



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:57 AM BST

PDB ID : 4GDI  
Title : A subtype N10 neuraminidase-like protein of A/little yellow-shouldered bat/  
Guatemala/164/2009  
Authors : Zhu, X.; Wilson, I.A.  
Deposited on : 2012-07-31  
Resolution : 1.95 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 : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

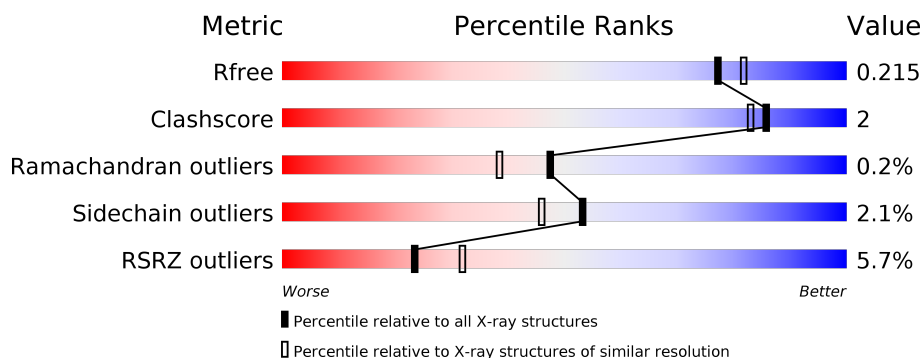
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	373	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div>•</div> </div> </div>
1	B	373	<div> <div>6%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>•</div> </div> </div>
1	C	373	<div> <div>10%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>••</div> </div> </div>
1	D	373	<div> <div>7%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>••</div> </div> </div>
1	E	373	<div> <div>6%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>••</div> </div> </div>
1	F	373	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	5	
3	H	6	
4	I	4	
4	K	4	
4	M	4	
5	J	3	
6	L	2	
7	N	3	

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	H	4	-	-	-	X
7	FUL	N	2	-	-	-	X
7	NAG	N	3	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 36150 atoms, of which 16780 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 Neuraminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	B	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	C	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	D	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	E	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			
1	F	367	Total	C	H	N	O	S	0	0	0
			5654	1816	2778	489	551	20			

There are 30 discrepancies between the modelled and reference sequences:

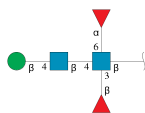
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	expression tag	UNP H6QM85
A	78	SER	-	expression tag	UNP H6QM85
A	79	PRO	-	expression tag	UNP H6QM85
A	80	SER	-	expression tag	UNP H6QM85
A	81	ARG	-	expression tag	UNP H6QM85
B	77	GLY	-	expression tag	UNP H6QM85
B	78	SER	-	expression tag	UNP H6QM85
B	79	PRO	-	expression tag	UNP H6QM85
B	80	SER	-	expression tag	UNP H6QM85
B	81	ARG	-	expression tag	UNP H6QM85
C	77	GLY	-	expression tag	UNP H6QM85
C	78	SER	-	expression tag	UNP H6QM85
C	79	PRO	-	expression tag	UNP H6QM85
C	80	SER	-	expression tag	UNP H6QM85
C	81	ARG	-	expression tag	UNP H6QM85
D	77	GLY	-	expression tag	UNP H6QM85
D	78	SER	-	expression tag	UNP H6QM85

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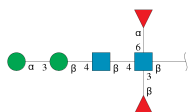
Chain	Residue	Modelled	Actual	Comment	Reference
D	79	PRO	-	expression tag	UNP H6QM85
D	80	SER	-	expression tag	UNP H6QM85
D	81	ARG	-	expression tag	UNP H6QM85
E	77	GLY	-	expression tag	UNP H6QM85
E	78	SER	-	expression tag	UNP H6QM85
E	79	PRO	-	expression tag	UNP H6QM85
E	80	SER	-	expression tag	UNP H6QM85
E	81	ARG	-	expression tag	UNP H6QM85
F	77	GLY	-	expression tag	UNP H6QM85
F	78	SER	-	expression tag	UNP H6QM85
F	79	PRO	-	expression tag	UNP H6QM85
F	80	SER	-	expression tag	UNP H6QM85
F	81	ARG	-	expression tag	UNP H6QM85

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



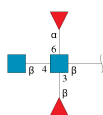
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	0	0	0
			59	34	2	23			

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



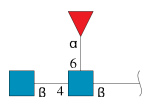
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	6	Total	C	N	O	0	0	0
			70	40	2	28			

- Molecule 4 is an oligosaccharide called beta-L-fucopyranose-(1-3)-[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	I	4	Total	C	N	O	0	0	0
			48	28	2	18			
4	K	4	Total	C	N	O	0	0	0
			48	28	2	18			
4	M	4	Total	C	N	O	0	0	0
			48	28	2	18			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



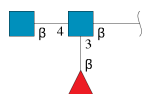
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



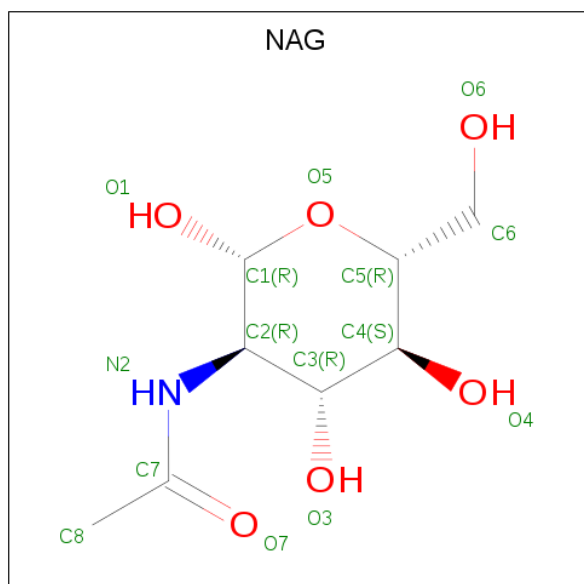
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 is an oligosaccharide called beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	N	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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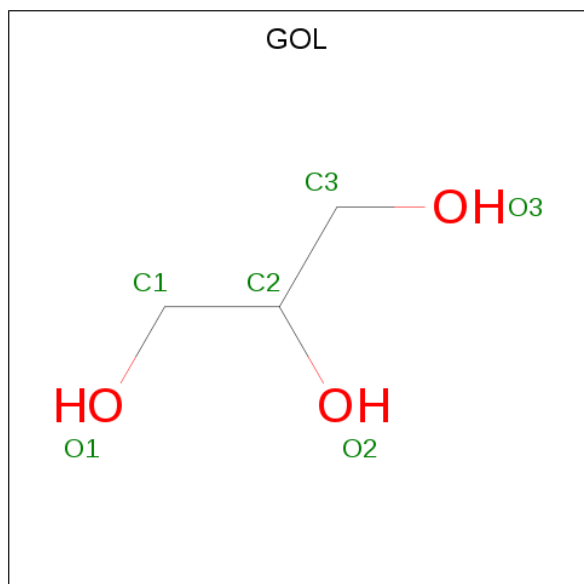
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Ca	0	0
			2	2		
9	E	2	Total	Ca	0	0
			2	2		
9	B	2	Total	Ca	0	0
			2	2		
9	C	2	Total	Ca	0	0
			2	2		
9	A	1	Total	Ca	0	0
			1	1		
9	F	2	Total	Ca	0	0
			2	2		

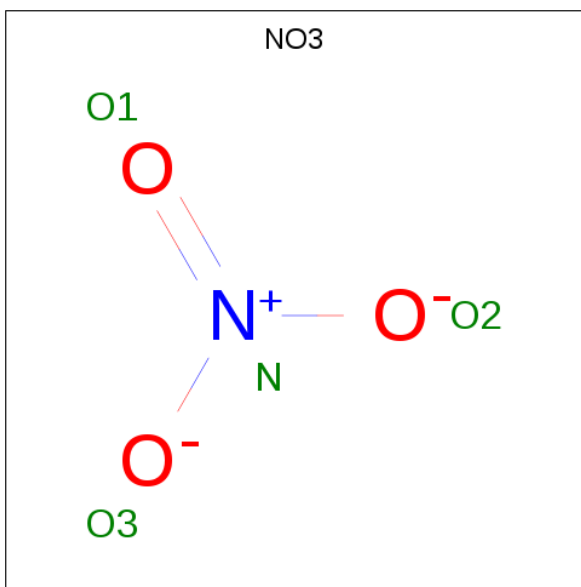
- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			14	3	8	3		
10	A	1	Total	C	H	O	0	0
			14	3	8	3		
10	A	1	Total	C	H	O	0	0
			14	3	8	3		
10	B	1	Total	C	H	O	0	0
			14	3	8	3		
10	B	1	Total	C	H	O	0	0
			14	3	8	3		
10	C	1	Total	C	H	O	0	0
			14	3	8	3		
10	D	1	Total	C	H	O	0	0
			14	3	8	3		
10	E	1	Total	C	H	O	0	0
			14	3	8	3		
10	E	1	Total	C	H	O	0	0
			14	3	8	3		
10	E	1	Total	C	H	O	0	0
			14	3	8	3		
10	F	1	Total	C	H	O	0	0
			14	3	8	3		
10	F	1	Total	C	H	O	0	0
			14	3	8	3		
10	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 11 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	N	O	0	0
			4	1	3		
11	A	1	Total	N	O	0	0
			4	1	3		
11	B	1	Total	N	O	0	0
			4	1	3		
11	B	1	Total	N	O	0	0
			4	1	3		
11	B	1	Total	N	O	0	0
			4	1	3		
11	B	1	Total	N	O	0	0
			4	1	3		
11	C	1	Total	N	O	0	0
			4	1	3		
11	C	1	Total	N	O	0	0
			4	1	3		
11	D	1	Total	N	O	0	0
			4	1	3		
11	D	1	Total	N	O	0	0
			4	1	3		
11	F	1	Total	N	O	0	0
			4	1	3		
11	F	1	Total	N	O	0	0
			4	1	3		
11	F	1	Total	N	O	0	0
			4	1	3		

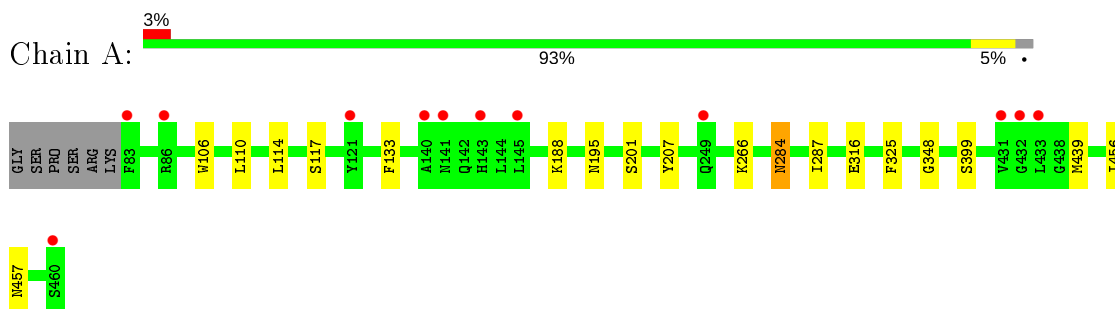
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	247	Total 247	O 247	0	0
12	B	246	Total 246	O 246	0	0
12	C	176	Total 176	O 176	0	0
12	D	213	Total 213	O 213	0	0
12	E	207	Total 207	O 207	0	0
12	F	319	Total 319	O 319	0	0

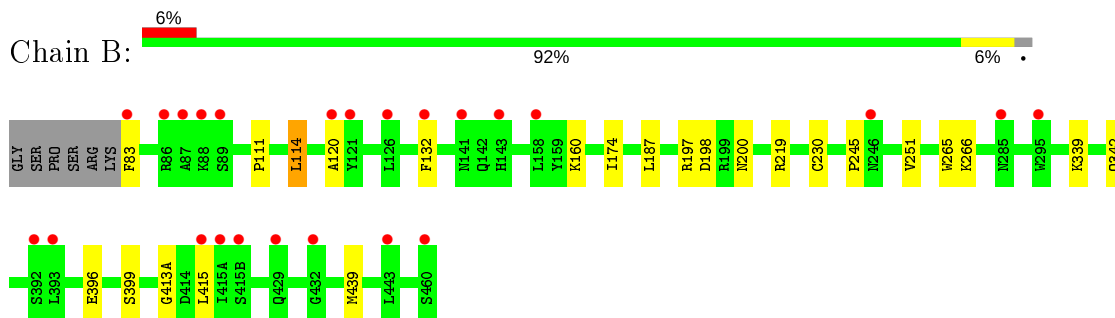
### 3 Residue-property plots

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.

