



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 04:10 PM BST

PDB ID : 1E6S  
Title : MYROSINASE FROM SINAPIS ALBA with bound gluco-hydroximolactam and sulfate  
Authors : Burmeister, W.P.  
Deposited on : 2000-08-23  
Resolution : 1.35 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)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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

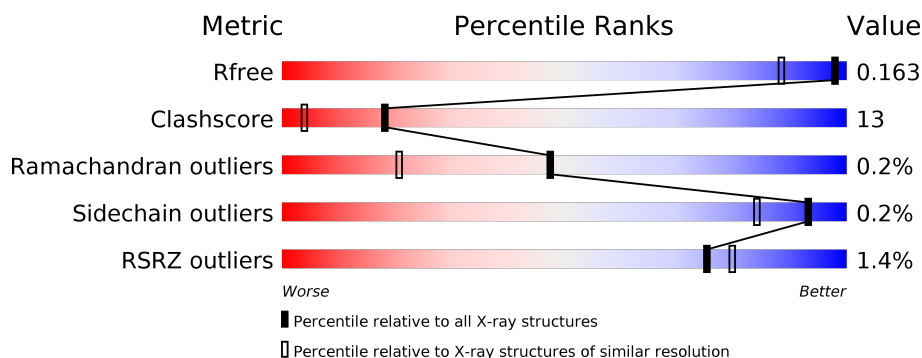
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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  $\geq 3$ , 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	M	501	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, orange 14%, yellow 83%, green 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">83% 14% .</div> </div> </div>
2	A	2	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, yellow 50%, orange 50%, red 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">50% 50%</div> </div> </div>
3	B	5	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, yellow 80%, orange 20%, red 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">80% 20%</div> </div> </div>
4	C	7	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, yellow 57%, orange 43%, red 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">57% 43%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BMA	C	3	-	-	X	-
4	MAN	C	6	X	-	X	-
5	NAG	M	905	-	-	X	-
5	NAG	M	918	-	-	-	X
5	NAG	M	919	-	-	-	X
8	SO4	M	925[A]	-	X	-	-
8	SO4	M	925[B]	-	-	X	-
8	SO4	M	927	-	X	-	-

## 2 Entry composition [i](#)

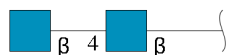
There are 10 unique types of molecules in this entry. The entry contains 5207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MYROSINASE MA1.

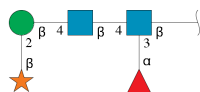
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	499	Total	C	N	O	S	0	21	0
			4082	2618	660	788	16			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



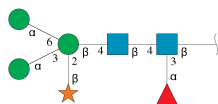
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



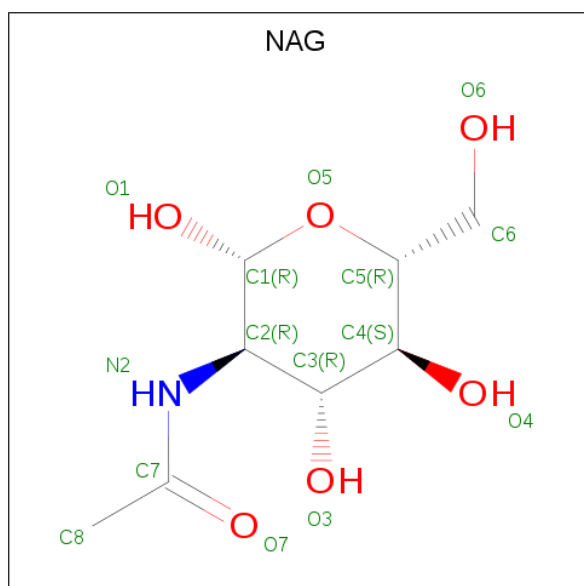
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	5	Total	C	N	O	0	0	0
			58	33	2	23			

- Molecule 4 is an oligosaccharide called beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



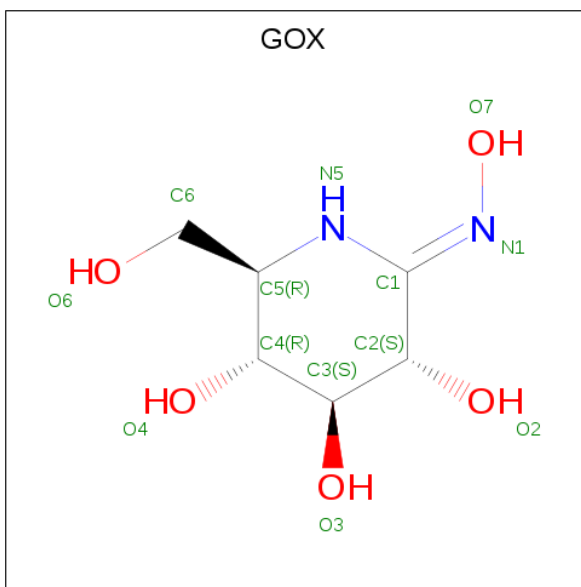
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	7	Total	C	N	O	0	0	0
			80	45	2	33			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is (2S,3S,4R,5R)-6-(HYDROXYAMINO)-2-(HYDROXYMETHYL)-2,3,4,5-TE TRAHYDROPYRIDINE-3,4,5-TRIOL (three-letter code: GOX) (formula:  $C_6H_{12}N_2O_5$ ).

