



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:55 PM UTC

PDB ID : 1OGS / pdb\_00001ogs  
Title : human acid-beta-glucosidase  
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Deposited on : 2003-05-13  
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

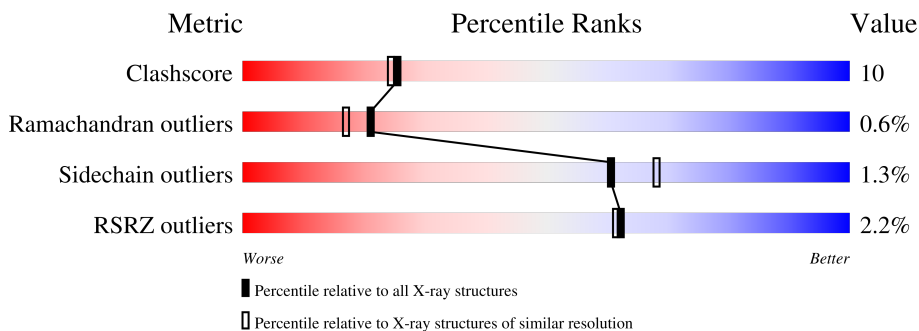
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

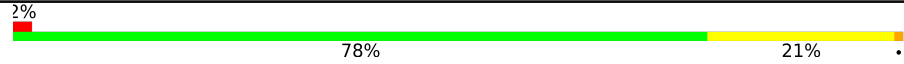
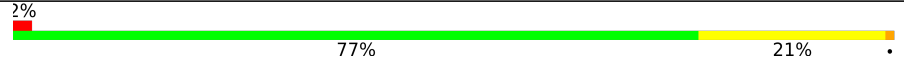
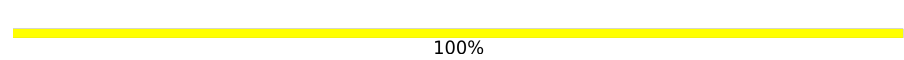
The reported resolution of this entry is 2.00 Å.

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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	 2% 78% 21%
1	B	497	 2% 77% 21%
2	C	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1997	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9020 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 Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3973	2556	678	723	16	0	5	0
1	B	497	3992	2565	684	727	16	0	7	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	495	HIS	ARG	conflict	UNP P04062
B	495	HIS	ARG	conflict	UNP P04062

- 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
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



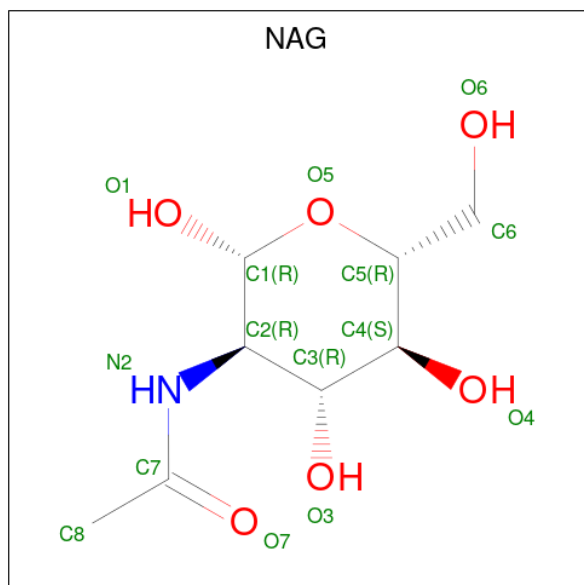
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total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

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

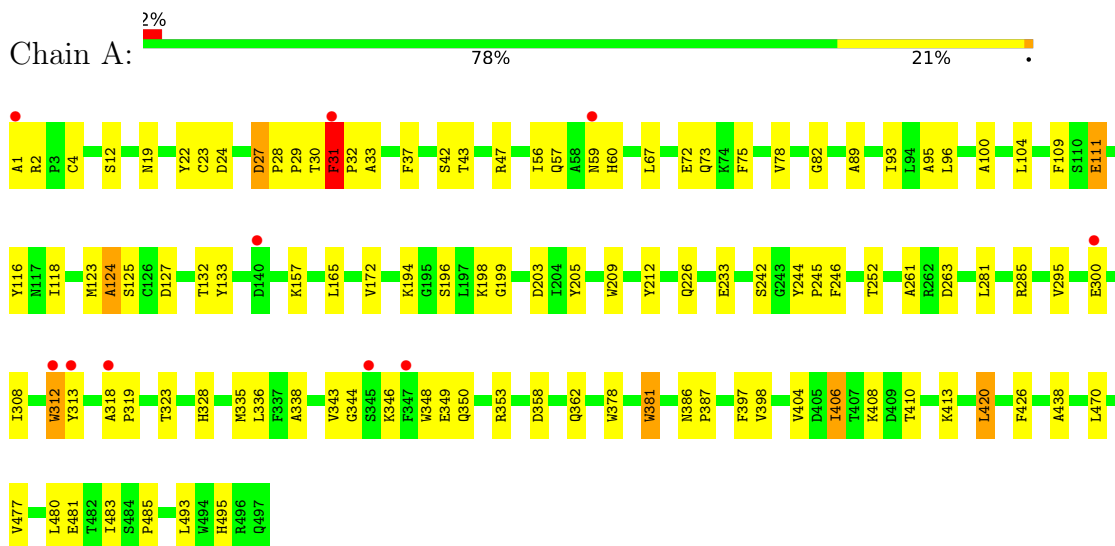
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	438	Total	O	0	0
			438	438		
5	B	500	Total	O	0	0
			500	500		

