

Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2020 – 09:55 AM BST

PDB ID : 3OY8

Title : Crystal structure of human galectin-1 in complex with lactobionic acid

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Deposited on : 2010-09-23

Resolution : 2.19 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 (i) symbol.

The following versions of software and data (see references (1)) 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)

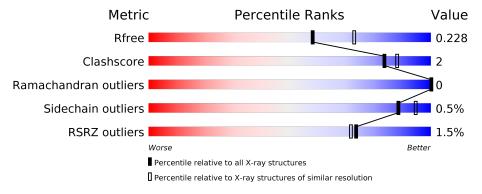
Validation Pipeline (wwPDB-VP) : 2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.19 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
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 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 <=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	134	96%	
2	В	134	93%	7% •
3	С	2	100%	
3	D	2	50% 50%	



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2276 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 Galectin-1.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	Λ	134	Total	С	N	О	S	0	9	0
1	A	104	1044	657	180	199	8	0	2	U

• Molecule 2 is a protein called Galectin-1.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
2	В	134	Total 1045	C 659	N 179	O 198	S 9	0	2	0

• Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-D-gluconic acid.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	С	2	Total (24 1	C O 12 12	0	0	0
3	D	2	Total 0 24 1	C O 12 12	0	0	0

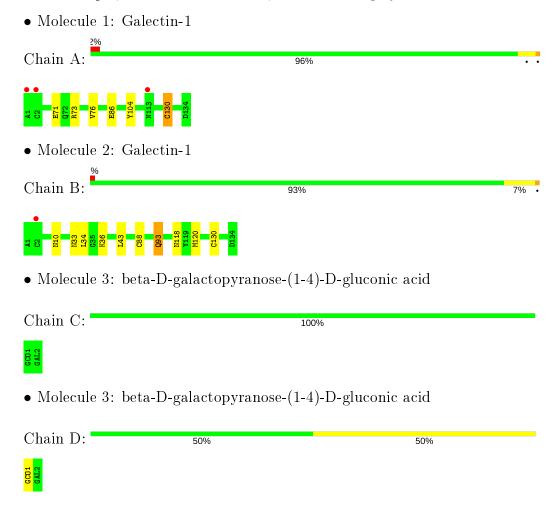
• Molecule 4 is water.

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
4	A	61	Total O 61 61	0	0
4	В	78	Total O 78 78	0	0



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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	44.71Å 58.57Å 111.62Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.81 - 2.19	Depositor
Resolution (A)	55.81 - 2.19	EDS
% Data completeness	94.6 (55.81-2.19)	Depositor
(in resolution range)	94.6 (55.81-2.19)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) > 1$	1.84 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D.	0.173 , 0.226	Depositor
R, R_{free}	0.172 , 0.228	DCC
R_{free} test set	752 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 39.7	EDS
L-test for twinning ²	$ < L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2276	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.80% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: CSO, GAL, CME, GCO

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		
WIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.39	0/1042	0.52	0/1405	
2	В	0.39	0/1043	0.52	0/1407	
All	All	0.39	0/2085	0.52	0/2812	

There are no bond length outliers.

There are no bond angle outliers.

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	1044	0	1013	3	0
2	В	1045	0	1017	6	0
3	С	24	0	20	0	0
3	D	24	0	20	1	0
4	A	61	0	0	0	0
4	В	78	0	0	1	0
All	All	2276	0	2070	10	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 2.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	Clash overlap (Å)
2:B:93[A]:GLN:HE21	2:B:93[A]:GLN:H	1.31	0.79
2:B:93[B]:GLN:OE1	2:B:93[B]:GLN:HA	1.89	0.72
1:A:76:VAL:HG21	1:A:104:TYR:CD2	2.35	0.60
1:A:71:GLU:OE1	1:A:73:ARG:NH1	2.44	0.49
2:B:36:LYS:HE3	4:B:186:HOH:O	2.14	0.48
2:B:34[B]:LEU:HD12	2:B:43:LEU:HD23	1.96	0.47
1:A:86:GLU:OE2	1:A:130:CME:HZ3	2.16	0.46
2:B:10:ASN:H	2:B:118:ASN:ND2	2.16	0.44
3:D:1:GCO:H5	3:D:1:GCO:H2	1.87	0.44
2:B:33:ASN:O	2:B:120:MET:HA	2.22	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	Perce	\mathbf{ntiles}
1	A	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
2	В	131/134 (98%)	127 (97%)	4 (3%)	0	100	100
All	All	$262/268 \; (98\%)$	254 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	108/106 (102%)	108 (100%)	0	100	100	
2	В	108/106 (102%)	106 (98%)	2 (2%)	57	71	
All	All	$216/212 \; (102\%)$	214 (99%)	2 (1%)	88	88	

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type	
2	В	93[A]	GLN	
2	В	93[B]	GLN	

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	72	GLN
1	A	118	ASN
2	В	56	ASN
2	В	118	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)

