



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:15 AM BST

PDB ID : 4Z3G
Title : Crystal structure of the lectin domain of PapG from E. coli BI47 in complex with 4-methoxyphenyl beta-D-galabiose in space group P212121
Authors : Jakob, R.P.; Navarra, G.; Zihlmann, P.; Stangier, K.; Preston, R.C.; Rabbani, S.; Maier, T.; Ernst, B.
Deposited on : 2015-03-31
Resolution : 1.45 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

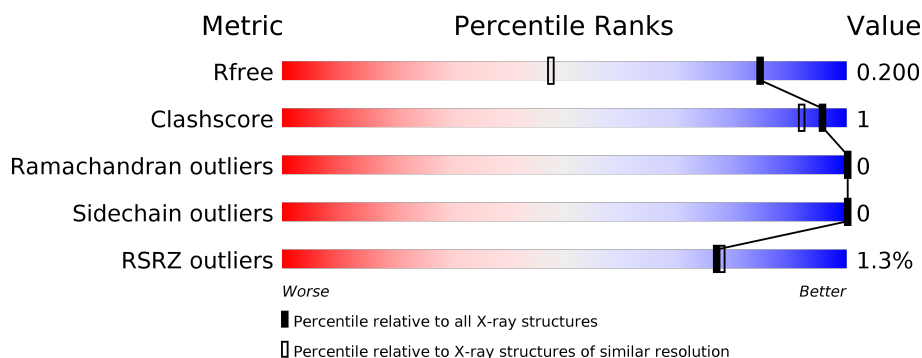
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	198	<div> <div>2%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
1	B	198	<div> <div>%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>100%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7124 atoms, of which 3208 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 PapG, lectin domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	H	N	O	S	0	8	0
			3196	1060	1566	271	294	5			
1	B	198	Total	C	H	N	O	S	1	8	0
			3189	1061	1560	268	295	5			

There are 4 discrepancies between the modelled and reference sequences:

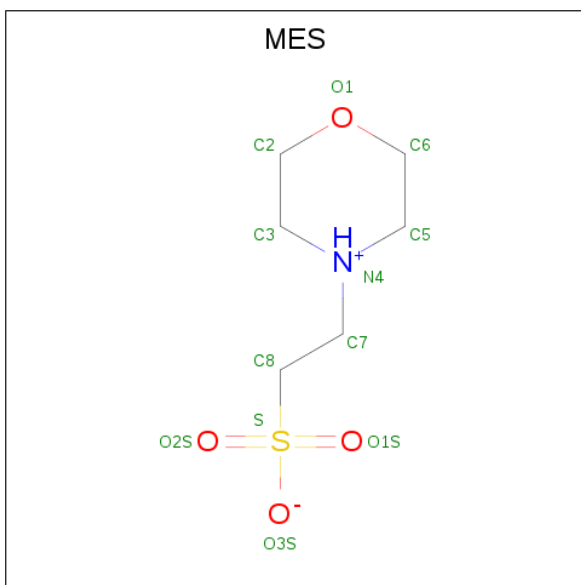
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP T7DCJ2
A	109	GLN	GLU	conflict	UNP T7DCJ2
B	-1	MET	-	expression tag	UNP T7DCJ2
B	109	GLN	GLU	conflict	UNP T7DCJ2

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



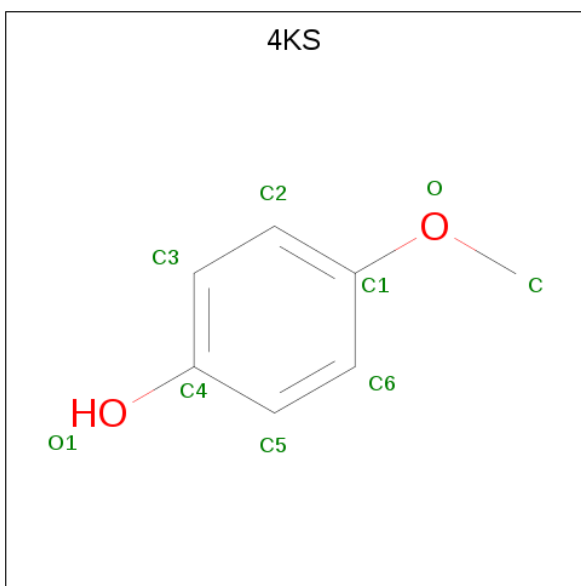
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	O	0	0	0
			43	12	21	10			
2	D	2	Total	C	H	O	0	0	0
			43	12	21	10			