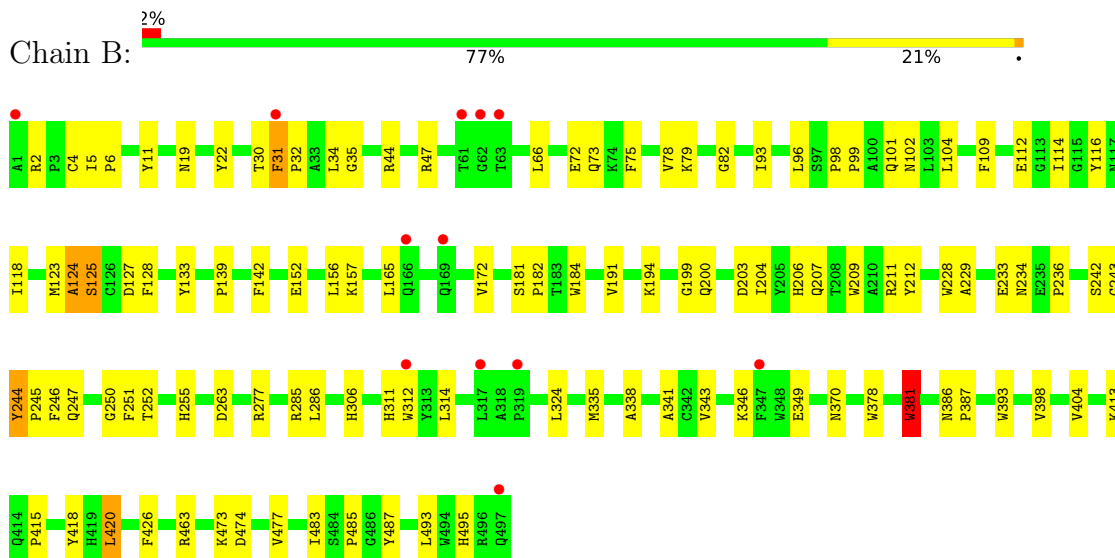
### 3 Residue-property plots [i](#)

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: Glucosylceramidase

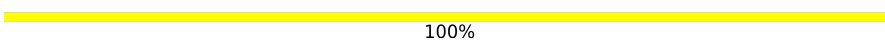


- Molecule 1: Glucosylceramidase



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

Chain C:



100%

MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.73Å 285.23Å 91.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.40 – 2.00 14.40 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (14.40-2.00) 93.2 (14.40-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 2.01Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.195 , 0.230 0.200 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtrriage
Anisotropy	0.891	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 65.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9020	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.36	0/4094	0.93	19/5582 (0.3%)
1	B	0.36	0/4113	0.93	15/5606 (0.3%)
All	All	0.36	0/8207	0.93	34/11188 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	THR	N-CA-C	-8.39	99.12	110.36
1	B	244	TYR	CA-C-N	7.99	127.91	119.05
1	B	244	TYR	C-N-CA	7.99	127.91	119.05
1	A	31	PHE	CA-C-N	7.63	127.58	120.03
1	A	31	PHE	C-N-CA	7.63	127.58	120.03
1	A	125	SER	N-CA-C	6.69	120.38	110.48
1	A	244	TYR	CA-C-N	6.51	125.94	118.85
1	A	244	TYR	C-N-CA	6.51	125.94	118.85
1	A	252	THR	N-CA-C	-6.36	100.85	110.39
1	A	56	ILE	N-CA-C	-6.16	98.10	106.85
1	B	114	ILE	N-CA-C	6.13	118.14	111.77
1	A	27	ASP	N-CA-C	-6.03	103.20	110.13
1	A	111	GLU	N-CA-C	-5.85	105.40	112.54
1	B	245	PRO	N-CA-C	5.82	121.62	113.53
1	B	109	PHE	N-CA-C	5.78	120.61	113.50
1	B	181	SER	N-CA-C	-5.74	103.42	110.31
1	B	157	LYS	N-CA-C	5.68	117.16	110.97
1	A	157	LYS	N-CA-C	5.57	117.04	110.97
1	A	406	ILE	N-CA-C	5.56	116.29	110.62
1	B	125	SER	N-CA-C	5.52	118.00	110.55
1	A	31	PHE	N-CA-C	5.46	116.83	109.24
1	B	112[A]	GLU	N-CA-C	-5.43	106.65	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112[B]	GLU	N-CA-C	-5.43	106.65	113.28
1	A	78	VAL	N-CA-C	5.43	116.59	109.21
1	A	109	PHE	N-CA-C	5.42	120.17	113.50
1	A	477	VAL	N-CA-C	5.42	115.90	111.62
1	A	245	PRO	N-CA-C	5.30	120.50	113.40
1	B	78	VAL	N-CA-C	5.28	116.19	108.58
1	B	250	GLY	N-CA-C	5.14	118.54	111.54
1	B	393	TRP	N-CA-C	5.13	118.64	112.38
1	A	12	SER	N-CA-C	5.13	117.61	111.71
1	A	263	ASP	N-CA-C	5.13	118.98	111.34
1	A	295	VAL	N-CA-C	5.02	115.69	110.82
1	B	263	ASP	N-CA-C	5.00	118.62	111.02

