



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2025 – 01:18 pm BST

PDB ID : 9GV9 / pdb\_00009gv9  
Title : Structure of Heparinase I from *Bacteroides eggerthii* in complex with calcium cofactor and delta-UA(1-4)Glc 3, 6, N-Sulphated disaccharide  
Authors : Mycroft-West, C.; Wu, L.  
Deposited on : 2024-09-23  
Resolution : 1.72 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

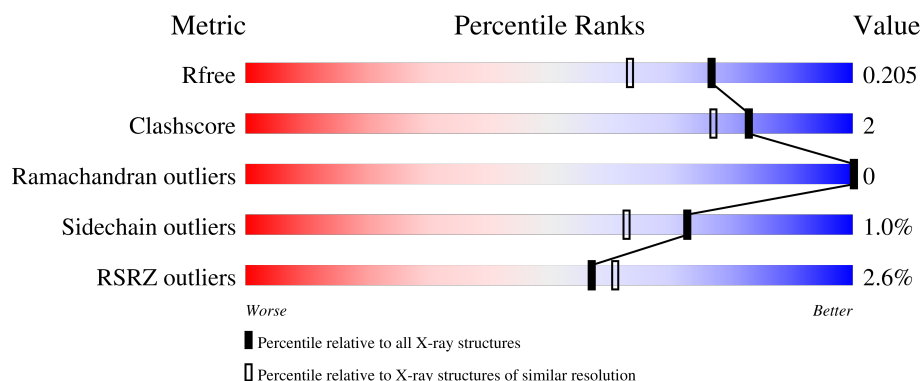
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 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))
$R_{free}$	164625	7106 (1.74-1.70)
Clashscore	180529	7746 (1.74-1.70)
Ramachandran outliers	177936	7654 (1.74-1.70)
Sidechain outliers	177891	7654 (1.74-1.70)
RSRZ outliers	164620	7104 (1.74-1.70)

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	A	382	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div></div> </div> </div>
1	B	382	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div></div> <div></div> </div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	G	2	<div> <div>50%</div> <div>50%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	410	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12526 atoms, of which 5879 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.

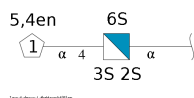
- Molecule 1 is a protein called Heparin lyase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	367	Total	C	H	N	O	S	83	0	0
			5858	1880	2914	505	549	10			
1	A	367	Total	C	H	N	O	S	85	2	0
			5877	1886	2923	508	550	10			

There are 18 discrepancies between the modelled and reference sequences:

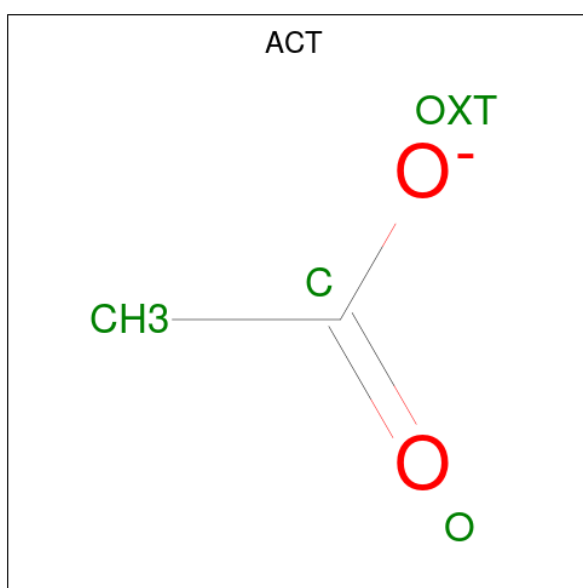
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP E5WZ15
B	375	LEU	-	expression tag	UNP E5WZ15
B	376	GLU	-	expression tag	UNP E5WZ15
B	377	HIS	-	expression tag	UNP E5WZ15
B	378	HIS	-	expression tag	UNP E5WZ15
B	379	HIS	-	expression tag	UNP E5WZ15
B	380	HIS	-	expression tag	UNP E5WZ15
B	381	HIS	-	expression tag	UNP E5WZ15
B	382	HIS	-	expression tag	UNP E5WZ15
A	1	MET	-	initiating methionine	UNP E5WZ15
A	375	LEU	-	expression tag	UNP E5WZ15
A	376	GLU	-	expression tag	UNP E5WZ15
A	377	HIS	-	expression tag	UNP E5WZ15
A	378	HIS	-	expression tag	UNP E5WZ15
A	379	HIS	-	expression tag	UNP E5WZ15
A	380	HIS	-	expression tag	UNP E5WZ15
A	381	HIS	-	expression tag	UNP E5WZ15
A	382	HIS	-	expression tag	UNP E5WZ15

- Molecule 2 is an oligosaccharide called 4-deoxy- $\alpha$ -L-threo-hex-4-enopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)- $\alpha$ -D-glucopyranose.



