



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2026 – 10:08 am BST

PDB ID : 9HHU / pdb\_00009hhu  
Title : Plant membrane receptor IGP1 in complex with celotriose  
Authors : Jimenez-Sandoval, P.; Santiago, J.  
Deposited on : 2024-11-22  
Resolution : 2.16 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

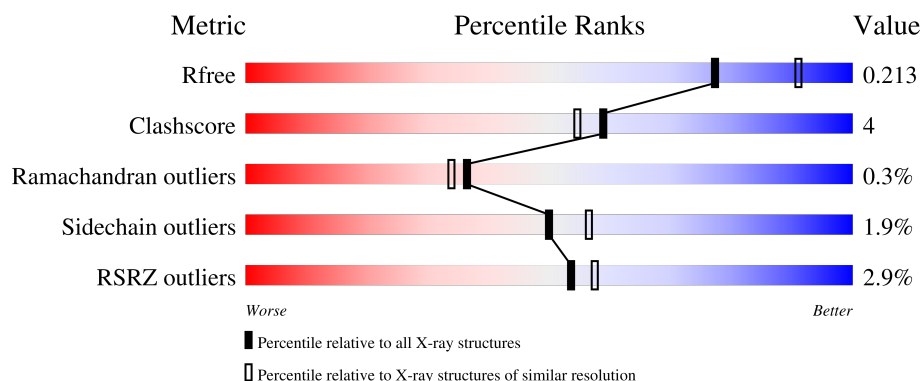
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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.



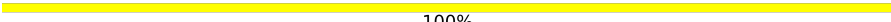
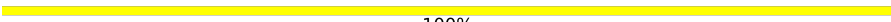

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 of 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	618	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>..</div> </div> </div>
2	B	3	<div> <div>100%</div> </div>
2	C	3	<div> <div>67%</div> <div>33%</div> </div>
3	D	2	<div> <div>100%</div> </div>
4	E	6	<div> <div>33%</div> <div>67%</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	2	 100%
5	G	2	 100%
6	H	3	 100%

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4956 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.

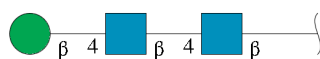
- Molecule 1 is a protein called non-specific serine/threonine protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	1	0
			4456	2841	747	850	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP C0LGH4
A	24	GLY	-	expression tag	UNP C0LGH4
A	631	LEU	-	expression tag	UNP C0LGH4
A	632	GLU	-	expression tag	UNP C0LGH4
A	633	GLY	-	expression tag	UNP C0LGH4
A	634	SER	-	expression tag	UNP C0LGH4
A	635	GLU	-	expression tag	UNP C0LGH4
A	636	ASN	-	expression tag	UNP C0LGH4
A	637	LEU	-	expression tag	UNP C0LGH4
A	638	TYR	-	expression tag	UNP C0LGH4
A	639	PHE	-	expression tag	UNP C0LGH4
A	640	GLN	-	expression tag	UNP C0LGH4

- 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.



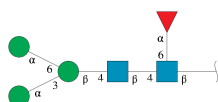
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 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
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	H	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



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 CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula:  $O_4S$ ).



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

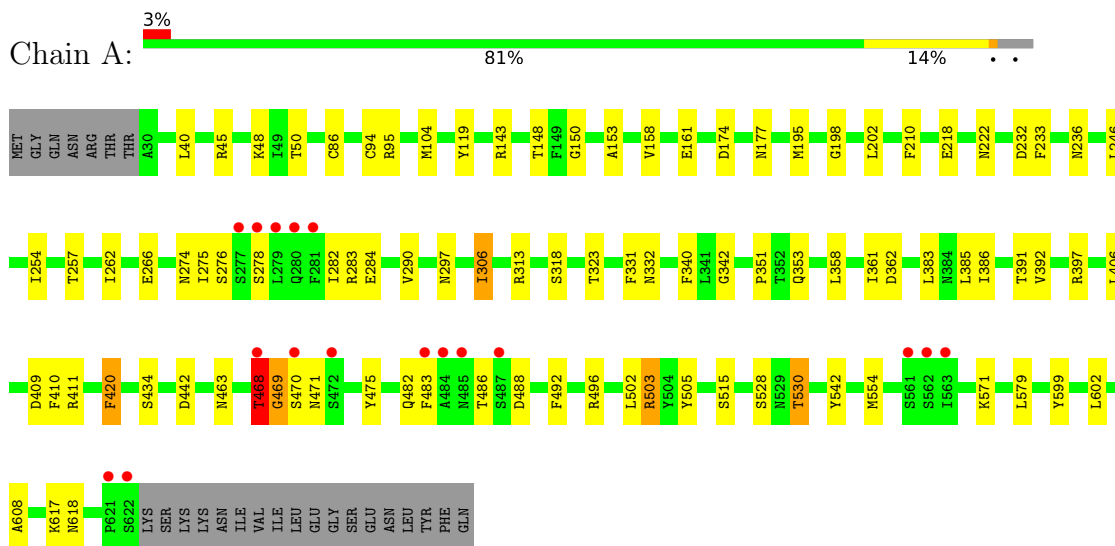
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	188	Total	O	0	0
			188	188		

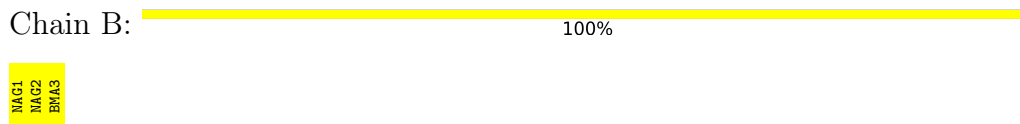
### 3 Residue-property plots [i](#)

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.

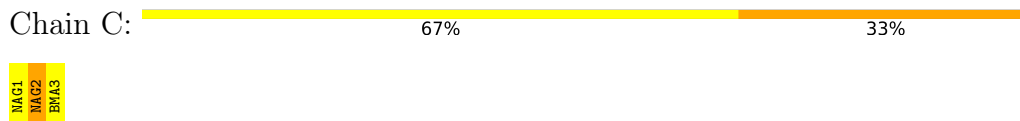
- Molecule 1: non-specific serine/threonine protein kinase



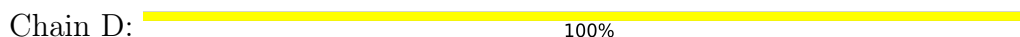
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose





MAG1  
FUC2

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

Chain E:  33% 67%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
FUC6

- Molecule 5: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain F:  100%

MAG1  
MAG2

- Molecule 5: 2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain G:  100%

MAG1  
MAG2

- Molecule 6:  $\beta$ -D-glucopyranose-(1-4)- $\beta$ -D-glucopyranose-(1-4)- $\beta$ -D-glucopyranose

Chain H:  100%

BGC1  
BGC2  
BGC3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.78Å 83.78Å 198.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.95 – 2.16 48.95 – 2.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.95-2.16) 99.9 (48.95-2.16)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, $R_{free}$	0.169 , 0.210 0.175 , 0.213	Depositor DCC
$R_{free}$ test set	2076 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.098 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage'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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, NAG, BMA, SO4, CA, BGC, 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	0.91	0/4549	1.42	32/6201 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	THR	CA-CB-OG1	-9.60	95.20	109.60
1	A	218	GLU	CB-CG-CD	8.04	126.28	112.60
1	A	468	THR	CA-CB-OG1	-7.95	97.67	109.60
1	A	218	GLU	CB-CA-C	7.54	121.24	110.24
1	A	530	THR	CA-CB-OG1	-7.50	98.35	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	411	ARG	Sidechain

## 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	4456	0	4314	40	0
2	B	39	0	34	0	0
2	C	39	0	34	2	0
3	D	24	0	22	0	0
4	E	71	0	61	0	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0
6	H	34	0	29	0	0
7	A	28	0	26	0	0
8	A	1	0	0	0	0
9	A	20	0	0	0	0
10	A	188	0	0	4	0
All	All	4956	0	4570	40	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 4.