6 non-standard protein/DNA/RNA residues 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	Tuno	Chain	Pos	Res Link Bond lengths			В	ond ang	gles	
10101	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CSO	В	16	2	3,6,7	0.73	0	0,6,8	0.00	-
1	CSO	A	16	1	3,6,7	0.73	0	0,6,8	0.00	-
2	CME	В	130	2	8,9,10	0.84	0	5,9,11	1.71	2 (40%)
1	CSO	A	88	1	3,6,7	0.65	0	0,6,8	0.00	-



Mol	Т	Chain	Dog	T : 1-	Bond lengths			Bond angles		
MIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	CME	A	130	1	8,9,10	0.87	0	5,9,11	1.89	2 (40%)
2	CME	В	88	2	8,9,10	0.80	0	5,9,11	1.51	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
2	CSO	В	16	2	-	0/1/5/7	-
1	CSO	A	16	1	_	0/1/5/7	_
2	CME	В	130	2	-	3/5/8/10	_
1	CSO	A	88	1	-	1/1/5/7	-
1	CME	A	130	1	-	2/5/8/10	_
2	CME	В	88	2	-	1/5/8/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	130	CME	CE-SD-SG	3.02	117.38	103.45
2	В	130	CME	CE-SD-SG	2.73	116.01	103.45
2	В	88	CME	CE-SD-SG	2.51	115.03	103.45
1	A	130	CME	CB-SG-SD	2.35	109.91	103.82
2	В	130	CME	CB-SG-SD	2.32	109.83	103.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	130	CME	CE-SD-SG-CB
2	В	130	CME	SD-CE-CZ-OH
2	В	88	CME	SD-CE-CZ-OH
1	A	130	CME	CE-SD-SG-CB
2	В	130	CME	CZ-CE-SD-SG
1	A	130	CME	CZ-CE-SD-SG
1	A	88	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	130	CME	1	0

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	Tuno	Chain	Dog	Res Link Bond lengths			Bond angles			
MIGI	Type	Chain	nes	LIIIK	Counts	RMSZ	$\mid \# Z > 2$	Counts	RMSZ	# Z > 2
3	GCO	С	1	3	9,12,12	0.39	0	12,16,16	0.59	0
3	GAL	С	2	3	11,11,12	0.58	0	15,15,17	0.71	0
3	GCO	D	1	3	9,12,12	0.49	0	12,16,16	0.75	0
3	GAL	D	2	3	11,11,12	0.58	0	15,15,17	0.85	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
3	GCO	С	1	3	-	1/14/18/18	-
3	GAL	С	2	3	-	0/2/19/22	0/1/1/1
3	GCO	D	1	3	-	5/14/18/18	-
3	GAL	D	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	GCO	C3-C4-C5-C6
3	D	1	GCO	O4-C4-C5-C6
3	D	1	GCO	C3-C4-C5-O5

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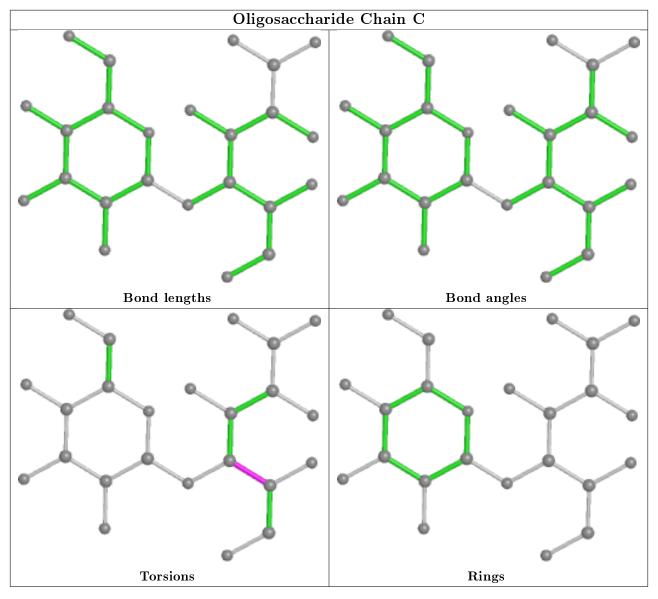
Mol	Chain	Res	Type	Atoms
3	D	1	GCO	O4-C4-C5-O5
3	D	1	GCO	C2-C3-C4-C5
3	С	1	GCO	C3-C4-C5-O5

There are no ring outliers.

