



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:53 PM BST

PDB ID : 1E70  
Title : 2-F-glucosylated MYROSINASE FROM SINAPIS ALBA  
Authors : Burmeister, W.P.  
Deposited on : 2000-08-23  
Resolution : 1.65 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 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

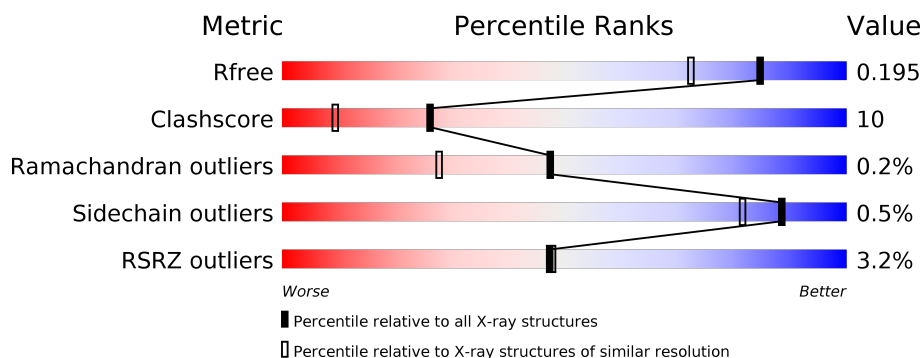
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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>3%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
2	A	2	<div> <div>50%</div> <div>50%</div> </div>
3	B	5	<div> <div>60%</div> <div>40%</div> </div>
4	C	6	<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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	C	3	X	-	-	-
4	XYP	C	4	-	-	-	X
4	MAN	C	5	-	-	-	X
5	NAG	M	961	X	-	-	X
5	NAG	M	971	-	-	-	X
5	NAG	M	991	X	-	-	X
8	SO4	M	1505	-	-	X	-
8	SO4	M	1507	-	-	-	X
8	SO4	M	1510	-	-	X	-
9	GOL	M	1513	-	X	-	-

## 2 Entry composition [i](#)

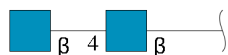
There are 10 unique types of molecules in this entry. The entry contains 5196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

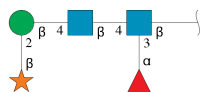
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	499	Total	C	N	O	S	0	22	0
			4086	2622	660	788	16			

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



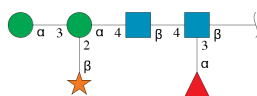
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



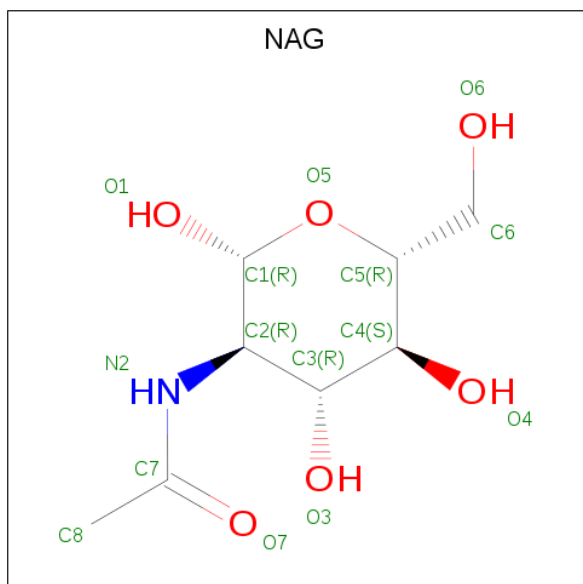
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	5	Total	C	N	O	0	0	0
			58	33	2	23			

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



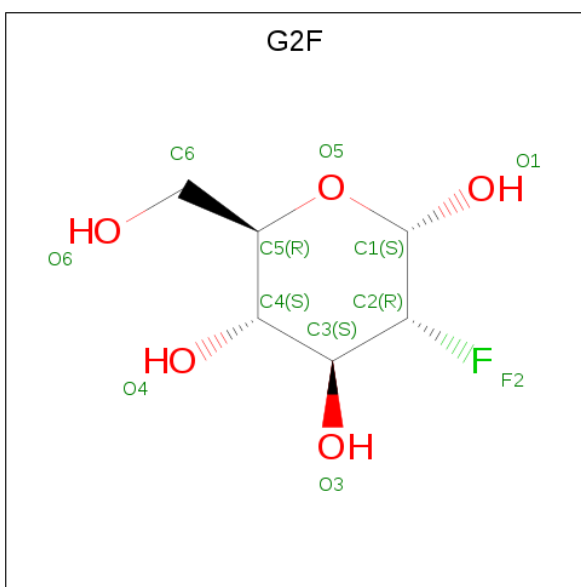
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	6	Total	C	N	O	0	0	0
			69	39	2	28			

- 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 2-deoxy-2-fluoro-alpha-D-glucopyranose (three-letter code: G2F) (formula:  $C_6H_{11}FO_5$ ).

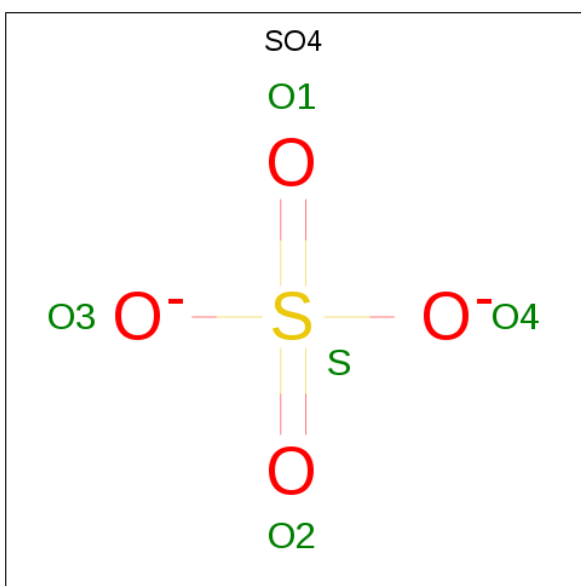


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	F	O	0	0
			11	6	1	4		

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

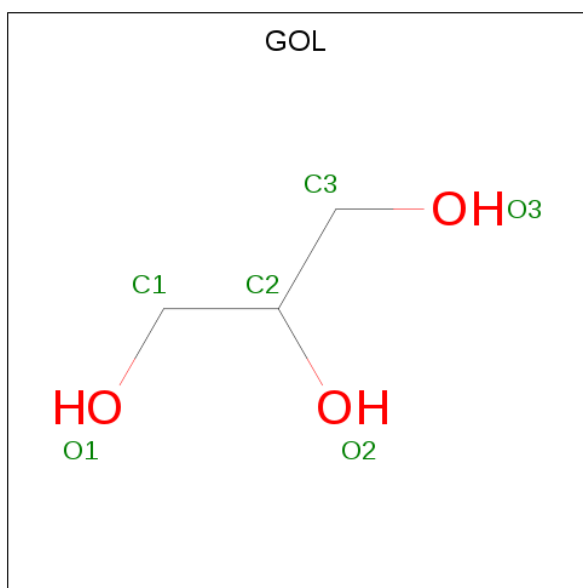
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Zn	0	0
			1	1		

