



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5MWK
Title : Glycoside hydrolase BT_0986
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Deposited on : 2017-01-18
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

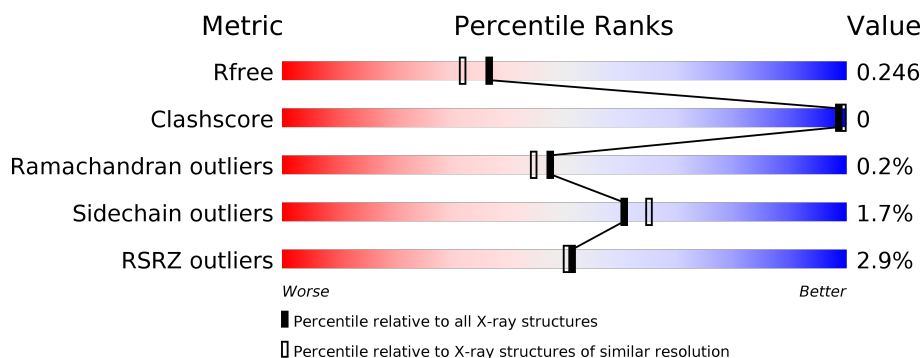
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1105	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>• 6%</div> </div> </div>
2	B	6	<div> <div>100%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8765 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 Glycoside hydrolase family 2, sugar binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1040	Total	C	N	O	S	0	1	0
			8297	5282	1431	1544	40			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	461	GLN	GLU	conflict	UNP Q8A931

- Molecule 2 is an oligosaccharide called alpha-L-rhamnopyranose-(1-2)-alpha-L-arabinopyranose-(1-4)-[4-O-[(1R)-1-hydroxyethyl]-2-O-methyl-alpha-L-fucopyranose-(1-2)]beta-D-galactopyranose-(1-2)-alpha-D-aceric acid-(1-3)-alpha-L-rhamnopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	6	Total	C	O	0	0	0
			63	36	27			

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	I	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Br	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	401	Total	O	0	0
			401	401		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.25Å 86.22Å 123.20Å 90.00° 99.38° 90.00°	Depositor
Resolution (Å)	45.40 – 2.00 45.40 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.40-2.00) 98.9 (45.40-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.199 , 0.239 0.207 , 0.246	Depositor DCC
R_{free} test set	4464 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8765	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 8PK, 8OQ, CA, RAM, ARA, GAL, BR, IOD

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	0.64	0/8512	0.77	12/11551 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1082	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	623	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	251	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	63	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	623	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	652	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	345	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	1081	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	850	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	850	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	742	MET	CA-CB-CG	5.22	122.17	113.30
1	A	251	ARG	NE-CZ-NH1	5.15	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

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	8297	0	8134	8	0
2	B	63	0	34	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	401	0	0	0	0
All	All	8765	0	8168	8	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 0.

All (8) 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:230:GLU:O	1:A:293:ARG:NH1	2.10	0.84
1:A:659:LYS:HD3	1:A:1018:THR:HG21	1.74	0.69
1:A:883:CYS:SG	1:A:916:VAL:HG21	2.50	0.51
1:A:157:GLY:H	1:A:387:THR:HG22	1.76	0.51
1:A:128:LEU:HD13	1:A:460:TRP:HA	1.95	0.49
1:A:154:LYS:HA	1:A:389:THR:HG22	1.97	0.47
1:A:883:CYS:SG	1:A:916:VAL:CG2	3.08	0.42
1:A:617:TYR:OH	1:A:668:ILE:HG23	2.21	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1035/1105 (94%)	999 (96%)	34 (3%)	2 (0%)	47	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	ASP
1	A	372	PRO