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	2	Total 47	C 12	H 12	N 1	O 19	S 3	1	0	0
2	G	2	Total 47	C 12	H 12	N 1	O 19	S 3	1	0	0

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	3	0
			7	2	3	2		
3	B	1	Total	C	H	O	3	0
			7	2	3	2		
3	B	1	Total	C	H	O	3	0
			7	2	3	2		
3	B	1	Total	C	H	O	3	0
			7	2	3	2		
3	A	1	Total	C	H	O	3	0
			7	2	3	2		
3	A	1	Total	C	H	O	3	0
			7	2	3	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula:  $O_4S$ ).



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

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

- Molecule 5 is CALCIUM ION (CCD ID: 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		

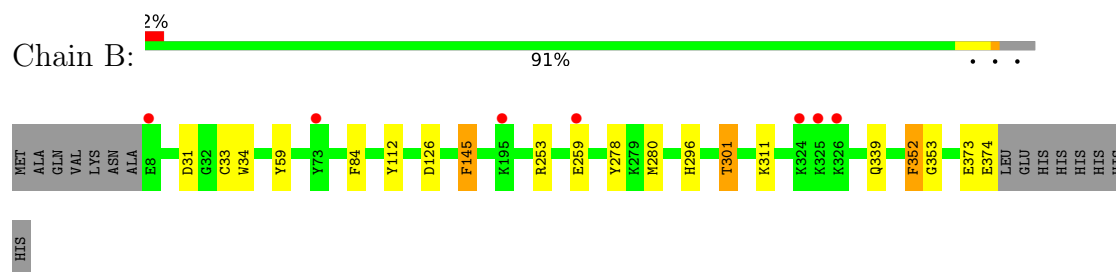
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	270	Total	O	0	0
			270	270		
6	A	308	Total	O	0	0
			308	308		

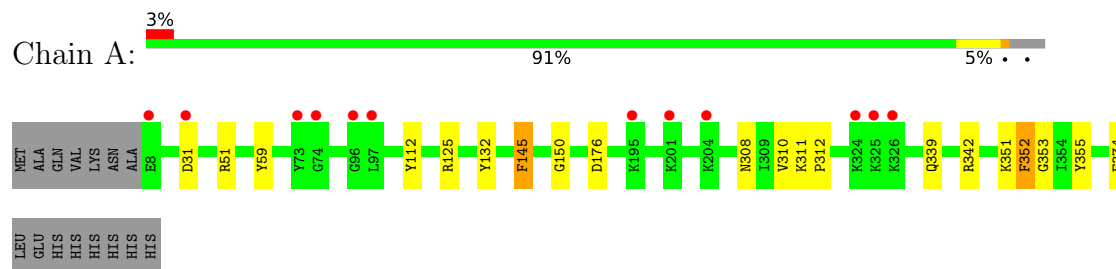
### 3 Residue-property plots [i](#)

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.

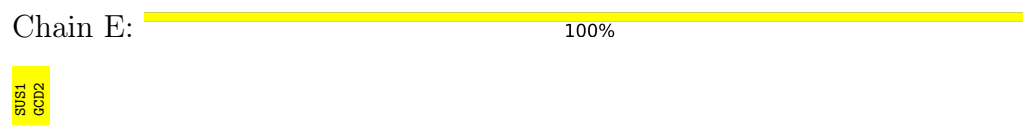
- Molecule 1: Heparin lyase I



- Molecule 1: Heparin lyase I



- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose



- Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-2-deoxy-3,6-di-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.59Å 91.56Å 73.44Å 90.00° 95.59° 90.00°	Depositor
Resolution (Å)	76.45 – 1.72 76.45 – 1.72	Depositor EDS
% Data completeness (in resolution range)	57.3 (76.45-1.72) 57.4 (76.45-1.72)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.204 , 0.241 0.205 , 0.205	Depositor DCC
$R_{free}$ test set	2782 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 31.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% 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: ACT, CA, SO4, SUS, GCD