- 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 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
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 6 3 3	0	0
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

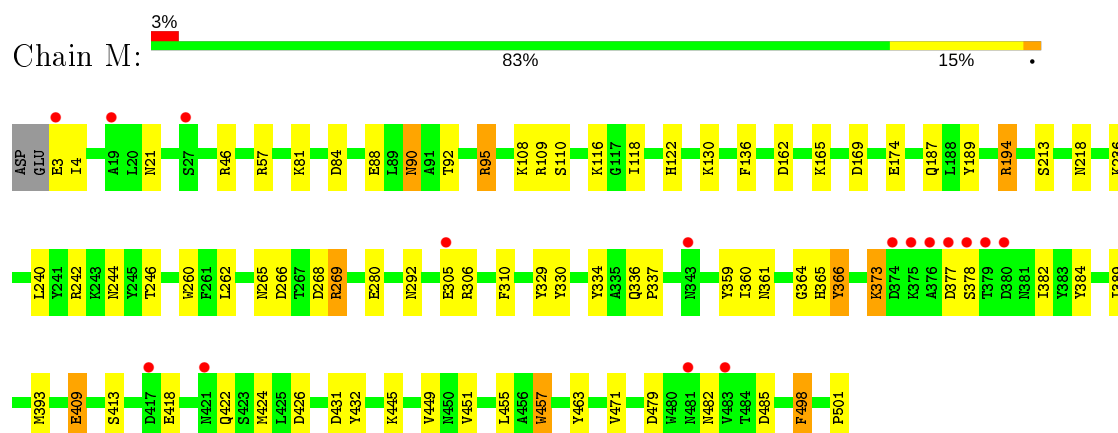
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	794	Total 794	O 794	0	0

### 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: 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-(1-4)-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, $\alpha$ , $\beta$ , $\gamma$	135.30 Å   137.20 Å   80.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 1.65 9.99 – 1.65	Depositor EDS
% Data completeness (in resolution range)	82.3 (10.00-1.65) 82.3 (9.99-1.65)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 1.65 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.169 , 0.195 0.177 , 0.195	Depositor DCC
$R_{free}$ test set	3755 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.49 , 72.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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, G2F, SO4, MAN, FUC

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	2.43	3/4299 (0.1%)	1.56	56/5845 (1.0%)

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	M	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	409[A]	GLU	CD-OE1	107.27	2.43	1.25
1	M	409[B]	GLU	CD-OE1	107.27	2.43	1.25
1	M	501	PRO	N-CD	5.46	1.55	1.47

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	426	ASP	CB-CG-OD1	15.70	132.43	118.30
1	M	109	ARG	NE-CZ-NH2	-15.33	112.63	120.30
1	M	409[A]	GLU	CG-CD-OE1	-15.30	87.70	118.30
1	M	409[B]	GLU	CG-CD-OE1	-15.30	87.70	118.30
1	M	46	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	M	269	ARG	NE-CZ-NH1	10.43	125.51	120.30
1	M	109	ARG	NH1-CZ-NH2	9.84	130.22	119.40
1	M	431	ASP	CB-CG-OD2	-9.69	109.58	118.30
1	M	463	TYR	CB-CG-CD1	9.69	126.81	121.00
1	M	57	ARG	NE-CZ-NH1	-9.29	115.66	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	330	TYR	CB-CG-CD1	-8.96	115.62	121.00
1	M	409[A]	GLU	OE1-CD-OE2	8.34	133.31	123.30
1	M	409[B]	GLU	OE1-CD-OE2	8.34	133.31	123.30
1	M	330	TYR	CB-CG-CD2	8.23	125.94	121.00
1	M	194	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	M	162	ASP	CB-CG-OD1	8.05	125.55	118.30
1	M	95	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	M	90	ASN	CB-CG-OD1	7.80	137.20	121.60
1	M	268	ASP	CB-CG-OD2	7.79	125.31	118.30
1	M	482	ASN	CB-CG-OD1	7.79	137.18	121.60
1	M	426	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	M	242	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	M	498	PHE	CB-CG-CD1	-6.93	115.95	120.80
1	M	457	TRP	O-C-N	-6.89	111.68	122.70
1	M	57	ARG	NH1-CZ-NH2	6.76	126.83	119.40
1	M	109	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	M	169[A]	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	M	169[B]	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	M	162	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	M	280	GLU	O-C-N	-5.98	113.13	122.70
1	M	426	ASP	O-C-N	-5.91	113.24	122.70
1	M	457	TRP	CA-C-O	-5.83	107.86	120.10
1	M	306	ARG	CD-NE-CZ	5.82	131.75	123.60
1	M	169[A]	ASP	CB-CG-OD1	5.79	123.51	118.30
1	M	169[B]	ASP	CB-CG-OD1	5.79	123.51	118.30
1	M	46	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	M	479	ASP	CB-CG-OD1	5.76	123.48	118.30
1	M	242	ARG	CD-NE-CZ	5.71	131.60	123.60
1	M	384	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	M	57	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	M	213[A]	SER	CA-C-O	-5.60	108.34	120.10
1	M	213[B]	SER	CA-C-O	-5.60	108.34	120.10
1	M	329	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	M	366[A]	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	M	366[B]	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	M	310	PHE	CB-CG-CD1	-5.47	116.97	120.80
1	M	485	ASP	CB-CG-OD1	5.45	123.20	118.30
1	M	432	TYR	CG-CD1-CE1	-5.37	117.00	121.30
1	M	457	TRP	N-CA-CB	5.37	120.27	110.60
1	M	189	TYR	CG-CD2-CE2	-5.35	117.02	121.30
1	M	92	THR	CA-CB-CG2	-5.29	104.99	112.40
1	M	463	TYR	CB-CG-CD2	-5.18	117.89	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	361	ASN	CB-CG-OD1	5.17	131.95	121.60
1	M	266	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	M	457	TRP	CA-C-N	5.10	128.42	117.20
1	M	426	ASP	CA-C-O	5.06	130.72	120.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	457	TRP	Mainchain,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	M	4086	0	3841	73	0
2	A	28	0	25	4	0
3	B	58	0	42	4	0
4	C	69	0	49	6	0
5	M	84	0	77	9	0
6	M	11	0	9	2	0
7	M	1	0	0	0	0
8	M	40	0	0	3	0
9	M	25	0	30	2	0
10	M	794	0	0	18	0
All	All	5196	0	4073	83	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 10.