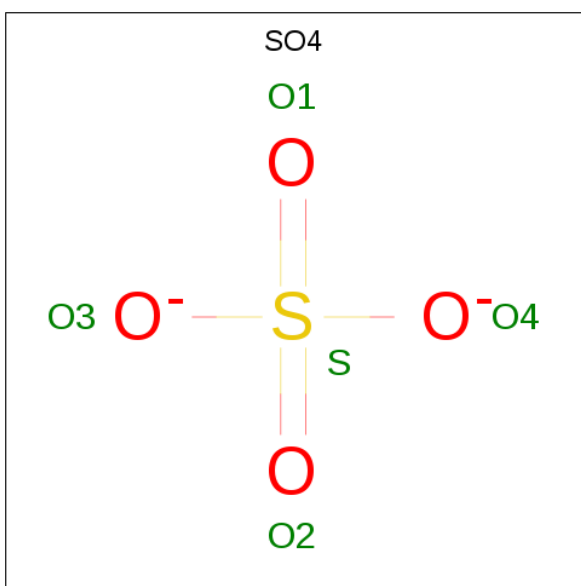


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			13	6	2	5		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

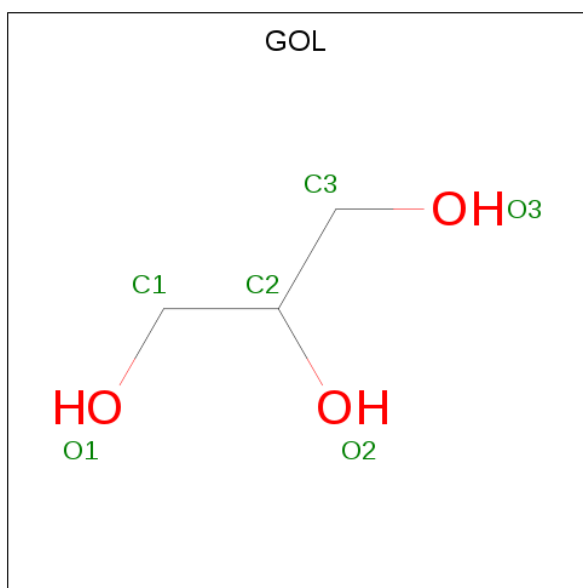
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Zn	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 10 8 2	0	1
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C O 7 3 4	0	1
9	M	1	Total C O 6 3 3	0	0
9	M	1	Total C O 6 3 3	0	0
9	M	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

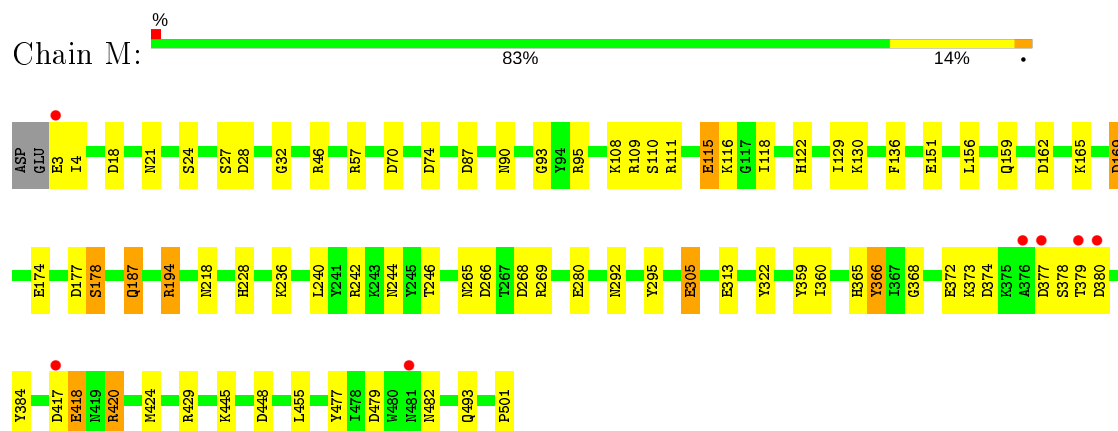
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	791	Total 791	O 791	0	0



