



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 07:12 AM EDT

PDB ID : 4FUS  
Title : The X-ray structure of Hahella chejuensis family 48 glycosyl hydrolase  
Authors : Alahuhta, P.M.; Lunin, V.V.  
Deposited on : 2012-06-28  
Resolution : 1.75 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

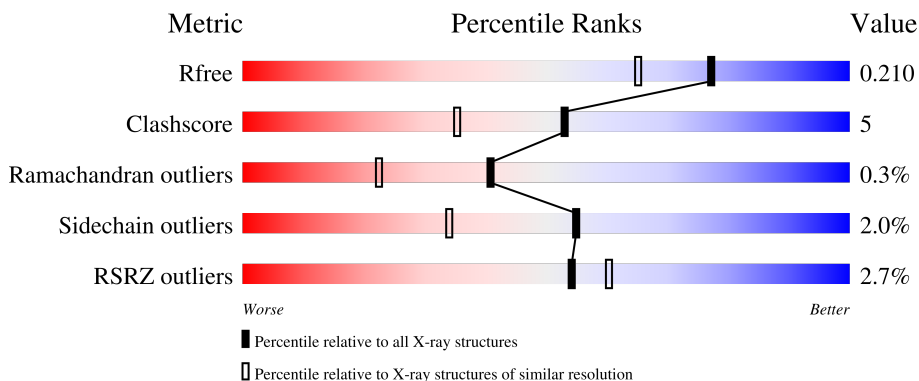
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	695	
2	B	2	

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	GOL	A	804	-	X	-	-
4	GOL	A	805	-	X	-	-

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 5837 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 RTX toxins and related Ca<sup>2+</sup>-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	635	5190	3321	852	988	29	0	14	0

There are 23 discrepancies between the modelled and reference sequences:

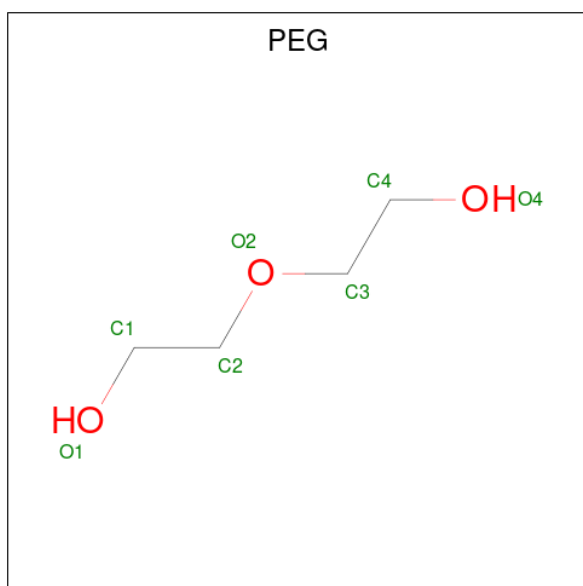
Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	expression tag	UNP Q2SJA2
A	11	GLY	-	expression tag	UNP Q2SJA2
A	12	SER	-	expression tag	UNP Q2SJA2
A	13	SER	-	expression tag	UNP Q2SJA2
A	14	HIS	-	expression tag	UNP Q2SJA2
A	15	HIS	-	expression tag	UNP Q2SJA2
A	16	HIS	-	expression tag	UNP Q2SJA2
A	17	HIS	-	expression tag	UNP Q2SJA2
A	18	HIS	-	expression tag	UNP Q2SJA2
A	19	HIS	-	expression tag	UNP Q2SJA2
A	20	SER	-	expression tag	UNP Q2SJA2
A	21	SER	-	expression tag	UNP Q2SJA2
A	22	GLY	-	expression tag	UNP Q2SJA2
A	23	LEU	-	expression tag	UNP Q2SJA2
A	24	VAL	-	expression tag	UNP Q2SJA2
A	25	PRO	-	expression tag	UNP Q2SJA2
A	26	ARG	-	expression tag	UNP Q2SJA2
A	27	GLY	-	expression tag	UNP Q2SJA2
A	28	SER	-	expression tag	UNP Q2SJA2
A	29	HIS	-	expression tag	UNP Q2SJA2
A	30	MET	-	expression tag	UNP Q2SJA2
A	31	ALA	-	expression tag	UNP Q2SJA2
A	32	SER	-	expression tag	UNP Q2SJA2