All (83) 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:360[B]:ILE:HD11	1:M:366[B]:TYR:CZ	1.24	1.70
1:M:21:ASN:HD21	5:M:901:NAG:C1	1.00	1.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:292:ASN:HD21	4:C:1:NAG:C1	1.00	1.62
1:M:265:ASN:HD21	3:B:1:NAG:C1	0.97	1.61
1:M:90:ASN:HD21	5:M:911:NAG:C1	0.97	1.58
1:M:218:ASN:HD21	2:A:1:NAG:C1	0.94	1.55
1:M:244:ASN:HD21	5:M:931:NAG:C1	1.00	1.52
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CZ	1.91	1.49
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:CE1	1.54	1.39
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE1	2.19	1.18
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CE1	2.30	1.14
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:OH	1.43	1.14
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CD1	1.88	1.07
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CZ	1.98	0.94
1:M:246:THR:HG22	10:M:2392:HOH:O	1.69	0.90
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CE1	2.01	0.87
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:OH	2.10	0.83
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CD1	2.63	0.74
1:M:165:LYS:NZ	5:M:931:NAG:H82	2.02	0.74
1:M:130:LYS:HG3	10:M:2253:HOH:O	1.89	0.72
1:M:130:LYS:HB3	10:M:2264:HOH:O	1.92	0.69
10:M:2741:HOH:O	4:C:3:MAN:C4	2.43	0.66
10:M:2741:HOH:O	4:C:3:MAN:C5	2.42	0.66
1:M:409[B]:GLU:CD	6:M:999:G2F:C1	2.66	0.63
1:M:218:ASN:HD21	2:A:1:NAG:C2	2.00	0.63
1:M:95:ARG:HB2	1:M:455:LEU:HD13	1.83	0.61
1:M:118[B]:ILE:HD12	1:M:174:GLU:HG3	1.81	0.61
1:M:360[B]:ILE:HG12	1:M:366[B]:TYR:CG	2.36	0.61
1:M:360[B]:ILE:HD13	1:M:366[B]:TYR:CE2	2.35	0.61
1:M:449[B]:VAL:HG23	1:M:451:VAL:HG23	1.84	0.60
10:M:2741:HOH:O	4:C:3:MAN:C6	2.50	0.60
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE2	2.76	0.59
1:M:360[B]:ILE:HD11	1:M:366[B]:TYR:HH	1.63	0.58
1:M:108:LYS:HE3	1:M:110:SER:OG	2.04	0.57
1:M:4:ILE:HD11	1:M:445:LYS:HD2	1.87	0.56
1:M:165:LYS:HZ1	5:M:931:NAG:H82	1.67	0.56
1:M:360[B]:ILE:HG13	1:M:366[B]:TYR:CE1	2.35	0.55
1:M:365:HIS:HE1	10:M:2552:HOH:O	1.89	0.55
1:M:90:ASN:ND2	5:M:911:NAG:C2	2.66	0.54
1:M:194:ARG:HD2	8:M:1510:SO4:O1	2.10	0.52
1:M:218:ASN:ND2	2:A:1:NAG:C2	2.68	0.52
1:M:122:HIS:HE1	1:M:174:GLU:O	1.93	0.52
5:M:991:NAG:H61	10:M:2682:HOH:O	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:265:ASN:ND2	3:B:1:NAG:O5	2.41	0.51
1:M:360[A]:ILE:HD11	1:M:364:GLY:HA2	1.91	0.51
1:M:265:ASN:ND2	3:B:1:NAG:C2	2.69	0.50
1:M:409[A]:GLU:CD	6:M:999:G2F:C1	2.80	0.50
9:M:1511:GOL:H11	10:M:2786:HOH:O	2.13	0.48
10:M:2453:HOH:O	4:C:5:MAN:H61	2.14	0.48
8:M:1505:SO4:O2	8:M:1510:SO4:O2	2.30	0.48
1:M:165:LYS:HD2	1:M:236:LYS:HE3	1.94	0.48
1:M:240:LEU:HA	5:M:931:NAG:H83	1.97	0.47
1:M:373:LYS:NZ	1:M:378:SER:OG	2.42	0.47
1:M:218:ASN:ND2	2:A:1:NAG:O5	2.43	0.47
1:M:418:GLU:HB3	1:M:422:GLN:HB2	1.96	0.46
1:M:292:ASN:ND2	4:C:1:NAG:O5	2.38	0.46
1:M:365:HIS:HD2	10:M:2256:HOH:O	1.98	0.45
1:M:336:GLN:HB2	1:M:337:PRO:HD2	1.98	0.45
9:M:1511:GOL:H31	10:M:2427:HOH:O	2.16	0.45
1:M:359:TYR:CZ	1:M:382:ILE:HG23	2.52	0.45
1:M:424:MET:HE3	10:M:2695:HOH:O	2.16	0.45
10:M:2424:HOH:O	3:B:2:NAG:H82	2.17	0.45
1:M:95:ARG:HA	1:M:136:PHE:O	2.17	0.45
1:M:165:LYS:HZ2	5:M:931:NAG:H82	1.79	0.45
1:M:269:ARG:NH2	10:M:2426:HOH:O	2.51	0.43
1:M:262:LEU:O	1:M:334:TYR:HA	2.18	0.43
1:M:389:ILE:O	1:M:393:MET:HG2	2.19	0.42
1:M:116:LYS:HG2	10:M:2234:HOH:O	2.20	0.42
1:M:21:ASN:HA	1:M:498:PHE:CD2	2.55	0.42
1:M:413:SER:HB2	1:M:471:VAL:HB	2.01	0.42
1:M:4:ILE:CD1	1:M:445:LYS:HD2	2.50	0.41
1:M:260:TRP:CE3	1:M:260:TRP:HA	2.55	0.41
1:M:84:ASP:O	1:M:88[B]:GLU:HG3	2.20	0.41
8:M:1505:SO4:O1	8:M:1510:SO4:O3	2.38	0.41
1:M:377:ASP:HA	10:M:2568:HOH:O	2.20	0.41
1:M:81:LYS:HD2	10:M:2167:HOH:O	2.21	0.41

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	M	519/501 (104%)	503 (97%)	15 (3%)	1 (0%)	47 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

### 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	M	457/437 (105%)	455 (100%)	2 (0%)	91 85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	3	GLU
1	M	373	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	90	ASN
1	M	122	HIS
1	M	218	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	M	244	ASN
1	M	265	ASN
1	M	292	ASN
1	M	365	HIS