The worst 5 of 40 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:468:THR:HG22	1:A:599:TYR:OH	1.80	0.80
1:A:483:PHE:O	1:A:486:THR:HG22	1.82	0.78
1:A:469:GLY:O	1:A:470:SER:C	2.35	0.67
1:A:383:LEU:HD11	1:A:385:LEU:HD21	1.77	0.65
1:A:528:SER:HB3	1:A:530:THR:HG22	1.81	0.62

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	592/618 (96%)	554 (94%)	36 (6%)	2 (0%)	36	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	SER
1	A	392	VAL

### 5.3.2 Protein sidechains ⓘ

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	472/529 (89%)	463 (98%)	9 (2%)	50	56

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	ASN
1	A	482	GLN
1	A	306	ILE
1	A	332	ASN
1	A	434	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	229	GLN
1	A	529	ASN
1	A	596	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 ⓘ

21 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	0.52	0	17,19,21	1.11	1 (5%)
2	NAG	B	2	2	14,14,15	0.64	0	17,19,21	2.03	4 (23%)
2	BMA	B	3	2	11,11,12	1.27	2 (18%)	15,15,17	2.81	8 (53%)
2	NAG	C	1	1,2	14,14,15	0.59	0	17,19,21	1.27	2 (11%)
2	NAG	C	2	2	14,14,15	0.53	0	17,19,21	1.96	5 (29%)
2	BMA	C	3	2	11,11,12	1.43	3 (27%)	15,15,17	2.70	7 (46%)
3	NAG	D	1	3,1	14,14,15	0.71	0	17,19,21	1.28	1 (5%)
3	FUC	D	2	3	10,10,11	0.88	0	14,14,16	1.86	4 (28%)
4	NAG	E	1	1,4	14,14,15	0.56	0	17,19,21	0.71	0
4	NAG	E	2	4	14,14,15	0.64	0	17,19,21	1.87	6 (35%)
4	BMA	E	3	4	11,11,12	0.60	0	15,15,17	0.87	0
4	MAN	E	4	4	11,11,12	1.53	1 (9%)	15,15,17	1.34	1 (6%)
4	MAN	E	5	4	11,11,12	1.13	2 (18%)	15,15,17	1.74	3 (20%)
4	FUC	E	6	4	10,10,11	0.99	1 (10%)	14,14,16	1.37	3 (21%)
5	NAG	F	1	5,1	14,14,15	0.66	0	17,19,21	1.38	2 (11%)
5	NAG	F	2	5	14,14,15	0.65	0	17,19,21	1.34	3 (17%)
5	NAG	G	1	5,1	14,14,15	0.79	0	17,19,21	1.80	3 (17%)
5	NAG	G	2	5	14,14,15	0.46	0	17,19,21	1.66	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BGC	H	1	6	12,12,12	0.57	0	17,17,17	1.49	3 (17%)
6	BGC	H	2	6	11,11,12	0.55	0	15,15,17	1.38	2 (13%)
6	BGC	H	3	6	11,11,12	0.69	0	15,15,17	1.68	4 (26%)

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	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	BMA	B	3	2	-	1/2/19/22	0/1/1/1
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	FUC	E	6	4	-	-	0/1/1/1
5	NAG	F	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	NAG	G	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
6	BGC	H	1	6	-	0/2/22/22	0/1/1/1
6	BGC	H	2	6	-	0/2/19/22	0/1/1/1
6	BGC	H	3	6	-	0/2/19/22	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4	MAN	C2-C3	3.35	1.57	1.52
2	C	3	BMA	O5-C5	2.65	1.48	1.43
4	E	6	FUC	C2-C3	2.64	1.56	1.52
2	B	3	BMA	C2-C3	2.51	1.56	1.52
2	C	3	BMA	C4-C5	2.42	1.58	1.53

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	O5-C5-C6	5.52	115.86	107.20
2	B	2	NAG	C1-O5-C5	5.27	119.33	112.19
2	B	3	BMA	C6-C5-C4	-5.13	100.98	113.00
2	C	3	BMA	O2-C2-C1	4.93	119.24	109.15
5	G	1	NAG	C1-O5-C5	4.87	118.79	112.19

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	2	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2

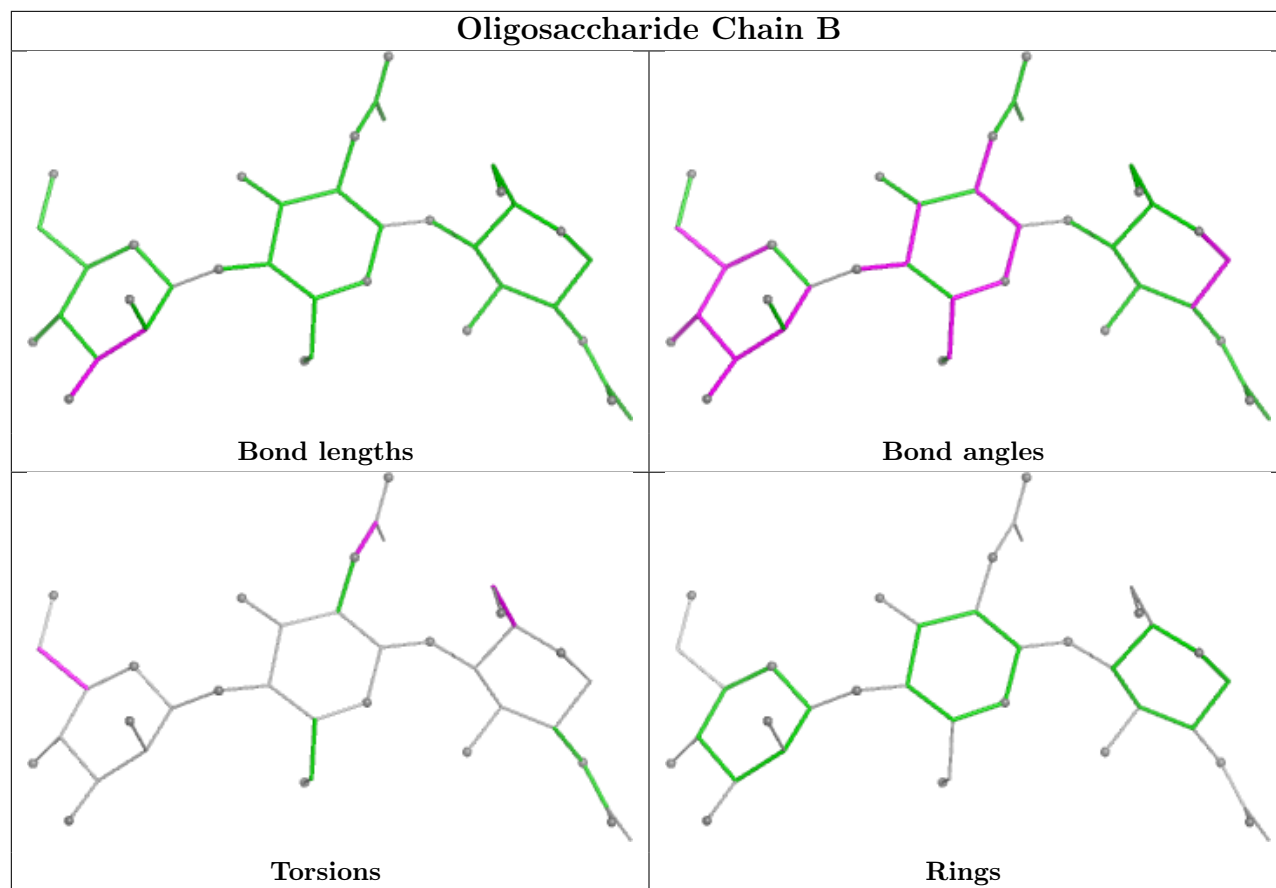
There are no ring outliers.