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



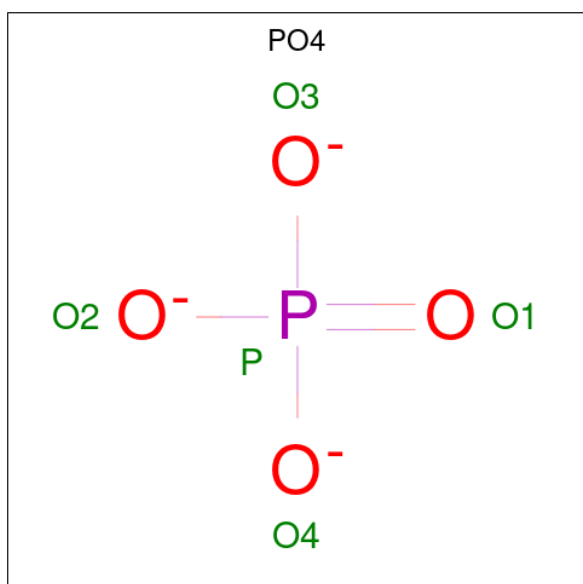
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	2	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



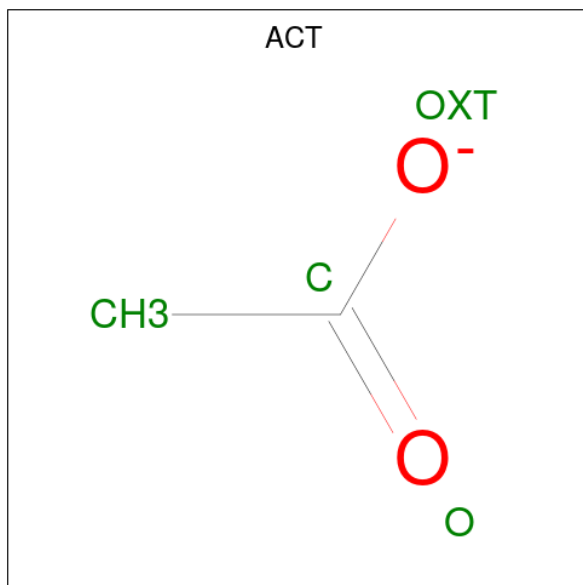
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 12 6 6	0	1

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



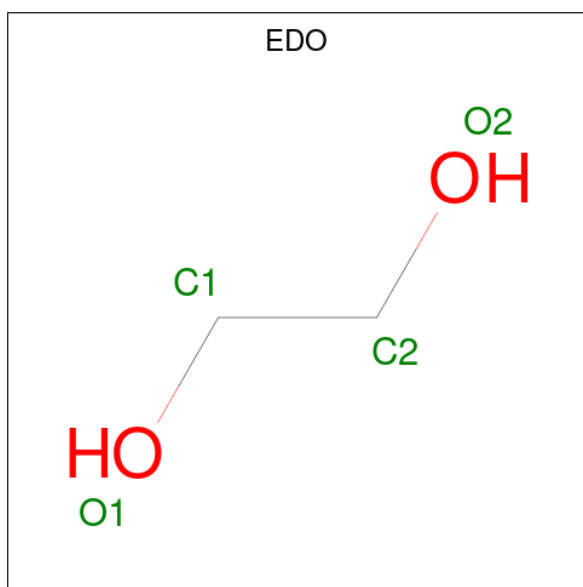
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 8 4 4	0	1
7	A	1	Total C O 8 4 4	0	1
7	A	1	Total C O 8 4 4	0	1
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 8 4 4	0	1
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0
7	A	1	Total C O 4 2 2	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total Na 2 2	0	0

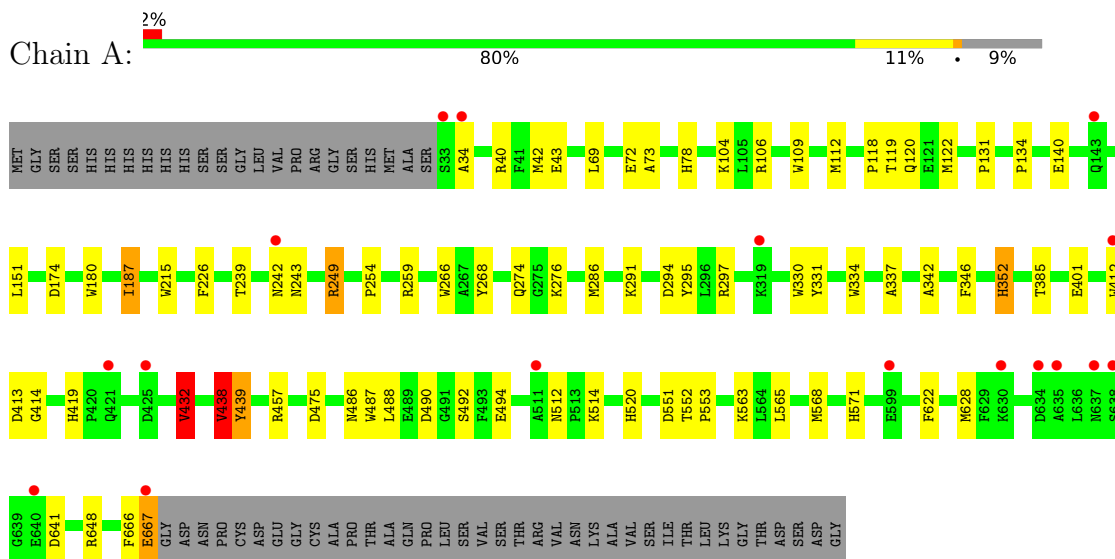
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	478	Total O 492 492	0	20