### 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 ⓘ

13 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	1,2	14,14,15	1.55	4 (28%)	17,19,21	3.30	9 (52%)
2	NAG	A	2	2	14,14,15	1.01	0	17,19,21	2.52	8 (47%)
3	NAG	B	1	1,3	14,14,15	1.19	2 (14%)	17,19,21	4.07	11 (64%)
3	NAG	B	2	3	14,14,15	1.22	2 (14%)	17,19,21	1.53	4 (23%)
3	BMA	B	3	3	11,11,12	1.88	2 (18%)	15,15,17	1.44	3 (20%)
3	XYP	B	4	3	9,9,10	0.81	0	10,12,14	3.03	3 (30%)
3	FUC	B	5	3	10,10,11	1.50	2 (20%)	14,14,16	1.92	6 (42%)
4	NAG	C	1	1,4	14,14,15	1.21	1 (7%)	17,19,21	2.87	5 (29%)
4	NAG	C	2	4	14,14,15	1.43	2 (14%)	17,19,21	2.41	7 (41%)
4	MAN	C	3	4	11,11,12	2.03	3 (27%)	15,15,17	6.46	10 (66%)
4	XYP	C	4	4	9,9,10	1.36	1 (11%)	10,12,14	3.76	5 (50%)
4	MAN	C	5	4	11,11,12	1.22	2 (18%)	15,15,17	1.96	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FUC	C	6	4	10,10,11	1.75	3 (30%)	14,14,16	2.46	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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	A	2	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1	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
4	NAG	C	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	2	4	-	0/6/23/26	0/1/1/1
4	MAN	C	3	4	1/1/4/5	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	FUC	C	6	4	-	-	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3	MAN	C2-C3	-4.66	1.45	1.52
3	B	3	BMA	C2-C3	-4.31	1.46	1.52
4	C	6	FUC	C2-C3	3.72	1.58	1.52
4	C	3	MAN	O5-C1	3.65	1.49	1.43
3	B	3	BMA	C4-C5	3.27	1.59	1.53
3	B	1	NAG	C3-C2	2.99	1.58	1.52
2	A	1	NAG	O5-C5	2.92	1.49	1.43
4	C	2	NAG	C1-C2	2.90	1.56	1.52
4	C	2	NAG	C3-C2	-2.87	1.46	1.52
4	C	1	NAG	O5-C5	2.76	1.49	1.43
4	C	3	MAN	O3-C3	2.69	1.49	1.43
2	A	1	NAG	C3-C2	2.52	1.57	1.52
3	B	2	NAG	O7-C7	2.45	1.28	1.23
4	C	6	FUC	C6-C5	2.42	1.57	1.51
3	B	5	FUC	C2-C3	2.38	1.56	1.52
2	A	1	NAG	C8-C7	2.31	1.55	1.50
4	C	5	MAN	O5-C5	2.26	1.48	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5	MAN	C4-C3	2.20	1.57	1.52
3	B	1	NAG	O5-C5	2.18	1.47	1.43
3	B	2	NAG	C1-C2	2.15	1.55	1.52
2	A	1	NAG	O7-C7	-2.13	1.18	1.23
4	C	4	XYP	C2-C3	2.08	1.55	1.52
3	B	5	FUC	C6-C5	2.07	1.56	1.51
4	C	6	FUC	O2-C2	2.04	1.47	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3	MAN	C6-C5-C4	13.10	143.68	113.00
4	C	3	MAN	O4-C4-C5	9.97	134.06	109.30
4	C	3	MAN	C1-O5-C5	-9.59	99.20	112.19
4	C	3	MAN	O5-C5-C6	-8.94	93.19	107.20
2	A	1	NAG	C1-O5-C5	-8.44	100.75	112.19
4	C	3	MAN	C3-C4-C5	8.38	125.19	110.24
4	C	1	NAG	O5-C1-C2	8.02	123.95	111.29
3	B	1	NAG	C8-C7-N2	-7.75	102.97	116.10
3	B	1	NAG	C1-O5-C5	-7.65	101.83	112.19
3	B	4	XYP	C1-C2-C3	7.52	118.91	109.67
4	C	4	XYP	O3-C3-C4	6.88	123.16	109.99
3	B	1	NAG	C2-N2-C7	-6.57	113.55	122.90
4	C	4	XYP	C4-C3-C2	-6.56	103.13	110.92
3	B	1	NAG	C4-C3-C2	-6.27	101.83	111.02
2	A	2	NAG	C1-O5-C5	-6.14	103.87	112.19
2	A	1	NAG	C8-C7-N2	-5.78	106.31	116.10
4	C	3	MAN	O4-C4-C3	-5.76	97.03	110.35
4	C	3	MAN	C2-C3-C4	-5.68	101.07	110.89
4	C	6	FUC	C1-C2-C3	-5.67	102.70	109.67
4	C	1	NAG	C1-O5-C5	-5.49	104.76	112.19
3	B	1	NAG	O7-C7-N2	5.19	131.50	121.95
4	C	2	NAG	O4-C4-C5	-5.03	96.81	109.30
3	B	4	XYP	O2-C2-C3	-4.97	100.19	110.14
2	A	1	NAG	O7-C7-N2	4.89	130.94	121.95
4	C	2	NAG	O4-C4-C3	-4.80	99.25	110.35
4	C	3	MAN	O2-C2-C3	-4.52	101.09	110.14
4	C	4	XYP	O4-C4-C3	4.02	118.19	110.14
4	C	4	XYP	O4-C4-C5	3.88	117.08	109.15
2	A	2	NAG	O5-C5-C4	-3.87	101.40	110.83
4	C	6	FUC	C6-C5-C4	-3.67	106.28	113.07
4	C	1	NAG	C8-C7-N2	-3.66	109.91	116.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5	MAN	O2-C2-C3	-3.52	103.08	110.14
3	B	1	NAG	C1-C2-N2	-3.51	104.48	110.49
4	C	4	XYP	O2-C2-C3	-3.46	103.21	110.14
4	C	2	NAG	C2-N2-C7	-3.43	118.01	122.90
4	C	3	MAN	O3-C3-C2	-3.39	103.50	109.99
3	B	2	NAG	O7-C7-N2	-3.39	115.73	121.95
4	C	3	MAN	C1-C2-C3	-3.33	105.57	109.67
2	A	2	NAG	O5-C1-C2	3.30	116.49	111.29
2	A	2	NAG	O5-C5-C6	-3.25	102.11	107.20
2	A	1	NAG	C2-N2-C7	-3.21	118.33	122.90
3	B	5	FUC	C6-C5-C4	-3.15	107.25	113.07
3	B	5	FUC	O3-C3-C2	-3.15	103.96	109.99
4	C	6	FUC	O3-C3-C2	-3.14	103.97	109.99
3	B	1	NAG	O5-C5-C4	-3.14	103.18	110.83
2	A	1	NAG	C4-C3-C2	-3.14	106.42	111.02
2	A	1	NAG	C1-C2-N2	-3.08	105.23	110.49
4	C	1	NAG	O5-C5-C6	-2.95	102.57	107.20
4	C	2	NAG	C8-C7-N2	-2.90	111.19	116.10
4	C	5	MAN	C1-C2-C3	2.89	113.22	109.67
4	C	5	MAN	C2-C3-C4	-2.88	105.91	110.89
3	B	1	NAG	O3-C3-C2	-2.87	103.52	109.47
4	C	2	NAG	O5-C5-C4	-2.86	103.86	110.83
2	A	1	NAG	O4-C4-C3	-2.83	103.81	110.35
2	A	2	NAG	O3-C3-C2	-2.76	103.76	109.47
2	A	1	NAG	O3-C3-C2	-2.64	104.00	109.47
4	C	2	NAG	O5-C1-C2	-2.63	107.14	111.29
4	C	5	MAN	O2-C2-C1	-2.62	103.80	109.15
3	B	5	FUC	O2-C2-C3	-2.61	104.90	110.14
4	C	5	MAN	O5-C1-C2	-2.61	106.75	110.77
3	B	3	BMA	O2-C2-C1	2.60	114.48	109.15
3	B	5	FUC	C1-C2-C3	-2.60	106.47	109.67
4	C	1	NAG	C3-C4-C5	2.54	114.78	110.24
2	A	1	NAG	O4-C4-C5	-2.52	103.04	109.30
4	C	6	FUC	C1-O5-C5	2.48	118.39	112.78
4	C	6	FUC	O3-C3-C4	-2.47	104.63	110.35
3	B	1	NAG	C6-C5-C4	2.47	118.79	113.00
3	B	4	XYP	O3-C3-C4	2.45	114.69	109.99
2	A	2	NAG	C6-C5-C4	-2.45	107.28	113.00
3	B	2	NAG	O5-C5-C6	-2.41	103.43	107.20
4	C	6	FUC	O2-C2-C1	-2.39	104.27	109.15
2	A	2	NAG	O6-C6-C5	-2.33	103.29	111.29
4	C	2	NAG	O5-C5-C6	2.29	110.80	107.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3	BMA	C1-C2-C3	2.25	112.43	109.67
3	B	1	NAG	O4-C4-C3	-2.25	105.15	110.35
3	B	5	FUC	O4-C4-C5	-2.25	104.68	109.67
3	B	3	BMA	C1-O5-C5	-2.23	109.17	112.19
3	B	1	NAG	C3-C4-C5	2.22	114.20	110.24
3	B	5	FUC	O5-C5-C6	-2.21	102.57	107.33
2	A	2	NAG	C8-C7-N2	-2.21	112.36	116.10
4	C	6	FUC	O2-C2-C3	-2.18	105.77	110.14
4	C	5	MAN	C3-C4-C5	-2.09	106.50	110.24
3	B	2	NAG	O7-C7-C8	-2.07	118.21	122.06
3	B	2	NAG	O3-C3-C2	-2.02	105.28	109.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	3	MAN	C1

