



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 10:24 AM BST

PDB ID : 5JBF
Title : 4,6-alpha-glucanotransferase GTFB (D1015N mutant) from *Lactobacillus reuteri* 121 complexed with maltopentaose
Authors : Pijning, T.; Dijkstra, B.W.; Bai, Y.; Gangoiti-Munecas, J.; Dijkhuizen, L.
Deposited on : 2016-04-13
Resolution : 2.19 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

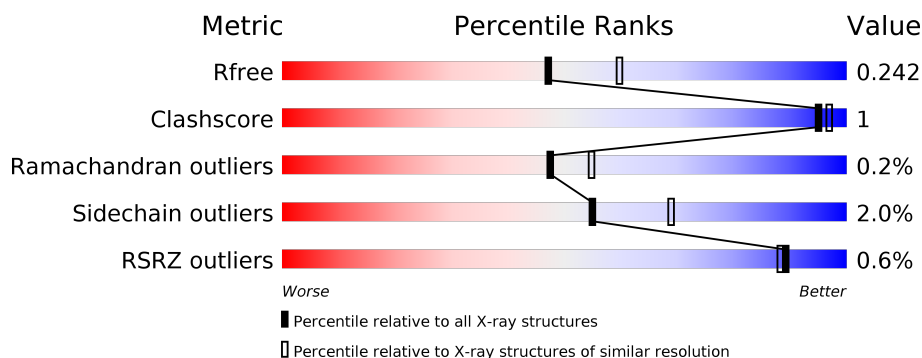
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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.




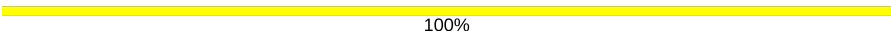
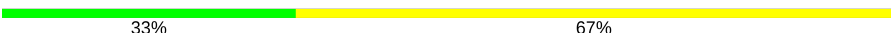
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	854	<div> <div></div> <div>96%</div> <div>.</div> </div>
1	B	854	<div> <div></div> <div>95%</div> <div>5%</div> <div>.</div> </div>
2	C	5	<div> <div>20%</div> <div>80%</div> </div>
2	F	5	<div> <div>20%</div> <div>80%</div> </div>
3	D	2	<div> <div>50%</div> <div>50%</div> </div>
3	E	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	 50%50%
3	H	2	 100%
4	I	3	 33%67%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14324 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 Inactive glucansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	854	Total	C	N	O	S	0	0	0
			6678	4151	1147	1354	26			
1	B	854	Total	C	N	O	S	0	0	0
			6678	4151	1147	1354	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	761	MET	LEU	cloning artifact	UNP Q5SBM0
A	1015	ASN	ASP	engineered mutation	UNP Q5SBM0
B	761	MET	LEU	cloning artifact	UNP Q5SBM0
B	1015	ASN	ASP	engineered mutation	UNP Q5SBM0

- Molecule 2 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
2	C	5	Total	C	O	0	0	0
			56	30	26			
2	F	5	Total	C	O	0	0	0
			56	30	26			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	2	Total	C	O	0	0	0
			23	12	11			
3	E	2	Total	C	O	0	0	0
			23	12	11			
3	G	2	Total	C	O	0	0	0
			23	12	11			
3	H	2	Total	C	O	0	0	0
			23	12	11			

- 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	I	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

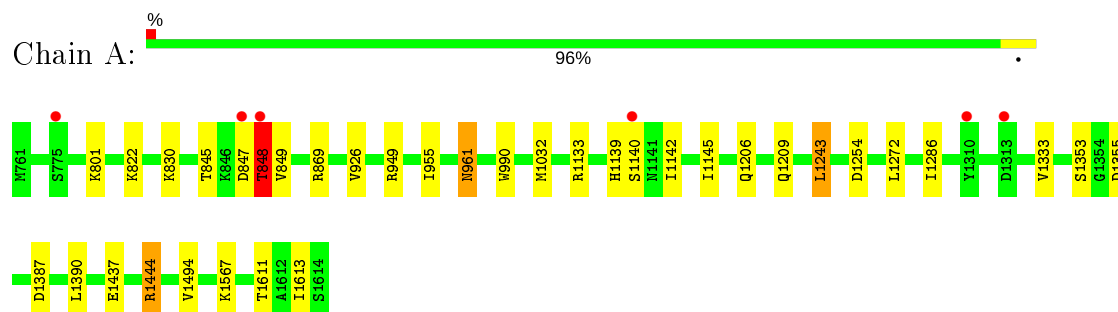
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	340	Total	O	0	0
			340	340		
7	B	363	Total	O	0	0
			363	363		

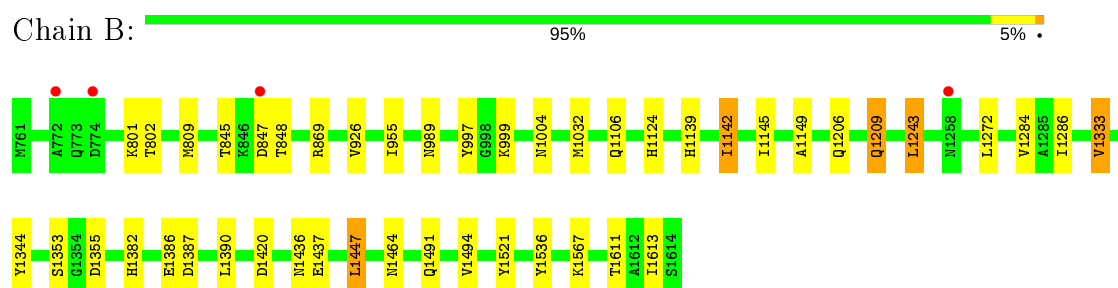
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Inactive glucansucrase



- Molecule 1: Inactive glucansucrase



- 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



- 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



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

Chain D:  50% 50%

GLC1
GLC2

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

Chain E:  50% 50%

GLC3
GLC2

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

Chain G:  50% 50%

GLC1
GLC2

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

Chain H:  100%

GLC1
GLC2

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

Chain I:  33% 67%

GLC1
GLC2
GLC3

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.48Å 58.14Å 150.38Å 90.00° 114.36° 90.00°	Depositor
Resolution (Å)	48.02 – 2.19 48.02 – 2.19	Depositor EDS
% Data completeness (in resolution range)	90.2 (48.02-2.19) 90.2 (48.02-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.194 , 0.237 0.199 , 0.242	Depositor DCC
R_{free} test set	4021 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.875	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14324	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 4.55% 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: CA, GLC, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.56	0/6815	0.72	6/9268 (0.1%)
1	B	0.58	0/6815	0.73	3/9268 (0.0%)
All	All	0.57	0/13630	0.72	9/18536 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1444	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	B	869	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	A	1444	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	869	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	B	1243	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	1133	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	1254	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	809	MET	CG-SD-CE	5.14	108.43	100.20
1	A	949	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1353	SER	Peptide
1	A	1613	ILE	Peptide
1	B	1353	SER	Peptide
1	B	1613	ILE	Peptide