### 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: RTX toxins and related Ca<sup>2+</sup>-binding protein



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.69Å 78.39Å 67.08Å 90.00° 98.94° 90.00°	Depositor
Resolution (Å)	25.00 – 1.75 33.13 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (25.00-1.75) 98.8 (33.13-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.94	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.154 , 0.205 0.162 , 0.210	Depositor DCC
$R_{free}$ test set	3165 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.9	Xtrriage
Anisotropy	0.500	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 61.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: EDO, BGC, CA, GOL, ACT, PEG, PO4, OHI, NA

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	1.17	9/5355 (0.2%)	1.04	17/7281 (0.2%)

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	A	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	439	TYR	C-N	10.75	1.58	1.34
1	A	438	VAL	C-N	10.72	1.58	1.34
1	A	334	TRP	CD2-CE2	8.27	1.51	1.41
1	A	215	TRP	CD2-CE2	6.06	1.48	1.41
1	A	412	TRP	CD2-CE2	5.83	1.48	1.41
1	A	266	TRP	CD2-CE2	5.64	1.48	1.41
1	A	266	TRP	NE1-CE2	-5.44	1.30	1.37
1	A	487	TRP	CD2-CE2	5.20	1.47	1.41
1	A	180	TRP	CD2-CE2	5.11	1.47	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	106	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	A	297	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	A	457	ARG	NE-CZ-NH1	6.43	123.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	40	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	457	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	432[A]	VAL	CB-CA-C	-5.93	100.12	111.40
1	A	432[B]	VAL	CB-CA-C	-5.93	100.12	111.40
1	A	439	TYR	CA-C-N	-5.52	105.05	117.20
1	A	641	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	439	TYR	N-CA-C	-5.49	96.19	111.00
1	A	439	TYR	CB-CA-C	5.45	121.29	110.40
1	A	648	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	475	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	226	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	A	294	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	TYR	Peptide
1	A	352	OHI	Mainchain
1	A	438	VAL	Mainchain
1	A	439	TYR	Mainchain
1	A	78	HIS	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	5190	0	4765	56	0
2	B	23	0	21	0	0
3	A	3	0	2	0	0
4	A	36	0	48	1	0
5	A	10	0	0	0	0
6	A	16	0	12	1	0
7	A	64	0	96	5	0
8	A	1	0	0	0	0
9	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	492	0	0	10	0
All	All	5837	0	4944	56	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 5.