### 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.

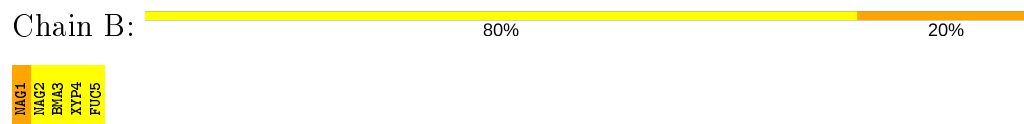
- Molecule 1: MYROSINASE MA1



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-xylopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.30Å 137.20Å 80.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.35 9.99 – 1.35	Depositor EDS
% Data completeness (in resolution range)	82.1 (10.00-1.35) 81.7 (9.99-1.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 1.35Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.120 , 0.152 0.137 , 0.163	Depositor DCC
$R_{free}$ test set	6736 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.9	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.51 , 62.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5207	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: XYP, GOL, ZN, BMA, NAG, SO4, FUC, MAN, GOX

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	M	0.98	5/4290 (0.1%)	1.50	56/5833 (1.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	24	SER	CB-OG	7.01	1.51	1.42
1	M	178	SER	CB-OG	6.19	1.50	1.42
1	M	151	GLU	CD-OE2	-5.99	1.19	1.25
1	M	115	GLU	CD-OE2	5.23	1.31	1.25
1	M	501	PRO	N-CD	5.02	1.54	1.47

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	109	ARG	NE-CZ-NH2	-18.31	111.14	120.30
1	M	269	ARG	NE-CZ-NH2	-13.15	113.73	120.30
1	M	115	GLU	OE1-CD-OE2	-13.02	107.67	123.30
1	M	109	ARG	NH1-CZ-NH2	10.98	131.48	119.40
1	M	57	ARG	NE-CZ-NH2	-9.36	115.62	120.30

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	M	4082	0	3835	97	0
2	A	28	0	25	6	0
3	B	58	0	42	6	0
4	C	80	0	58	18	0
5	M	84	0	77	22	0
6	M	13	0	12	1	0
7	M	1	0	0	0	0
8	M	45	0	0	5	0
9	M	25	0	29	1	0
10	M	791	0	0	33	1
All	All	5207	0	4078	114	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 13.

The worst 5 of 114 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:M:21:ASN:HD21	5:M:901:NAG:C1	0.92	1.56
1:M:244:ASN:HD21	5:M:905:NAG:C1	0.96	1.54
1:M:90:ASN:HD21	5:M:902:NAG:C1	0.92	1.54
1:M:265:ASN:HD21	3:B:1:NAG:C1	0.88	1.51
1:M:218:ASN:HD21	2:A:1:NAG:C1	0.86	1.49

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)
10:M:1004:HOH:O	10:M:1556:HOH:O[6_565]	1.95	0.25

## 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	M	518/501 (103%)	503 (97%)	14 (3%)	1 (0%)	47 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

### 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	M	456/437 (104%)	455 (100%)	1 (0%)	93 84

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

Mol	Chain	Res	Type
1	M	3	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	218	ASN
1	M	365	HIS
1	M	244	ASN
1	M	122	HIS
1	M	265	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 ⓘ

14 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	NAG	A	1	2	14,14,15	2.62	7 (50%)	17,19,21	3.42	9 (52%)
2	NAG	A	2	2	14,14,15	2.34	4 (28%)	17,19,21	4.44	8 (47%)
3	NAG	B	1	3	14,14,15	1.07	1 (7%)	17,19,21	3.00	7 (41%)
3	NAG	B	2	3	14,14,15	1.43	1 (7%)	17,19,21	1.69	4 (23%)
3	BMA	B	3	3	11,11,12	2.00	3 (27%)	15,15,17	1.57	3 (20%)
3	XYP	B	4	3	9,9,10	1.31	1 (11%)	10,12,14	2.14	4 (40%)
3	FUC	B	5	3	10,10,11	2.06	4 (40%)	14,14,16	2.23	3 (21%)
4	NAG	C	1	4	14,14,15	1.58	2 (14%)	17,19,21	3.07	5 (29%)
4	NAG	C	2	4	14,14,15	1.47	2 (14%)	17,19,21	2.24	7 (41%)
4	BMA	C	3	4	11,11,12	2.45	3 (27%)	15,15,17	4.86	9 (60%)
4	XYP	C	4	4	9,9,10	2.12	2 (22%)	10,12,14	3.67	6 (60%)
4	MAN	C	5	4	11,11,12	1.59	3 (27%)	15,15,17	2.54	6 (40%)
4	MAN	C	6	4	11,11,12	2.86	5 (45%)	15,15,17	7.64	12 (80%)
4	FUC	C	7	4	10,10,11	2.18	5 (50%)	14,14,16	2.81	7 (50%)