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	6678	0	6331	12	0
1	B	6678	0	6331	19	0
2	C	56	0	48	0	0
2	F	56	0	48	0	0
3	D	23	0	21	0	0
3	E	23	0	21	0	0
3	G	23	0	21	0	0
3	H	23	0	21	0	0
4	I	34	0	30	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	15	0	0	1	0
6	B	10	0	0	1	0
7	A	340	0	0	1	0
7	B	363	0	0	1	0
All	All	14324	0	12872	31	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 1.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:997:TYR:CE1	1:B:1447:LEU:HD22	2.18	0.77
1:B:989:ASN:HD21	1:B:1536:TYR:H	1.35	0.75
1:B:1004:ASN:HD22	1:B:1464:ASN:HD22	1.39	0.71
1:B:1206:GLN:HB2	1:B:1209:GLN:HG3	1.84	0.60
1:B:1004:ASN:HD22	1:B:1464:ASN:ND2	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:LEU:HD21	1:A:1286:ILE:HD11	1.87	0.55
1:B:845:THR:OG1	1:B:847:ASP:O	2.24	0.55
1:A:845:THR:OG1	1:A:847:ASP:O	2.24	0.55
1:B:1272:LEU:HD21	1:B:1286:ILE:HD11	1.88	0.54
1:B:1124:HIS:HD2	1:B:1386:GLU:OE2	1.91	0.54
1:B:1491:GLN:HG3	1:B:1521:TYR:CE1	2.42	0.54
1:A:1206:GLN:HB2	1:A:1209:GLN:HG3	1.92	0.50
1:B:1124:HIS:CD2	1:B:1386:GLU:OE2	2.64	0.50
1:A:1611:THR:HG23	6:A:1706:SO4:O1	2.15	0.47
1:B:1436:ASN:ND2	7:B:1810:HOH:O	2.48	0.47
1:B:997:TYR:CE1	1:B:1447:LEU:CD2	2.94	0.47
1:A:847:ASP:O	1:A:848:THR:HB	2.14	0.47
1:A:990:TRP:CZ2	1:A:1444:ARG:HG2	2.51	0.44
1:B:1142:ILE:CD1	1:B:1149:ALA:HB1	2.48	0.44
1:B:1142:ILE:O	1:B:1142:ILE:HG13	2.17	0.44
1:A:1390:LEU:CD2	1:A:1437:GLU:HG3	2.48	0.43
1:B:1333:VAL:HG22	1:B:1344:TYR:CE2	2.53	0.43
1:B:1611:THR:HG23	6:B:1705:SO4:O3	2.19	0.42
1:B:1390:LEU:CD2	1:B:1437:GLU:HG3	2.49	0.42
1:A:961:ASN:ND2	7:A:1805:HOH:O	2.53	0.41
1:B:1382:HIS:HD2	1:B:1420:ASP:OD2	2.03	0.41
1:A:1243:LEU:C	1:A:1243:LEU:HD23	2.41	0.41
1:A:830:LYS:HG2	1:A:849:VAL:HG13	2.02	0.41
1:B:1139:HIS:HB2	1:B:1145:ILE:CD1	2.50	0.40
1:A:1139:HIS:HB3	1:A:1142:ILE:HD12	2.02	0.40
1:A:1139:HIS:HB2	1:A:1145:ILE:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	852/854 (100%)	822 (96%)	28 (3%)	2 (0%)	47	55
1	B	852/854 (100%)	824 (97%)	26 (3%)	2 (0%)	47	55
All	All	1704/1708 (100%)	1646 (97%)	54 (3%)	4 (0%)	47	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	848	THR
1	A	848	THR
1	A	955	ILE
1	B	955	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	720/720 (100%)	707 (98%)	13 (2%)	59	72
1	B	720/720 (100%)	704 (98%)	16 (2%)	52	65
All	All	1440/1440 (100%)	1411 (98%)	29 (2%)	55	69

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	801	LYS
1	A	822	LYS
1	A	848	THR
1	A	926	VAL
1	A	961	ASN
1	A	1032	MET
1	A	1140	SER
1	A	1243	LEU
1	A	1333	VAL
1	A	1355	ASP
1	A	1387	ASP
1	A	1494	VAL

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Mol	Chain	Res	Type
1	A	1567	LYS
1	B	801	LYS
1	B	802	THR
1	B	926	VAL
1	B	999	LYS
1	B	1032	MET
1	B	1106	GLN
1	B	1142	ILE
1	B	1209	GLN
1	B	1243	LEU
1	B	1284	VAL
1	B	1333	VAL
1	B	1355	ASP
1	B	1387	ASP
1	B	1447	LEU
1	B	1494	VAL
1	B	1567	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	961	ASN
1	A	1083	ASN
1	A	1090	ASN
1	A	1139	HIS
1	A	1382	HIS
1	B	779	ASN
1	B	952	ASN
1	B	956	ASN
1	B	974	ASN
1	B	989	ASN
1	B	1019	ASN
1	B	1061	GLN
1	B	1068	ASN
1	B	1090	ASN
1	B	1106	GLN
1	B	1117	ASN
1	B	1124	HIS
1	B	1139	HIS
1	B	1177	ASN
1	B	1256	ASN
1	B	1326	ASN

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Mol	Chain	Res	Type
1	B	1356	GLN
1	B	1382	HIS
1	B	1436	ASN
1	B	1464	ASN
1	B	1527	ASN
1	B	1543	ASN
1	B	1580	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 ⓘ

