



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 18, 2025 – 05:16 PM EDT

PDB ID : 9BEV / pdb\_00009bev  
Title : Structure of GH110A in complex with a lambda-carrageenan oligosaccharide  
Authors : Hettle, J.A.; Vickers, C.; Boraston, A.B.  
Deposited on : 2024-04-16  
Resolution : 2.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

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<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 Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

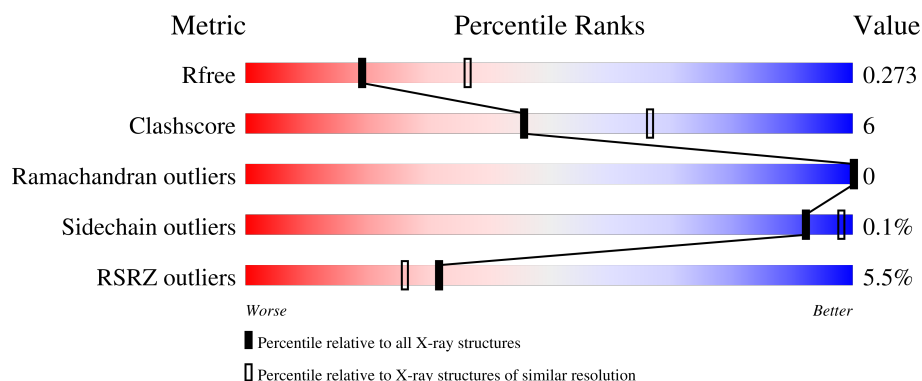
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	600	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div></div> </div> </div>
1	B	600	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div></div> </div> </div>
2	G	3	<div> <div></div> <div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>
2	H	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </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
3	CL	A	702	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9591 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 GH110A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4549	2885	782	874	8			
1	B	577	Total	C	N	O	S	0	1	0
			4565	2904	777	876	8			

- Molecule 2 is an oligosaccharide called 6-O-sulfo-alpha-D-galactopyranose-(1-3)-2-O-sulfo-beta-D-galactopyranose-(1-4)-2,6-di-O-sulfo-alpha-D-galactopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	H	3	Total	C	O	S	0	0	0
			50	18	28	4			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		
3	B	4	Total	Cl	0	0
			4	4		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

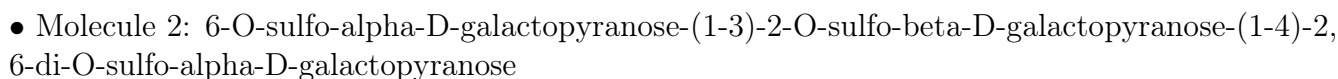
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	168	Total 168	O 168	0	0
5	B	200	Total 200	O 200	0	0



- Molecule 1: GH110A



Chain G:  33% 33% 33%



- Molecule 2: 6-O-sulfo-alpha-D-galactopyranose-(1-3)-2-O-sulfo-beta-D-galactopyranose-(1-4)-2,6-di-O-sulfo-alpha-D-galactopyranose

Chain H:  67% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.51Å 77.48Å 116.04Å 90.00° 113.21° 90.00°	Depositor
Resolution (Å)	28.81 – 2.59 28.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.3 (28.81-2.59) 96.3 (28.81-2.59)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.236 , 0.272 0.237 , 0.273	Depositor DCC
$R_{free}$ test set	2819 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9591	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.17% 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: MG, CL, A1APB, A1APC, A1APD

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	0.10	0/4650	0.30	0/6312
1	B	0.10	0/4671	0.30	0/6338
All	All	0.10	0/9321	0.30	0/12650

There are no bond length outliers.

There are no bond angle outliers.

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	4549	0	4333	53	0
1	B	4565	0	4346	48	0
2	G	50	0	0	1	0
2	H	50	0	0	1	0
3	A	3	0	0	2	0
3	B	4	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	168	0	0	1	0
5	B	200	0	0	1	0
All	All	9591	0	8679	102	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 6.

