



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 10, 2020 – 12:36 PM BST

PDB ID : 5O7V  
Title : Crystal structure of the 5F-tryptophan RSL lectin in complex with Lewis x tetrasaccharide  
Authors : Varrot, A.  
Deposited on : 2017-06-09  
Resolution : 1.28 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](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.dev3  
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.dev3

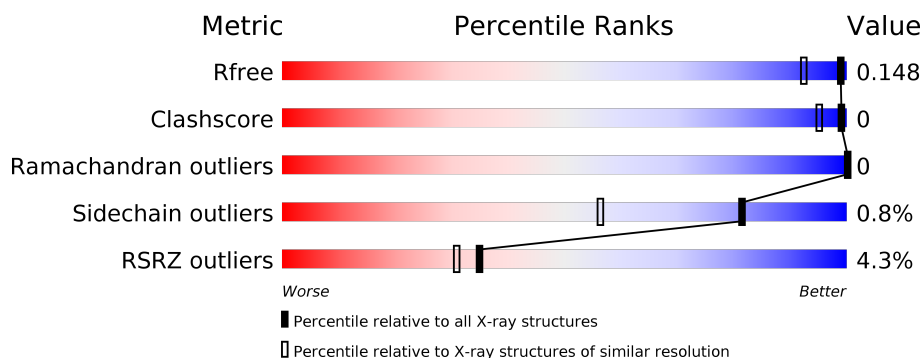
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.28 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	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (1.30-1.26)

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	90	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	B	90	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
3	D	4	<div> <div></div> <div>100%</div> </div>
3	F	4	<div> <div>25%</div> <div>75%</div> </div>
4	E	3	<div> <div>67%</div> <div>33%</div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 1747 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 Fucose-binding lectin protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	89	Total	C	F	N	O	S	0	4	0
			719	444	7	123	143	2			
1	B	89	Total	C	F	N	O	S	0	2	0
			700	433	7	119	139	2			

There are 2 discrepancies between the modelled and reference sequences:

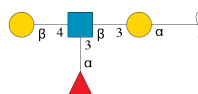
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	THR	SER	conflict	UNP A0A0S4VQ74
B	67	THR	SER	conflict	UNP A0A0S4VQ74

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



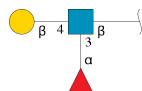
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			25	14	1	10			

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



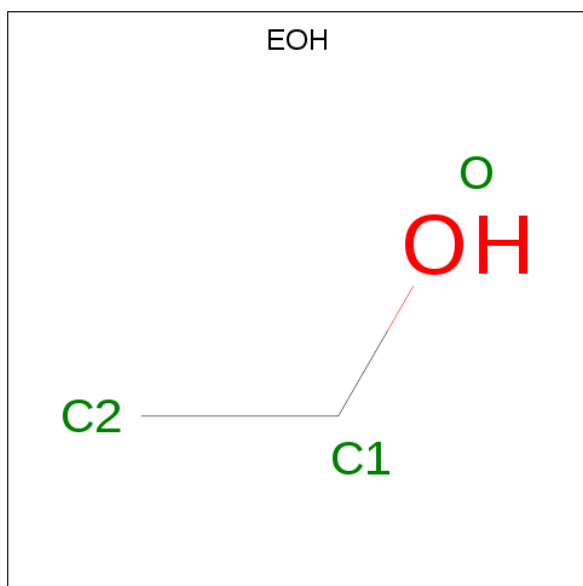
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	4	Total	C	N	O	0	0	0
			47	26	1	20			
3	F	4	Total	C	N	O	0	1	0
			53	29	1	23			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			36	20	1	15			

- Molecule 5 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	2	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	Na 1	0	0
7	A	3	Total 3	Na 3	0	0

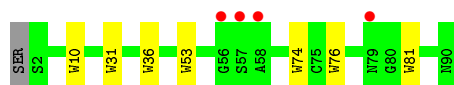
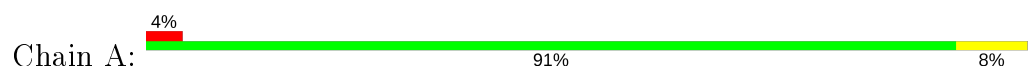
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	82	Total 85	O 85	0	3
8	B	71	Total 74	O 74	0	3

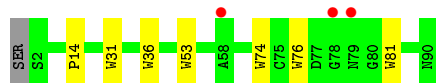
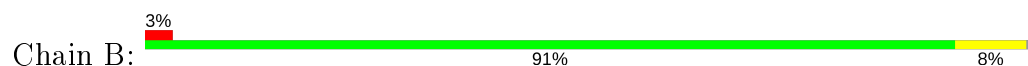
### 3 Residue-property plots [i](#)

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.

- Molecule 1: Fucose-binding lectin protein



- Molecule 1: Fucose-binding lectin protein



- Molecule 2: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-galactopyranose



- Molecule 3: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-alpha-D-galactopyranose



- Molecule 4: alpha-L-fucopyranose-(1-3)-[beta-D-galactopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  67% 33%

 MAG1  
FUC2  
GAL3

## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.88Å 129.88Å 129.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.92 – 1.28 45.92 – 1.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.92-1.28) 100.0 (45.92-1.28)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 1.28Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.122 , 0.148 0.123 , 0.148	Depositor DCC
$R_{free}$ test set	2369 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 77.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	1747	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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 96.73 % 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 3.9390e-10. 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FTR, NAG, CL, GLA, EOH, GAL, FUC, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.64	0/614	0.78	0/825
1	B	0.65	0/595	0.79	0/800
All	All	0.65	0/1209	0.78	0/1625

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	719	0	633	0	0
1	B	700	0	612	0	0
2	C	25	0	24	0	0
3	D	47	0	42	0	0
3	F	53	0	43	0	0
4	E	36	0	33	0	0
5	A	3	0	6	0	0
6	A	1	0	0	1	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
8	A	85	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	74	0	0	0	0
All	All	1747	0	1393	1	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (1) 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)
6:A:102:CL:CL	8:A:236[B]:HOH:O	2.44	0.71

