



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 01:50 PM BST

PDB ID : 6VFT  
Title : Crystal structure of human delta protocadherin 17 EC1-EC4  
Authors : Harrison, O.J.; Brasch, J.; Shapiro, L.  
Deposited on : 2020-01-06  
Resolution : 3.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

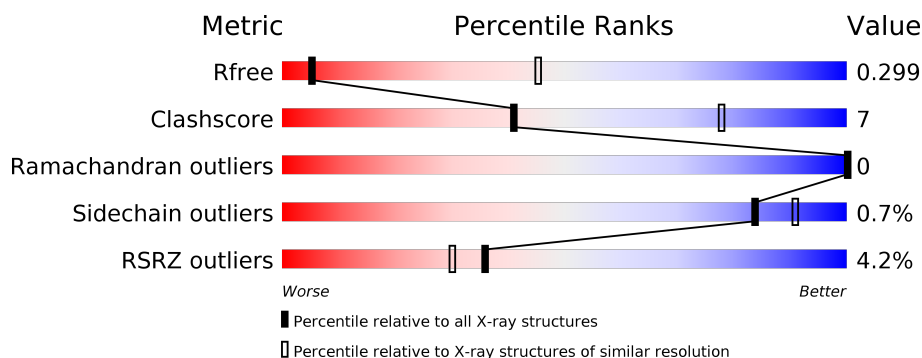
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.71 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.





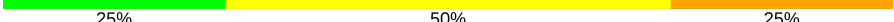
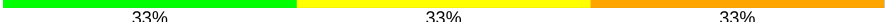
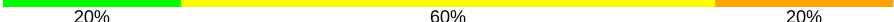
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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	453	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>9%</div> </div> </div>
1	B	453	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>9%</div> </div> </div>
1	C	453	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>7%</div> </div> </div>
1	D	453	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>8%</div> </div> </div>
2	E	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
2	F	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	L	2	 50% 50%
4	H	4	 50% 50%
4	K	4	 25% 50% 25%
5	I	3	 33% 33% 33%
6	J	5	 20% 60% 20%

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
2	FUC	E	3	-	-	-	X
4	FUC	H	4	-	-	-	X
5	NAG	I	2	-	-	-	X
5	BMA	I	3	-	-	-	X
8	MAN	B	511	-	-	-	X
8	MAN	D	517	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25685 atoms, of which 12355 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 Protocadherin-17.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	413	Total	C	H	N	O	S	0	0	0
			6153	1977	2969	558	641	8			
1	B	414	Total	C	H	N	O	S	0	0	0
			6218	1981	3027	559	643	8			
1	C	420	Total	C	H	N	O	S	0	0	0
			6215	2007	2979	569	652	8			
1	D	418	Total	C	H	N	O	S	0	0	0
			6176	1994	2962	563	649	8			

There are 24 discrepancies between the modelled and reference sequences:

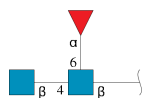
Chain	Residue	Modelled	Actual	Comment	Reference
A	448	HIS	-	expression tag	UNP O14917
A	449	HIS	-	expression tag	UNP O14917
A	450	HIS	-	expression tag	UNP O14917
A	451	HIS	-	expression tag	UNP O14917
A	452	HIS	-	expression tag	UNP O14917
A	453	HIS	-	expression tag	UNP O14917
B	448	HIS	-	expression tag	UNP O14917
B	449	HIS	-	expression tag	UNP O14917
B	450	HIS	-	expression tag	UNP O14917
B	451	HIS	-	expression tag	UNP O14917
B	452	HIS	-	expression tag	UNP O14917
B	453	HIS	-	expression tag	UNP O14917
C	448	HIS	-	expression tag	UNP O14917
C	449	HIS	-	expression tag	UNP O14917
C	450	HIS	-	expression tag	UNP O14917
C	451	HIS	-	expression tag	UNP O14917
C	452	HIS	-	expression tag	UNP O14917
C	453	HIS	-	expression tag	UNP O14917
D	448	HIS	-	expression tag	UNP O14917
D	449	HIS	-	expression tag	UNP O14917
D	450	HIS	-	expression tag	UNP O14917

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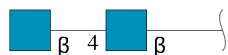
Chain	Residue	Modelled	Actual	Comment	Reference
D	451	HIS	-	expression tag	UNP O14917
D	452	HIS	-	expression tag	UNP O14917
D	453	HIS	-	expression tag	UNP O14917

- Molecule 2 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.



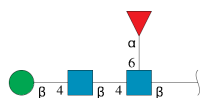
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	3	Total 75	C 22	H 37	N 2	O 14	0	0	0
2	F	3	Total 74	C 22	H 36	N 2	O 14	0	0	0

- Molecule 3 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
3	G	2	Total 54	C 16	H 26	N 2	O 10	0	0	0
3	L	2	Total 53	C 16	H 25	N 2	O 10	0	0	0

- Molecule 4 is an oligosaccharide called 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	H	4	Total	C	H	N	O	0	0	0
			84	28	35	2	19			

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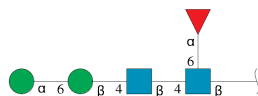
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	4	Total	C	H	N	O	0	0	0
			95	28	46	2	19			

- Molecule 5 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
5	I	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			

- Molecule 6 is an oligosaccharide called 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
6	J	5	Total	C	H	N	O	0	0	0
			115	34	55	2	24			

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	10	Total	Ca	0	0
			10	10		
7	A	10	Total	Ca	0	0
			10	10		
7	D	10	Total	Ca	0	0
			10	10		
7	C	10	Total	Ca	0	0
			10	10		

- Molecule 8 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			21	6	10	5		
8	A	1	Total	C	H	O	0	0
			21	6	10	5		
8	B	1	Total	C	H	O	0	0
			21	6	10	5		
8	B	1	Total	C	H	O	0	0
			21	6	10	5		
8	C	1	Total	C	H	O	0	0
			21	6	10	5		
8	C	1	Total	C	H	O	0	0
			21	6	10	5		
8	D	1	Total	C	H	O	0	0
			21	6	10	5		
8	D	1	Total	C	H	O	0	0
			21	6	10	5		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
9	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
9	C	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 10 is water.

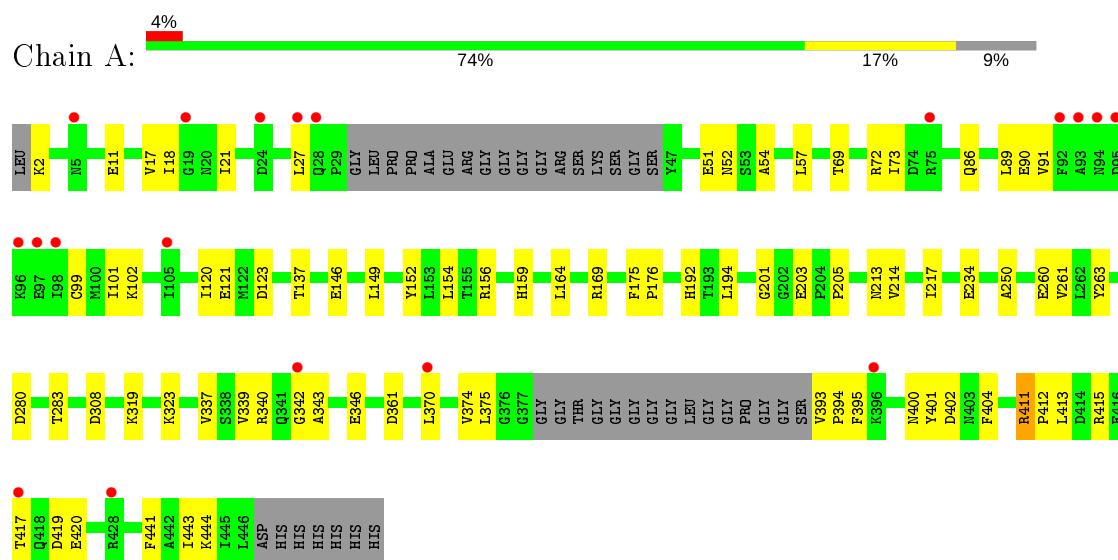
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			1	1		
10	B	3	Total	O	0	0
			3	3		
10	D	2	Total	O	0	0
			2	2		



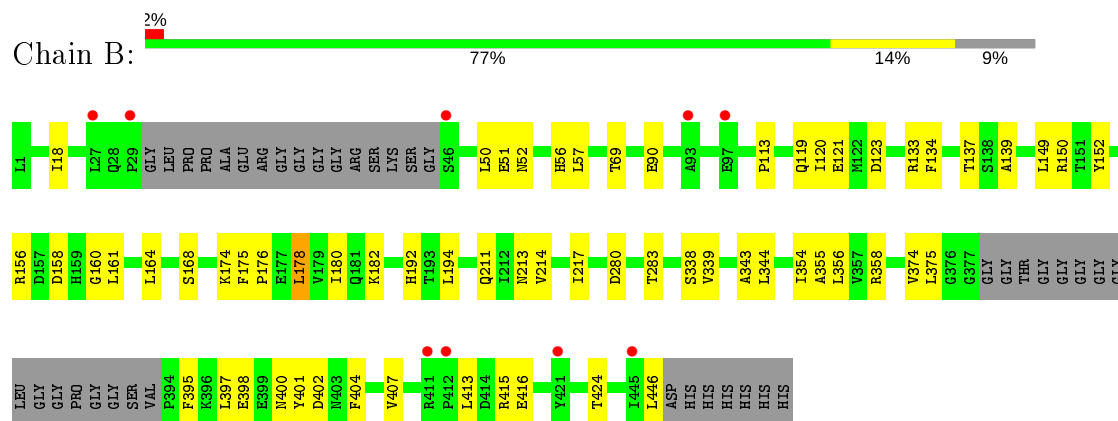
### 3 Residue-property plots

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.

