



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 08:14 AM BST

PDB ID : 5E65  
Title : The complex structure of Hemagglutinin-esterase-fusion mutant protein from the influenza D virus with receptor analog 9-O-Ac-3'SLN (Tr322)  
Authors : Song, H.; Qi, J.; Shi, Y.; Gao, G.F.  
Deposited on : 2015-10-09  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

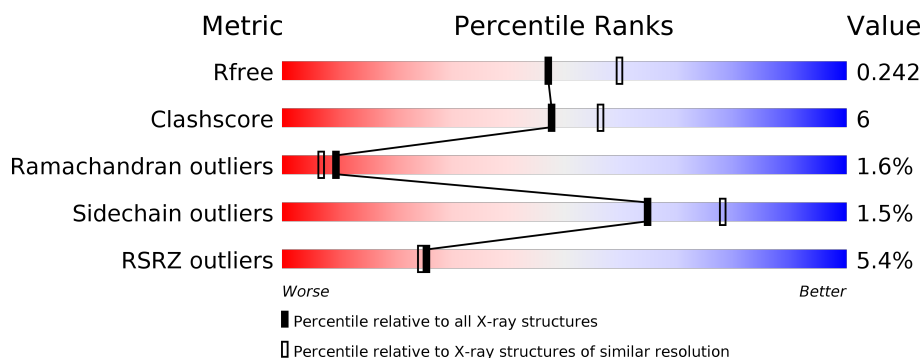
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	427	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	C	427	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
2	B	166	<div> <div>11%</div> <div> <div></div> <div>66%</div> <div>21%</div> <div>.</div> <div>10%</div> </div> </div>
2	D	166	<div> <div>11%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>..</div> <div>10%</div> </div> </div>
3	E	6	<div> <div></div> <div> <div>33%</div> <div>50%</div> <div>17%</div> </div> </div>
3	F	6	<div> <div></div> <div> <div>17%</div> <div>33%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	J	6	 33% 67%
4	G	2	 50% 50%
4	I	2	 50% 50%
4	K	2	 100%
4	L	2	 100%
4	N	2	 50% 50%
5	H	2	 50% 50%
5	M	2	 100%

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
6	NAG	D	703	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9829 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3240	2039	540	639	22			
1	C	424	Total	C	N	O	S	0	0	0
			3240	2039	540	639	22			

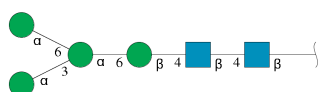
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	SER	engineered mutation	UNP K9LG83
A	356	ALA	ASP	engineered mutation	UNP K9LG83
A	359	ALA	HIS	engineered mutation	UNP K9LG83
C	57	ALA	SER	engineered mutation	UNP K9LG83
C	356	ALA	ASP	engineered mutation	UNP K9LG83
C	359	ALA	HIS	engineered mutation	UNP K9LG83

- Molecule 2 is a protein called Hemagglutinin-esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total	C	N	O	S	0	0	0
			1110	695	194	217	4			
2	D	149	Total	C	N	O	S	0	0	0
			1110	695	194	217	4			

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



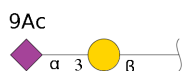
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	F	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	J	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	2	Total	C	N	O	0	0	0
			35	19	1	15			
5	M	2	Total	C	N	O	0	0	0
			35	19	1	15			