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	3973	0	3870	72	0
1	B	3992	0	3886	81	0
2	C	28	0	25	0	0
3	A	50	0	0	0	0
3	B	25	0	0	2	0
4	A	14	0	13	1	0
5	A	438	0	0	12	0
5	B	500	0	0	11	0
All	All	9020	0	7794	152	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 (152) 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:31:PHE:HD2	1:B:32:PRO:HD2	1.22	1.03
1:B:285:ARG:HB3	1:B:312:TRP:HZ3	1.23	0.98
1:B:207:GLN:HB3	1:B:211[A]:ARG:HH12	1.36	0.89
1:B:31:PHE:CD2	1:B:32:PRO:HD2	2.10	0.87
1:B:207:GLN:HB3	1:B:211[A]:ARG:NH1	1.89	0.86
1:B:285:ARG:HB3	1:B:312:TRP:CZ3	2.10	0.85
1:B:200:GLN:HB3	5:B:2267:HOH:O	1.84	0.76
1:A:1:ALA:HB3	5:A:2001:HOH:O	1.87	0.74
1:B:165:LEU:HD22	1:B:172:VAL:HB	1.72	0.72
1:A:408:LYS:O	1:A:410:THR:HG23	1.90	0.72
1:B:34:LEU:HD23	1:B:35:GLY:N	2.05	0.72
1:B:30:THR:HB	5:B:2054:HOH:O	1.91	0.70
1:A:57[B]:GLN:HG3	1:A:59:ASN:O	1.93	0.68
1:B:314:LEU:HB2	1:B:343:VAL:HG12	1.76	0.68
1:B:156:LEU:HD13	5:B:2138:HOH:O	1.93	0.68
1:A:312:TRP:CE3	1:A:312:TRP:HA	2.29	0.67
1:A:346:LYS:HB2	1:A:349:GLU:HB2	1.78	0.66
1:A:165:LEU:HD22	1:A:172:VAL:HB	1.81	0.63
1:A:95:ALA:HB1	1:A:406:ILE:HD12	1.80	0.63
1:B:312:TRP:NE1	1:B:370:ASN:HD21	1.97	0.62
1:B:346:LYS:HB2	1:B:349:GLU:HG3	1.81	0.61
1:A:226:GLN:NE2	5:A:2238:HOH:O	2.14	0.61
1:A:328:HIS:HD2	5:A:2306:HOH:O	1.82	0.61
1:A:483:ILE:O	1:A:485:PRO:HD3	2.01	0.60
1:A:1:ALA:HB2	1:A:27:ASP:OD1	2.02	0.60
1:A:312:TRP:HA	1:A:312:TRP:HE3	1.65	0.60
1:B:229:ALA:HB2	1:B:277:ARG:HB2	1.83	0.60
1:B:206:HIS:NE2	1:B:255:HIS:HE1	1.99	0.59
1:A:410:THR:HG21	5:A:2177:HOH:O	2.03	0.58
1:A:312:TRP:CZ2	1:A:318:ALA:HB2	2.39	0.58
1:B:73[B]:GLN:HG2	1:B:75:PHE:CE1	2.38	0.58
1:B:306:HIS:HE1	5:B:2491:HOH:O	1.86	0.58
4:A:1997:NAG:H2	5:A:2434:HOH:O	2.03	0.57
1:B:152:GLU:HA	1:B:156:LEU:HD12	1.86	0.57
1:B:194:LYS:HB2	1:B:242:SER:HA	1.88	0.56
1:A:438:ALA:HB2	5:A:2192:HOH:O	2.04	0.56
1:A:31:PHE:HB3	1:A:495:HIS:HE1	1.71	0.55
1:B:312:TRP:NE1	1:B:370:ASN:ND2	2.55	0.55
1:A:30:THR:HG21	1:B:204:ILE:HG21	1.89	0.55
1:B:98:PRO:HB2	1:B:99:PRO:HD3	1.88	0.54
1:B:44:ARG:HD2	3:B:1501:SO4:O2	2.07	0.54
1:A:319:PRO:HB2	5:A:2297:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LYS:HB2	1:A:242:SER:HA	1.90	0.54
1:B:142:PHE:O	1:B:211[B]:ARG:NH2	2.41	0.53
1:B:66:LEU:HD11	1:B:473:LYS:HB2	1.90	0.53
1:A:346:LYS:HD3	1:A:348:TRP:CZ2	2.44	0.53
1:A:387:PRO:HD3	1:A:404:VAL:O	2.09	0.52
1:A:23:CYS:SG	1:A:413:LYS:HE3	2.50	0.52
1:A:123:MET:O	1:A:124:ALA:HB3	2.09	0.52
