



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 02:39 PM BST

PDB ID : 4NO4  
Title : Crystal Structure of Galectin-1 L11A mutant  
Authors : Dessau, M.  
Deposited on : 2013-11-19  
Resolution : 1.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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

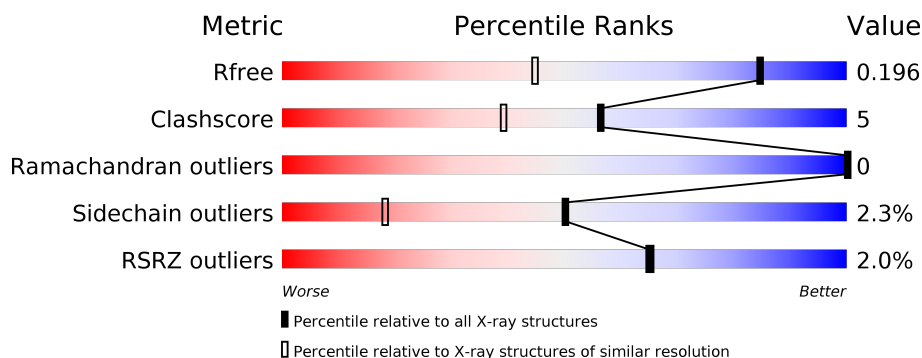
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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  $\geq 3$ , 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	134	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 89%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>89%</span> <span>11%</span> </div> </div>
1	B	134	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 90%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>90%</span> <span>10%</span> </div> </div>
1	C	134	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 6%, green 94%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>94%</span> <span>6%</span> </div> </div>
1	D	134	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 7%, green 93%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>93%</span> <span>7%</span> </div> </div>
1	E	134	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 12%, green 87%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>87%</span> <span>12%</span> </div> </div>
1	F	134	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 89%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>89%</span> <span>11%</span> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	H	2	 50%50%
2	I	2	 50%50%
2	J	2	 50%50%
2	K	2	 100%
2	L	2	 100%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14006 atoms, of which 6253 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	A	134	Total	C	H	N	O	S	0	3	0
			2058	657	1009	181	203	8			
1	B	134	Total	C	H	N	O	S	0	6	0
			2103	669	1043	181	202	8			
1	C	134	Total	C	H	N	O	S	0	1	0
			2032	650	996	178	200	8			
1	D	134	Total	C	H	N	O	S	0	2	0
			2033	650	995	179	201	8			
1	E	134	Total	C	H	N	O	S	0	4	0
			2071	660	1021	181	201	8			
1	F	134	Total	C	H	N	O	S	0	3	0
			2054	656	1010	179	201	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	LEU	engineered mutation	UNP P11762
B	12	ALA	LEU	engineered mutation	UNP P11762
C	12	ALA	LEU	engineered mutation	UNP P11762
D	12	ALA	LEU	engineered mutation	UNP P11762
E	12	ALA	LEU	engineered mutation	UNP P11762
F	12	ALA	LEU	engineered mutation	UNP P11762

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	H	O	0	0	0
			45	12	22	11			

*Continued on next page...*

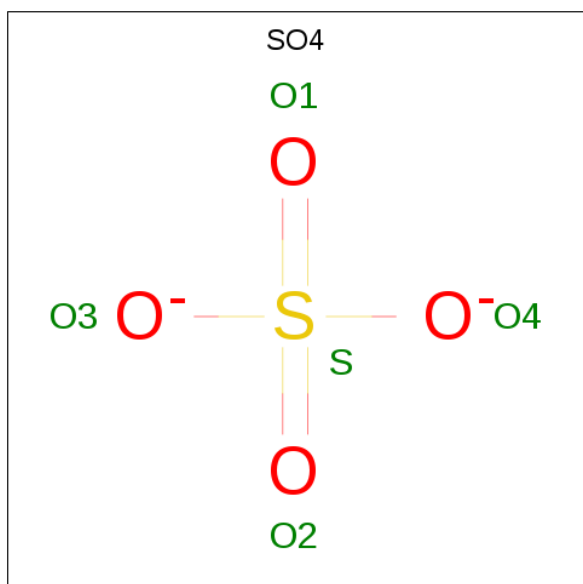
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	2	Total	C	H	O	0	0	0
			45	12	22	11			
2	I	2	Total	C	H	O	0	0	0
			45	12	22	11			
2	J	2	Total	C	H	O	0	0	0
			45	12	22	11			
2	K	2	Total	C	H	O	0	0	0
			45	12	22	11			
2	L	2	Total	C	H	O	0	0	0
			45	12	22	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			13	3	7	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	E	1	Total	C	H	O	0	0
			14	3	8	3		
5	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	220	Total	O	0	0
			220	220		
6	B	211	Total	O	0	0
			211	211		

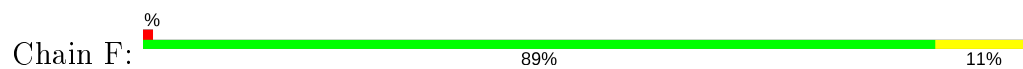
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	209	Total 209	O 209	0	0
6	D	209	Total 209	O 209	0	0
6	E	216	Total 216	O 216	0	0
6	F	224	Total 224	O 224	0	0







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



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



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



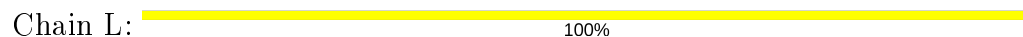
- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.52Å 193.83Å 108.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.97 – 1.40 28.97 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.97-1.40) 98.2 (28.97-1.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 1.40Å)	Xtriage
Refinement program	PHENIX dev_1593, REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.188 , 0.197 0.188 , 0.196	Depositor DCC
$R_{free}$ test set	11365 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.50 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.048 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.047 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14006	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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 31.30 % 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 1.1327e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, MG, BGC, GAL, SO4

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	0.45	0/1077	0.59	0/1457
1	B	0.46	0/1100	0.59	0/1486
1	C	0.42	0/1061	0.57	0/1435
1	D	0.42	0/1073	0.58	0/1451
1	E	0.46	0/1091	0.62	0/1473
1	F	0.47	0/1075	0.59	0/1454
All	All	0.45	0/6477	0.59	0/8756

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	1049	1009	1009	14	0
1	B	1060	1043	1043	13	0
1	C	1036	996	997	6	0
1	D	1038	995	986	6	0
1	E	1050	1021	1012	11	0
1	F	1044	1010	1010	15	0
2	G	23	22	21	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	23	22	21	0	0
2	I	23	22	21	0	0
2	J	23	22	21	0	0
2	K	23	22	21	0	0
2	L	23	22	21	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
4	A	5	0	0	0	0
4	E	5	0	0	0	0
5	A	12	16	15	0	0
5	B	6	7	8	0	0
5	C	6	8	7	0	0
5	E	6	8	8	0	0
5	F	6	8	8	0	0
6	A	220	0	0	11	4
6	B	211	0	0	10	2
6	C	209	0	0	3	2
6	D	209	0	0	3	5
6	E	216	0	0	7	2
6	F	224	0	0	8	1
All	All	7753	6253	6229	64	10

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.