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



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

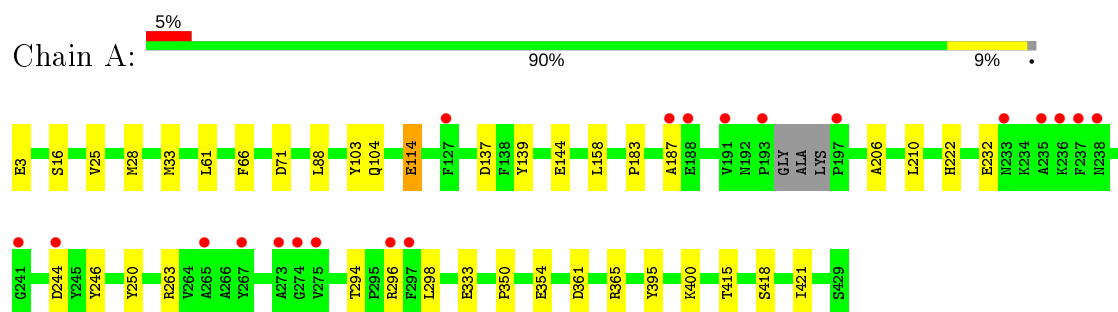
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	264	Total	O	0	0
			264	264		
7	B	68	Total	O	0	0
			68	68		
7	C	304	Total	O	0	0
			304	304		
7	D	39	Total	O	0	0
			39	39		

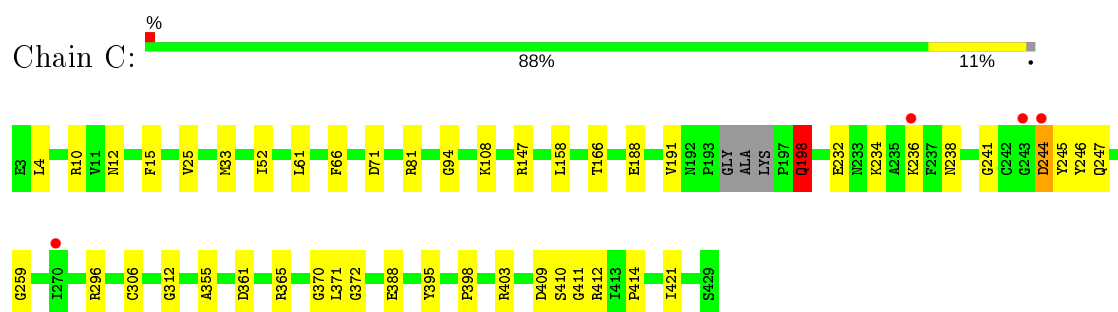
### 3 Residue-property plots

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.

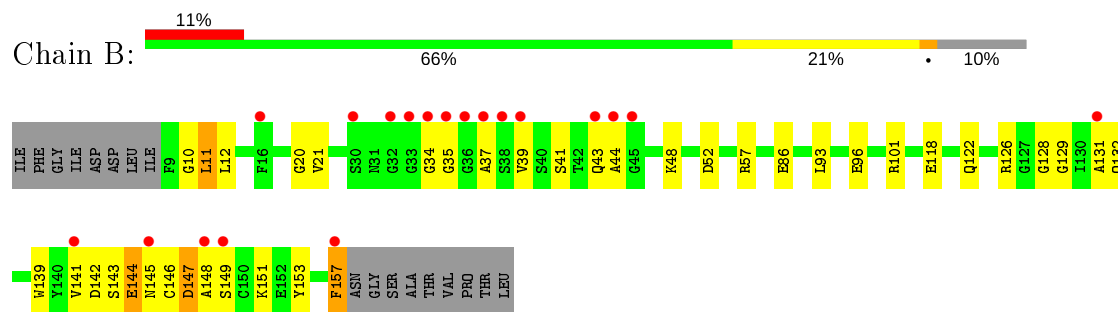
#### • Molecule 1: Hemagglutinin-esterase



#### • Molecule 1: Hemagglutinin-esterase

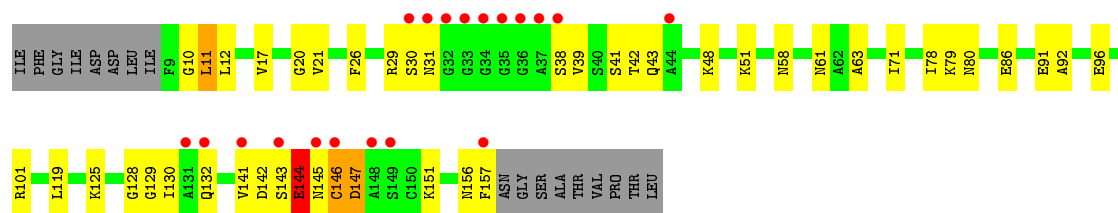


#### • Molecule 2: Hemagglutinin-esterase



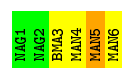
#### • Molecule 2: Hemagglutinin-esterase






