



# wwPDB X-ray Structure Validation Summary Report

Aug 8, 2020 – 04:37 PM BST

PDB ID : 1XC6  
Title : Native Structure Of Beta-Galactosidase from Penicillium sp. in complex with Galactose  
Authors : Rojas, A.L.; Nagem, R.A.P.; Neustroev, K.N.; Arand, M.; Adamska, M.; Eneyskaya, E.V.; Kulminskaya, A.A.; Garratt, R.C.; Golubev, A.M.; Polikarpov, I.  
Deposited on : 2004-09-01  
Resolution : 2.10 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.

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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 : 2.13.1  
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

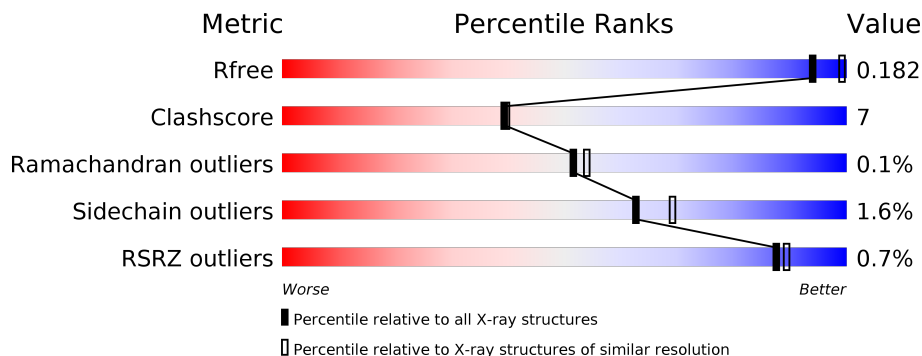
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	971	
2	B	3	
3	C	9	
4	D	2	
5	E	5	
6	F	7	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
11	IOD	A	9022	-	-	X	-
11	IOD	A	9056	-	-	X	-
11	IOD	A	9058	-	-	X	-
11	IOD	A	9059	-	-	X	-

## 2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 8894 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 Beta-Galactosidase.

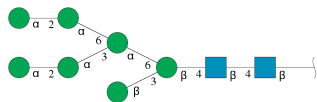
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	971	7484	4776	1241	1457	10	24	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	105	58	2	45	0	0	0

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



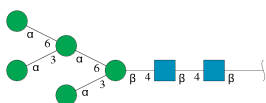
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	5	61	34	2	25	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



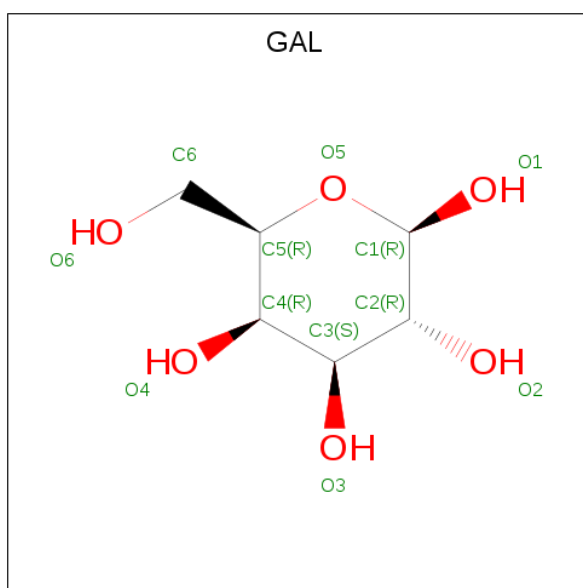
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	F	7	83	46	2	35	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is beta-D-galactopyranose (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).

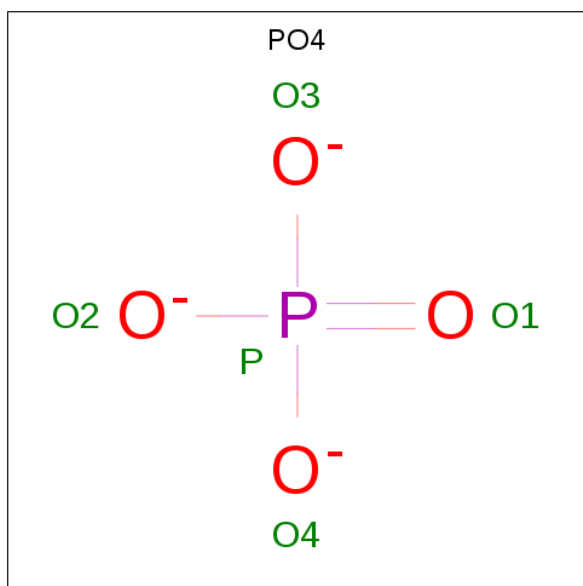


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O		
			12	6	6	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Na 1 1	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

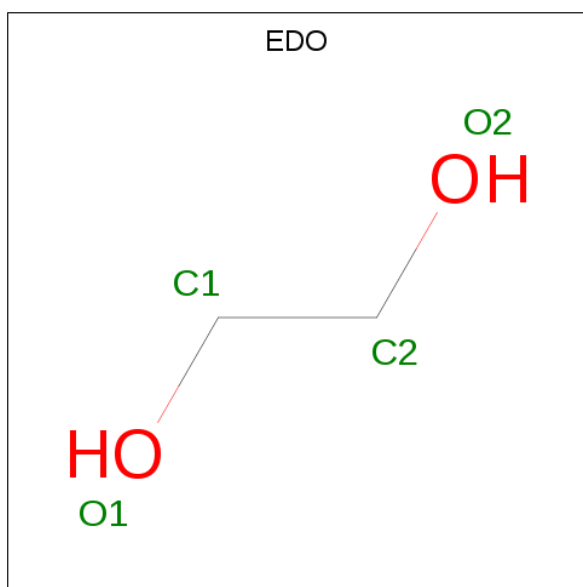


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total O P 5 4 1	0	0

- Molecule 11 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	52	Total I 52 52	0	0

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 13 is water.