The worst 5 of 64 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:E:40:ASN:ND2	6:E:440:HOH:O	1.88	1.04
1:A:61:CYS:SG	6:A:513:HOH:O	2.16	1.01
1:F:73:GLN:O	6:F:478:HOH:O	1.87	0.91
1:F:13:LYS:NZ	6:F:498:HOH:O	2.04	0.90
1:A:94:GLN:NE2	6:A:434:HOH:O	1.91	0.87

The worst 5 of 10 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:486:HOH:O	6:B:486:HOH:O[3_655]	1.51	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:458:HOH:O	6:F:458:HOH:O[3_555]	1.52	0.68
6:E:474:HOH:O	6:E:492:HOH:O[3_555]	1.55	0.65
6:C:391:HOH:O	6:E:327:HOH:O[2_555]	1.96	0.24
6:B:430:HOH:O	6:D:426:HOH:O[6_555]	1.98	0.22

## 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	135/134 (101%)	132 (98%)	3 (2%)	0	100	100
1	B	138/134 (103%)	137 (99%)	1 (1%)	0	100	100
1	C	133/134 (99%)	131 (98%)	2 (2%)	0	100	100
1	D	134/134 (100%)	132 (98%)	2 (2%)	0	100	100
1	E	136/134 (102%)	134 (98%)	2 (2%)	0	100	100
1	F	135/134 (101%)	132 (98%)	3 (2%)	0	100	100
All	All	811/804 (101%)	798 (98%)	13 (2%)	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	114/111 (103%)	110 (96%)	4 (4%)	36	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	117/111 (105%)	115 (98%)	2 (2%)	60	31
1	C	112/111 (101%)	110 (98%)	2 (2%)	59	28
1	D	113/111 (102%)	111 (98%)	2 (2%)	59	28
1	E	115/111 (104%)	111 (96%)	4 (4%)	36	7
1	F	114/111 (103%)	112 (98%)	2 (2%)	59	28
All	All	685/666 (103%)	669 (98%)	16 (2%)	50	18

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	134	PHE
1	D	127	PHE
1	E	127	PHE
1	C	127	PHE
1	E	134	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	94	GLN

### 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 ⓘ

12 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	G	1	2	12,12,12	1.09	1 (8%)	17,17,17	0.95	1 (5%)
2	GAL	G	2	2	11,11,12	1.00	0	15,15,17	0.52	0
2	BGC	H	1	2	12,12,12	0.88	0	17,17,17	0.96	0
2	GAL	H	2	2	11,11,12	1.28	2 (18%)	15,15,17	0.52	0
2	BGC	I	1	2	12,12,12	0.80	0	17,17,17	0.92	0
2	GAL	I	2	2	11,11,12	1.16	1 (9%)	15,15,17	0.62	0
2	BGC	J	1	2	12,12,12	1.00	1 (8%)	17,17,17	1.02	1 (5%)
2	GAL	J	2	2	11,11,12	1.10	0	15,15,17	0.45	0
2	BGC	K	1	2	12,12,12	0.90	1 (8%)	17,17,17	0.97	1 (5%)
2	GAL	K	2	2	11,11,12	1.08	1 (9%)	15,15,17	0.65	0
2	BGC	L	1	2	12,12,12	0.88	0	17,17,17	0.91	1 (5%)
2	GAL	L	2	2	11,11,12	1.04	1 (9%)	15,15,17	0.59	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	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	BGC	I	1	2	-	0/2/22/22	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	BGC	J	1	2	-	0/2/22/22	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	BGC	K	1	2	-	0/2/22/22	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	BGC	L	1	2	-	0/2/22/22	0/1/1/1
2	GAL	L	2	2	-	0/2/19/22	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	GAL	O5-C1	-2.58	1.39	1.43
2	G	1	BGC	O2-C2	-2.37	1.37	1.43
2	I	2	GAL	O5-C1	-2.29	1.40	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	2	GAL	O5-C1	-2.28	1.40	1.43
2	H	2	GAL	O2-C2	-2.26	1.38	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1	BGC	O1-C1-C2	-2.87	100.95	109.03
2	J	1	BGC	O1-C1-C2	-2.31	102.52	109.03
2	L	1	BGC	O1-C1-C2	-2.03	103.33	109.03
2	G	1	BGC	O1-C1-C2	-2.02	103.33	109.03

There are no chirality outliers.

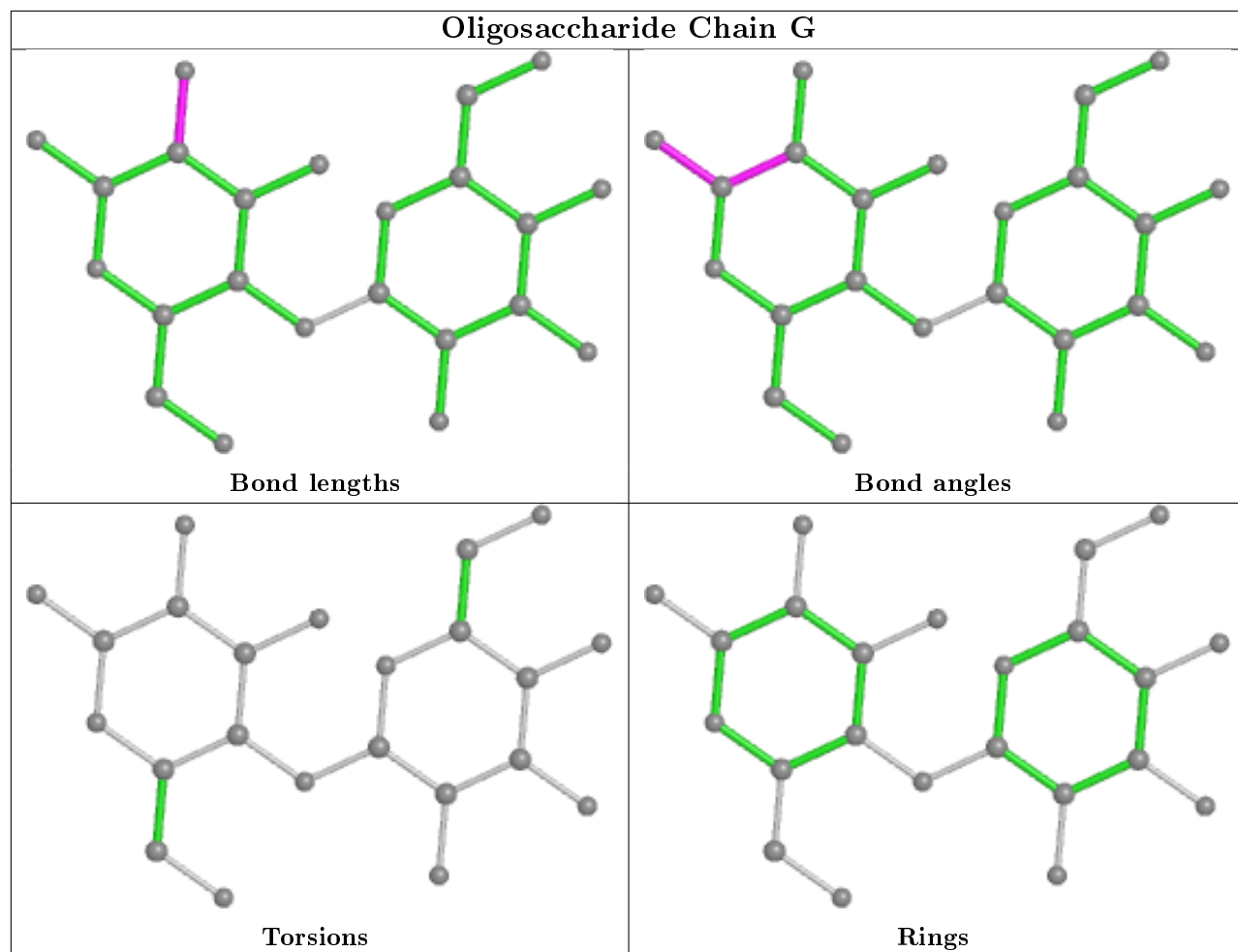
There are no torsion outliers.