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	84/90 (93%)	83 (99%)	1 (1%)	0	100	100
1	B	82/90 (91%)	81 (99%)	1 (1%)	0	100	100
All	All	166/180 (92%)	164 (99%)	2 (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	67/65 (103%)	67 (100%)	0	100	100
1	B	64/65 (98%)	63 (98%)	1 (2%)	62	26
All	All	131/130 (101%)	130 (99%)	1 (1%)	81	56

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	14	PRO

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 ⓘ

14 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FTR	A	74	1	14,16,17	1.29	1 (7%)	14,22,24	2.23	4 (28%)
1	FTR	B	76	1	14,16,17	1.20	2 (14%)	14,22,24	2.15	5 (35%)
1	FTR	A	10	1	14,16,17	1.15	0	14,22,24	1.01	1 (7%)
1	FTR	B	81	1	14,16,17	1.15	1 (7%)	14,22,24	1.21	2 (14%)
1	FTR	A	81	1	14,16,17	1.29	3 (21%)	14,22,24	1.30	3 (21%)
1	FTR	B	53	1	14,16,17	1.24	2 (14%)	14,22,24	1.27	3 (21%)
1	FTR	A	31	1	14,16,17	0.90	0	14,22,24	1.39	2 (14%)
1	FTR	B	36	1	14,16,17	1.13	1 (7%)	14,22,24	1.50	2 (14%)
1	FTR	B	74	1	14,16,17	1.26	2 (14%)	14,22,24	2.22	5 (35%)
1	FTR	B	10	1	14,16,17	1.22	0	14,22,24	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FTR	A	36	1	14,16,17	1.10	1 (7%)	14,22,24	1.96	4 (28%)
1	FTR	B	31	1	14,16,17	1.08	1 (7%)	14,22,24	1.59	3 (21%)
1	FTR	A	53	1	14,16,17	1.41	2 (14%)	14,22,24	1.11	1 (7%)
1	FTR	A	76	1	14,16,17	1.23	1 (7%)	14,22,24	2.28	5 (35%)

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
1	FTR	A	74	1	-	1/4/6/8	0/2/2/2
1	FTR	B	76	1	-	0/4/6/8	0/2/2/2
1	FTR	A	10	1	-	0/4/6/8	0/2/2/2
1	FTR	B	81	1	-	0/4/6/8	0/2/2/2
1	FTR	A	81	1	-	0/4/6/8	0/2/2/2
1	FTR	B	53	1	-	0/4/6/8	0/2/2/2
1	FTR	A	31	1	-	0/4/6/8	0/2/2/2
1	FTR	B	36	1	-	0/4/6/8	0/2/2/2
1	FTR	B	74	1	-	1/4/6/8	0/2/2/2
1	FTR	B	10	1	-	0/4/6/8	0/2/2/2
1	FTR	A	36	1	-	0/4/6/8	0/2/2/2
1	FTR	B	31	1	-	0/4/6/8	0/2/2/2
1	FTR	A	53	1	-	0/4/6/8	0/2/2/2
1	FTR	A	76	1	-	0/4/6/8	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	FTR	CE3-CZ3	3.17	1.41	1.36
1	A	53	FTR	CZ2-CE2	-3.13	1.36	1.41
1	B	81	FTR	CE3-CZ3	2.87	1.40	1.36
1	B	31	FTR	CE3-CZ3	2.82	1.40	1.36
1	A	36	FTR	CE3-CZ3	2.65	1.40	1.36
1	B	74	FTR	CE3-CZ3	2.56	1.40	1.36
1	B	76	FTR	CE3-CD2	-2.53	1.37	1.42
1	B	36	FTR	CE3-CZ3	2.36	1.40	1.36
1	B	53	FTR	CH2-CZ3	2.32	1.41	1.37
1	A	81	FTR	CE3-CD2	-2.25	1.37	1.42
1	B	74	FTR	CZ2-CH2	2.23	1.41	1.36
1	B	76	FTR	CE3-CZ3	2.22	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	FTR	CZ2-CE2	-2.20	1.38	1.41
1	A	81	FTR	CE3-CZ3	2.17	1.39	1.36
1	A	76	FTR	CE3-CD2	-2.14	1.37	1.42
1	A	53	FTR	CH2-CZ3	2.03	1.41	1.37
1	A	81	FTR	CH2-CZ3	2.00	1.41	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	FTR	CZ3-CE3-CD2	-5.55	114.45	118.80
1	A	76	FTR	CZ2-CH2-CZ3	4.70	124.13	118.74
1	A	76	FTR	CE3-CD2-CE2	4.09	123.85	118.26
1	B	76	FTR	CZ3-CE3-CD2	-4.08	115.61	118.80
1	B	74	FTR	CZ2-CH2-CZ3	4.02	123.34	118.74
1	B	76	FTR	CE3-CD2-CE2	3.97	123.69	118.26
1	B	74	FTR	CE3-CD2-CE2	3.86	123.54	118.26
1	A	36	FTR	CZ3-CE3-CD2	-3.78	115.84	118.80
1	A	74	FTR	CE3-CD2-CE2	3.74	123.38	118.26
1	B	74	FTR	CH2-CZ3-CE3	-3.50	119.37	123.23
1	B	36	FTR	CZ3-CE3-CD2	-3.46	116.09	118.80
1	B	76	FTR	CZ2-CH2-CZ3	3.41	122.64	118.74
1	A	36	FTR	CZ2-CH2-CZ3	3.29	122.50	118.74
1	A	76	FTR	CH2-CZ2-CE2	-3.16	116.87	120.84
1	A	36	FTR	CE3-CD2-CE2	3.11	122.51	118.26
1	A	74	FTR	CZ2-CH2-CZ3	3.04	122.22	118.74
1	B	74	FTR	CZ2-CE2-CD2	-3.02	115.24	120.76
1	A	31	FTR	CZ2-CH2-CZ3	2.94	122.11	118.74
1	A	81	FTR	CZ3-CE3-CD2	-2.93	116.51	118.80
1	B	31	FTR	CZ3-CE3-CD2	-2.91	116.52	118.80
1	B	31	FTR	CZ2-CH2-CZ3	2.90	122.06	118.74
1	A	36	FTR	CH2-CZ2-CE2	-2.88	117.21	120.84
1	B	76	FTR	CH2-CZ2-CE2	-2.81	117.30	120.84
1	A	74	FTR	CH2-CZ2-CE2	-2.74	117.39	120.84
1	B	36	FTR	CE3-CD2-CE2	2.61	121.83	118.26
1	B	76	FTR	CG-CB-CA	-2.59	110.52	114.53
1	A	76	FTR	CH2-CZ3-CE3	-2.59	120.37	123.23
1	B	81	FTR	CZ3-CE3-CD2	-2.55	116.80	118.80
1	A	81	FTR	CE3-CD2-CE2	2.40	121.55	118.26
1	B	53	FTR	CH2-CZ3-CE3	-2.37	120.62	123.23
1	B	31	FTR	CE3-CD2-CE2	2.36	121.48	118.26
1	B	74	FTR	CG-CB-CA	-2.33	110.93	114.53
1	A	81	FTR	CH2-CZ2-CE2	-2.26	117.99	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	FTR	CZ3-CE3-CD2	-2.15	117.12	118.80
1	B	81	FTR	CG-CB-CA	-2.14	111.22	114.53
1	A	53	FTR	CE3-CD2-CE2	2.13	121.17	118.26
1	A	10	FTR	CZ2-CH2-CZ3	2.12	121.17	118.74
1	A	31	FTR	CZ3-CE3-CD2	-2.12	117.14	118.80
1	B	53	FTR	CZ3-CE3-CD2	2.06	120.41	118.80
1	B	53	FTR	CZ2-CE2-NE1	2.03	136.43	130.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	74	FTR	O-C-CA-CB
1	B	74	FTR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