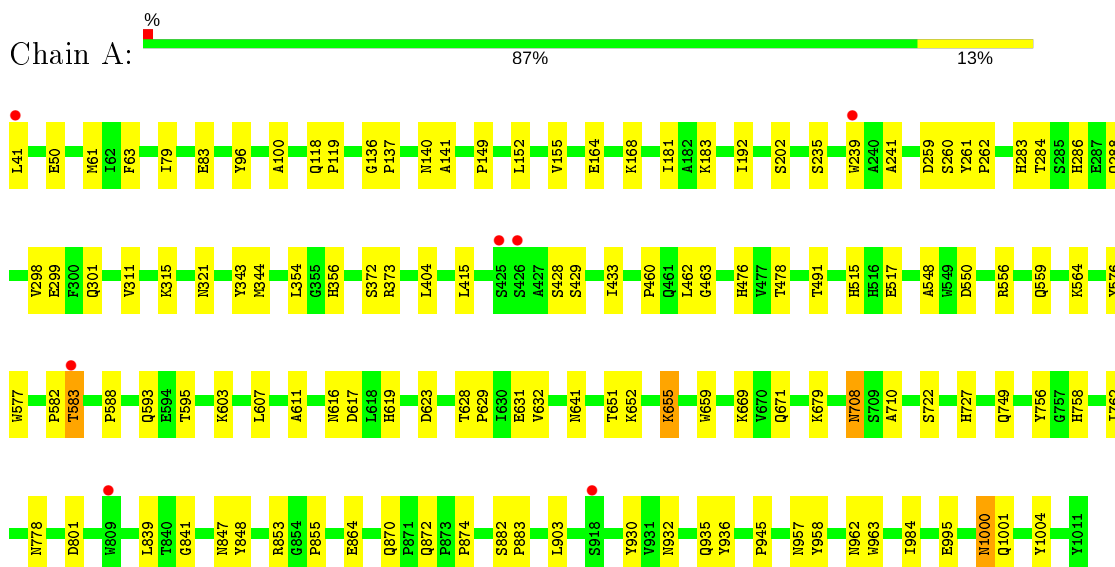
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	952	Total O 952 952	0	0



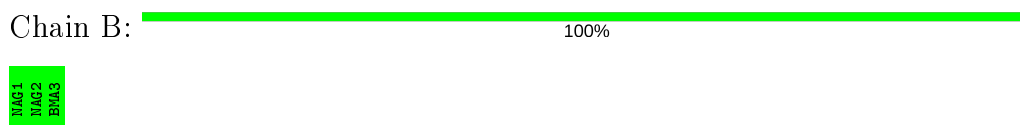
### 3 Residue-property plots

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: Beta-Galactosidase




- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain D:  100%

MAG1  
MAG2

● Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  20% 60% 20%

MAG1  
MAG2  
BGLU3  
MAN14  
MAN15

● Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  57% 43%

MAG1  
MAG2  
BGLU3  
MAN14  
MAN15  
MAN16  
MAN17

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.96Å 110.96Å 161.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.40 – 2.10 110.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.40-2.10) 99.9 (110.96-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.10Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.171 , 0.186 0.167 , 0.182	Depositor DCC
$R_{free}$ test set	2249 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtrriage
Anisotropy	0.227	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 71.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: BMA, NAG, NA, PO4, EDO, GAL, IOD, MAN

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	0.33	0/7698	0.62	1/10501 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	841	GLY	N-CA-C	-5.02	100.55	113.10

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	7484	0	7126	98	0
2	B	39	0	34	0	0
3	C	105	0	88	2	0
4	D	28	0	25	2	0
5	E	61	0	52	5	0
6	F	83	0	70	3	0
7	A	28	0	26	1	0
8	A	12	0	12	1	0
9	A	1	0	0	0	0
10	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	52	0	0	25	0
12	A	44	0	66	0	0
13	A	952	0	0	23	0
All	All	8894	0	7499	114	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 7.

The worst 5 of 114 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:299:GLU:OE1	8:A:9011:GAL:H1	1.60	1.02
1:A:778:ASN:HD21	5:E:1:NAG:HN2	1.24	0.83
1:A:462:LEU:HB2	11:A:9056:IOD:I	2.50	0.81
11:A:9034:IOD:I	11:A:9058:IOD:I	3.43	0.77
1:A:515:HIS:HE1	11:A:9056:IOD:I	2.38	0.76

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	969/971 (100%)	940 (97%)	28 (3%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ASN

### 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	795/795 (100%)	782 (98%)	13 (2%)	62 69

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	655	LYS
1	A	708	ASN
1	A	936	TYR
1	A	583	THR
1	A	935	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	708	ASN
1	A	778	ASN
1	A	959	HIS
1	A	621	GLN
1	A	985	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](#)

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

## 5.5 Carbohydrates [i](#)

26 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	NAG	B	1	1,2	14,14,15	0.58	0	17,19,21	0.73	0
2	NAG	B	2	2	14,14,15	0.59	0	17,19,21	0.60	0
2	BMA	B	3	2	11,11,12	0.45	0	15,15,17	0.28	0
3	NAG	C	1	1,3	14,14,15	0.57	0	17,19,21	0.64	0
3	NAG	C	2	3	14,14,15	0.55	0	17,19,21	0.64	0
3	BMA	C	3	3	11,11,12	0.58	0	15,15,17	0.40	0
3	MAN	C	4	3	11,11,12	0.47	0	15,15,17	0.70	1 (6%)
3	MAN	C	5	3	11,11,12	0.48	0	15,15,17	0.54	0
3	MAN	C	6	3	11,11,12	0.46	0	15,15,17	0.58	0
3	MAN	C	7	3	11,11,12	0.50	0	15,15,17	0.67	1 (6%)
3	MAN	C	8	3	11,11,12	0.48	0	15,15,17	0.62	1 (6%)
3	BMA	C	9	3	11,11,12	0.59	0	15,15,17	1.01	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.56	0	17,19,21	0.72	1 (5%)
4	NAG	D	2	4	14,14,15	0.47	0	17,19,21	0.65	0
5	NAG	E	1	1,5	14,14,15	0.46	0	17,19,21	0.65	0
5	NAG	E	2	5	14,14,15	0.48	0	17,19,21	0.70	1 (5%)
5	BMA	E	3	5	11,11,12	0.45	0	15,15,17	0.35	0
5	MAN	E	4	5	11,11,12	0.54	0	15,15,17	0.53	0
5	MAN	E	5	5	11,11,12	0.48	0	15,15,17	0.56	0
6	NAG	F	1	1,9,6	14,14,15	0.54	0	17,19,21	0.67	0
6	NAG	F	2	6	14,14,15	0.55	0	17,19,21	0.67	0
6	BMA	F	3	6	11,11,12	0.52	0	15,15,17	0.40	0
6	MAN	F	4	6	11,11,12	0.52	0	15,15,17	0.69	1 (6%)
6	MAN	F	5	6	11,11,12	0.52	0	15,15,17	0.44	0
6	MAN	F	6	6	11,11,12	0.54	0	15,15,17	0.51	0
6	MAN	F	7	6	11,11,12	0.46	0	15,15,17	0.53	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	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
3	MAN	C	7	3	-	0/2/19/22	0/1/1/1
3	MAN	C	8	3	-	0/2/19/22	0/1/1/1
3	BMA	C	9	3	-	0/2/19/22	1/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	2/2/19/22	0/1/1/1
6	NAG	F	1	1,9,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	0/2/19/22	0/1/1/1
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	MAN	F	6	6	-	2/2/19/22	0/1/1/1
6	MAN	F	7	6	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	9	BMA	C1-O5-C5	3.21	116.55	112.19
3	C	4	MAN	C1-O5-C5	2.16	115.11	112.19
5	E	2	NAG	C2-N2-C7	-2.11	119.90	122.90
4	D	1	NAG	C2-N2-C7	-2.11	119.90	122.90
6	F	4	MAN	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
6	F	6	MAN	O5-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
5	E	5	MAN	O5-C5-C6-O6
5	E	5	MAN	C4-C5-C6-O6
4	D	2	NAG	O7-C7-N2-C2