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
3	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 4 is 4-methoxyphenol (three-letter code: 4KS) (formula: C₇H₈O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			16	7	7	2		
4	B	1	Total	C	H	O	0	0
			16	7	7	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	278	Total 278	O 278	0	0
5	B	293	Total 293	O 293	0	0

3 Residue-property plots

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: PapG, lectin domain



- Molecule 1: PapG, lectin domain



- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose



- Molecule 2: alpha-D-galactopyranose-(1-4)-beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.27Å 72.61Å 94.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.66 – 1.45 57.66 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (57.66-1.45) 99.2 (57.66-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.45Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.169 , 0.189 0.178 , 0.200	Depositor DCC
R_{free} test set	3494 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7124	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2860e-04.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, GAL, 4KS, MES

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	0.41	0/1758	0.66	0/2394
1	B	0.42	0/1749	0.65	0/2383
All	All	0.41	0/3507	0.65	0/4777

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

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	1630	1566	1520	4	0
1	B	1629	1560	1528	2	0
2	C	22	21	19	0	0
2	D	22	21	19	0	0
3	A	12	13	13	4	0
3	B	12	13	13	0	0
4	A	9	7	0	0	0
4	B	9	7	0	0	0
5	A	278	0	0	1	0
5	B	293	0	0	0	0
All	All	3916	3208	3112	7	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 1.

All (7) 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:148:ASP:O	3:A:201:MES:H52	1.89	0.73
1:A:73:LYS:HB2	3:A:201:MES:H21	1.96	0.48
1:A:148:ASP:O	3:A:201:MES:C5	2.63	0.45
3:A:201:MES:H61	5:A:526:HOH:O	2.19	0.43
1:B:150:SER:HA	1:B:190:LEU:HD23	2.02	0.42
1:A:52:GLY:HA2	1:A:113:ASP:HA	2.02	0.41
1:B:180:THR:O	1:B:180:THR:HG22	2.20	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	205/198 (104%)	203 (99%)	2 (1%)	0	100	100
1	B	205/198 (104%)	203 (99%)	2 (1%)	0	100	100
All	All	410/396 (104%)	406 (99%)	4 (1%)	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	178/170 (105%)	178 (100%)	0	100	100
1	B	178/170 (105%)	178 (100%)	0	100	100
All	All	356/340 (105%)	356 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 ⓘ

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	$\# Z > 2$
2	GAL	C	1	2,4	11,11,12	0.35	0	15,15,17	0.66	0
2	GLA	C	2	2	11,11,12	0.36	0	15,15,17	0.77	1 (6%)
2	GAL	D	1	2,4	11,11,12	0.30	0	15,15,17	0.63	0
2	GLA	D	2	2	11,11,12	0.36	0	15,15,17	0.67	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
2	GAL	C	1	2,4	-	1/2/19/22	0/1/1/1
2	GLA	C	2	2	-	0/2/19/22	0/1/1/1
2	GAL	D	1	2,4	-	1/2/19/22	0/1/1/1
2	GLA	D	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	2	GLA	C1-O5-C5	2.39	115.44	112.19

There are no chirality outliers.