1:A:261:ALA:HB1	1:A:300:GLU:HG2	1.92	0.52
1:A:350:GLN:H	1:A:350:GLN:CD	2.18	0.52
1:A:426:PHE:HB3	1:A:493:LEU:HD21	1.92	0.52
1:A:33:ALA:HB2	1:B:139:PRO:O	2.11	0.51
1:A:348:TRP:H	1:A:348:TRP:CD1	2.28	0.51
1:A:67:LEU:HG	1:A:470:LEU:HD11	1.92	0.51
1:B:47:ARG:NH1	5:B:2084:HOH:O	2.41	0.51
1:B:338:ALA:HB3	1:B:378:TRP:HA	1.92	0.51
1:B:123:MET:O	1:B:124:ALA:HB3	2.10	0.51
1:A:381:TRP:HA	1:A:381:TRP:CE3	2.45	0.51
1:B:312:TRP:HE1	1:B:370:ASN:CG	2.20	0.50
1:A:32:PRO:HD2	5:A:2414:HOH:O	2.11	0.50
1:B:312:TRP:HH2	1:B:324:LEU:HD21	1.77	0.50
1:A:73[B]:GLN:HG2	1:A:75:PHE:CE1	2.47	0.50
1:A:397:PHE:CD1	1:A:398:VAL:HG13	2.47	0.50
1:A:31:PHE:CD1	1:A:31:PHE:N	2.80	0.50
1:B:483:ILE:O	1:B:485:PRO:HD3	2.12	0.49
1:A:381:TRP:HA	1:A:381:TRP:HE3	1.77	0.49
1:A:19:ASN:HB2	5:A:2436:HOH:O	2.12	0.49
1:A:285:ARG:HD2	1:A:323:THR:OG1	2.12	0.49
1:B:31:PHE:CD1	1:B:495:HIS:HE1	2.30	0.49
1:B:72:GLU:OE2	1:B:72:GLU:HA	2.11	0.48
1:B:413:LYS:HE3	1:B:418:TYR:OH	2.13	0.48
1:A:31:PHE:HB3	1:A:495:HIS:CE1	2.49	0.48
1:A:72:GLU:OE2	1:A:72:GLU:HA	2.14	0.48
1:B:381:TRP:HA	1:B:381:TRP:CE3	2.48	0.48
1:B:381:TRP:HA	1:B:381:TRP:HE3	1.79	0.48
1:B:116:TYR:OH	1:B:420:LEU:HD13	2.14	0.47
1:B:311:HIS:O	1:B:312:TRP:CE3	2.67	0.47
1:A:82:GLY:HA3	1:A:118:ILE:O	2.15	0.47
1:B:199:GLY:HA3	1:B:203:ASP:OD2	2.15	0.47
1:B:127:ASP:HB3	1:B:246:PHE:CG	2.50	0.47
1:B:463:ARG:HD2	5:B:2236:HOH:O	2.14	0.47
1:A:37:PHE:CD2	1:A:480:LEU:HG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ILE:HG22	5:A:2348:HOH:O	2.14	0.46
1:B:128:PHE:CZ	1:B:398:VAL:HG22	2.51	0.46
1:B:2:ARG:NH1	5:B:2002:HOH:O	2.49	0.46
1:A:2:ARG:HD3	1:A:22:TYR:CE1	2.51	0.46
1:A:199:GLY:HA3	1:A:203:ASP:OD2	2.16	0.46
1:B:128:PHE:HZ	1:B:398:VAL:HG22	1.81	0.46
1:B:346:LYS:HB2	1:B:349:GLU:CG	2.47	0.45
1:B:426:PHE:HB3	1:B:493:LEU:HD21	1.97	0.45
1:A:343:VAL:HG22	1:A:344:GLY:N	2.31	0.45
1:A:312:TRP:CZ2	1:A:318:ALA:CB	2.99	0.45
1:A:338:ALA:HB3	1:A:378:TRP:HA	1.98	0.45
1:B:19:ASN:HB2	5:B:2032:HOH:O	2.17	0.45
1:B:209:TRP:O	1:B:212:TYR:HB3	2.16	0.45
1:B:93:ILE:O	1:B:101:GLN:HG2	2.16	0.45
1:A:116:TYR:OH	1:A:420:LEU:HD13	2.17	0.44
1:A:308:ILE:HB	1:A:336:LEU:HD23	1.99	0.43
1:A:89:ALA:O	1:A:93:ILE:HG13	2.17	0.43
1:B:312:TRP:O	1:B:341:ALA:HA	2.18	0.43
1:B:312:TRP:CZ2	1:B:370:ASN:OD1	2.71	0.43
1:B:82:GLY:HA3	1:B:118:ILE:O	2.19	0.43
1:A:358[B]:ASP:O	1:A:362:GLN:HG3	2.19	0.43
1:B:102[A]:ASN:ND2	5:B:2153:HOH:O	2.51	0.43
1:B:312:TRP:HE1	1:B:370:ASN:ND2	2.15	0.43