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

Chain E: 



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

Chain F: 



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

Chain J: 



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

Chain G: 



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

Chain I: 





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

Chain K:  100%



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

Chain L:  100%



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

Chain N:  50% 50%



- Molecule 5: 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-3)-beta-D-galactopyranose

Chain H:  50% 50%



- Molecule 5: 9-O-acetyl-5-acetamido-3,5-dideoxy-D-glycero-alpha-D-galacto-non-2-ulopyranosonic acid-(2-3)-beta-D-galactopyranose

Chain M:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.90Å 164.90Å 164.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.60 – 2.20 47.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.60-2.20) 99.6 (47.60-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.203 , 0.243 0.206 , 0.242	Depositor DCC
$R_{free}$ test set	3800 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9829	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: GAL, BMA, NAG, 5N6, 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	0.28	0/3315	0.46	0/4494
1	C	0.29	0/3315	0.49	1/4494 (0.0%)
2	B	0.29	0/1127	0.46	0/1515
2	D	0.32	0/1127	0.49	0/1515
All	All	0.29	0/8884	0.47	1/12018 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	GLN	CA-CB-CG	5.78	126.12	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	244	ASP	Peptide
2	D	144	GLU	Peptide

## 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	3240	0	3114	29	0
1	C	3240	0	3114	34	0
2	B	1110	0	1067	23	0
2	D	1110	0	1067	33	0
3	E	72	0	61	1	0
3	F	72	0	61	2	0
3	J	72	0	61	0	0
4	G	28	0	25	1	0
4	I	28	0	25	1	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	N	28	0	25	0	0
5	H	35	0	11	1	0
5	M	35	0	11	1	0
6	B	14	0	13	0	0
6	D	14	0	13	2	0
7	A	264	0	0	9	1
7	B	68	0	0	2	0
7	C	304	0	0	4	0
7	D	39	0	0	3	0
All	All	9829	0	8718	109	1

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 6.

The worst 5 of 109 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)
5:H:2:5N6:O10	5:H:2:5N6:O7	1.89	0.90
3:F:2:NAG:O3	3:F:3:BMA:H2	1.81	0.81
2:D:63:ALA:O	7:D:801:HOH:O	2.02	0.76
1:A:415:THR:O	2:B:101:ARG:NH1	2.19	0.75
7:B:801:HOH:O	4:I:2:NAG:O4	2.07	0.73

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1061:HOH:O	7:A:1063:HOH:O[9_555]	2.04	0.16

## 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	420/427 (98%)	403 (96%)	17 (4%)	0	100	100
1	C	420/427 (98%)	398 (95%)	20 (5%)	2 (0%)	29	31
2	B	147/166 (89%)	122 (83%)	15 (10%)	10 (7%)	1	0
2	D	147/166 (89%)	124 (84%)	17 (12%)	6 (4%)	3	1
All	All	1134/1186 (96%)	1047 (92%)	69 (6%)	18 (2%)	9	7

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ASP
1	C	245	TYR
2	D	11	LEU
2	D	143	SER
2	B	11	LEU

### 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	357/358 (100%)	354 (99%)	3 (1%)	81	90
1	C	357/358 (100%)	354 (99%)	3 (1%)	81	90
2	B	109/123 (89%)	106 (97%)	3 (3%)	43	56
2	D	109/123 (89%)	104 (95%)	5 (5%)	27	34
All	All	932/962 (97%)	918 (98%)	14 (2%)	65	78

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	158	LEU
1	C	198	GLN
2	D	144	GLU
2	B	157	PHE
2	D	39	VAL

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

Mol	Chain	Res	Type
1	A	104	GLN
2	B	73	HIS
1	C	198	GLN
2	D	61	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 ⓘ