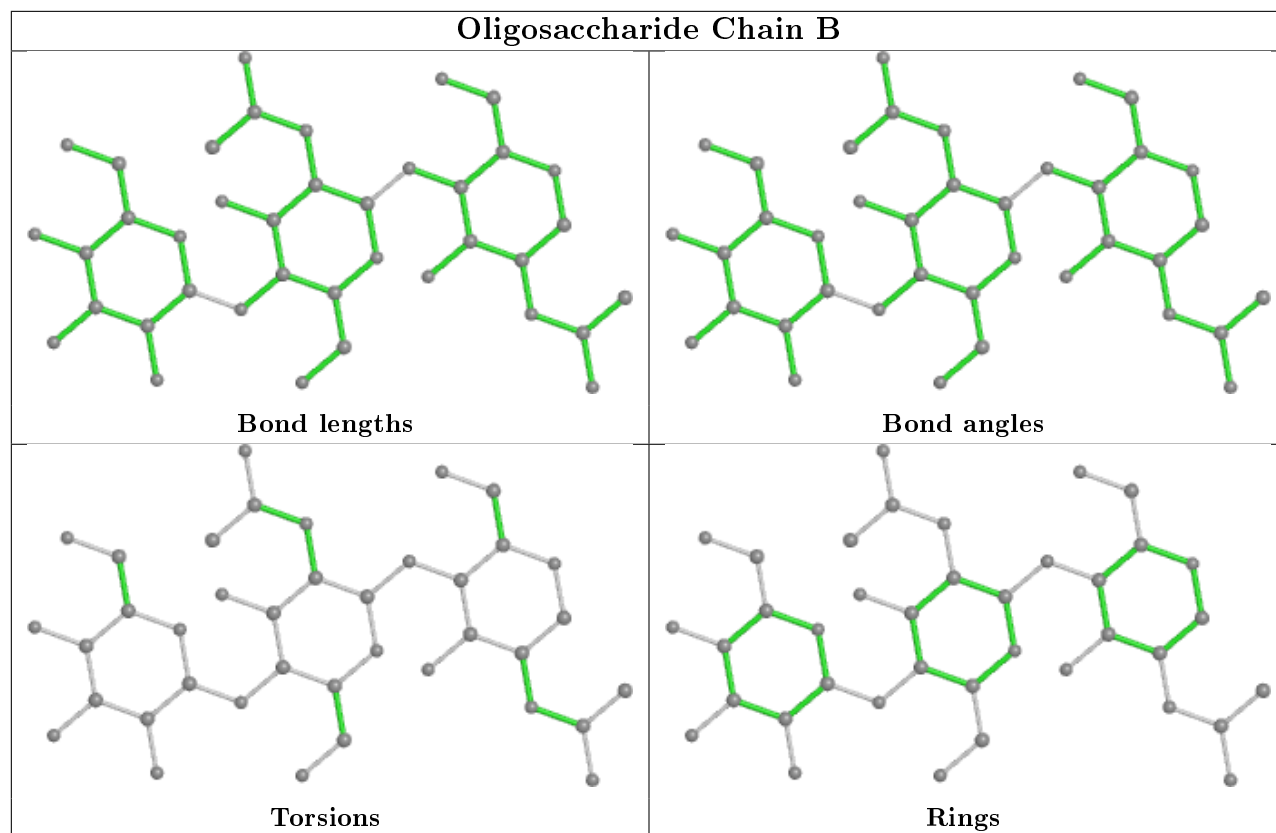
All (1) ring outliers are listed below:

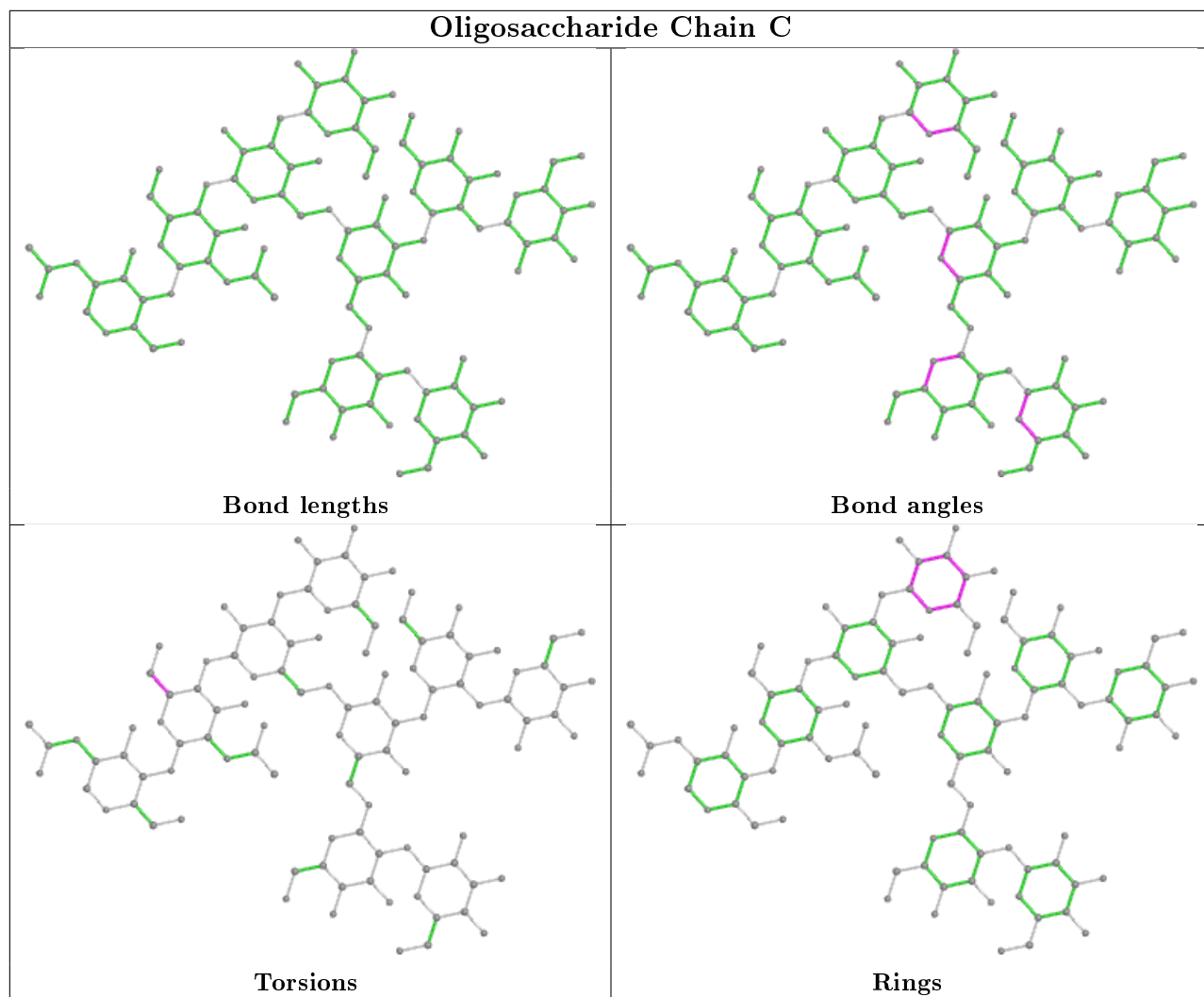
Mol	Chain	Res	Type	Atoms
3	C	9	BMA	C1-C2-C3-C4-C5-O5