14 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	C	1	2	15,15,15	0.73	0	21,21,21	1.60	4 (19%)
2	FUC	C	2	2	10,10,11	0.52	0	14,14,16	1.33	1 (7%)
3	GLA	D	1	3	12,12,12	0.47	0	17,17,17	1.07	1 (5%)
3	NAG	D	2	3	14,14,15	0.84	0	17,19,21	1.61	5 (29%)
3	FUC	D	3	3	10,10,11	0.52	0	14,14,16	0.89	1 (7%)
3	GAL	D	4	3	11,11,12	1.33	2 (18%)	15,15,17	2.47	4 (26%)
4	NAG	E	1	4	15,15,15	0.57	0	21,21,21	1.15	2 (9%)
4	FUC	E	2	4	10,10,11	0.57	0	14,14,16	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GAL	E	3	4	11,11,12	0.74	0	15,15,17	0.99	0
3	GLA	F	1	3	12,12,12	0.61	0	17,17,17	1.49	3 (17%)
3	NAG	F	2[A]	3	14,14,15	0.71	0	17,19,21	1.67	5 (29%)
3	NAG	F	2[B]	3	14,14,15	0.71	0	17,19,21	1.17	2 (11%)
3	FUC	F	3	3	10,10,11	0.67	0	14,14,16	0.80	0
3	GAL	F	4	3	11,11,12	1.13	1 (9%)	15,15,17	1.81	3 (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	NAG	C	1	2	-	2/6/26/26	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1
3	GLA	D	1	3	-	0/2/22/22	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	FUC	D	3	3	-	-	0/1/1/1
3	GAL	D	4	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4	-	0/6/26/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
4	GAL	E	3	4	-	0/2/19/22	0/1/1/1
3	GLA	F	1	3	-	2/2/22/22	0/1/1/1
3	NAG	F	2[A]	3	-	2/6/23/26	0/1/1/1
3	NAG	F	2[B]	3	-	2/6/23/26	0/1/1/1
3	FUC	F	3	3	-	-	0/1/1/1
3	GAL	F	4	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	GAL	O2-C2	3.07	1.49	1.43
3	F	4	GAL	O2-C2	2.40	1.48	1.43
3	D	4	GAL	O5-C1	2.10	1.47	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	GAL	C1-C2-C3	-6.27	101.95	109.67
3	D	4	GAL	O2-C2-C1	4.92	119.23	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	GAL	C1-C2-C3	-4.24	104.46	109.67
2	C	1	NAG	C1-C2-N2	-4.06	106.02	110.73
3	F	4	GAL	O2-C2-C1	3.65	116.62	109.15
2	C	1	NAG	O3-C3-C2	3.53	116.79	109.66
3	D	4	GAL	O5-C1-C2	3.40	116.03	110.77
2	C	2	FUC	C1-C2-C3	3.39	113.83	109.67
3	F	1	GLA	O3-C3-C2	-3.32	102.68	110.35
3	F	2[A]	NAG	O5-C5-C6	3.20	112.22	107.20
3	D	2	NAG	C3-C4-C5	3.11	115.79	110.24
3	F	1	GLA	C1-O5-C5	3.10	119.51	113.66
3	F	2[A]	NAG	C3-C4-C5	3.06	115.69	110.24
3	F	2[A]	NAG	C1-O5-C5	2.74	115.91	112.19
3	D	4	GAL	O3-C3-C4	-2.71	104.08	110.35
3	F	2[A]	NAG	O4-C4-C3	2.70	116.59	110.35
3	F	2[B]	NAG	C3-C4-C5	2.49	114.68	110.24
3	D	2	NAG	O4-C4-C3	2.45	116.02	110.35
3	D	2	NAG	C1-O5-C5	2.38	115.41	112.19
4	E	1	NAG	C1-C2-C3	-2.36	107.32	110.54
3	F	2[B]	NAG	O4-C4-C3	2.35	115.78	110.35
2	C	1	NAG	C3-C4-C5	2.27	114.30	110.24
3	F	2[A]	NAG	O5-C5-C4	-2.26	105.32	110.83
3	D	2	NAG	O5-C5-C4	-2.26	105.33	110.83
3	F	1	GLA	C3-C4-C5	2.22	114.20	110.24
4	E	1	NAG	C1-C2-N2	-2.20	108.18	110.73
3	F	4	GAL	O3-C3-C2	-2.17	105.84	109.99
2	C	1	NAG	C3-C2-N2	2.17	114.71	110.62
3	D	1	GLA	O4-C4-C3	-2.16	105.34	110.35
3	D	2	NAG	O3-C3-C4	-2.16	105.34	110.35
3	D	3	FUC	O4-C4-C5	-2.09	105.04	109.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	F	1	GLA	C4-C5-C6-O6
3	F	2[A]	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	F	1	GLA	O5-C5-C6-O6
3	F	2[A]	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	F	2[B]	NAG	O5-C5-C6-O6