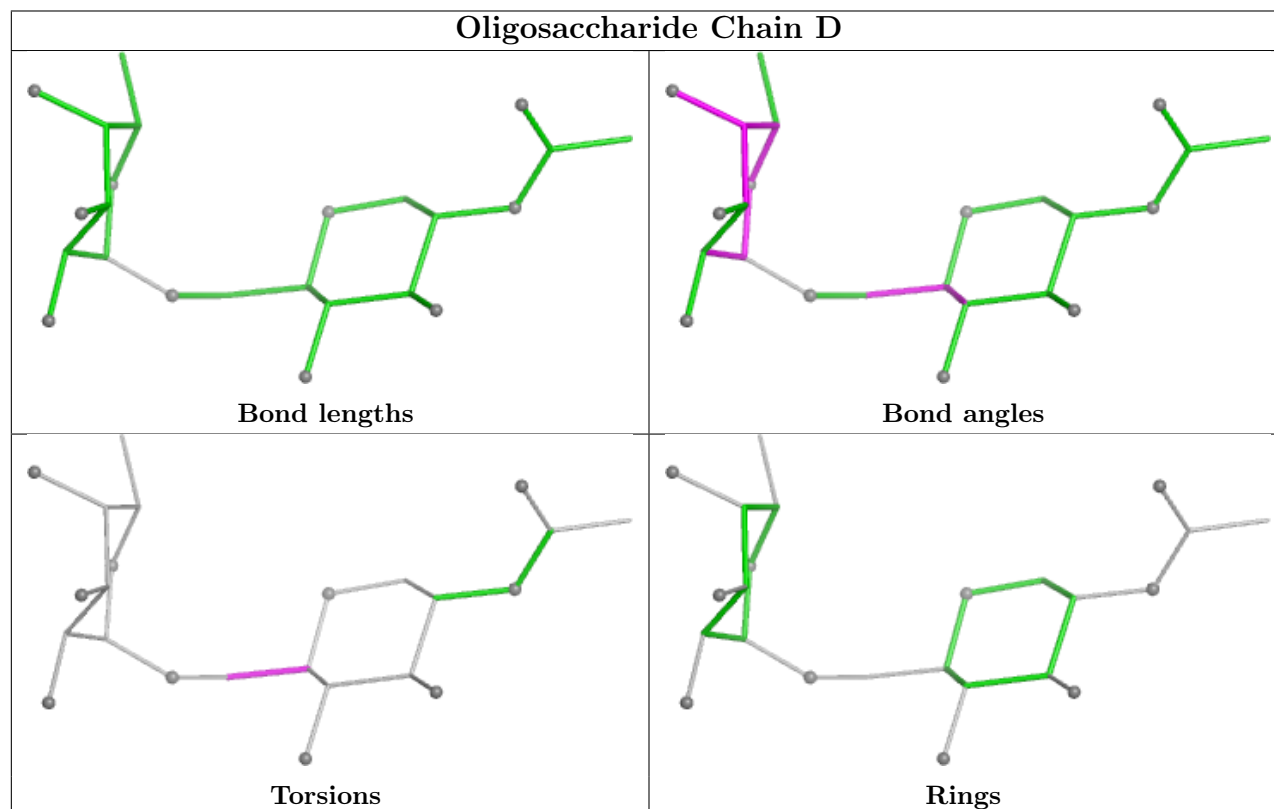
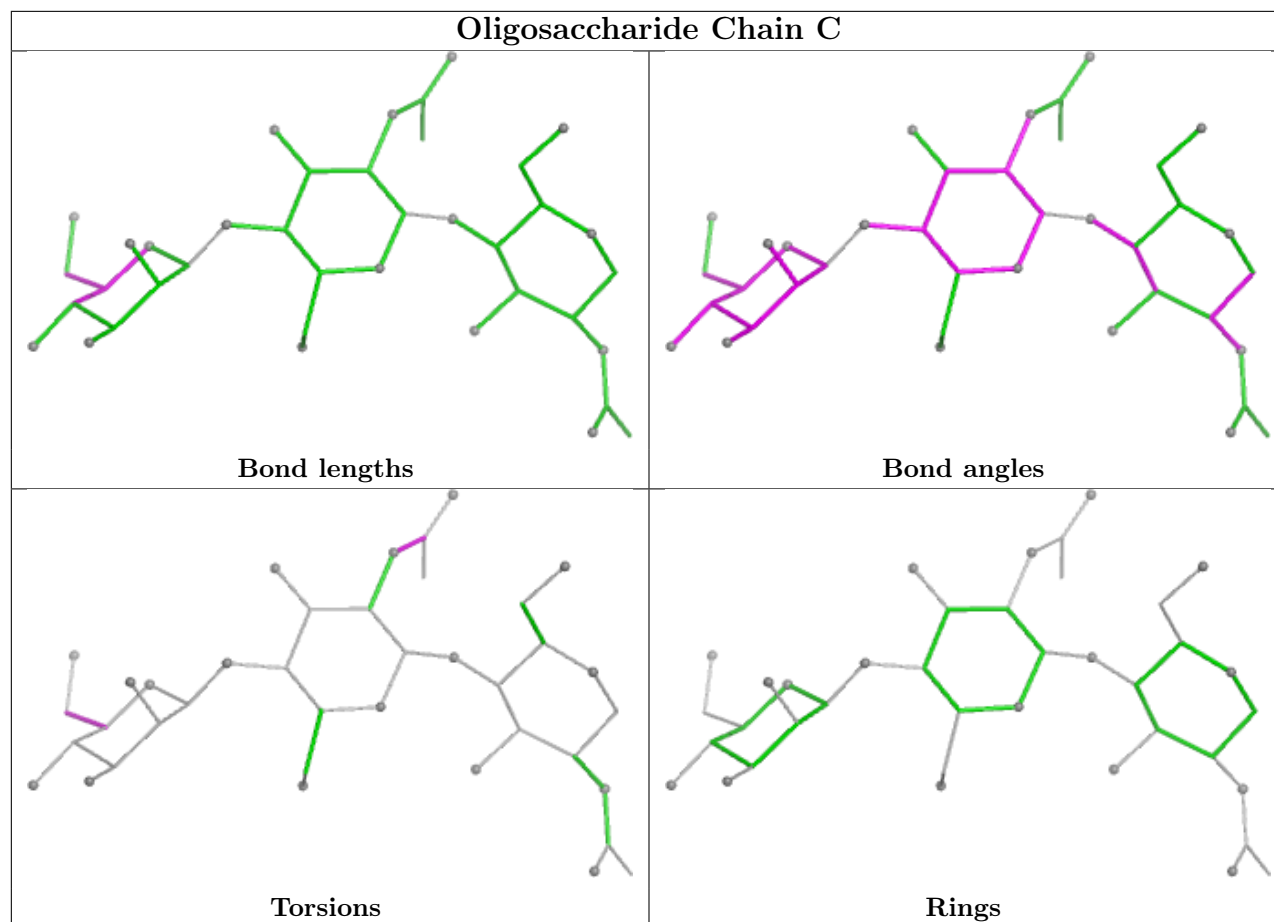
1 monomer is involved in 2 short contacts:

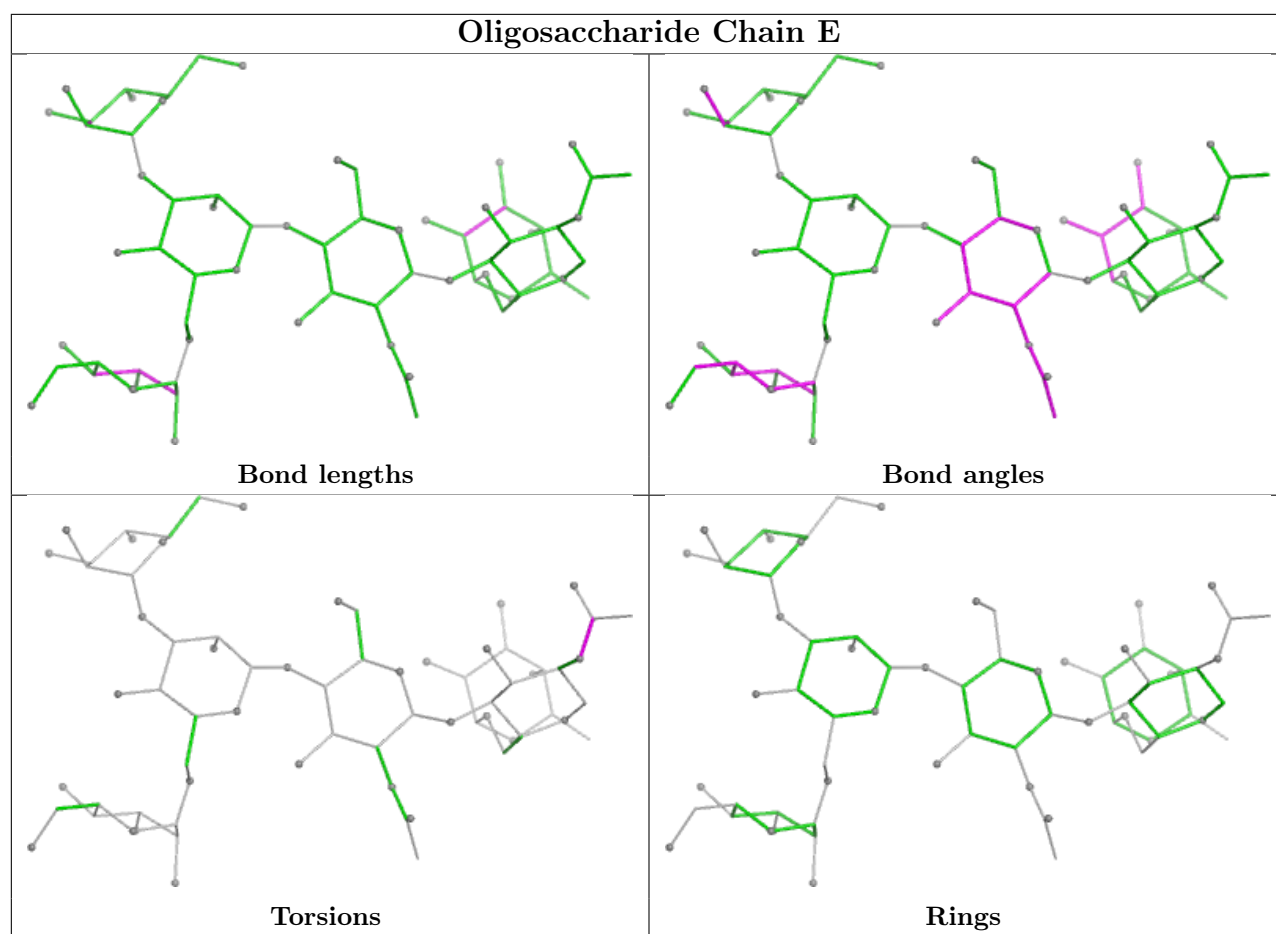
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0