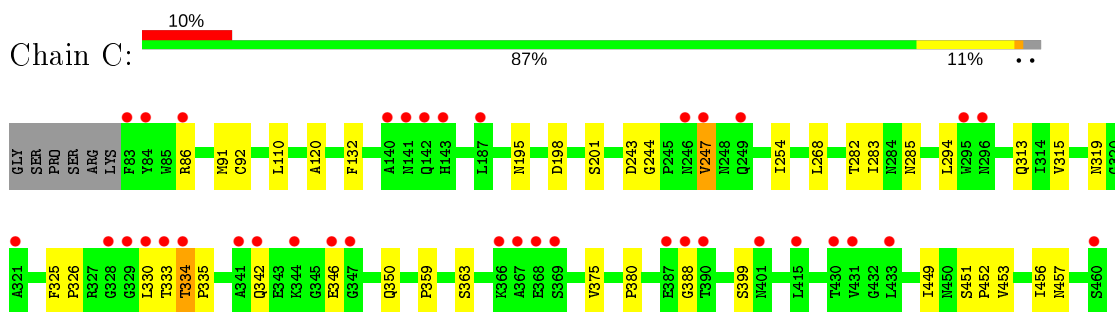
- Molecule 1: Neuraminidase



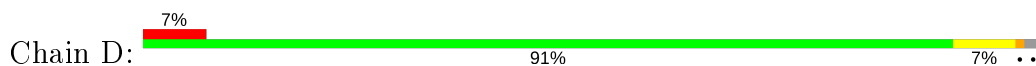
- Molecule 1: Neuraminidase

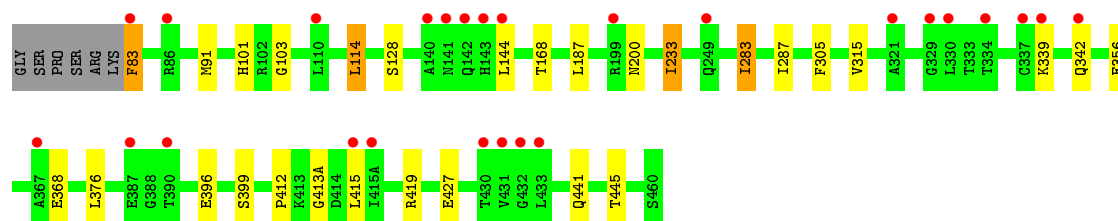


- Molecule 1: Neuraminidase

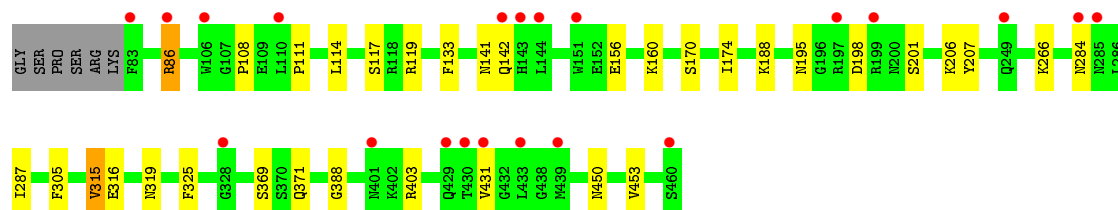
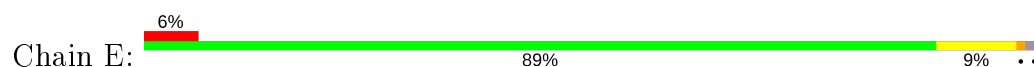


- Molecule 1: Neuraminidase

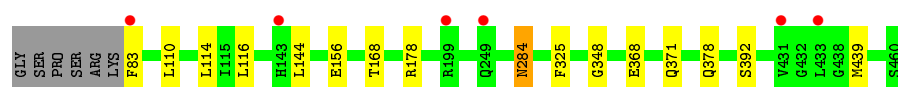
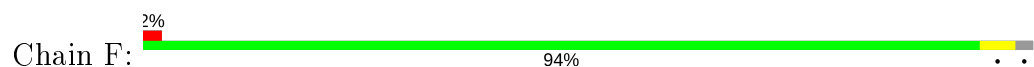




• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



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



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



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



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

Chain K:  25% 75%



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

Chain M:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



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

Chain L:  100%



- Molecule 7: beta-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  67% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.32Å 176.32Å 193.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.11 – 1.95 40.11 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.11-1.95) 98.6 (40.11-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.180 , 0.223 0.172 , 0.215	Depositor DCC
$R_{free}$ test set	10567 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	36150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: GOL, BMA, NAG, CA, FUC, FUL, NO3, 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	0.39	0/2945	0.58	0/3990
1	B	0.40	0/2945	0.58	0/3990
1	C	0.35	0/2945	0.55	0/3990
1	D	0.37	0/2945	0.55	0/3990
1	E	0.37	0/2945	0.56	0/3990
1	F	0.42	0/2945	0.59	0/3990
All	All	0.39	0/17670	0.57	0/23940

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	2876	2778	2775	9	0
1	B	2876	2778	2776	12	0
1	C	2876	2778	2776	19	0
1	D	2876	2778	2776	15	0
1	E	2876	2778	2775	14	0
1	F	2876	2778	2775	8	0
2	G	59	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	70	0	61	1	0
4	I	48	0	43	0	0
4	K	48	0	43	0	0
4	M	48	0	43	0	0
5	J	38	0	34	0	0
6	L	24	0	22	0	0
7	N	38	0	34	0	0
8	A	42	0	39	0	0
8	B	28	0	26	0	0
8	C	28	0	26	0	0
8	D	28	0	26	0	0
8	E	28	0	26	1	0
8	F	28	0	26	0	0
9	A	1	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	2	0	0	0	0
9	E	2	0	0	0	0
9	F	2	0	0	0	0
10	A	18	24	24	2	0
10	B	12	16	16	0	0
10	C	6	8	8	0	0
10	D	6	8	8	1	0
10	E	18	24	24	1	0
10	F	24	32	32	0	0
11	A	8	0	0	1	0
11	B	20	0	0	1	0
11	C	8	0	0	1	0
11	D	8	0	0	0	0
11	F	12	0	0	0	0
12	A	247	0	0	0	0
12	B	246	0	0	1	0
12	C	176	0	0	0	0
12	D	213	0	0	1	0
12	E	207	0	0	1	0
12	F	319	0	0	1	0
All	All	19370	16780	17266	78	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 2.

All (78) 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:C:451:SER:HB2	1:C:452:PRO:CD	2.29	0.63
1:E:108:PRO:HB2	1:E:431:VAL:HG13	1.82	0.60
1:D:91:MET:HE1	1:D:356:GLU:HG3	1.84	0.59
1:B:396:GLU:OE2	1:B:399:SER:OG	2.19	0.58
1:D:103:GLY:O	10:D:508:GOL:O3	2.21	0.57
1:A:399:SER:OG	1:A:457:ASN:ND2	2.38	0.56
1:C:350:GLN:N	11:C:510:NO3:O1	2.33	0.56
1:D:287:ILE:HD13	1:D:305:PHE:CE2	2.41	0.56
1:F:325:PHE:CE1	1:F:371:GLN:HG3	2.43	0.54
1:D:91:MET:CE	1:D:356:GLU:HG3	2.38	0.54
1:C:399:SER:OG	1:C:457:ASN:ND2	2.41	0.53
1:A:456:ILE:HG12	1:B:200:ASN:HB3	1.90	0.52
1:D:427:GLU:OE1	1:D:441:GLN:HG3	2.10	0.52
1:E:119:ARG:NH2	1:E:156:GLU:OE2	2.43	0.52
1:E:117:SER:HB3	1:E:133:PHE:CD2	2.46	0.51
1:F:116:LEU:HD12	1:F:144:LEU:HD21	1.94	0.50
8:E:505:NAG:O7	10:E:511:GOL:O1	2.29	0.50
1:D:412:PRO:HG2	1:D:419:ARG:NH2	2.27	0.49
1:F:156:GLU:OE2	1:F:178:ARG:NH1	2.45	0.49
1:F:284:ASN:O	1:F:284:ASN:ND2	2.40	0.48
1:C:195:ASN:O	1:C:201:SER:HA	2.13	0.48
1:D:396:GLU:OE2	1:D:399:SER:OG	2.29	0.48
1:B:111:PRO:HG2	1:B:114:LEU:HD12	1.95	0.48
1:A:117:SER:HB3	1:A:133:PHE:CD2	2.49	0.48
1:C:333:THR:OG1	1:C:334:THR:N	2.42	0.47
1:E:325:PHE:CE1	1:E:371:GLN:HG3	2.50	0.47
1:F:325:PHE:O	1:F:348:GLY:HA2	2.15	0.47
1:B:83:PHE:HB3	1:B:187:LEU:HD11	1.97	0.47
1:C:282:THR:O	1:C:283:ILE:HG23	2.14	0.47
1:C:451:SER:HB2	1:C:452:PRO:HD2	1.96	0.46
1:A:188:LYS:HB2	1:A:207:TYR:CZ	2.50	0.46
1:B:219:ARG:HG3	1:B:251:VAL:HG21	1.97	0.46
10:A:511:GOL:H32	11:A:513:NO3:O2	2.14	0.46
1:C:325:PHE:HA	1:C:326:PRO:C	2.36	0.46
1:C:449:ILE:HD11	1:C:453:VAL:HB	1.97	0.46
1:A:325:PHE:O	1:A:348:GLY:HA2	2.16	0.45
1:E:111:PRO:HG2	1:E:114:LEU:HD13	1.98	0.45
1:E:195:ASN:O	1:E:201:SER:HA	2.16	0.45
1:D:233:ILE:HD11	1:D:287:ILE:HD11	1.98	0.45
1:B:160:LYS:HB2	1:B:174:ILE:HD11	1.99	0.45
1:E:86:ARG:NH1	12:E:688:HOH:O	2.50	0.45
1:C:247:VAL:HG21	1:C:294:LEU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:N	1:A:287:ILE:HD12	2.31	0.44
1:D:101:HIS:HB3	1:D:445:THR:OG1	2.16	0.44
1:E:141:ASN:O	1:E:142:GLN:HB2	2.17	0.44
1:B:265:TRP:NE1	11:B:517:NO3:O2	2.49	0.44
1:A:316:GLU:HB2	10:A:512:GOL:H32	2.00	0.44
1:C:91:MET:HG2	1:C:92:CYS:O	2.18	0.44
1:C:313:GLN:HG2	1:C:315:VAL:HG23	2.00	0.43
1:C:359:PRO:HB3	1:C:380:PRO:HA	2.00	0.43
1:C:120:ALA:HA	1:C:132:PHE:O	2.19	0.43
1:C:456:ILE:CD1	1:D:200:ASN:HB3	2.48	0.43
1:E:160:LYS:HB2	1:E:174:ILE:HD11	2.01	0.42
1:A:106:TRP:NE1	1:A:114:LEU:HD21	2.34	0.42
1:D:283:ILE:HD11	1:D:356:GLU:OE2	2.18	0.42
3:H:3:BMA:H3	3:H:4:MAN:H2	1.41	0.42
1:E:188:LYS:HB2	1:E:207:TYR:CZ	2.55	0.42
1:A:195:ASN:O	1:A:201:SER:HA	2.20	0.42
1:B:197:ARG:HA	1:B:197:ARG:HD2	1.70	0.42
1:D:83:PHE:HB3	1:D:187:LEU:HD11	2.01	0.42
1:C:363:SER:HA	1:C:375:VAL:O	2.20	0.41
1:D:339:LYS:HE3	12:D:752:HOH:O	2.20	0.41
1:B:339:LYS:HD3	1:B:339:LYS:HA	1.86	0.41
1:E:450:ASN:C	1:E:450:ASN:OD1	2.59	0.41
1:B:413(A):GLY:O	1:B:415:LEU:N	2.53	0.41
1:B:245:PRO:HD2	12:B:721:HOH:O	2.19	0.41
1:C:243:ASP:OD1	1:C:244:GLY:N	2.51	0.41
1:E:315:VAL:CG1	1:E:316:GLU:N	2.84	0.41
1:F:114:LEU:HD23	1:F:168:THR:HG22	2.02	0.41
1:B:120:ALA:HA	1:B:132:PHE:O	2.21	0.41
1:F:378:GLN:OE1	1:F:392:SER:OG	2.32	0.41
1:D:114:LEU:HD22	1:D:168:THR:HG22	2.02	0.40
1:E:287:ILE:HD12	1:E:305:PHE:CE2	2.55	0.40
1:C:319:ASN:HB3	1:C:388:GLY:HA3	2.04	0.40
1:F:368:GLU:OE1	12:F:847:HOH:O	2.22	0.40
1:C:254:ILE:HG13	1:C:268:LEU:HD21	2.03	0.40
1:D:413(A):GLY:O	1:D:415:LEU:HG	2.22	0.40
1:E:319:ASN:HB3	1:E:388:GLY:HA3	2.03	0.40

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	365/373 (98%)	354 (97%)	10 (3%)	1 (0%)	41	30
1	B	365/373 (98%)	353 (97%)	12 (3%)	0	100	100
1	C	365/373 (98%)	349 (96%)	13 (4%)	3 (1%)	19	9
1	D	365/373 (98%)	353 (97%)	12 (3%)	0	100	100
1	E	365/373 (98%)	351 (96%)	13 (4%)	1 (0%)	41	30
1	F	365/373 (98%)	352 (96%)	13 (4%)	0	100	100
All	All	2190/2238 (98%)	2112 (96%)	73 (3%)	5 (0%)	47	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	ASN
1	C	198	ASP
1	C	285	ASN
1	E	198	ASP
1	C	335	PRO