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	NAG	A	1	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	XYP	B	4	3	-	-	0/1/1/1
3	FUC	B	5	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1	4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	XYP	C	4	4	-	-	0/1/1/1
4	MAN	C	5	4	-	0/2/19/22	0/1/1/1
4	MAN	C	6	4	1/1/4/5	1/2/19/22	0/1/1/1
4	FUC	C	7	4	-	-	0/1/1/1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	NAG	C4-C5	6.66	1.67	1.53
4	C	6	MAN	O5-C5	6.52	1.56	1.43
4	C	3	BMA	C2-C3	-6.43	1.43	1.52
2	A	1	NAG	O7-C7	-5.02	1.11	1.23
4	C	4	XYP	C2-C3	4.81	1.59	1.52

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	6	MAN	C6-C5-C4	15.27	148.77	113.00
2	A	2	NAG	C1-O5-C5	-13.90	93.36	112.19
4	C	6	MAN	O5-C5-C6	-13.84	85.50	107.20
4	C	6	MAN	C1-O5-C5	-13.39	94.05	112.19
4	C	3	BMA	O4-C4-C5	12.04	139.19	109.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	6	MAN	C5

All (2) torsion outliers are listed below:

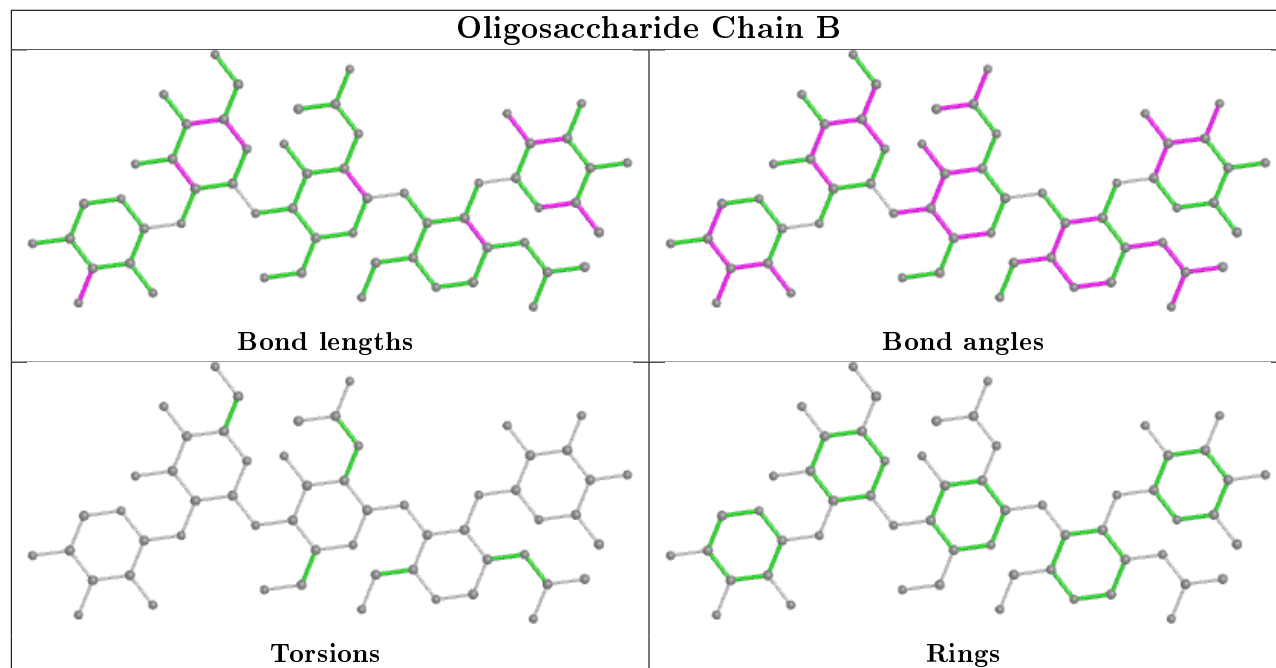
Mol	Chain	Res	Type	Atoms
4	C	6	MAN	O5-C5-C6-O6
2	A	2	NAG	O5-C5-C6-O6

There are no ring outliers.

