



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:01 AM BST

PDB ID : 3EQO  
Title : Crystal structure of beta-1,3-glucanase from *Phanerochaete chrysosporium* (Lam55A) gluconolactone complex  
Authors : Ishida, T.; Fushinobu, S.; Kawai, R.; Kitaoka, M.; Igarashi, K.; Samejima, M.  
Deposited on : 2008-10-01  
Resolution : 2.25 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.

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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

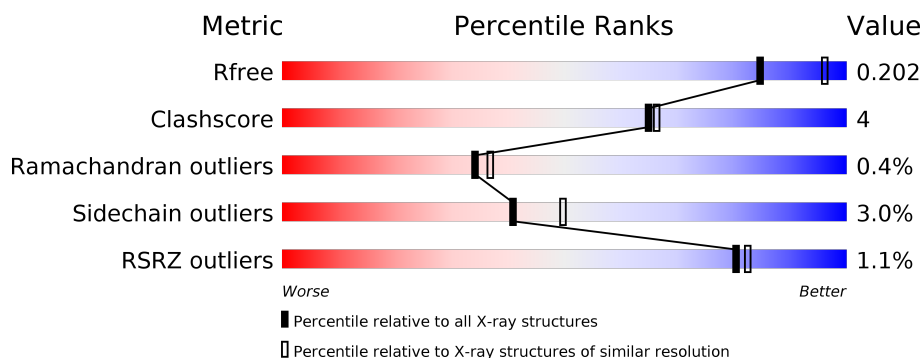
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	A	758	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>88%</span> <span>10% ..</span> </div> </div>
1	B	758	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>87%</span> <span>11% ..</span> </div> </div>
2	C	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span></span> <span>100%</span> </div> </div>
2	D	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span></span> <span>100%</span> </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
2	BMA	D	3	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12519 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 Glucan 1,3-beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	752	Total	C	N	O	S	0	0	0
			5611	3526	973	1096	16			
1	B	752	Total	C	N	O	S	0	0	0
			5611	3526	973	1096	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLU	-	expression tag	UNP Q2Z1W1
A	-4	ALA	-	expression tag	UNP Q2Z1W1
A	-3	GLU	-	expression tag	UNP Q2Z1W1
A	-2	ALA	-	expression tag	UNP Q2Z1W1
A	-1	GLU	-	expression tag	UNP Q2Z1W1
A	0	PHE	-	expression tag	UNP Q2Z1W1
B	-5	GLU	-	expression tag	UNP Q2Z1W1
B	-4	ALA	-	expression tag	UNP Q2Z1W1
B	-3	GLU	-	expression tag	UNP Q2Z1W1
B	-2	ALA	-	expression tag	UNP Q2Z1W1
B	-1	GLU	-	expression tag	UNP Q2Z1W1
B	0	PHE	-	expression tag	UNP Q2Z1W1

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

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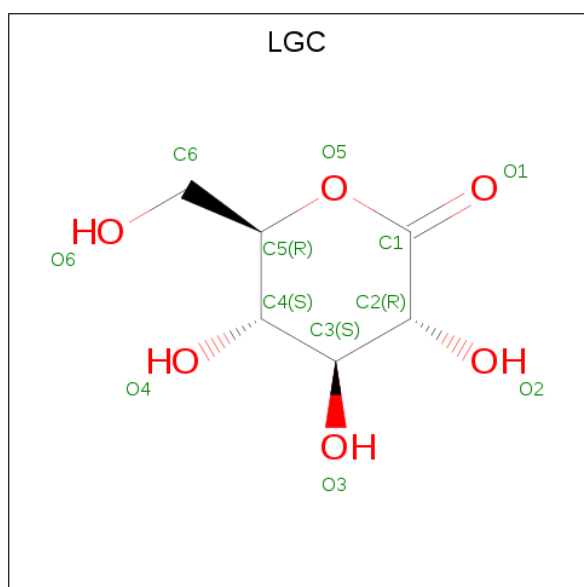
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is D-glucono-1,5-lactone (three-letter code: LGC) (formula: C<sub>6</sub>H<sub>10</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		