### 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	320/325 (98%)	316 (99%)	4 (1%)	69	65
1	B	320/325 (98%)	314 (98%)	6 (2%)	57	50
1	C	320/325 (98%)	313 (98%)	7 (2%)	52	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	320/325 (98%)	310 (97%)	10 (3%)	40	28
1	E	320/325 (98%)	311 (97%)	9 (3%)	43	33
1	F	320/325 (98%)	316 (99%)	4 (1%)	69	65
All	All	1920/1950 (98%)	1880 (98%)	40 (2%)	53	46

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	A	266	LYS
1	A	284	ASN
1	A	439	MET
1	B	114	LEU
1	B	198	ASP
1	B	230	CYS
1	B	266	LYS
1	B	342	GLN
1	B	439	MET
1	C	86	ARG
1	C	110	LEU
1	C	247	VAL
1	C	330	LEU
1	C	334	THR
1	C	342	GLN
1	C	346	GLU
1	D	83	PHE
1	D	114	LEU
1	D	128	SER
1	D	144	LEU
1	D	233	ILE
1	D	283	ILE
1	D	315	VAL
1	D	342	GLN
1	D	368	GLU
1	D	376	LEU
1	E	86	ARG
1	E	170	SER
1	E	206	LYS
1	E	266	LYS
1	E	284	ASN
1	E	315	VAL

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Mol	Chain	Res	Type
1	E	369	SER
1	E	403	ARG
1	E	453	VAL
1	F	83	PHE
1	F	110	LEU
1	F	284	ASN
1	F	439	MET

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

Mol	Chain	Res	Type
1	C	143	HIS

### 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 ⓘ

31 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	G	1	1,2	14,14,15	0.55	0	17,19,21	1.29	3 (17%)
2	NAG	G	2	2	14,14,15	0.45	0	17,19,21	0.70	0
2	BMA	G	3	2	11,11,12	0.62	0	15,15,17	0.68	0
2	FUL	G	4	2	10,10,11	0.75	0	14,14,16	2.14	4 (28%)
2	FUC	G	5	2	10,10,11	0.67	0	14,14,16	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	H	1	1,3	14,14,15	0.62	0	17,19,21	1.56	3 (17%)
3	NAG	H	2	3	14,14,15	0.47	0	17,19,21	0.59	0
3	BMA	H	3	3	11,11,12	0.66	0	15,15,17	0.65	0
3	MAN	H	4	3	11,11,12	0.56	0	15,15,17	1.03	1 (6%)
3	FUL	H	5	3	10,10,11	0.82	0	14,14,16	2.68	5 (35%)
3	FUC	H	6	3	10,10,11	0.68	0	14,14,16	1.05	1 (7%)
4	NAG	I	1	1,4	14,14,15	0.65	0	17,19,21	1.24	3 (17%)
4	FUL	I	2	4	10,10,11	0.69	0	14,14,16	0.62	0
4	NAG	I	3	4	14,14,15	0.44	0	17,19,21	0.92	0
4	FUC	I	4	4	10,10,11	0.62	0	14,14,16	0.86	0
5	NAG	J	1	1,5	14,14,15	0.61	0	17,19,21	1.07	0
5	NAG	J	2	5	14,14,15	0.44	0	17,19,21	0.80	0
5	FUC	J	3	5	10,10,11	0.60	0	14,14,16	0.69	0
4	NAG	K	1	1,4	14,14,15	0.56	0	17,19,21	1.07	2 (11%)
4	FUL	K	2	4	10,10,11	0.73	0	14,14,16	2.29	4 (28%)
4	NAG	K	3	4	14,14,15	0.49	0	17,19,21	0.70	0
4	FUC	K	4	4	10,10,11	0.65	0	14,14,16	0.89	1 (7%)
6	NAG	L	1	1,6	14,14,15	0.53	0	17,19,21	1.10	2 (11%)
6	FUC	L	2	6	10,10,11	0.79	0	14,14,16	1.16	1 (7%)
4	NAG	M	1	1,4	14,14,15	0.50	0	17,19,21	1.23	1 (5%)
4	FUL	M	2	4	10,10,11	0.71	0	14,14,16	1.88	3 (21%)
4	NAG	M	3	4	14,14,15	0.52	0	17,19,21	0.90	0
4	FUC	M	4	4	10,10,11	0.70	0	14,14,16	1.04	0
7	NAG	N	1	1,7	14,14,15	0.60	0	17,19,21	1.30	4 (23%)
7	FUL	N	2	7	10,10,11	0.70	0	14,14,16	0.56	0
7	NAG	N	3	7	14,14,15	0.49	0	17,19,21	0.85	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	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	BMA	G	3	2	-	1/2/19/22	0/1/1/1
2	FUL	G	4	2	-	-	0/1/1/1
2	FUC	G	5	2	-	-	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	H	3	3	-	0/2/19/22	1/1/1/1
3	MAN	H	4	3	-	1/2/19/22	1/1/1/1
3	FUL	H	5	3	-	-	0/1/1/1
3	FUC	H	6	3	-	-	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	FUL	I	2	4	-	-	0/1/1/1
4	NAG	I	3	4	-	1/6/23/26	0/1/1/1
4	FUC	I	4	4	-	-	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	FUC	J	3	5	-	-	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	FUL	K	2	4	-	-	0/1/1/1
4	NAG	K	3	4	-	0/6/23/26	0/1/1/1
4	FUC	K	4	4	-	-	0/1/1/1
6	NAG	L	1	1,6	-	2/6/23/26	0/1/1/1
6	FUC	L	2	6	-	-	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	FUL	M	2	4	-	-	0/1/1/1
4	NAG	M	3	4	-	0/6/23/26	0/1/1/1
4	FUC	M	4	4	-	-	0/1/1/1
7	NAG	N	1	1,7	-	2/6/23/26	0/1/1/1
7	FUL	N	2	7	-	-	0/1/1/1
7	NAG	N	3	7	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	5	FUL	C1-C2-C3	-7.21	100.80	109.67
4	K	2	FUL	C1-C2-C3	-6.17	102.09	109.67
2	G	4	FUL	C1-C2-C3	-5.52	102.88	109.67
4	M	2	FUL	C1-C2-C3	-4.58	104.03	109.67
4	K	2	FUL	O5-C1-C2	-3.76	104.96	110.77
3	H	5	FUL	C3-C4-C5	3.74	115.59	109.77
4	M	2	FUL	C1-O5-C5	-3.64	104.53	112.78
2	G	4	FUL	O5-C1-C2	-3.33	105.63	110.77
3	H	1	NAG	O3-C3-C2	-3.32	102.60	109.47
3	H	5	FUL	O5-C1-C2	-3.29	105.69	110.77
6	L	2	FUC	O5-C1-C2	-3.19	105.85	110.77
4	M	1	NAG	O3-C3-C2	-3.12	103.01	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	NAG	C2-N2-C7	-3.05	118.57	122.90
3	H	1	NAG	O5-C1-C2	-2.97	106.61	111.29
4	M	2	FUL	O5-C1-C2	-2.94	106.23	110.77
3	H	5	FUL	C1-O5-C5	-2.89	106.22	112.78
2	G	4	FUL	C3-C4-C5	2.77	114.09	109.77
3	H	6	FUC	C6-C5-C4	-2.66	108.15	113.07
3	H	4	MAN	C1-O5-C5	2.60	115.71	112.19
3	H	1	NAG	C2-N2-C7	-2.59	119.22	122.90
2	G	1	NAG	O3-C3-C2	-2.48	104.33	109.47
3	H	5	FUL	O5-C5-C4	2.44	113.91	109.52
2	G	4	FUL	C1-O5-C5	-2.39	107.37	112.78
7	N	1	NAG	O5-C1-C2	-2.37	107.54	111.29
4	I	1	NAG	O3-C3-C4	-2.36	104.90	110.35
7	N	1	NAG	C4-C3-C2	2.35	114.47	111.02
2	G	1	NAG	O5-C1-C2	-2.34	107.59	111.29
6	L	1	NAG	C1-O5-C5	2.32	115.33	112.19
7	N	1	NAG	O5-C5-C6	2.26	110.74	107.20
6	L	1	NAG	C2-N2-C7	-2.23	119.73	122.90
4	K	2	FUL	C1-O5-C5	-2.23	107.72	112.78
4	I	1	NAG	C4-C3-C2	2.22	114.27	111.02
4	K	4	FUC	C6-C5-C4	-2.21	108.98	113.07
4	K	1	NAG	C2-N2-C7	-2.18	119.80	122.90
7	N	1	NAG	C1-O5-C5	2.17	115.13	112.19
4	I	1	NAG	C3-C4-C5	2.15	114.07	110.24
4	K	2	FUL	C3-C4-C5	2.11	113.07	109.77
4	K	1	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	1	NAG	C4-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
7	N	1	NAG	C8-C7-N2-C2
7	N	3	NAG	C4-C5-C6-O6
2	G	3	BMA	O5-C5-C6-O6
7	N	1	NAG	O7-C7-N2-C2
3	H	4	MAN	C4-C5-C6-O6
5	J	1	NAG	C8-C7-N2-C2
7	N	3	NAG	O5-C5-C6-O6
5	J	1	NAG	O7-C7-N2-C2
4	I	3	NAG	C4-C5-C6-O6

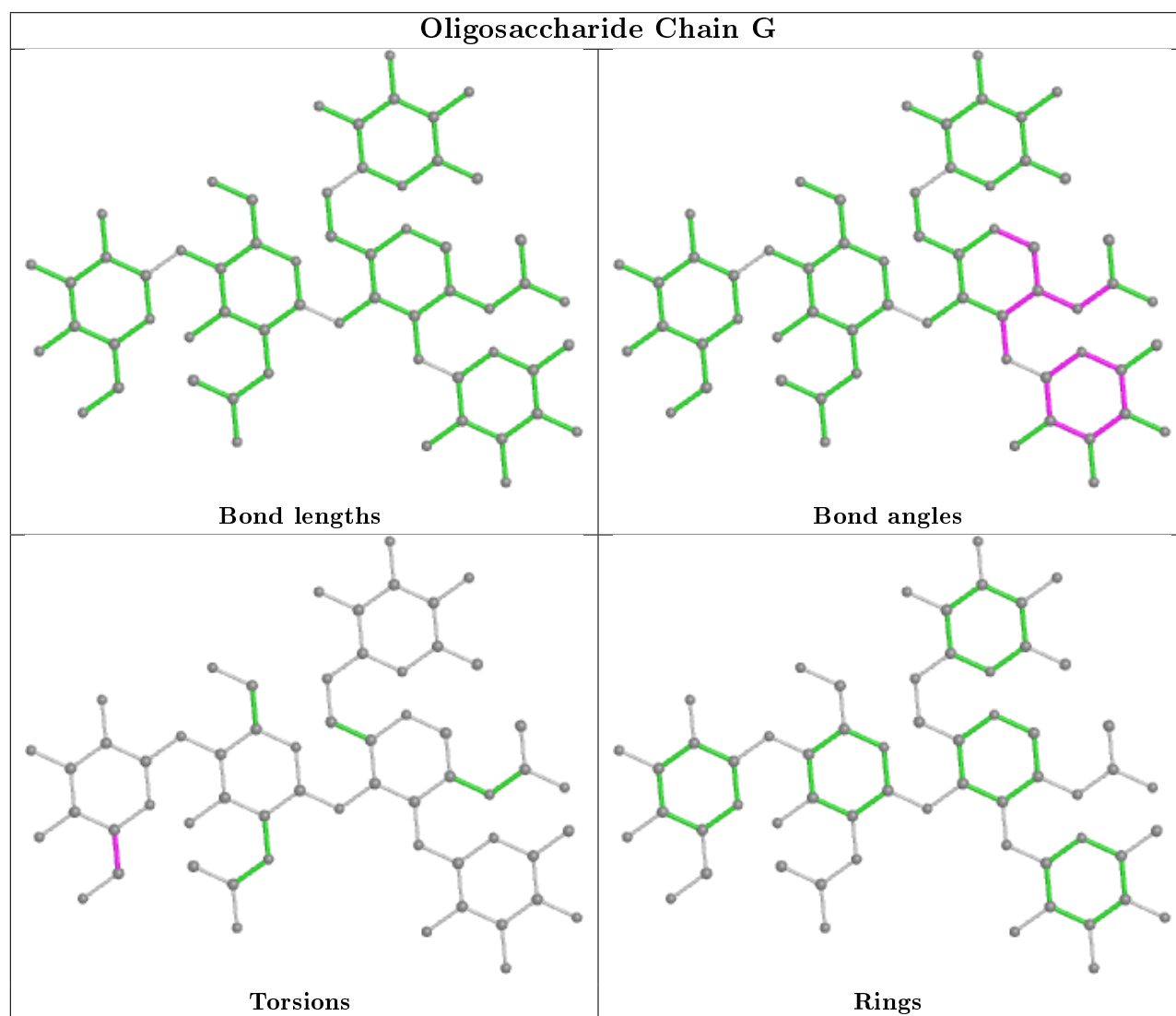
All (2) ring outliers are listed below:

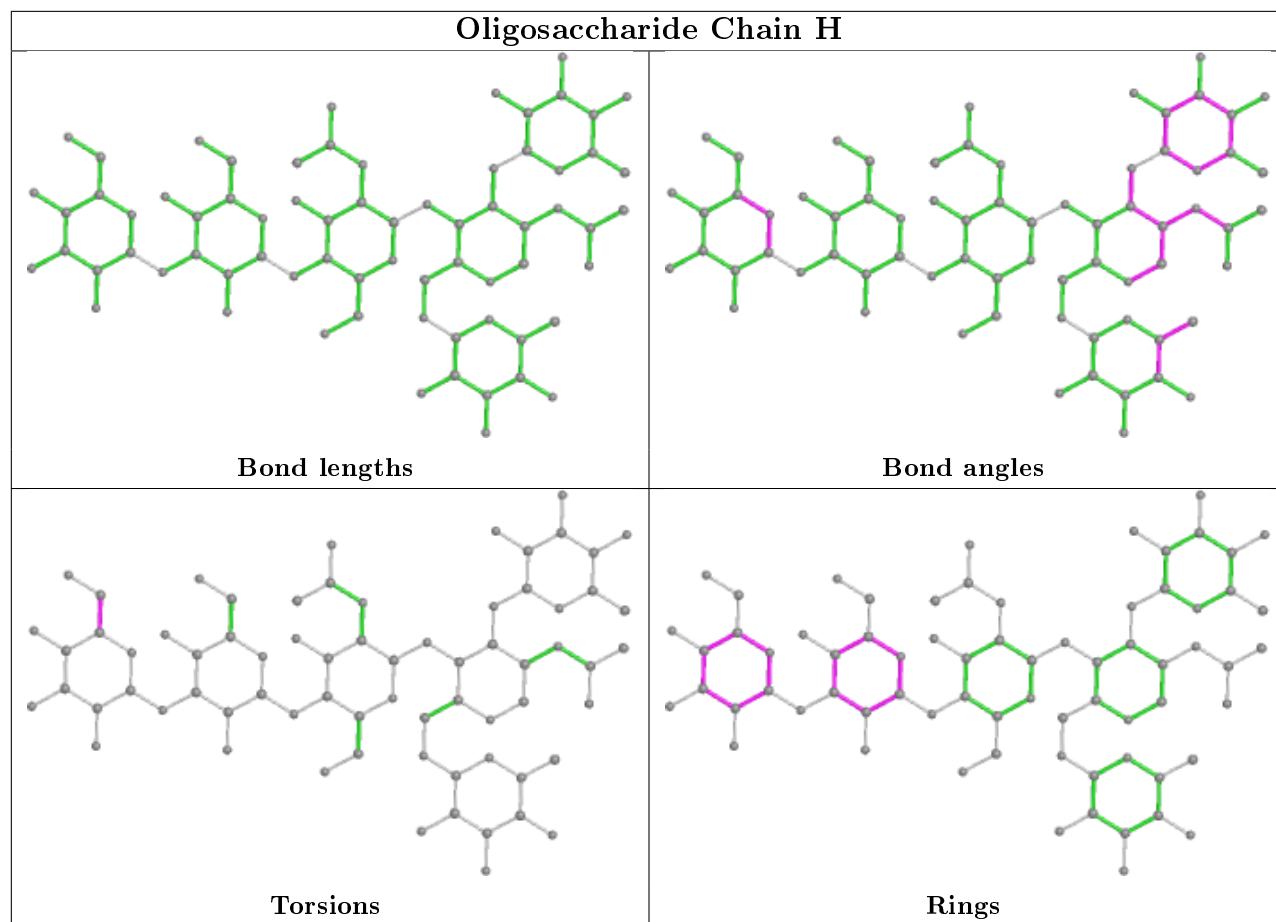
Mol	Chain	Res	Type	Atoms
3	H	3	BMA	C1-C2-C3-C4-C5-O5
3	H	4	MAN	C1-C2-C3-C4-C5-O5

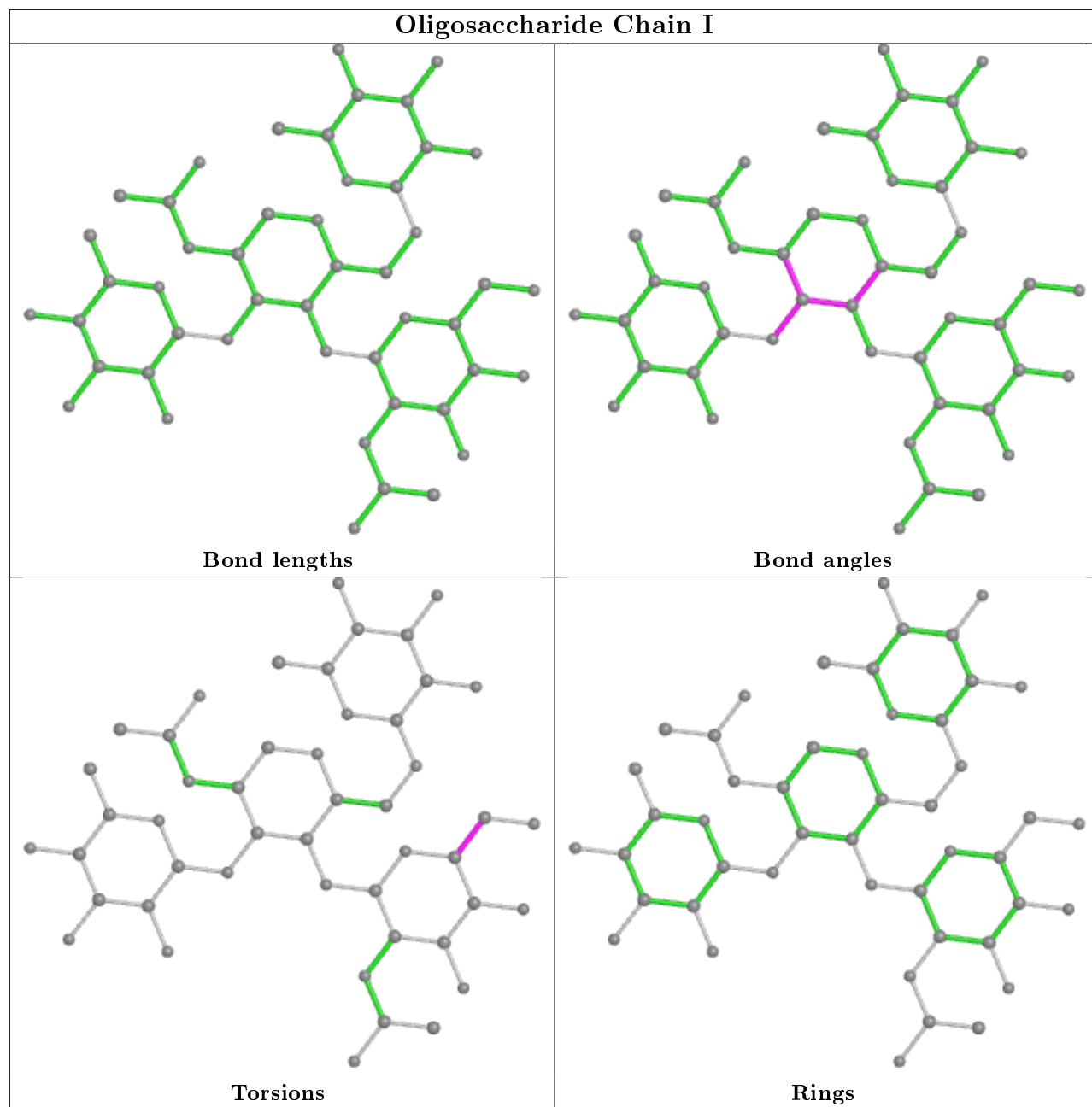
2 monomers are involved in 1 short contact:

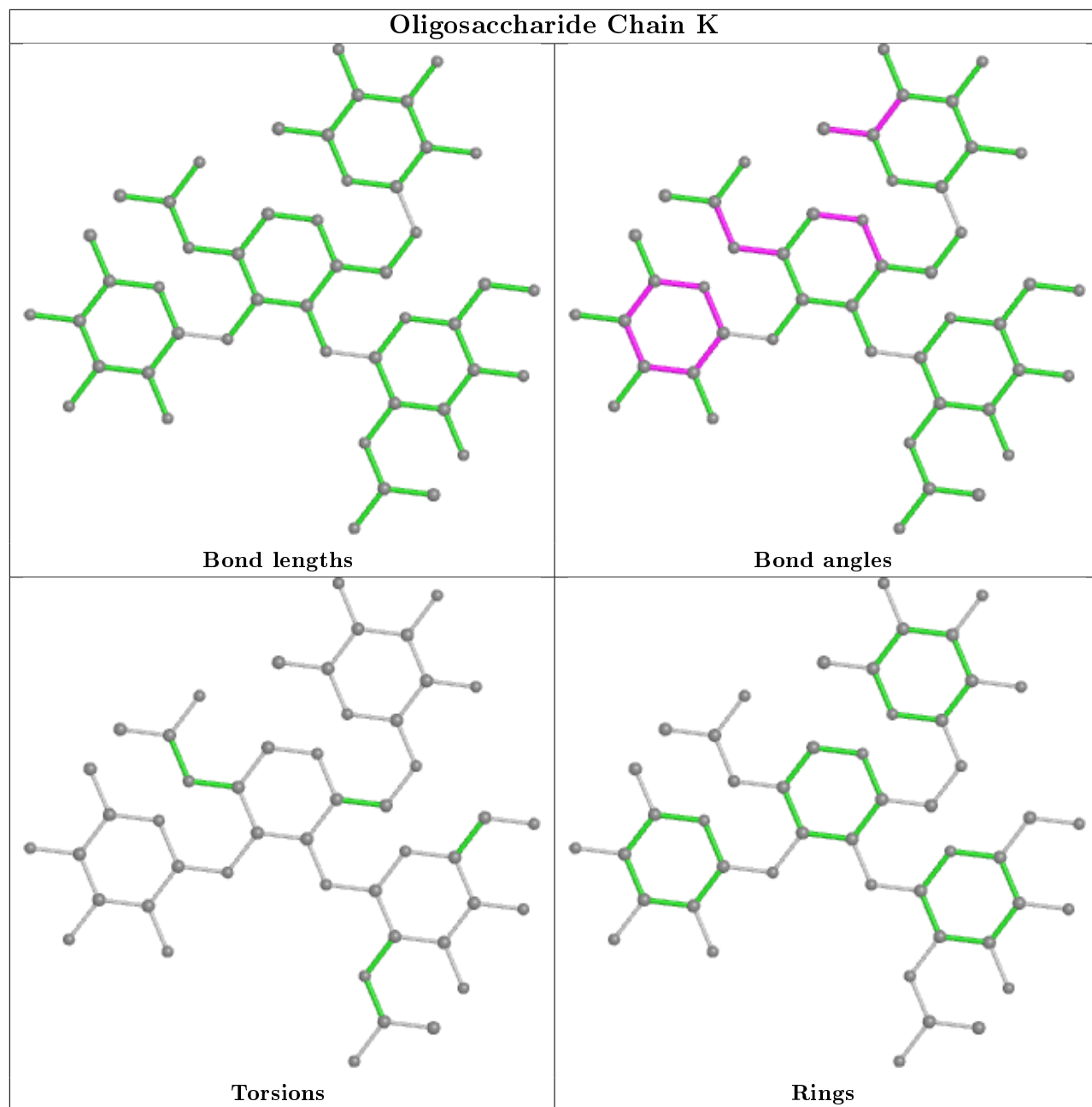
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	3	BMA	1	0
3	H	4	MAN	1	0