32 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
3	NAG	E	1	1,3	14,14,15	0.36	0	17,19,21	0.42	0
3	NAG	E	2	3	14,14,15	0.57	0	17,19,21	0.55	0
3	BMA	E	3	3	11,11,12	0.76	0	15,15,17	1.25	2 (13%)
3	MAN	E	4	3	11,11,12	0.91	1 (9%)	15,15,17	1.07	2 (13%)
3	MAN	E	5	3	11,11,12	0.99	0	15,15,17	1.14	1 (6%)
3	MAN	E	6	3	11,11,12	0.87	0	15,15,17	1.18	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.29	0	17,19,21	0.39	0
3	NAG	F	2	3	14,14,15	0.21	0	17,19,21	0.86	1 (5%)
3	BMA	F	3	3	11,11,12	1.34	2 (18%)	15,15,17	1.44	2 (13%)
3	MAN	F	4	3	11,11,12	0.93	1 (9%)	15,15,17	2.05	4 (26%)
3	MAN	F	5	3	11,11,12	0.90	1 (9%)	15,15,17	0.96	1 (6%)
3	MAN	F	6	3	11,11,12	1.21	1 (9%)	15,15,17	0.88	0
4	NAG	G	1	1,4	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	G	2	4	14,14,15	0.34	0	17,19,21	0.52	0
5	GAL	H	1	5	12,12,12	1.15	1 (8%)	17,17,17	1.29	3 (17%)
5	5N6	H	2	5	20,23,24	1.98	7 (35%)	25,32,35	1.57	5 (20%)
4	NAG	I	1	2,4	14,14,15	0.48	0	17,19,21	0.49	0
4	NAG	I	2	4	14,14,15	0.22	0	17,19,21	0.65	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.39	0	17,19,21	0.42	0
3	NAG	J	2	3	14,14,15	0.68	1 (7%)	17,19,21	0.56	0
3	BMA	J	3	3	11,11,12	0.77	0	15,15,17	1.10	1 (6%)
3	MAN	J	4	3	11,11,12	0.91	0	15,15,17	1.33	1 (6%)
3	MAN	J	5	3	11,11,12	0.83	0	15,15,17	0.92	0
3	MAN	J	6	3	11,11,12	0.95	1 (9%)	15,15,17	0.97	1 (6%)
4	NAG	K	1	1,4	14,14,15	0.32	0	17,19,21	0.57	0
4	NAG	K	2	4	14,14,15	0.21	0	17,19,21	0.62	0
4	NAG	L	1	1,4	14,14,15	0.39	0	17,19,21	0.58	0
4	NAG	L	2	4	14,14,15	0.34	0	17,19,21	0.55	0
5	GAL	M	1	5	12,12,12	1.43	3 (25%)	17,17,17	1.16	1 (5%)
5	5N6	M	2	5	20,23,24	2.37	11 (55%)	25,32,35	1.42	4 (16%)
4	NAG	N	1	2,4	14,14,15	0.43	0	17,19,21	0.55	0
4	NAG	N	2	4	14,14,15	0.31	0	17,19,21	0.63	1 (5%)

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
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1
5	GAL	H	1	5	-	2/2/22/22	0/1/1/1
5	5N6	H	2	5	-	9/17/37/41	0/1/1/1
4	NAG	I	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	MAN	J	4	3	-	0/2/19/22	0/1/1/1
3	MAN	J	5	3	-	2/2/19/22	0/1/1/1
3	MAN	J	6	3	-	2/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
5	GAL	M	1	5	-	2/2/22/22	0/1/1/1
5	5N6	M	2	5	-	0/17/37/41	0/1/1/1
4	NAG	N	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	2	5N6	O4-C4	-4.98	1.32	1.43
5	M	2	5N6	C4-C5	-4.02	1.49	1.53
5	M	2	5N6	C7-C6	-3.83	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	6	MAN	O5-C1	-3.58	1.38	1.43
5	H	2	5N6	C3-C2	-3.41	1.47	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	C1-O5-C5	5.93	120.23	112.19
3	F	3	BMA	C2-C3-C4	-3.90	104.14	110.89
3	J	4	MAN	C1-O5-C5	3.82	117.36	112.19
5	H	2	5N6	C9-O9-CAG	-3.80	107.56	117.10
3	J	3	BMA	C1-O5-C5	3.10	116.40	112.19