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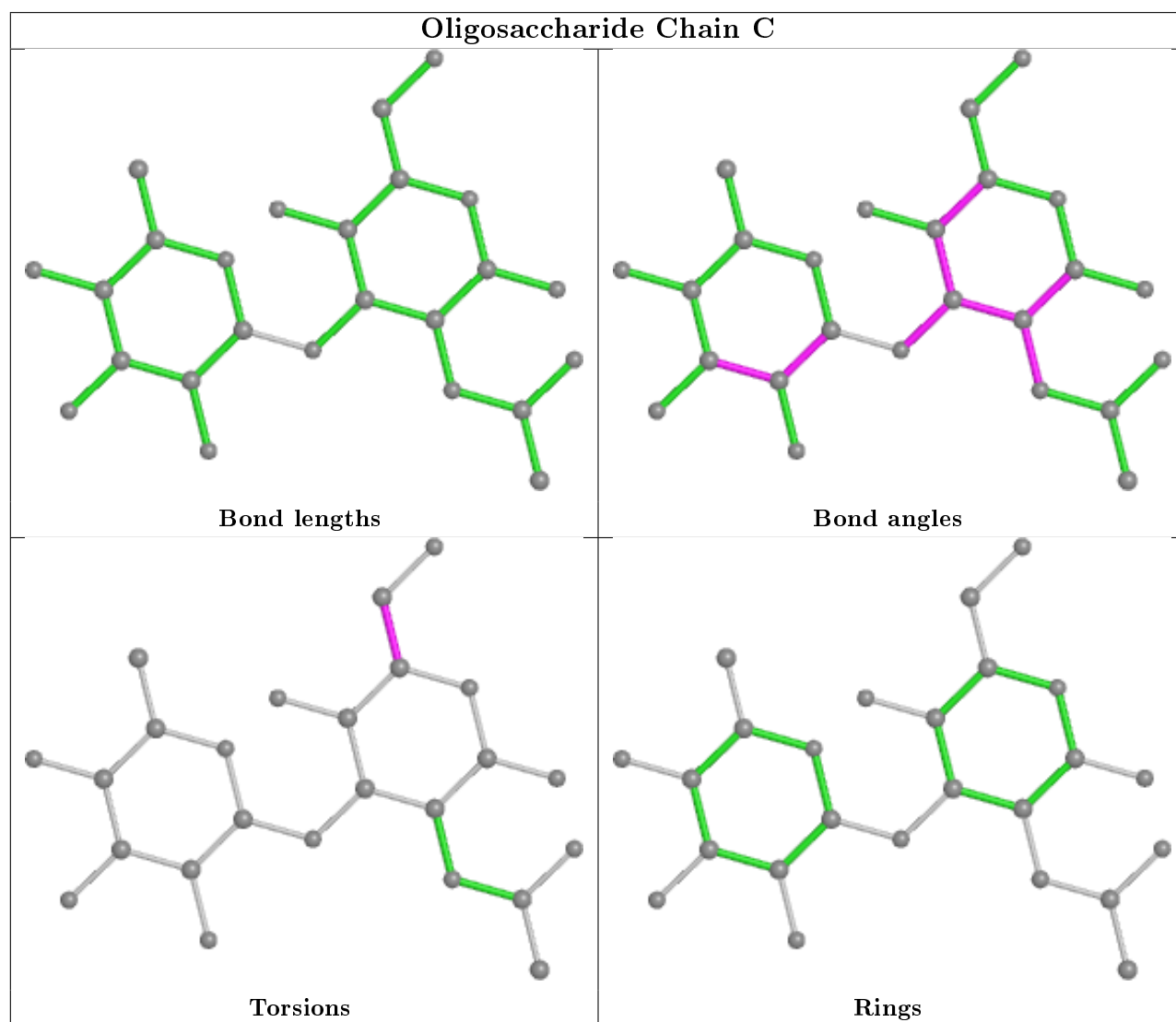
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Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
3	F	2[B]	NAG	C4-C5-C6-O6

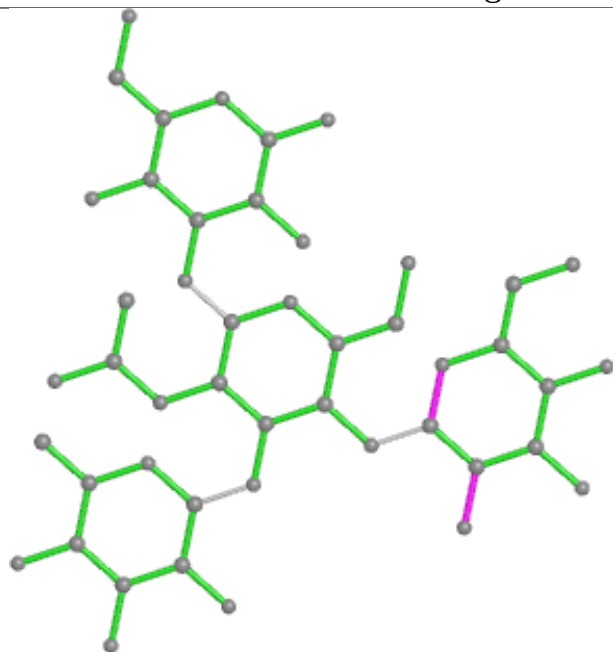
There are no ring outliers.

No monomer is involved in short contacts.