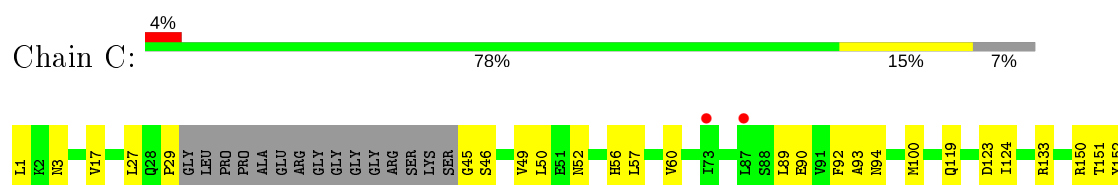
#### • Molecule 1: Protocadherin-17

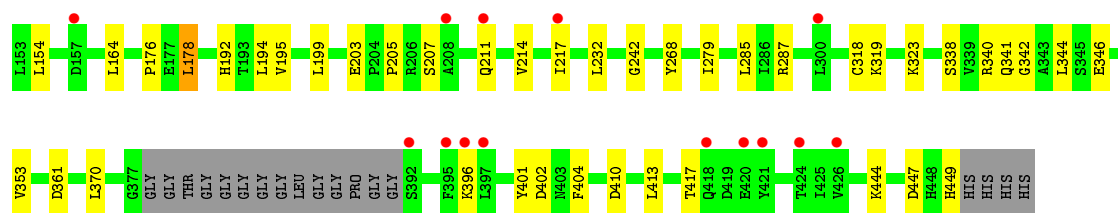


#### • Molecule 1: Protocadherin-17

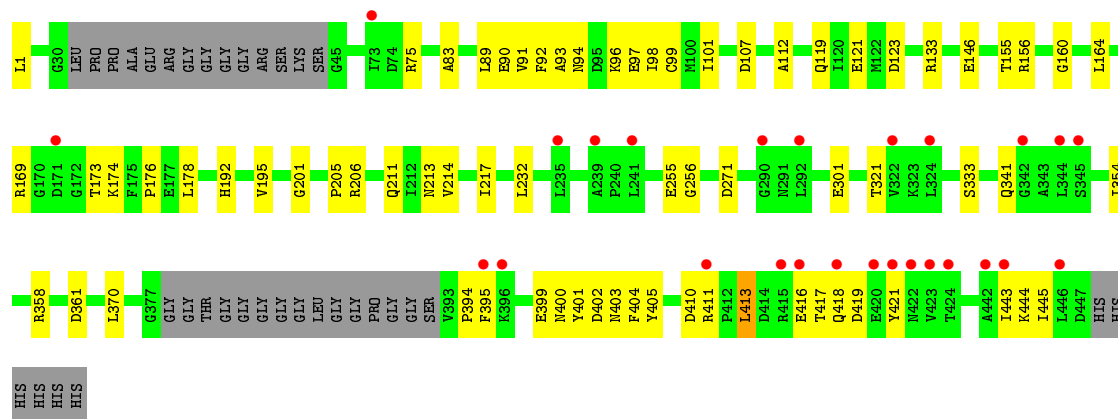
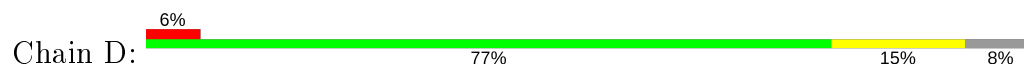


#### • Molecule 1: Protocadherin-17





• Molecule 1: Protocadherin-17



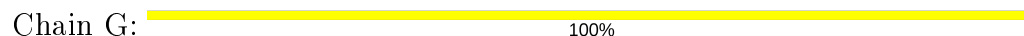
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%



- Molecule 4: 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 H:  50% 50%



- Molecule 4: 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 K:  25% 50% 25%



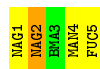
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 33% 33%



- Molecule 6: 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 J:  20% 60% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.55Å 105.84Å 101.40Å 90.00° 101.04° 90.00°	Depositor
Resolution (Å)	19.94 – 3.71 39.13 – 3.71	Depositor EDS
% Data completeness (in resolution range)	96.3 (19.94-3.71) 86.9 (39.13-3.71)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.63 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.253 , 0.300 0.259 , 0.299	Depositor DCC
$R_{free}$ test set	1140 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 66.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	25685	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CA, BMA, NAG, FUC

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	0.29	1/3238 (0.0%)	0.52	1/4401 (0.0%)
1	B	0.27	0/3245	0.51	0/4409
1	C	0.27	0/3292	0.52	0/4474
1	D	0.28	0/3268	0.52	0/4441
All	All	0.28	1/13043 (0.0%)	0.52	1/17725 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	VAL	C-N	5.86	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	ARG	CG-CD-NE	-5.05	101.20	111.80

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3184	2969	3114	55	0
1	B	3191	3027	3125	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3236	2979	3159	52	0
1	D	3214	2962	3144	45	0
2	E	38	37	34	1	0
2	F	38	36	34	0	0
3	G	28	26	25	0	0
3	L	28	25	25	0	0
4	H	49	35	43	0	0
4	K	49	46	43	2	0
5	I	39	36	34	1	0
6	J	60	55	52	2	0
7	A	10	0	0	0	0
7	B	10	0	0	0	0
7	C	10	0	0	0	0
7	D	10	0	0	0	0
8	A	22	20	20	0	0
8	B	22	20	20	0	0
8	C	22	20	20	0	0
8	D	22	20	20	0	0
9	B	14	14	13	0	0
9	C	28	28	26	0	0
10	A	1	0	0	0	0
10	B	3	0	0	0	0
10	D	2	0	0	0	0
All	All	13330	12355	12951	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 187 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:B:339:VAL:H	1:C:1:LEU:HD13	1.38	0.89
1:D:400:ASN:OD1	1:D:401:TYR:N	2.15	0.80
1:B:400:ASN:OD1	1:B:401:TYR:N	2.18	0.76
6:J:2:NAG:O7	6:J:2:NAG:O3	2.03	0.75
1:C:150:ARG:NH1	1:C:151:THR:OG1	2.19	0.74

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	407/453 (90%)	389 (96%)	18 (4%)	0	100	100
1	B	408/453 (90%)	386 (95%)	22 (5%)	0	100	100
1	C	414/453 (91%)	393 (95%)	21 (5%)	0	100	100
1	D	412/453 (91%)	393 (95%)	19 (5%)	0	100	100
All	All	1641/1812 (91%)	1561 (95%)	80 (5%)	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	356/378 (94%)	353 (99%)	3 (1%)	81	89
1	B	357/378 (94%)	355 (99%)	2 (1%)	86	92
1	C	362/378 (96%)	360 (99%)	2 (1%)	86	92
1	D	359/378 (95%)	356 (99%)	3 (1%)	81	89
All	All	1434/1512 (95%)	1424 (99%)	10 (1%)	84	91

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	194	LEU
1	C	178	LEU
1	D	205	PRO

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Mol	Chain	Res	Type
1	B	178	LEU
1	C	449	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	305	GLN
1	D	94	ASN
1	C	3	ASN
1	A	192	HIS
1	C	52	ASN

### 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 ⓘ

26 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	E	1	1,2	14,14,15	0.23	0	17,19,21	0.36	0
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	1.04	1 (5%)
2	FUC	E	3	2	10,10,11	0.74	0	14,14,16	0.82	0
2	NAG	F	1	1,2	14,14,15	0.49	0	17,19,21	0.91	1 (5%)
2	NAG	F	2	2	14,14,15	0.37	0	17,19,21	0.40	0
2	FUC	F	3	2	10,10,11	1.20	2 (20%)	14,14,16	1.48	3 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	G	1	1,3	14,14,15	0.84	1 (7%)	17,19,21	0.82	1 (5%)
3	NAG	G	2	3	14,14,15	0.86	1 (7%)	17,19,21	0.61	0
4	NAG	H	1	1,4	14,14,15	0.76	1 (7%)	17,19,21	0.59	0
4	NAG	H	2	4	14,14,15	0.23	0	17,19,21	0.51	0
4	BMA	H	3	4	11,11,12	0.57	0	15,15,17	0.77	0
4	FUC	H	4	4	10,10,11	1.18	1 (10%)	14,14,16	1.10	2 (14%)
5	NAG	I	1	1,5	14,14,15	0.79	1 (7%)	17,19,21	0.60	0
5	NAG	I	2	5	14,14,15	0.84	1 (7%)	17,19,21	1.10	2 (11%)
5	BMA	I	3	5	11,11,12	0.65	0	15,15,17	0.78	0
6	NAG	J	1	1,6	14,14,15	0.82	1 (7%)	17,19,21	0.84	1 (5%)
6	NAG	J	2	6	14,14,15	0.81	1 (7%)	17,19,21	0.72	0
6	BMA	J	3	6	11,11,12	0.63	0	15,15,17	0.78	0
6	MAN	J	4	6	11,11,12	1.06	1 (9%)	15,15,17	1.13	2 (13%)
6	FUC	J	5	6	10,10,11	1.64	2 (20%)	14,14,16	2.04	2 (14%)
4	NAG	K	1	1,4	14,14,15	0.40	0	17,19,21	0.45	0
4	NAG	K	2	4	14,14,15	0.91	1 (7%)	17,19,21	0.68	0
4	BMA	K	3	4	11,11,12	0.64	0	15,15,17	0.72	0
4	FUC	K	4	4	10,10,11	0.73	0	14,14,16	1.23	2 (14%)
3	NAG	L	1	1,3	14,14,15	0.67	0	17,19,21	2.22	3 (17%)
3	NAG	L	2	3	14,14,15	0.45	0	17,19,21	0.42	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	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	5/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1
2	NAG	F	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	FUC	F	3	2	-	-	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1