All (3) torsion outliers are listed below:

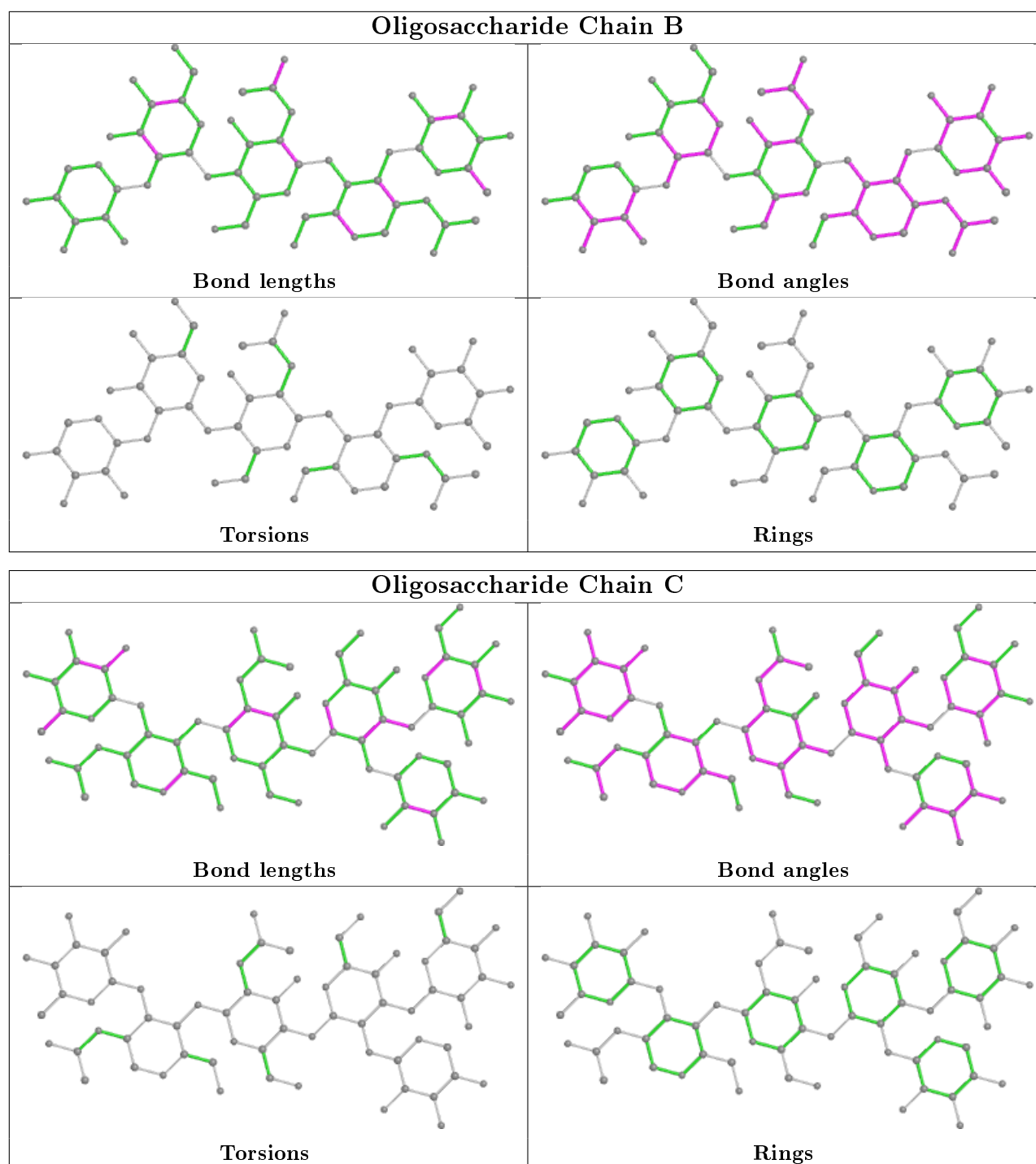
Mol	Chain	Res	Type	Atoms
2	A	1	NAG	O5-C5-C6-O6
2	A	1	NAG	C4-C5-C6-O6
2	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	4	0
3	B	1	NAG	3	0
3	B	2	NAG	1	0
4	C	5	MAN	1	0
4	C	3	MAN	3	0
4	C	1	NAG	2	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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	1505	-	4,4,4	0.61	0	6,6,6	0.30	0
5	NAG	M	931	1	14,14,15	1.71	2 (14%)	17,19,21	7.71	10 (58%)
5	NAG	M	961	1	14,14,15	1.47	2 (14%)	17,19,21	2.46	5 (29%)
5	NAG	M	901	1	14,14,15	1.08	1 (7%)	17,19,21	1.64	5 (29%)
5	NAG	M	991	1	14,14,15	1.29	1 (7%)	17,19,21	1.93	6 (35%)
9	GOL	M	1513	-	5,5,5	3.95	4 (80%)	5,5,5	2.47	3 (60%)
8	SO4	M	1509	-	4,4,4	0.63	0	6,6,6	0.23	0
8	SO4	M	1503	-	4,4,4	0.47	0	6,6,6	0.37	0
5	NAG	M	911	1	14,14,15	1.19	1 (7%)	17,19,21	1.97	4 (23%)
8	SO4	M	1506	-	4,4,4	0.49	0	6,6,6	1.65	1 (16%)
8	SO4	M	1508	-	4,4,4	0.75	0	6,6,6	0.68	0
8	SO4	M	1510	-	4,4,4	0.53	0	6,6,6	0.43	0
9	GOL	M	1511	-	5,5,5	0.32	0	5,5,5	0.55	0
8	SO4	M	1507	-	4,4,4	0.78	0	6,6,6	1.41	1 (16%)
8	SO4	M	1504	-	4,4,4	0.60	0	6,6,6	0.28	0
5	NAG	M	971	1	14,14,15	1.34	1 (7%)	17,19,21	1.36	2 (11%)
9	GOL	M	1512[B]	-	5,5,5	0.73	0	5,5,5	2.11	2 (40%)
9	GOL	M	1514	-	5,5,5	0.25	0	5,5,5	0.79	0
9	GOL	M	1512[A]	-	5,5,5	0.75	0	5,5,5	1.79	1 (20%)
6	G2F	M	999	-	11,11,12	1.86	2 (18%)	10,15,17	2.71	4 (40%)