21 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	C	1	2	12,12,12	0.61	0	17,17,17	1.60	3 (17%)
2	GLC	C	2	2	11,11,12	0.33	0	15,15,17	1.22	1 (6%)
2	GLC	C	3	2	11,11,12	0.45	0	15,15,17	1.10	1 (6%)
2	GLC	C	4	2	11,11,12	0.50	0	15,15,17	1.17	2 (13%)
2	GLC	C	5	2	11,11,12	0.37	0	15,15,17	0.88	0
3	GLC	D	1	3	12,12,12	0.61	0	17,17,17	0.78	0
3	GLC	D	2	3	11,11,12	0.47	0	15,15,17	1.01	1 (6%)
3	GLC	E	1	3	12,12,12	0.52	0	17,17,17	0.85	0
3	GLC	E	2	3	11,11,12	0.51	0	15,15,17	1.11	1 (6%)
2	GLC	F	1	2	12,12,12	0.63	0	17,17,17	1.78	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	F	2	2	11,11,12	0.32	0	15,15,17	1.01	1 (6%)
2	GLC	F	3	2	11,11,12	0.47	0	15,15,17	1.20	1 (6%)
2	GLC	F	4	2	11,11,12	0.48	0	15,15,17	0.96	1 (6%)
2	GLC	F	5	2	11,11,12	0.27	0	15,15,17	0.99	0
3	GLC	G	1	3	12,12,12	0.70	0	17,17,17	0.71	0
3	GLC	G	2	3	11,11,12	0.55	0	15,15,17	1.39	2 (13%)
3	GLC	H	1	3	12,12,12	0.56	0	17,17,17	0.77	1 (5%)
3	GLC	H	2	3	11,11,12	0.30	0	15,15,17	1.05	2 (13%)
4	GLC	I	1	4	12,12,12	0.64	0	17,17,17	0.82	0
4	GLC	I	2	4	11,11,12	0.38	0	15,15,17	1.04	1 (6%)
4	GLC	I	3	4	11,11,12	0.50	0	15,15,17	0.95	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	2/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1
3	GLC	E	1	3	-	2/2/22/22	0/1/1/1
3	GLC	E	2	3	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	2/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	3	2	-	0/2/19/22	0/1/1/1
2	GLC	F	4	2	-	0/2/19/22	0/1/1/1
2	GLC	F	5	2	-	1/2/19/22	0/1/1/1
3	GLC	G	1	3	-	2/2/22/22	0/1/1/1
3	GLC	G	2	3	-	1/2/19/22	0/1/1/1
3	GLC	H	1	3	-	0/2/22/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
4	GLC	I	1	4	-	0/2/22/22	0/1/1/1
4	GLC	I	2	4	-	1/2/19/22	0/1/1/1
4	GLC	I	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3	GLC	C1-O5-C5	3.78	117.31	112.19
3	E	2	GLC	C1-C2-C3	3.41	113.86	109.67
2	F	1	GLC	O4-C4-C5	-3.28	101.15	109.30
2	F	1	GLC	C3-C4-C5	3.27	116.08	110.24
2	C	2	GLC	C1-O5-C5	3.16	116.48	112.19
2	F	1	GLC	C4-C3-C2	3.11	116.26	110.82
2	C	1	GLC	C3-C4-C5	3.07	115.71	110.24
3	G	2	GLC	C1-C2-C3	3.01	113.36	109.67
2	C	1	GLC	O5-C5-C4	2.97	115.09	109.69
3	D	2	GLC	C1-O5-C5	2.75	115.92	112.19
3	G	2	GLC	C1-O5-C5	2.72	115.88	112.19
2	C	4	GLC	C1-C2-C3	2.63	112.90	109.67
2	C	3	GLC	C1-O5-C5	2.62	115.74	112.19
2	C	1	GLC	O2-C2-C1	2.58	115.14	109.16
3	H	2	GLC	C1-C2-C3	2.50	112.74	109.67
2	F	2	GLC	C1-O5-C5	2.40	115.45	112.19
4	I	3	GLC	C1-O5-C5	2.37	115.40	112.19
2	F	1	GLC	O5-C5-C6	2.33	112.24	106.44
4	I	2	GLC	C1-O5-C5	2.20	115.17	112.19
4	I	3	GLC	O5-C5-C6	2.18	110.62	107.20
2	F	4	GLC	C1-C2-C3	2.14	112.30	109.67
3	H	1	GLC	C1-O5-C5	2.11	117.64	113.66
2	F	1	GLC	O3-C3-C2	-2.09	105.52	110.35
3	H	2	GLC	C1-O5-C5	2.08	115.00	112.19
2	C	4	GLC	O5-C5-C6	2.03	110.38	107.20

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

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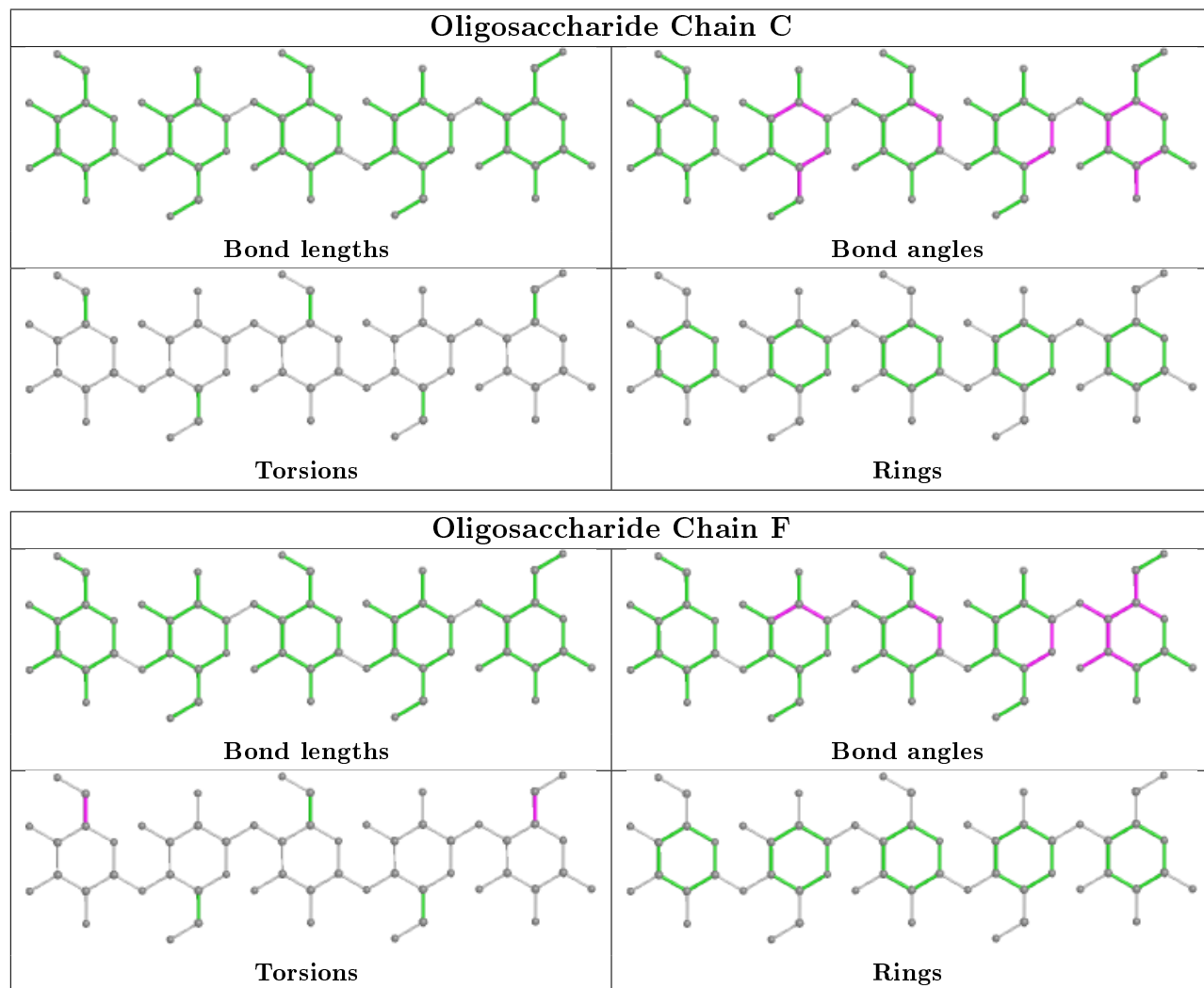
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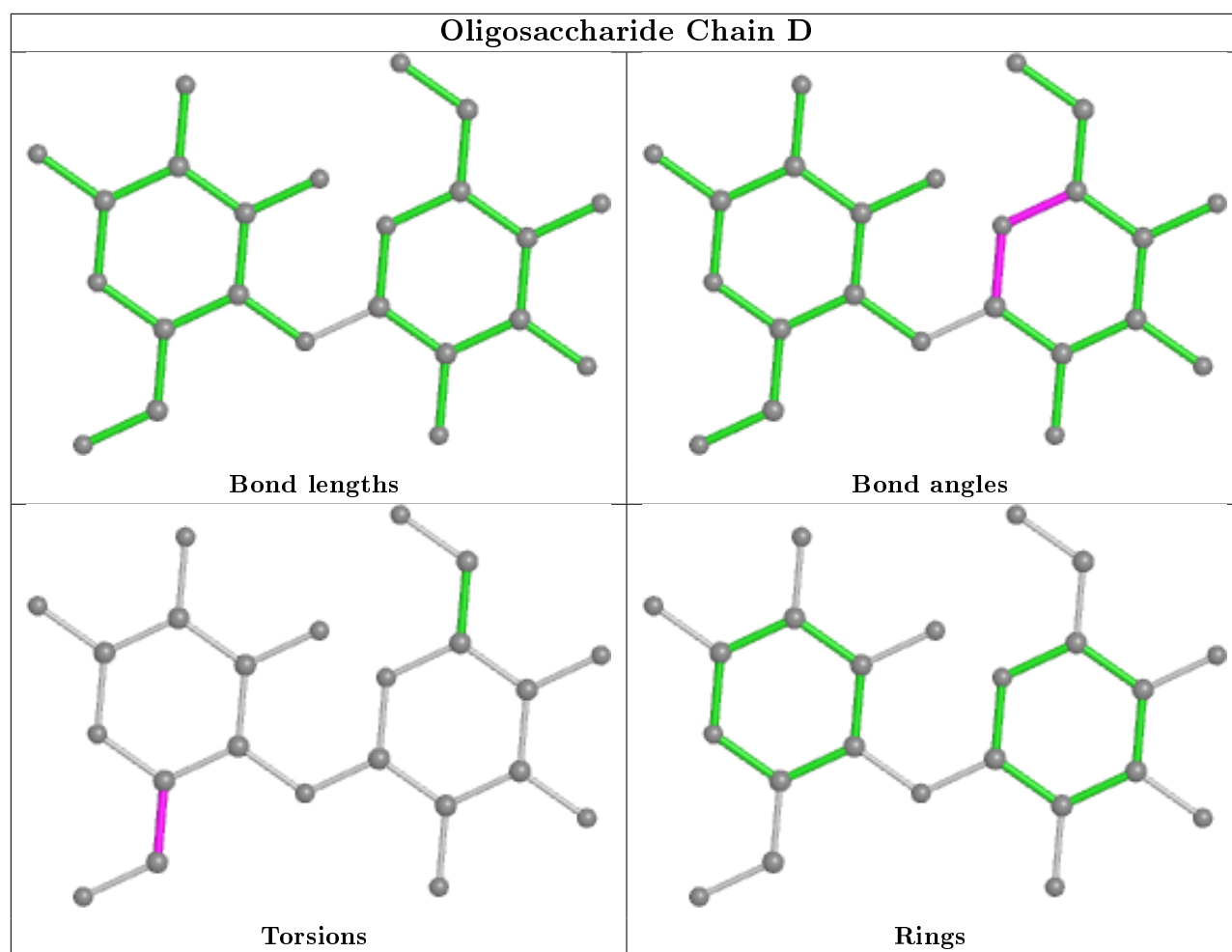
Mol	Chain	Res	Type	Atoms
3	E	1	GLC	C4-C5-C6-O6