The worst 5 of 102 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:59:LYS:NZ	5:A:801:HOH:O	2.16	0.77
1:B:186:LEU:HD22	1:B:431:ARG:HG3	1.68	0.76
1:A:186:LEU:HD22	1:A:431:ARG:HG3	1.77	0.67
1:B:100:GLY:HA3	1:B:127:ILE:HG23	1.76	0.67
1:B:422:MET:HE1	1:B:435:VAL:HG21	1.78	0.66

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	575/600 (96%)	551 (96%)	24 (4%)	0	100	100
1	B	576/600 (96%)	554 (96%)	22 (4%)	0	100	100
All	All	1151/1200 (96%)	1105 (96%)	46 (4%)	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	488/533 (92%)	488 (100%)	0	100	100
1	B	488/533 (92%)	487 (100%)	1 (0%)	92	98
All	All	976/1066 (92%)	975 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	324	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	161	GLN
1	B	496	ASN
1	B	527	ASN
1	A	280	GLN
1	A	373	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 ⓘ

6 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	A1APD	G	1	2	20,20,20	1.07	0	27,31,31	0.89	1 (3%)
2	A1APB	G	2	2	15,15,16	1.12	1 (6%)	17,22,24	0.93	1 (5%)
2	A1APC	G	3	2	15,15,16	0.92	0	21,22,24	0.72	0
2	A1APD	H	1	2	20,20,20	1.09	0	27,31,31	0.90	0
2	A1APB	H	2	2	15,15,16	1.11	1 (6%)	17,22,24	0.94	1 (5%)
2	A1APC	H	3	2	15,15,16	0.95	0	21,22,24	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1APD	G	1	2	-	1/11/31/31	0/1/1/1
2	A1APB	G	2	2	-	3/7/24/27	0/1/1/1
2	A1APC	G	3	2	-	0/6/23/26	0/1/1/1
2	A1APD	H	1	2	-	8/11/31/31	0/1/1/1
2	A1APB	H	2	2	-	3/7/24/27	0/1/1/1
2	A1APC	H	3	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	A1APB	O2-C2	-2.68	1.43	1.47
2	G	2	A1APB	O2-C2	-2.51	1.43	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	A1APB	O2-C2-C3	2.46	110.39	106.95
2	G	2	A1APB	O2-C2-C3	2.45	110.37	106.95
2	G	1	A1APD	O5-C5-C6	2.20	111.07	106.69

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	A1APD	O5-C5-C6-O6
2	H	2	A1APB	C2-O2-S1-O8
2	H	2	A1APB	C2-O2-S1-O9

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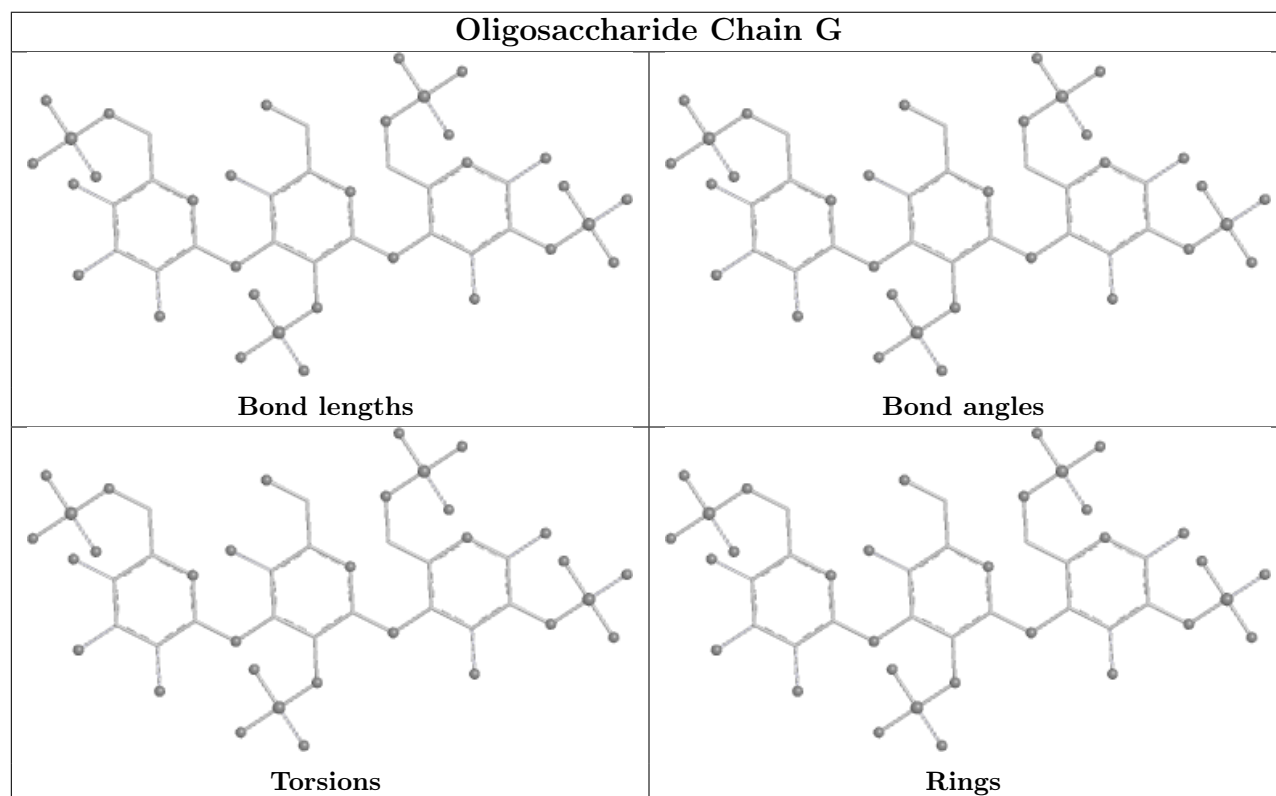
Mol	Chain	Res	Type	Atoms
2	G	2	A1APB	C2-O2-S1-O7
2	G	2	A1APB	C2-O2-S1-O8

