



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 11:46 PM EDT

PDB ID : 3GBN  
Title : Crystal Structure of Fab CR6261 in Complex with the 1918 H1N1 influenza virus hemagglutinin  
Authors : Ekiert, D.C.; Elsliger, M.A.; Wilson, I.A.  
Deposited on : 2009-02-20  
Resolution : 2.20 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

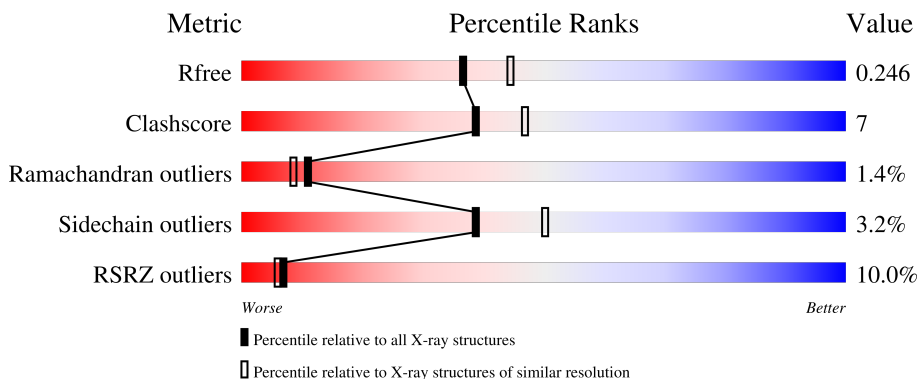
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	331	 10% 85% 12% ..
2	B	179	 3% 88% 7% ...
3	H	226	 6% 60% 9% . 29%
4	L	221	 14% 52% 14% . 32%
5	C	4	 50% 50%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	NAG	C	1	-	-	-	X
6	NAG	B	180	X	-	-	-
7	EDO	B	185	-	-	X	-
8	GOL	A	332	-	-	X	-
9	ETX	A	333	-	-	X	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6618 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	2501	1577	427	486	11	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q9WFX3
A	8	ASP	-	expression tag	UNP Q9WFX3
A	9	PRO	-	expression tag	UNP Q9WFX3
A	10	GLY	-	expression tag	UNP Q9WFX3

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	173	1399	873	240	280	6	0	2	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP Q9WFX3
B	178	GLY	-	expression tag	UNP Q9WFX3
B	179	ARG	-	expression tag	UNP Q9WFX3

- Molecule 3 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	160	1209	774	196	231	8	0	0	0

- Molecule 4 is a protein called Fab Lambda Light Chain.

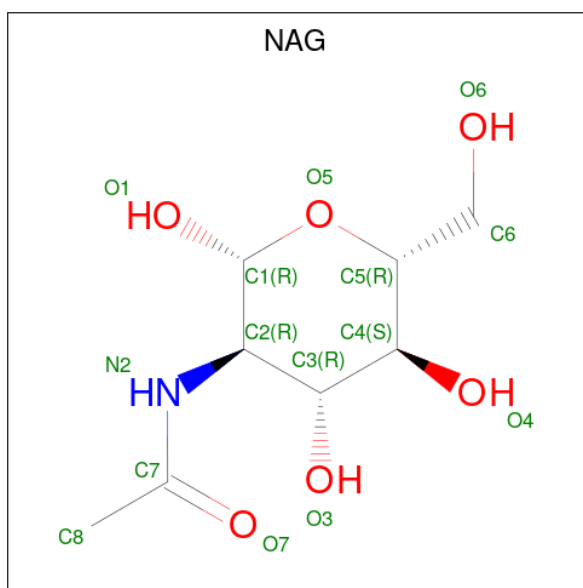
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	151	1085	677	180	224	4	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
			Total	C	N	O	S			
5	C	4	50	28	2	20		0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