1:A:4:CYS:HA	1:A:24:ASP:HB3	2.00	0.42
1:A:209:TRP:O	1:A:212:TYR:HB3	2.20	0.42
1:B:314:LEU:HB2	1:B:343:VAL:CG1	2.47	0.42
1:A:209:TRP:HA	1:A:209:TRP:CE3	2.55	0.42
1:B:206:HIS:NE2	1:B:255:HIS:CE1	2.84	0.42
1:B:34:LEU:HD23	1:B:35:GLY:H	1.82	0.42
1:B:79:LYS:HE2	1:B:228:TRP:CE2	2.54	0.42
1:A:196:SER:HB2	5:A:2251:HOH:O	2.19	0.42
1:B:286:LEU:HG	5:B:2334:HOH:O	2.20	0.42
1:A:132:THR:O	1:A:133:TYR:HB3	2.19	0.42
1:A:42:SER:HA	1:A:47:ARG:O	2.19	0.42
1:B:5:ILE:HG12	1:B:22:TYR:CE2	2.55	0.42
1:B:34:LEU:HB2	5:B:2059:HOH:O	2.20	0.41
1:A:313:TYR:CD1	1:A:313:TYR:N	2.89	0.41
1:A:37:PHE:CD1	1:A:37:PHE:C	2.98	0.41
1:A:104:LEU:HD23	1:A:104:LEU:C	2.46	0.41
1:B:191:VAL:O	1:B:247:GLN:HA	2.21	0.41
1:A:31:PHE:HA	1:A:32:PRO:HD3	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ASP:C	1:B:203:ASP:OD1	2.63	0.41
1:A:29:PRO:HD3	1:A:111:GLU:HG2	2.02	0.41
1:B:11:TYR:HB3	3:B:1500:SO4:O3	2.21	0.41
1:B:104:LEU:C	1:B:104:LEU:HD23	2.45	0.41
1:A:43:THR:HB	5:A:2058:HOH:O	2.20	0.41
1:A:386:ASN:HB2	1:A:387:PRO:CD	2.51	0.41
1:B:22:TYR:CD2	1:B:22:TYR:C	2.99	0.41
1:B:211[A]:ARG:HG3	1:B:211[A]:ARG:HH11	1.85	0.41
1:B:234:ASN:OD1	1:B:311:HIS:HE1	2.04	0.41
1:A:60:HIS:HD2	1:A:481:GLU:OE2	2.03	0.41
1:A:198:LYS:HB2	1:A:205:TYR:CD2	2.56	0.41
1:B:243:GLY:O	1:B:244:TYR:C	2.62	0.41
1:A:28:PRO:HA	1:A:29:PRO:HD3	1.97	0.41
1:A:73[B]:GLN:HG2	1:A:75:PHE:CZ	2.56	0.40
1:A:349:GLU:HG2	1:A:353:ARG:NH2	2.36	0.40
1:B:4:CYS:O	1:B:6:PRO:HD3	2.21	0.40
1:B:44:ARG:NH1	1:B:487:TYR:CE1	2.89	0.40
1:B:312:TRP:HZ2	1:B:370:ASN:OD1	2.05	0.40
1:A:127:ASP:HB3	1:A:246:PHE:CD2	2.55	0.40
1:B:236:PRO:HB2	1:B:251:PHE:HB2	2.03	0.40
1:A:96:LEU:HB3	1:A:100:ALA:HB3	2.02	0.40
1:B:125:SER:HB3	1:B:133:TYR:CE2	2.56	0.40
1:B:386:ASN:HB2	1:B:387:PRO:CD	2.52	0.40
1:B:387:PRO:HD3	1:B:404:VAL:O	2.21	0.40
1:B:474:ASP:HB3	1:B:477:VAL:HG22	2.04	0.40
1:A:29:PRO:HD3	1:A:111:GLU:CG	2.52	0.40
1:B:96:LEU:HD21	1:B:404:VAL:HG13	2.04	0.40
1:B:184:TRP:CD1	1:B:184:TRP:H	2.39	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	500/497 (101%)	473 (95%)	24 (5%)	3 (1%)	21	17
1	B	502/497 (101%)	482 (96%)	17 (3%)	3 (1%)	21	17
All	All	1002/994 (101%)	955 (95%)	41 (4%)	6 (1%)	21	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	GLU
1	A	124	ALA
1	B	124	ALA
1	B	233	GLU
1	A	281	LEU
1	B	381	TRP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/424 (101%)	424 (99%)	5 (1%)	63	70
1	B	431/424 (102%)	425 (99%)	6 (1%)	59	66
All	All	860/848 (101%)	849 (99%)	11 (1%)	61	68

