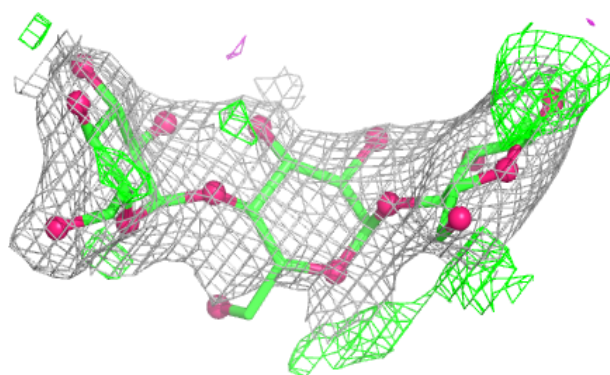
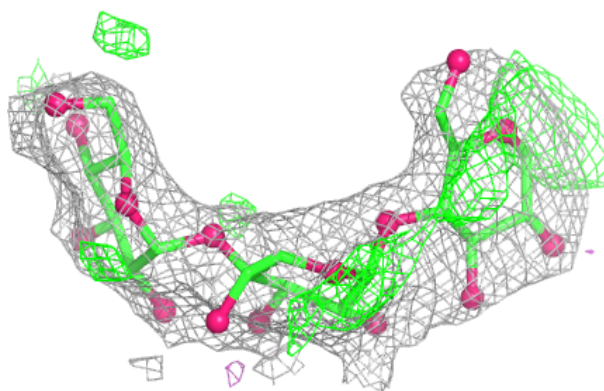
**Electron density around Chain C:**

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

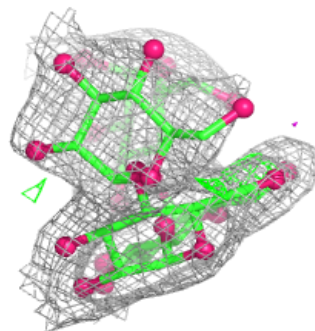
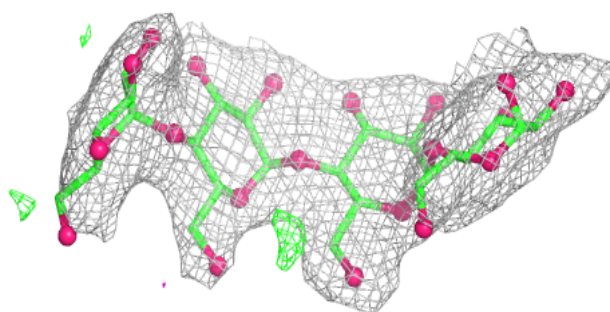
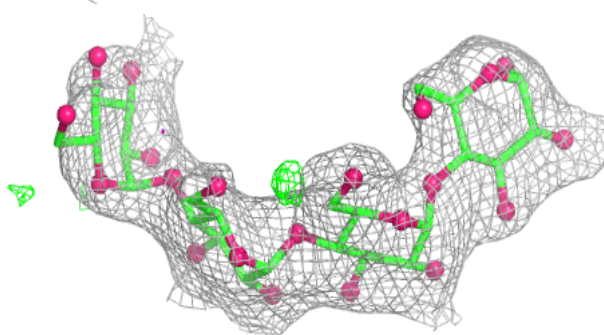


Electron density around Chain G:

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

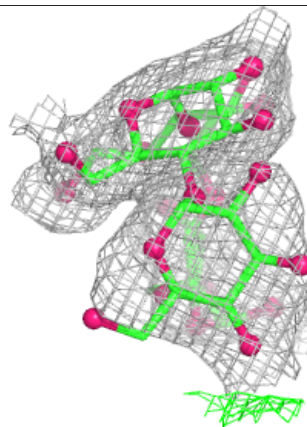
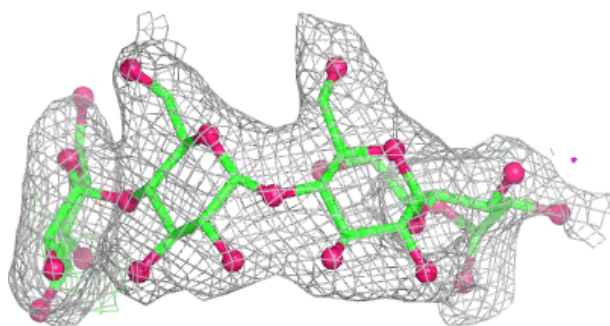
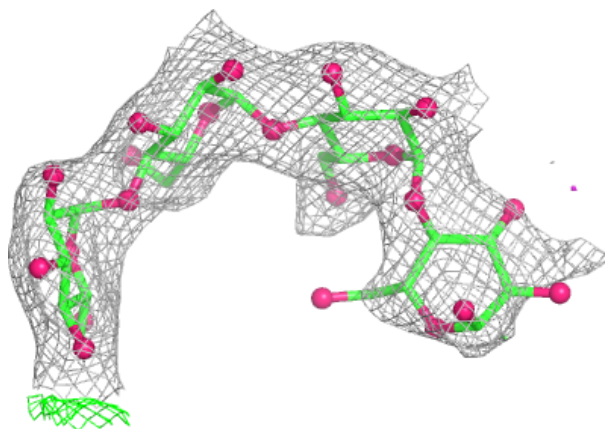
**Electron density around Chain D:**