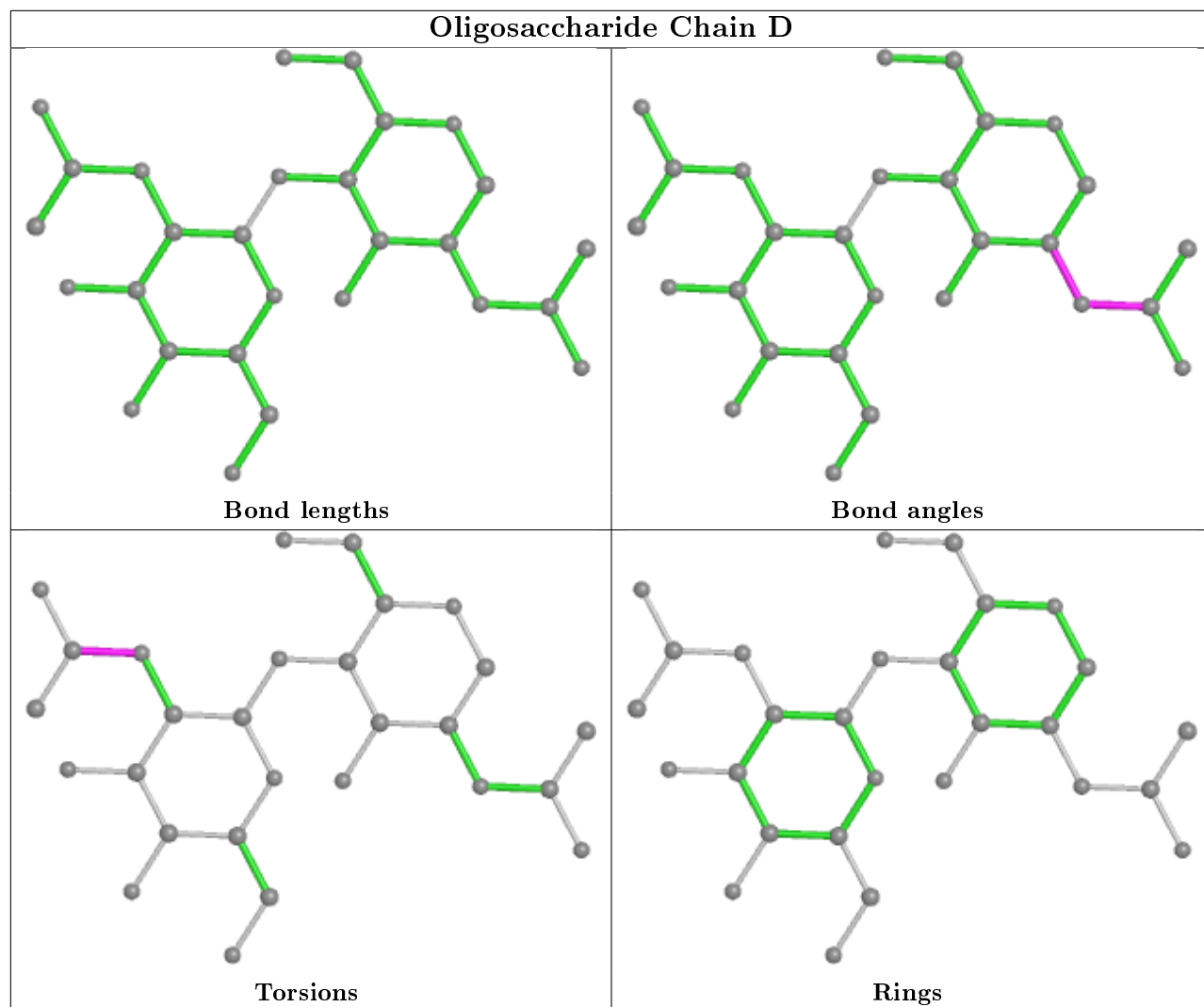
10 monomers are involved in 12 short contacts:

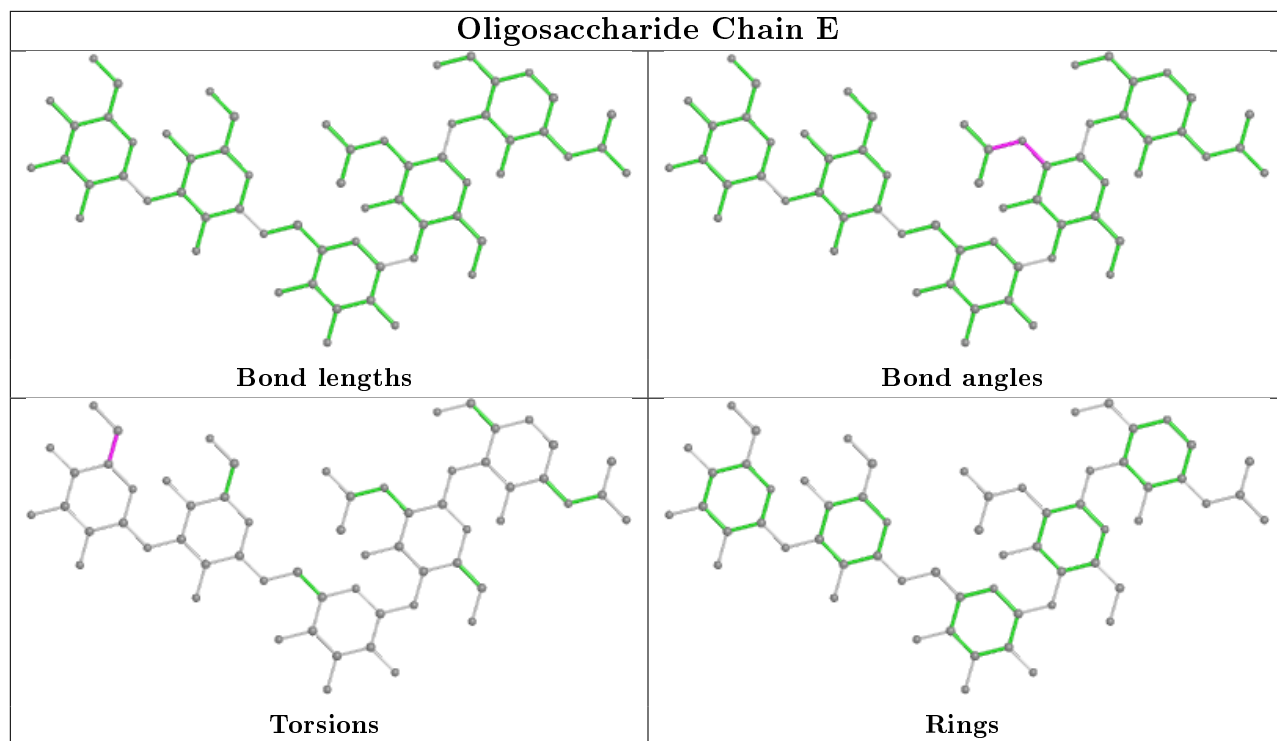
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	2	0
3	C	2	NAG	1	0
4	D	2	NAG	2	0
6	F	6	MAN	2	0
5	E	4	MAN	1	0
3	C	9	BMA	1	0
6	F	7	MAN	1	0
3	C	3	BMA	1	0
5	E	5	MAN	1	0
5	E	2	NAG	2	0