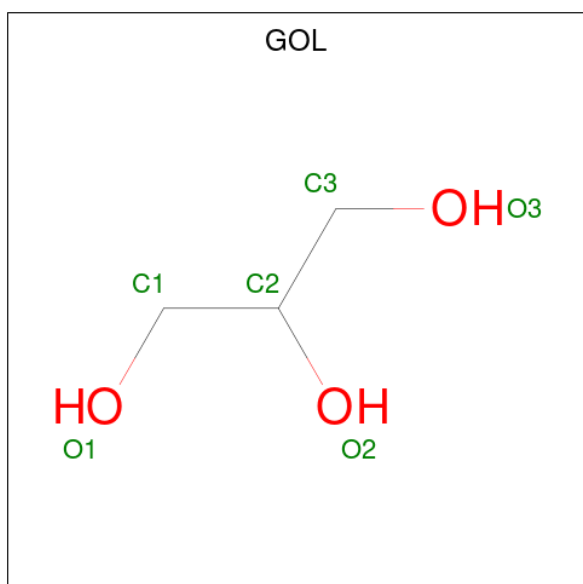
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	14	8	1	5		0	0
6	B	1	14	8	1	5		0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



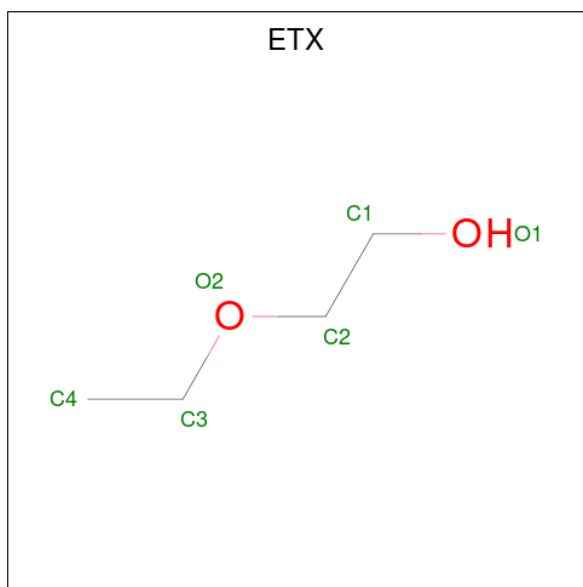
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	B	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 2-ETHOXYETHANOL (three-letter code: ETX) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Cl	0	0
			1	1		

- Molecule 11 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

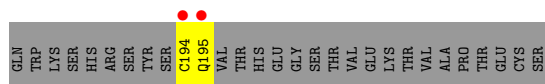
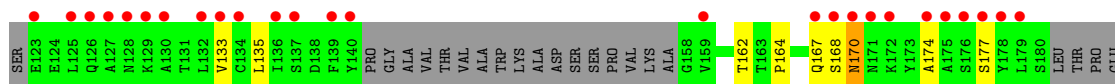
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	O	0	0
			14	14		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	82	Total O 82 82	0	0
12	B	124	Total O 124 124	0	0
12	H	79	Total O 79 79	0	0
12	L	8	Total O 8 8	0	0







- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.92Å 202.25Å 202.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.72 – 2.20 39.72 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (39.72-2.20) 94.8 (39.72-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.205 , 0.241 0.206 , 0.246	Depositor DCC
$R_{free}$ test set	3391 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.017 for -l,-k,-h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: GOL, ETX, UNL, MAN, CL, EDO, 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	0.73	0/2565	0.71	1/3505 (0.0%)
2	B	1.04	2/1432 (0.1%)	0.89	3/1929 (0.2%)
3	H	0.93	1/1238 (0.1%)	0.85	1/1676 (0.1%)
4	L	0.70	0/1103	0.73	0/1503
All	All	0.85	3/6338 (0.0%)	0.79	5/8613 (0.1%)

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
3	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	92	CYS	CB-SG	-6.96	1.70	1.82
2	B	1	GLY	N-CA	5.59	1.54	1.46
2	B	78	GLU	CD-OE2	-5.13	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	153	ARG	NE-CZ-NH2	-11.40	114.60	120.30
2	B	153	ARG	NE-CZ-NH1	8.43	124.52	120.30
3	H	42	GLY	N-CA-C	-6.63	96.51	113.10
1	A	315	ARG	NE-CZ-NH2	-6.53	117.03	120.30
2	B	19	ASP	CB-CG-OD2	5.38	123.14	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	150	GLU	Peptide

## 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	2501	0	2365	41	0
2	B	1399	0	1305	13	0
3	H	1209	0	1191	13	0
4	L	1085	0	1005	27	0
5	C	50	0	43	1	0
6	A	14	0	13	1	0
6	B	14	0	13	0	0
7	A	4	0	6	2	0
7	B	12	0	18	6	0
7	H	4	0	6	0	0
8	A	6	0	8	7	0
8	B	6	0	8	0	0
9	A	6	0	10	7	0
10	B	1	0	0	0	0
11	B	14	0	0	0	0
12	A	82	0	0	1	0
12	B	124	0	0	1	0
12	H	79	0	0	1	0
12	L	8	0	0	0	0
All	All	6618	0	5991	92	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 7.