All (56) 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:A:419:HIS:CG	1:A:432[B]:VAL:HG21	1.94	1.00
1:A:119:THR:H	1:A:122[A]:MET:HE3	1.33	0.91
1:A:42[B]:MET:SD	10:A:1187[B]:HOH:O	2.35	0.85
1:A:419:HIS:CE1	1:A:432[B]:VAL:HG23	2.12	0.85
1:A:34:ALA:HB2	1:A:667:GLU:HB2	1.64	0.80
1:A:419:HIS:CG	1:A:432[B]:VAL:CG2	2.67	0.77
1:A:419:HIS:CE1	1:A:432[B]:VAL:CG2	2.68	0.77
1:A:419:HIS:ND1	1:A:432[B]:VAL:CG2	2.49	0.74
1:A:120:GLN:HG3	10:A:929:HOH:O	1.88	0.74
1:A:512:ASN:ND2	1:A:514:LYS:HE3	2.03	0.73
1:A:119:THR:H	1:A:122[A]:MET:CE	2.05	0.69
1:A:151:LEU:HD11	10:A:1350[A]:HOH:O	1.95	0.65
1:A:187:ILE:HG23	10:A:1312:HOH:O	1.98	0.64
1:A:118:PRO:HA	1:A:122[A]:MET:HE1	1.84	0.59
1:A:122[A]:MET:CE	10:A:911:HOH:O	2.52	0.58
1:A:122[A]:MET:HE1	10:A:911:HOH:O	2.03	0.57
1:A:34:ALA:HB2	1:A:667:GLU:CB	2.35	0.56
1:A:419:HIS:CD2	1:A:432[B]:VAL:HG21	2.41	0.55
1:A:385:THR:HG23	6:A:811:ACT:H1	1.90	0.53
1:A:419:HIS:NE2	1:A:432[B]:VAL:HG23	2.24	0.53
1:A:131:PRO:HB2	7:A:819[A]:EDO:H21	1.92	0.51
1:A:43:GLU:OE2	7:A:825:EDO:O1	2.23	0.51
1:A:419:HIS:CD2	1:A:432[B]:VAL:CG2	2.95	0.50
1:A:628[A]:MET:HE2	10:A:979:HOH:O	2.11	0.50
1:A:69:LEU:H	1:A:628[A]:MET:CE	2.24	0.49
1:A:486:ASN:HB2	1:A:494:GLU:HG2	1.93	0.49
1:A:69:LEU:HB3	1:A:628[B]:MET:HE2	1.92	0.49
1:A:291:LYS:NZ	10:A:1090:HOH:O	2.22	0.47
1:A:337:ALA:HB1	1:A:342:ALA:HB3	1.97	0.47
1:A:551[C]:ASP:CG	1:A:552:THR:N	2.68	0.46
1:A:330:TRP:CD2	1:A:438:VAL:HG21	2.51	0.46
1:A:72:GLU:HA	4:A:804:GOL:H12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLN:OE1	1:A:276[A]:LYS:NZ	2.46	0.45
1:A:552:THR:HG22	1:A:553:PRO:HD2	2.00	0.44
1:A:486:ASN:HB2	1:A:494:GLU:CG	2.47	0.44
1:A:174:ASP:OD2	7:A:816[B]:EDO:O1	2.28	0.43
1:A:286[B]:MET:HG2	10:A:921:HOH:O	2.17	0.43
1:A:187:ILE:HD12	1:A:622:PHE:CZ	2.53	0.43
1:A:488:LEU:HD12	1:A:492[B]:SER:OG	2.18	0.43
1:A:239:THR:HG23	10:A:1345:HOH:O	2.19	0.43
1:A:109:TRP:CH2	1:A:112[A]:MET:HE1	2.54	0.43
1:A:69:LEU:H	1:A:628[A]:MET:HE1	1.84	0.42
1:A:187:ILE:CD1	1:A:622:PHE:CE1	3.02	0.42
1:A:109:TRP:CZ2	1:A:112[A]:MET:HE1	2.55	0.42
1:A:131:PRO:HB2	7:A:819[B]:EDO:H12	2.02	0.42
1:A:134:PRO:O	1:A:346:PHE:HA	2.20	0.41
1:A:565:LEU:HD23	1:A:568:MET:CE	2.51	0.41
1:A:140:GLU:HB2	1:A:414:GLY:HA3	2.02	0.41
1:A:295:TYR:HH	7:A:817[A]:EDO:HO2	1.64	0.41
1:A:666:PHE:C	1:A:667:GLU:HG2	2.41	0.41
1:A:401:GLU:OE1	1:A:520:HIS:HA	2.20	0.41
1:A:330:TRP:CG	1:A:438:VAL:HG21	2.56	0.40
1:A:268:TYR:CD1	1:A:286[B]:MET:HE2	2.56	0.40
1:A:490:ASP:O	1:A:571:HIS:CE1	2.75	0.40
1:A:490:ASP:O	1:A:571:HIS:HE1	2.03	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	646/695 (93%)	625 (97%)	19 (3%)	2 (0%)	41 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	ALA
1	A	438	VAL