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

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	5	FUC	C2-C3	3.42	1.57	1.52
6	J	4	MAN	C1-C2	3.08	1.59	1.52
6	J	5	FUC	C1-C2	3.08	1.59	1.52
3	G	1	NAG	O5-C1	-3.03	1.38	1.43
5	I	2	NAG	O5-C1	-2.92	1.39	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	C1-O5-C5	7.99	123.02	112.19
6	J	5	FUC	C1-C2-C3	6.16	117.23	109.67
2	E	2	NAG	C2-N2-C7	3.38	127.72	122.90
5	I	2	NAG	C3-C4-C5	3.25	116.04	110.24
6	J	4	MAN	C1-O5-C5	3.22	116.55	112.19

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	2	NAG	C3-C2-N2-C7

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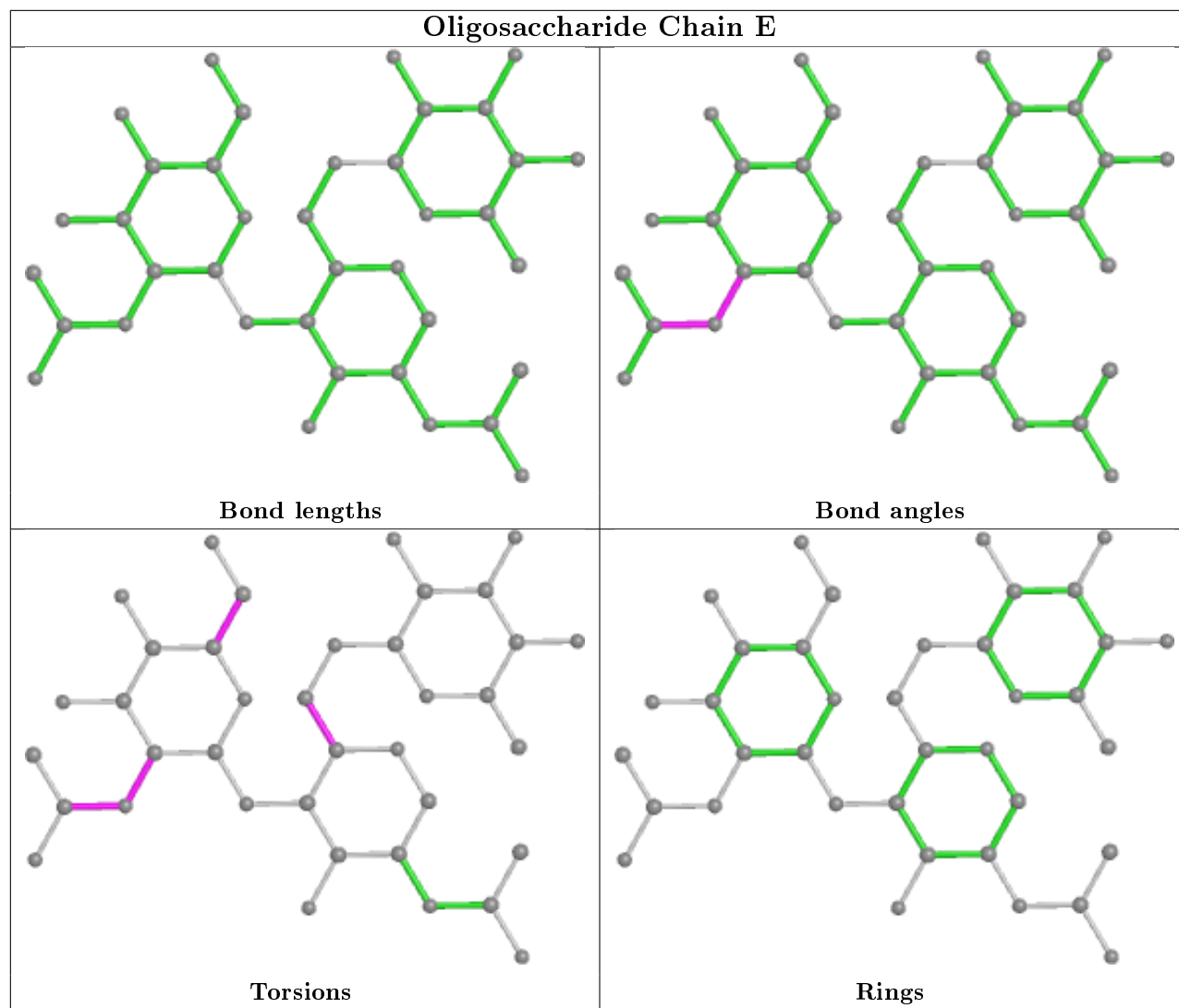
Mol	Chain	Res	Type	Atoms
4	K	2	NAG	C1-C2-N2-C7
4	K	3	BMA	O5-C5-C6-O6
6	J	4	MAN	C4-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6

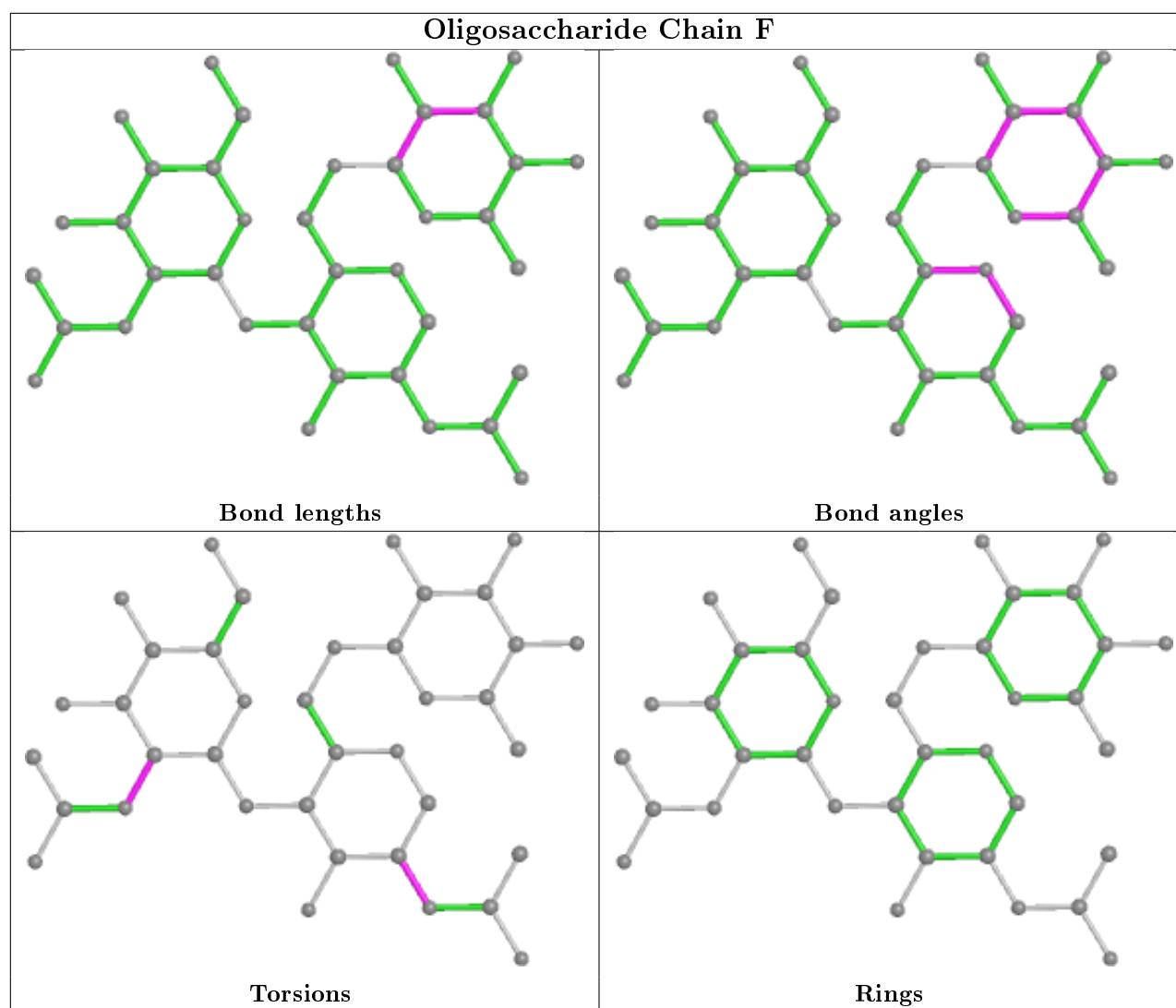
There are no ring outliers.