All (92) 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)
4:L:9:SER:C	4:L:11:VAL:N	2.12	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HE	8:A:332:GOL:H31	1.23	1.01
1:A:321:ARG:HE	8:A:332:GOL:C3	1.77	0.96
1:A:321:ARG:NE	8:A:332:GOL:H31	1.83	0.93
3:H:174:PHE:CE2	4:L:135:LEU:HD23	2.06	0.89
2:B:29:GLU:H	7:B:185:EDO:H12	1.38	0.88
3:H:177:VAL:HG12	3:H:186:SER:O	1.77	0.84
3:H:180:SER:C	3:H:182:SER:N	2.31	0.83
1:A:70:LEU:HD11	1:A:112:LEU:HD11	1.67	0.76
1:A:134:GLY:CA	1:A:135:VAL:O	2.35	0.74
1:A:134:GLY:HA2	1:A:135:VAL:O	1.87	0.73
1:A:29:VAL:HB	9:A:333:ETX:H22	1.70	0.72
4:L:133:VAL:HG12	4:L:135:LEU:HD12	1.71	0.72
2:B:29:GLU:N	7:B:185:EDO:H12	2.08	0.67
3:H:147:TYR:CD2	3:H:185:TYR:O	2.47	0.67
3:H:147:TYR:CE2	3:H:185:TYR:O	2.48	0.67
4:L:91:TRP:CZ2	4:L:95(B):ALA:HB1	2.30	0.67
4:L:9:SER:O	4:L:11:VAL:N	2.27	0.66
1:A:321:ARG:NE	8:A:332:GOL:C3	2.49	0.64
2:B:19:ASP:OD1	2:B:19:ASP:N	2.28	0.64
1:A:188:GLY:CA	1:A:217:ILE:HD11	2.28	0.64
1:A:54:LEU:HD23	1:A:279:THR:O	1.98	0.63
4:L:13:ALA:HB1	4:L:17:GLN:HG2	1.82	0.62
1:A:60[A]:GLN:HE21	1:A:62:GLY:H	1.47	0.61
4:L:133:VAL:HG12	4:L:135:LEU:CD1	2.32	0.60
1:A:186:PRO:O	1:A:187:THR:C	2.41	0.59
1:A:188:GLY:HA3	1:A:217:ILE:HD11	1.85	0.59
4:L:104:LEU:HD23	4:L:104:LEU:C	2.24	0.58
3:H:52:ILE:HD13	3:H:52:ILE:N	2.18	0.58
1:A:310:ARG:NH1	2:B:90:ASP:OD1	2.32	0.57
1:A:188:GLY:HA2	1:A:189:THR:HB	1.88	0.56
1:A:321:ARG:HE	8:A:332:GOL:H32	1.63	0.56
4:L:167:GLN:HE21	4:L:174:ALA:HB2	1.71	0.55
2:B:143:LYS:NZ	7:B:185:EDO:H11	2.23	0.54
3:H:146:ASP:HB3	3:H:184:LEU:HD13	1.89	0.54
4:L:15:PRO:HA	4:L:78:LEU:O	2.06	0.54
1:A:134:GLY:HA3	1:A:135:VAL:O	2.05	0.54
2:B:145:ASP:HA	7:B:185:EDO:H21	1.88	0.53
4:L:13:ALA:HB1	4:L:17:GLN:CG	2.37	0.53
1:A:29:VAL:CB	9:A:333:ETX:H22	2.37	0.53
1:A:125(A):LYS:HG2	1:A:125(B):THR:HG23	1.91	0.52
4:L:4:LEU:HD11	4:L:90:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:HG2	6:A:330:NAG:H82	1.92	0.52
1:A:29:VAL:HB	9:A:333:ETX:C2	2.40	0.52
1:A:29:VAL:CG1	9:A:333:ETX:H22	2.39	0.51
1:A:321:ARG:CD	8:A:332:GOL:H31	2.40	0.51
4:L:94:ARG:CB	4:L:95:PRO:CD	2.87	0.51
1:A:238:GLU:HG3	1:A:239:PRO:HD2	1.93	0.50
1:A:138:ALA:O	1:A:224:ARG:NH1	2.44	0.49
3:H:108:THR:HG22	12:H:261:HOH:O	2.10	0.49