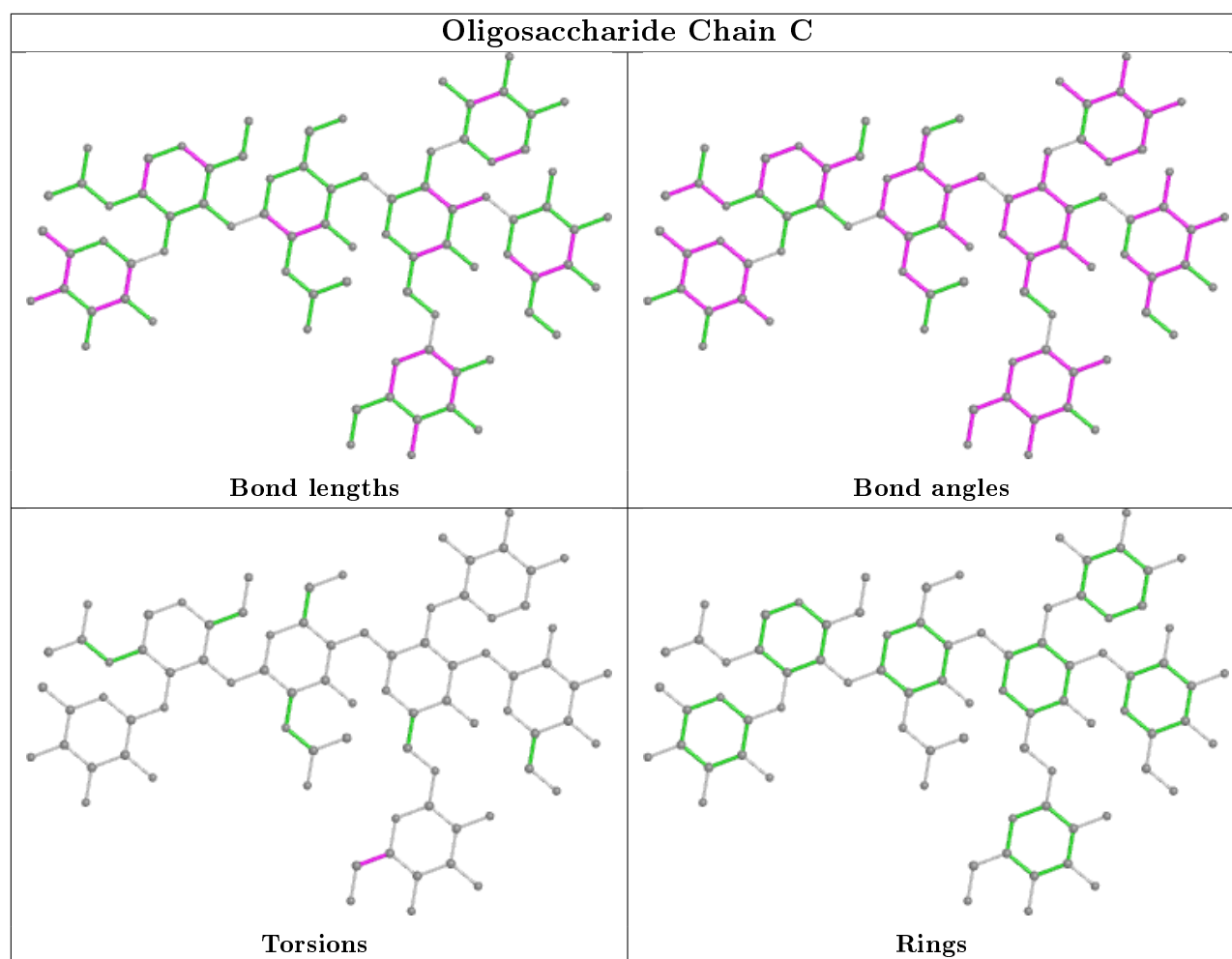
5 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	6	0
3	B	1	NAG	6	0
4	C	3	BMA	10	0
4	C	6	MAN	12	0
4	C	1	NAG	3	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 22 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
8	SO4	M	924	-	4,4,4	0.50	0	6,6,6	0.49	0
5	NAG	M	905	-	14,14,15	1.72	3 (21%)	17,19,21	7.06	11 (64%)
8	SO4	M	923	-	4,4,4	0.76	0	6,6,6	1.30	1 (16%)
5	NAG	M	901	-	14,14,15	1.23	2 (14%)	17,19,21	2.35	6 (35%)
6	GOX	M	921	-	11,13,13	1.31	2 (18%)	14,18,18	3.98	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	M	928	-	4,4,4	0.96	0	6,6,6	1.54	1 (16%)
5	NAG	M	918	1	14,14,15	1.38	2 (14%)	17,19,21	2.42	6 (35%)
5	NAG	M	902	-	14,14,15	1.46	2 (14%)	17,19,21	2.43	5 (29%)
8	SO4	M	926	-	4,4,4	0.50	0	6,6,6	0.25	0
8	SO4	M	929	-	4,4,4	0.74	0	6,6,6	0.37	0
9	GOL	M	933	-	5,5,5	0.24	0	5,5,5	1.13	0
5	NAG	M	920	1	14,14,15	1.26	1 (7%)	17,19,21	2.30	5 (29%)
8	SO4	M	925[A]	-	4,4,4	1.48	1 (25%)	6,6,6	2.63	4 (66%)
8	SO4	M	927	-	4,4,4	1.86	1 (25%)	6,6,6	2.39	4 (66%)