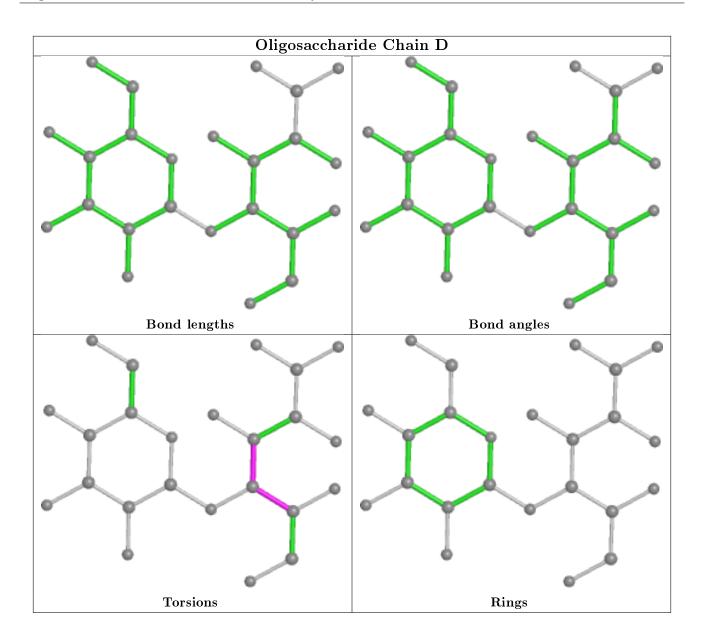
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	GCO	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)

There are no ligands in this entry.

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^{th} 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 $>$	$\# \mathrm{RSRZ} {>} 2$	$OWAB(Å^2)$	Q < 0.9
1	A	131/134 (97%)	-0.32	3 (2%) 60 58	14, 27, 48, 69	0
2	В	131/134 (97%)	-0.36	1 (0%) 86 85	15, 26, 44, 77	0
All	All	262/268 (97%)	-0.34	4 (1%) 73 72	14, 26, 47, 77	0

All (4) RSRZ outliers are listed below:

Mol	Chain	${f Res}$	Type	RSRZ
1	A	2	CYS	4.1
2	В	2	CYS	4.0
1	A	1	ALA	2.8
1	A	113	ASN	2.3

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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	CSO	В	16	7/8	0.92	0.12	22,25,28,31	0
2	CME	В	88	10/11	0.92	0.10	15,26,38,40	0
1	CSO	A	16	7/8	0.94	0.10	26,30,37,38	0
2	CME	В	130	10/11	0.95	0.12	16,29,45,49	0
1	CME	A	130	10/11	0.96	0.11	19,31,42,45	0
1	CSO	A	88	7/8	0.97	0.08	20,24,32,35	0

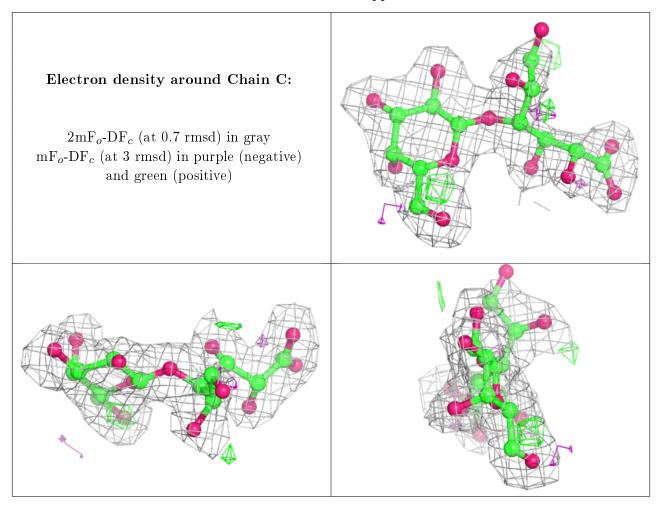


6.3 Carbohydrates (i)

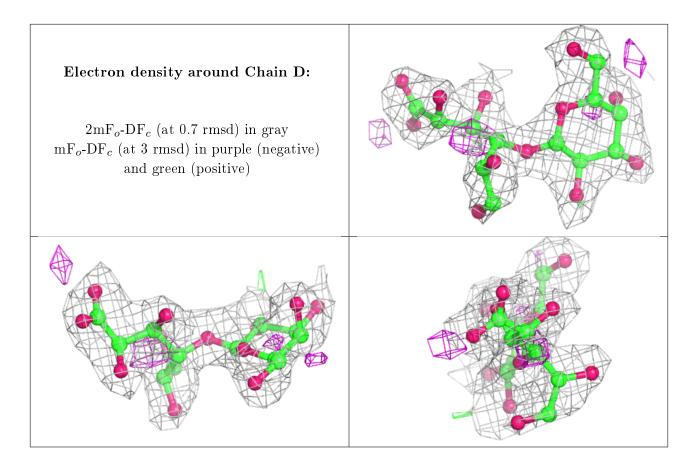
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	${f Res}$	Atoms	RSCC	RSR	${f B-factors(\AA^2)}$	Q<0.9
3	GAL	D	2	11/12	0.87	0.14	39,42,43,44	0
3	GCO	D	1	13/13	0.88	0.19	43,46,50,52	0
3	GAL	С	2	11/12	0.90	0.12	31,34,36,36	0
3	GCO	С	1	13/13	0.92	0.15	38,40,46,49	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