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

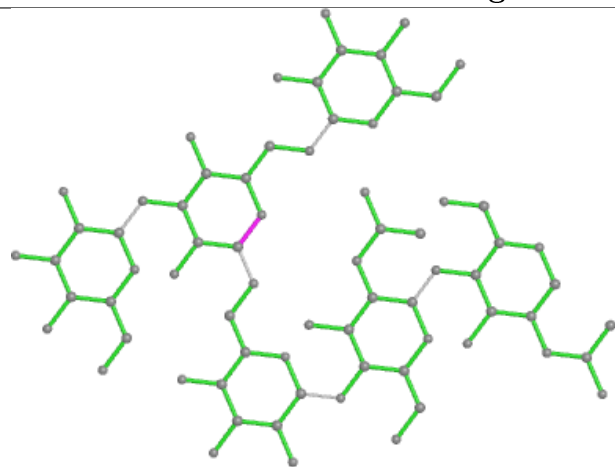
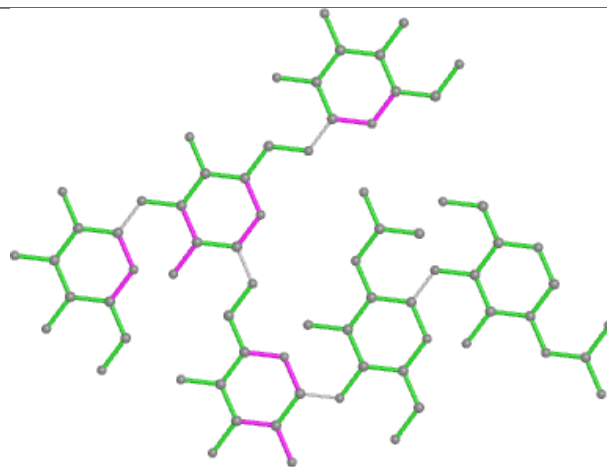
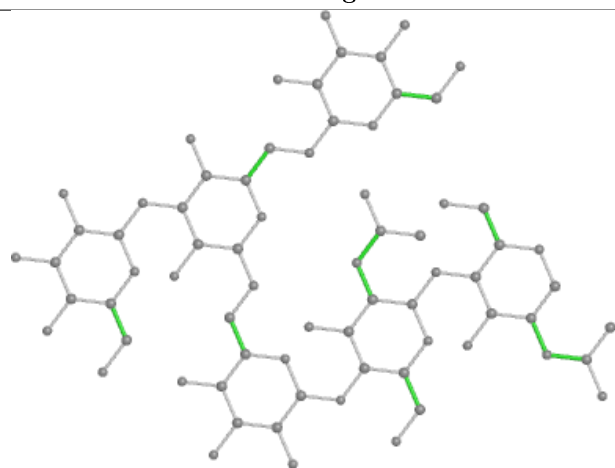
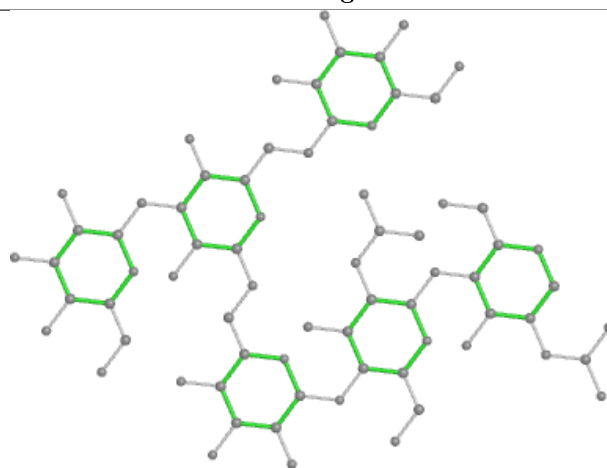
Mol	Chain	Res	Type	Atoms
5	H	2	5N6	C7-C8-C9-O9
5	H	2	5N6	O8-C8-C9-O9
5	H	2	5N6	O6-C6-C7-C8
5	H	2	5N6	O6-C6-C7-O7
5	H	2	5N6	CAF-CAG-O9-C9