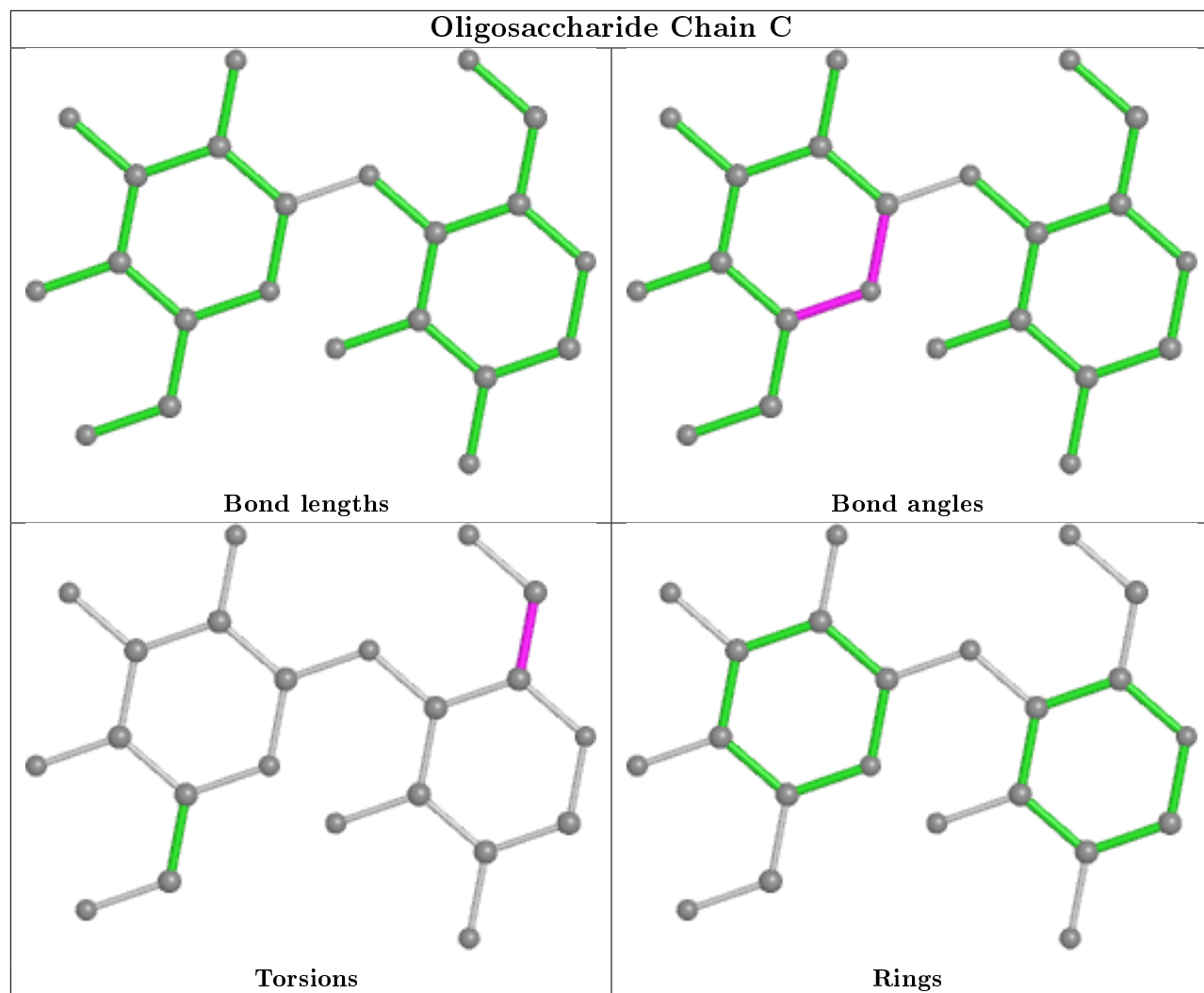
All (2) torsion outliers are listed below:

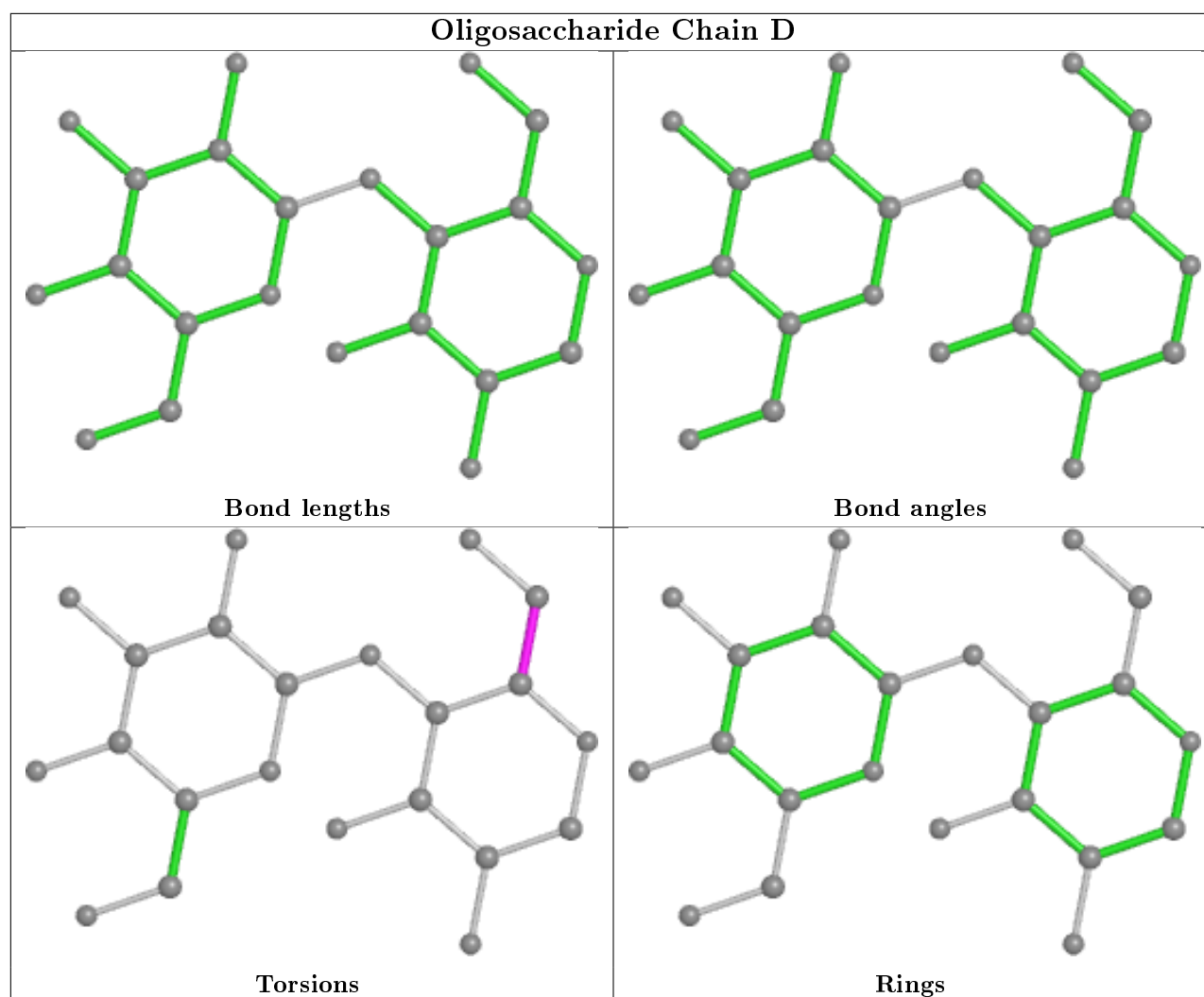
Mol	Chain	Res	Type	Atoms
2	C	1	GAL	O5-C5-C6-O6
2	D	1	GAL	O5-C5-C6-O6

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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	MES	A	201	-	12,12,12	0.73	0	14,16,16	0.57	0
3	MES	B	201	-	12,12,12	0.70	0	14,16,16	0.47	0
4	4KS	A	202	2	9,9,9	1.13	0	11,11,11	1.27	1 (9%)
4	4KS	B	202	2	9,9,9	1.56	2 (22%)	11,11,11	1.00	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	MES	A	201	-	-	0/6/14/14	0/1/1/1
3	MES	B	201	-	-	5/6/14/14	0/1/1/1
4	4KS	A	202	2	-	0/2/2/2	0/1/1/1
4	4KS	B	202	2	-	0/2/2/2	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	4KS	C2-C1	3.10	1.44	1.38
4	B	202	4KS	C3-C4	2.50	1.43	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	202	4KS	O1-C4-C3	-2.15	113.90	120.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	201	MES	C8-C7-N4-C3
3	B	201	MES	C7-C8-S-O2S
3	B	201	MES	C7-C8-S-O3S
3	B	201	MES	C7-C8-S-O1S
3	B	201	MES	N4-C7-C8-S