### 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	521/556 (94%)	510 (98%)	11 (2%)	53 31

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

Mol	Chain	Res	Type
1	A	104	LYS
1	A	187	ILE
1	A	242	ASN
1	A	243	ASN
1	A	249	ARG
1	A	254	PRO
1	A	413	ASP
1	A	432[A]	VAL
1	A	432[B]	VAL
1	A	563	LYS
1	A	667	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	A	314	ASN
1	A	341	ASN
1	A	398	GLN
1	A	472	GLN
1	A	484	ASN
1	A	512	ASN
1	A	571	HIS
1	A	661	ASN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
1	OHI	A	352	1	8,11,12	1.81	2 (25%)	5,14,16	1.55	1 (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
1	OHI	A	352	1	-	0/3/15/17	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	OHI	O12-CE1	3.18	1.28	1.24
1	A	352	OHI	CB-CA	-2.69	1.47	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	OHI	CB-CA-C	2.25	115.69	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	BGC	B	1	2	12,12,12	0.45	0	17,17,17	1.78	4 (23%)
2	BGC	B	2	2	11,11,12	0.90	0	15,15,17	1.42	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
2	BGC	B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	B	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	BGC	C1-O5-C5	-4.78	104.65	113.66
2	B	2	BGC	O3-C3-C2	-3.07	104.11	109.99
2	B	1	BGC	C1-C2-C3	-2.83	104.44	110.31
2	B	2	BGC	O5-C1-C2	2.44	114.54	110.77
2	B	1	BGC	O5-C1-C2	-2.19	106.39	110.28
2	B	2	BGC	O2-C2-C1	-2.12	104.82	109.15
2	B	1	BGC	O2-C2-C1	-2.09	104.32	109.16

There are no chirality outliers.

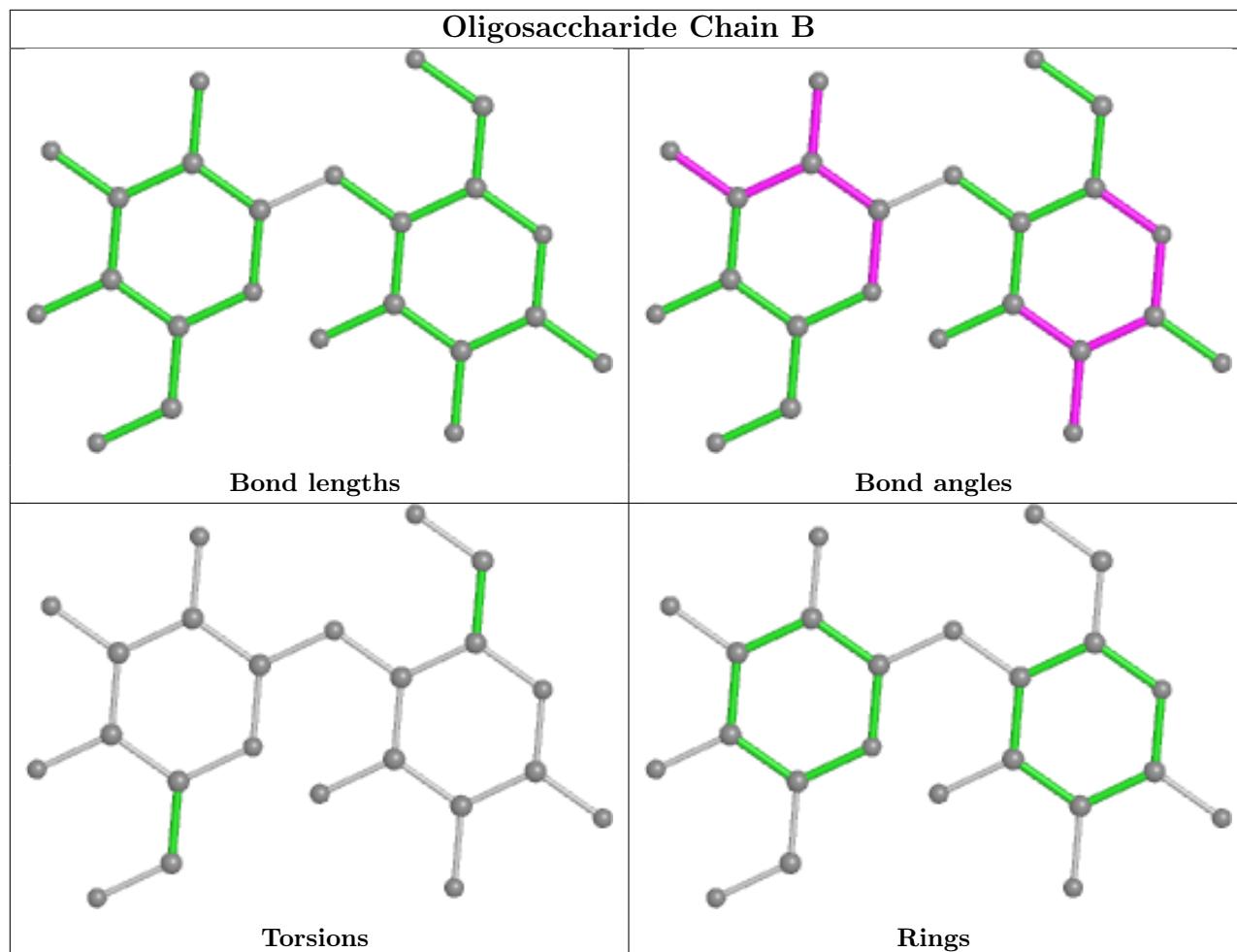
There are no torsion outliers.