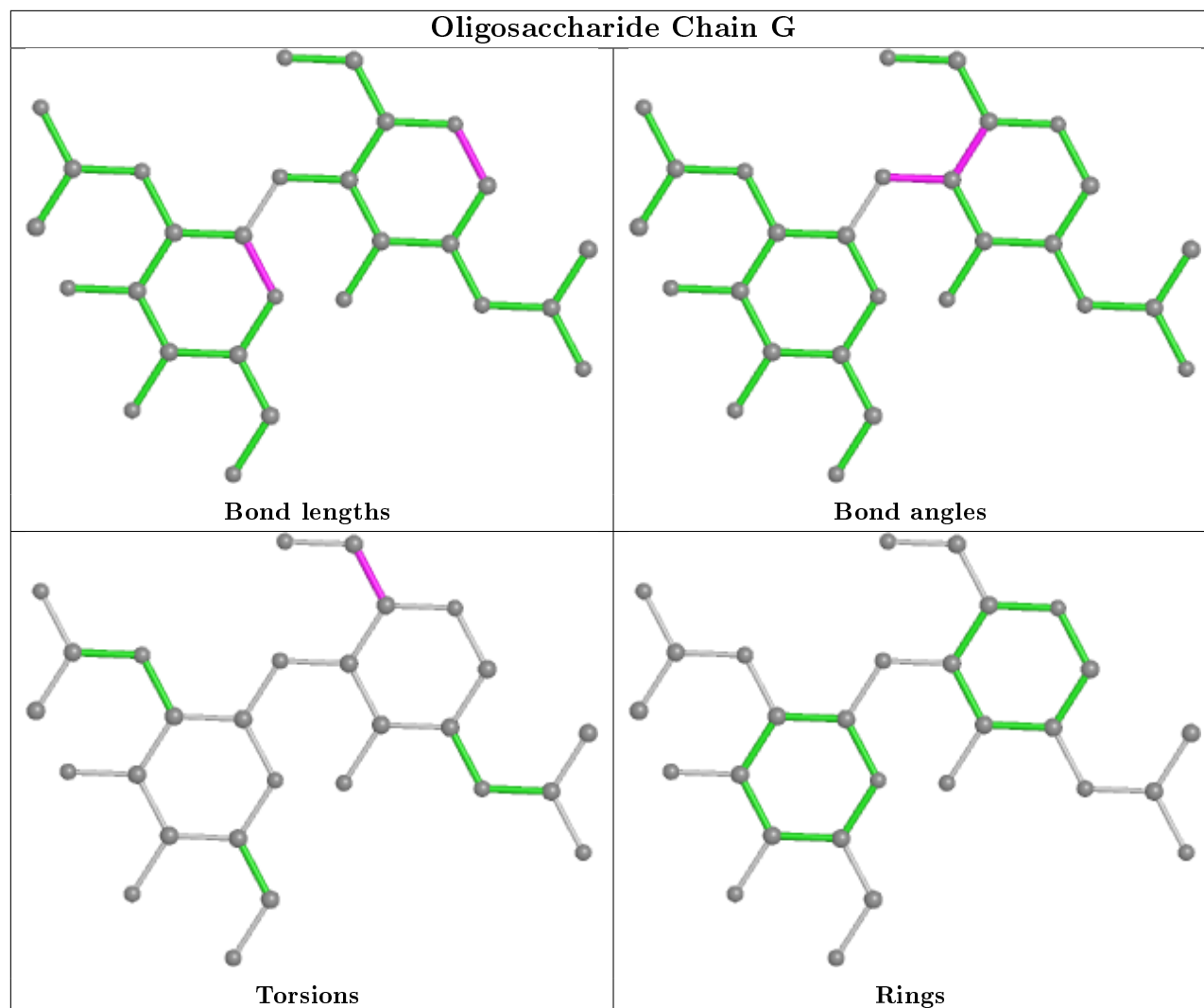
5 monomers are involved in 6 short contacts:

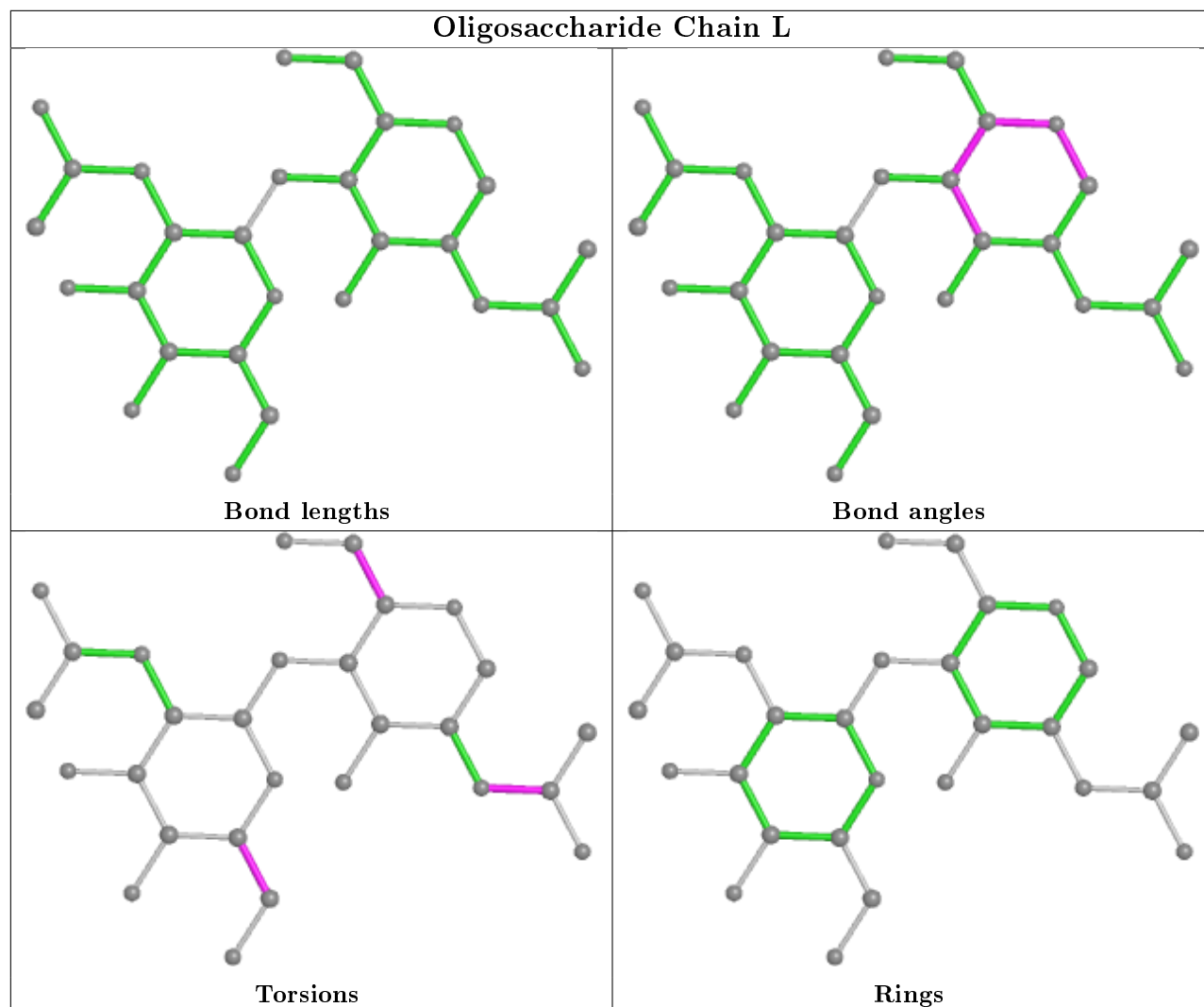
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	2	NAG	2	0
4	K	3	BMA	1	0
4	K	2	NAG	2	0
5	I	1	NAG	1	0
2	E	2	NAG	1	0