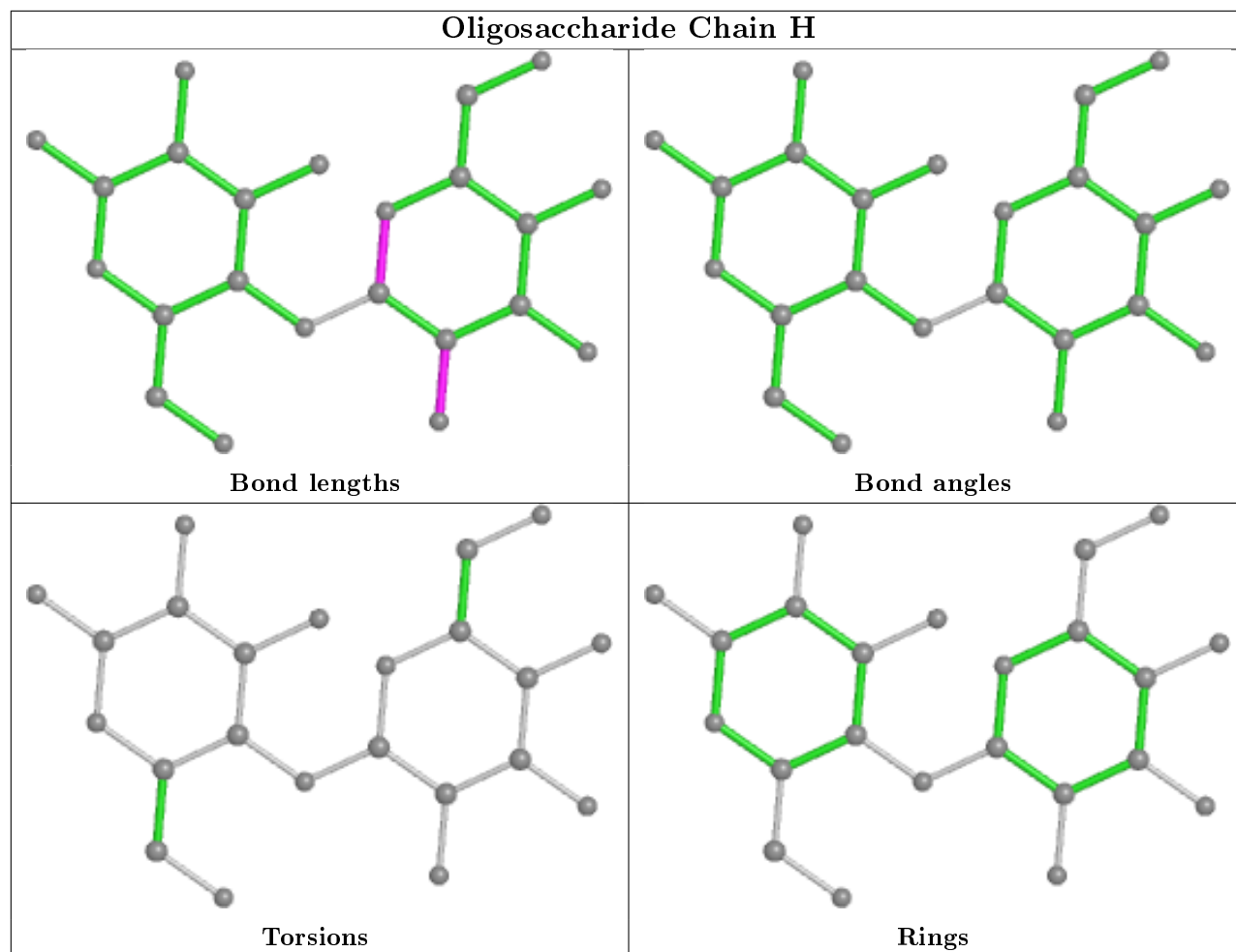
There are no ring outliers.