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 32 ligands modelled in this entry, 3 are monoatomic - leaving 29 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	$\# Z  > 2$
6	ACT	A	812	-	3,3,3	0.81	0	3,3,3	1.10	0
7	EDO	A	819[A]	-	3,3,3	0.31	0	2,2,2	0.86	0
7	EDO	A	815[A]	-	3,3,3	0.65	0	2,2,2	0.15	0
7	EDO	A	816[B]	-	3,3,3	0.69	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	807[B]	-	5,5,5	0.68	0	5,5,5	0.87	0
7	EDO	A	825	-	3,3,3	0.41	0	2,2,2	0.40	0
7	EDO	A	817[B]	-	3,3,3	0.60	0	2,2,2	0.24	0
6	ACT	A	813	8	3,3,3	1.53	1 (33%)	3,3,3	1.49	1 (33%)
6	ACT	A	810	-	3,3,3	0.77	0	3,3,3	0.66	0
4	GOL	A	805	-	5,5,5	1.19	1 (20%)	5,5,5	1.85	2 (40%)
6	ACT	A	811	-	3,3,3	0.77	0	3,3,3	0.78	0
7	EDO	A	823	-	3,3,3	0.20	0	2,2,2	0.62	0
7	EDO	A	824	-	3,3,3	0.60	0	2,2,2	0.59	0
5	PO4	A	808	-	4,4,4	0.46	0	6,6,6	1.04	0
7	EDO	A	822	-	3,3,3	0.53	0	2,2,2	0.20	0
7	EDO	A	820	-	3,3,3	0.29	0	2,2,2	0.43	0
7	EDO	A	816[A]	-	3,3,3	0.40	0	2,2,2	0.41	0
4	GOL	A	807[A]	-	5,5,5	0.43	0	5,5,5	1.53	2 (40%)
7	EDO	A	819[B]	-	3,3,3	0.41	0	2,2,2	0.37	0
7	EDO	A	814	-	3,3,3	0.70	0	2,2,2	0.31	0
7	EDO	A	815[B]	-	3,3,3	0.54	0	2,2,2	0.19	0
7	EDO	A	818	-	3,3,3	0.36	0	2,2,2	0.74	0
7	EDO	A	817[A]	-	3,3,3	0.63	0	2,2,2	0.26	0
7	EDO	A	821	-	3,3,3	0.37	0	2,2,2	0.24	0
4	GOL	A	806	-	5,5,5	0.21	0	5,5,5	1.15	1 (20%)
4	GOL	A	803	-	5,5,5	0.54	0	5,5,5	1.25	0
5	PO4	A	809	-	4,4,4	0.92	0	6,6,6	0.67	0
3	PEG	A	801	1	2,2,6	0.39	0	1,1,5	0.01	0
4	GOL	A	804	-	5,5,5	0.48	0	5,5,5	1.79	2 (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
7	EDO	A	819[A]	-	-	1/1/1/1	-
7	EDO	A	815[A]	-	-	1/1/1/1	-
7	EDO	A	816[B]	-	-	0/1/1/1	-
4	GOL	A	807[B]	-	-	2/4/4/4	-
7	EDO	A	825	-	-	0/1/1/1	-
7	EDO	A	817[B]	-	-	1/1/1/1	-
4	GOL	A	805	-	-	4/4/4/4	-
7	EDO	A	823	-	-	0/1/1/1	-
7	EDO	A	824	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	822	-	-	0/1/1/1	-
7	EDO	A	820	-	-	1/1/1/1	-
7	EDO	A	816[A]	-	-	0/1/1/1	-
4	GOL	A	807[A]	-	-	2/4/4/4	-
7	EDO	A	819[B]	-	-	1/1/1/1	-
7	EDO	A	814	-	-	1/1/1/1	-
7	EDO	A	815[B]	-	-	1/1/1/1	-
7	EDO	A	818	-	-	0/1/1/1	-
7	EDO	A	817[A]	-	-	1/1/1/1	-
7	EDO	A	821	-	-	1/1/1/1	-
4	GOL	A	803	-	-	0/4/4/4	-
4	GOL	A	806	-	-	0/4/4/4	-
4	GOL	A	804	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	805	GOL	O3-C3	2.18	1.51	1.42
6	A	813	ACT	O-C	2.09	1.31	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	805	GOL	O1-C1-C2	2.88	124.03	110.20
4	A	804	GOL	O2-C2-C1	-2.74	97.07	109.12
4	A	805	GOL	O2-C2-C1	2.49	120.08	109.12
4	A	804	GOL	O2-C2-C3	2.40	119.71	109.12
4	A	806	GOL	C3-C2-C1	-2.28	102.84	111.70
4	A	807[A]	GOL	O2-C2-C1	2.13	118.50	109.12
4	A	807[A]	GOL	C3-C2-C1	-2.11	103.49	111.70
6	A	813	ACT	OXT-C-CH3	-2.00	106.90	115.18