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	876/934 (94%)	861 (98%)	15 (2%)	60	65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	274	GLN
1	A	373	PHE
1	A	385	THR
1	A	397	LEU
1	A	458	ASP
1	A	534	GLN
1	A	535	PHE
1	A	699	PRO
1	A	743	SER
1	A	894	ASP
1	A	947	THR
1	A	953	GLU
1	A	997	LYS
1	A	1102	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	RAM	B	1	2	11,11,11	1.08	1 (9%)	15,16,16	1.21	1 (6%)
2	8OQ	B	2	2	7,11,12	1.00	1 (14%)	5,17,19	4.18	2 (40%)
2	GAL	B	3	2	11,11,12	0.63	0	15,15,17	1.97	5 (33%)
2	ARA	B	4	2	9,9,10	1.11	1 (11%)	10,12,14	1.69	2 (20%)
2	RAM	B	5	2,4	10,10,11	0.84	0	14,14,16	1.91	3 (21%)
2	8PK	B	6	2	11,11,15	1.00	1 (9%)	15,15,21	1.13	1 (6%)

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	RAM	B	1	2	-	-	0/1/1/1
2	8OQ	B	2	2	-	0/0/23/26	0/1/1/1
2	GAL	B	3	2	-	0/2/19/22	0/1/1/1
2	ARA	B	4	2	-	-	0/1/1/1
2	RAM	B	5	2,4	-	-	0/1/1/1
2	8PK	B	6	2	-	0/2/19/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	RAM	O1-C1	2.09	1.46	1.39
2	B	2	8OQ	C3-C2	-2.08	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	ARA	C4-C3	2.08	1.55	1.52
2	B	6	8PK	C1-C2	2.02	1.54	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	8OQ	O2-C2-C3	8.70	131.99	112.57
2	B	5	RAM	C1-C2-C3	4.82	115.59	109.67
2	B	4	ARA	C1-C2-C3	-3.99	104.76	109.67
2	B	3	GAL	O4-C4-C5	3.76	118.63	109.30
2	B	3	GAL	C6-C5-C4	2.96	119.94	113.00
2	B	5	RAM	O2-C2-C3	-2.80	104.52	110.14
2	B	3	GAL	O2-C2-C1	-2.72	103.59	109.15
2	B	5	RAM	C2-C3-C4	2.65	115.47	110.89
2	B	3	GAL	C1-C2-C3	2.63	112.90	109.67
2	B	2	8OQ	O2-C2-C1	2.48	116.87	110.26
2	B	6	8PK	O4-C4-C3	-2.40	104.81	110.35
2	B	4	ARA	O3-C3-C4	2.14	114.08	109.99
2	B	3	GAL	O5-C1-C2	2.05	113.94	110.77
2	B	1	RAM	O1-C1-C2	2.04	114.77	109.03