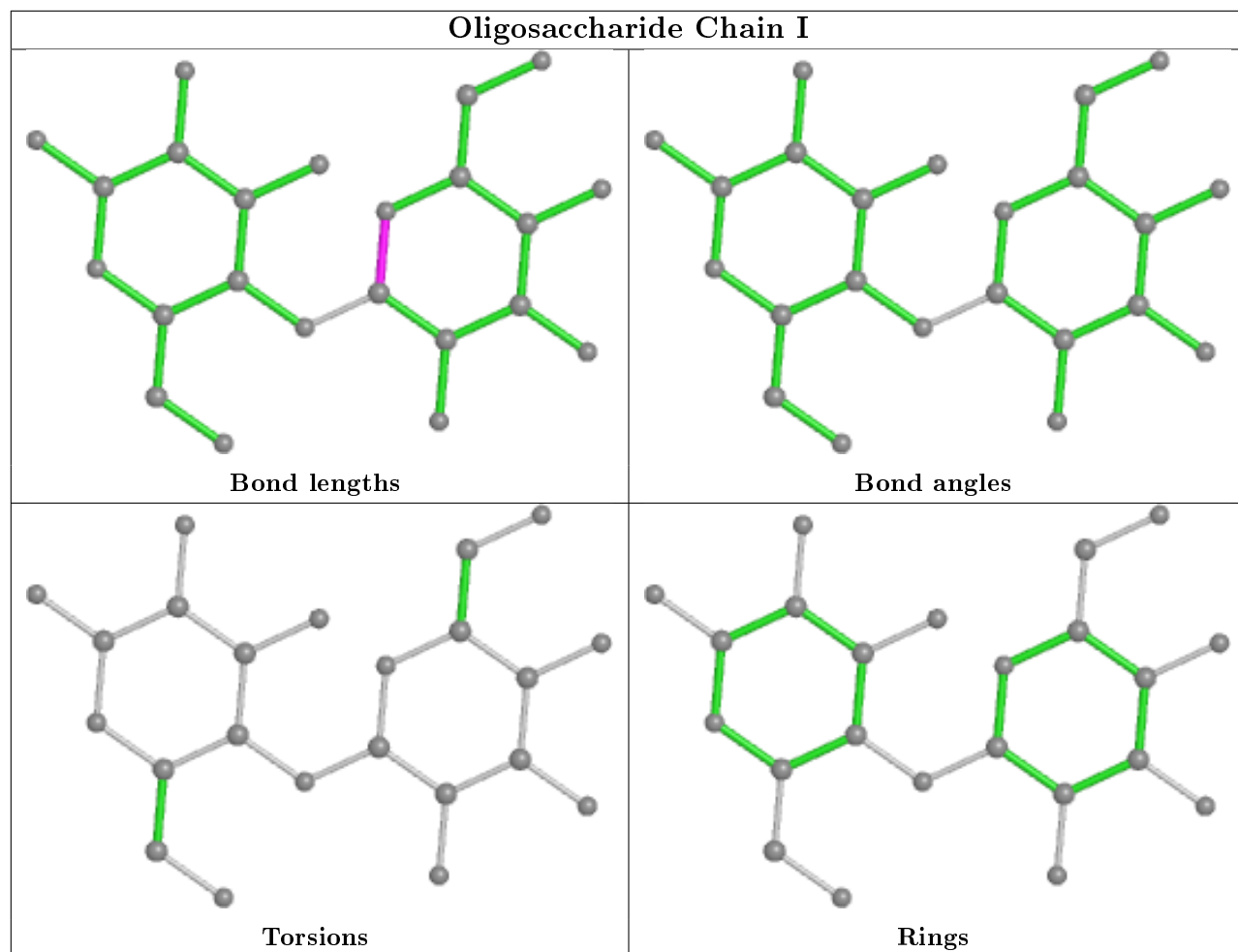
No monomer is involved in short contacts.

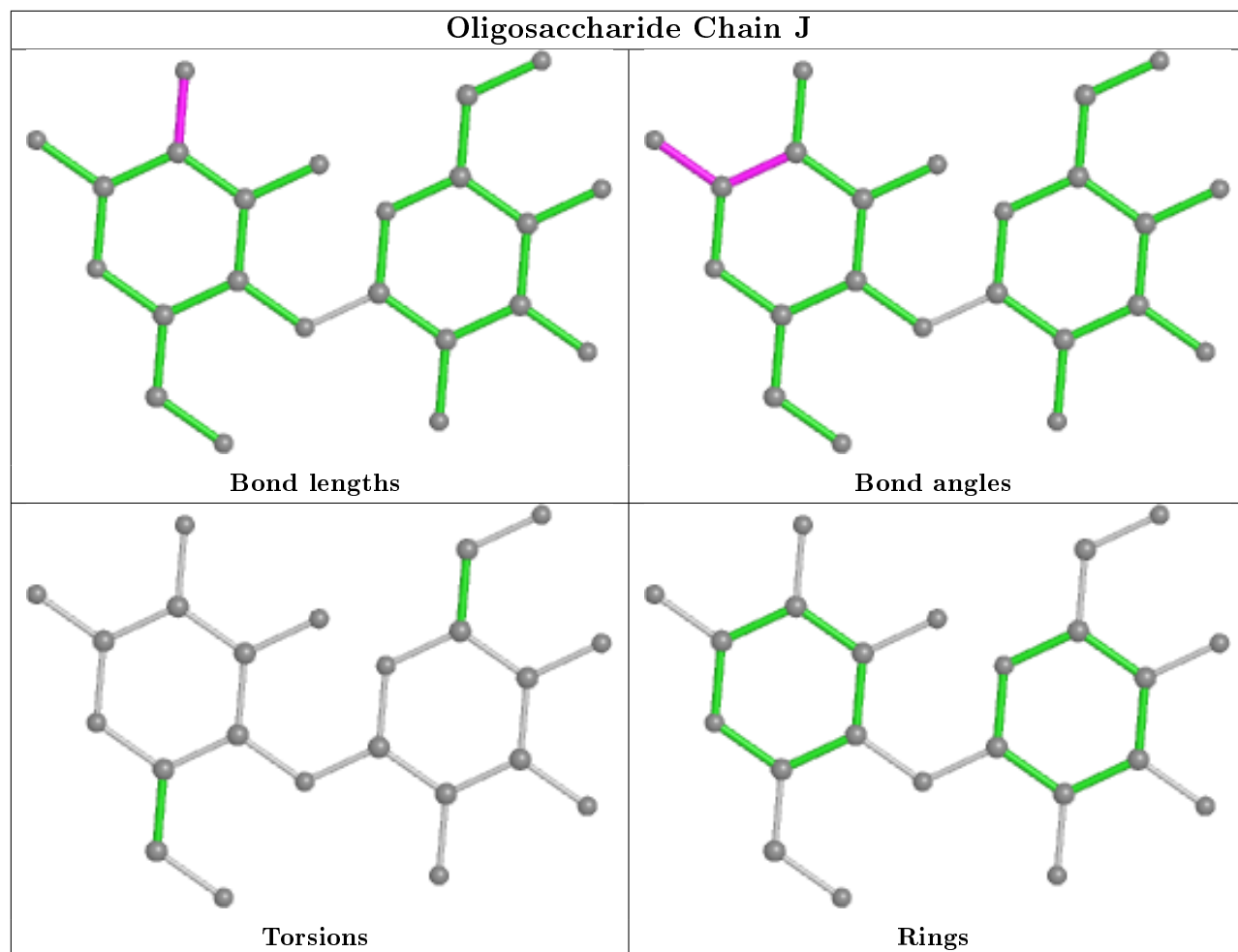
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