1:A:8:ASP:N	1:A:9:PRO:CD	2.75	0.49
2:B:9:PHE:O	2:B:135:ASN:HA	2.13	0.49
3:H:119:PRO:HB2	3:H:144:VAL:HG13	1.94	0.49
1:A:152:LEU:HD23	1:A:154:LEU:HD21	1.94	0.49
1:A:313:LYS:HE2	7:A:331:EDO:H12	1.95	0.48
1:A:161:TYR:HB3	1:A:197:ASN:ND2	2.28	0.48
3:H:150:GLU:HG2	3:H:151:PRO:HD3	1.95	0.48
4:L:39:LEU:HD23	4:L:39:LEU:N	2.29	0.48
1:A:152:LEU:HD23	1:A:154:LEU:CD2	2.44	0.48
4:L:69:THR:CG2	4:L:69:THR:O	2.62	0.47
9:A:333:ETX:C1	2:B:105:GLU:HG2	2.46	0.46
4:L:164:PRO:HA	4:L:174:ALA:O	2.16	0.46
1:A:301:THR:HB	1:A:305:CYS:SG	2.56	0.45
4:L:69:THR:O	4:L:69:THR:HG23	2.17	0.45
1:A:321:ARG:CZ	8:A:332:GOL:H12	2.47	0.45
1:A:60[A]:GLN:NE2	1:A:62:GLY:H	2.13	0.45
9:A:333:ETX:H11	2:B:105:GLU:HG2	1.99	0.45
4:L:9:SER:CA	4:L:11:VAL:N	2.78	0.45
4:L:48:ILE:HD13	4:L:73:LEU:HD13	1.98	0.45
1:A:11:ASP:OD1	7:B:185:EDO:O1	2.35	0.45
2:B:1:GLY:H2	7:B:184:EDO:C2	2.31	0.44
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.99	0.44
4:L:167:GLN:NE2	4:L:174:ALA:HB2	2.33	0.44
3:H:187:LEU:C	3:H:187:LEU:HD12	2.38	0.44
9:A:333:ETX:H32	12:B:226:HOH:O	2.18	0.44
1:A:7:ALA:N	2:B:139:GLU:OE1	2.52	0.43
1:A:186:PRO:O	1:A:188:GLY:N	2.52	0.43
4:L:3:VAL:HG12	4:L:4:LEU:N	2.33	0.43
2:B:21:TRP:CZ2	3:H:53:ILE:HG21	2.54	0.42
4:L:104:LEU:C	4:L:104:LEU:CD2	2.88	0.42
4:L:94:ARG:O	4:L:95:PRO:C	2.57	0.42
1:A:191:GLN:HB2	1:A:217:ILE:HD12	2.01	0.42
4:L:168:SER:C	4:L:170:ASN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:150:GLU:CB	3:H:151:PRO:HD3	2.49	0.41
1:A:60[B]:GLN:NE2	12:A:369:HOH:O	2.46	0.41
1:A:135:VAL:HG13	1:A:145:SER:C	2.40	0.41
1:A:313:LYS:HE2	7:A:331:EDO:C1	2.50	0.41
4:L:194:CYS:O	4:L:195:GLN:C	2.59	0.41
1:A:133(A):LYS:HA	1:A:134:GLY:HA2	1.96	0.41
5:C:2:NAG:H61	5:C:3:BMA:C1	2.50	0.41
4:L:104:LEU:HD23	4:L:105:THR:N	2.37	0.40
4:L:14:ALA:O	4:L:17:GLN:HB3	2.21	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	328/331 (99%)	308 (94%)	13 (4%)	7 (2%)	7	4
2	B	173/179 (97%)	169 (98%)	4 (2%)	0	100	100
3	H	152/226 (67%)	146 (96%)	4 (3%)	2 (1%)	12	9
4	L	139/221 (63%)	129 (93%)	8 (6%)	2 (1%)	11	8
All	All	792/957 (83%)	752 (95%)	29 (4%)	11 (1%)	11	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
3	H	152	VAL
4	L	94	ARG
1	A	187	THR
3	H	151	PRO
1	A	125(C)	SER