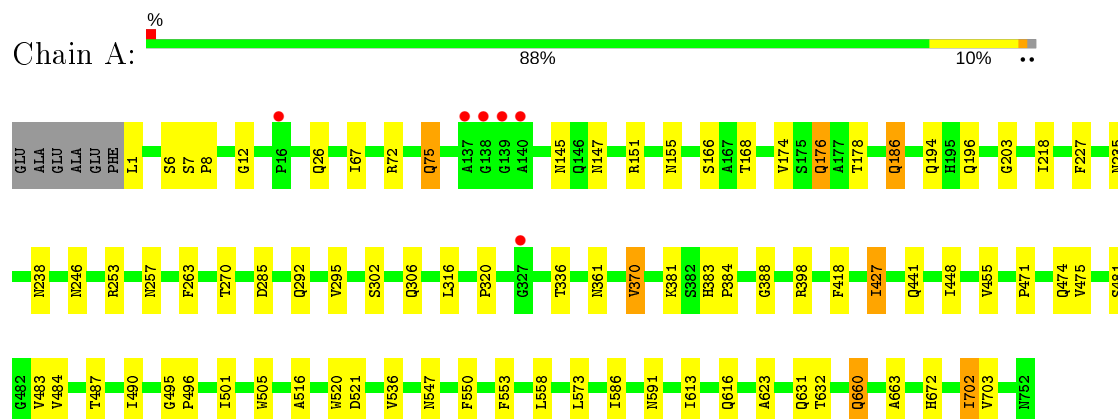
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	609	Total	O	0	0
			609	609		
5	B	584	Total	O	0	0
			584	584		

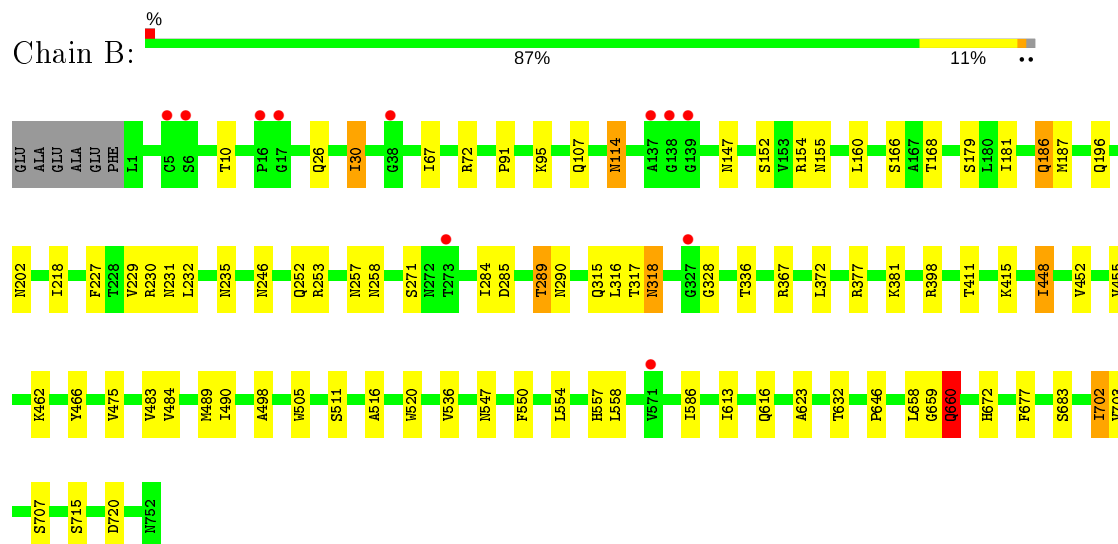
### 3 Residue-property plots [i](#)

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.

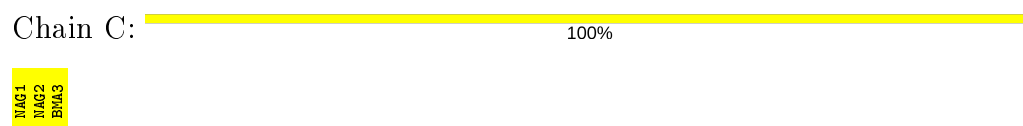
#### • Molecule 1: Glucan 1,3-beta-glucosidase



#### • Molecule 1: Glucan 1,3-beta-glucosidase



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



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

Chain D:

100%

MAG1  
MAG2  
EMJ3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.53 Å   67.15 Å   109.78 Å 93.94°   106.76°   97.08°	Depositor
Resolution (Å)	31.50 – 2.25 31.49 – 2.25	Depositor EDS
% Data completeness (in resolution range)	91.5 (31.50-2.25) 91.5 (31.49-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.26 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.142   ,   0.200 0.144   ,   0.202	Depositor DCC
$R_{free}$ test set	3875 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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: LGC, ZN, BMA, NAG