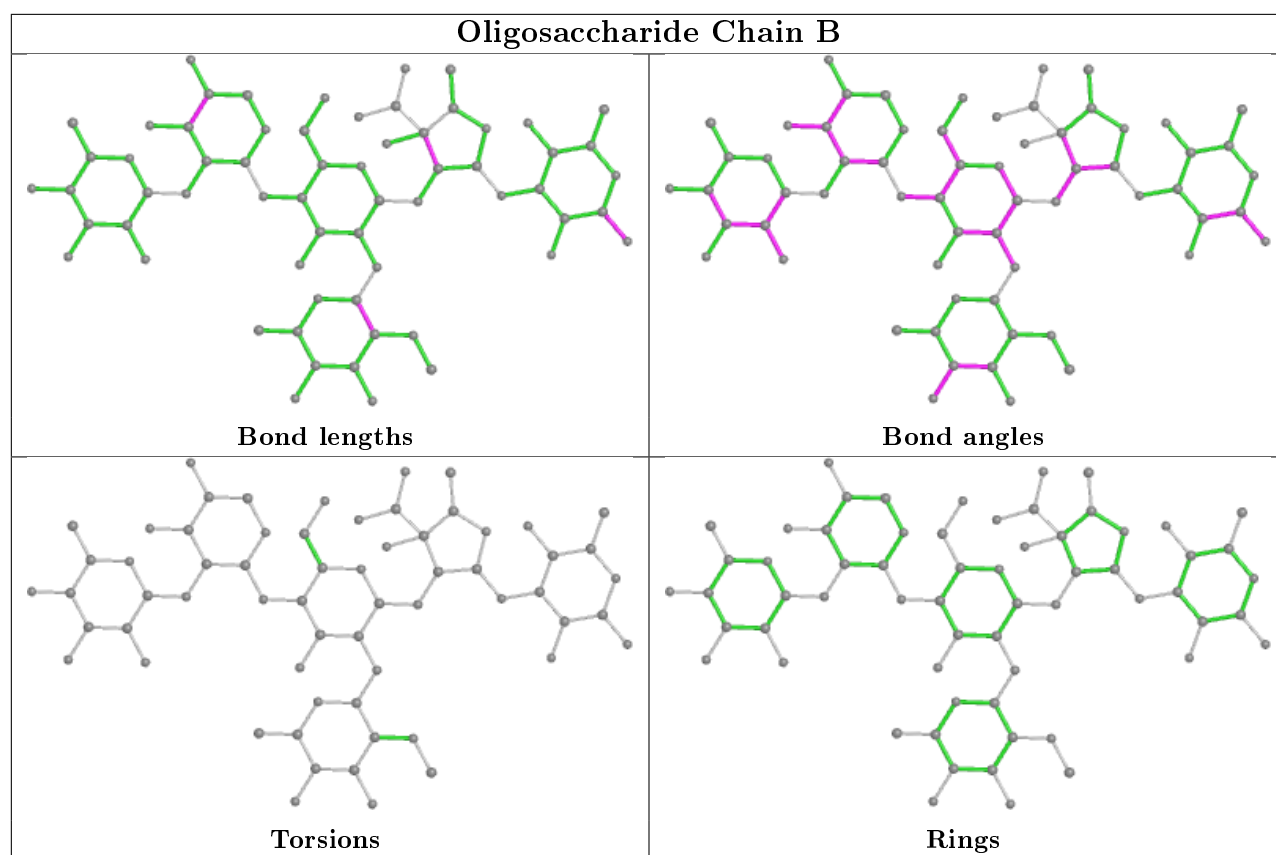
There are no chirality outliers.

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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 ²)	Q<0.9
1	A	1040/1105 (94%)	-0.07	30 (2%) 51 50	17, 28, 54, 95	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	ASN	6.8
1	A	202	HIS	4.9
1	A	373	PHE	4.3
1	A	1003	ASP	3.6
1	A	159	HIS	3.5
1	A	968	GLN	3.3
1	A	997	LYS	3.2
1	A	949	LEU	3.1
1	A	393	GLY	3.0
1	A	383	GLU	2.9
1	A	200	GLY	2.8
1	A	392	LYS	2.8
1	A	156	LYS	2.7
1	A	922	ALA	2.7
1	A	158	LEU	2.7
1	A	384	ARG	2.6
1	A	30	LEU	2.6
1	A	153	GLY	2.4
1	A	389	THR	2.4
1	A	390	LEU	2.3
1	A	995	ARG	2.3
1	A	199	THR	2.2
1	A	37	ASN	2.1
1	A	998	SER	2.1
1	A	391	PRO	2.1
1	A	950	GLU	2.1
1	A	152	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	540	VAL	2.1
1	A	90	ASN	2.1
1	A	154	LYS	2.0