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Mol	Chain	Res	Type
1	A	163	LYS
1	A	189	THR
1	A	133(A)	LYS
4	L	95	PRO
1	A	158	GLY

### 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	270/285 (95%)	264 (98%)	6 (2%)	52	65
2	B	148/152 (97%)	147 (99%)	1 (1%)	84	91
3	H	132/189 (70%)	126 (96%)	6 (4%)	27	34
4	L	115/182 (63%)	107 (93%)	8 (7%)	15	16
All	All	665/808 (82%)	644 (97%)	21 (3%)	39	50

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	102	PHE
1	A	118	PHE
1	A	136	THR
1	A	207	SER
1	A	320	LEU
2	B	19	ASP
3	H	4	LEU
3	H	120	SER
3	H	142	CYS
3	H	153	THR
3	H	180	SER
3	H	187	LEU
4	L	12	SER
4	L	19	VAL
4	L	56	SER

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Mol	Chain	Res	Type
4	L	69	THR
4	L	103	LYS
4	L	162	THR
4	L	170	ASN
4	L	177	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	ASN
4	L	170	ASN
4	L	195	GLN

### 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](#)

4 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
5	NAG	C	1	5,1	14,14,15	0.72	0	17,19,21	2.59	6 (35%)
5	NAG	C	2	5	14,14,15	0.49	0	17,19,21	1.95	5 (29%)
5	BMA	C	3	5	11,11,12	0.47	0	15,15,17	1.54	2 (13%)
5	MAN	C	4	5	11,11,12	1.19	1 (9%)	15,15,17	1.38	3 (20%)

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
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	4	MAN	C2-C3	-2.02	1.49	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	C4-C3-C2	-7.31	100.31	111.02
5	C	1	NAG	C2-N2-C7	-4.62	116.33	122.90
5	C	2	NAG	O5-C5-C6	4.51	114.28	107.20
5	C	3	BMA	C2-C3-C4	-4.37	103.33	110.89
5	C	2	NAG	C6-C5-C4	-3.80	104.11	113.00
5	C	1	NAG	O4-C4-C3	3.02	117.33	110.35
5	C	2	NAG	C1-C2-N2	2.85	115.35	110.49
5	C	1	NAG	O3-C3-C4	2.71	116.62	110.35
5	C	1	NAG	O5-C1-C2	-2.48	107.37	111.29
5	C	4	MAN	O2-C2-C3	-2.46	105.21	110.14
5	C	3	BMA	C1-O5-C5	2.46	115.52	112.19
5	C	2	NAG	O5-C1-C2	-2.29	107.67	111.29
5	C	2	NAG	O7-C7-C8	-2.27	117.85	122.06
5	C	4	MAN	O4-C4-C5	2.20	114.75	109.30
5	C	1	NAG	C8-C7-N2	2.06	119.59	116.10
5	C	4	MAN	O4-C4-C3	-2.01	105.70	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

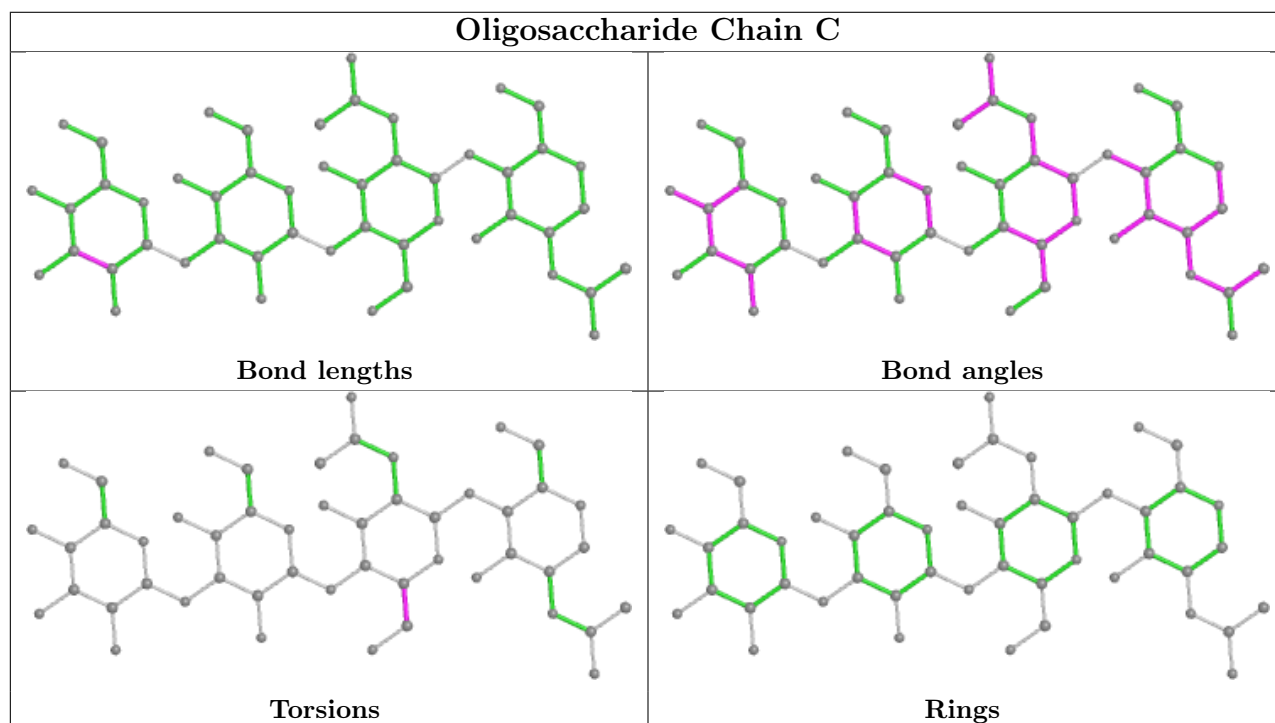
Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	3	BMA	1	0
5	C	2	NAG	1	0