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	MES	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	198/198 (100%)	-0.49	4 (2%) 65 67	14, 21, 34, 47	0
1	B	198/198 (100%)	-0.42	1 (0%) 91 93	15, 21, 35, 53	0
All	All	396/396 (100%)	-0.46	5 (1%) 77 78	14, 21, 35, 53	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	MET	5.1
1	A	-1	MET	4.3
1	A	52	GLY	3.2
1	A	180	THR	2.2
1	A	54	TRP	2.1

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

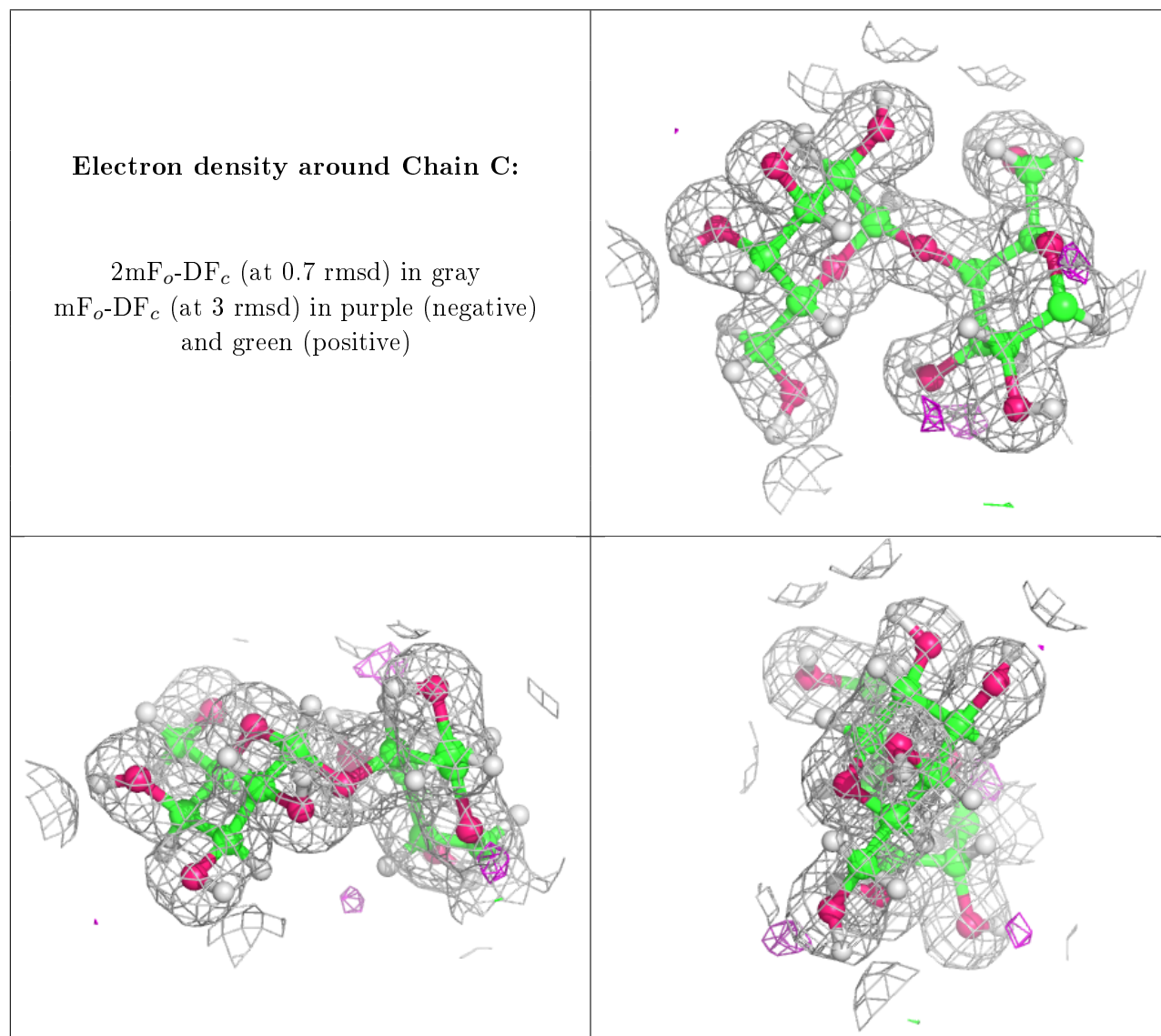
There are no non-standard protein/DNA/RNA residues in this entry.