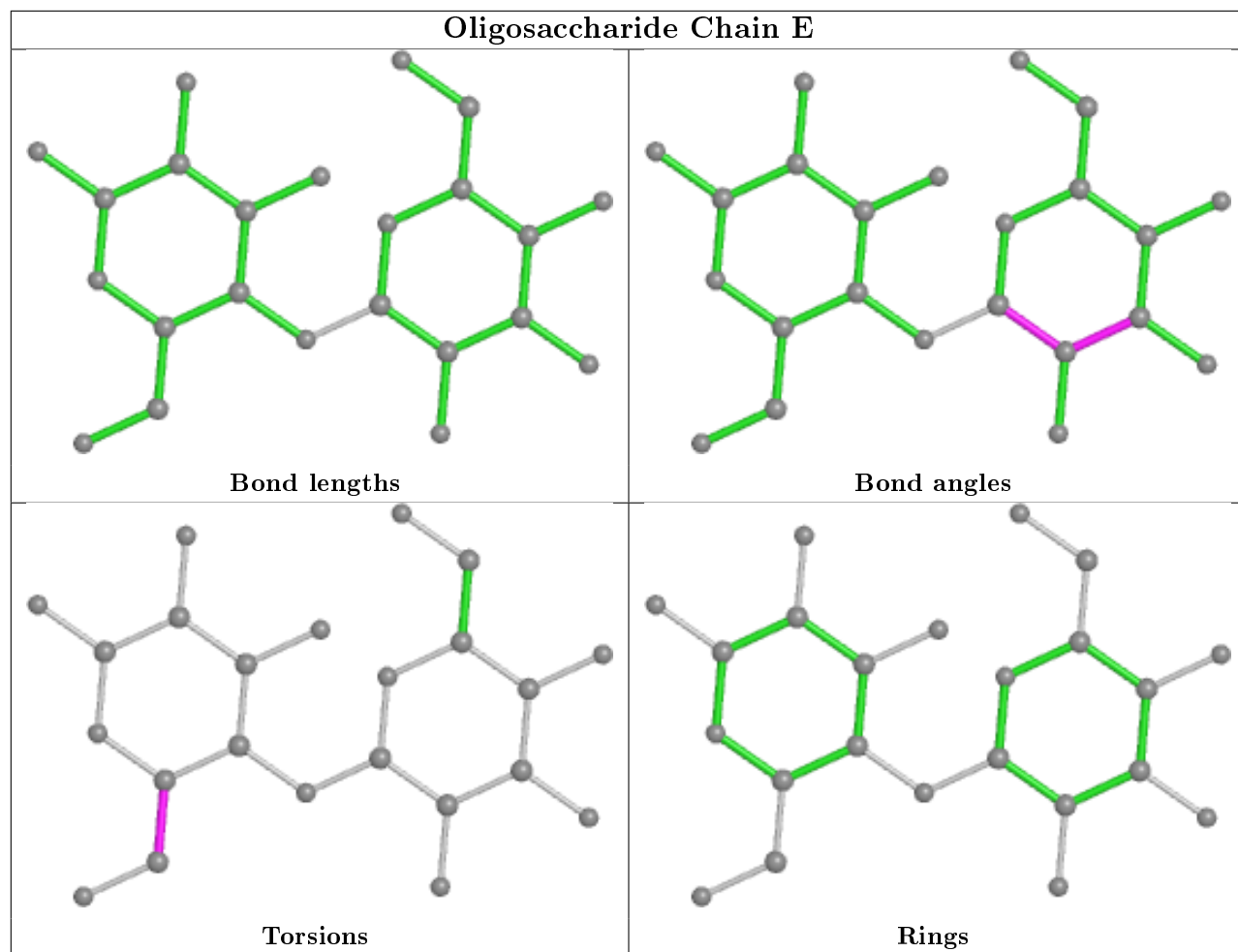
There are no ring outliers.