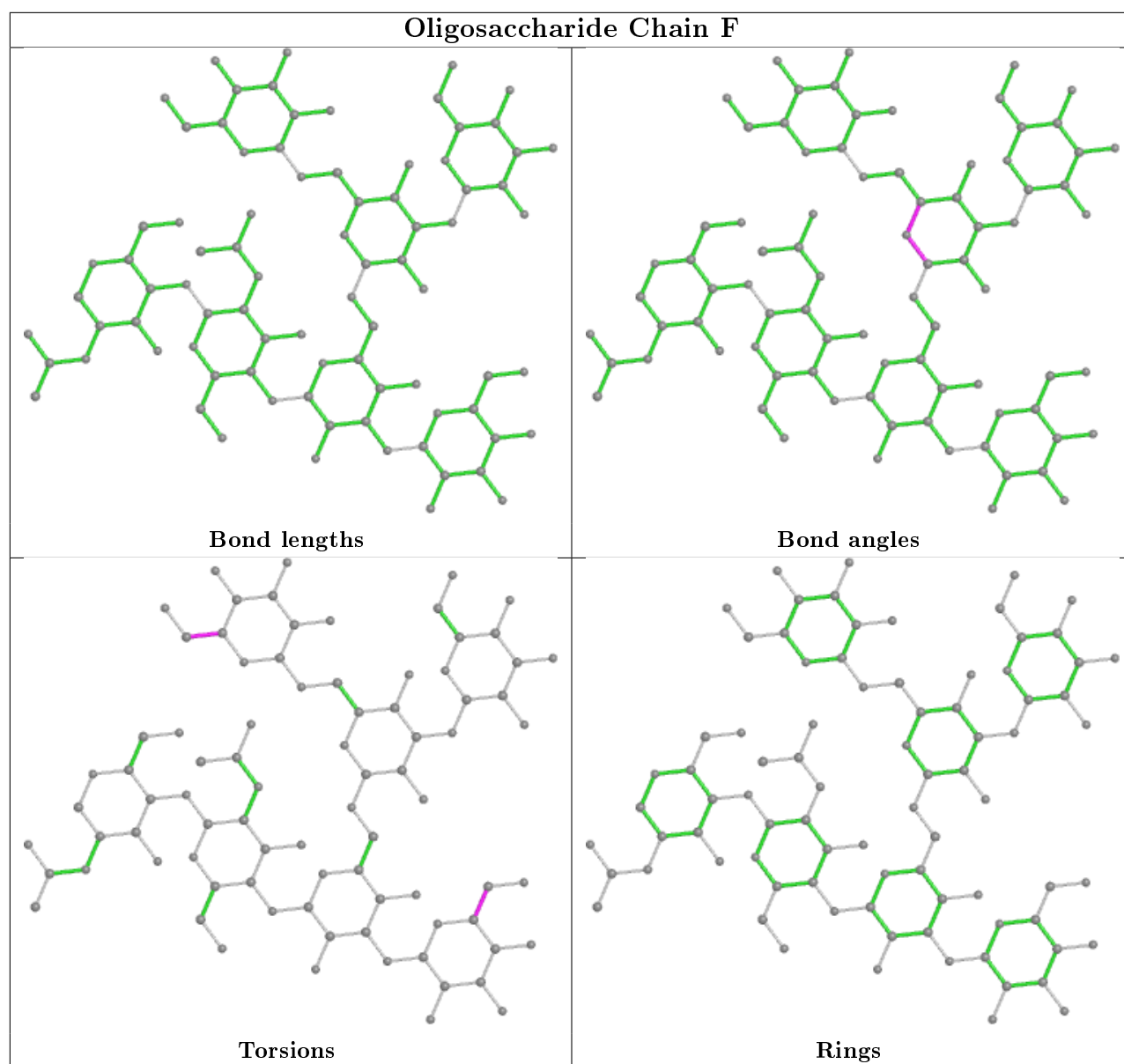
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 53 are monoatomic - leaving 15 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
12	EDO	A	9002	-	3,3,3	0.55	0	2,2,2	0.42	0
8	GAL	A	9011	-	12,12,12	0.39	0	17,17,17	0.39	0
12	EDO	A	9007	-	3,3,3	0.59	0	2,2,2	0.44	0
10	PO4	A	8002	-	4,4,4	1.68	0	6,6,6	0.43	0
12	EDO	A	9003	-	3,3,3	0.57	0	2,2,2	0.43	0
7	NAG	A	4001	1	14,14,15	0.48	0	17,19,21	0.64	0
12	EDO	A	9081	-	3,3,3	0.58	0	2,2,2	0.43	0
12	EDO	A	9004	-	3,3,3	0.54	0	2,2,2	0.42	0
12	EDO	A	9005	-	3,3,3	0.66	0	2,2,2	0.42	0
12	EDO	A	9001	-	3,3,3	0.56	0	2,2,2	0.43	0
7	NAG	A	2001	1	14,14,15	0.49	0	17,19,21	0.60	0
12	EDO	A	9008	-	3,3,3	0.71	0	2,2,2	0.46	0
12	EDO	A	9080	-	3,3,3	0.49	0	2,2,2	0.43	0
12	EDO	A	9006	-	3,3,3	0.54	0	2,2,2	0.43	0
12	EDO	A	9009	-	3,3,3	0.61	0	2,2,2	0.43	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
12	EDO	A	9002	-	-	0/1/1/1	-
8	GAL	A	9011	-	-	1/2/22/22	0/1/1/1
12	EDO	A	9007	-	-	0/1/1/1	-
12	EDO	A	9080	-	-	0/1/1/1	-
12	EDO	A	9003	-	-	0/1/1/1	-
7	NAG	A	4001	1	-	0/6/23/26	0/1/1/1
12	EDO	A	9081	-	-	0/1/1/1	-
12	EDO	A	9004	-	-	0/1/1/1	-
12	EDO	A	9005	-	-	0/1/1/1	-
12	EDO	A	9001	-	-	0/1/1/1	-
7	NAG	A	2001	1	-	5/6/23/26	0/1/1/1
12	EDO	A	9008	-	-	0/1/1/1	-
12	EDO	A	9006	-	-	0/1/1/1	-
12	EDO	A	9009	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2001	NAG	C8-C7-N2-C2
7	A	2001	NAG	O7-C7-N2-C2
7	A	2001	NAG	C4-C5-C6-O6
7	A	2001	NAG	O5-C5-C6-O6
8	A	9011	GAL	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	9011	GAL	1	0
7	A	2001	NAG	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	971/971 (100%)	-0.37	7 (0%) 87   89	7, 18, 34, 51	18 (1%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	SER	4.0
1	A	41	LEU	3.2
1	A	809	TRP	3.1
1	A	239	TRP	3.0
1	A	918	SER	2.9