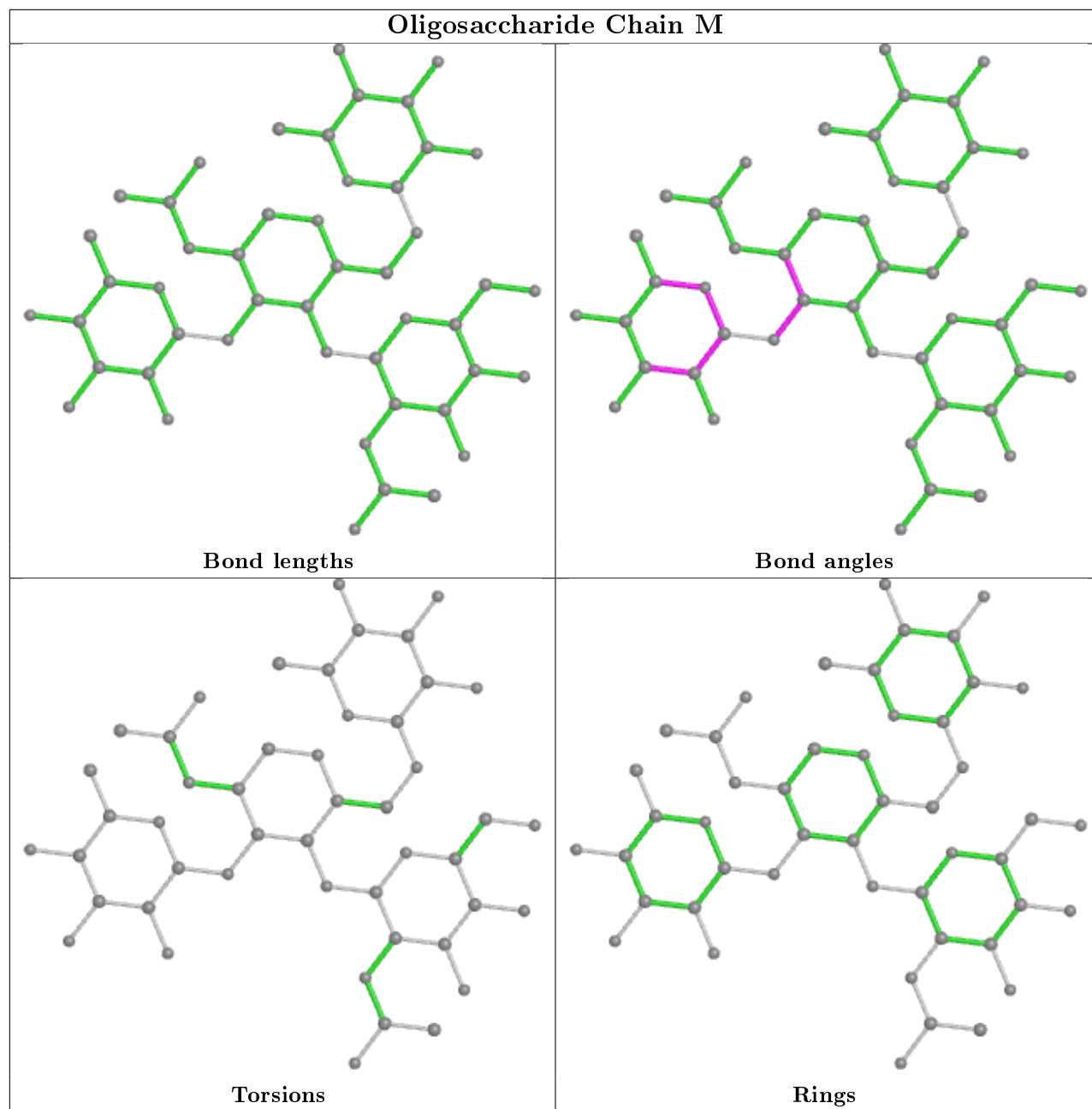
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

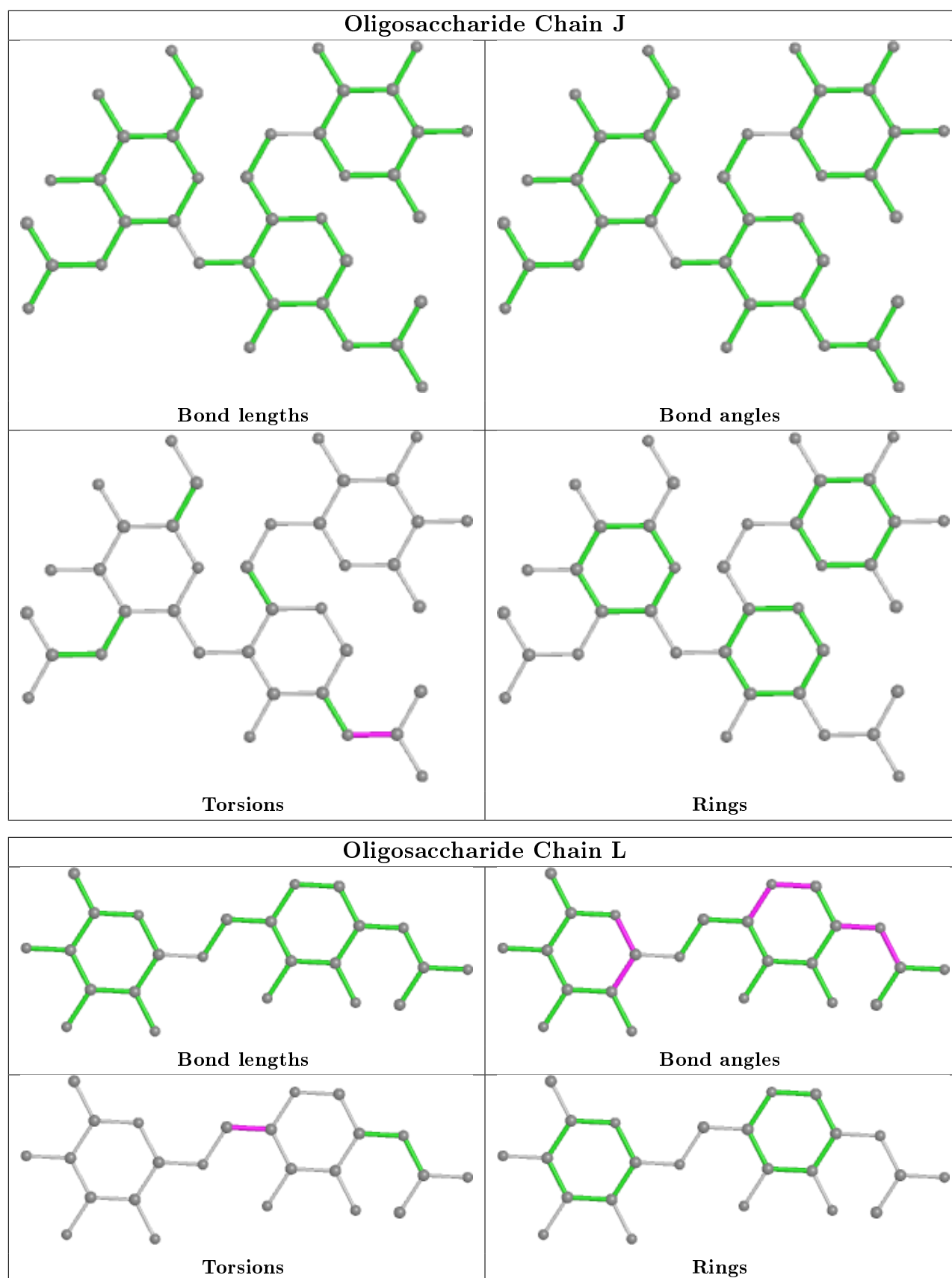


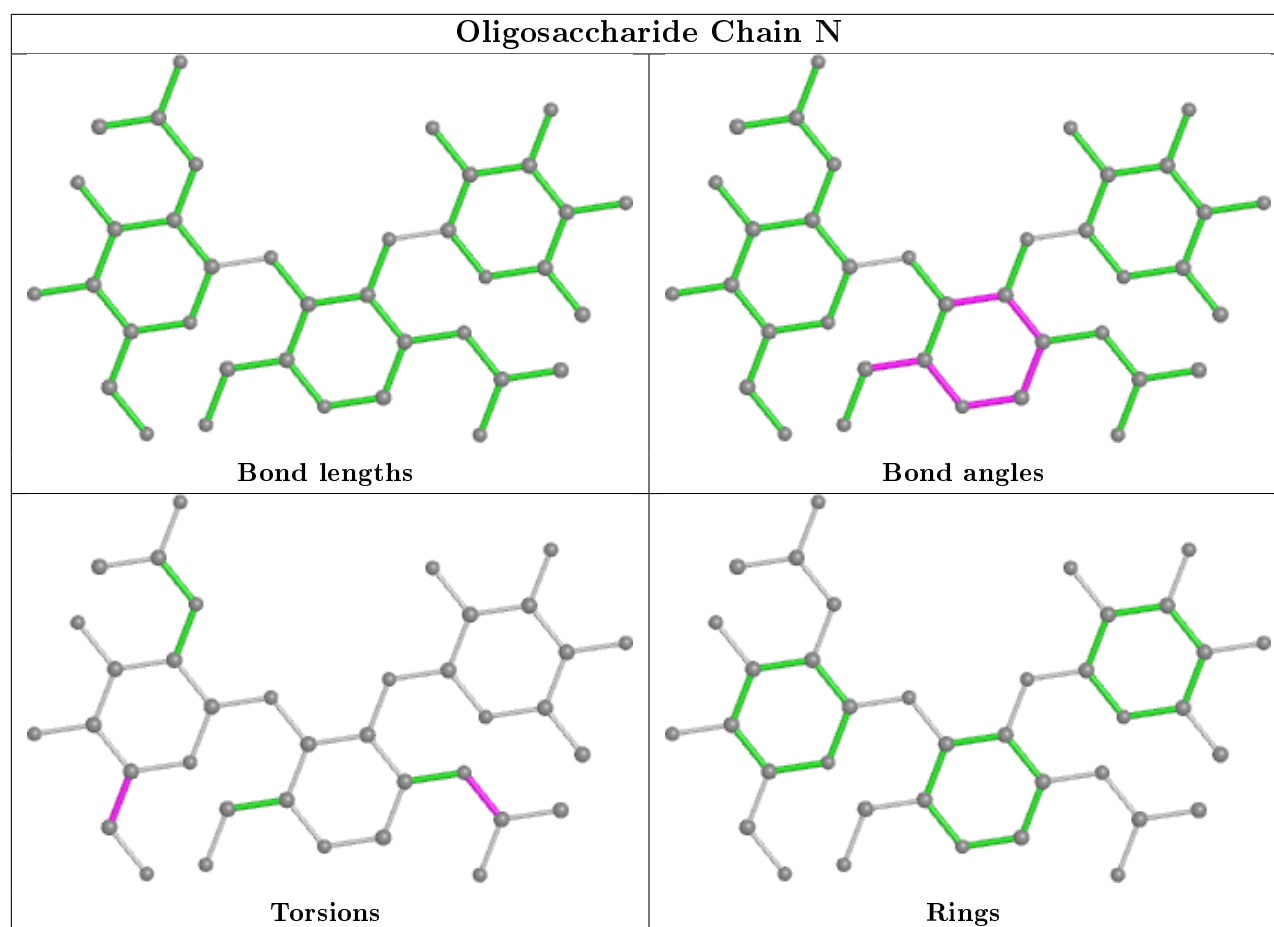












## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 11 are monoatomic - leaving 41 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	$\# Z  > 2$
11	NO3	C	510	-	1,3,3	3.34	1 (100%)	0,3,3	0.00	-
11	NO3	B	517	-	1,3,3	3.53	1 (100%)	0,3,3	0.00	-
11	NO3	F	518	-	1,3,3	3.45	1 (100%)	0,3,3	0.00	-
11	NO3	D	510	-	1,3,3	3.55	1 (100%)	0,3,3	0.00	-
8	NAG	D	504	1	14,14,15	0.54	0	17,19,21	1.39	1 (5%)
10	GOL	A	512	-	5,5,5	0.43	0	5,5,5	0.18	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	B	508	1	14,14,15	0.54	0	17,19,21	0.84	0
8	NAG	A	508	1	14,14,15	0.57	0	17,19,21	1.04	1 (5%)
11	NO3	B	513	-	1,3,3	3.65	1 (100%)	0,3,3	0.00	-
10	GOL	B	512	-	5,5,5	0.31	0	5,5,5	0.30	0
11	NO3	D	509	-	1,3,3	3.41	1 (100%)	0,3,3	0.00	-
10	GOL	A	510	-	5,5,5	0.31	0	5,5,5	0.44	0
8	NAG	A	507	1	14,14,15	0.42	0	17,19,21	1.31	3 (17%)
8	NAG	A	506	1	14,14,15	0.52	0	17,19,21	1.10	1 (5%)
10	GOL	C	509	-	5,5,5	0.34	0	5,5,5	0.50	0
11	NO3	A	514	-	1,3,3	3.61	1 (100%)	0,3,3	0.00	-
10	GOL	D	508	-	5,5,5	0.37	0	5,5,5	0.37	0
11	NO3	B	516	-	1,3,3	3.29	1 (100%)	0,3,3	0.00	-
8	NAG	F	506	1	14,14,15	0.52	0	17,19,21	0.92	1 (5%)
10	GOL	F	512	-	5,5,5	0.54	0	5,5,5	0.60	0
8	NAG	F	505	1	14,14,15	0.58	0	17,19,21	0.85	1 (5%)
11	NO3	C	511	-	1,3,3	3.46	1 (100%)	0,3,3	0.00	-
8	NAG	B	507	1	14,14,15	0.64	0	17,19,21	0.96	0
11	NO3	B	514	-	1,3,3	3.44	1 (100%)	0,3,3	0.00	-
10	GOL	F	513	-	5,5,5	0.34	0	5,5,5	0.48	0
10	GOL	E	511	-	5,5,5	0.33	0	5,5,5	0.43	0
8	NAG	C	505	1	14,14,15	0.57	0	17,19,21	0.85	0
11	NO3	F	517	-	1,3,3	3.74	1 (100%)	0,3,3	0.00	-
10	GOL	B	511	-	5,5,5	0.31	0	5,5,5	0.40	0
11	NO3	F	516	-	1,3,3	3.53	1 (100%)	0,3,3	0.00	-
10	GOL	E	513	-	5,5,5	0.35	0	5,5,5	0.26	0
10	GOL	F	515	-	5,5,5	0.34	0	5,5,5	0.49	0
10	GOL	F	514	-	5,5,5	0.34	0	5,5,5	0.31	0
11	NO3	B	515	-	1,3,3	3.70	1 (100%)	0,3,3	0.00	-
10	GOL	A	511	-	5,5,5	0.45	0	5,5,5	0.20	0
8	NAG	C	506	1	14,14,15	0.66	0	17,19,21	1.15	1 (5%)
8	NAG	E	505	1	14,14,15	0.63	0	17,19,21	0.86	0
8	NAG	D	505	1	14,14,15	0.59	0	17,19,21	1.18	2 (11%)
10	GOL	E	512	-	5,5,5	0.47	0	5,5,5	0.25	0
11	NO3	A	513	-	1,3,3	3.49	1 (100%)	0,3,3	0.00	-
8	NAG	E	508	1	14,14,15	0.68	0	17,19,21	1.23	2 (11%)