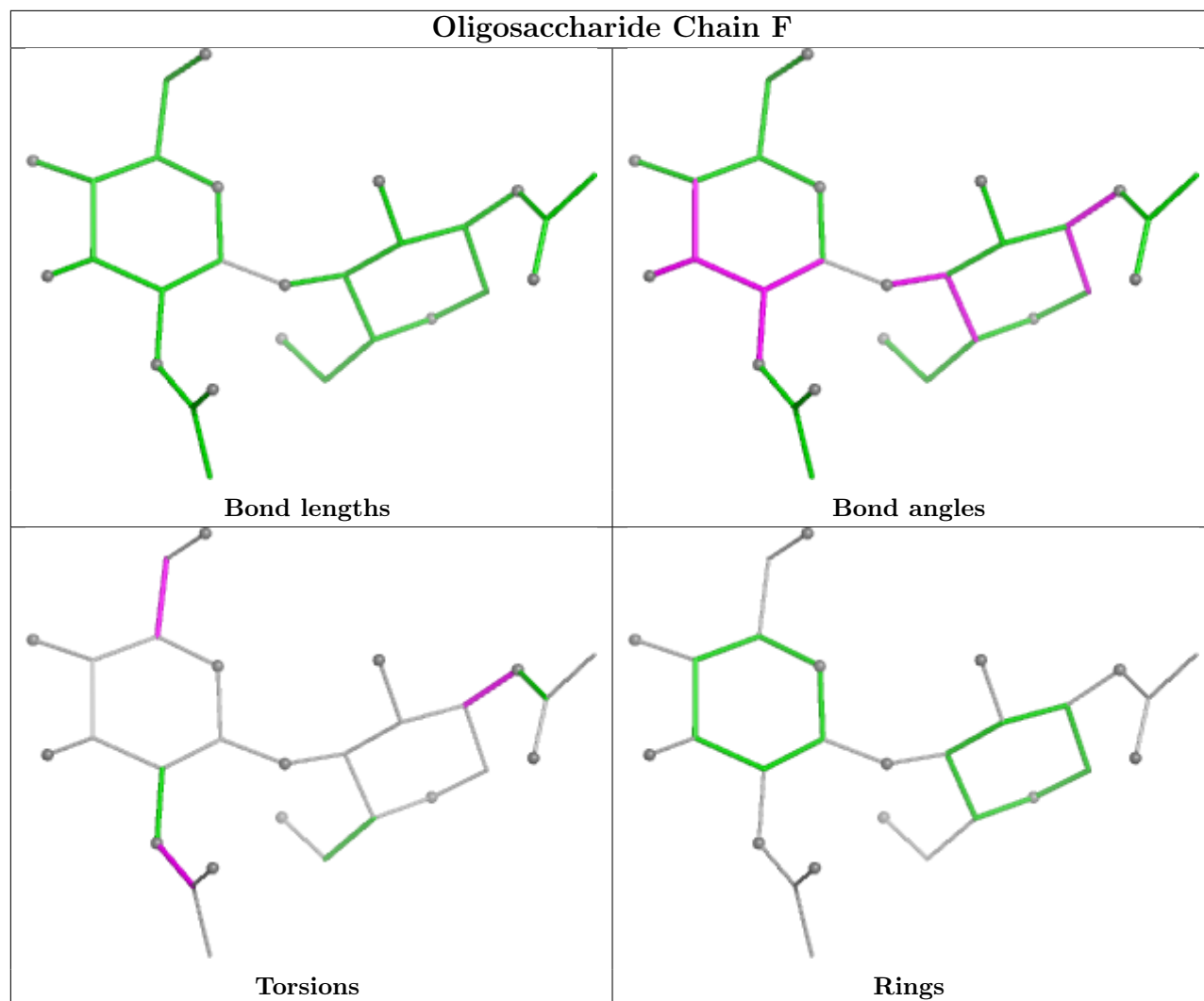
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

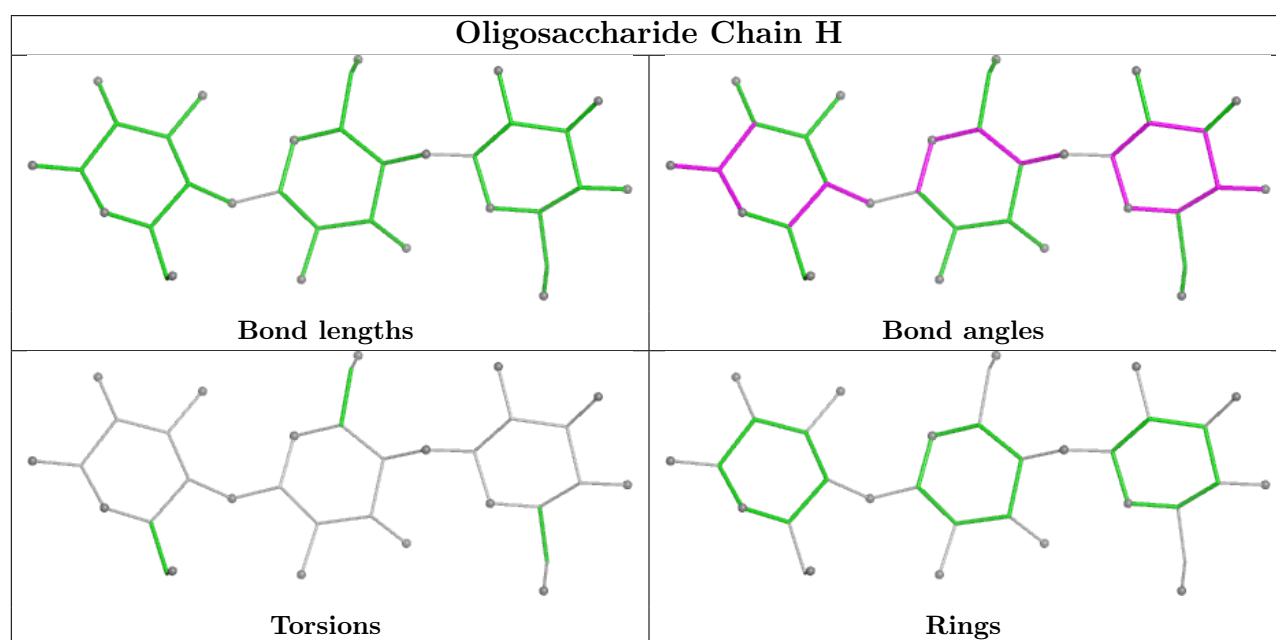
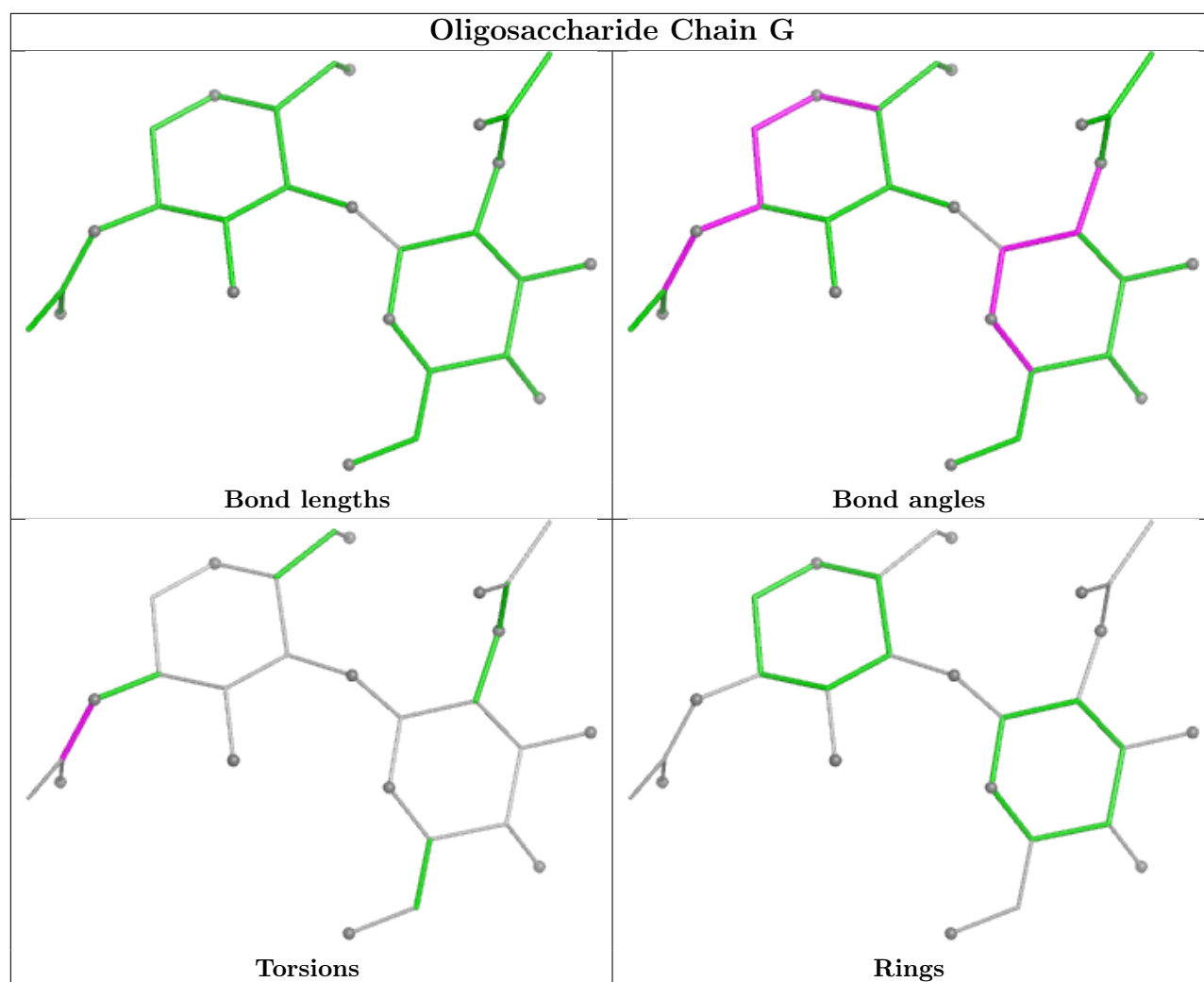












## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
9	SO4	A	707	-	4,4,4	0.44	0	6,6,6	0.61	0
7	NAG	A	701	1	14,14,15	0.58	0	17,19,21	1.19	2 (11%)
9	SO4	A	705	-	4,4,4	0.22	0	6,6,6	0.46	0
9	SO4	A	704	-	4,4,4	0.26	0	6,6,6	0.42	0
7	NAG	A	702	1	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
9	SO4	A	706	-	4,4,4	0.31	0	6,6,6	0.38	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
7	NAG	A	701	1	-	0/6/23/26	0/1/1/1
7	NAG	A	702	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	701	NAG	C2-N2-C7	2.57	126.56	122.90
7	A	702	NAG	C3-C4-C5	-2.20	106.31	110.24
7	A	701	NAG	O4-C4-C5	2.17	114.68	109.30

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 [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	593/618 (95%)	-0.19	17 (2%) 53 57	21, 48, 82, 133	1 (0%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	SER	4.4
1	A	485	ASN	3.9
1	A	622	SER	3.8
1	A	562	SER	3.8
1	A	484	ALA	3.6

### 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
5	NAG	G	2	14/15	0.59	0.14	85,133,166,186	0
5	NAG	F	2	14/15	0.67	0.16	74,102,123,130	0
4	MAN	E	4	11/12	0.72	0.12	84,107,126,130	0
2	BMA	B	3	11/12	0.74	0.12	75,101,112,117	0
5	NAG	G	1	14/15	0.75	0.13	76,106,136,158	0
2	BMA	C	3	11/12	0.80	0.12	65,95,106,110	0
5	NAG	F	1	14/15	0.82	0.12	58,86,99,100	0

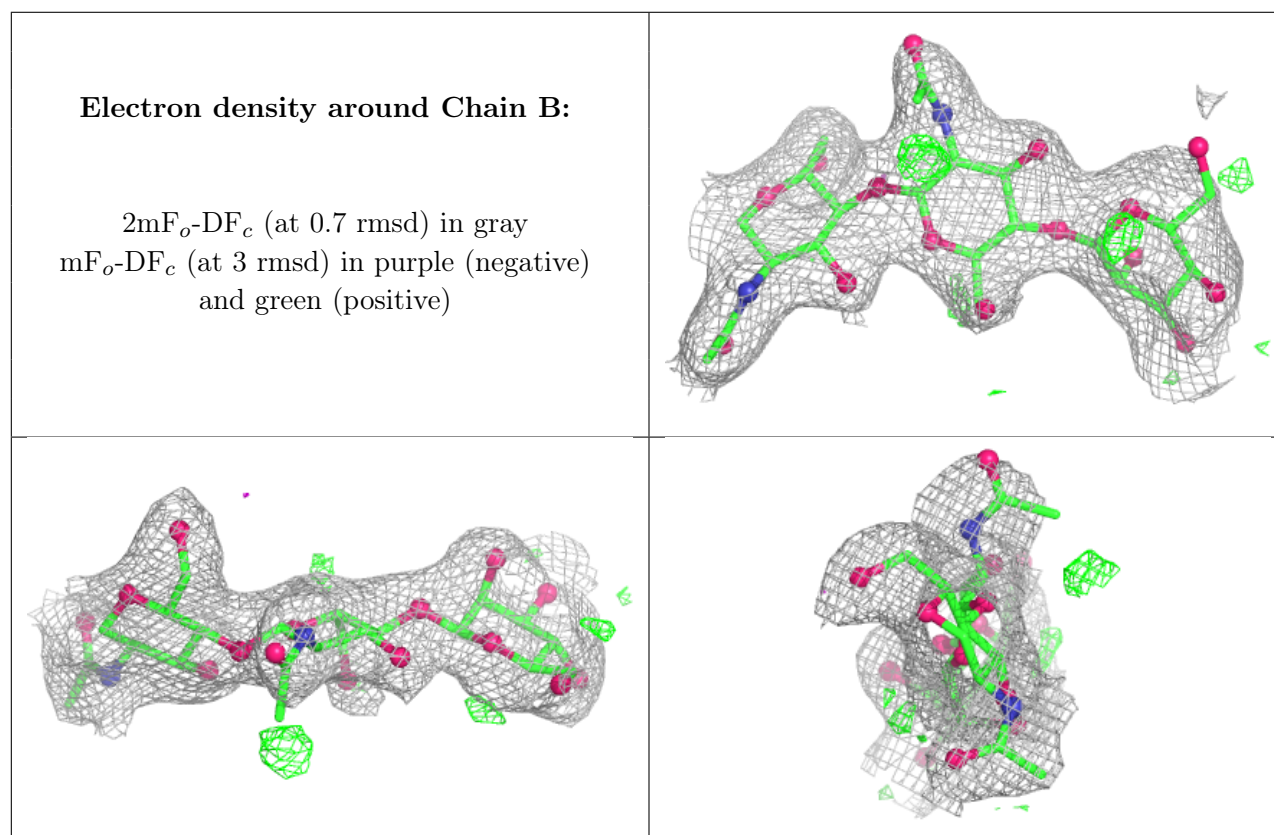
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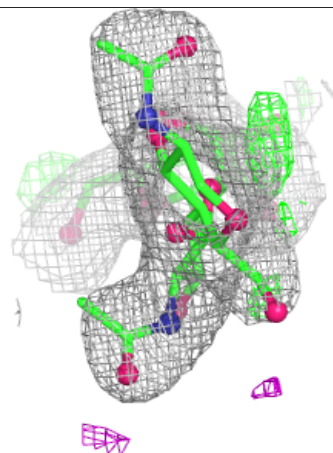
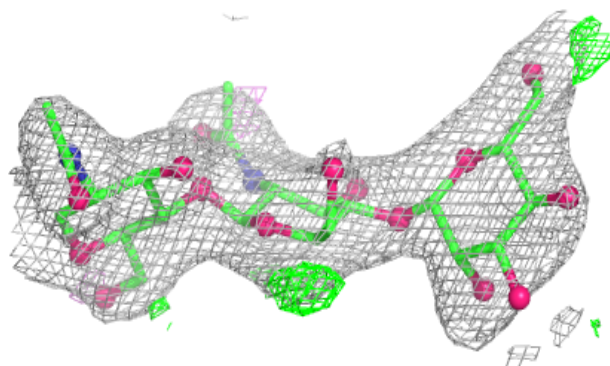
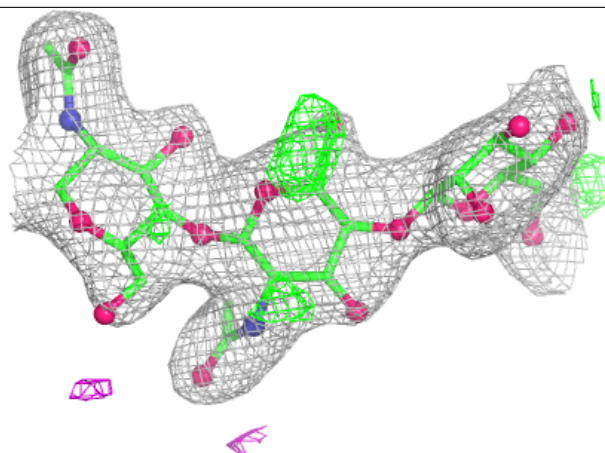
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	2	14/15	0.86	0.12	56,79,85,92	0
2	NAG	C	2	14/15	0.87	0.12	61,75,102,105	0
4	NAG	E	2	14/15	0.88	0.10	42,79,90,97	0
4	FUC	E	6	10/11	0.88	0.13	73,96,113,113	0
4	MAN	E	5	11/12	0.89	0.09	63,82,96,99	0
3	NAG	D	1	14/15	0.89	0.10	50,68,83,86	0
4	BMA	E	3	11/12	0.92	0.09	67,82,88,94	0
3	FUC	D	2	10/11	0.93	0.11	61,83,91,96	0
2	NAG	C	1	14/15	0.93	0.09	52,66,76,81	0
4	NAG	E	1	14/15	0.95	0.07	62,76,99,105	0
2	NAG	B	1	14/15	0.95	0.07	40,48,52,60	0
6	BGC	H	2	11/12	0.96	0.05	35,40,43,48	0
6	BGC	H	3	11/12	0.96	0.06	37,39,42,45	0
6	BGC	H	1	12/12	0.98	0.05	35,41,46,47	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.