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	1513	-	-	3/4/4/4	-
9	GOL	M	1514	-	-	1/4/4/4	-
5	NAG	M	901	1	-	2/6/23/26	0/1/1/1
5	NAG	M	991	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	M	931	1	-	3/6/23/26	0/1/1/1
5	NAG	M	911	1	-	0/6/23/26	0/1/1/1
9	GOL	M	1511	-	-	1/4/4/4	-
5	NAG	M	971	1	-	2/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	M	1512[B]	-	-	2/4/4/4	-
5	NAG	M	961	1	1/1/5/7	0/6/23/26	0/1/1/1
9	GOL	M	1512[A]	-	-	0/4/4/4	-
6	G2F	M	999	-	-	0/2/19/22	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1513	GOL	O2-C2	6.33	1.62	1.43
5	M	931	NAG	O7-C7	-4.38	1.13	1.23
9	M	1513	GOL	O1-C1	4.22	1.60	1.42
6	M	999	G2F	C2-C3	4.06	1.57	1.51
5	M	971	NAG	O7-C7	-4.01	1.14	1.23
5	M	961	NAG	O7-C7	-3.93	1.14	1.23
5	M	911	NAG	O7-C7	-3.75	1.14	1.23
5	M	991	NAG	O7-C7	-3.61	1.15	1.23
9	M	1513	GOL	C1-C2	3.45	1.65	1.51
5	M	901	NAG	O7-C7	-3.10	1.16	1.23
6	M	999	G2F	O5-C1	2.85	1.48	1.43
9	M	1513	GOL	C3-C2	2.81	1.63	1.51
5	M	931	NAG	C2-N2	-2.70	1.41	1.46
5	M	961	NAG	C2-N2	2.65	1.50	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	931	NAG	C2-N2-C7	28.95	164.12	122.90
5	M	931	NAG	O5-C1-C2	8.55	124.78	111.29
5	M	961	NAG	C1-O5-C5	7.90	122.89	112.19
5	M	931	NAG	O7-C7-N2	-6.27	110.43	121.95
6	M	999	G2F	C1-O5-C5	-5.11	105.27	112.19
5	M	911	NAG	C4-C3-C2	-4.92	103.81	111.02
6	M	999	G2F	O5-C5-C6	-4.56	100.05	107.20
5	M	971	NAG	O5-C1-C2	-4.13	104.76	111.29
5	M	991	NAG	C4-C3-C2	-3.96	105.21	111.02
5	M	961	NAG	C1-C2-N2	-3.90	103.83	110.49
6	M	999	G2F	C3-C4-C5	-3.90	103.29	110.24
5	M	991	NAG	O5-C1-C2	3.78	117.26	111.29
9	M	1512[B]	GOL	O2-C2-C1	3.76	125.69	109.12
9	M	1512[A]	GOL	O2-C2-C1	3.76	125.69	109.12
5	M	931	NAG	O7-C7-C8	3.59	128.72	122.06
9	M	1513	GOL	O3-C3-C2	3.54	127.16	110.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	931	NAG	C4-C3-C2	-3.46	105.95	111.02
5	M	901	NAG	C1-O5-C5	-3.45	107.52	112.19
5	M	901	NAG	O5-C1-C2	3.22	116.38	111.29
8	M	1506	SO4	O4-S-O3	-3.17	95.51	109.06
5	M	911	NAG	C1-O5-C5	-3.12	107.97	112.19
5	M	991	NAG	C2-N2-C7	-2.93	118.73	122.90
5	M	911	NAG	O3-C3-C2	-2.81	103.66	109.47
5	M	931	NAG	C8-C7-N2	2.80	120.85	116.10
9	M	1513	GOL	C3-C2-C1	2.79	122.56	111.70
5	M	901	NAG	C4-C3-C2	-2.69	107.07	111.02
5	M	911	NAG	O5-C5-C4	-2.68	104.32	110.83
9	M	1513	GOL	O1-C1-C2	2.60	122.67	110.20
5	M	991	NAG	C1-O5-C5	2.56	115.66	112.19
9	M	1512[B]	GOL	O1-C1-C2	2.51	122.24	110.20
5	M	961	NAG	C4-C3-C2	2.47	114.64	111.02
5	M	971	NAG	O5-C5-C4	-2.40	104.98	110.83
5	M	991	NAG	O5-C5-C4	-2.38	105.04	110.83
5	M	931	NAG	C3-C4-C5	2.38	114.48	110.24
5	M	931	NAG	C1-O5-C5	-2.34	109.02	112.19
8	M	1507	SO4	O3-S-O1	2.33	121.49	109.31
5	M	931	NAG	O4-C4-C5	-2.33	103.52	109.30
5	M	931	NAG	O5-C5-C4	-2.31	105.20	110.83
5	M	901	NAG	O3-C3-C4	2.21	115.46	110.35
5	M	901	NAG	O3-C3-C2	-2.19	104.93	109.47
6	M	999	G2F	C6-C5-C4	2.13	117.99	113.00
5	M	991	NAG	C6-C5-C4	-2.11	108.06	113.00
5	M	961	NAG	C8-C7-N2	-2.09	112.56	116.10
5	M	961	NAG	O3-C3-C2	-2.09	105.15	109.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	991	NAG	C1
5	M	961	NAG	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	1512[B]	GOL	O1-C1-C2-C3
5	M	971	NAG	O5-C5-C6-O6
5	M	971	NAG	C4-C5-C6-O6
5	M	931	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	M	901	NAG	C4-C5-C6-O6
5	M	901	NAG	O5-C5-C6-O6
5	M	991	NAG	O5-C5-C6-O6
5	M	931	NAG	C4-C5-C6-O6
9	M	1514	GOL	O1-C1-C2-C3
9	M	1513	GOL	O1-C1-C2-C3
9	M	1512[B]	GOL	O1-C1-C2-O2
9	M	1513	GOL	O1-C1-C2-O2
5	M	931	NAG	C3-C2-N2-C7
5	M	991	NAG	C4-C5-C6-O6
9	M	1513	GOL	C1-C2-C3-O3
9	M	1511	GOL	O1-C1-C2-C3