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
8	NAG	D	504	1	-	0/6/23/26	0/1/1/1
10	GOL	A	512	-	-	1/4/4/4	-
8	NAG	B	508	1	-	0/6/23/26	0/1/1/1
8	NAG	A	508	1	-	2/6/23/26	0/1/1/1
10	GOL	B	512	-	-	2/4/4/4	-
10	GOL	A	510	-	-	2/4/4/4	-
8	NAG	A	507	1	-	2/6/23/26	0/1/1/1
8	NAG	A	506	1	-	4/6/23/26	0/1/1/1
10	GOL	C	509	-	-	2/4/4/4	-
10	GOL	D	508	-	-	2/4/4/4	-
10	GOL	F	515	-	-	3/4/4/4	-
10	GOL	F	512	-	-	2/4/4/4	-
8	NAG	F	505	1	-	0/6/23/26	0/1/1/1
8	NAG	B	507	1	-	0/6/23/26	0/1/1/1
10	GOL	F	513	-	-	2/4/4/4	-
10	GOL	E	511	-	-	4/4/4/4	-
8	NAG	C	505	1	-	0/6/23/26	0/1/1/1
10	GOL	B	511	-	-	0/4/4/4	-
8	NAG	F	506	1	-	0/6/23/26	0/1/1/1
10	GOL	E	513	-	-	4/4/4/4	-
10	GOL	F	514	-	-	3/4/4/4	-
10	GOL	A	511	-	-	0/4/4/4	-
8	NAG	C	506	1	-	0/6/23/26	0/1/1/1
8	NAG	E	505	1	-	0/6/23/26	0/1/1/1
8	NAG	D	505	1	-	0/6/23/26	0/1/1/1
10	GOL	E	512	-	-	4/4/4/4	-
8	NAG	E	508	1	-	2/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	517	NO3	O1-N	3.74	1.41	1.24
11	B	515	NO3	O1-N	3.70	1.41	1.24
11	B	513	NO3	O1-N	3.65	1.40	1.24
11	A	514	NO3	O1-N	3.61	1.40	1.24
11	D	510	NO3	O1-N	3.55	1.40	1.24
11	F	516	NO3	O1-N	3.53	1.40	1.24
11	B	517	NO3	O1-N	3.53	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	513	NO3	O1-N	3.49	1.40	1.24
11	C	511	NO3	O1-N	3.46	1.40	1.24
11	F	518	NO3	O1-N	3.45	1.40	1.24
11	B	514	NO3	O1-N	3.44	1.39	1.24
11	D	509	NO3	O1-N	3.41	1.39	1.24
11	C	510	NO3	O1-N	3.34	1.39	1.24
11	B	516	NO3	O1-N	3.29	1.39	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	504	NAG	C1-O5-C5	4.47	118.25	112.19
8	A	506	NAG	O5-C1-C2	-3.18	106.27	111.29
8	D	505	NAG	C4-C3-C2	3.09	115.55	111.02
8	A	507	NAG	C4-C3-C2	-3.06	106.53	111.02
8	E	508	NAG	C2-N2-C7	-3.03	118.59	122.90
8	C	506	NAG	C4-C3-C2	2.91	115.28	111.02
8	A	508	NAG	O5-C5-C6	2.63	111.33	107.20
8	E	508	NAG	C1-O5-C5	-2.53	108.77	112.19
8	A	507	NAG	O5-C5-C6	2.49	111.11	107.20
8	A	507	NAG	C1-O5-C5	2.33	115.35	112.19
8	D	505	NAG	O5-C5-C6	2.23	110.69	107.20
8	F	505	NAG	O5-C5-C6	2.18	110.61	107.20
8	F	506	NAG	C2-N2-C7	-2.13	119.86	122.90

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	507	NAG	O7-C7-N2-C2
10	C	509	GOL	O1-C1-C2-C3
10	D	508	GOL	O1-C1-C2-C3
10	E	511	GOL	O1-C1-C2-C3
10	E	513	GOL	O1-C1-C2-O2
10	E	513	GOL	O1-C1-C2-C3
8	A	507	NAG	C8-C7-N2-C2
8	A	506	NAG	C8-C7-N2-C2
8	A	506	NAG	O7-C7-N2-C2
10	C	509	GOL	O1-C1-C2-O2
10	E	511	GOL	O1-C1-C2-O2
10	A	510	GOL	O1-C1-C2-C3
10	F	512	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
10	F	513	GOL	O1-C1-C2-C3
10	E	513	GOL	C1-C2-C3-O3
10	F	515	GOL	O1-C1-C2-C3
10	F	515	GOL	C1-C2-C3-O3
10	F	514	GOL	O1-C1-C2-C3
10	E	512	GOL	O1-C1-C2-C3
10	E	512	GOL	C1-C2-C3-O3
10	D	508	GOL	O1-C1-C2-O2
10	E	513	GOL	O2-C2-C3-O3
10	F	515	GOL	O1-C1-C2-O2
8	A	508	NAG	C8-C7-N2-C2
10	A	510	GOL	O1-C1-C2-O2
10	F	513	GOL	O1-C1-C2-O2
10	E	512	GOL	O1-C1-C2-O2
8	A	506	NAG	C4-C5-C6-O6
10	F	512	GOL	O2-C2-C3-O3
10	E	511	GOL	O2-C2-C3-O3
8	A	508	NAG	O7-C7-N2-C2
8	E	508	NAG	C4-C5-C6-O6
10	B	512	GOL	O1-C1-C2-O2
8	E	508	NAG	O5-C5-C6-O6
10	F	514	GOL	O1-C1-C2-O2
10	F	514	GOL	O2-C2-C3-O3
8	A	506	NAG	O5-C5-C6-O6
10	E	512	GOL	O2-C2-C3-O3
10	A	512	GOL	O1-C1-C2-C3
10	B	512	GOL	O1-C1-C2-C3
10	E	511	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	510	NO3	1	0
11	B	517	NO3	1	0
10	A	512	GOL	1	0
10	D	508	GOL	1	0
10	E	511	GOL	1	0
10	A	511	GOL	1	0
8	E	505	NAG	1	0
11	A	513	NO3	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	367/373 (98%)	0.32	12 (3%)	46 56	19, 30, 52, 77	0
1	B	367/373 (98%)	0.41	24 (6%)	18 27	20, 32, 61, 93	0
1	C	367/373 (98%)	0.57	37 (10%)	7 11	23, 39, 66, 85	0
1	D	367/373 (98%)	0.47	26 (7%)	16 24	23, 36, 62, 88	0
1	E	367/373 (98%)	0.43	21 (5%)	23 32	22, 36, 60, 92	0
1	F	367/373 (98%)	0.19	6 (1%)	72 79	18, 28, 49, 76	0
All	All	2202/2238 (98%)	0.40	126 (5%)	23 32	18, 33, 60, 93	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	83	PHE	7.4
1	C	83	PHE	6.9
1	E	83	PHE	6.4
1	F	83	PHE	6.2
1	A	83	PHE	6.1
1	B	83	PHE	6.1
1	E	431	VAL	5.4
1	B	415(A)	ILE	5.1
1	D	143	HIS	4.6
1	D	330	LEU	4.5
1	E	143	HIS	4.4
1	C	329	GLY	4.3
1	C	330	LEU	4.2
1	D	415	LEU	4.2
1	E	460	SER	4.1
1	C	431	VAL	4.1
1	D	415(A)	ILE	4.0
1	D	431	VAL	3.9
1	A	431	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	295	TRP	3.8
1	E	151	TRP	3.8
1	C	321	ALA	3.8
1	C	341	ALA	3.8
1	E	433	LEU	3.6
1	A	460	SER	3.5
1	D	199	ARG	3.3
1	D	367	ALA	3.3
1	C	140	ALA	3.3
1	C	84	TYR	3.3
1	C	415	LEU	3.2
1	C	460	SER	3.2
1	C	369	SER	3.2
1	C	296	ASN	3.2
1	C	334	THR	3.2
1	C	433	LEU	3.1
1	C	143	HIS	3.1
1	B	415	LEU	3.1
1	B	86	ARG	3.1
1	F	431	VAL	3.0
1	C	342	GLN	2.9
1	C	344	LYS	2.9
1	D	390	THR	2.9
1	A	433	LEU	2.9
1	D	433	LEU	2.9
1	E	110	LEU	2.9
1	C	387	GLU	2.9
1	B	415(B)	SER	2.8
1	C	388	GLY	2.8
1	A	141	ASN	2.8
1	C	187	LEU	2.8
1	C	141	ASN	2.8
1	C	333	THR	2.7
1	C	390	THR	2.7
1	C	368	GLU	2.7
1	C	328	GLY	2.7
1	B	88	LYS	2.7
1	E	328	GLY	2.7
1	B	158	LEU	2.7
1	F	143	HIS	2.7
1	A	140	ALA	2.6
1	B	121	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	367	ALA	2.6
1	C	249	GLN	2.6
1	D	342	GLN	2.6
1	F	249	GLN	2.6
1	B	143	HIS	2.6
1	E	106	TRP	2.5
1	A	86	ARG	2.5
1	D	141	ASN	2.5
1	B	141	ASN	2.5
1	C	247	VAL	2.5
1	D	249	GLN	2.5
1	E	142	GLN	2.5
1	C	430	THR	2.5
1	C	366	LYS	2.4
1	C	86	ARG	2.4
1	E	249	GLN	2.4
1	D	86	ARG	2.4
1	F	199	ARG	2.4
1	E	285	ASN	2.4
1	D	142	GLN	2.4
1	A	249	GLN	2.3
1	D	321	ALA	2.3
1	B	295	TRP	2.3
1	D	144	LEU	2.3
1	F	433	LEU	2.3
1	E	197	ARG	2.3
1	E	429	GLN	2.3
1	E	86	ARG	2.3
1	A	145	LEU	2.3
1	B	460	SER	2.3
1	C	347	GLY	2.3
1	E	199	ARG	2.3
1	B	120	ALA	2.3
1	B	132	PHE	2.2
1	A	143	HIS	2.2
1	B	432	GLY	2.2
1	B	87	ALA	2.2
1	A	432	GLY	2.2
1	B	429	GLN	2.2
1	D	329	GLY	2.2
1	C	401	ASN	2.2
1	B	246	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	285	ASN	2.2
1	B	443	LEU	2.2
1	D	430	THR	2.1
1	E	284	ASN	2.1
1	D	337	CYS	2.1
1	D	140	ALA	2.1
1	D	387	GLU	2.1
1	C	246	ASN	2.1
1	D	334	THR	2.1
1	E	430	THR	2.1
1	C	142	GLN	2.1
1	E	439	MET	2.1
1	D	339	LYS	2.1
1	B	393	LEU	2.1
1	B	89	SER	2.1
1	C	346	GLU	2.1
1	E	144	LEU	2.1
1	B	392	SER	2.0
1	E	401	ASN	2.0
1	D	432	GLY	2.0
1	D	110	LEU	2.0
1	A	121	TYR	2.0
1	B	126	LEU	2.0

## 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
3	MAN	H	4	11/12	0.54	0.46	106,118,121,124	0
2	BMA	G	3	11/12	0.66	0.28	102,115,122,126	0
7	FUL	N	2	10/11	0.68	0.45	103,113,123,131	0
7	NAG	N	3	14/15	0.69	0.43	90,105,113,114	0
4	FUL	K	2	10/11	0.75	0.30	73,80,87,88	0