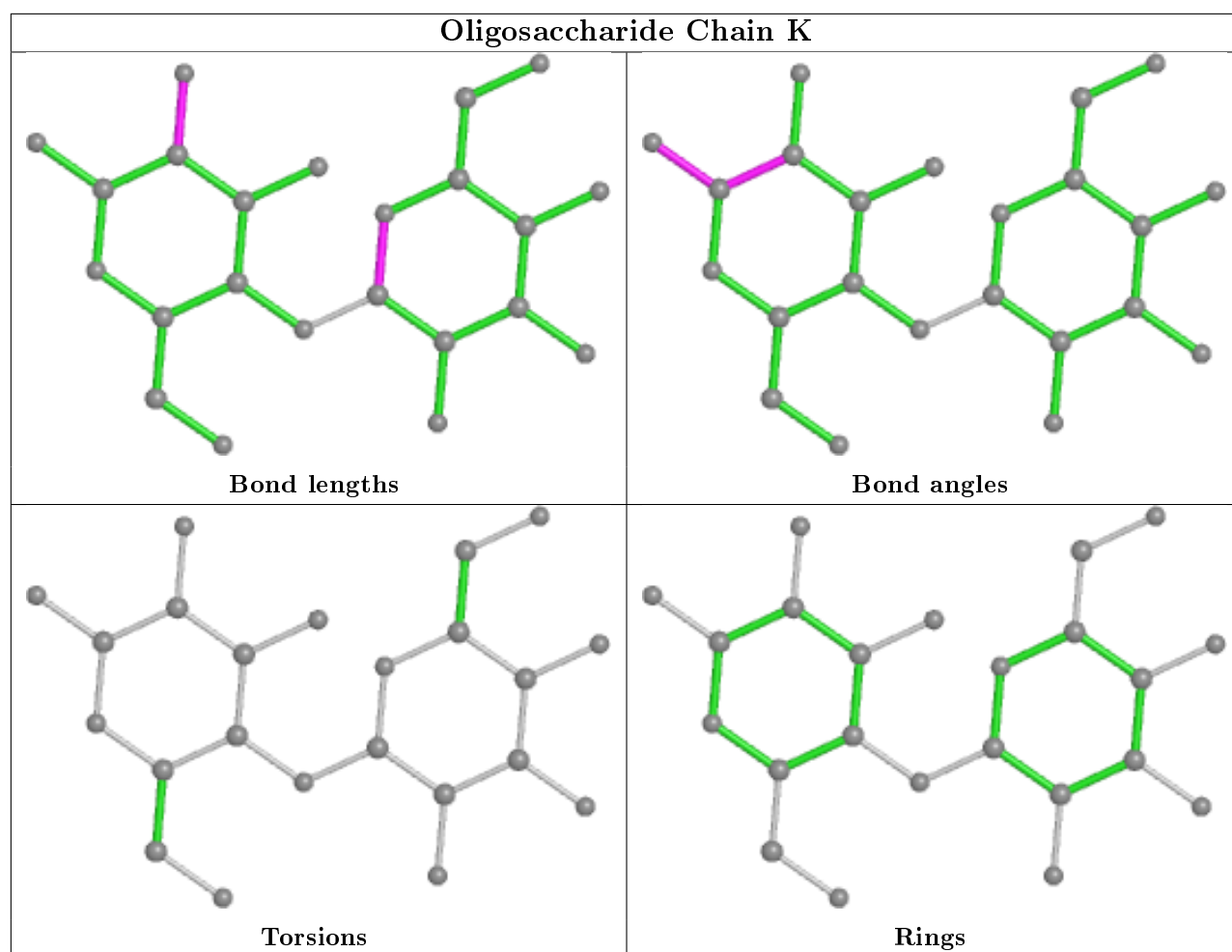


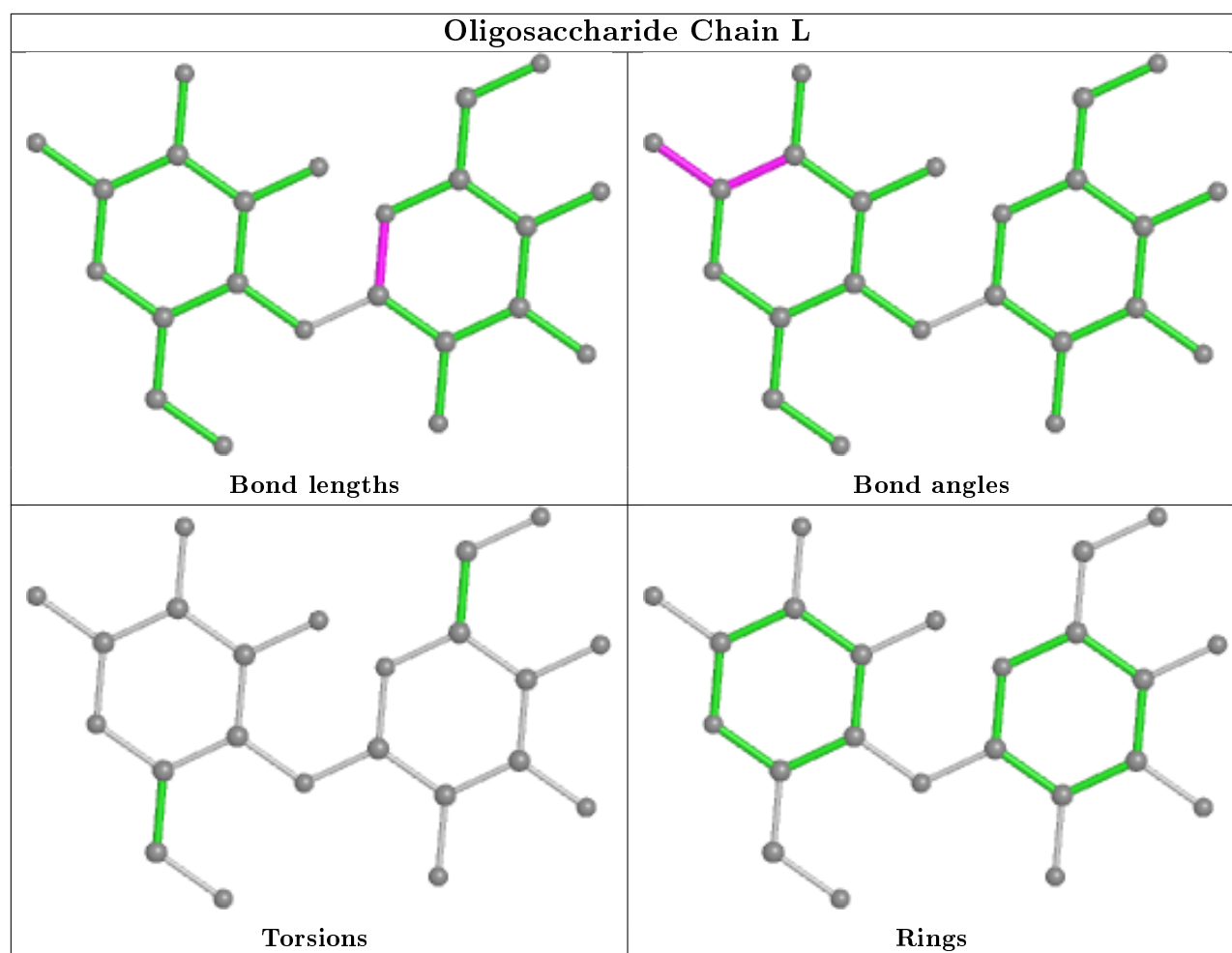












## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\# Z  > 2$
5	GOL	B	201	-	5,5,5	0.37	0	5,5,5	0.66	0
5	GOL	F	202	-	5,5,5	0.33	0	5,5,5	0.76	0
4	SO4	A	202	-	4,4,4	0.18	0	6,6,6	0.13	0
5	GOL	A	204	3	5,5,5	0.98	0	5,5,5	1.05	0
5	GOL	A	203	-	5,5,5	0.33	0	5,5,5	0.45	0
4	SO4	E	201	-	4,4,4	0.13	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	E	202	-	5,5,5	0.41	0	5,5,5	0.60	0
5	GOL	C	202	-	5,5,5	0.71	0	5,5,5	1.22	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
5	GOL	B	201	-	-	0/4/4/4	-
5	GOL	F	202	-	-	0/4/4/4	-
5	GOL	A	204	3	-	0/4/4/4	-
5	GOL	A	203	-	-	0/4/4/4	-
5	GOL	E	202	-	-	2/4/4/4	-
5	GOL	C	202	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	202	GOL	C3-C2-C1	-2.39	102.41	111.70