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	0.49	0/3038	0.86	3/4105 (0.1%)
1	B	0.49	0/3019	0.85	2/4079 (0.0%)
All	All	0.49	0/6057	0.86	5/8184 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	PHE	CA-CB-CG	7.67	121.47	113.80
1	B	352	PHE	CA-CB-CG	7.57	121.37	113.80
1	A	145	PHE	CA-CB-CG	5.47	119.27	113.80
1	A	176	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	145	PHE	CA-CB-CG	5.39	119.19	113.80

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	2954	2923	2902	12	0
1	B	2944	2914	2906	14	0
2	E	35	12	12	0	0
2	G	35	12	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	6	6	0	0
3	B	16	12	12	0	0
4	A	40	0	0	2	0
4	B	35	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	308	0	0	3	1
6	B	270	0	0	3	1
All	All	6647	5879	5850	27	1

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 2.

All (27) 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:31:ASP:OD2	1:A:59:TYR:OH	2.00	0.79
1:B:31:ASP:OD2	1:B:59:TYR:OH	1.99	0.77
1:A:351:LYS:NZ	4:A:410:SO4:O2	2.33	0.61
4:B:409:SO4:O4	6:B:501:HOH:O	2.16	0.59
1:B:301:THR:HG23	1:B:311:LYS:H	1.67	0.59
1:A:374:GLU:HA	6:A:605:HOH:O	2.06	0.55
1:B:373:GLU:O	1:B:374:GLU:C	2.55	0.50
1:A:312:PRO:HB3	6:A:517:HOH:O	2.15	0.47
1:A:339:GLN:OE1	1:A:339:GLN:HA	2.15	0.47
1:B:339:GLN:HA	1:B:339:GLN:OE1	2.15	0.46
1:B:259:GLU:HG3	6:B:573:HOH:O	2.15	0.45
1:B:278:TYR:OH	1:B:280:MET:HE2	2.17	0.44
1:B:145:PHE:HA	1:B:353:GLY:O	2.18	0.43
1:A:145:PHE:HA	1:A:353:GLY:O	2.18	0.43
1:A:51:ARG:HD3	1:A:132:TYR:CD1	2.54	0.43
1:B:33:CYS:HG	1:B:34:TRP:CD1	2.37	0.43
1:A:339:GLN:NE2	6:A:517:HOH:O	2.50	0.43
1:A:125:ARG:HG3	1:A:374:GLU:HG2	2.01	0.42
1:B:253:ARG:HH21	2:G:2:GCD:C6	2.32	0.41
1:A:355:TYR:CZ	4:A:410:SO4:O3	2.73	0.41
1:B:374:GLU:HB3	6:B:718:HOH:O	2.20	0.41
1:A:150:GLY:HA3	1:A:342:ARG:HD3	2.02	0.41
1:B:34:TRP:CE3	1:B:84:PHE:HB3	2.56	0.41
1:A:310:VAL:HG12	1:A:311:LYS:HG3	2.02	0.40
1:B:126:ASP:OD1	1:B:296:HIS:ND1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:THR:CG2	1:B:311:LYS:HB2	2.51	0.40
1:B:301:THR:HG23	1:B:311:LYS:N	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:709:HOH:O	6:A:725:HOH:O[1_556]	2.08	0.12

## 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	367/382 (96%)	356 (97%)	11 (3%)	0	100	100
1	B	365/382 (96%)	356 (98%)	9 (2%)	0	100	100
All	All	732/764 (96%)	712 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	317/328 (97%)	314 (99%)	3 (1%)	75	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	315/328 (96%)	312 (99%)	3 (1%)	73	63
All	All	632/656 (96%)	626 (99%)	6 (1%)	73	67

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	112	TYR
1	B	301	THR
1	B	352	PHE
1	A	112	TYR
1	A	308	ASN
1	A	352	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	GLN
1	A	46	GLN

### 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 ⓘ

4 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	SUS	E	1	2	23,24,24	1.24	3 (13%)	26,38,38	1.46	3 (11%)
2	GCD	E	2	2	10,11,12	0.88	0	13,15,17	1.27	2 (15%)
2	SUS	G	1	2	23,24,24	1.25	3 (13%)	26,38,38	1.61	5 (19%)
2	GCD	G	2	2	10,11,12	0.81	0	13,15,17	1.08	1 (7%)