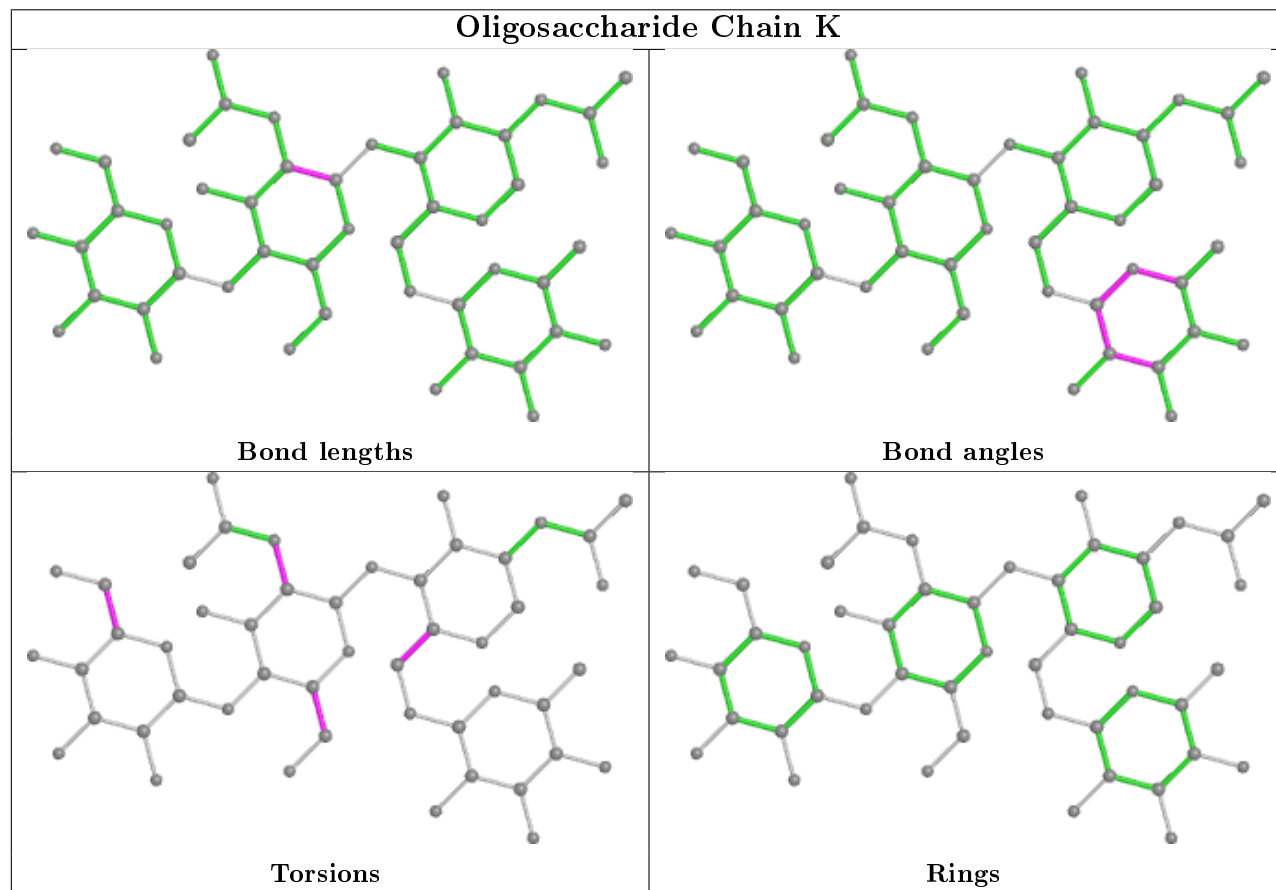
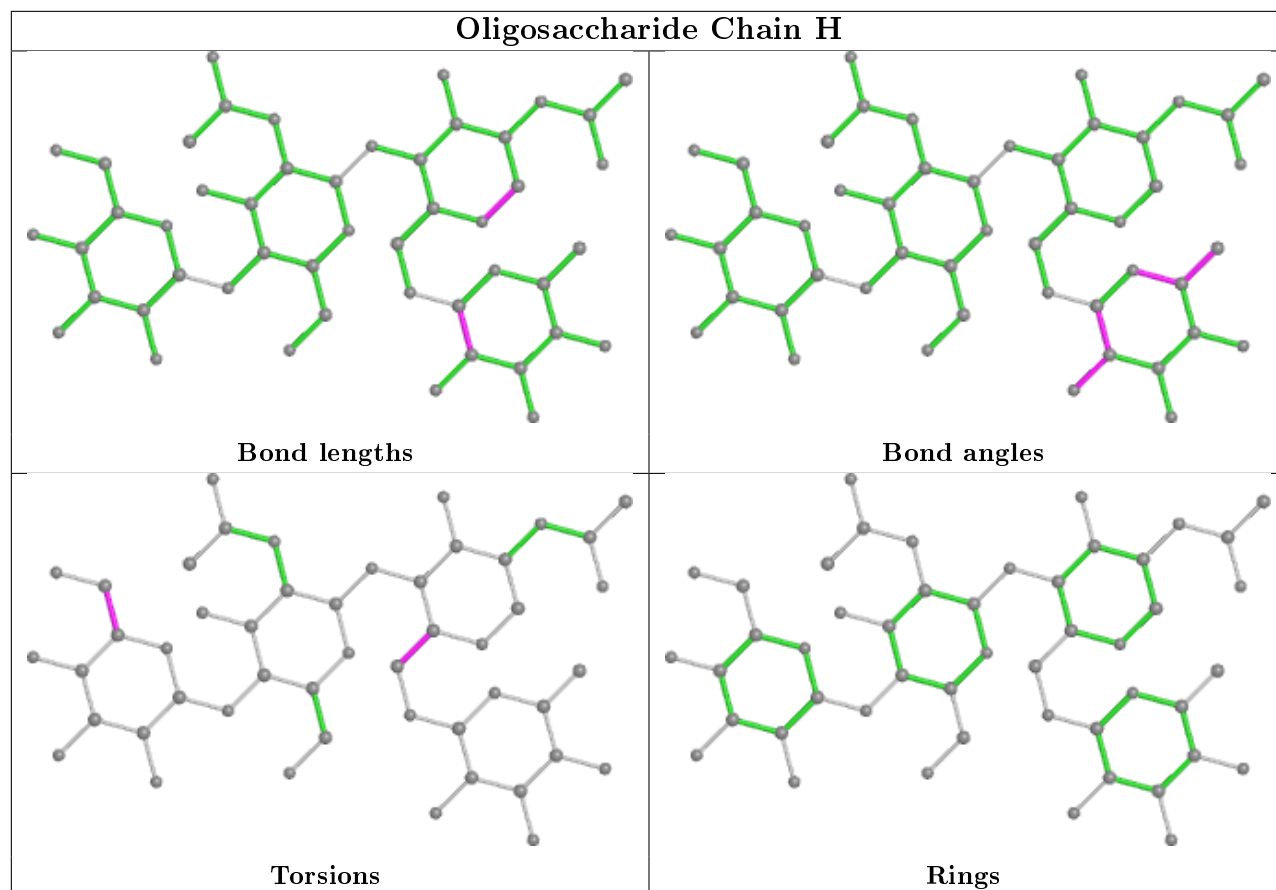
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



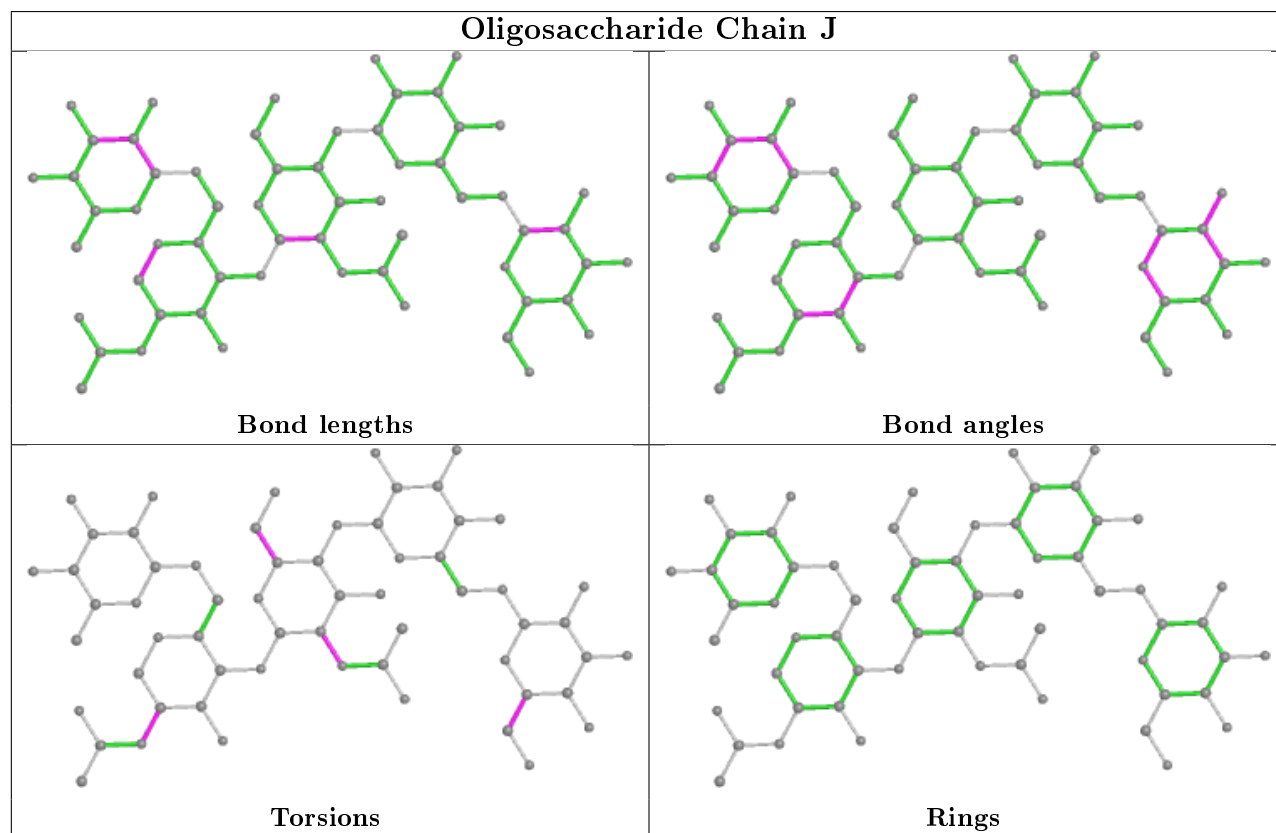
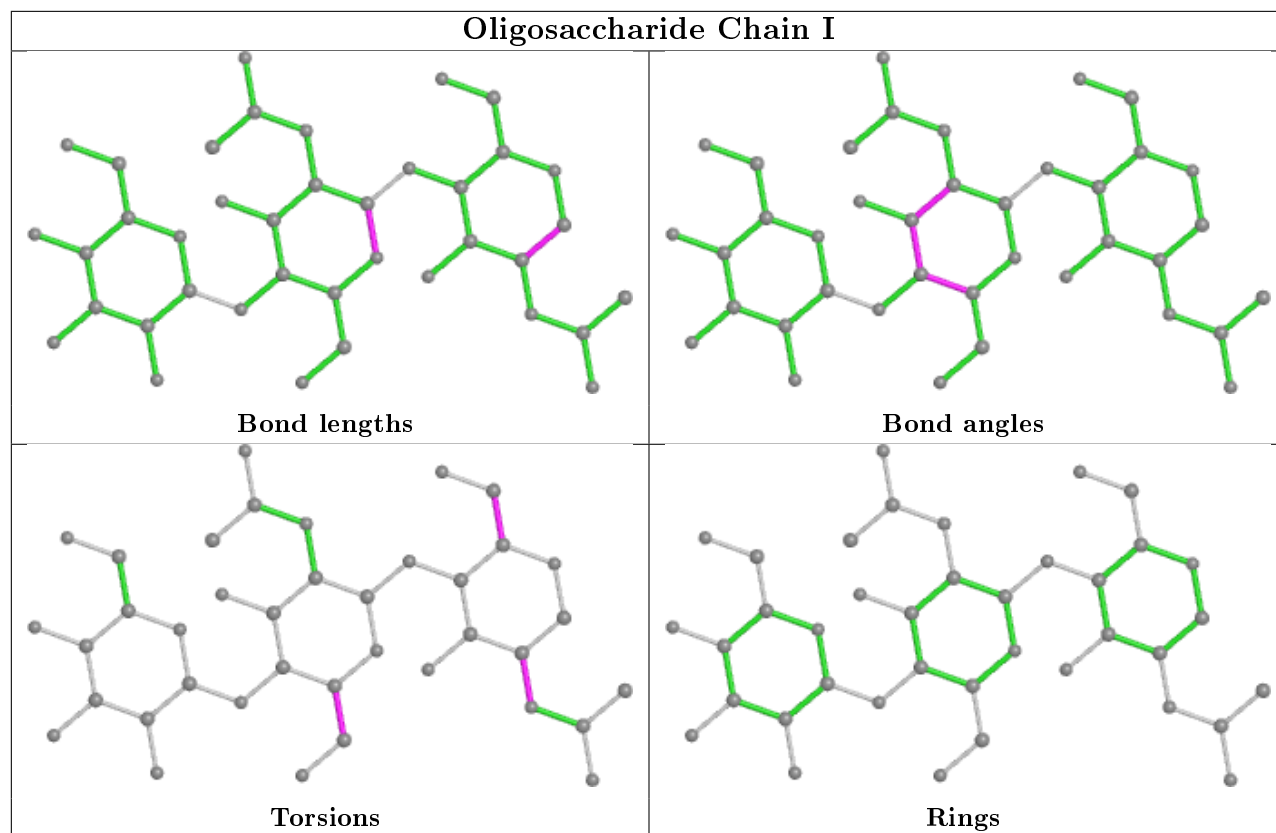