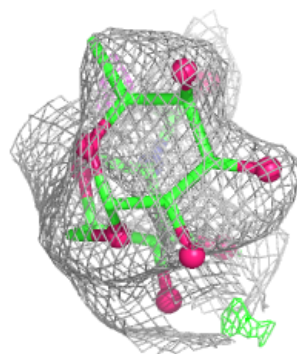
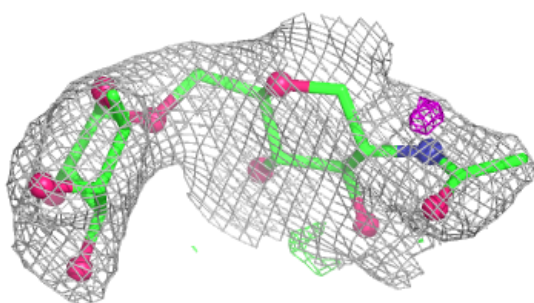
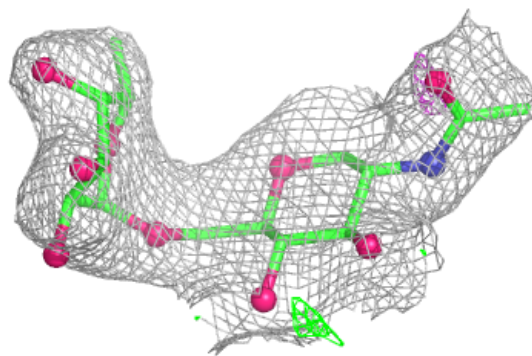
**Electron density around Chain C:**

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

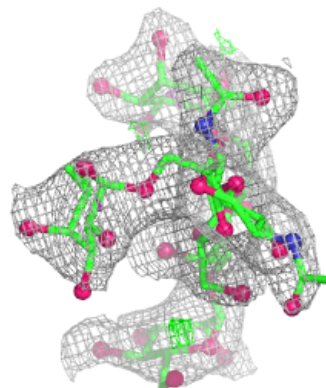
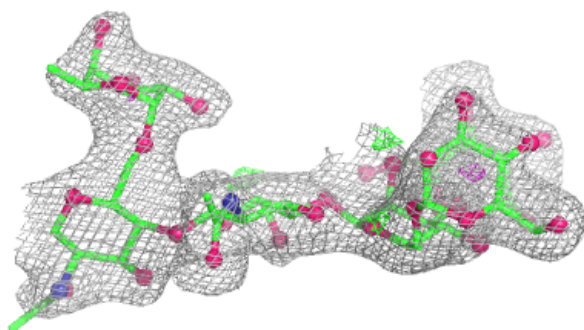
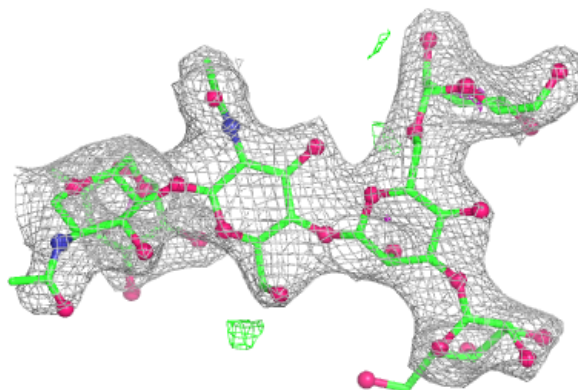


**Electron density around Chain D:**

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

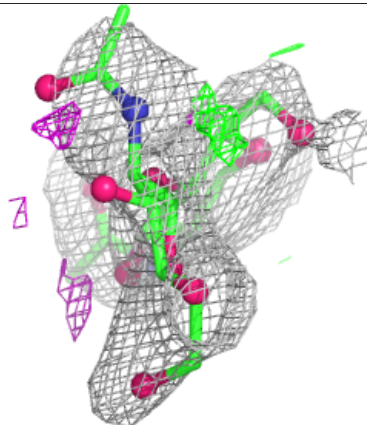
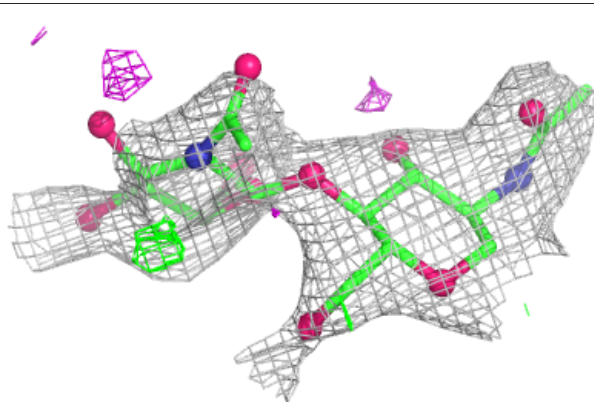
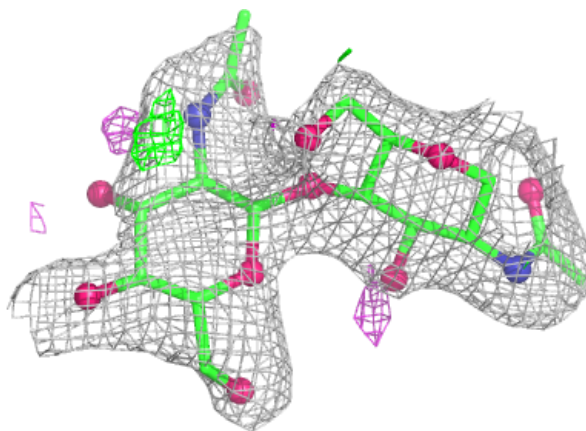
**Electron density around Chain E:**