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	202	GOL	O1-C1-C2-C3
5	E	202	GOL	O1-C1-C2-O2

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 [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	134/134 (100%)	0.00	1 (0%) 87 86	13, 18, 31, 46	0
1	B	134/134 (100%)	0.13	1 (0%) 87 86	14, 20, 36, 49	0
1	C	134/134 (100%)	0.01	4 (2%) 50 49	15, 19, 35, 45	0
1	D	134/134 (100%)	0.02	3 (2%) 62 61	14, 19, 36, 48	0
1	E	134/134 (100%)	0.03	5 (3%) 41 41	14, 19, 34, 48	0
1	F	134/134 (100%)	-0.12	2 (1%) 73 72	13, 18, 31, 43	0
All	All	804/804 (100%)	0.01	16 (1%) 65 65	13, 19, 35, 49	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ALA	7.5
1	A	2	ALA	5.9
1	C	2	ALA	5.5
1	E	2	ALA	5.4
1	D	2	ALA	5.4

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

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

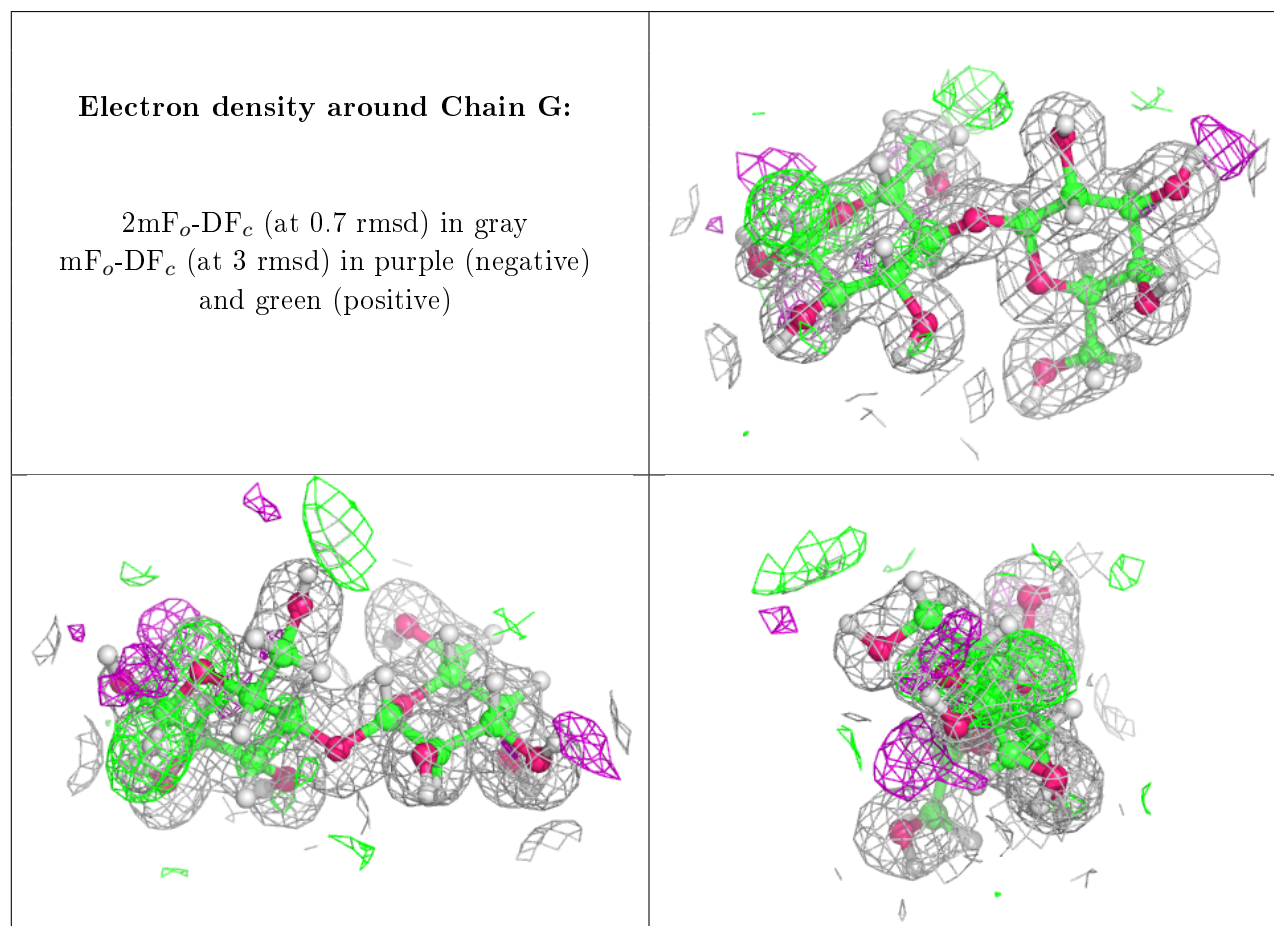
### 6.3 Carbohydrates [i](#)

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.