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	PHE
1	A	312	TRP
1	A	335	MET
1	A	381	TRP
1	A	420	LEU
1	B	31	PHE
1	B	182	PRO
1	B	335	MET
1	B	381	TRP
1	B	415	PRO

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Mol	Chain	Res	Type
1	B	420	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	GLN
1	A	223	HIS
1	A	328	HIS
1	A	362	GLN
1	A	495	HIS
1	B	166	GLN
1	B	169	GLN
1	B	255	HIS
1	B	306	HIS
1	B	495	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

2 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	0.49	0	17,19,21	0.73	1 (5%)
2	NAG	C	2	2	14,14,15	0.56	0	17,19,21	0.70	1 (5%)

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	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C2-N2-C7	-2.24	119.89	122.90
2	C	2	NAG	C2-N2-C7	-2.08	120.11	122.90

There are no chirality outliers.

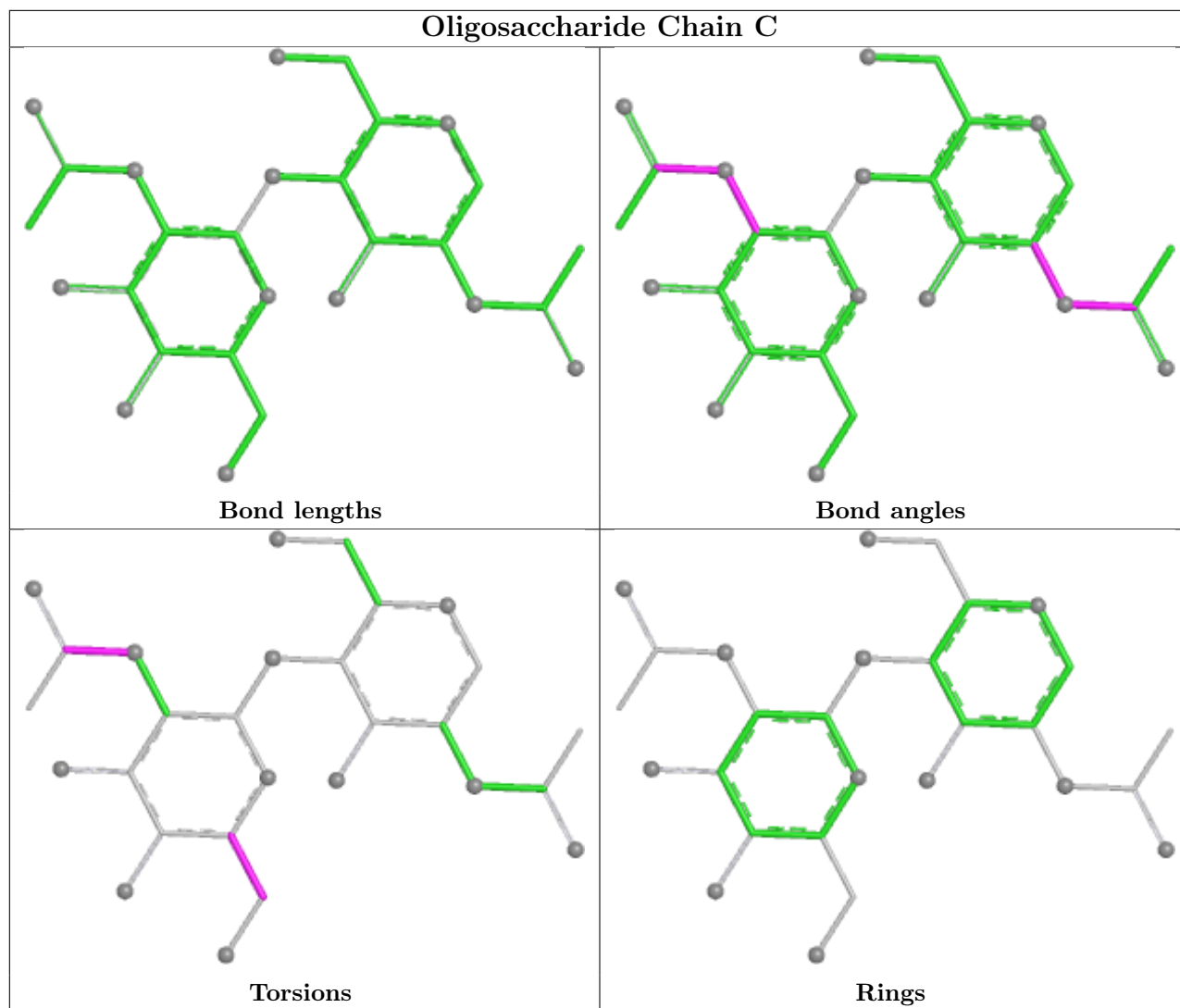
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2