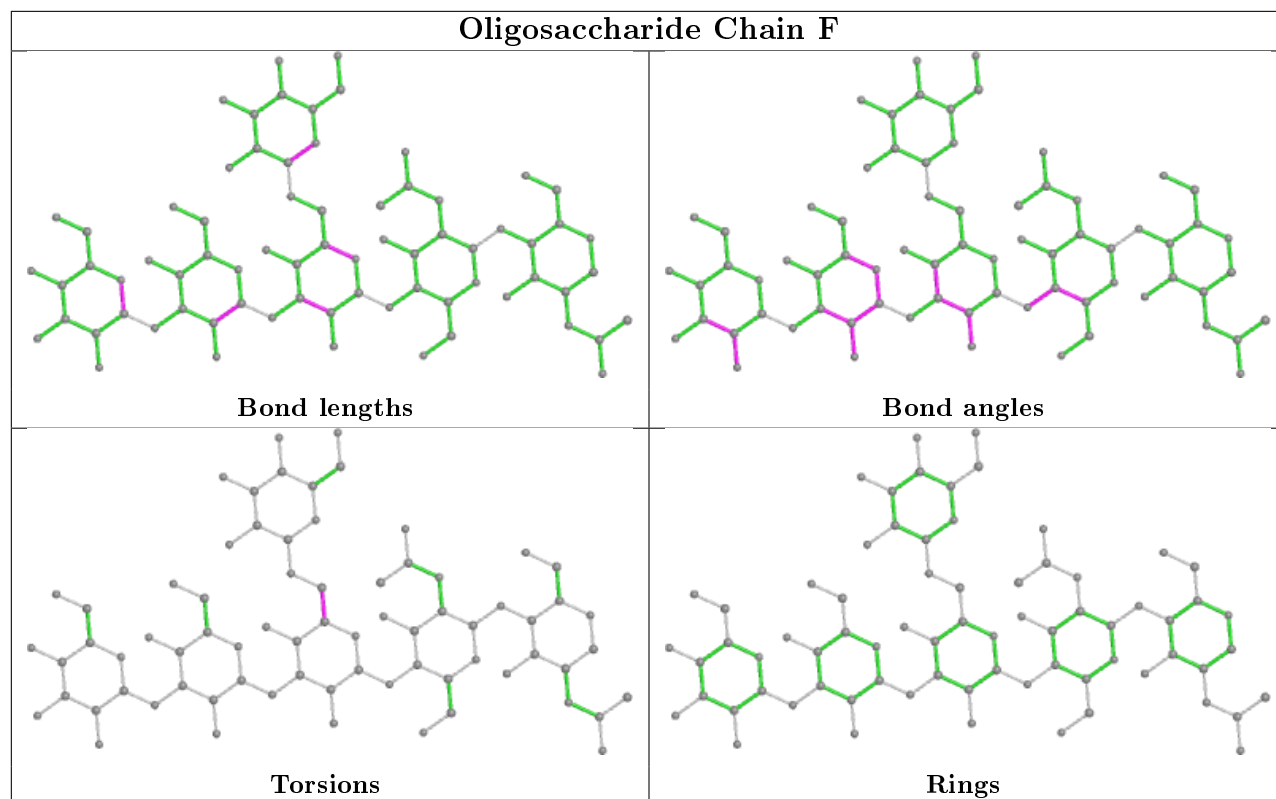
There are no ring outliers.