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

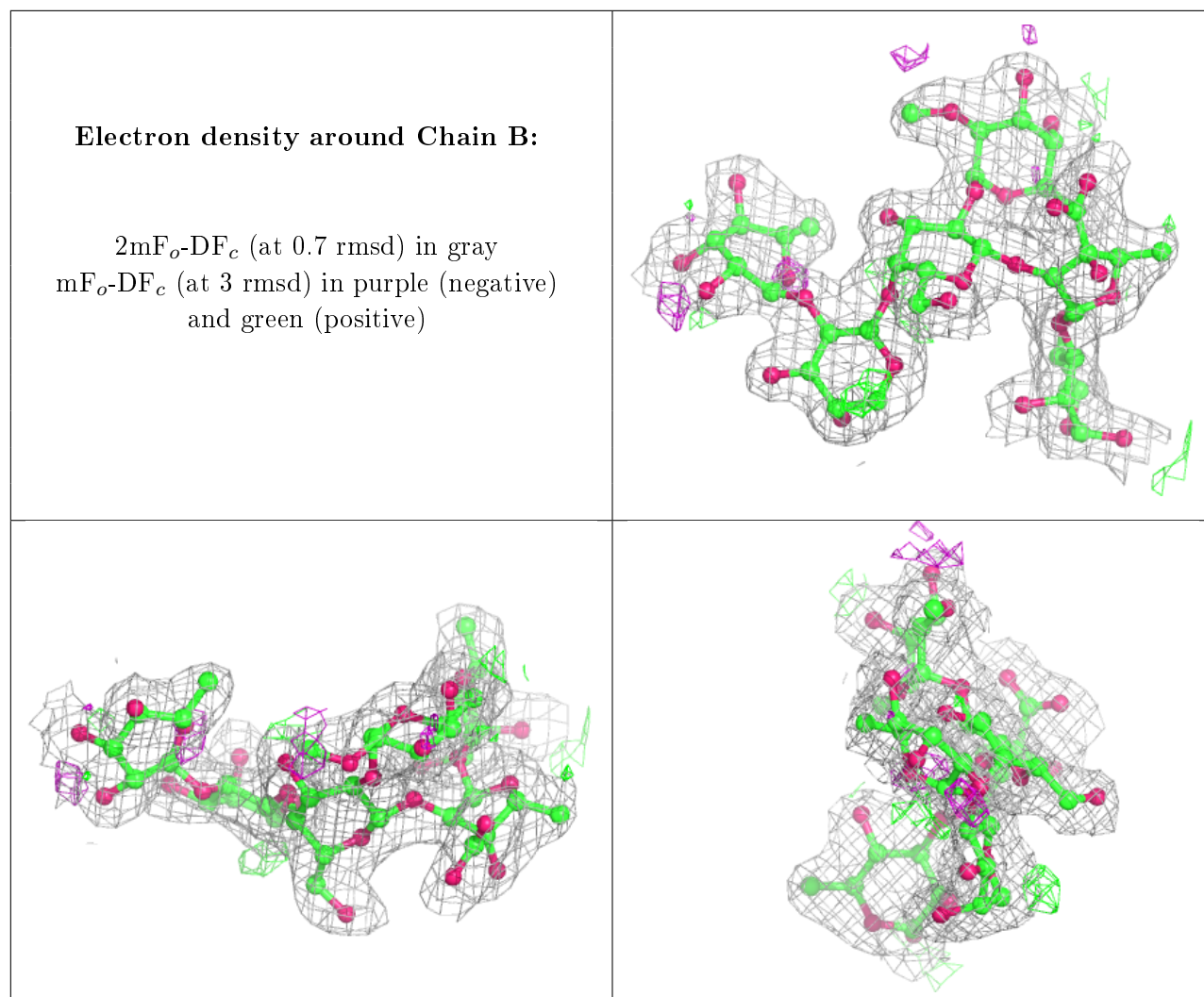
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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(\AA^2)	Q<0.9
2	RAM	B	5	10/11	0.81	0.18	35,41,44,44	0
2	ARA	B	4	9/10	0.86	0.15	29,31,35,39	0
2	RAM	B	1	11/11	0.91	0.10	27,28,31,35	0
2	8OQ	B	2	11/12	0.91	0.10	33,38,42,42	0
2	8PK	B	6	11/15	0.92	0.11	25,29,30,31	0
2	GAL	B	3	11/12	0.94	0.10	29,34,36,38	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, 95th 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(\AA^2)	Q<0.9
4	CA	A	1208	1/1	0.90	0.07	52,52,52,52	0
5	BR	A	1210	1/1	0.99	0.06	38,38,38,38	0
3	IOD	A	1207	1/1	0.99	0.05	37,37,37,37	0
5	BR	A	1209	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.