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](#)

16 ligands 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	$\# Z  > 2$
3	SO4	A	1503	-	4,4,4	0.37	0	6,6,6	0.10	0
3	SO4	B	1499	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	A	1498	-	4,4,4	0.39	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	1498	-	4,4,4	0.35	0	6,6,6	0.09	0
3	SO4	B	1502	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	A	1507	-	4,4,4	0.37	0	6,6,6	0.11	0
3	SO4	B	1501	-	4,4,4	0.35	0	6,6,6	0.09	0
3	SO4	A	1506	-	4,4,4	0.33	0	6,6,6	0.12	0
3	SO4	A	1504	-	4,4,4	0.37	0	6,6,6	0.11	0
3	SO4	A	1500	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	A	1502	-	4,4,4	0.37	0	6,6,6	0.11	0
3	SO4	A	1505	-	4,4,4	0.35	0	6,6,6	0.08	0
3	SO4	B	1500	-	4,4,4	0.33	0	6,6,6	0.08	0
3	SO4	A	1501	-	4,4,4	0.37	0	6,6,6	0.09	0
4	NAG	A	1997	1	14,14,15	0.68	0	17,19,21	0.77	0
3	SO4	A	1499	-	4,4,4	0.38	0	6,6,6	0.06	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
4	NAG	A	1997	1	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1997	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1997	NAG	C8-C7-N2-C2
4	A	1997	NAG	O7-C7-N2-C2
4	A	1997	NAG	C4-C5-C6-O6
4	A	1997	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1501	SO4	1	0
3	B	1500	SO4	1	0
4	A	1997	NAG	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	497/497 (100%)	-0.19	10 (2%) 65 64	14, 25, 43, 57	5 (1%)
1	B	497/497 (100%)	-0.29	12 (2%) 59 59	11, 23, 42, 57	7 (1%)
All	All	994/994 (100%)	-0.24	22 (2%) 62 61	11, 24, 43, 57	12 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	TRP	6.7
1	A	31	PHE	4.7
1	A	312	TRP	4.2
1	B	31	PHE	3.8
1	B	317	LEU	3.4
1	B	169	GLN	3.3
1	B	1	ALA	3.1
1	A	347	PHE	3.0
1	A	1	ALA	3.0
1	A	313	TYR	2.8
1	B	319	PRO	2.7
1	B	63	THR	2.6
1	B	347	PHE	2.5
1	B	61	THR	2.4
1	B	62	GLY	2.3
1	A	345	SER	2.2
1	B	497	GLN	2.2
1	A	59	ASN	2.2
1	A	318	ALA	2.2
1	B	166	GLN	2.1
1	A	300	GLU	2.1
1	A	140	ASP	2.0