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	0.95	0/5755	0.83	2/7869 (0.0%)
1	B	0.95	0/5755	0.83	2/7869 (0.0%)
All	All	0.95	0/11510	0.83	4/15738 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	660	GLN	N-CA-C	7.07	130.08	111.00
1	A	151	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	370	VAL	CB-CA-C	-5.82	100.35	111.40
1	B	328	GLY	N-CA-C	-5.06	100.45	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	659	GLY	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5611	0	5302	44	0
1	B	5611	0	5300	46	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	10	1	0
4	B	12	0	10	0	0
5	A	609	0	0	5	0
5	B	584	0	0	3	0
All	All	12519	0	10690	90	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 4.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:ILE:HD11	1:B:489:MET:HG3	1.58	0.84
1:B:547:ASN:HD22	1:B:550:PHE:HE2	1.32	0.78
1:B:505:TRP:HB3	1:B:558:LEU:HD23	1.69	0.73
1:B:257:ASN:HD22	1:B:289:THR:HB	1.59	0.67
1:A:616:GLN:HG3	1:A:632:THR:HB	1.79	0.64
1:A:176:GLN:H	1:A:176:GLN:HE21	1.45	0.63
1:A:441:GLN:NE2	1:A:474:GLN:OE1	2.25	0.62
1:A:418:PHE:HE1	1:A:448:ILE:HD11	1.63	0.61
1:B:381:LYS:HG2	1:B:520:TRP:HZ2	1.67	0.60
1:B:616:GLN:HG3	1:B:632:THR:HB	1.83	0.60
1:A:547:ASN:HD22	1:A:550:PHE:HE2	1.49	0.59
1:B:107:GLN:HG2	1:B:152:SER:HB3	1.83	0.59
1:B:229:VAL:CG1	1:B:232:LEU:HD22	2.33	0.58
1:B:229:VAL:HG11	1:B:232:LEU:HD22	1.87	0.57
1:A:194:GLN:NE2	5:A:1331:HOH:O	2.38	0.56
1:B:455:VAL:HG22	1:B:490:ILE:HB	1.88	0.54
1:A:235:ASN:HD22	1:A:257:ASN:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ALA:HA	1:A:672:HIS:O	2.08	0.54
1:B:231:ASN:HA	1:B:253:ARG:O	2.07	0.53
1:A:1:LEU:N	5:A:777:HOH:O	2.41	0.53
1:A:487:THR:HG22	1:A:520:TRP:HB2	1.90	0.53
1:B:381:LYS:HG2	1:B:520:TRP:CZ2	2.44	0.53
1:B:95:LYS:HE2	5:B:1044:HOH:O	2.10	0.52
1:B:448:ILE:CD1	1:B:489:MET:HG3	2.35	0.51
1:B:623:ALA:HA	1:B:672:HIS:O	2.11	0.51
1:A:427:ILE:HB	1:A:448:ILE:HD13	1.93	0.51
1:A:455:VAL:HG22	1:A:490:ILE:HB	1.94	0.49
1:A:381:LYS:HD3	1:A:520:TRP:HZ2	1.77	0.49
1:B:186:GLN:HA	1:B:186:GLN:HE21	1.76	0.49
1:A:536:VAL:HA	1:A:586:ILE:HG22	1.94	0.49
1:A:613:ILE:O	1:A:663:ALA:HB2	2.11	0.49
1:B:196:GLN:HA	1:B:218:ILE:O	2.13	0.48
1:B:702:ILE:HG23	1:B:703:VAL:HG23	1.95	0.48
1:B:317:THR:O	1:B:318:ASN:HB2	2.13	0.47
1:A:381:LYS:HD3	1:A:520:TRP:CZ2	2.49	0.47
1:B:67:ILE:O	1:B:72:ARG:HD3	2.15	0.47
1:A:246:ASN:OD1	1:A:246:ASN:C	2.54	0.47
1:B:554:LEU:HD23	1:B:557:HIS:HB2	1.98	0.46
1:A:702:ILE:HG23	1:A:703:VAL:HG23	1.97	0.46
1:A:270:THR:HG23	1:A:306:GLN:HG3	1.98	0.46
1:B:613:ILE:CD1	1:B:646:PRO:HD2	2.45	0.46