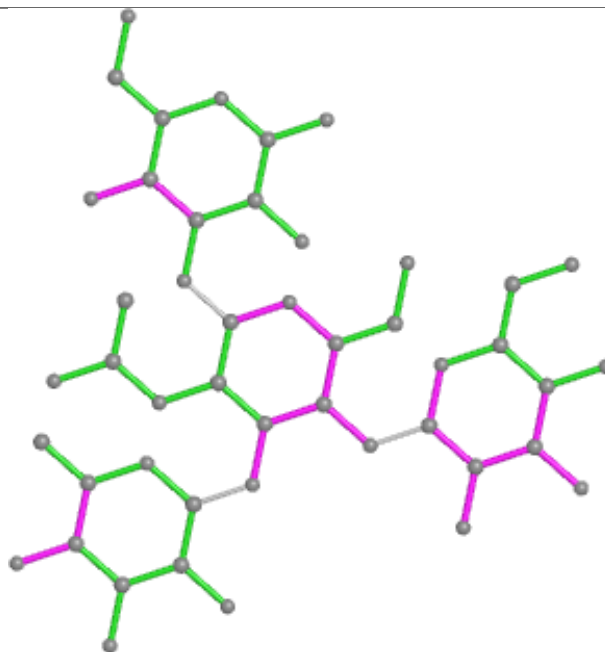
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