5	NAG	M	919	1	14,14,15	1.29	1 (7%)	17,19,21	2.35	5 (29%)
8	SO4	M	934	-	4,4,4	0.64	0	6,6,6	0.81	0
9	GOL	M	932	-	5,5,5	0.79	0	5,5,5	1.55	1 (20%)
9	GOL	M	930[B]	-	5,5,5	0.95	0	5,5,5	2.82	2 (40%)
9	GOL	M	930[A]	-	5,5,5	0.84	0	5,5,5	1.18	1 (20%)
9	GOL	M	931	-	5,5,5	0.89	0	5,5,5	1.08	0
8	SO4	M	925[B]	-	4,4,4	0.82	0	6,6,6	1.03	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
9	GOL	M	930[A]	-	-	0/4/4/4	-
5	NAG	M	905	-	-	2/6/23/26	0/1/1/1
5	NAG	M	901	-	-	0/6/23/26	0/1/1/1
6	GOX	M	921	-	-	0/3/24/24	0/1/1/1
5	NAG	M	918	1	-	0/6/23/26	0/1/1/1
5	NAG	M	902	-	-	0/6/23/26	0/1/1/1
9	GOL	M	933	-	-	3/4/4/4	-
5	NAG	M	920	1	-	0/6/23/26	0/1/1/1
5	NAG	M	919	1	-	2/6/23/26	0/1/1/1
9	GOL	M	932	-	-	0/4/4/4	-
9	GOL	M	930[B]	-	-	2/4/4/4	-
9	GOL	M	931	-	-	0/4/4/4	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	919	NAG	O7-C7	-4.17	1.13	1.23
5	M	902	NAG	O7-C7	-3.98	1.14	1.23
5	M	920	NAG	O7-C7	-3.81	1.14	1.23
5	M	918	NAG	O7-C7	-3.78	1.14	1.23
8	M	927	SO4	O2-S	3.53	1.65	1.46