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	SUS	E	1	2	-	0/16/36/36	0/1/1/1
2	GCD	E	2	2	-	4/4/17/20	0/1/1/1
2	SUS	G	1	2	-	0/16/36/36	0/1/1/1
2	GCD	G	2	2	-	4/4/17/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	SUS	O3S-S1	3.58	1.46	1.42
2	E	1	SUS	O1S-S1	3.37	1.46	1.42
2	E	1	SUS	O3S-S1	3.37	1.46	1.42
2	G	1	SUS	O1S-S1	3.10	1.45	1.42
2	G	1	SUS	S1-N2	2.49	1.62	1.59
2	E	1	SUS	S1-N2	2.38	1.62	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	SUS	O3S-S1-N2	-4.34	100.96	108.87
2	G	1	SUS	O1S-S1-O3S	-3.44	112.04	120.16
2	G	1	SUS	C1-C2-N2	3.42	114.75	110.67
2	G	1	SUS	O3S-S1-N2	-3.20	103.04	108.87
2	G	1	SUS	O5-C1-C2	3.09	112.62	109.52
2	E	1	SUS	O1S-S1-O3S	-3.03	113.00	120.16
2	E	2	GCD	O6A-C6-C5	-2.56	113.70	120.48
2	G	2	GCD	O6B-C6-O6A	2.14	128.49	123.61
2	E	2	GCD	O6B-C6-O6A	2.13	128.48	123.61
2	E	1	SUS	O5-C1-C2	2.13	111.65	109.52
2	G	1	SUS	O6S-S2-O5S	2.03	115.55	108.49

There are no chirality outliers.

All (8) torsion outliers are listed below:

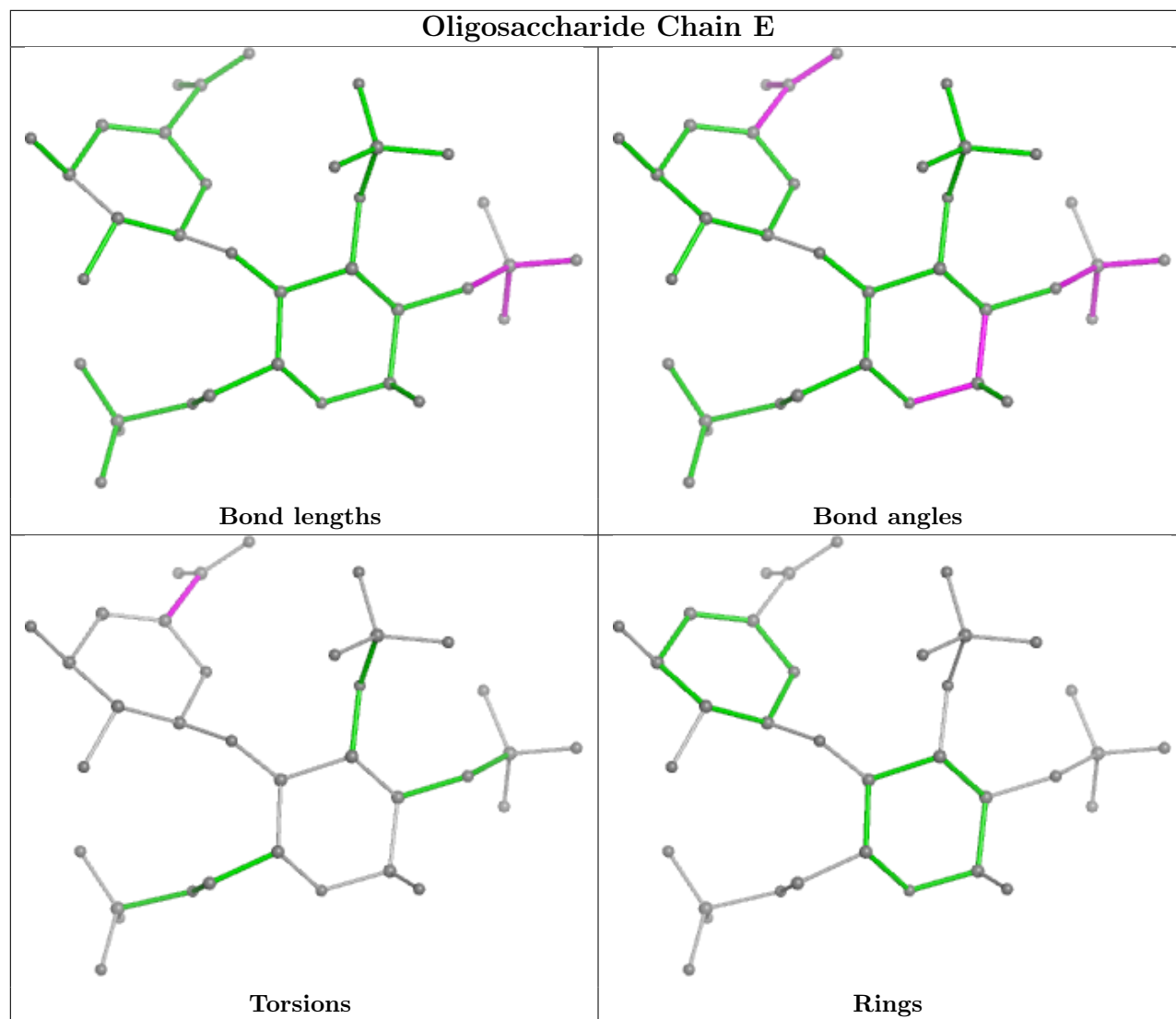
Mol	Chain	Res	Type	Atoms
2	E	2	GCD	C4-C5-C6-O6A
2	E	2	GCD	C4-C5-C6-O6B
2	E	2	GCD	O5-C5-C6-O6A
2	E	2	GCD	O5-C5-C6-O6B
2	G	2	GCD	C4-C5-C6-O6A
2	G	2	GCD	C4-C5-C6-O6B
2	G	2	GCD	O5-C5-C6-O6A
2	G	2	GCD	O5-C5-C6-O6B