1:A:418:PHE:CE1	1:A:448:ILE:HD11	2.49	0.46
1:A:186:GLN:HE21	1:A:186:GLN:HA	1.81	0.46
1:B:202:ASN:HB2	5:B:1133:HOH:O	2.15	0.45
1:A:475:VAL:HG13	1:A:484:VAL:HG11	1.97	0.45
1:A:660:GLN:HG3	1:A:660:GLN:O	2.16	0.45
1:A:12:GLY:HA3	1:A:388:GLY:O	2.17	0.45
1:B:285:ASP:HB3	1:B:377:ARG:HD2	1.98	0.44
1:B:235:ASN:HD22	1:B:257:ASN:HB2	1.83	0.44
1:B:258:ASN:HA	1:B:290:ASN:O	2.18	0.44
1:A:483:VAL:HG22	1:A:516:ALA:HB1	1.99	0.44
1:B:536:VAL:HA	1:B:586:ILE:HG22	2.00	0.44
1:A:383:HIS:ND1	1:A:521:ASP:OD2	2.50	0.44
1:A:505:TRP:HB3	1:A:558:LEU:HD23	2.00	0.44
1:B:168:THR:HA	1:B:196:GLN:O	2.17	0.44
1:A:196:GLN:HA	1:A:218:ILE:O	2.18	0.43
1:A:7:SER:HB2	1:A:8:PRO:CD	2.48	0.43
1:B:160:LEU:HD12	1:B:187:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:THR:HG22	1:B:415:LYS:HE2	2.00	0.43
1:A:145:ASN:HD22	1:A:203:GLY:HA2	1.84	0.43
1:B:154:ARG:HA	1:B:181:ILE:O	2.18	0.43
1:B:483:VAL:HG22	1:B:516:ALA:HB1	2.01	0.43
1:B:91:PRO:HG3	1:B:114:ASN:HB3	2.01	0.42
1:B:498:ALA:HB2	1:B:550:PHE:CG	2.54	0.42
1:A:316:LEU:O	1:A:336:THR:HA	2.20	0.42
1:A:67:ILE:O	1:A:72:ARG:HD3	2.19	0.42
1:B:317:THR:O	1:B:318:ASN:CB	2.67	0.42
1:B:284:ILE:HB	1:B:677:PHE:CE2	2.55	0.42
1:B:230:ARG:HA	1:B:252:GLN:O	2.19	0.42
1:A:75:GLN:HB2	5:A:1314:HOH:O	2.18	0.41
1:A:292:GLN:NE2	1:A:320:PRO:HG2	2.35	0.41
4:A:757:LGC:C1	5:A:1186:HOH:O	2.68	0.41
1:A:361:ASN:HD22	1:B:511:SER:HB3	1.86	0.41
1:B:462:LYS:HG3	1:B:462:LYS:O	2.20	0.41
1:A:263:PHE:HB2	1:A:295:VAL:HG22	2.02	0.41
1:A:553:PHE:O	1:A:591:ASN:HB3	2.21	0.41
1:B:475:VAL:HG13	1:B:484:VAL:HG11	2.03	0.41
1:A:481:SER:HB2	5:A:1227:HOH:O	2.21	0.41
1:A:573:LEU:C	1:A:573:LEU:HD13	2.41	0.41
1:A:174:VAL:HB	1:A:178:THR:HG21	2.03	0.41
1:A:495:GLY:HA2	1:A:496:PRO:C	2.40	0.41
1:A:253:ARG:HA	1:A:285:ASP:O	2.21	0.40
1:B:152:SER:HA	1:B:179:SER:O	2.22	0.40
1:B:316:LEU:O	1:B:336:THR:HA	2.21	0.40
1:B:683:SER:O	1:B:720:ASP:HB2	2.21	0.40
1:B:246:ASN:OD1	1:B:246:ASN:C	2.59	0.40
1:A:168:THR:HA	1:A:196:GLN:O	2.21	0.40
1:B:367:ARG:HB3	1:B:372:LEU:HD21	2.03	0.40
1:A:471:PRO:HA	1:A:501:ILE:O	2.21	0.40
1:B:30:ILE:HG22	5:B:866:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	750/758 (99%)	710 (95%)	38 (5%)	2 (0%)	41	46
1	B	750/758 (99%)	708 (94%)	38 (5%)	4 (0%)	29	29
All	All	1500/1516 (99%)	1418 (94%)	76 (5%)	6 (0%)	34	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	660	GLN
1	A	155	ASN
1	B	155	ASN
1	A	702	ILE
1	B	452	VAL
1	B	702	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	590/594 (99%)	574 (97%)	16 (3%)	44	54
1	B	590/594 (99%)	571 (97%)	19 (3%)	39	47
All	All	1180/1188 (99%)	1145 (97%)	35 (3%)	41	50