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

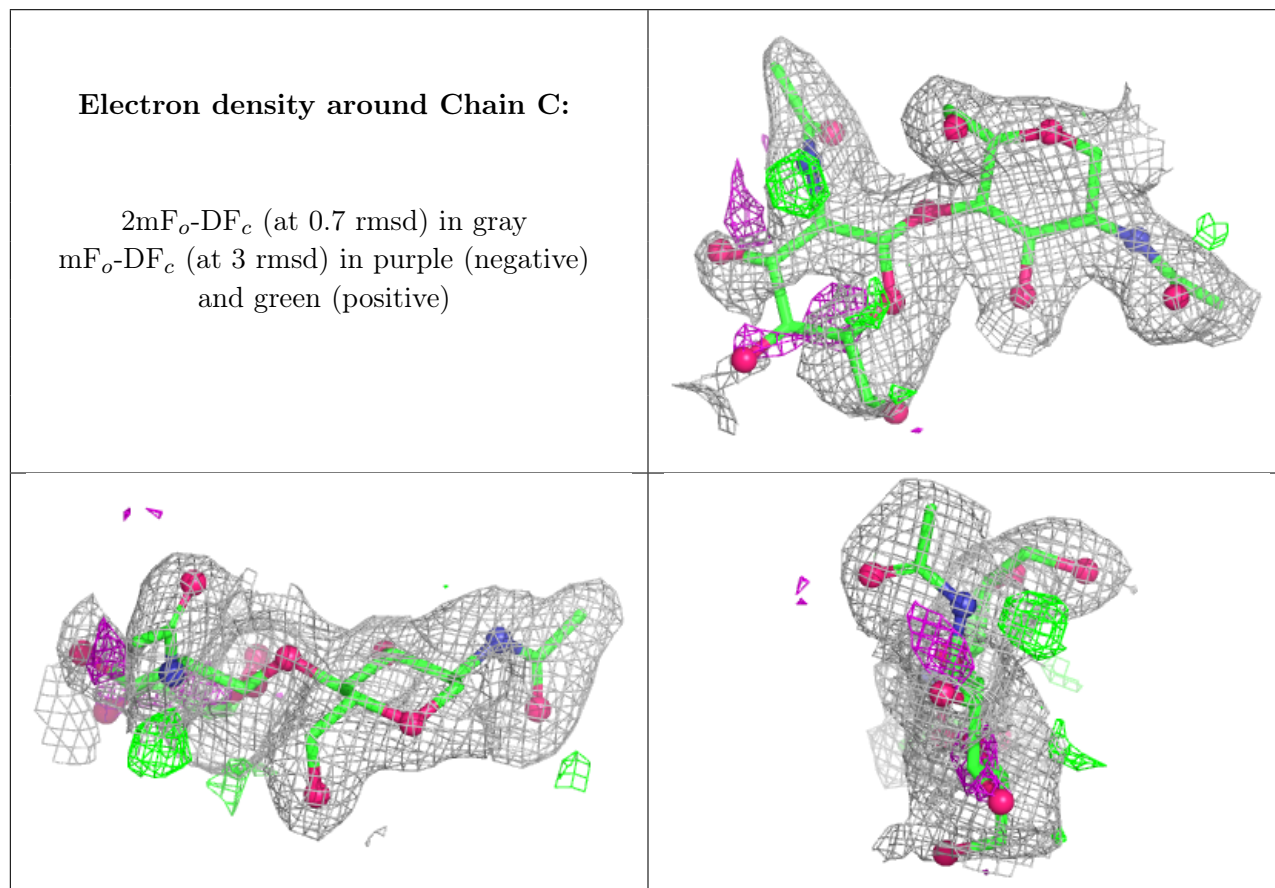
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	C	2	14/15	0.72	0.15	46,50,54,56	0
2	NAG	C	1	14/15	0.91	0.08	33,36,38,43	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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	1500	5/5	0.68	0.17	95,96,96,97	0
3	SO4	A	1499	5/5	0.71	0.21	85,85,86,86	0
3	SO4	A	1498	5/5	0.75	0.22	94,95,95,96	0
4	NAG	A	1997	14/15	0.75	0.14	42,48,53,55	0
3	SO4	A	1502	5/5	0.76	0.17	89,89,89,90	0
3	SO4	A	1501	5/5	0.82	0.12	84,84,85,85	0
3	SO4	A	1503	5/5	0.84	0.16	71,72,72,72	0
3	SO4	B	1502	5/5	0.86	0.14	75,75,76,76	0
3	SO4	B	1501	5/5	0.86	0.16	65,66,67,67	0
3	SO4	A	1505	5/5	0.90	0.12	60,60,61,63	0
3	SO4	A	1507	5/5	0.93	0.09	65,65,65,65	0
3	SO4	A	1506	5/5	0.93	0.10	53,53,54,55	0
3	SO4	B	1498	5/5	0.95	0.08	58,59,59,60	0
3	SO4	B	1499	5/5	0.96	0.07	42,42,42,44	0
3	SO4	A	1504	5/5	0.96	0.07	34,34,35,38	0
3	SO4	B	1500	5/5	0.97	0.07	31,31,34,35	0

## 6.5 Other polymers

There are no such residues in this entry.