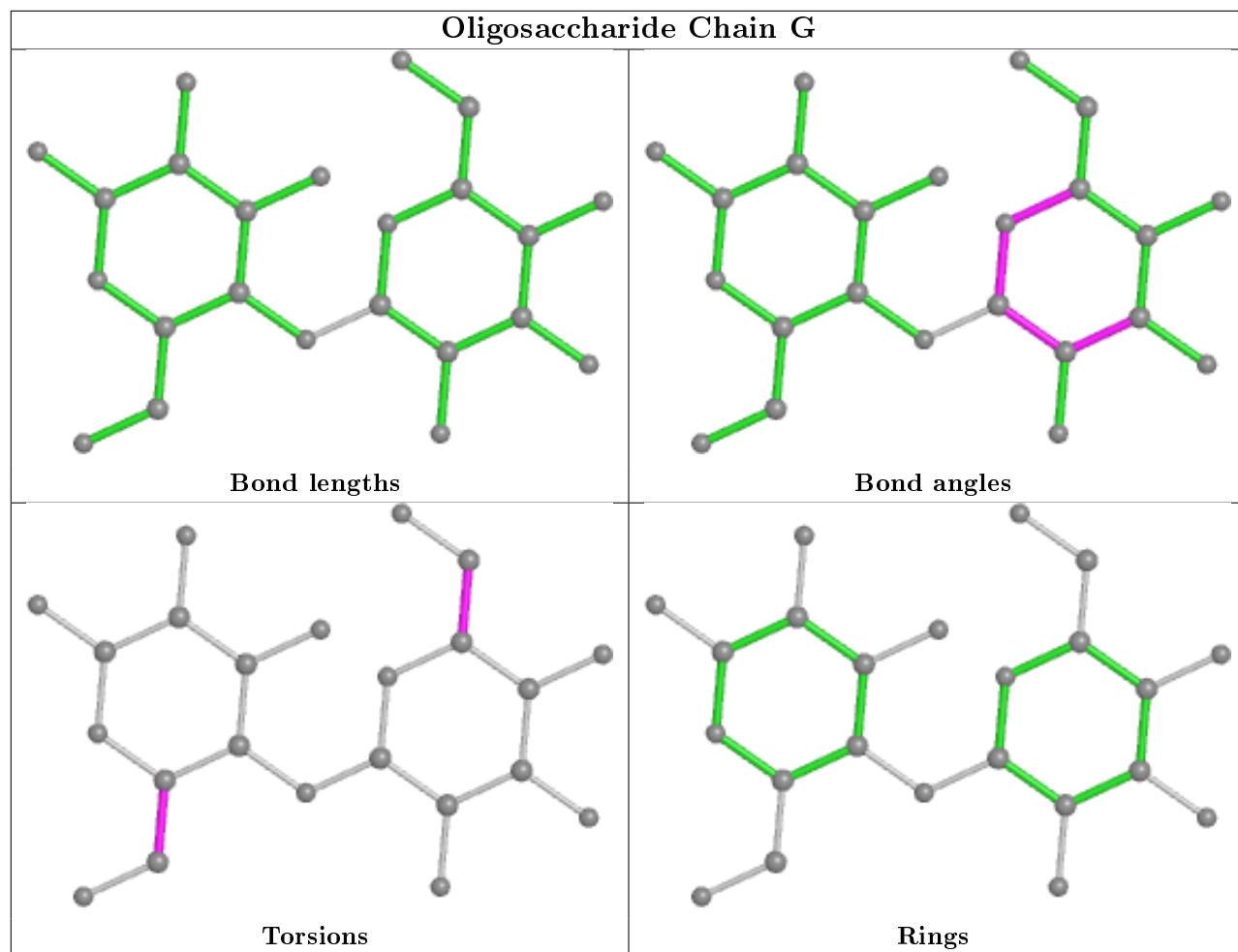
No monomer is involved in short contacts.

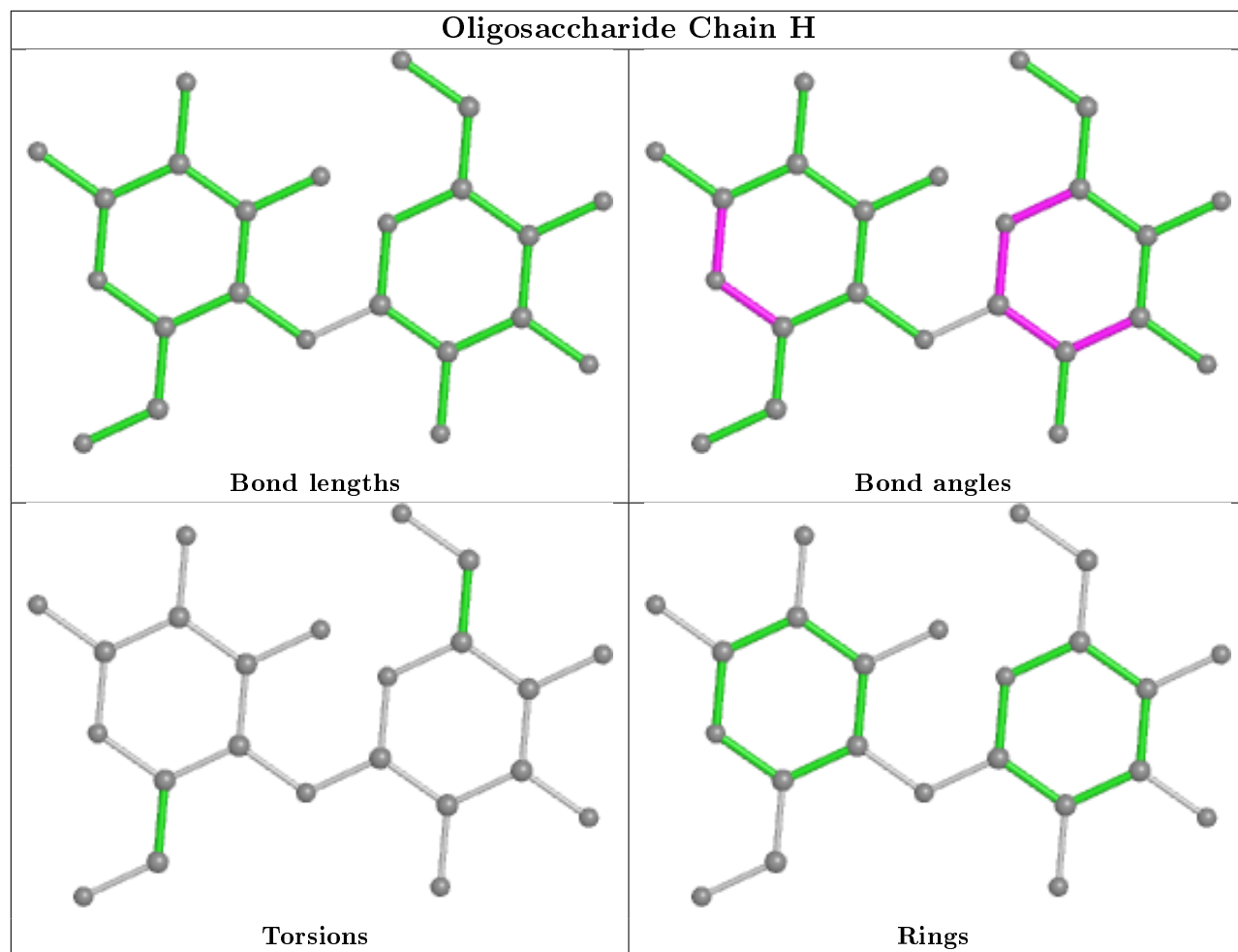
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