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



## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic and 1 is unknown - leaving 10 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	$\# Z  > 2$
9	ETX	A	333	-	5,5,5	0.46	0	4,4,4	1.51	1 (25%)
7	EDO	B	184	-	3,3,3	0.60	0	2,2,2	0.07	0
7	EDO	B	185	-	3,3,3	0.33	0	2,2,2	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	B	183	-	3,3,3	0.61	0	2,2,2	0.52	0
6	NAG	A	330	1	14,14,15	0.72	1 (7%)	17,19,21	1.40	1 (5%)
7	EDO	H	228	-	3,3,3	0.30	0	2,2,2	0.34	0
8	GOL	A	332	-	5,5,5	1.10	1 (20%)	5,5,5	1.32	1 (20%)
8	GOL	B	181	-	5,5,5	0.49	0	5,5,5	1.34	0
7	EDO	A	331	-	3,3,3	0.92	0	2,2,2	0.70	0
6	NAG	B	180	2	14,14,15	0.81	1 (7%)	17,19,21	1.64	2 (11%)

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	ETX	A	333	-	-	1/3/3/3	-
7	EDO	B	184	-	-	0/1/1/1	-
7	EDO	B	185	-	-	1/1/1/1	-
7	EDO	B	183	-	-	1/1/1/1	-
6	NAG	A	330	1	-	2/6/23/26	0/1/1/1
7	EDO	H	228	-	-	1/1/1/1	-
8	GOL	A	332	-	-	2/4/4/4	-
8	GOL	B	181	-	-	1/4/4/4	-
7	EDO	A	331	-	-	1/1/1/1	-
6	NAG	B	180	2	1/1/5/7	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	180	NAG	C1-C2	2.34	1.55	1.52
6	A	330	NAG	C1-C2	2.12	1.55	1.52
8	A	332	GOL	O2-C2	-2.10	1.37	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	180	NAG	C1-O5-C5	4.77	118.66	112.19
6	A	330	NAG	C1-O5-C5	4.40	118.15	112.19
9	A	333	ETX	C3-O2-C2	-2.89	102.53	112.90
6	B	180	NAG	C1-C2-N2	-2.49	106.23	110.49
8	A	332	GOL	C3-C2-C1	2.35	120.84	111.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	180	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	330	NAG	O5-C5-C6-O6
6	A	330	NAG	C4-C5-C6-O6
7	B	185	EDO	O1-C1-C2-O2
7	H	228	EDO	O1-C1-C2-O2
7	A	331	EDO	O1-C1-C2-O2
8	A	332	GOL	O1-C1-C2-O2
7	B	183	EDO	O1-C1-C2-O2
8	A	332	GOL	O1-C1-C2-C3
8	B	181	GOL	O1-C1-C2-C3
9	A	333	ETX	C1-C2-O2-C3

There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	333	ETX	7	0
7	B	184	EDO	1	0
7	B	185	EDO	5	0
6	A	330	NAG	1	0
8	A	332	GOL	7	0
7	A	331	EDO	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	L	2
3	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	168:SER	C	170:ASN	N	2.74
1	H	180:SER	C	182:SER	N	2.31
1	L	9:SER	C	11:VAL	N	2.12