### 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(Å <sup>2</sup> )	Q<0.9
4	NAG	D	2	14/15	0.68	0.27	49,52,55,55	14
2	BMA	B	3	11/12	0.68	0.29	51,57,59,60	0
3	BMA	C	9	11/12	0.71	0.24	41,47,51,52	0
5	MAN	E	5	11/12	0.77	0.23	48,49,51,51	11
3	MAN	C	8	11/12	0.80	0.13	35,37,37,38	11
5	BMA	E	3	11/12	0.80	0.17	44,47,49,50	0
5	MAN	E	4	11/12	0.83	0.19	43,46,47,49	11

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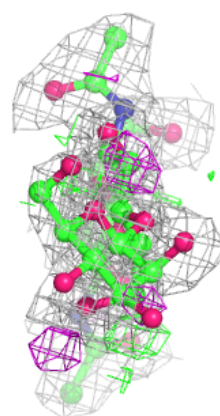
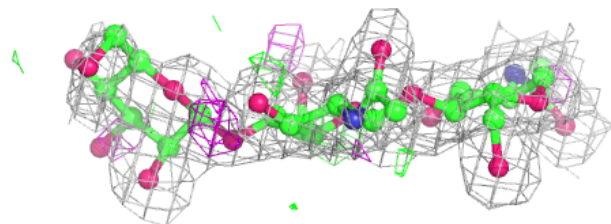
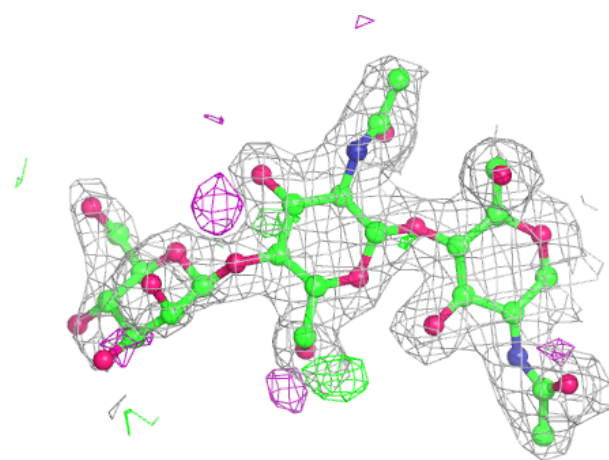
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MAN	F	6	11/12	0.85	0.20	36,41,43,43	0
3	MAN	C	7	11/12	0.85	0.16	22,30,33,34	11
5	NAG	E	2	14/15	0.86	0.21	41,46,49,50	0
6	MAN	F	5	11/12	0.92	0.12	30,33,35,37	0
2	NAG	B	2	14/15	0.93	0.13	24,31,40,44	0
4	NAG	D	1	14/15	0.93	0.13	37,41,45,47	0
5	NAG	E	1	14/15	0.94	0.12	18,25,35,35	0
3	NAG	C	2	14/15	0.94	0.10	15,17,24,32	0
3	MAN	C	6	11/12	0.94	0.12	30,32,35,36	0
6	MAN	F	7	11/12	0.95	0.11	25,29,33,39	0
6	MAN	F	4	11/12	0.95	0.10	21,23,29,30	0
6	NAG	F	1	14/15	0.96	0.11	14,17,22,31	0
3	NAG	C	1	14/15	0.97	0.10	14,18,27,27	0
3	MAN	C	5	11/12	0.97	0.09	16,21,23,26	0
3	MAN	C	4	11/12	0.97	0.10	19,20,23,27	0
6	NAG	F	2	14/15	0.97	0.10	12,17,23,23	0
6	BMA	F	3	11/12	0.97	0.09	16,18,20,20	0
2	NAG	B	1	14/15	0.97	0.11	15,19,20,23	0
3	BMA	C	3	11/12	0.98	0.10	18,20,24,32	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.

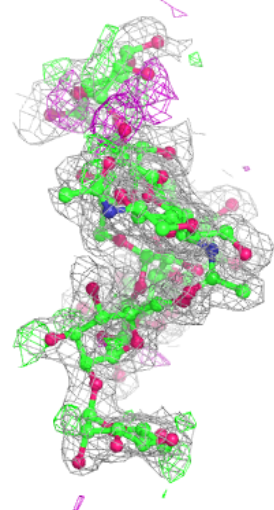
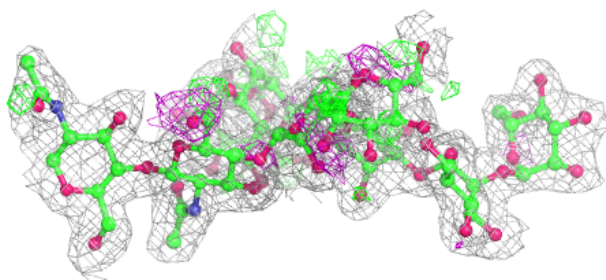
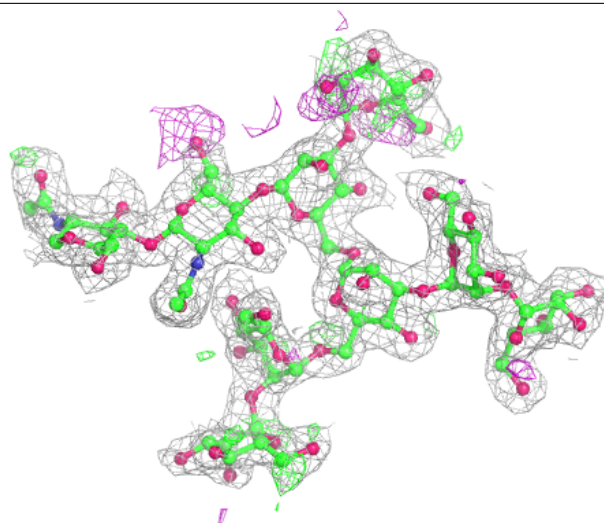
**Electron density around Chain B:**