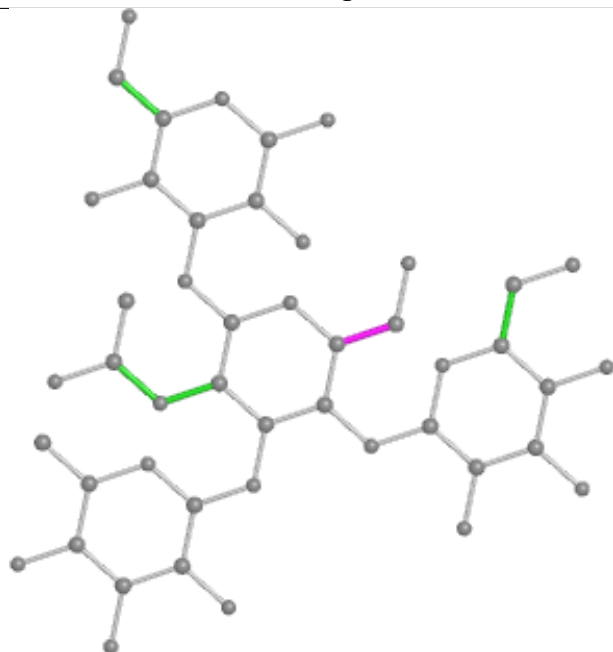
## Oligosaccharide Chain D



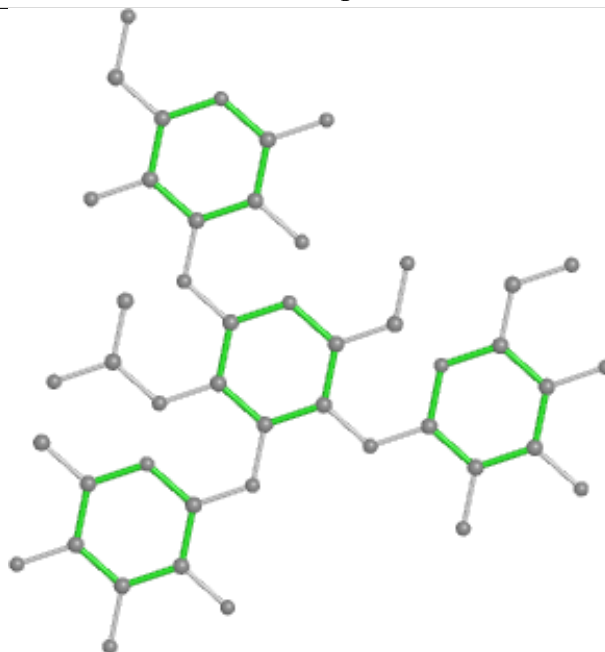
Bond lengths



Bond angles

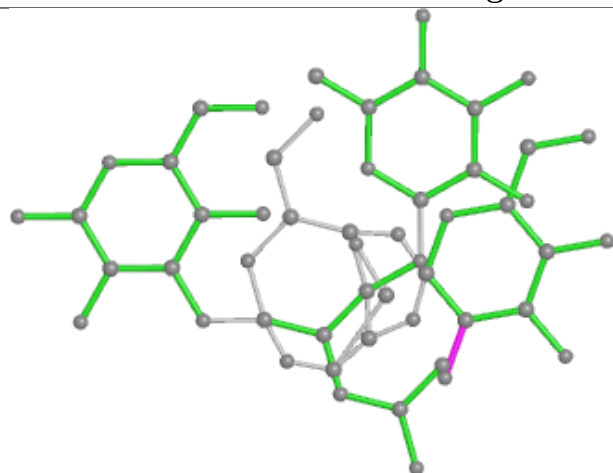


Torsions

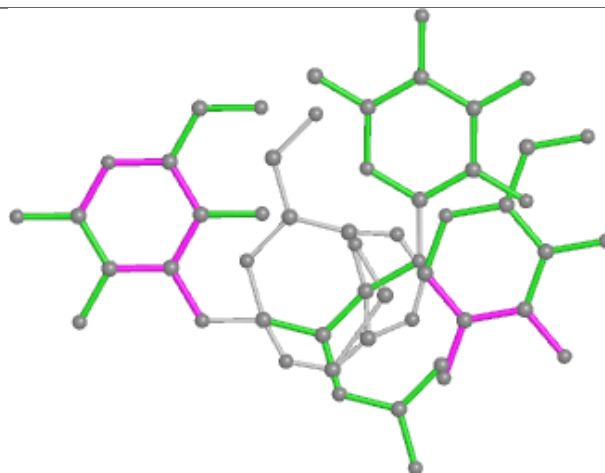


Rings

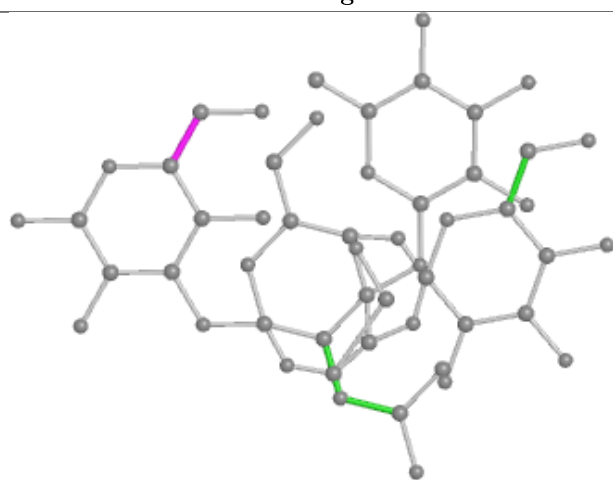
## Oligosaccharide Chain F



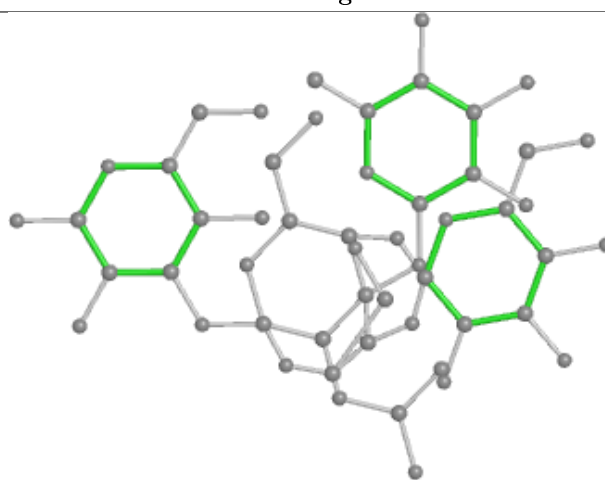
Bond lengths



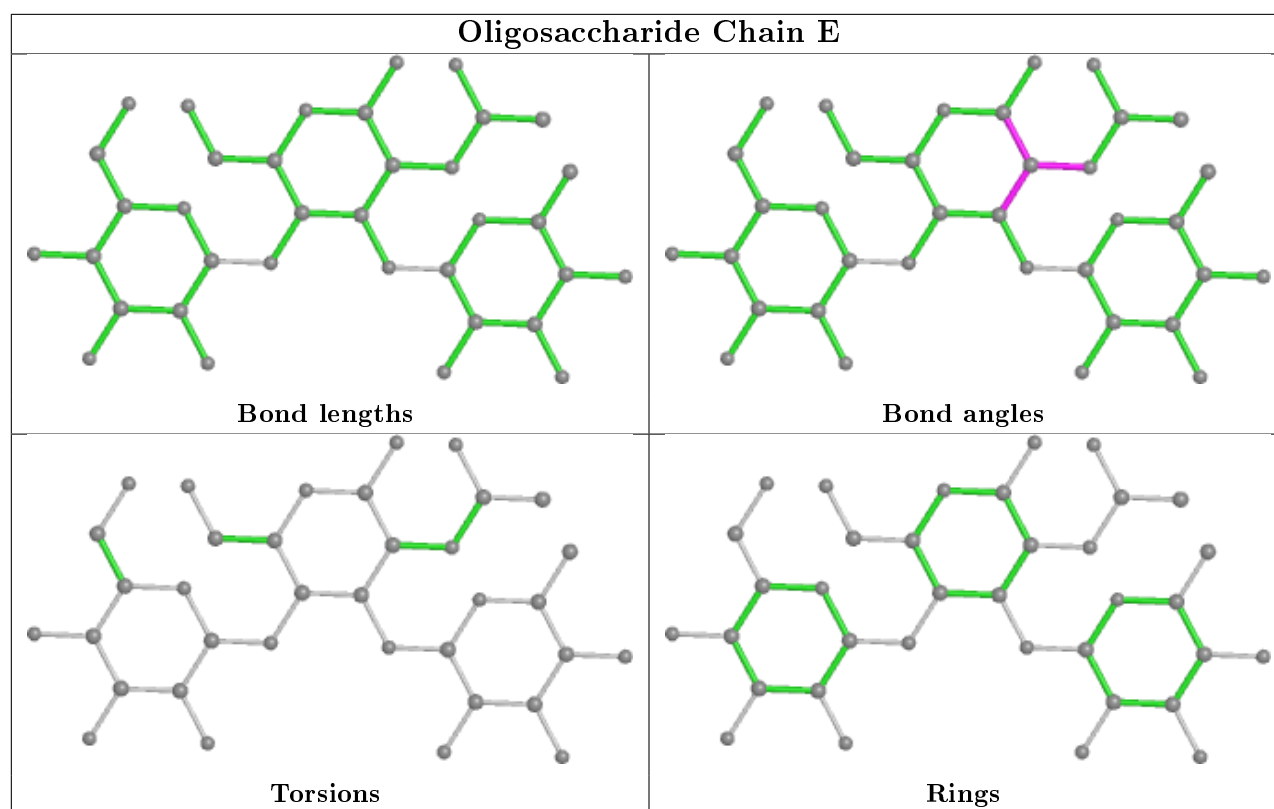
Bond angles



Torsions



Rings



## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	EOH	A	101	-	2,2,2	0.43	0	1,1,1	0.36	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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, 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	82/90 (91%)	-0.17	4 (4%) 29 26	7, 12, 23, 39	4 (4%)
1	B	82/90 (91%)	-0.27	3 (3%) 41 36	7, 13, 25, 40	5 (6%)
All	All	164/180 (91%)	-0.22	7 (4%) 35 31	7, 12, 25, 40	9 (5%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ALA	4.5
1	A	57	SER	3.7
1	B	79	ASN	3.2
1	B	58	ALA	2.8
1	A	79	ASN	2.6
1	A	56	GLY	2.2
1	B	78	GLY	2.1

### 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<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
1	FTR	B	74	15/16	0.92	0.09	9,12,22,24	0
1	FTR	A	81	15/16	0.93	0.08	9,10,13,15	0
1	FTR	B	81	15/16	0.94	0.07	9,11,14,16	0
1	FTR	B	76	15/16	0.95	0.08	10,12,14,18	0
1	FTR	A	74	15/16	0.95	0.08	8,11,15,19	0
1	FTR	A	76	15/16	0.95	0.06	9,11,17,20	0
1	FTR	B	31	15/16	0.97	0.05	8,10,11,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	FTR	B	36	15/16	0.98	0.05	8,8,9,10	0
1	FTR	A	10	15/16	0.98	0.05	8,9,11,12	0
1	FTR	B	10	15/16	0.98	0.05	8,10,11,12	0
1	FTR	A	36	15/16	0.98	0.05	8,8,9,10	0
1	FTR	B	53	15/16	0.98	0.05	9,11,13,14	0
1	FTR	A	53	15/16	0.98	0.05	9,11,12,13	0
1	FTR	A	31	15/16	0.98	0.05	8,9,11,12	0