## 5.6 Ligand geometry

Of 51 ligands modelled in this entry, 40 are monoatomic - leaving 11 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
8	MAN	D	517	1	11,11,12	1.13	1 (9%)	15,15,17	1.23	2 (13%)
8	MAN	B	511	1	11,11,12	0.90	1 (9%)	15,15,17	1.01	2 (13%)
9	NAG	C	513	1	14,14,15	0.21	0	17,19,21	0.43	0
8	MAN	A	510	1	11,11,12	1.45	2 (18%)	15,15,17	1.49	3 (20%)
8	MAN	D	516	1	11,11,12	0.66	0	15,15,17	1.43	3 (20%)
8	MAN	C	510	1	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
8	MAN	A	514	1	11,11,12	0.79	0	15,15,17	1.21	3 (20%)
9	NAG	B	519	1	14,14,15	0.22	0	17,19,21	0.32	0
8	MAN	C	511	1	11,11,12	0.61	0	15,15,17	1.09	2 (13%)
9	NAG	C	512	1	14,14,15	0.29	0	17,19,21	0.32	0
8	MAN	B	510	1	11,11,12	0.75	0	15,15,17	1.29	2 (13%)

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	MAN	D	517	1	-	2/2/19/22	0/1/1/1
8	MAN	B	511	1	-	2/2/19/22	0/1/1/1
9	NAG	C	513	1	-	0/6/23/26	0/1/1/1
8	MAN	A	510	1	-	1/2/19/22	0/1/1/1
8	MAN	D	516	1	-	2/2/19/22	0/1/1/1
8	MAN	C	510	1	-	2/2/19/22	0/1/1/1
8	MAN	A	514	1	-	0/2/19/22	0/1/1/1
9	NAG	B	519	1	-	2/6/23/26	0/1/1/1
8	MAN	C	511	1	-	2/2/19/22	0/1/1/1
9	NAG	C	512	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	B	510	1	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	510	MAN	O5-C1	-3.93	1.37	1.43
8	D	517	MAN	O5-C1	-3.02	1.38	1.43
8	B	511	MAN	O5-C1	-2.59	1.39	1.43
8	A	510	MAN	C4-C5	2.03	1.57	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	510	MAN	C1-O5-C5	3.77	117.31	112.19
8	D	516	MAN	C1-O5-C5	3.24	116.58	112.19
8	A	510	MAN	C3-C4-C5	3.18	115.92	110.24
8	C	511	MAN	C1-O5-C5	2.83	116.03	112.19
8	D	516	MAN	O5-C1-C2	2.81	115.11	110.77

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	511	MAN	O5-C5-C6-O6
8	D	516	MAN	O5-C5-C6-O6
8	C	511	MAN	C4-C5-C6-O6
8	D	516	MAN	C4-C5-C6-O6
9	B	519	NAG	O5-C5-C6-O6

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	413/453 (91%)	0.25	19 (4%) 32 27	57, 95, 198, 343	1 (0%)
1	B	414/453 (91%)	0.19	9 (2%) 62 55	58, 97, 198, 271	1 (0%)
1	C	420/453 (92%)	0.31	16 (3%) 40 33	71, 109, 169, 217	1 (0%)
1	D	418/453 (92%)	0.44	26 (6%) 20 16	78, 118, 191, 283	1 (0%)
All	All	1665/1812 (91%)	0.30	70 (4%) 36 30	57, 108, 191, 343	4 (0%)

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	421	TYR	8.0
1	A	97	GLU	6.3
1	A	27	LEU	5.6
1	A	96	LYS	5.0
1	D	420	GLU	4.5

### 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
2	NAG	F	2	14/15	0.43	0.38	200,210,252,256	0
5	BMA	I	3	11/12	0.59	0.41	156,166,197,199	0

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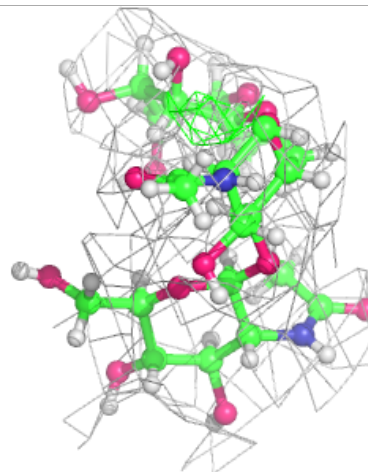
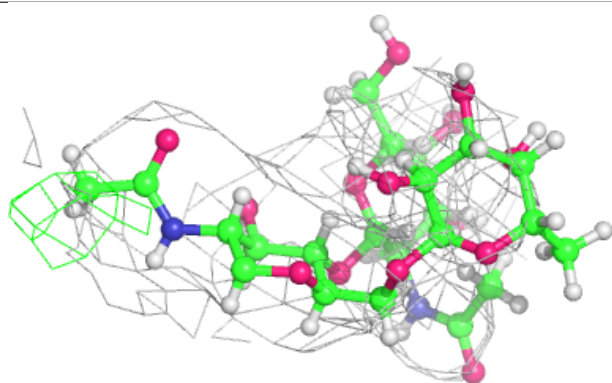
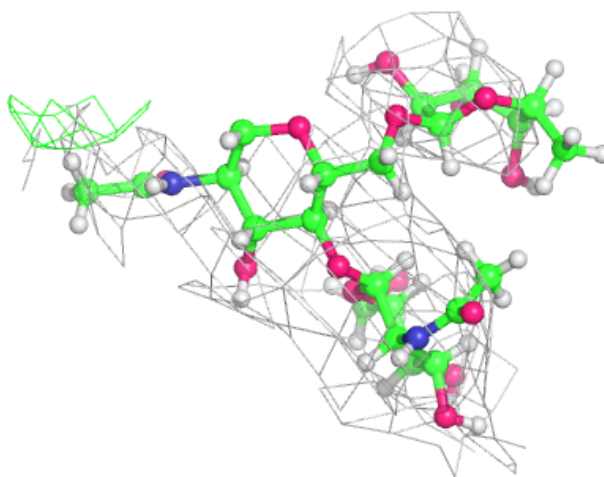
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	BMA	H	3	11/12	0.62	0.33	166,174,206,210	0
3	NAG	L	1	14/15	0.62	0.32	172,186,223,224	0
4	FUC	H	4	10/11	0.63	0.46	158,161,166,167	0
5	NAG	I	2	14/15	0.64	0.47	168,180,219,219	0
4	NAG	H	2	14/15	0.67	0.29	148,178,213,216	0
2	NAG	F	1	14/15	0.67	0.30	173,187,218,225	0
4	BMA	K	3	11/12	0.69	0.23	159,167,200,203	0
3	NAG	L	2	14/15	0.70	0.32	166,176,209,210	0
6	MAN	J	4	11/12	0.70	0.35	147,162,188,204	0
4	FUC	K	4	10/11	0.72	0.32	146,171,189,205	0
4	NAG	K	1	14/15	0.73	0.23	149,157,186,189	0
3	NAG	G	1	14/15	0.75	0.27	170,179,213,216	0
5	NAG	I	1	14/15	0.76	0.25	167,191,229,231	0
2	FUC	F	3	10/11	0.77	0.22	169,176,209,211	0
2	FUC	E	3	10/11	0.78	0.46	167,175,208,208	0
6	NAG	J	1	14/15	0.78	0.28	146,167,196,211	0
4	NAG	K	2	14/15	0.78	0.20	154,181,211,232	0
3	NAG	G	2	14/15	0.80	0.26	154,165,194,198	0
4	NAG	H	1	14/15	0.82	0.29	120,159,198,207	0
6	BMA	J	3	11/12	0.83	0.21	143,151,179,181	0
2	NAG	E	2	14/15	0.83	0.24	127,151,176,181	0
2	NAG	E	1	14/15	0.83	0.20	94,124,156,172	0
6	NAG	J	2	14/15	0.85	0.26	146,156,185,190	0
6	FUC	J	5	10/11	0.86	0.30	154,162,193,194	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.