There are no ring outliers.

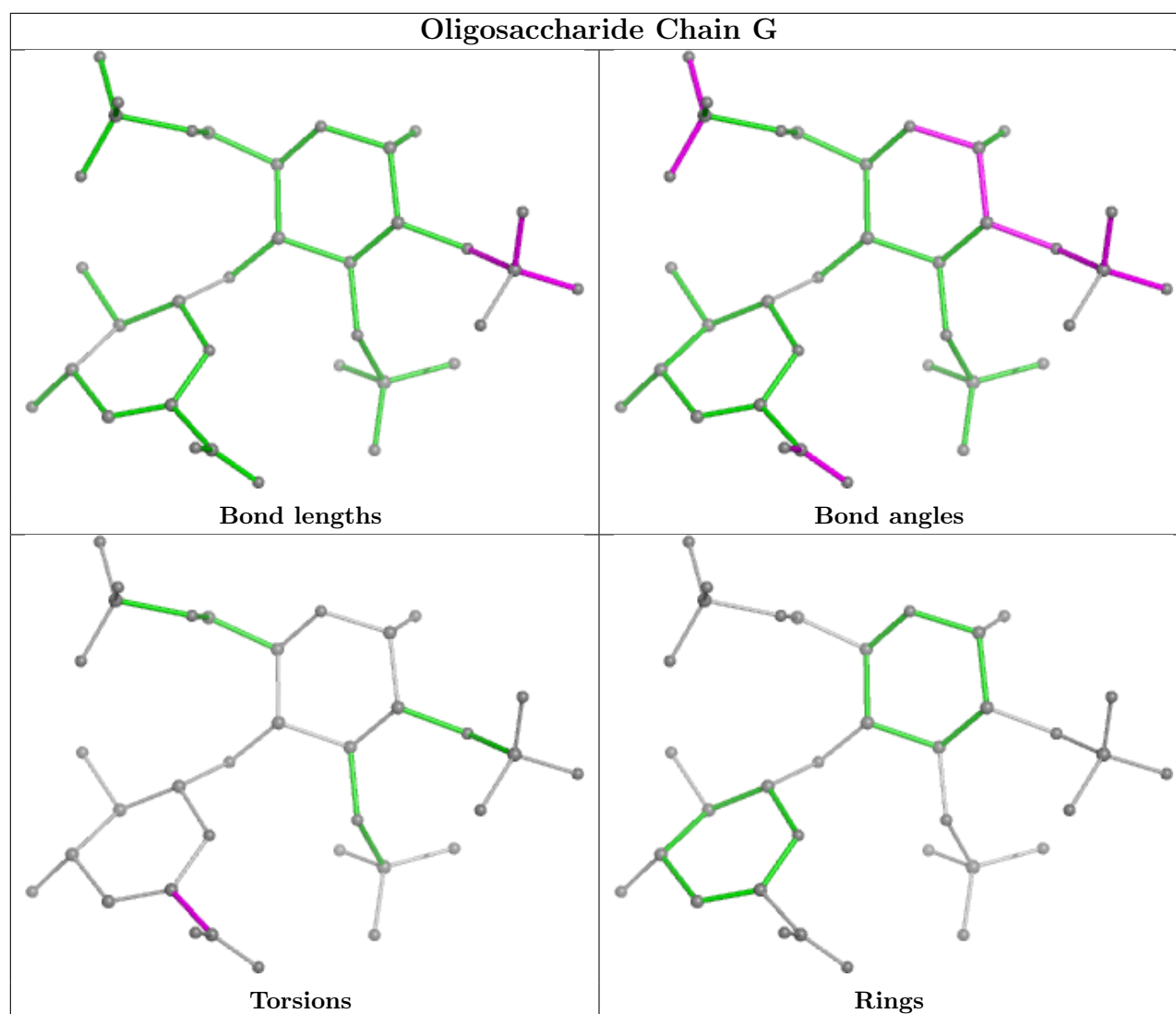
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	GCD	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](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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	$\# Z  > 2$
4	SO4	A	404	-	4,4,4	0.38	0	6,6,6	0.06	0
3	ACT	A	402	-	3,3,3	1.17	0	3,3,3	0.69	0
3	ACT	B	401	-	3,3,3	0.99	0	3,3,3	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACT	A	401	-	3,3,3	0.81	0	3,3,3	0.85	0
3	ACT	B	402	-	3,3,3	0.86	0	3,3,3	0.94	0
4	SO4	B	411	-	4,4,4	0.36	0	6,6,6	0.06	0
4	SO4	B	407	-	4,4,4	0.37	0	6,6,6	0.14	0
4	SO4	A	403	-	4,4,4	0.47	0	6,6,6	0.18	0
4	SO4	A	408	-	4,4,4	0.40	0	6,6,6	0.06	0
4	SO4	B	408	-	4,4,4	0.46	0	6,6,6	0.07	0
3	ACT	B	404	-	3,3,3	1.08	0	3,3,3	0.78	0
4	SO4	B	409	-	4,4,4	0.39	0	6,6,6	0.07	0
4	SO4	B	406	-	4,4,4	0.40	0	6,6,6	0.09	0
4	SO4	A	406	-	4,4,4	0.40	0	6,6,6	0.10	0
4	SO4	A	407	-	4,4,4	0.38	0	6,6,6	0.08	0