## 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	328/331 (99%)	0.30	33 (10%) <b>7</b> <b>6</b>	15, 37, 55, 60	0
2	B	173/179 (96%)	0.22	5 (2%) 51 49	18, 26, 39, 59	0
3	H	160/226 (70%)	0.44	13 (8%) <b>12</b> <b>10</b>	17, 30, 47, 58	0
4	L	151/221 (68%)	0.83	30 (19%) <b>1</b> <b>1</b>	25, 40, 61, 97	0
All	All	812/957 (84%)	0.41	81 (9%) <b>7</b> <b>6</b>	15, 34, 55, 97	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	142	CYS	9.7
3	H	143	LEU	6.9
4	L	136	ILE	6.5
4	L	125	LEU	6.2
4	L	139	PHE	5.9
3	H	120	SER	5.8
4	L	140	TYR	5.6
1	A	187	THR	5.5
1	A	225	ASP	5.1
4	L	175	ALA	4.9
4	L	137	SER	4.8
3	H	152	VAL	4.7
1	A	142	ALA	4.7
3	H	188	SER	4.6
3	H	174	PHE	4.6
4	L	174	ALA	4.5
1	A	144	ALA	4.0
4	L	126	GLN	3.9
3	H	122	PHE	3.9
4	L	168	SER	3.8
3	H	144	VAL	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	L	127	ALA	3.8
4	L	159	VAL	3.8
1	A	125(B)	THR	3.7
3	H	173	THR	3.5
1	A	98	TYR	3.5
1	A	197	ASN	3.4
1	A	190	ASP	3.3
1	A	195	TYR	3.3
1	A	160	SER	3.3
1	A	326	ILE	3.2
4	L	170	ASN	3.2
4	L	132	LEU	3.2
4	L	11	VAL	3.1
1	A	141	TYR	3.0
4	L	194	CYS	2.9
1	A	196	GLN	2.9
1	A	143	GLY	2.9
1	A	161	TYR	2.9
2	B	102	LEU	2.8
3	H	124	LEU	2.8
1	A	133(A)	LYS	2.8
1	A	247	ALA	2.8
4	L	129	LYS	2.8
4	L	177	SER	2.7
1	A	325	SER	2.7
1	A	128	PRO	2.7
1	A	131	GLU	2.7
1	A	248	THR	2.6
2	B	2	LEU	2.6
4	L	176	SER	2.6
4	L	134	CYS	2.6
1	A	240	GLY	2.6
1	A	159	SER	2.6
3	H	145	LYS	2.6
2	B	99	LEU	2.6
1	A	7	ALA	2.6
1	A	30	LEU	2.5
1	A	189	THR	2.4
4	L	133	VAL	2.4
4	L	128	ASN	2.4
4	L	195	GLN	2.4
4	L	123	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	H	175	PRO	2.4
1	A	157	LYS	2.4
1	A	158	GLY	2.3
3	H	121	VAL	2.3
1	A	137	ALA	2.3
4	L	167	GLN	2.2
2	B	113	SER	2.2
1	A	155	THR	2.2
4	L	179	LEU	2.2
2	B	3	PHE	2.2
4	L	130	ALA	2.1
4	L	106(A)	LEU	2.1
1	A	198	ALA	2.1
1	A	127	TRP	2.1
1	A	223	VAL	2.1
4	L	171	ASN	2.1
4	L	172	LYS	2.0
4	L	178	TYR	2.0