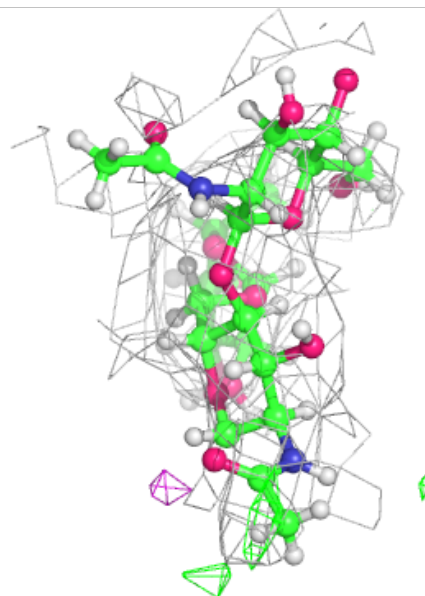
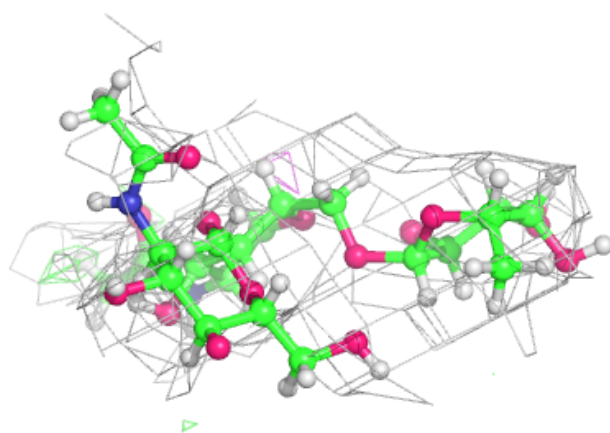
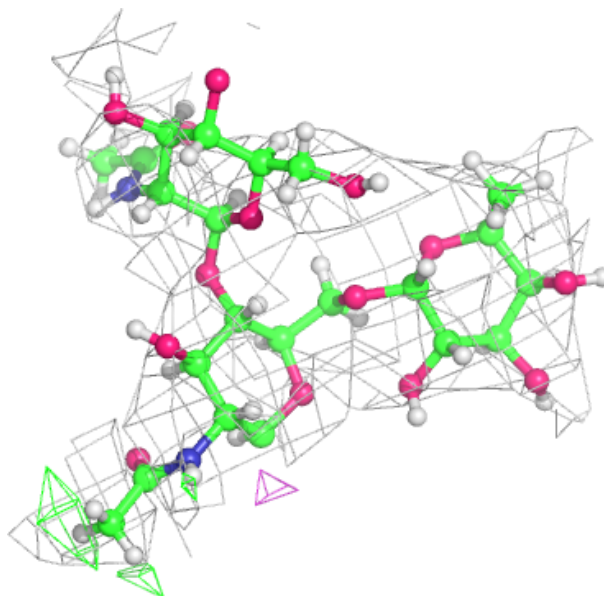
**Electron density around Chain E:**

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



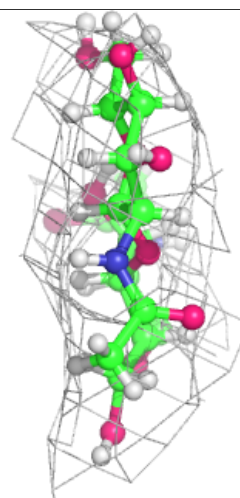
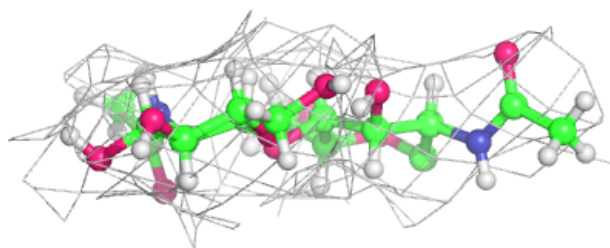
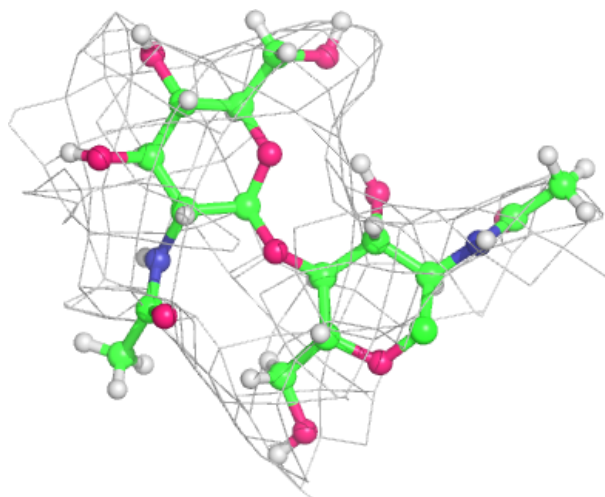
**Electron density around Chain F:**

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



**Electron density around Chain G:**

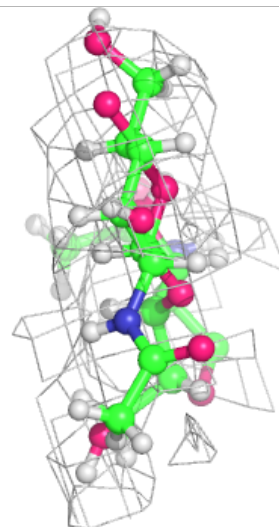
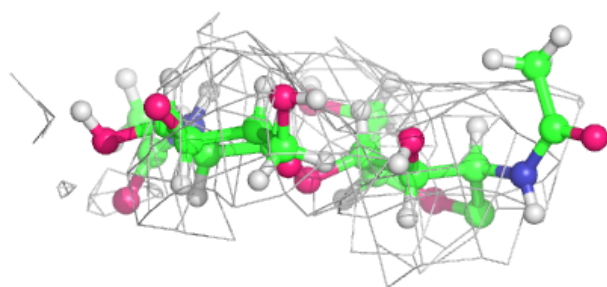
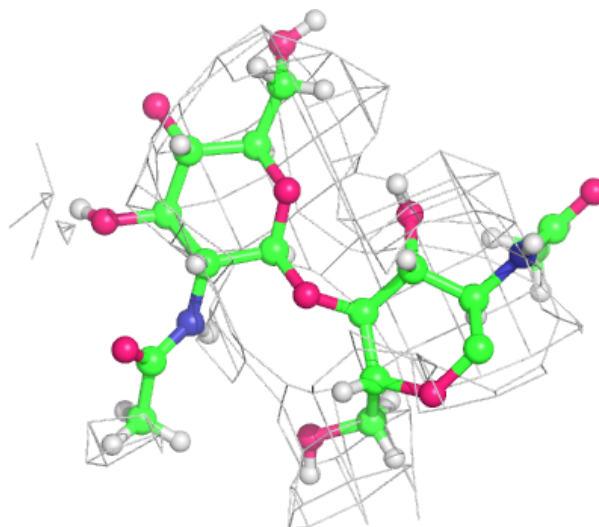
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





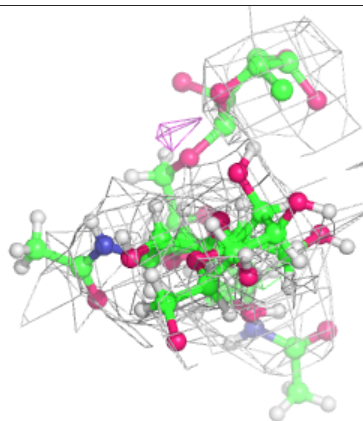
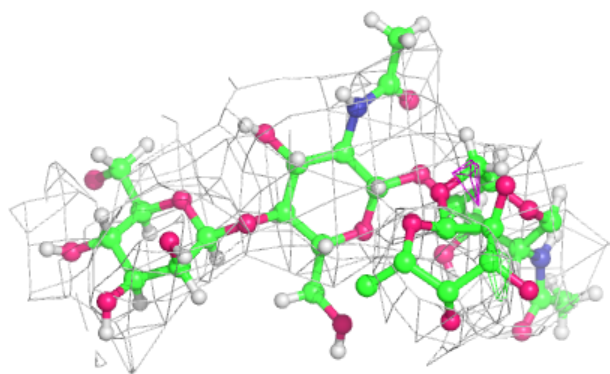
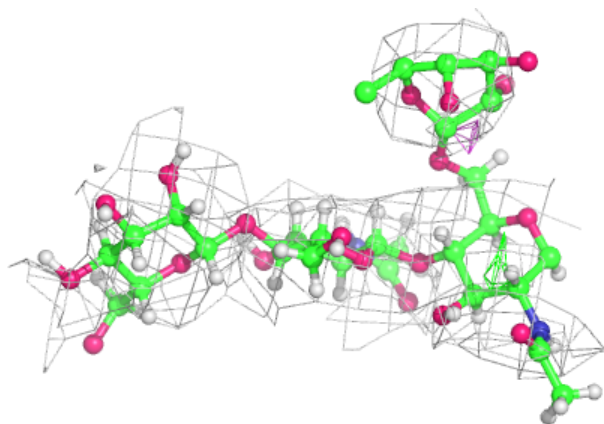
**Electron density around Chain L:**