4	SO4	A	409	-	4,4,4	0.31	0	6,6,6	0.08	0
4	SO4	B	410	-	4,4,4	0.39	0	6,6,6	0.07	0
4	SO4	A	405	-	4,4,4	0.39	0	6,6,6	0.06	0
4	SO4	A	410	-	4,4,4	0.38	0	6,6,6	0.18	0
4	SO4	B	405	-	4,4,4	0.40	0	6,6,6	0.07	0
3	ACT	B	403	-	3,3,3	1.09	0	3,3,3	0.71	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	409	SO4	1	0
4	A	410	SO4	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	367/382 (96%)	0.04	12 (3%) 49 54	7, 17, 35, 58	1 (0%)
1	B	367/382 (96%)	0.04	7 (1%) 66 70	9, 18, 34, 56	1 (0%)
All	All	734/764 (96%)	0.04	19 (2%) 57 61	7, 17, 35, 58	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	GLY	3.8
1	A	325	LYS	3.6
1	A	324	LYS	3.4
1	B	324	LYS	3.1
1	A	97	LEU	3.0
1	B	8	GLU	2.9
1	B	73	TYR	2.8
1	B	326	LYS	2.7
1	A	204	LYS	2.4
1	B	195	LYS	2.3
1	A	326	LYS	2.3
1	A	195	LYS	2.2
1	A	8	GLU	2.2
1	B	325	LYS	2.1
1	A	201	LYS	2.1
1	A	74	GLY	2.1
1	A	73	TYR	2.1
1	B	259	GLU	2.0
1	A	31	ASP	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