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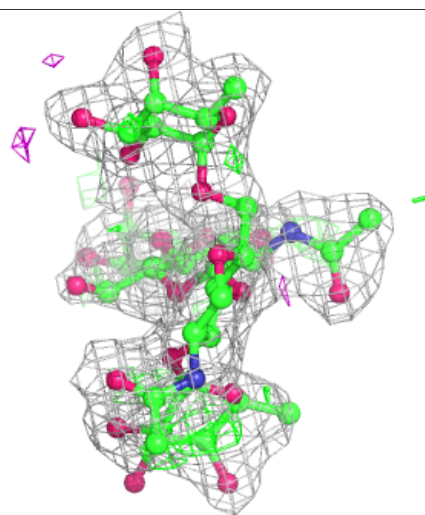
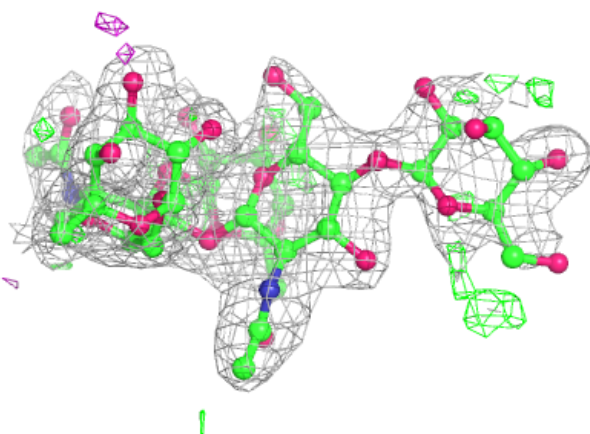
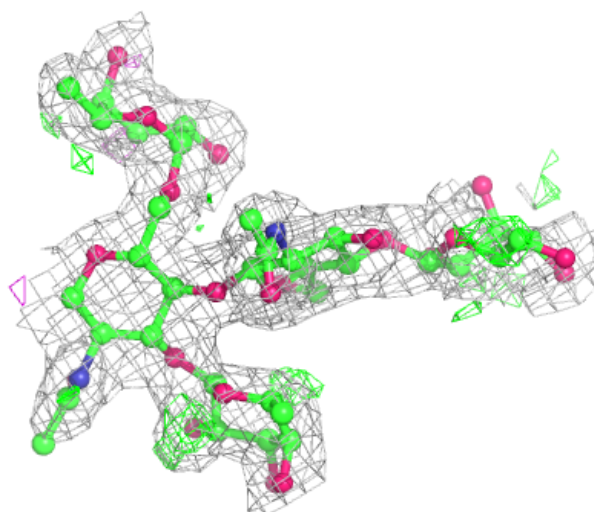
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FUL	I	2	10/11	0.75	0.30	100,113,123,132	0
3	BMA	H	3	11/12	0.77	0.38	98,112,119,120	0
3	FUL	H	5	10/11	0.78	0.30	63,76,83,83	0
4	NAG	I	3	14/15	0.78	0.28	72,83,94,98	0
5	NAG	J	1	14/15	0.79	0.23	50,64,73,92	0
2	FUL	G	4	10/11	0.79	0.23	59,70,83,96	0
7	NAG	N	1	14/15	0.79	0.25	53,72,95,97	0
4	FUL	M	2	10/11	0.82	0.19	66,72,76,90	0
5	NAG	J	2	14/15	0.83	0.37	71,78,90,96	0
4	NAG	I	1	14/15	0.84	0.19	64,72,87,101	0
6	FUC	L	2	10/11	0.87	0.24	87,96,100,100	0
6	NAG	L	1	14/15	0.87	0.19	48,55,72,75	0
4	FUC	I	4	10/11	0.87	0.16	47,64,80,86	0
3	NAG	H	2	14/15	0.89	0.17	46,54,72,83	0
4	NAG	K	1	14/15	0.89	0.16	39,45,68,70	0
2	FUC	G	5	10/11	0.90	0.15	23,39,45,49	0
4	NAG	M	3	14/15	0.91	0.18	41,58,67,89	0
3	NAG	H	1	14/15	0.92	0.13	40,43,55,59	0
5	FUC	J	3	10/11	0.92	0.21	49,55,64,70	0
2	NAG	G	1	14/15	0.93	0.16	38,47,53,63	0
4	NAG	K	3	14/15	0.93	0.23	53,64,80,89	0
2	NAG	G	2	14/15	0.93	0.14	48,62,76,87	0
4	FUC	K	4	10/11	0.93	0.16	35,41,50,56	0
4	NAG	M	1	14/15	0.93	0.10	28,35,51,57	0
3	FUC	H	6	10/11	0.94	0.10	30,45,49,51	0
4	FUC	M	4	10/11	0.96	0.10	27,35,40,47	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.

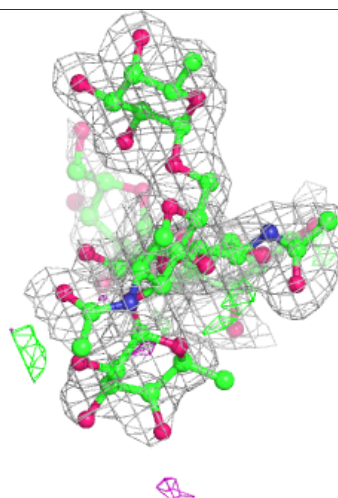
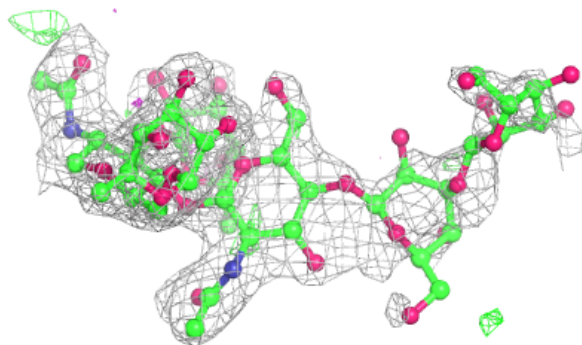
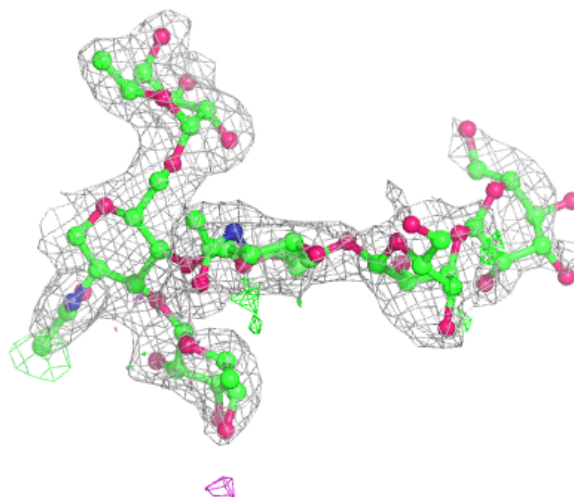
**Electron density around Chain G:**

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



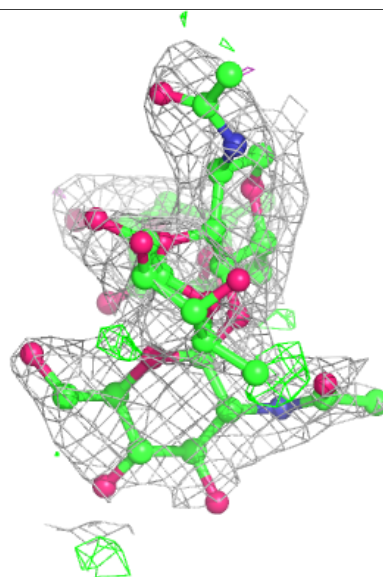
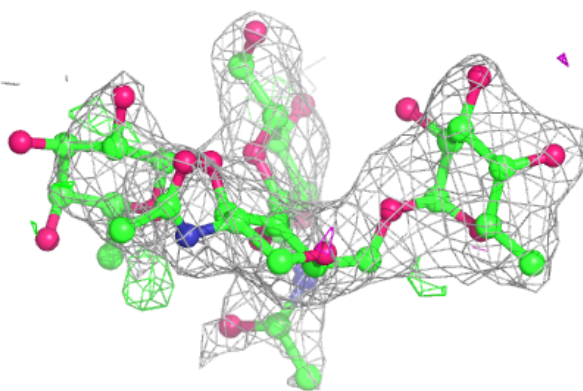
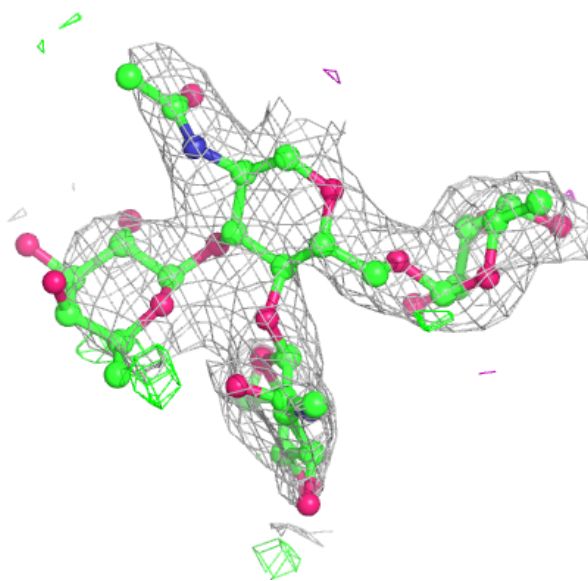
**Electron density around Chain H:**

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



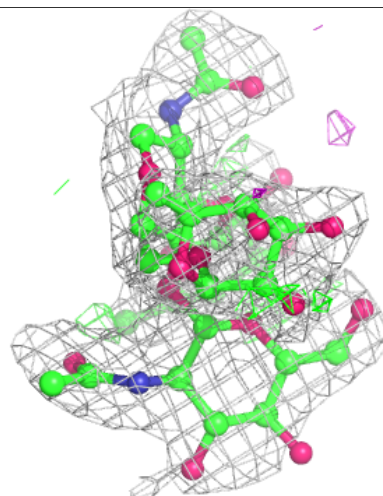
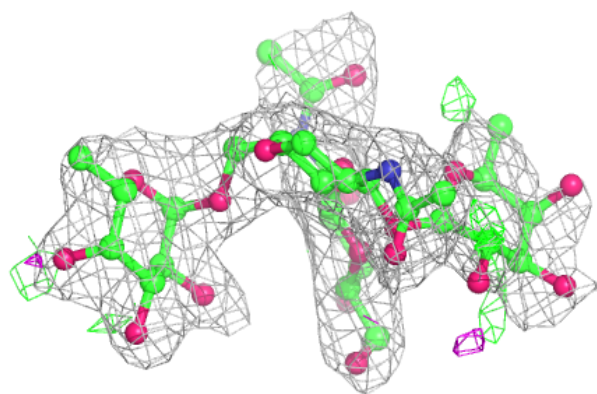
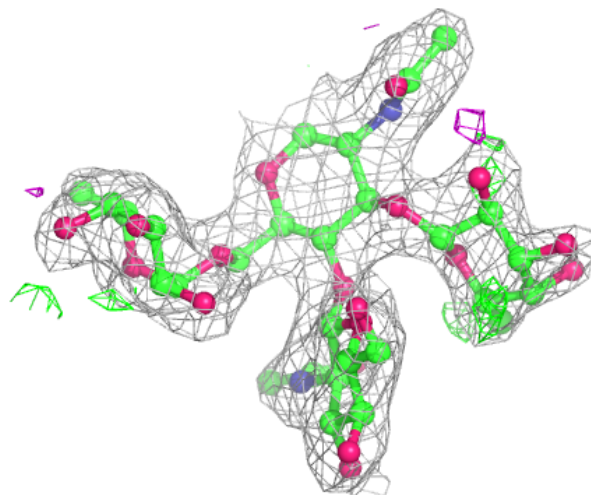
**Electron density around Chain I:**

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



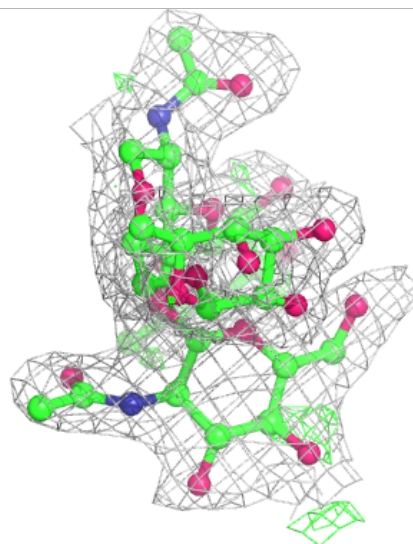
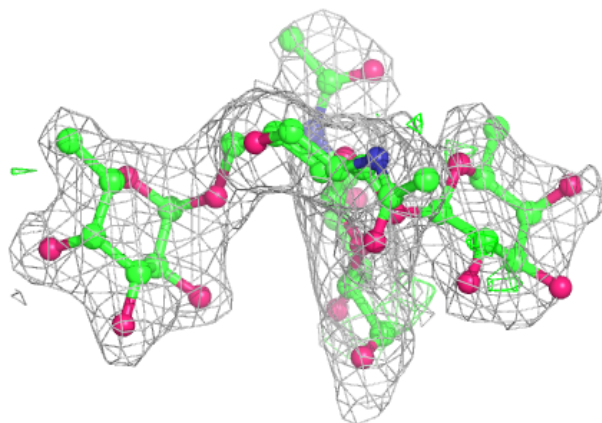
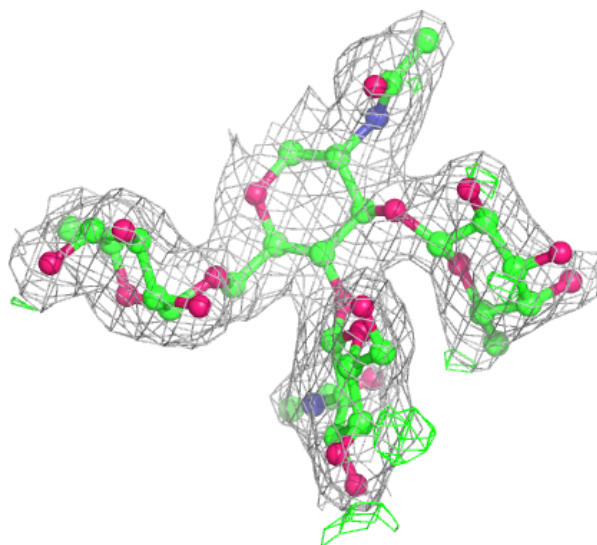
**Electron density around Chain K:**