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	GOL	O1-C1-C2-C3
4	A	804	GOL	C1-C2-C3-O3
4	A	805	GOL	C1-C2-C3-O3
4	A	805	GOL	O1-C1-C2-C3
4	A	807[B]	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	805	GOL	O2-C2-C3-O3
7	A	819[A]	EDO	O1-C1-C2-O2
7	A	821	EDO	O1-C1-C2-O2
4	A	805	GOL	O1-C1-C2-O2
7	A	817[B]	EDO	O1-C1-C2-O2
4	A	804	GOL	O2-C2-C3-O3
4	A	807[A]	GOL	O1-C1-C2-O2
7	A	820	EDO	O1-C1-C2-O2
7	A	815[A]	EDO	O1-C1-C2-O2
7	A	824	EDO	O1-C1-C2-O2
4	A	807[B]	GOL	O2-C2-C3-O3
7	A	815[B]	EDO	O1-C1-C2-O2
7	A	817[A]	EDO	O1-C1-C2-O2
7	A	819[B]	EDO	O1-C1-C2-O2
4	A	807[A]	GOL	O1-C1-C2-C3
7	A	814	EDO	O1-C1-C2-O2
4	A	804	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	819[A]	EDO	1	0
7	A	816[B]	EDO	1	0
7	A	825	EDO	1	0
6	A	811	ACT	1	0
7	A	819[B]	EDO	1	0
7	A	817[A]	EDO	1	0
4	A	804	GOL	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 [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	A	634/695 (91%)	-0.00	17 (2%) 54 60	4, 13, 30, 55	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	ALA	3.9
1	A	242	ASN	3.8
1	A	421	GLN	3.8
1	A	34	ALA	3.4
1	A	637	ASN	3.0
1	A	667	GLU	2.9
1	A	640	GLU	2.8
1	A	634	ASP	2.5
1	A	599[A]	GLU	2.4
1	A	630	LYS	2.3
1	A	319	LYS	2.3
1	A	638	SER	2.3
1	A	143	GLN	2.2
1	A	412	TRP	2.2
1	A	33	SER	2.1
1	A	425	ASP	2.1
1	A	635	ALA	2.0

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

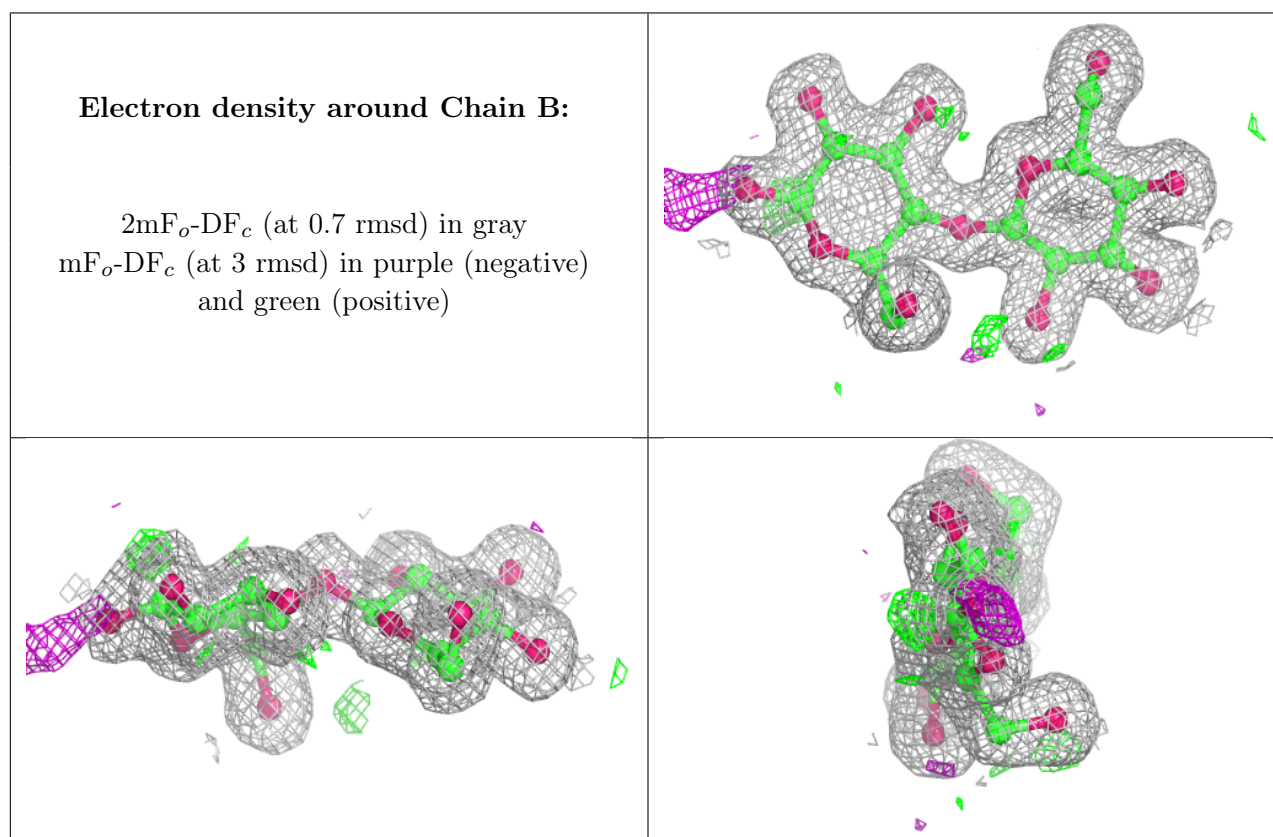
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	OHI	A	352	11/12	0.93	0.12	10,15,26,29	1