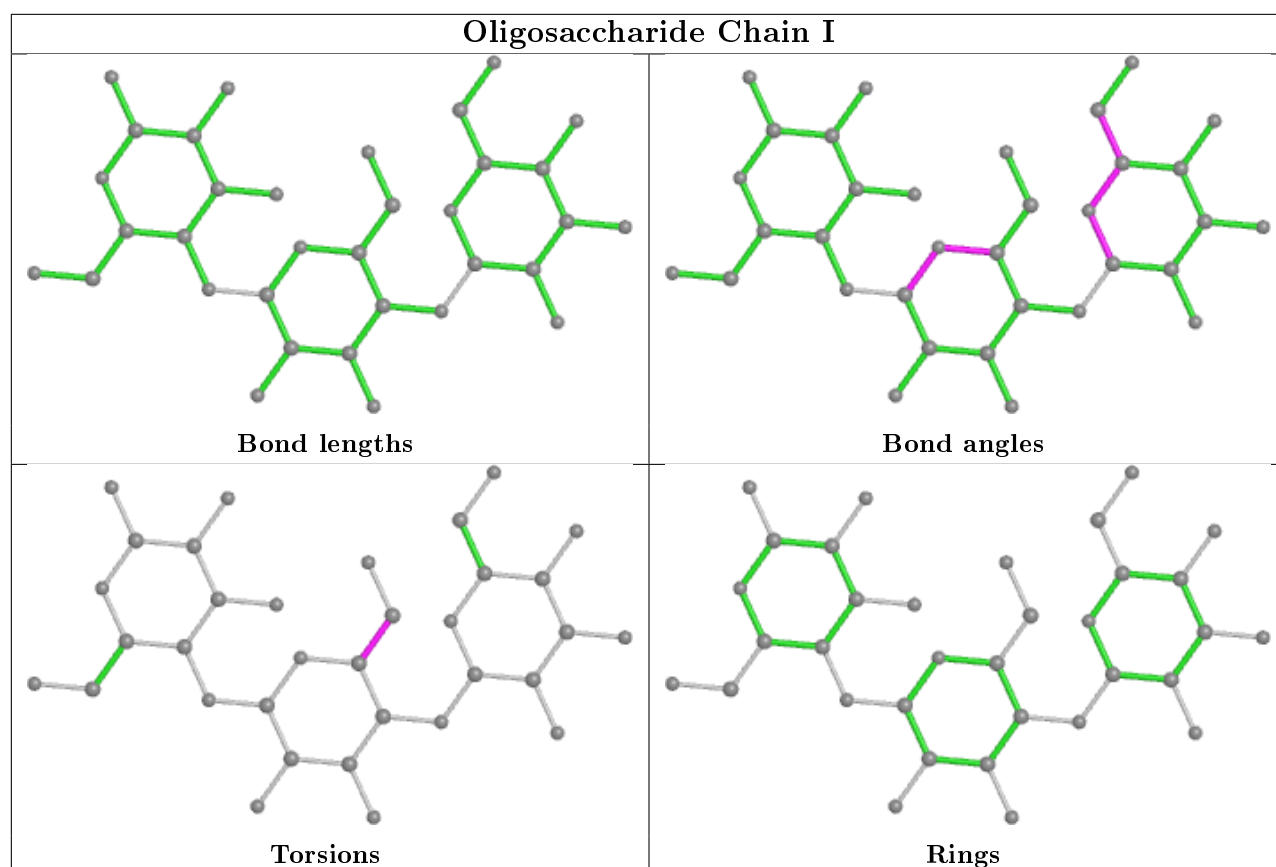












5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	B	1705	-	4,4,4	0.26	0	6,6,6	0.38	0
6	SO4	A	1705	-	4,4,4	0.34	0	6,6,6	0.11	0
6	SO4	A	1707	-	4,4,4	0.35	0	6,6,6	0.09	0
6	SO4	A	1706	-	4,4,4	0.34	0	6,6,6	0.30	0
6	SO4	B	1706	-	4,4,4	0.39	0	6,6,6	0.32	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1705	SO4	1	0
6	A	1706	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	854/854 (100%)	-0.02	6 (0%) 87 86	28, 41, 61, 82	0
1	B	854/854 (100%)	-0.08	4 (0%) 91 90	30, 41, 58, 79	0
All	All	1708/1708 (100%)	-0.05	10 (0%) 89 88	28, 41, 59, 82	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	848	THR	3.0
1	A	775	SER	2.9
1	A	1313	ASP	2.6
1	A	1310	TYR	2.5
1	B	1258	ASN	2.3
1	A	1140	SER	2.3
1	B	772	ALA	2.2
1	B	847	ASP	2.2
1	A	847	ASP	2.1
1	B	774	ASP	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 ⓘ

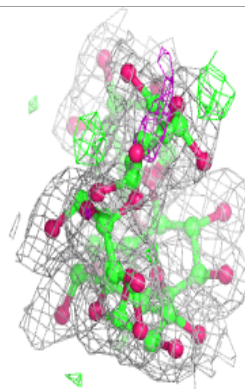
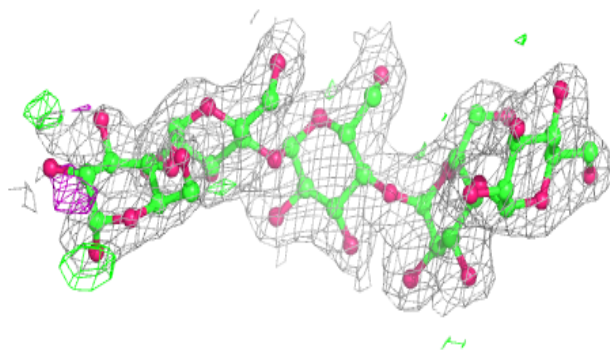
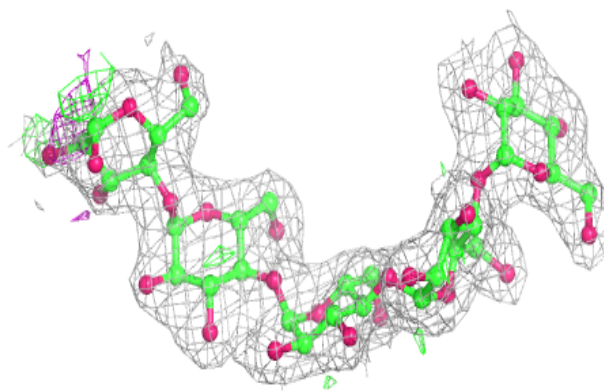
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLC	G	2	11/12	0.79	0.15	51,53,54,56	0
3	GLC	E	1	12/12	0.86	0.23	52,54,55,55	0
2	GLC	C	1	12/12	0.88	0.21	40,54,60,68	0
3	GLC	G	1	12/12	0.88	0.17	60,64,66,67	0
3	GLC	D	1	12/12	0.89	0.10	42,44,47,48	0
2	GLC	F	3	11/12	0.89	0.13	36,40,45,45	0
4	GLC	I	1	12/12	0.89	0.11	45,52,55,56	0
3	GLC	H	1	12/12	0.89	0.12	46,46,48,50	0
2	GLC	F	1	12/12	0.89	0.15	41,50,53,56	0
4	GLC	I	3	11/12	0.89	0.14	37,44,47,52	0
3	GLC	D	2	11/12	0.90	0.11	49,51,53,53	0
3	GLC	E	2	11/12	0.91	0.17	46,49,53,55	0
4	GLC	I	2	11/12	0.93	0.14	43,48,52,54	0
2	GLC	F	2	11/12	0.94	0.17	35,37,41,42	0
3	GLC	H	2	11/12	0.94	0.10	45,48,54,58	0
2	GLC	F	4	11/12	0.94	0.10	40,42,42,43	0
2	GLC	C	2	11/12	0.95	0.14	31,36,39,42	0
2	GLC	C	4	11/12	0.95	0.09	35,38,42,43	0
2	GLC	C	5	11/12	0.96	0.09	34,37,40,40	0
2	GLC	C	3	11/12	0.96	0.08	37,38,40,42	0
2	GLC	F	5	11/12	0.96	0.09	36,40,43,43	0