## 6.3 Carbohydrates

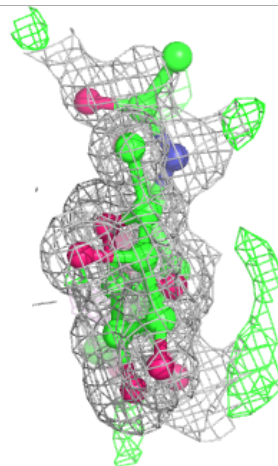
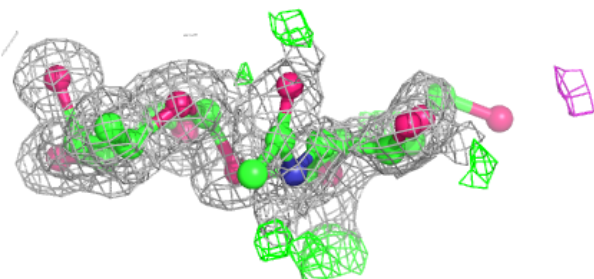
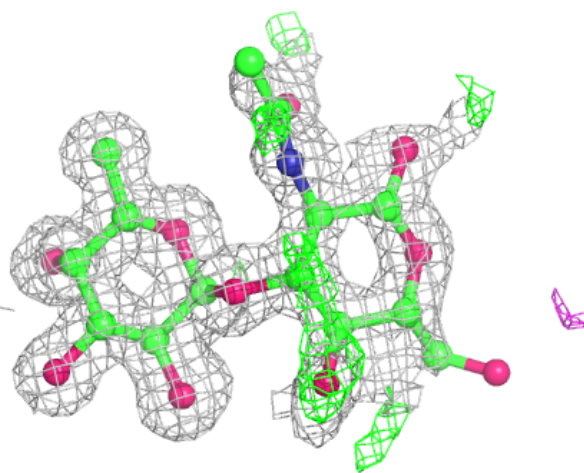
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	GLA	D	1	12/12	0.76	0.17	23,29,38,39	12
4	GAL	E	3	11/12	0.78	0.29	19,23,26,33	11
3	GLA	F	1	12/12	0.82	0.20	22,28,39,44	12
3	GAL	D	4	11/12	0.85	0.11	17,24,26,26	0
3	GAL	F	4	11/12	0.88	0.10	17,22,25,26	0
3	NAG	D	2	14/15	0.89	0.10	13,20,27,35	0
3	NAG	F	2[B]	14/15	0.94	0.09	13,19,25,25	6
4	NAG	E	1	15/15	0.94	0.17	13,22,29,36	1
3	NAG	F	2[A]	14/15	0.94	0.09	13,19,25,29	6
2	NAG	C	1	15/15	0.94	0.22	15,31,43,46	0
3	FUC	D	3	10/11	0.97	0.06	9,10,10,12	0
2	FUC	C	2	10/11	0.98	0.04	10,11,12,13	0
3	FUC	F	3	10/11	0.99	0.05	10,11,11,13	0
4	FUC	E	2	10/11	0.99	0.04	10,11,12,12	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 C:**

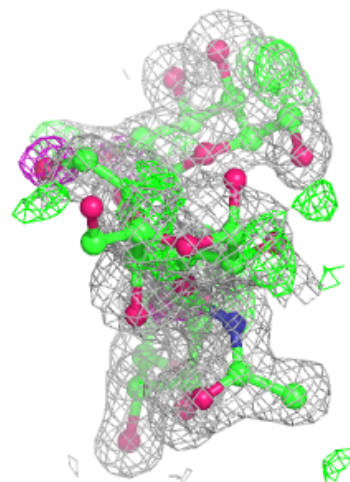
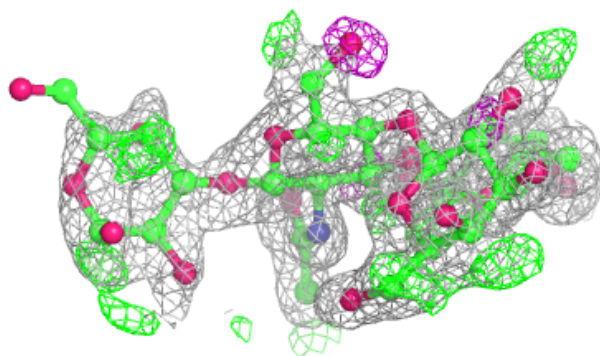
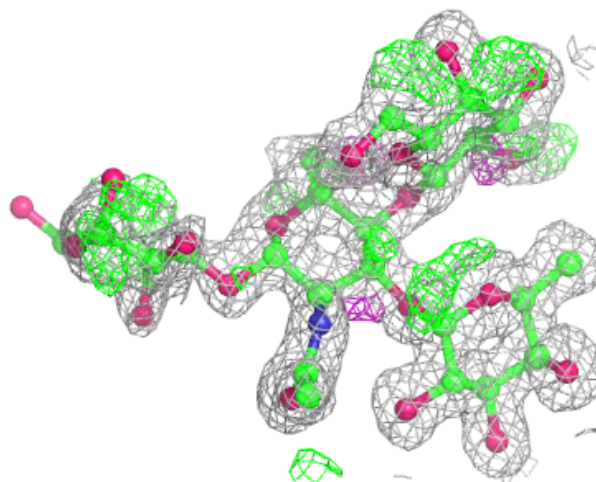
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