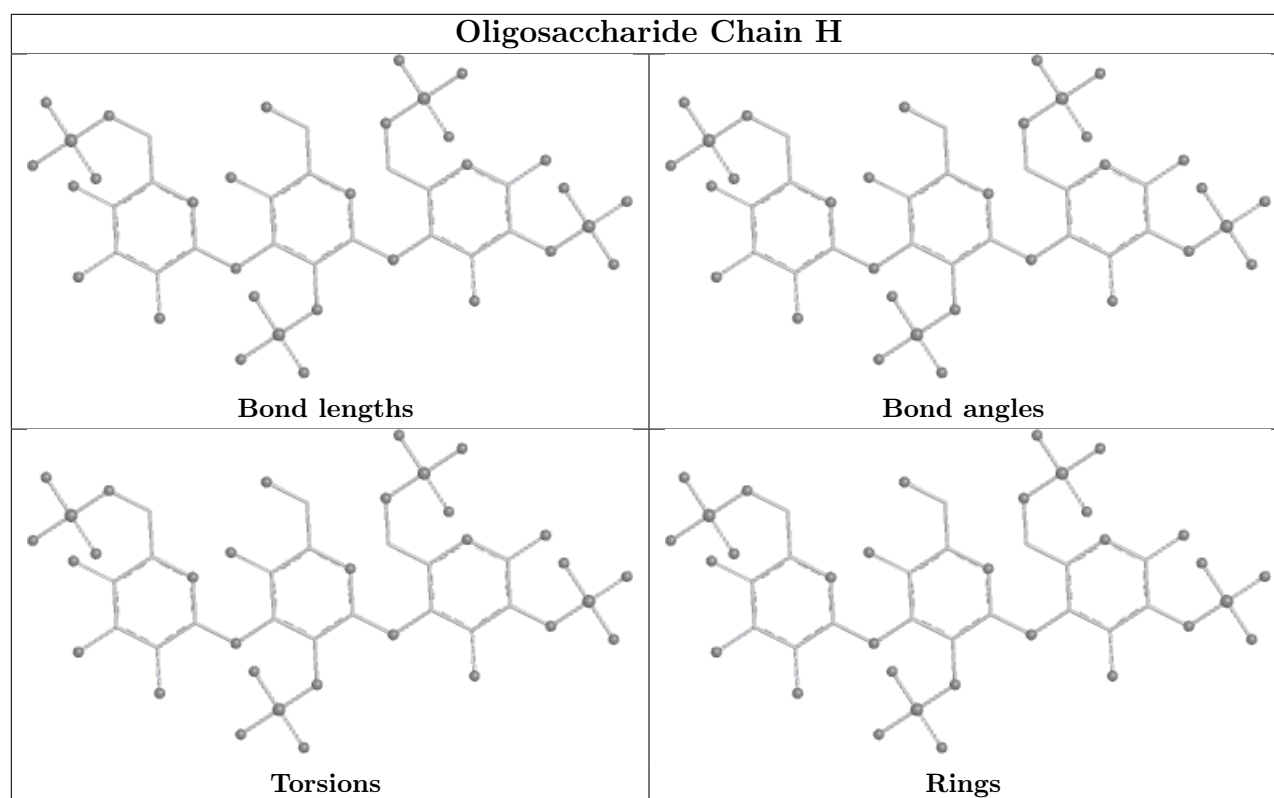
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	2	A1APB	1	0
2	H	2	A1APB	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 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

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.