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.

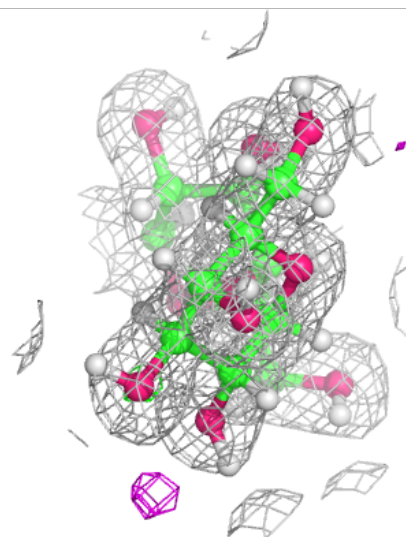
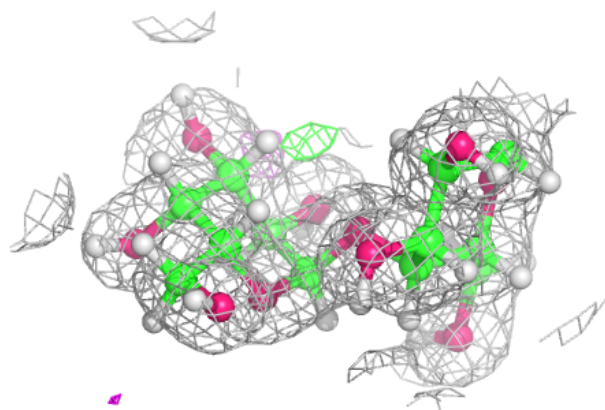
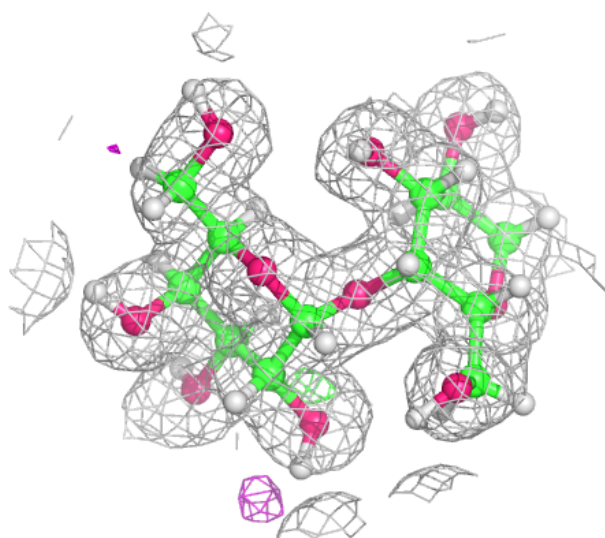
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLA	C	2	11/12	0.96	0.07	12,17,18,20	0
2	GAL	C	1	11/12	0.97	0.06	14,17,18,19	0
2	GAL	D	1	11/12	0.98	0.06	14,17,19,21	0
2	GLA	D	2	11/12	0.98	0.05	15,17,19,20	0

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.



Electron density around Chain D:

2mF_o-DF_c (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)

**6.4 Ligands** ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å ²)	Q<0.9
3	MES	A	201	12/12	0.73	0.31	36,44,66,67	0
3	MES	B	201	12/12	0.73	0.32	59,66,68,68	0
4	4KS	A	202	9/9	0.97	0.09	20,23,30,30	0
4	4KS	B	202	9/9	0.97	0.07	17,19,24,24	0

6.5 Other polymers

There are no such residues in this entry.