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	26	GLN
1	A	75	GLN
1	A	147	ASN
1	A	166	SER
1	A	176	GLN

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Mol	Chain	Res	Type
1	A	186	GLN
1	A	227	PHE
1	A	238	ASN
1	A	302	SER
1	A	370	VAL
1	A	384	PRO
1	A	398	ARG
1	A	427	ILE
1	A	631	GLN
1	A	660	GLN
1	B	10	THR
1	B	26	GLN
1	B	30	ILE
1	B	114	ASN
1	B	147	ASN
1	B	166	SER
1	B	186	GLN
1	B	227	PHE
1	B	271	SER
1	B	289	THR
1	B	315	GLN
1	B	318	ASN
1	B	398	ARG
1	B	448	ILE
1	B	466	TYR
1	B	658	LEU
1	B	660	GLN
1	B	707	SER
1	B	715	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	145	ASN
1	A	147	ASN
1	A	176	GLN
1	A	186	GLN
1	A	194	GLN
1	A	214	ASN
1	A	235	ASN
1	A	242	ASN

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Mol	Chain	Res	Type
1	A	257	ASN
1	A	292	GLN
1	A	361	ASN
1	A	508	HIS
1	A	547	ASN
1	A	631	GLN
1	A	652	ASN
1	B	186	GLN
1	B	214	ASN
1	B	235	ASN
1	B	242	ASN
1	B	257	ASN
1	B	315	GLN
1	B	468	ASN
1	B	547	ASN
1	B	696	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 ⓘ

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	NAG	C	1	1,2	14,14,15	0.81	0	17,19,21	1.84	4 (23%)
2	NAG	C	2	2	14,14,15	0.58	0	17,19,21	1.75	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BMA	C	3	2	11,11,12	1.29	1 (9%)	15,15,17	1.63	1 (6%)
2	NAG	D	1	1,2	14,14,15	0.77	0	17,19,21	1.43	3 (17%)
2	NAG	D	2	2	14,14,15	0.80	0	17,19,21	1.47	2 (11%)
2	BMA	D	3	2	11,11,12	0.89	0	15,15,17	1.53	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	BMA	C2-C3	2.56	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	5.08	119.07	112.19
2	C	3	BMA	C1-C2-C3	4.70	115.44	109.67
2	D	2	NAG	C1-O5-C5	4.61	118.44	112.19
2	C	2	NAG	C1-O5-C5	3.27	116.62	112.19
2	D	1	NAG	C2-N2-C7	2.94	127.09	122.90
2	D	3	BMA	O5-C5-C6	2.80	111.59	107.20
2	C	1	NAG	O5-C1-C2	-2.66	107.09	111.29
2	C	1	NAG	C2-N2-C7	-2.57	119.24	122.90
2	C	2	NAG	C4-C3-C2	2.54	114.74	111.02
2	C	2	NAG	C2-N2-C7	-2.53	119.30	122.90
2	C	1	NAG	C4-C3-C2	2.48	114.66	111.02
2	D	1	NAG	O5-C1-C2	-2.46	107.40	111.29
2	C	2	NAG	C8-C7-N2	2.40	120.17	116.10
2	D	1	NAG	O5-C5-C6	2.22	110.69	107.20
2	C	2	NAG	C3-C4-C5	-2.21	106.30	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O5-C5-C6	2.16	110.58	107.20
2	D	3	BMA	O5-C5-C4	-2.12	105.67	110.83
2	D	2	NAG	C1-C2-N2	-2.11	106.89	110.49

There are no chirality outliers.

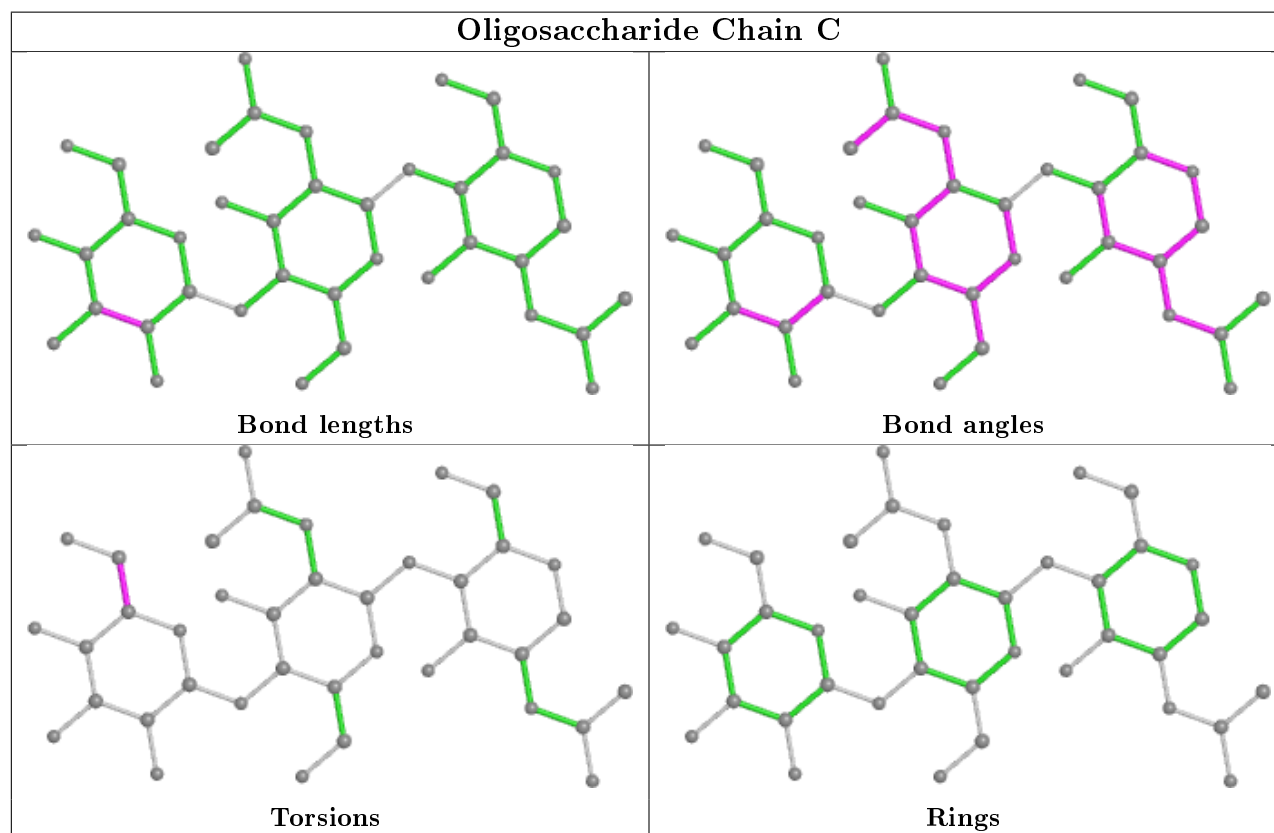
All (5) torsion outliers are listed below:

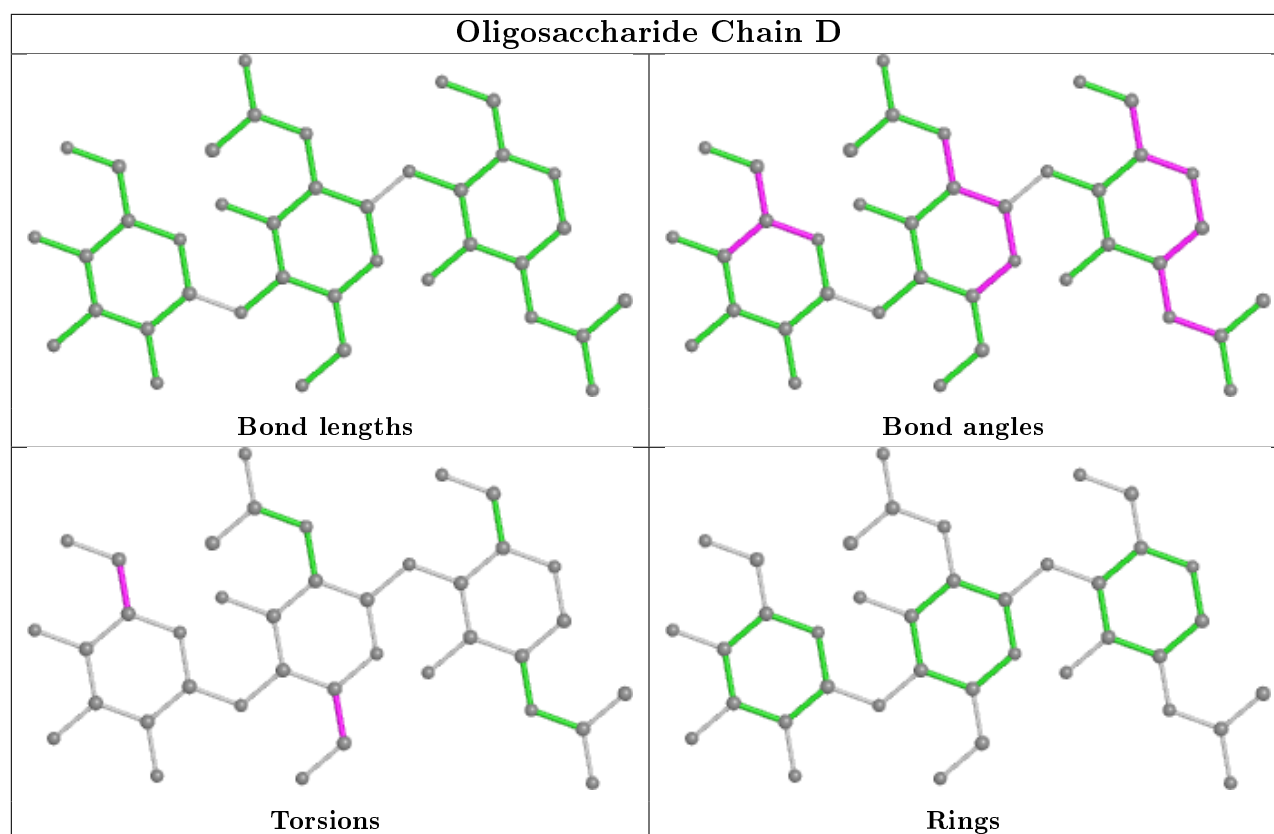
Mol	Chain	Res	Type	Atoms
2	D	3	BMA	O5-C5-C6-O6
2	D	3	BMA	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	LGC	B	757	-	12,12,12	2.34	1 (8%)	15,17,17	1.43	3 (20%)
4	LGC	A	757	-	12,12,12	2.78	2 (16%)	15,17,17	1.43	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LGC	B	757	-	-	0/2/22/22	0/1/1/1
4	LGC	A	757	-	-	2/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	757	LGC	O5-C1	8.48	1.47	1.34
4	B	757	LGC	O5-C1	7.52	1.45	1.34
4	A	757	LGC	O5-C5	-3.92	1.41	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	757	LGC	O4-C4-C5	-2.68	102.63	109.30
4	B	757	LGC	O5-C5-C4	2.64	114.42	109.73
4	A	757	LGC	O6-C6-C5	-2.56	102.49	111.29
4	A	757	LGC	O4-C4-C5	-2.37	103.40	109.30
4	B	757	LGC	O2-C2-C3	2.30	115.29	110.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	757	LGC	C4-C5-C6-O6
4	A	757	LGC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	757	LGC	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	752/758 (99%)	-0.57	6 (0%) 86 87	10, 18, 28, 41	0
1	B	752/758 (99%)	-0.48	11 (1%) 73 75	12, 20, 31, 48	0
All	All	1504/1516 (99%)	-0.52	17 (1%) 80 82	10, 19, 30, 48	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	GLY	3.5
1	B	327	GLY	3.3
1	B	6	SER	3.3
1	B	273	THR	3.3
1	B	138	GLY	3.3
1	B	139	GLY	3.1
1	A	16	PRO	3.0
1	B	16	PRO	2.9
1	A	139	GLY	2.8
1	B	17	GLY	2.7
1	B	137	ALA	2.4
1	A	140	ALA	2.3
1	B	38	GLY	2.2
1	A	327	GLY	2.2
1	B	571	VAL	2.2
1	B	5	CYS	2.1
1	A	137	ALA	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