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



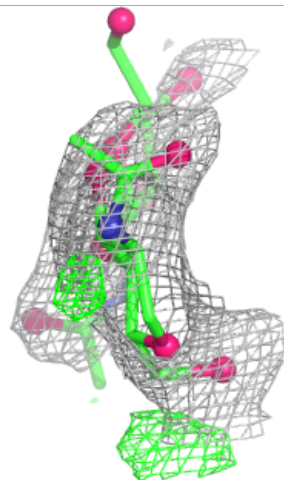
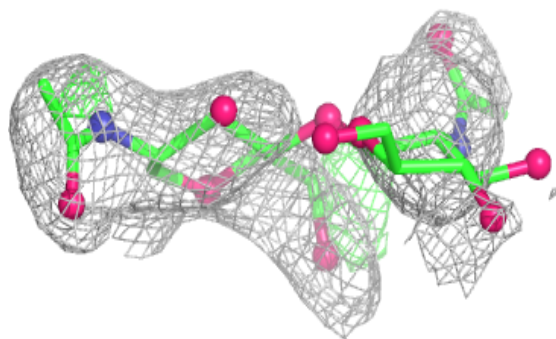
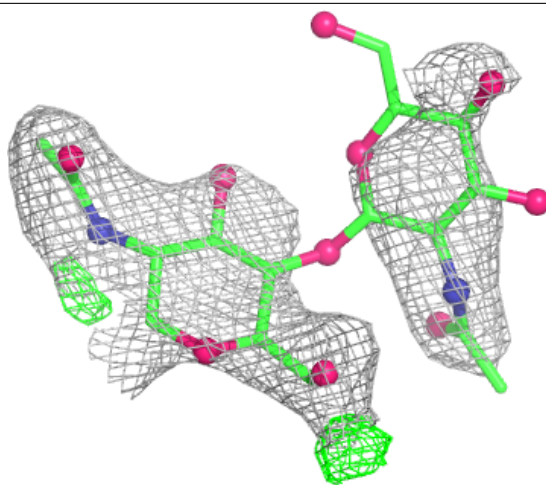
**Electron density around Chain F:**

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

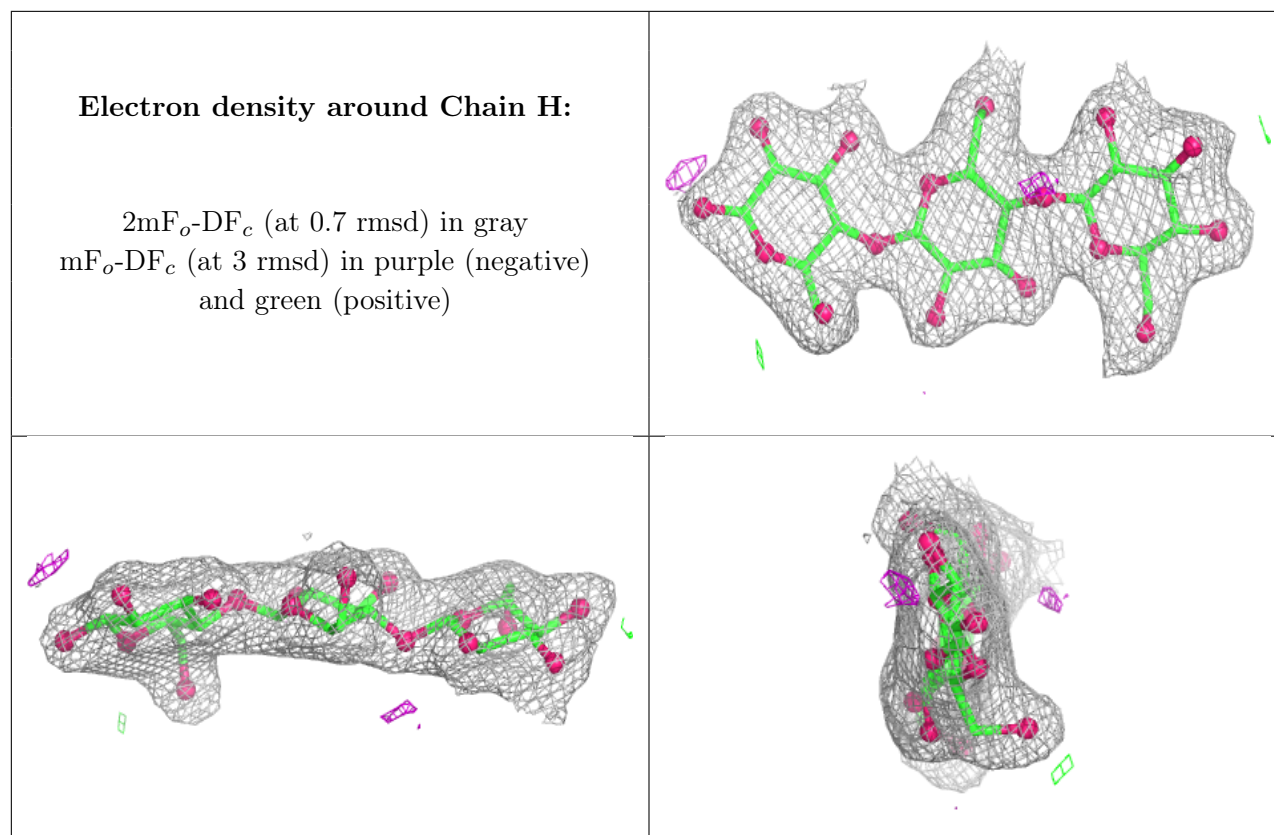


**Electron density around Chain G:**

$2mF_o-DF_c$  (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( $\text{\AA}^2$ )	Q<0.9
9	SO4	A	707	5/5	0.69	0.14	75,80,91,92	0
7	NAG	A	701	14/15	0.87	0.10	63,75,89,93	0
9	SO4	A	706	5/5	0.88	0.08	71,76,88,95	0
7	NAG	A	702	14/15	0.91	0.09	62,77,109,112	0
9	SO4	A	705	5/5	0.93	0.07	61,74,76,89	0
8	CA	A	703	1/1	0.97	0.12	59,59,59,59	0
9	SO4	A	704	5/5	0.99	0.06	42,46,54,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.