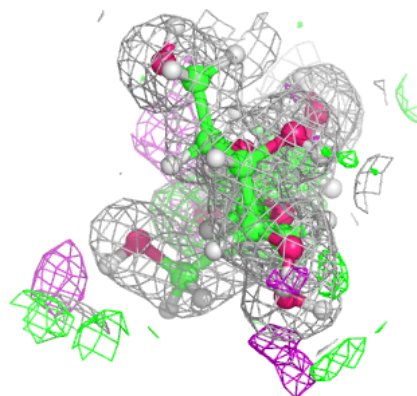
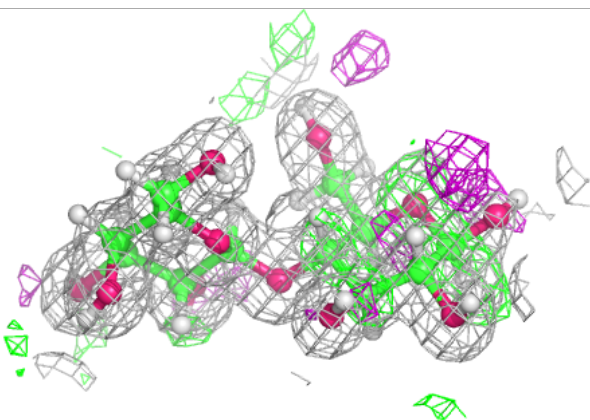
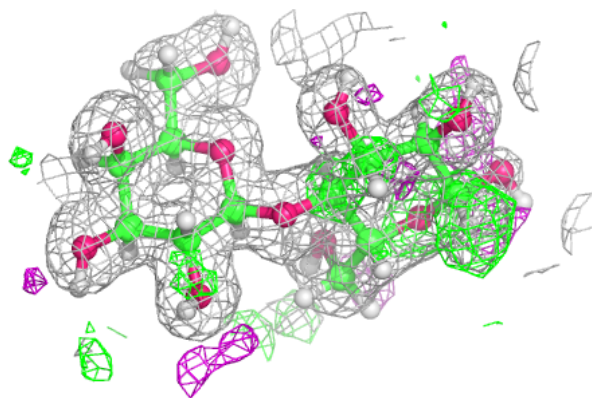
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	H	1	12/12	0.81	0.13	14,22,58,67	0
2	BGC	J	1	12/12	0.81	0.13	15,22,61,72	0
2	BGC	G	1	12/12	0.84	0.12	16,22,74,89	0
2	BGC	I	1	12/12	0.85	0.12	16,22,68,84	0
2	BGC	L	1	12/12	0.85	0.13	13,20,75,90	0
2	BGC	K	1	12/12	0.87	0.12	16,21,76,91	0
2	GAL	J	2	11/12	0.98	0.06	15,18,20,23	0
2	GAL	H	2	11/12	0.98	0.05	14,17,20,22	0
2	GAL	I	2	11/12	0.98	0.05	15,18,19,21	0
2	GAL	K	2	11/12	0.98	0.06	15,18,19,22	0
2	GAL	G	2	11/12	0.98	0.05	13,16,18,22	0
2	GAL	L	2	11/12	0.98	0.05	13,16,17,21	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.



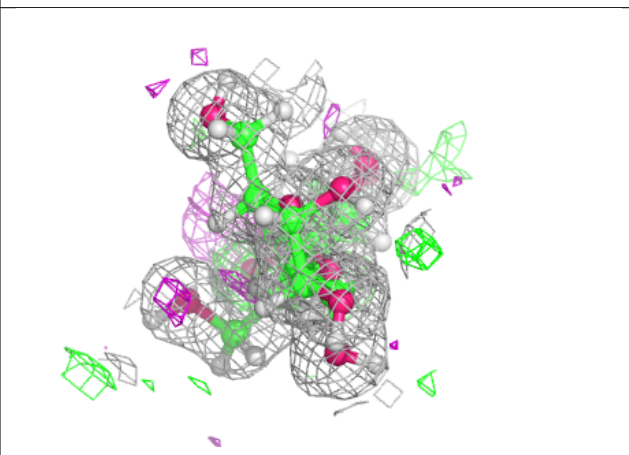
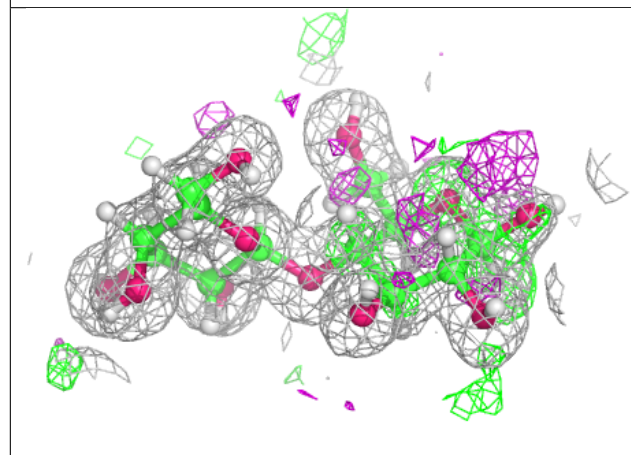
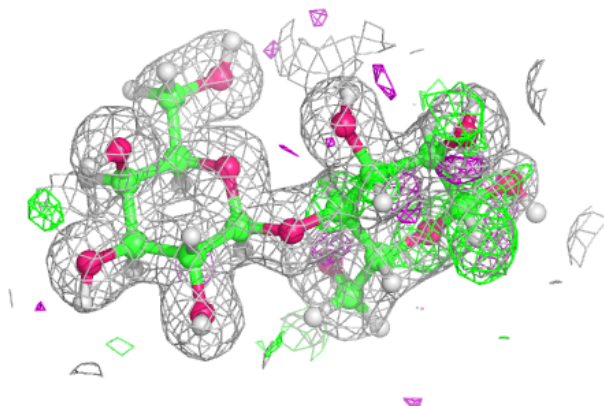
**Electron density around Chain H:**

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



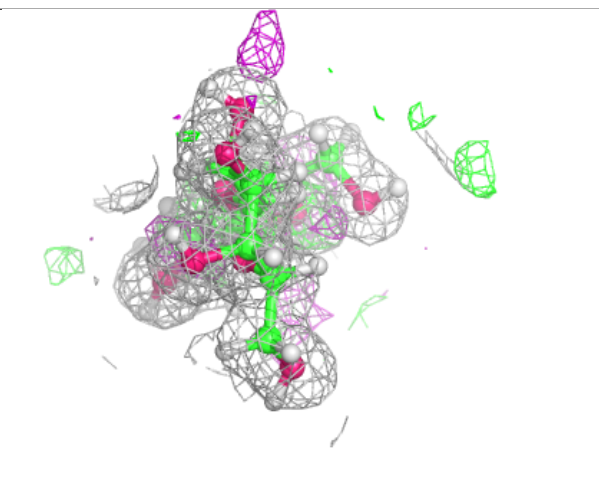
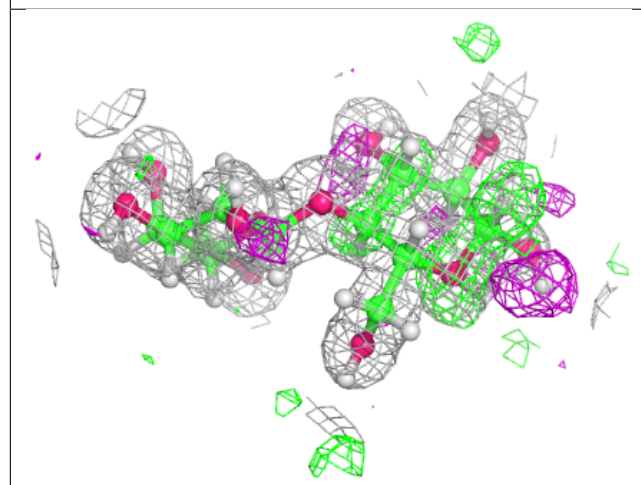
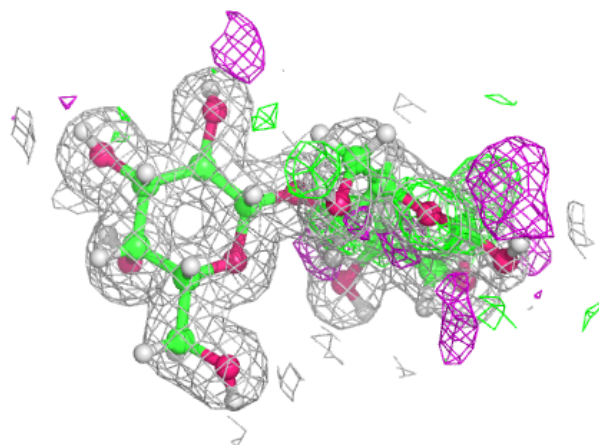
**Electron density around Chain I:**