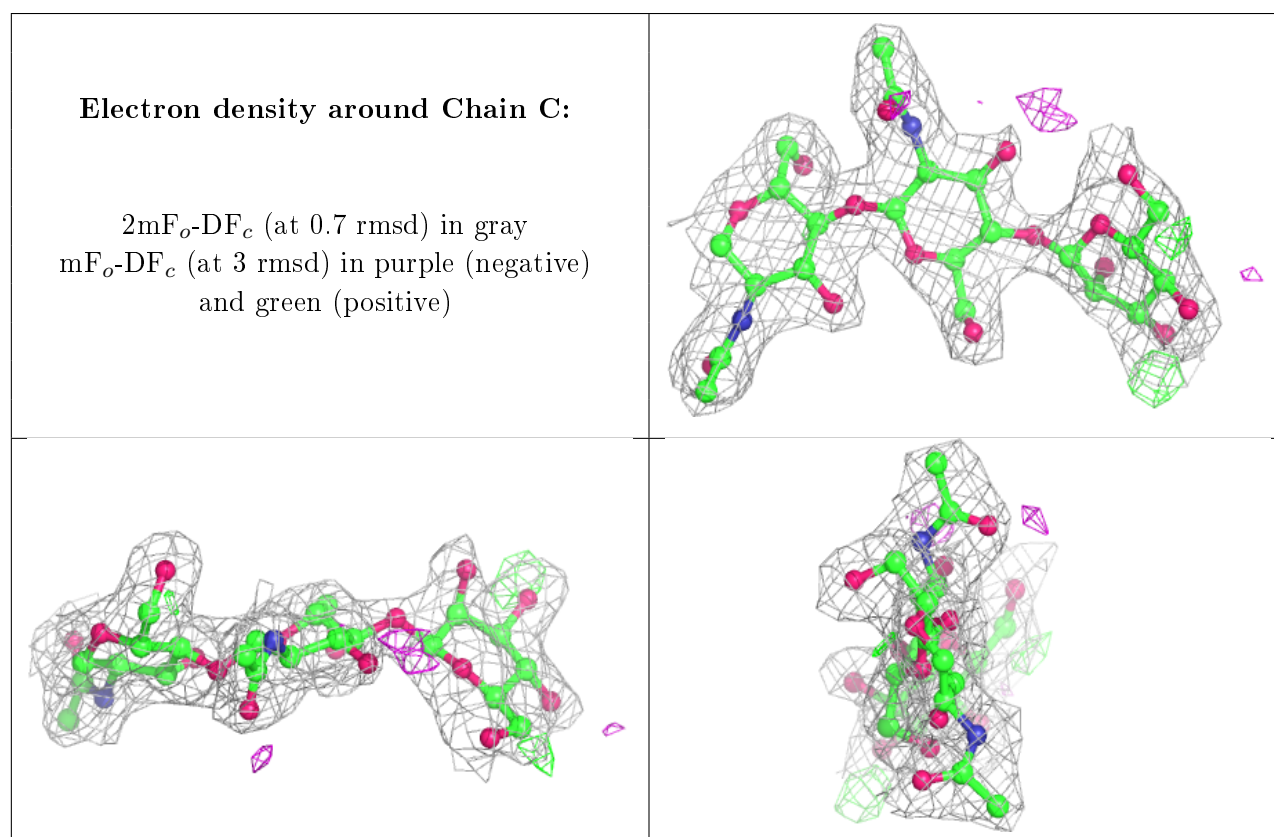
There are no non-standard protein/DNA/RNA residues in this entry.