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



**Electron density around Chain M:**

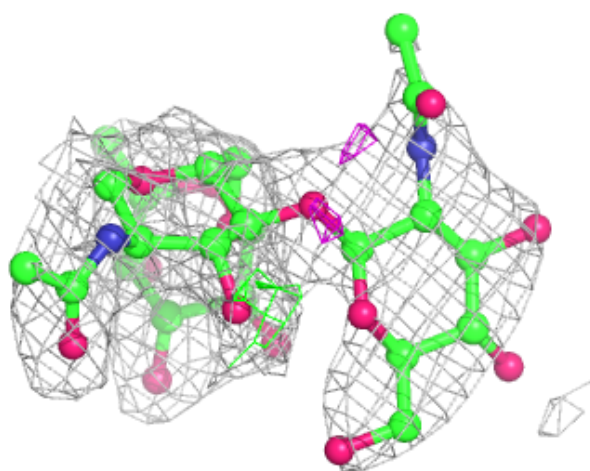
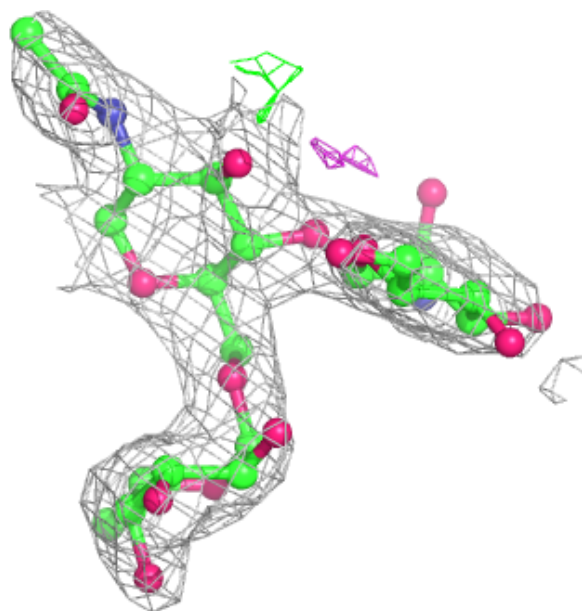
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around Chain J:**

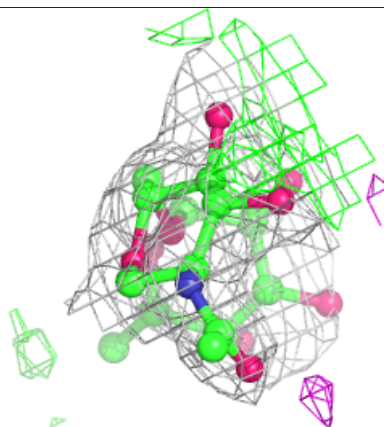
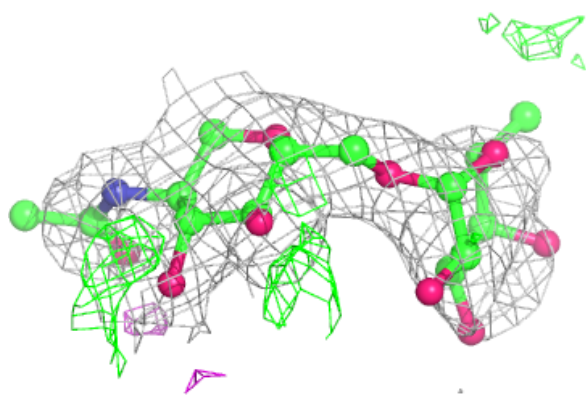
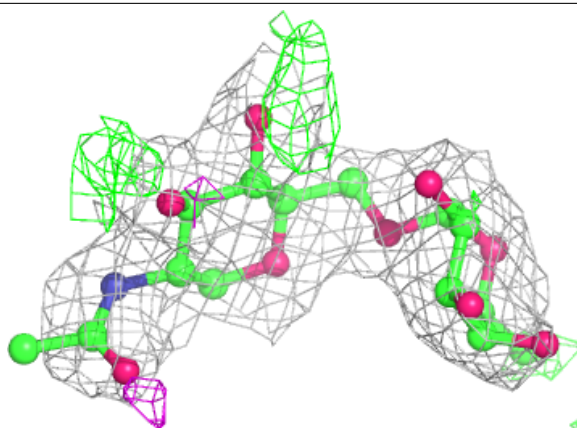
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

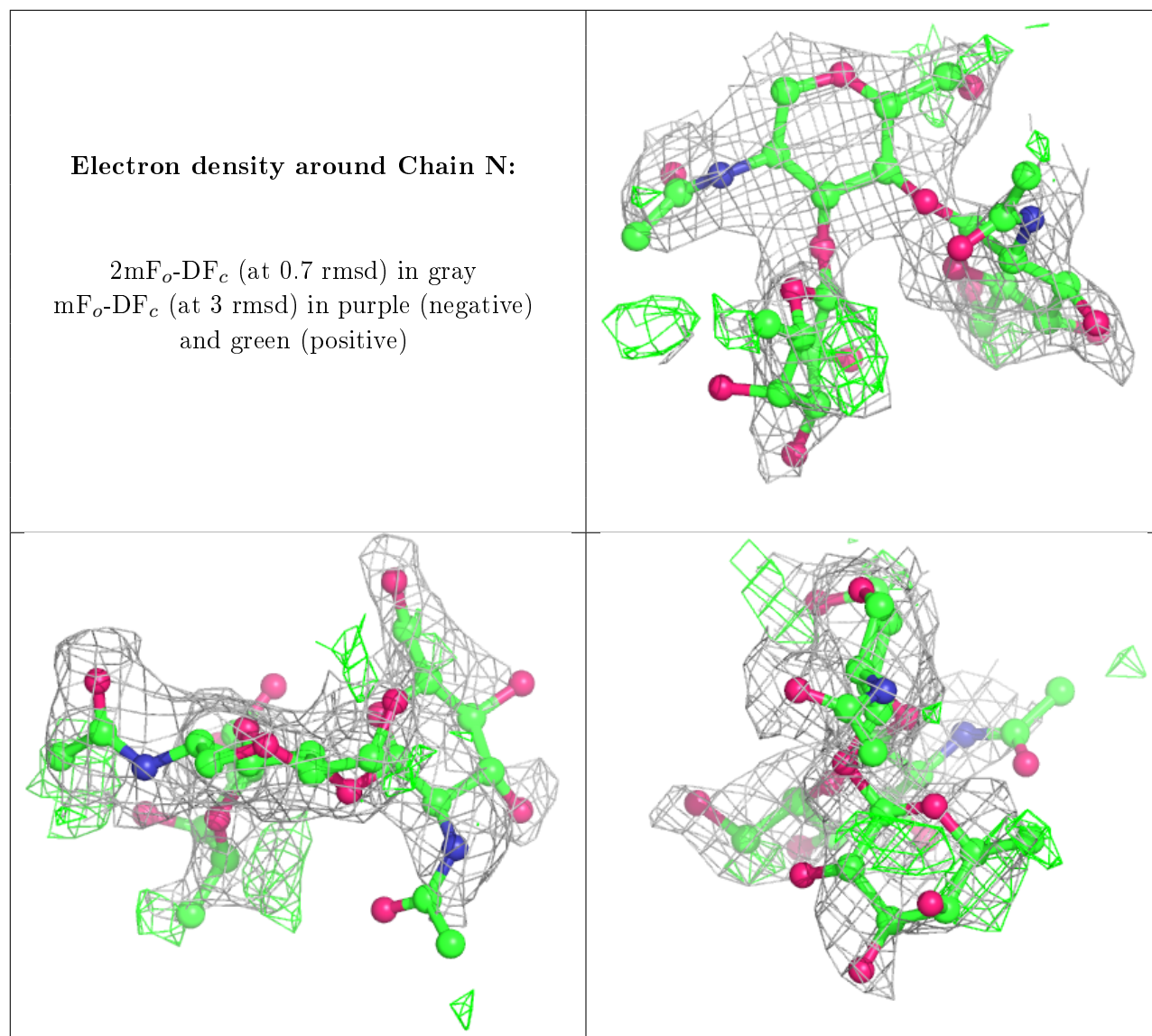




**Electron density around Chain L:**

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





## 6.4 Ligands ⓘ

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
10	GOL	B	511	6/6	0.54	0.22	37,64,76,77	0
10	GOL	E	511	6/6	0.67	0.26	62,74,80,87	0
8	NAG	D	505	14/15	0.68	0.33	56,75,86,92	0
8	NAG	E	508	14/15	0.68	0.29	68,87,102,114	0
8	NAG	A	506	14/15	0.73	0.29	47,82,97,105	0
8	NAG	A	508	14/15	0.73	0.27	65,82,93,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	C	505	14/15	0.73	0.29	62,73,80,87	0
8	NAG	F	506	14/15	0.74	0.36	66,80,88,95	0
8	NAG	C	506	14/15	0.74	0.31	65,74,98,101	0
9	CA	C	508	1/1	0.76	0.06	75,75,75,75	0
10	GOL	D	508	6/6	0.76	0.20	54,73,85,87	0
8	NAG	B	508	14/15	0.77	0.32	68,73,90,92	0
11	NO3	F	517	4/4	0.81	0.16	62,66,73,74	0
8	NAG	A	507	14/15	0.81	0.26	67,79,88,89	0
10	GOL	E	513	6/6	0.81	0.16	73,88,97,97	0
8	NAG	B	507	14/15	0.84	0.22	65,86,92,100	0
8	NAG	F	505	14/15	0.85	0.22	50,67,74,92	0
8	NAG	E	505	14/15	0.85	0.20	35,55,63,68	0
8	NAG	D	504	14/15	0.86	0.18	37,54,69,73	0
10	GOL	B	512	6/6	0.86	0.18	43,60,74,75	0
10	GOL	F	512	6/6	0.88	0.25	33,58,76,92	0
9	CA	D	507	1/1	0.89	0.05	55,55,55,55	0
10	GOL	F	515	6/6	0.89	0.16	47,56,58,58	0
11	NO3	A	514	4/4	0.90	0.25	26,46,53,69	0
9	CA	E	510	1/1	0.91	0.10	69,69,69,69	0
10	GOL	F	513	6/6	0.92	0.12	31,52,68,70	0
11	NO3	D	509	4/4	0.92	0.19	46,48,54,61	0
11	NO3	C	510	4/4	0.92	0.21	37,54,59,70	0
10	GOL	E	512	6/6	0.92	0.15	33,43,74,88	0
11	NO3	B	517	4/4	0.92	0.22	53,57,58,72	0
10	GOL	F	514	6/6	0.93	0.11	28,40,70,84	0
11	NO3	A	513	4/4	0.93	0.18	37,46,49,50	0
10	GOL	A	512	6/6	0.93	0.23	42,58,69,69	0
11	NO3	F	516	4/4	0.94	0.12	55,66,66,76	0
9	CA	C	507	1/1	0.94	0.07	48,48,48,48	0
9	CA	B	510	1/1	0.94	0.04	59,59,59,59	0
10	GOL	C	509	6/6	0.95	0.13	36,49,58,66	0
10	GOL	A	510	6/6	0.96	0.12	26,39,55,66	0
10	GOL	A	511	6/6	0.96	0.16	32,61,82,89	0
11	NO3	B	513	4/4	0.97	0.15	27,50,51,69	0
11	NO3	C	511	4/4	0.97	0.15	42,45,49,52	0
11	NO3	F	518	4/4	0.97	0.20	36,48,50,62	0
9	CA	F	511	1/1	0.97	0.05	45,45,45,45	0
9	CA	E	509	1/1	0.97	0.07	32,32,32,32	0
11	NO3	D	510	4/4	0.97	0.19	50,57,61,64	0
11	NO3	B	515	4/4	0.97	0.19	37,38,43,61	0
9	CA	D	506	1/1	0.98	0.06	33,33,33,33	0
11	NO3	B	516	4/4	0.98	0.15	32,35,37,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	NO3	B	514	4/4	0.98	0.16	36,41,47,50	0
9	CA	F	510	1/1	0.99	0.09	22,22,22,22	0
9	CA	B	509	1/1	0.99	0.08	25,25,25,25	0
9	CA	A	509	1/1	1.00	0.10	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.