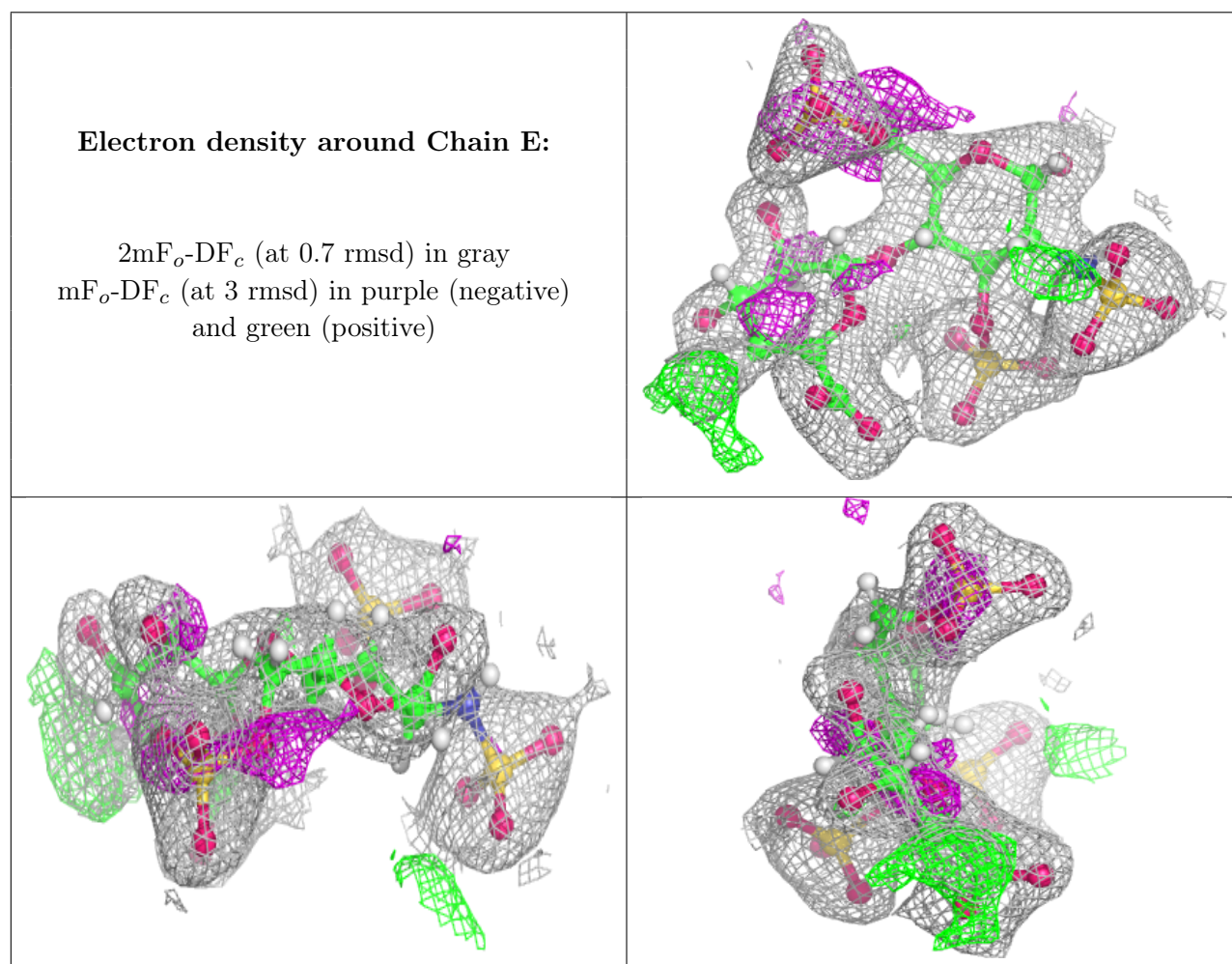
There are no non-standard protein/DNA/RNA residues in this entry.