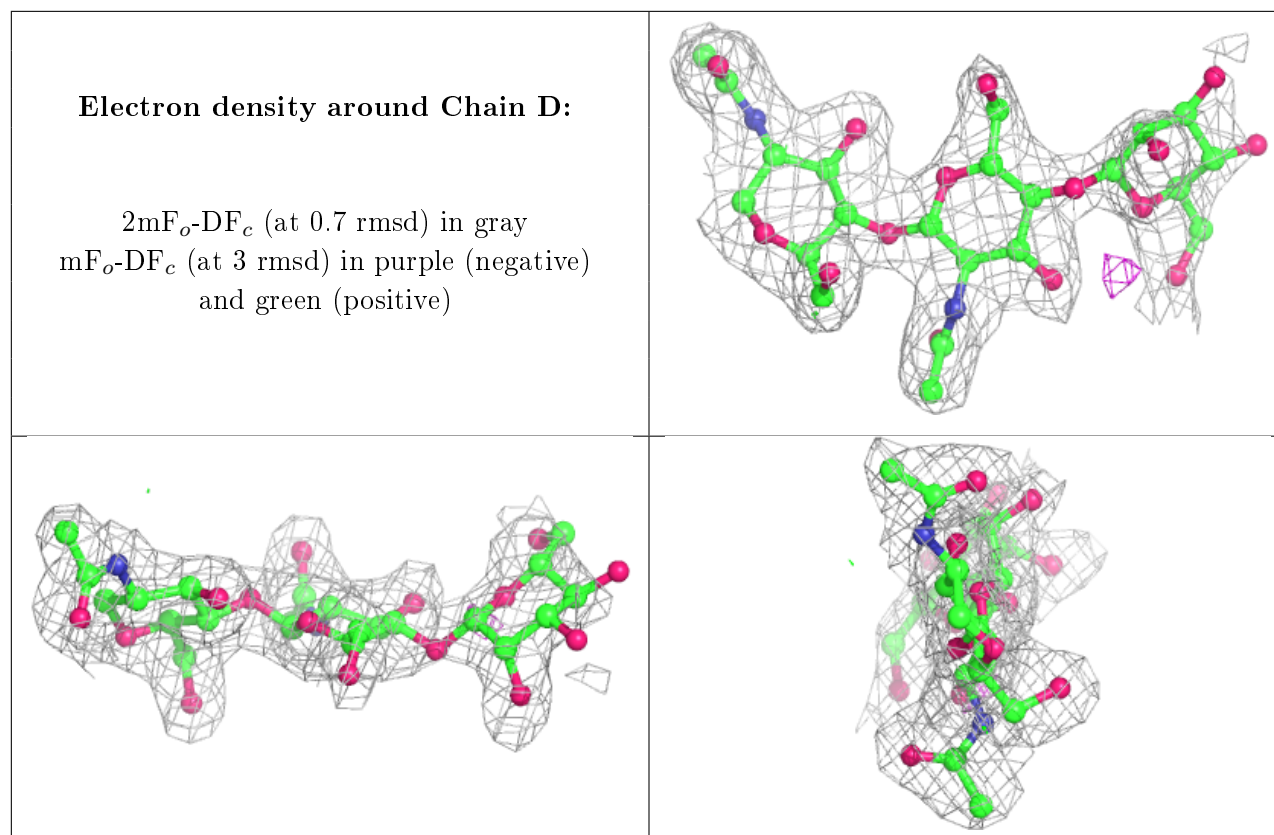
## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	BMA	C	3	11/12	0.72	0.30	60,62,63,63	0
2	BMA	D	3	11/12	0.72	0.45	65,69,71,72	0
2	NAG	C	2	14/15	0.85	0.20	41,44,50,56	0
2	NAG	D	2	14/15	0.91	0.24	31,43,52,60	0
2	NAG	C	1	14/15	0.96	0.10	21,28,30,36	0
2	NAG	D	1	14/15	0.97	0.11	20,24,29,36	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( $\text{\AA}^2$ )	Q<0.9
4	LGC	B	757	12/12	0.95	0.10	21,26,30,31	0
4	LGC	A	757	12/12	0.95	0.10	16,24,28,28	0
3	ZN	A	756	1/1	0.98	0.08	38,38,38,38	0
3	ZN	B	756	1/1	0.99	0.06	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.