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 [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	577/600 (96%)	0.69	32 (5%) 32 26	34, 48, 73, 87	0
1	B	577/600 (96%)	0.63	31 (5%) 32 27	25, 46, 64, 80	2 (0%)
All	All	1154/1200 (96%)	0.66	63 (5%) 32 26	25, 47, 68, 87	2 (0%)

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352[A]	PHE	5.4
1	A	432	ALA	5.0
1	B	432	ALA	4.9
1	A	203	LYS	3.5
1	A	470	GLY	3.4

### 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 [i](#)

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

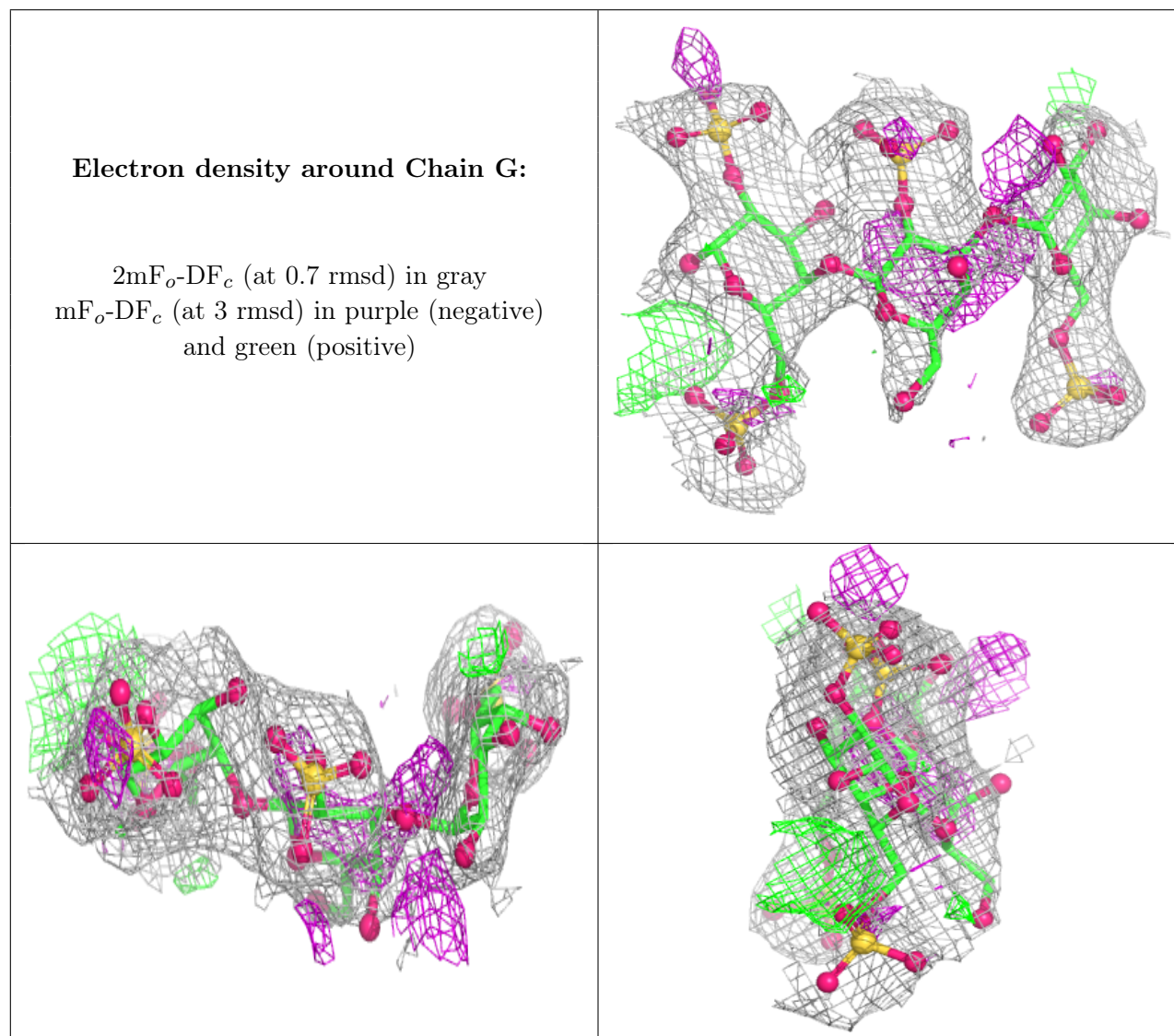
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	A1APD	G	1	20/20	-	-	73,84,114,133	0
2	A1APB	G	2	15/16	-	-	59,63,72,74	0
2	A1APC	G	3	15/16	-	-	46,50,53,55	0
2	A1APD	H	1	20/20	-	-	75,91,119,132	0
2	A1APB	H	2	15/16	-	-	62,71,78,80	0