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



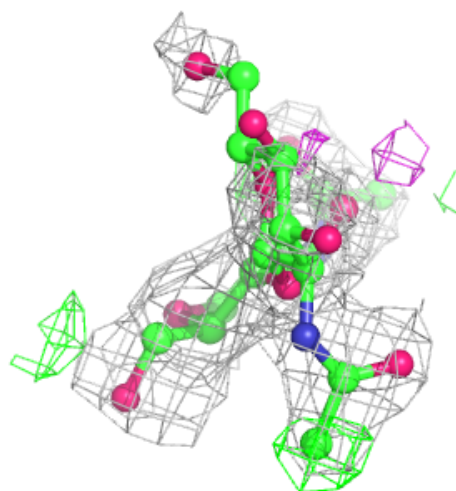
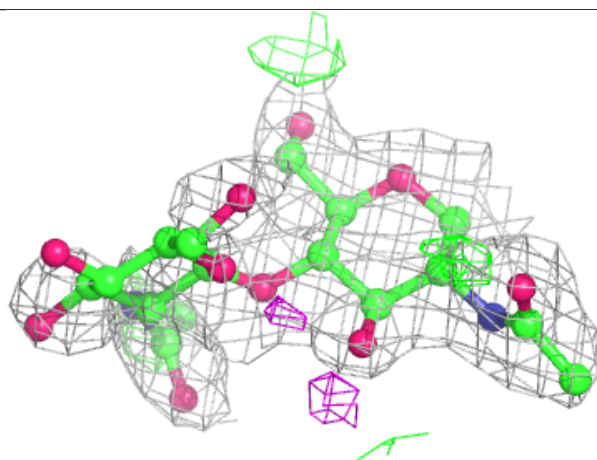
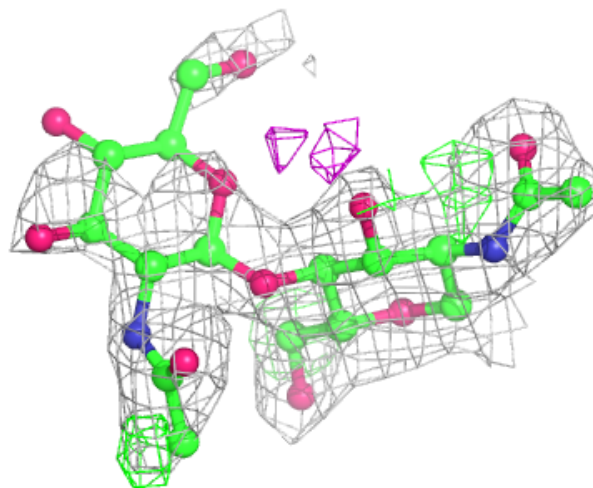
**Electron density around Chain C:**

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



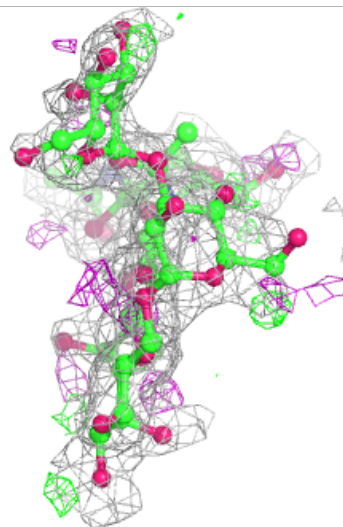
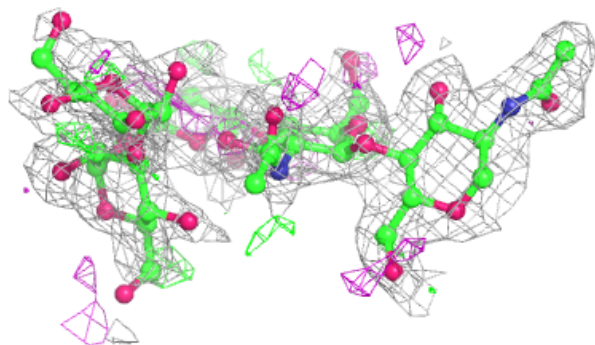
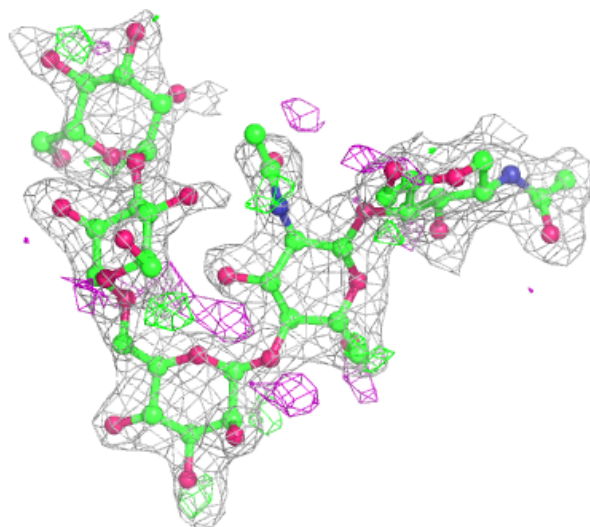
**Electron density around Chain D:**

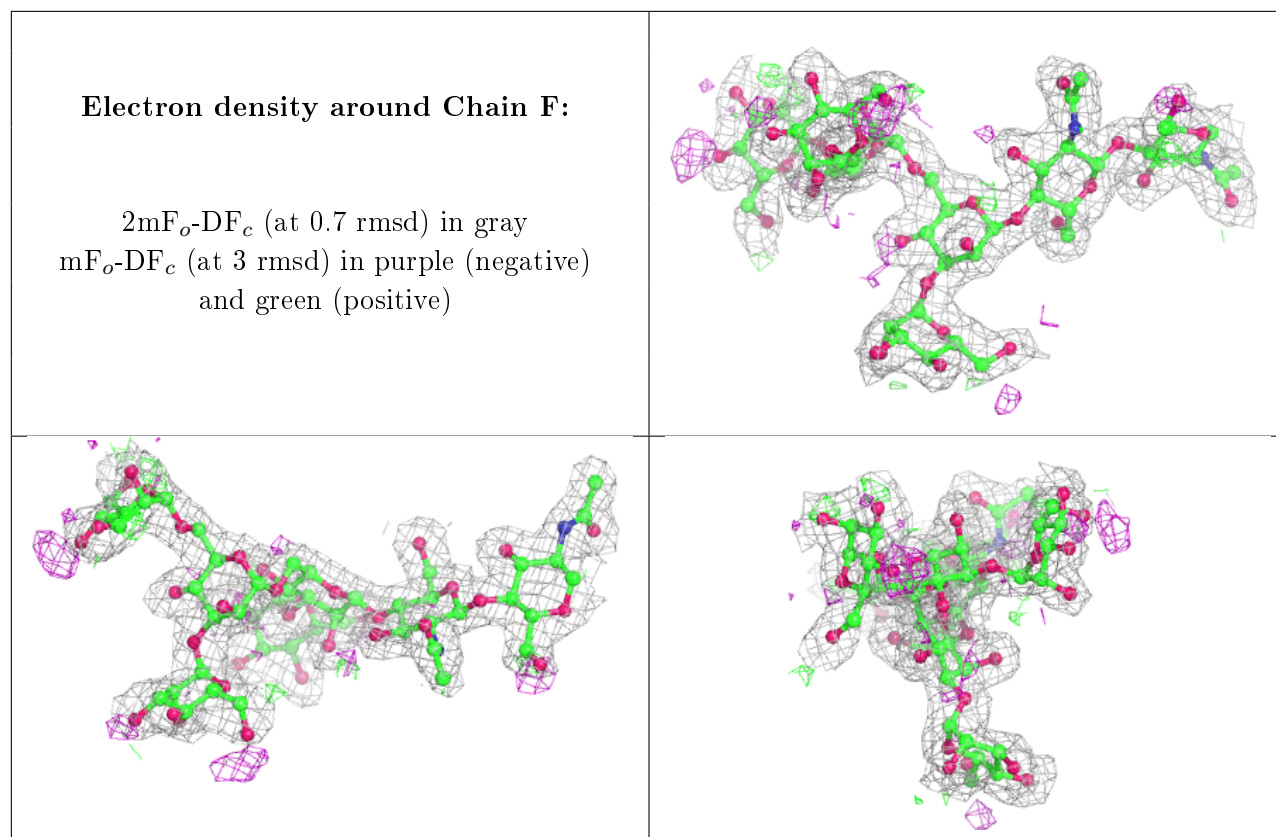
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain E:**