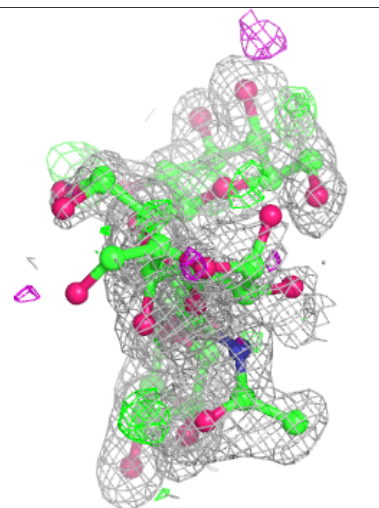
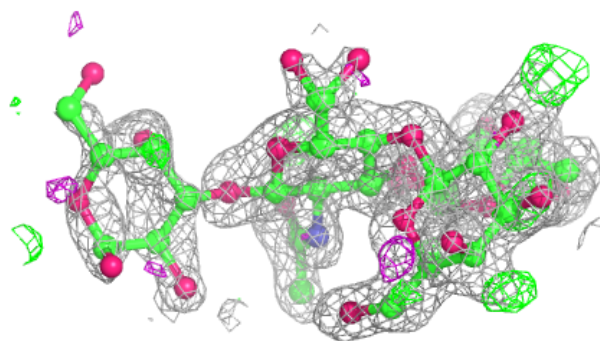
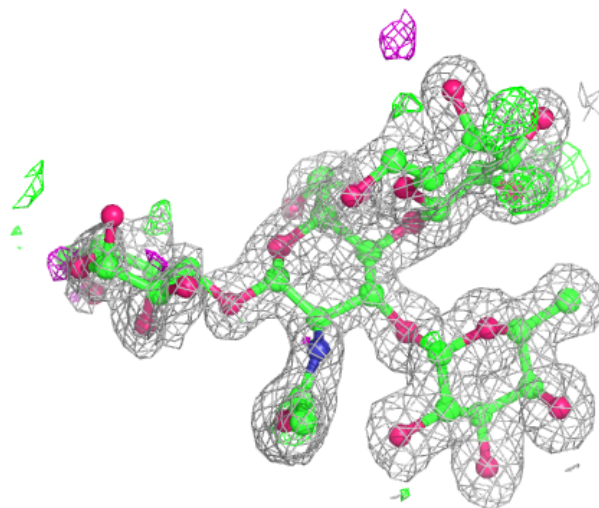
**Electron density around Chain D:**

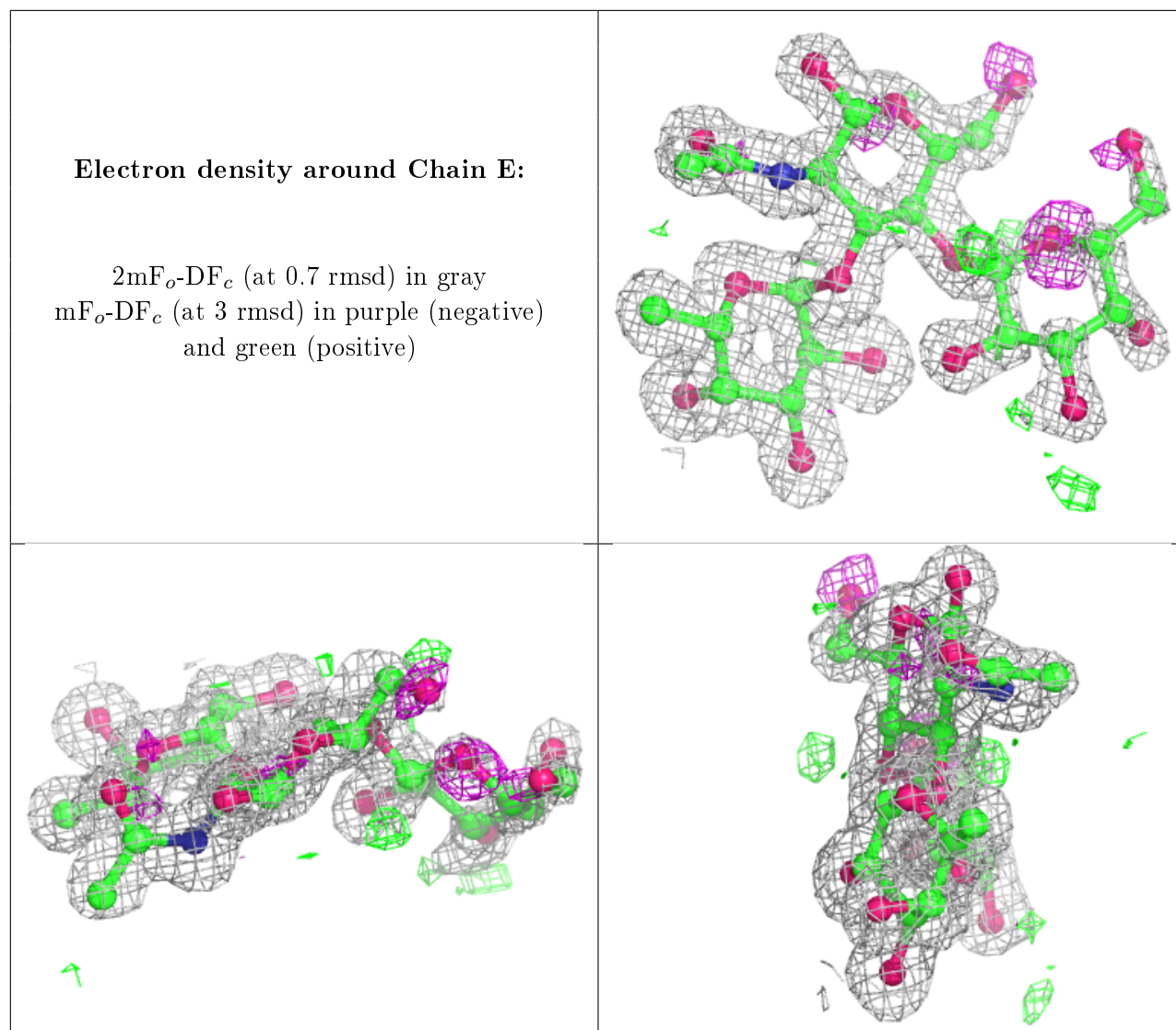
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain F:**

$2mF_o-DF_c$  (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, 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
5	EOH	A	101	3/3	0.74	0.17	24,24,24,32	0
7	NA	A	111	1/1	0.99	0.06	20,20,20,20	0
6	CL	A	102	1/1	0.99	0.06	16,16,16,16	1
7	NA	B	101	1/1	1.00	0.06	11,11,11,11	0
7	NA	A	104	1/1	1.00	0.06	12,12,12,12	0
7	NA	A	103	1/1	1.00	0.05	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.