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1505	SO4	2	0
5	M	931	NAG	5	0
5	M	901	NAG	1	0
5	M	991	NAG	1	0
5	M	911	NAG	2	0
8	M	1510	SO4	3	0
9	M	1511	GOL	2	0
6	M	999	G2F	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	M	499/501 (99%)	-0.13	16 (3%)	47 48	20, 25, 39, 66	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	376	ALA	9.0
1	M	380	ASP	5.6
1	M	375	LYS	4.7
1	M	374	ASP	4.3
1	M	417	ASP	3.9
1	M	378	SER	3.8
1	M	377	ASP	3.4
1	M	3	GLU	3.3
1	M	379	THR	3.2
1	M	27	SER	2.9
1	M	421	ASN	2.7
1	M	481	ASN	2.4
1	M	483	VAL	2.2
1	M	305[A]	GLU	2.1
1	M	343	ASN	2.1
1	M	19	ALA	2.1

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

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

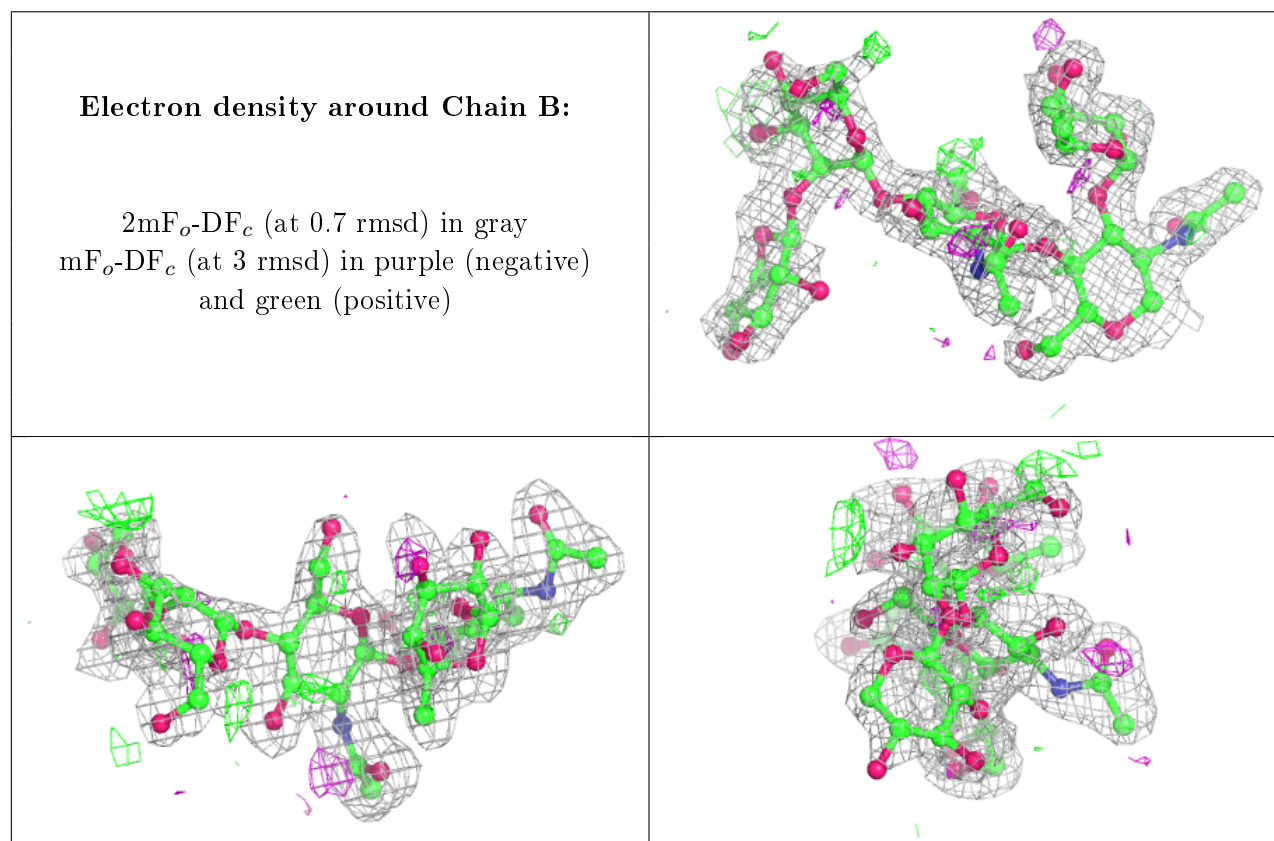
### 6.3 Carbohydrates [i](#)