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	905	NAG	C8-C7-N2	17.66	146.00	116.10
6	M	921	GOX	O7-N1-C1	13.27	122.65	110.18
5	M	905	NAG	O5-C1-C2	11.40	129.28	111.29
5	M	905	NAG	O7-C7-N2	-10.96	101.80	121.95
5	M	905	NAG	C2-N2-C7	10.55	137.92	122.90

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	905	NAG	C8-C7-N2-C2
9	M	933	GOL	C1-C2-C3-O3
9	M	930[B]	GOL	O1-C1-C2-C3
5	M	919	NAG	O5-C5-C6-O6
5	M	905	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	905	NAG	13	0
5	M	901	NAG	5	0
6	M	921	GOX	1	0
5	M	902	NAG	4	0
9	M	933	GOL	1	0
8	M	925[B]	SO4	5	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	M	499/501 (99%)	-0.36	7 (1%) 75 80	8, 12, 23, 51	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	376	ALA	6.0
1	M	380	ASP	4.3
1	M	3	GLU	4.2
1	M	379	THR	3.3
1	M	481	ASN	2.8

### 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.

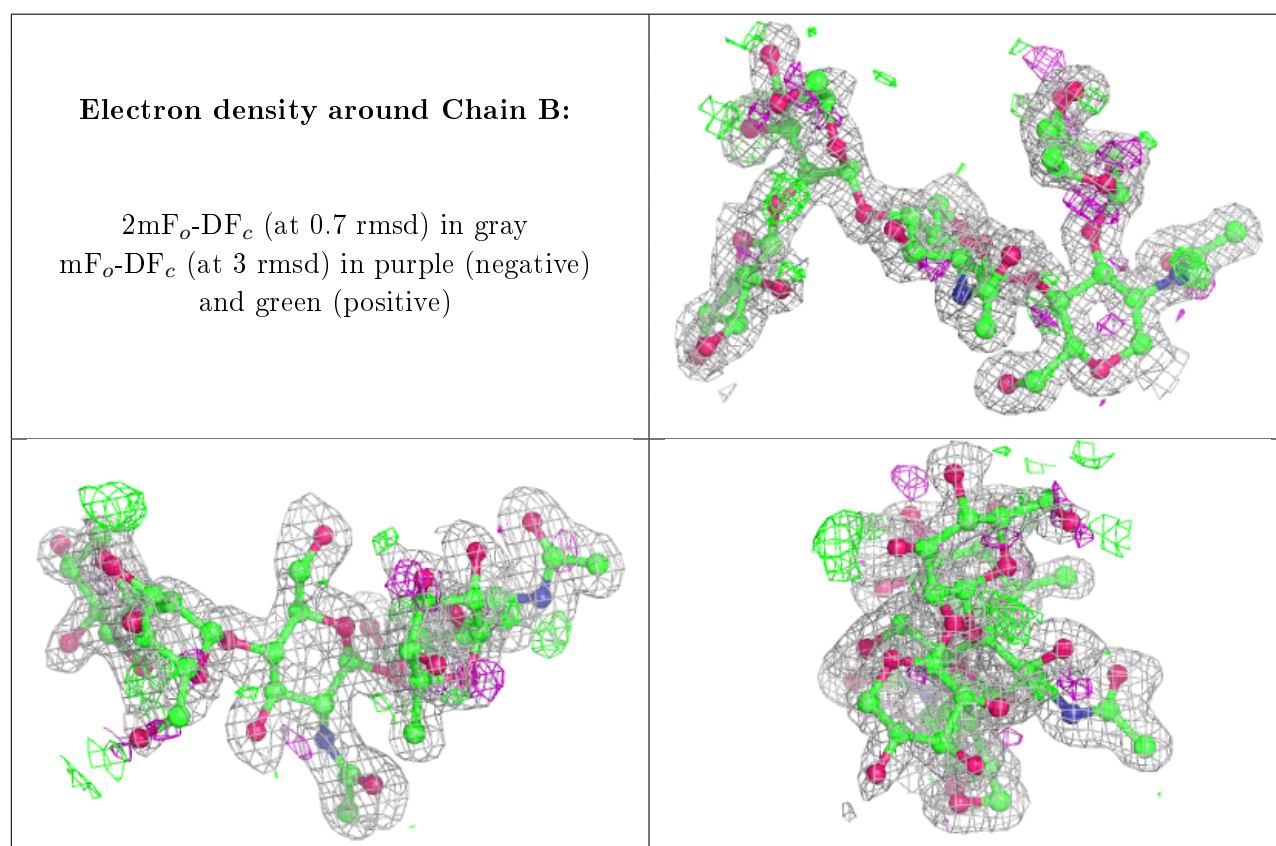
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	XYP	C	4	9/10	0.52	0.26	34,37,40,42	0
2	NAG	A	2	14/15	0.56	0.33	36,41,47,48	0
4	MAN	C	6	11/12	0.69	0.34	32,41,47,52	0
4	MAN	C	5	11/12	0.70	0.24	22,32,38,38	0
3	XYP	B	4	9/10	0.77	0.30	38,39,40,41	0
3	BMA	B	3	11/12	0.78	0.30	33,37,41,43	0
3	FUC	B	5	10/11	0.85	0.20	24,28,33,36	0