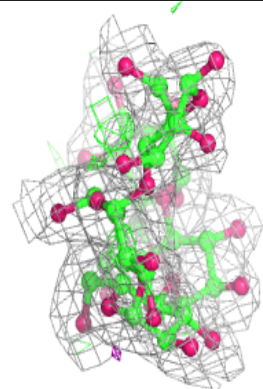
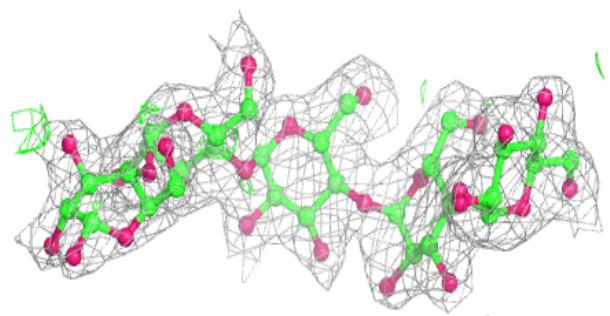
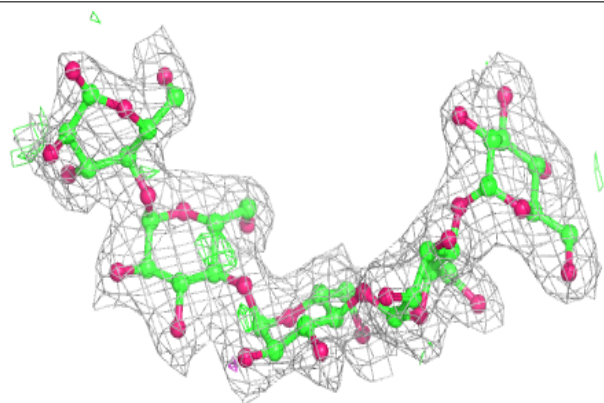
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

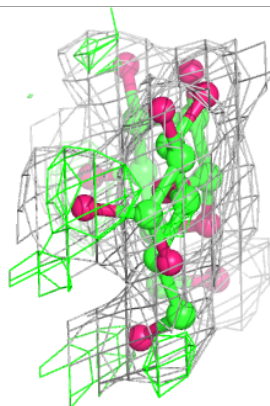
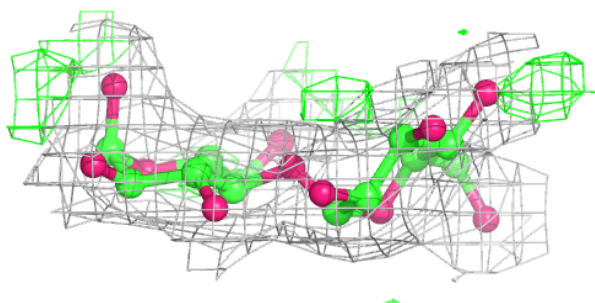
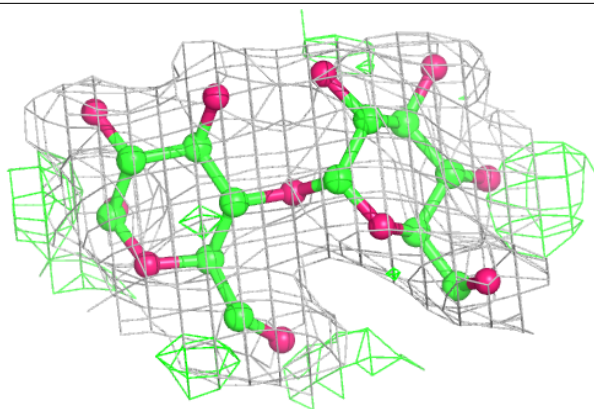
**Electron density around Chain F:**

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

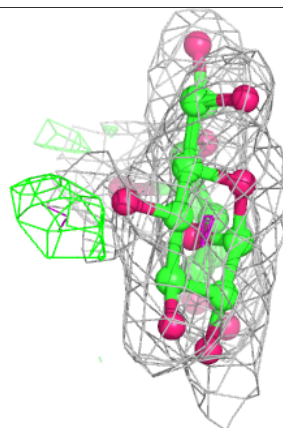
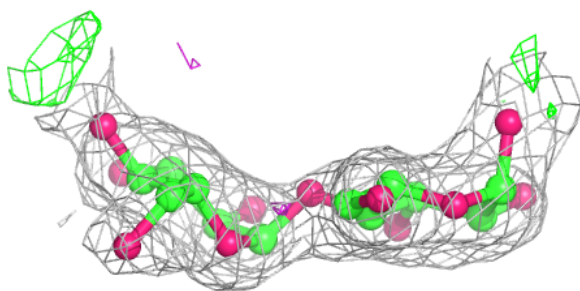
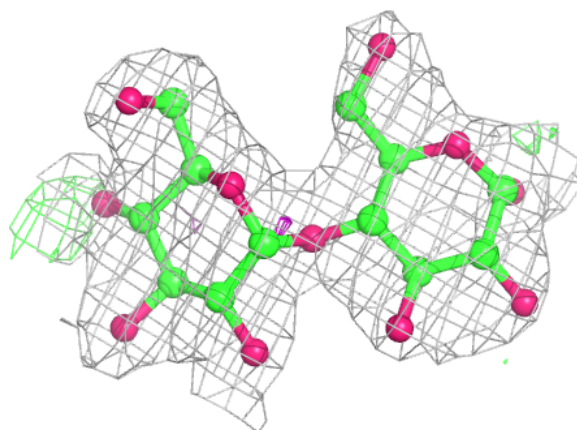


Electron density around Chain D:

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

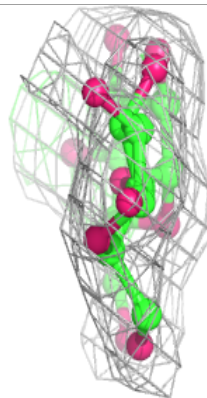
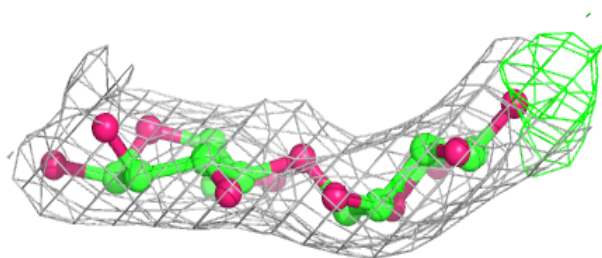
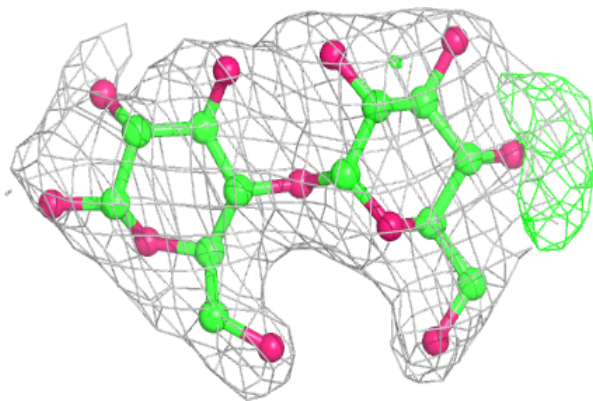
**Electron density around Chain E:**

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

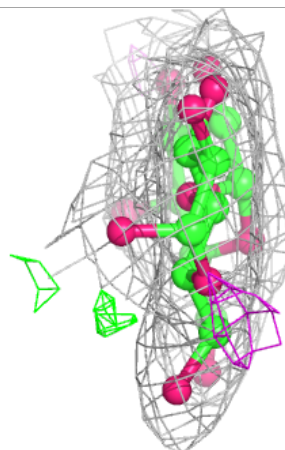
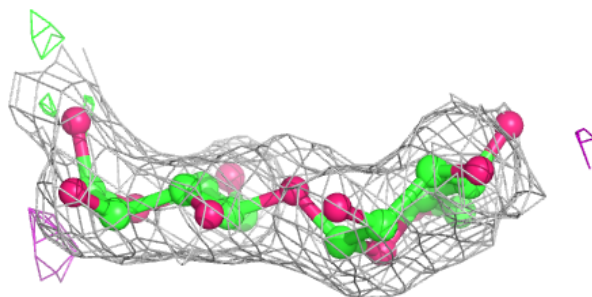
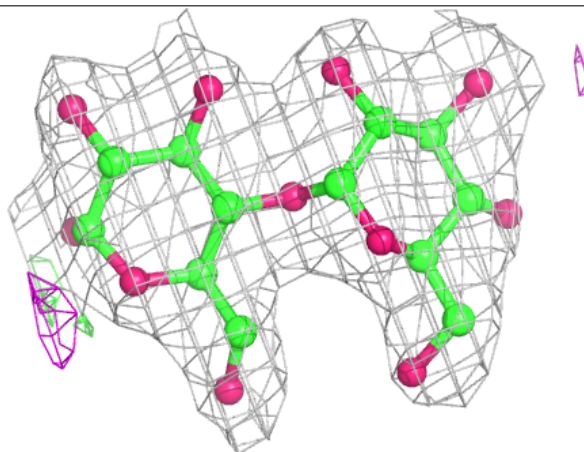


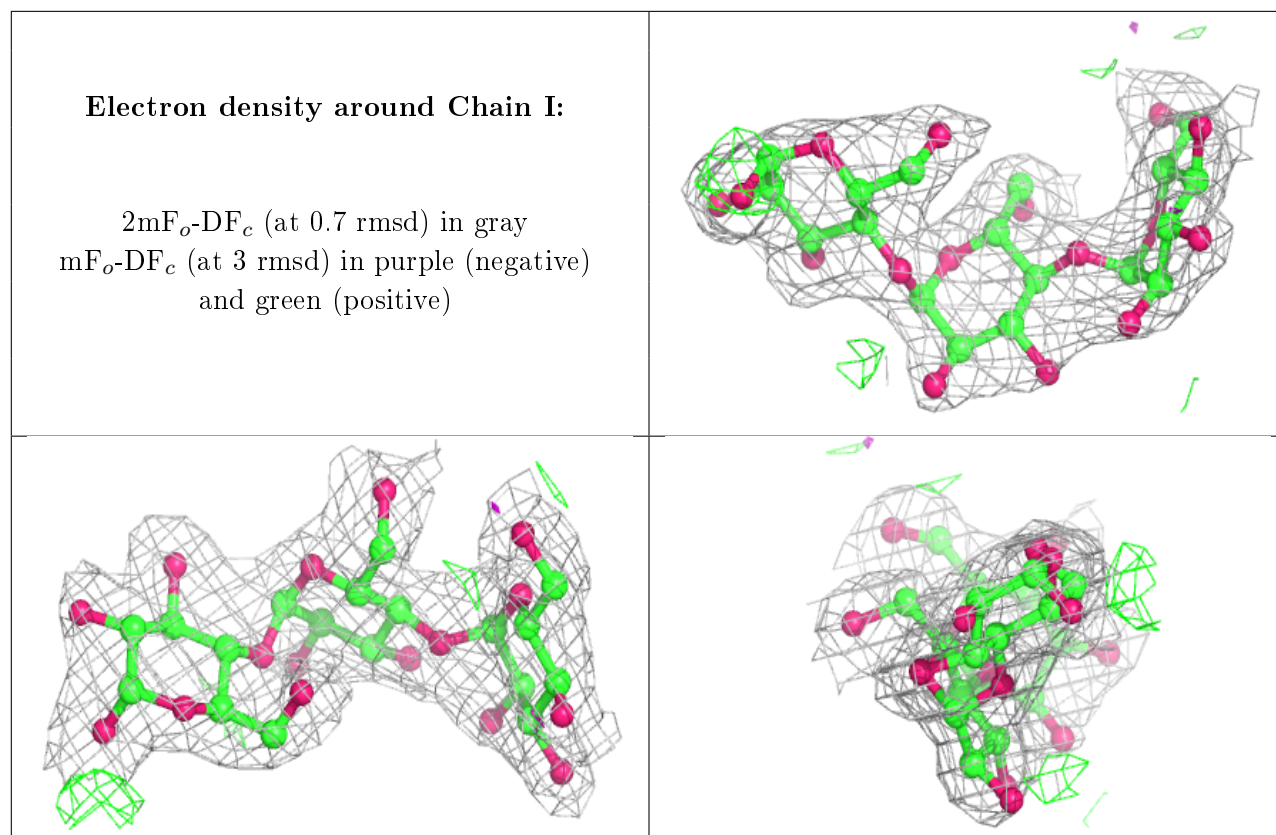
Electron density around Chain G:

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

**Electron density around Chain H:**

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
6	SO4	B	1706	5/5	0.93	0.13	65,65,69,70	0
6	SO4	A	1705	5/5	0.95	0.18	65,68,70,75	0
6	SO4	A	1707	5/5	0.95	0.10	78,80,83,84	0
6	SO4	B	1705	5/5	0.97	0.13	52,55,56,57	0
6	SO4	A	1706	5/5	0.97	0.09	68,68,68,70	0
5	CA	A	1704	1/1	0.97	0.12	28,28,28,28	0
5	CA	B	1704	1/1	0.98	0.11	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.