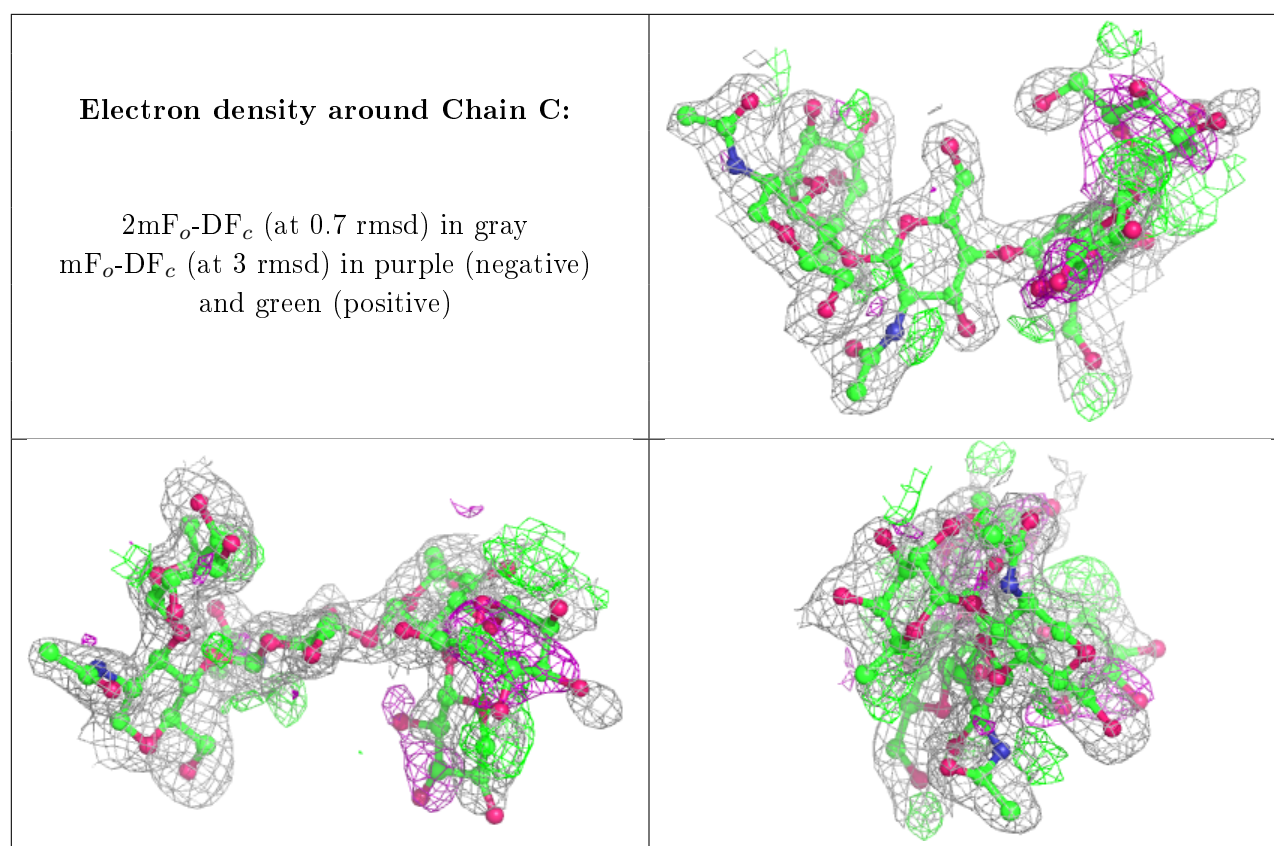
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	MAN	C	5	11/12	0.24	0.50	42,55,57,57	0
4	XYP	C	4	9/10	0.44	0.43	56,59,60,62	0
2	NAG	A	2	14/15	0.53	0.38	49,52,56,58	0
3	BMA	B	3	11/12	0.71	0.36	53,57,59,59	0
4	MAN	C	3	11/12	0.72	0.16	44,48,52,54	0
3	XYP	B	4	9/10	0.74	0.39	59,60,62,62	0
3	FUC	B	5	10/11	0.83	0.21	41,43,47,49	0
3	NAG	B	2	14/15	0.87	0.14	39,43,48,49	0
4	FUC	C	6	10/11	0.87	0.15	38,39,43,43	0
4	NAG	C	2	14/15	0.90	0.12	34,37,40,42	0
2	NAG	A	1	14/15	0.90	0.10	29,34,38,42	0
3	NAG	B	1	14/15	0.91	0.08	30,33,36,36	0
4	NAG	C	1	14/15	0.92	0.09	30,32,35,36	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
5	NAG	M	961	14/15	0.36	0.56	59,63,66,67	0
5	NAG	M	991	14/15	0.43	0.62	57,58,63,64	0
8	SO4	M	1507	5/5	0.46	0.47	50,52,53,54	5
5	NAG	M	971	14/15	0.54	0.50	69,75,76,76	0
9	GOL	M	1511	6/6	0.60	0.34	55,56,56,56	6
5	NAG	M	931	14/15	0.64	0.34	53,58,60,60	0
8	SO4	M	1508	5/5	0.68	0.29	42,46,47,47	5
9	GOL	M	1514	6/6	0.68	0.29	57,59,59,60	6
5	NAG	M	901	14/15	0.71	0.20	42,45,50,52	0
8	SO4	M	1505	5/5	0.74	0.34	54,56,56,58	5
9	GOL	M	1513	6/6	0.76	0.29	20,26,29,36	0
8	SO4	M	1509	5/5	0.77	0.30	54,55,55,55	5
5	NAG	M	911	14/15	0.83	0.21	36,40,41,45	0
8	SO4	M	1510	5/5	0.87	0.37	62,62,63,64	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	GOL	M	1512[B]	6/6	0.91	0.14	23,26,28,29	2
9	GOL	M	1512[A]	6/6	0.91	0.14	16,23,28,28	2
6	G2F	M	999	11/12	0.91	0.10	27,32,35,37	0
8	SO4	M	1506	5/5	0.94	0.12	35,36,37,40	0
8	SO4	M	1504	5/5	0.96	0.15	36,39,41,41	5
8	SO4	M	1503	5/5	0.98	0.14	37,40,41,43	5
7	ZN	M	1502	1/1	0.99	0.02	21,21,21,21	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.