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

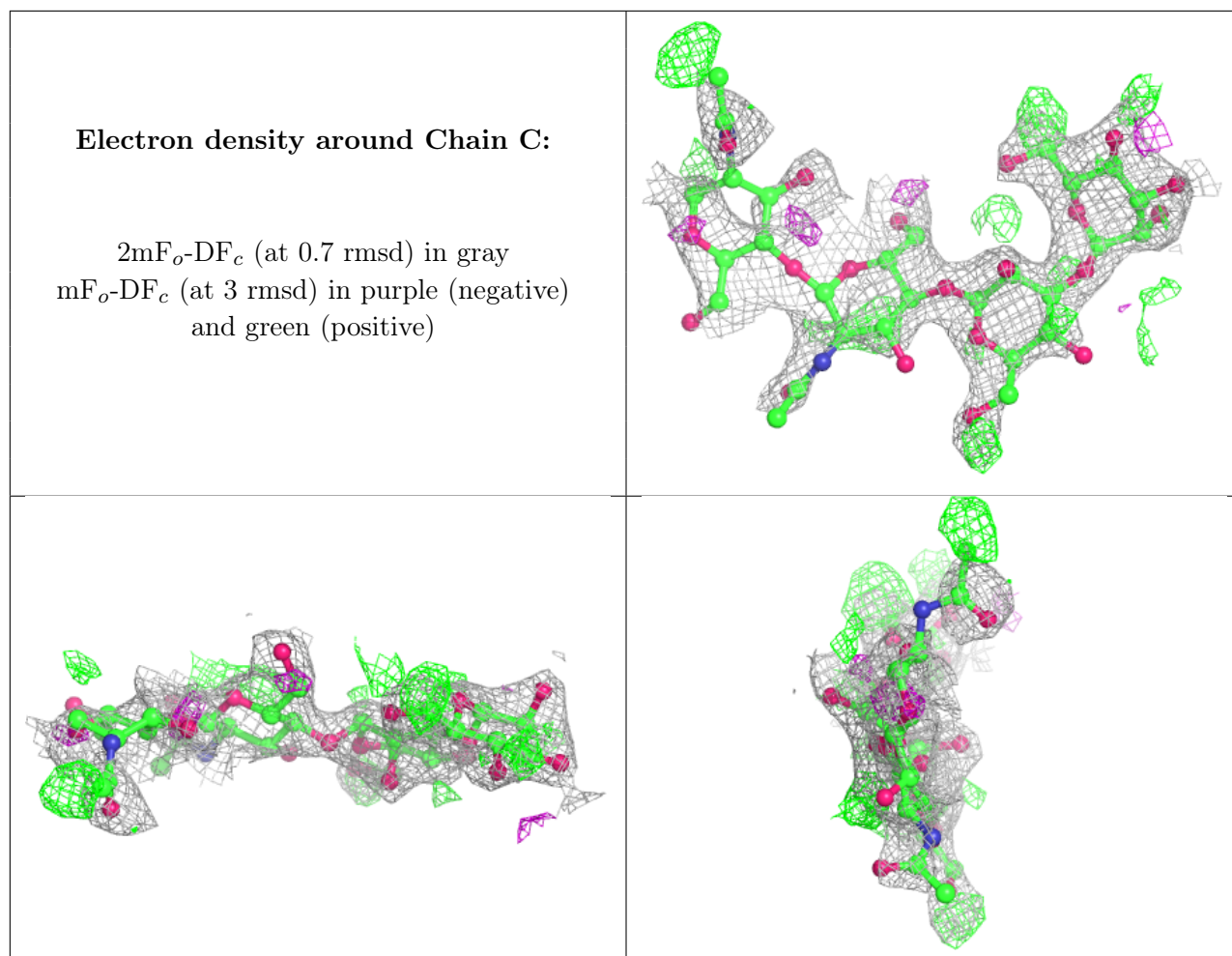
There are no non-standard protein/DNA/RNA residues in this entry.

## 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
5	NAG	C	1	14/15	0.79	0.44	28,49,62,66	14
5	BMA	C	3	11/12	0.86	0.18	40,46,56,57	11
5	NAG	C	2	14/15	0.87	0.28	24,47,61,62	14
5	MAN	C	4	11/12	0.91	0.18	23,27,36,48	11

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
8	GOL	A	332	6/6	0.82	0.23	36,57,59,61	0
11	UNL	B	186	14/-	0.83	0.18	66,84,91,97	0
6	NAG	B	180	14/15	0.86	0.22	53,74,80,81	0
7	EDO	A	331	4/4	0.89	0.18	32,59,63,65	0
7	EDO	B	183	4/4	0.89	0.18	36,48,51,56	0
6	NAG	A	330	14/15	0.90	0.21	73,81,86,89	0
9	ETX	A	333	6/6	0.92	0.26	21,40,51,62	0
7	EDO	B	184	4/4	0.93	0.26	41,54,62,67	0
8	GOL	B	181	6/6	0.94	0.20	33,55,57,63	0
7	EDO	B	185	4/4	0.95	0.21	46,53,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	H	228	4/4	0.97	0.18	39,48,52,55	0
10	CL	B	182	1/1	0.99	0.14	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.