$2mF_o-DF_c$  (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
11	IOD	A	9070	1/1	0.70	0.20	68,68,68,68	1
11	IOD	A	9069	1/1	0.79	0.14	65,65,65,65	1
7	NAG	A	2001	14/15	0.79	0.22	56,61,65,65	0
11	IOD	A	9056	1/1	0.81	0.22	79,79,79,79	1
12	EDO	A	9007	4/4	0.86	0.22	36,42,44,47	0
9	NA	A	8001	1/1	0.87	0.12	40,40,40,40	0
11	IOD	A	9058	1/1	0.88	0.15	58,58,58,58	1
11	IOD	A	9060	1/1	0.88	0.21	59,59,59,59	1
11	IOD	A	9072	1/1	0.88	0.15	65,65,65,65	1
11	IOD	A	9048	1/1	0.89	0.15	66,66,66,66	1
12	EDO	A	9005	4/4	0.90	0.15	30,34,35,36	0
11	IOD	A	9028	1/1	0.90	0.10	47,47,47,47	1
11	IOD	A	9045	1/1	0.90	0.07	61,61,61,61	1
11	IOD	A	9063	1/1	0.90	0.41	67,67,67,67	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	PO4	A	8002	5/5	0.91	0.20	57,57,58,58	5
12	EDO	A	9006	4/4	0.91	0.17	38,39,39,42	0
7	NAG	A	4001	14/15	0.92	0.12	29,33,39,42	0
11	IOD	A	9051	1/1	0.92	0.09	62,62,62,62	1
11	IOD	A	9061	1/1	0.92	0.13	64,64,64,64	1
12	EDO	A	9081	4/4	0.92	0.18	33,36,39,40	0
11	IOD	A	9022	1/1	0.93	0.12	27,27,27,27	1
11	IOD	A	9066	1/1	0.93	0.07	72,72,72,72	1
8	GAL	A	9011	12/12	0.93	0.15	13,18,23,25	0
12	EDO	A	9003	4/4	0.93	0.17	44,44,44,46	0
11	IOD	A	9037	1/1	0.93	0.07	47,47,47,47	1
11	IOD	A	9068	1/1	0.94	0.14	67,67,67,67	1
12	EDO	A	9080	4/4	0.94	0.15	17,20,22,24	0
11	IOD	A	9035	1/1	0.94	0.09	50,50,50,50	1
11	IOD	A	9067	1/1	0.94	0.06	67,67,67,67	1
11	IOD	A	9062	1/1	0.94	0.10	59,59,59,59	1
11	IOD	A	9071	1/1	0.95	0.08	75,75,75,75	1
11	IOD	A	9049	1/1	0.95	0.16	47,47,47,47	1
11	IOD	A	9050	1/1	0.95	0.06	68,68,68,68	1
12	EDO	A	9004	4/4	0.95	0.21	30,30,31,31	0
12	EDO	A	9002	4/4	0.95	0.11	25,26,27,27	0
11	IOD	A	9059	1/1	0.95	0.16	58,58,58,58	1
11	IOD	A	9064	1/1	0.96	0.24	57,57,57,57	1
11	IOD	A	9046	1/1	0.96	0.12	45,45,45,45	1
11	IOD	A	9057	1/1	0.96	0.10	69,69,69,69	1
11	IOD	A	9032	1/1	0.96	0.08	56,56,56,56	1
12	EDO	A	9009	4/4	0.96	0.10	25,28,29,30	0
12	EDO	A	9001	4/4	0.96	0.17	34,34,35,38	0
12	EDO	A	9008	4/4	0.97	0.10	12,17,18,19	0
11	IOD	A	9030	1/1	0.97	0.08	38,38,38,38	1
11	IOD	A	9065	1/1	0.97	0.18	56,56,56,56	1
11	IOD	A	9025	1/1	0.97	0.12	32,32,32,32	1
11	IOD	A	9039	1/1	0.97	0.10	37,37,37,37	1
11	IOD	A	9052	1/1	0.97	0.06	67,67,67,67	1
11	IOD	A	9036	1/1	0.98	0.11	40,40,40,40	1
11	IOD	A	9029	1/1	0.98	0.14	29,29,29,29	1
11	IOD	A	9026	1/1	0.98	0.12	32,32,32,32	1
11	IOD	A	9044	1/1	0.98	0.09	37,37,37,37	1
11	IOD	A	9055	1/1	0.98	0.05	68,68,68,68	1
11	IOD	A	9054	1/1	0.98	0.06	62,62,62,62	1
11	IOD	A	9027	1/1	0.98	0.10	37,37,37,37	1
11	IOD	A	9038	1/1	0.98	0.06	56,56,56,56	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	IOD	A	9053	1/1	0.98	0.12	65,65,65,65	1
11	IOD	A	9021	1/1	0.99	0.07	27,27,27,27	1
11	IOD	A	9024	1/1	0.99	0.10	29,29,29,29	1
11	IOD	A	9023	1/1	0.99	0.07	28,28,28,28	1
11	IOD	A	9047	1/1	0.99	0.11	33,33,33,33	1
11	IOD	A	9031	1/1	0.99	0.13	23,23,23,23	1
11	IOD	A	9040	1/1	0.99	0.11	43,43,43,43	1
11	IOD	A	9043	1/1	0.99	0.10	45,45,45,45	1
11	IOD	A	9033	1/1	0.99	0.12	28,28,28,28	0
11	IOD	A	9042	1/1	0.99	0.15	21,21,21,21	1
11	IOD	A	9041	1/1	0.99	0.09	29,29,29,29	1
11	IOD	A	9034	1/1	1.00	0.11	20,20,20,20	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.