### 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( $\text{\AA}^2$ )	Q<0.9
2	BGC	B	1	12/12	0.94	0.09	9,13,18,21	0
2	BGC	B	2	11/12	0.98	0.12	6,8,10,11	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
6	ACT	A	810	4/4	0.78	0.13	45,45,50,53	0
4	GOL	A	807[B]	6/6	0.84	0.20	22,24,26,28	6
4	GOL	A	807[A]	6/6	0.84	0.20	23,25,27,30	6
6	ACT	A	811	4/4	0.84	0.20	39,41,48,48	0
6	ACT	A	812	4/4	0.85	0.25	37,38,44,46	0
4	GOL	A	805	6/6	0.89	0.19	21,26,31,35	0
3	PEG	A	801	3/7	0.90	0.14	26,26,27,31	0
7	EDO	A	818	4/4	0.90	0.17	28,29,32,34	0
4	GOL	A	806	6/6	0.91	0.10	26,30,35,35	0
5	PO4	A	808	5/5	0.91	0.17	36,37,42,43	0
7	EDO	A	820	4/4	0.91	0.12	38,38,38,40	0
7	EDO	A	825	4/4	0.91	0.12	22,23,25,28	0
7	EDO	A	819[A]	4/4	0.92	0.23	25,26,26,29	4
7	EDO	A	822	4/4	0.92	0.16	26,26,27,32	0
7	EDO	A	819[B]	4/4	0.92	0.23	10,11,11,11	4
7	EDO	A	816[A]	4/4	0.93	0.14	15,17,18,20	4
7	EDO	A	816[B]	4/4	0.93	0.14	17,17,18,19	4
5	PO4	A	809	5/5	0.93	0.24	42,46,57,58	0
7	EDO	A	824	4/4	0.93	0.13	24,28,33,38	0
6	ACT	A	813	4/4	0.93	0.14	19,25,27,31	0
7	EDO	A	821	4/4	0.94	0.11	23,24,24,24	0
4	GOL	A	804	6/6	0.94	0.11	18,31,35,45	0
7	EDO	A	817[A]	4/4	0.95	0.10	22,23,24,24	4
7	EDO	A	817[B]	4/4	0.95	0.10	12,13,13,13	4
4	GOL	A	803	6/6	0.96	0.07	13,17,19,25	0
7	EDO	A	823	4/4	0.96	0.18	17,21,24,30	0
7	EDO	A	815[A]	4/4	0.96	0.10	17,17,17,17	4
7	EDO	A	815[B]	4/4	0.96	0.10	17,17,18,18	4
9	NA	A	828	1/1	0.96	0.19	23,23,23,23	0
8	CA	A	826	1/1	0.97	0.21	42,42,42,42	0
7	EDO	A	814	4/4	0.97	0.09	11,12,13,16	0
9	NA	A	827	1/1	1.00	0.04	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.