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



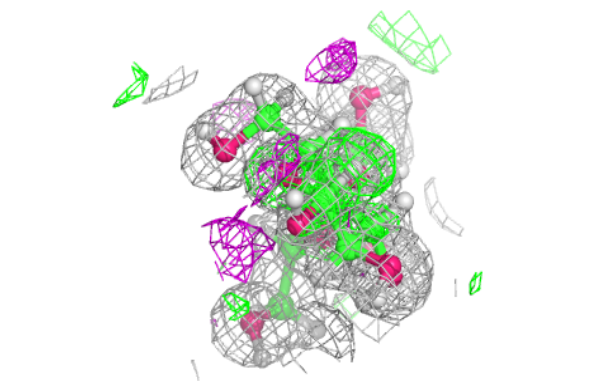
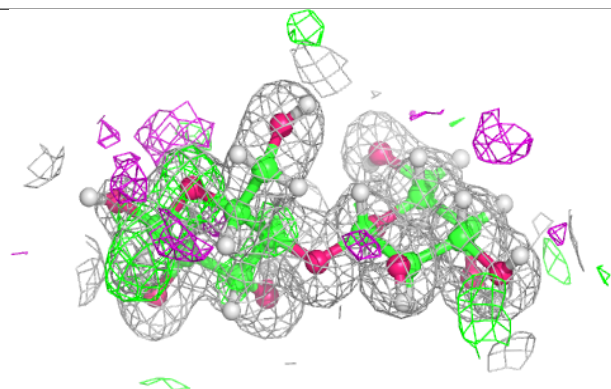
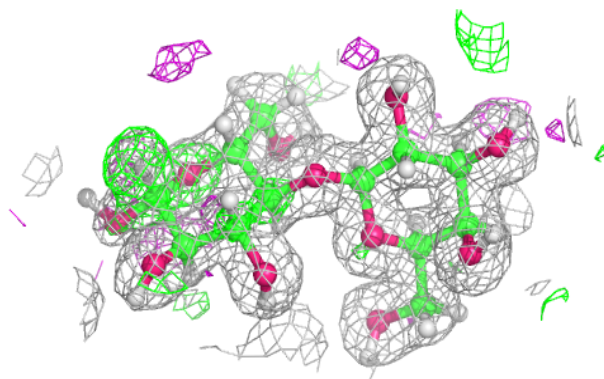
**Electron density around Chain J:**

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

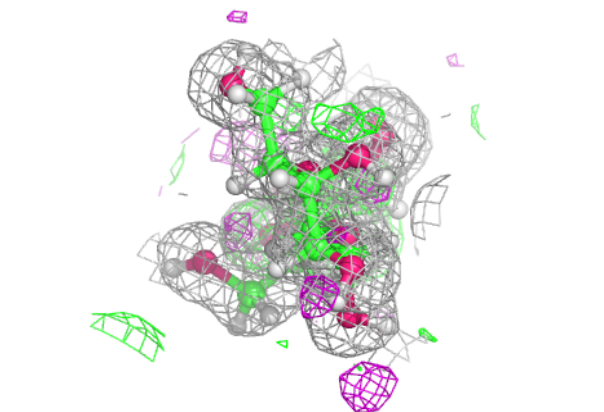
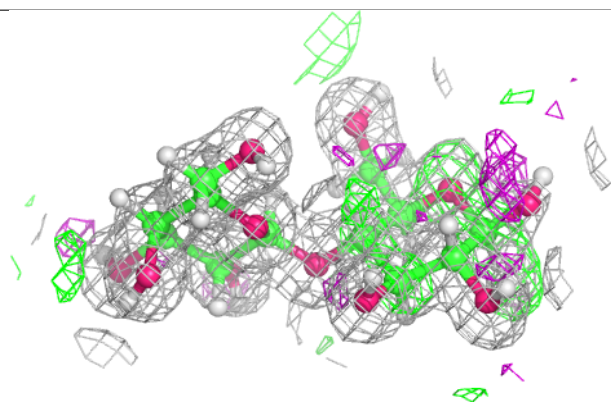
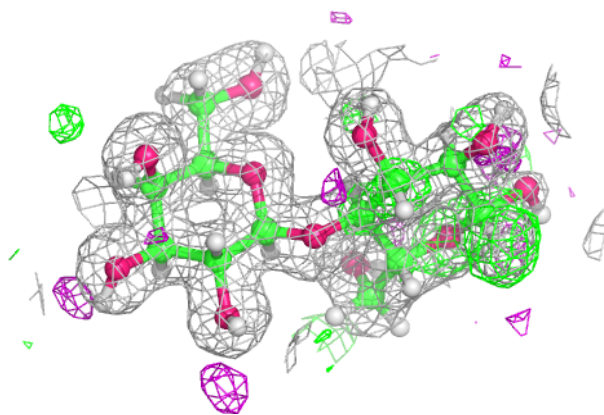


**Electron density around Chain K:**

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

**Electron density around Chain L:**

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





## 6.4 Ligands [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
3	MG	C	201	1/1	0.80	0.43	65,65,65,65	0
5	GOL	C	202	6/6	0.86	0.13	29,49,65,65	0
3	MG	F	201	1/1	0.87	0.71	76,76,76,76	0
5	GOL	A	204	6/6	0.88	0.13	31,48,63,64	0
5	GOL	E	202	6/6	0.89	0.12	35,44,63,63	0
5	GOL	F	202	6/6	0.89	0.12	26,41,49,58	0
5	GOL	B	201	6/6	0.89	0.11	24,36,46,46	0
5	GOL	A	203	6/6	0.94	0.13	22,40,56,58	0
4	SO4	A	202	5/5	0.96	0.15	21,23,25,32	5
4	SO4	E	201	5/5	0.98	0.13	41,41,59,60	0
3	MG	A	201	1/1	0.98	0.05	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.