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



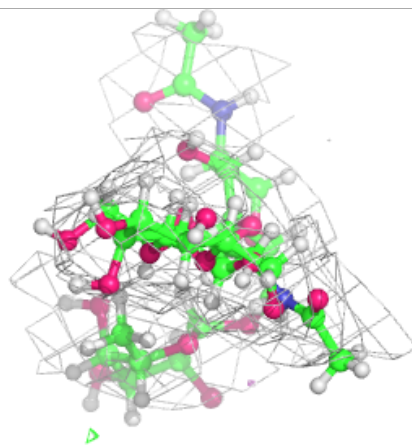
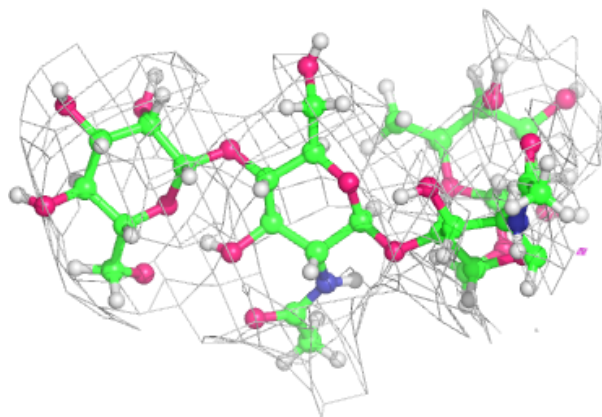
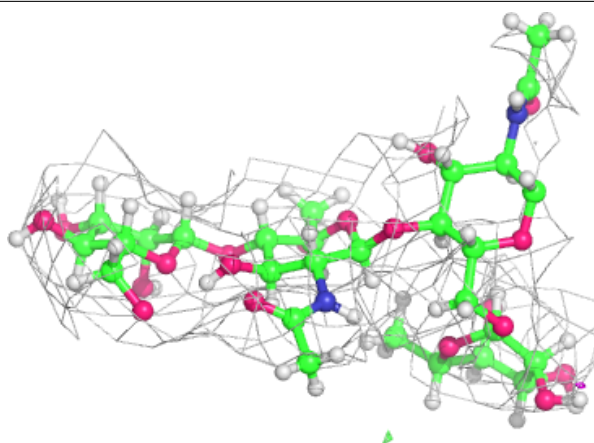
**Electron density around Chain H:**

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



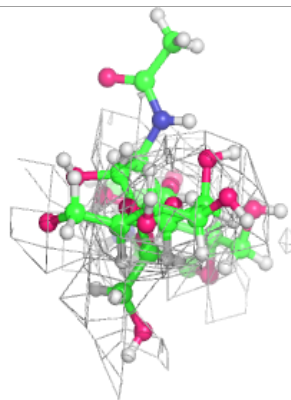
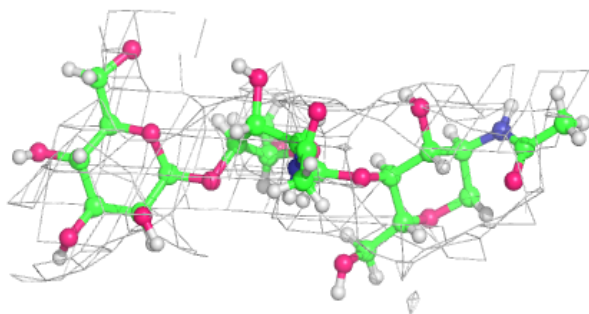
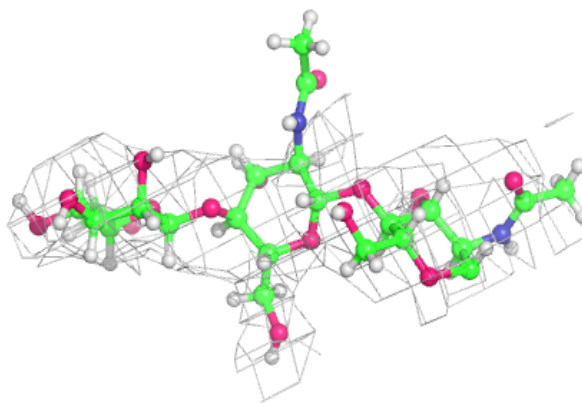
**Electron density around Chain K:**

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

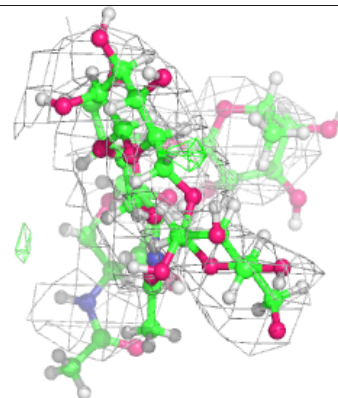
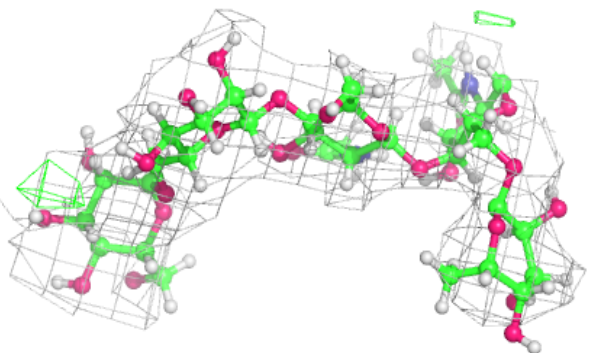
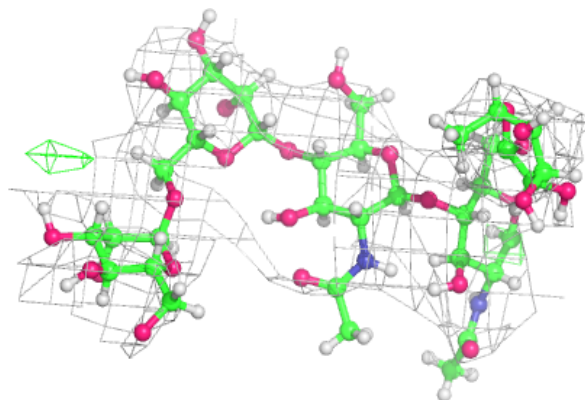


**Electron density around Chain I:**

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

**Electron density around Chain J:**

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



## 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
9	NAG	C	513	14/15	0.66	0.38	156,187,220,229	0
9	NAG	C	512	14/15	0.69	0.32	152,165,197,199	0
8	MAN	B	511	11/12	0.72	0.45	138,151,178,189	0
8	MAN	C	511	11/12	0.75	0.36	153,157,189,191	0
8	MAN	D	517	11/12	0.75	0.42	140,148,177,179	0
7	CA	D	503	1/1	0.77	0.11	92,92,92,92	0
7	CA	B	506	1/1	0.79	0.18	79,79,79,79	0
8	MAN	D	516	11/12	0.79	0.27	131,145,173,176	0
9	NAG	B	519	14/15	0.81	0.35	129,154,175,185	0
7	CA	B	503	1/1	0.82	0.19	79,79,79,79	0
8	MAN	A	510	11/12	0.82	0.36	115,139,166,167	0
7	CA	C	505	1/1	0.85	0.16	94,94,94,94	0
7	CA	D	508	1/1	0.86	0.07	92,92,92,92	0
7	CA	D	505	1/1	0.86	0.12	82,82,82,82	0
8	MAN	C	510	11/12	0.86	0.22	125,131,156,158	0
8	MAN	B	510	11/12	0.87	0.26	112,130,146,156	0
7	CA	C	501	1/1	0.88	0.10	81,81,81,81	0
7	CA	C	519	1/1	0.90	0.22	92,92,92,92	0
7	CA	B	508	1/1	0.91	0.07	112,112,112,112	0
7	CA	B	504	1/1	0.91	0.17	79,79,79,79	0
7	CA	D	509	1/1	0.91	0.07	110,110,110,110	0
7	CA	A	509	1/1	0.91	0.09	81,81,81,81	0
7	CA	B	507	1/1	0.91	0.17	82,82,82,82	0
7	CA	B	505	1/1	0.91	0.14	80,80,80,80	0
7	CA	A	502	1/1	0.91	0.13	79,79,79,79	0
7	CA	C	503	1/1	0.92	0.09	101,101,101,101	0
8	MAN	A	514	11/12	0.92	0.20	121,132,158,159	0
7	CA	B	520	1/1	0.92	0.22	79,79,79,79	0
7	CA	C	509	1/1	0.92	0.11	97,97,97,97	0
7	CA	D	507	1/1	0.93	0.06	101,101,101,101	0
7	CA	C	506	1/1	0.93	0.13	81,81,81,81	0
7	CA	D	518	1/1	0.93	0.14	85,85,85,85	0
7	CA	B	501	1/1	0.93	0.13	80,80,80,80	0
7	CA	B	502	1/1	0.94	0.20	79,79,79,79	0
7	CA	A	506	1/1	0.94	0.07	79,79,79,79	0
7	CA	D	501	1/1	0.94	0.04	82,82,82,82	0
7	CA	C	504	1/1	0.94	0.25	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CA	A	501	1/1	0.94	0.08	81,81,81,81	0
7	CA	C	508	1/1	0.95	0.20	122,122,122,122	0
7	CA	A	507	1/1	0.95	0.08	79,79,79,79	0
7	CA	A	508	1/1	0.95	0.11	81,81,81,81	0
7	CA	A	505	1/1	0.95	0.13	79,79,79,79	0
7	CA	A	520	1/1	0.96	0.26	79,79,79,79	0
7	CA	D	502	1/1	0.96	0.07	83,83,83,83	0
7	CA	A	503	1/1	0.97	0.08	79,79,79,79	0
7	CA	D	506	1/1	0.97	0.24	85,85,85,85	0
7	CA	C	507	1/1	0.97	0.08	105,105,105,105	0
7	CA	C	502	1/1	0.97	0.10	79,79,79,79	0
7	CA	A	504	1/1	0.97	0.12	95,95,95,95	0
7	CA	D	504	1/1	0.98	0.15	113,113,113,113	0
7	CA	B	509	1/1	0.98	0.12	79,79,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.