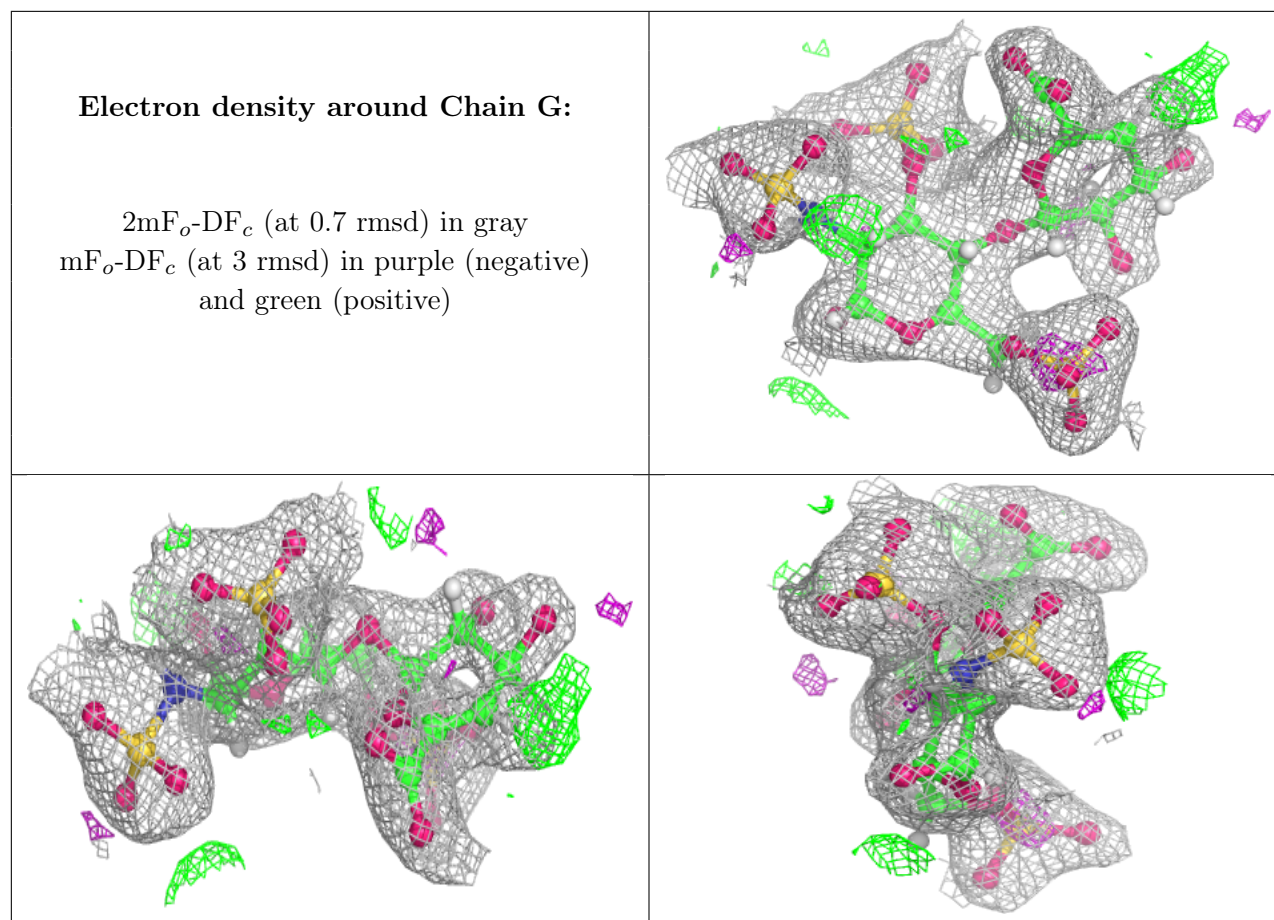
### 6.3 Carbohydrates ⓘ

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	SUS	E	1	24/24	-	-	23,26,29,30	1
2	GCD	E	2	11/12	-	-	28,31,32,33	0
2	SUS	G	1	24/24	-	-	23,25,29,30	1
2	GCD	G	2	11/12	-	-	27,29,30,31	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.





## 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, 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
4	SO4	B	411	5/5	0.72	0.20	33,33,33,34	5
3	ACT	A	402	4/4	0.77	0.18	30,30,35,37	3
3	ACT	B	403	4/4	0.81	0.22	30,30,33,34	3
4	SO4	B	406	5/5	0.84	0.17	26,26,27,28	5
3	ACT	B	402	4/4	0.86	0.17	30,30,32,33	3
4	SO4	A	404	5/5	0.86	0.18	22,22,23,24	5
4	SO4	B	409	5/5	0.88	0.16	30,30,31,31	5
4	SO4	A	407	5/5	0.88	0.13	25,26,27,28	5
4	SO4	A	410	5/5	0.88	0.17	28,31,31,31	5
3	ACT	B	404	4/4	0.89	0.15	27,30,30,30	3
4	SO4	A	408	5/5	0.90	0.20	28,28,29,30	5
4	SO4	B	407	5/5	0.91	0.12	26,27,28,29	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	A	401	4/4	0.92	0.10	15,16,30,30	3
4	SO4	B	408	5/5	0.92	0.13	23,24,24,25	5
4	SO4	A	406	5/5	0.93	0.17	31,32,35,35	0
4	SO4	B	410	5/5	0.93	0.11	32,32,33,33	5
3	ACT	B	401	4/4	0.95	0.10	16,17,30,30	3
4	SO4	A	405	5/5	0.95	0.08	33,33,35,36	0
4	SO4	A	409	5/5	0.96	0.10	30,30,32,33	0
4	SO4	A	403	5/5	0.96	0.08	26,27,28,29	0
4	SO4	B	405	5/5	0.98	0.05	24,25,25,26	0
5	CA	B	412	1/1	1.00	0.01	12,12,12,12	0
5	CA	A	411	1/1	1.00	0.01	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.