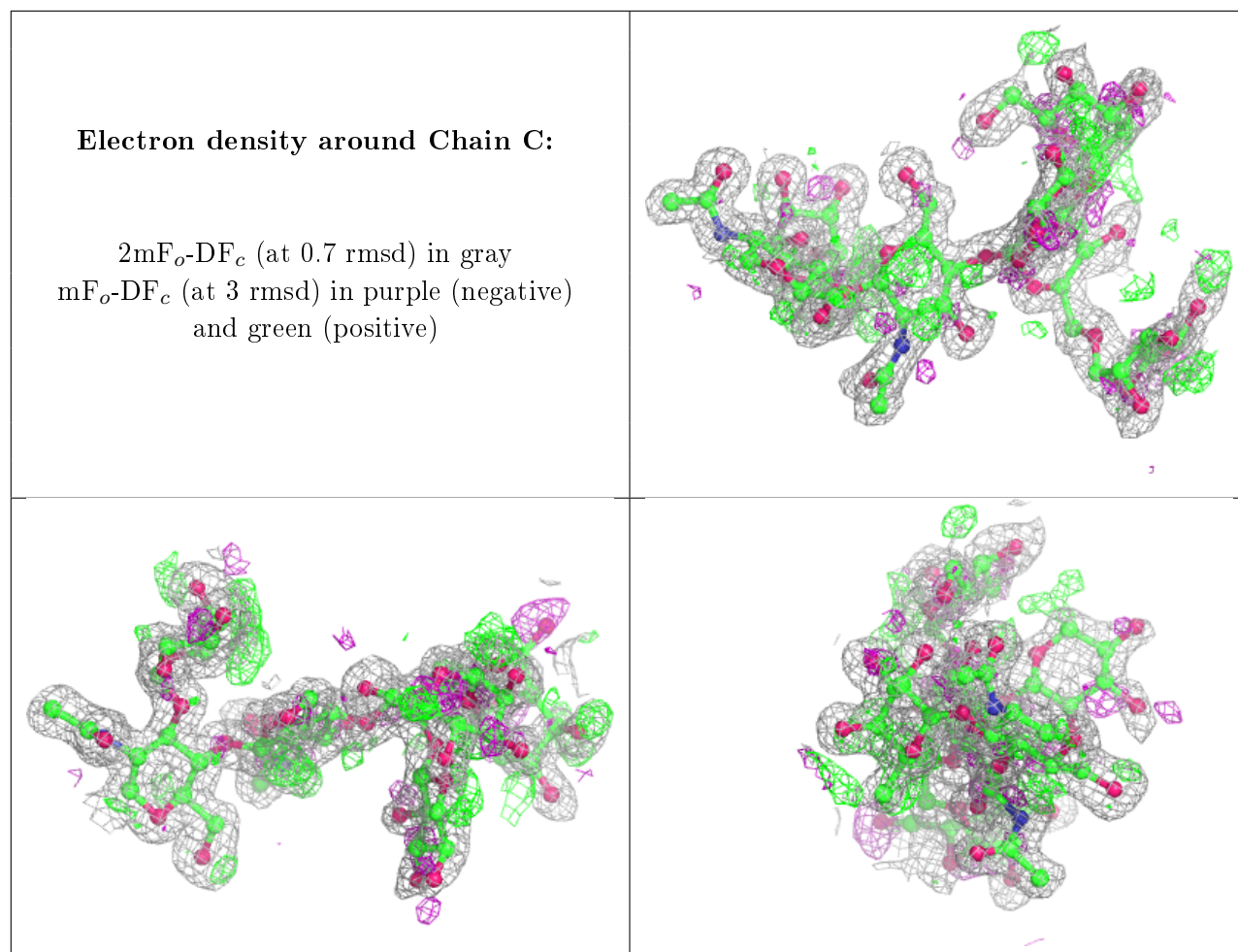
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	C	2	14/15	0.89	0.11	18,20,27,29	0
4	BMA	C	3	11/12	0.89	0.10	20,25,29,30	0
3	NAG	B	2	14/15	0.93	0.09	20,24,29,33	0
4	NAG	C	1	14/15	0.93	0.07	15,16,20,24	0
4	FUC	C	7	10/11	0.93	0.10	16,18,21,23	0
2	NAG	A	1	14/15	0.94	0.08	17,21,29,30	0
3	NAG	B	1	14/15	0.94	0.07	15,18,21,21	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( $\text{\AA}^2$ )	Q<0.9
5	NAG	M	918	14/15	0.57	0.42	28,35,43,45	0
5	NAG	M	919	14/15	0.61	0.48	53,61,64,66	0
9	GOL	M	933	6/6	0.69	0.30	37,39,41,44	6
5	NAG	M	905	14/15	0.70	0.28	31,40,45,47	0
8	SO4	M	928	5/5	0.72	0.22	21,28,30,31	5
5	NAG	M	920	14/15	0.73	0.34	30,35,44,46	0
5	NAG	M	901	14/15	0.74	0.16	27,30,35,38	0
9	GOL	M	932	6/6	0.77	0.17	28,29,30,33	6
8	SO4	M	925[B]	5/5	0.84	0.21	37,39,40,41	5
8	SO4	M	925[A]	5/5	0.84	0.21	23,27,27,27	5
5	NAG	M	902	14/15	0.85	0.17	22,24,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SO4	M	929	5/5	0.88	0.17	34,36,37,37	5
8	SO4	M	927	5/5	0.91	0.16	25,25,29,30	5
9	GOL	M	930[A]	6/6	0.94	0.11	9,13,15,16	2
9	GOL	M	930[B]	6/6	0.94	0.11	9,13,16,16	2
8	SO4	M	924	5/5	0.95	0.12	18,24,30,30	5
6	GOX	M	921	13/13	0.96	0.07	11,12,15,19	0
9	GOL	M	931	6/6	0.97	0.07	11,16,18,25	6
8	SO4	M	923	5/5	0.99	0.13	19,20,26,27	5
8	SO4	M	926	5/5	0.99	0.05	14,14,22,24	0
8	SO4	M	934	5/5	0.99	0.13	16,20,23,25	0
7	ZN	M	922	1/1	1.00	0.03	9,9,9,9	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.