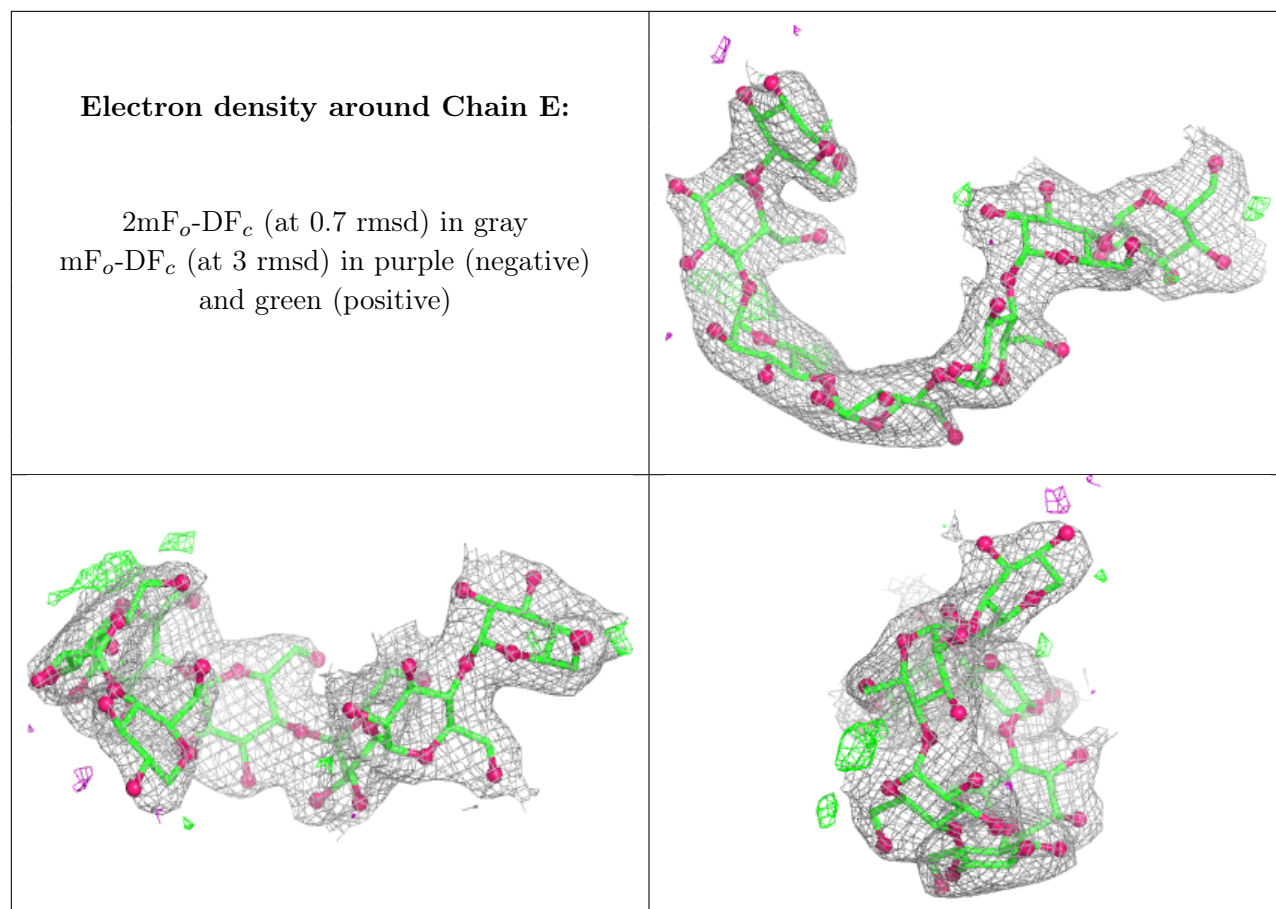
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
6	GOL	A	824	6/6	0.88	0.17	58,60,65,69	0
6	GOL	A	825	6/6	0.94	0.12	49,56,61,64	0
7	MG	A	826	1/1	0.99	0.04	51,51,51,51	0
7	MG	A	827	1/1	0.99	0.02	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.