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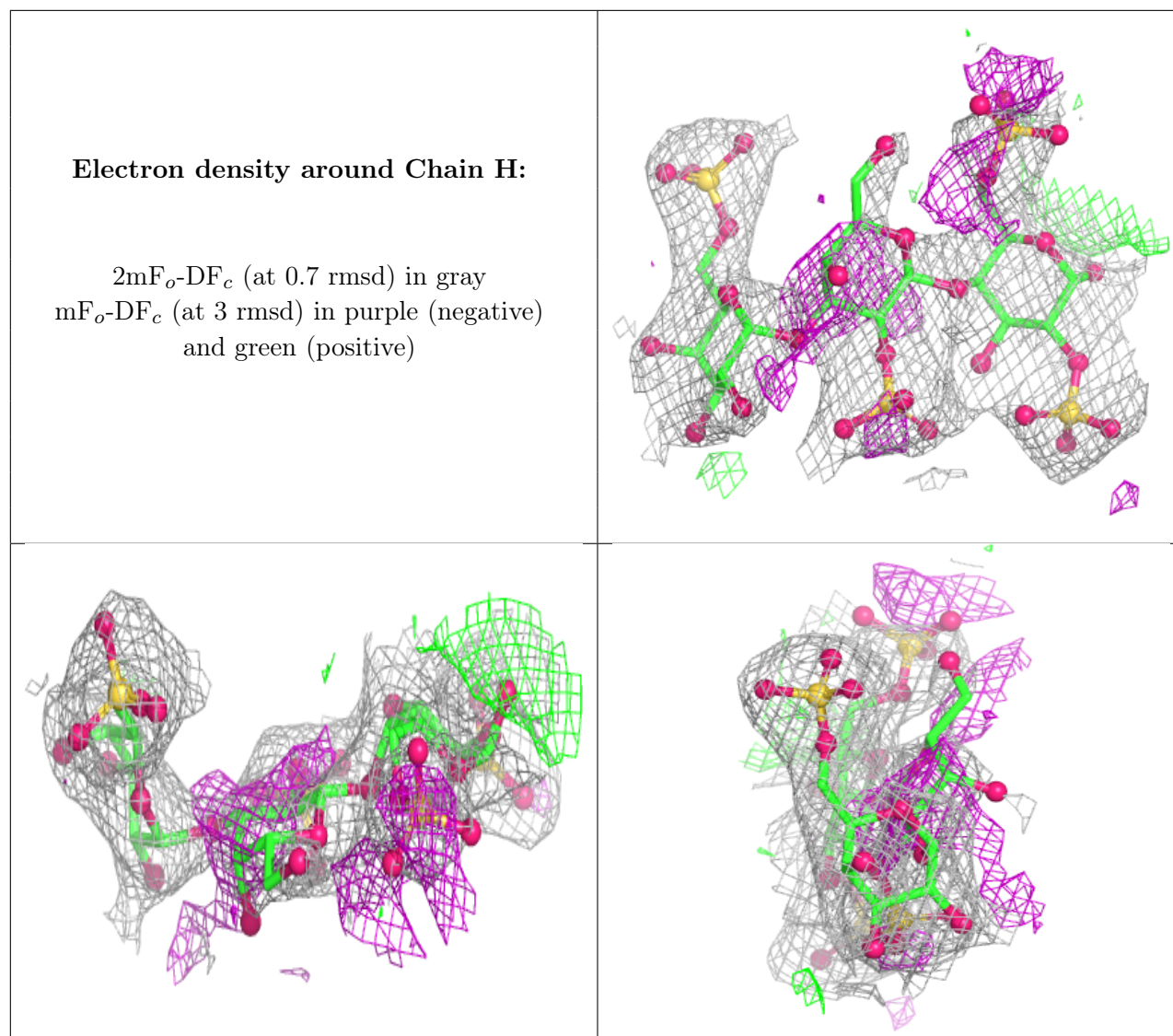
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1APC	H	3	15/16	-	-	47,52,54,55	0

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
3	CL	B	704	1/1	0.86	0.12	71,71,71,71	0
4	MG	A	704	1/1	0.91	0.07	42,42,42,42	0
3	CL	B	702	1/1	0.93	0.08	55,55,55,55	0
3	CL	B	701	1/1	0.94	0.06	49,49,49,49	0
3	CL	A	702	1/1	0.94	0.08	54,54,54,54	0
3	CL	A	703	1/1	0.95	0.11	68,68,68,68	0
3	CL	B	703	1/1	0.96	0.06	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	A	701	1/1	0.97	0.07	50,50,50,50	0
4	MG	B	705	1/1	0.98	0.03	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.