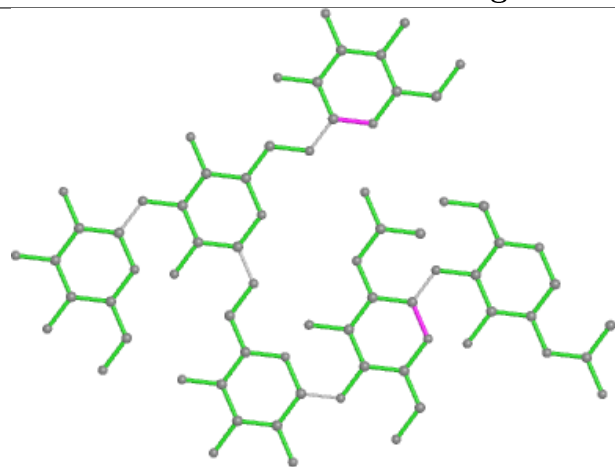
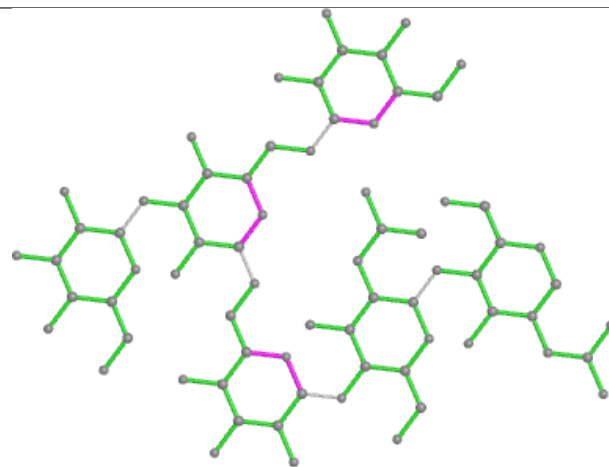
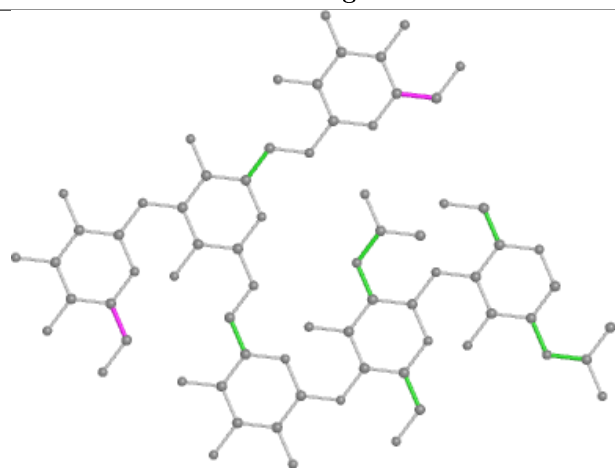
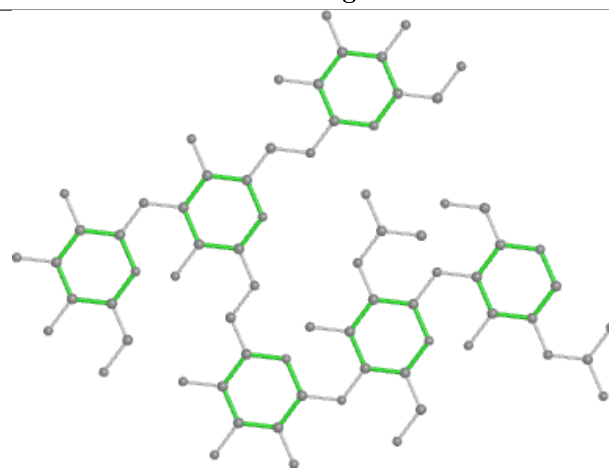
9 monomers are involved in 7 short contacts:

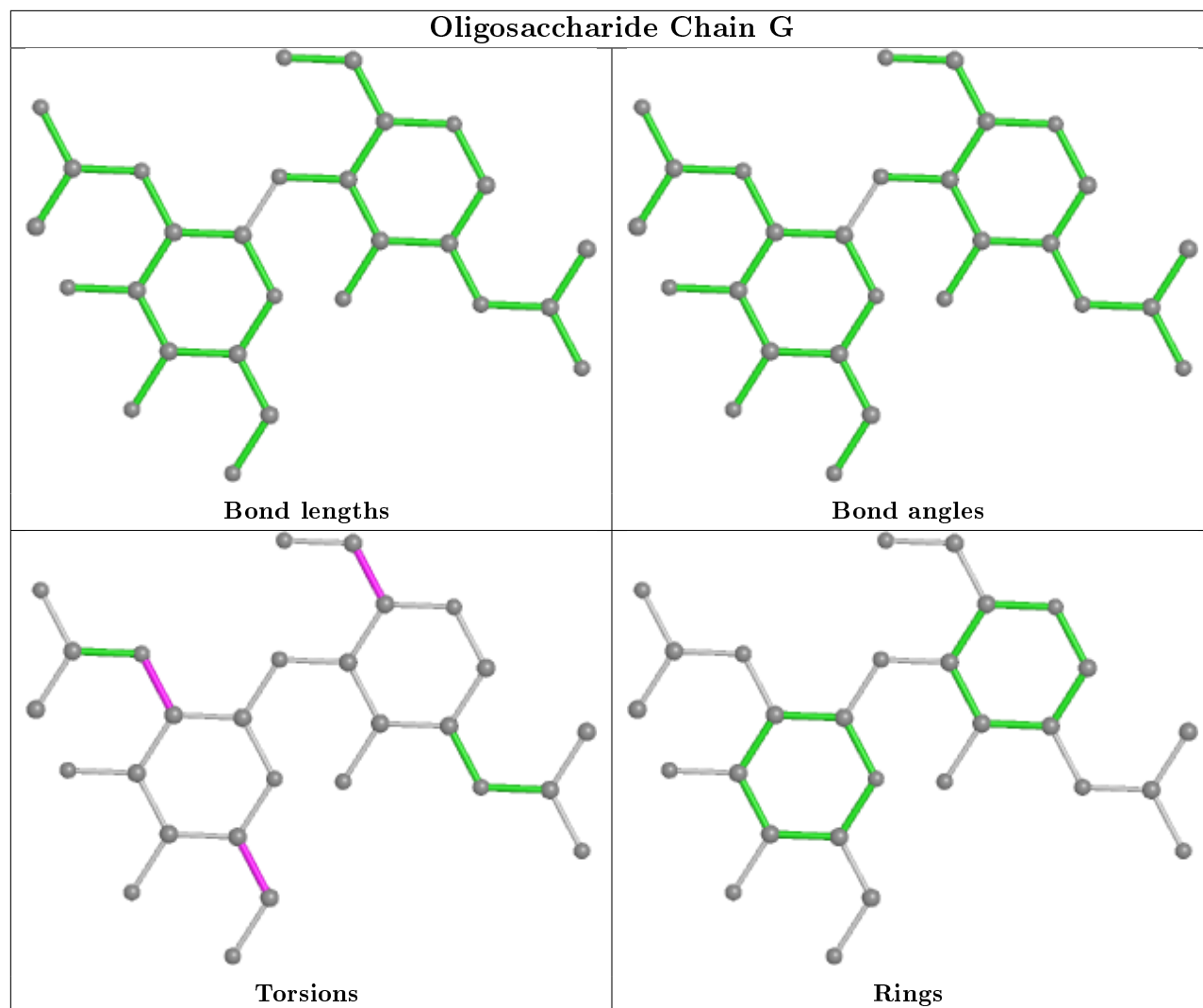
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	MAN	1	0
3	F	3	BMA	1	0
4	G	1	NAG	1	0
5	M	1	GAL	1	0
3	F	2	NAG	1	0
3	F	6	MAN	1	0
5	M	2	5N6	1	0
5	H	2	5N6	1	0
4	I	2	NAG	1	0

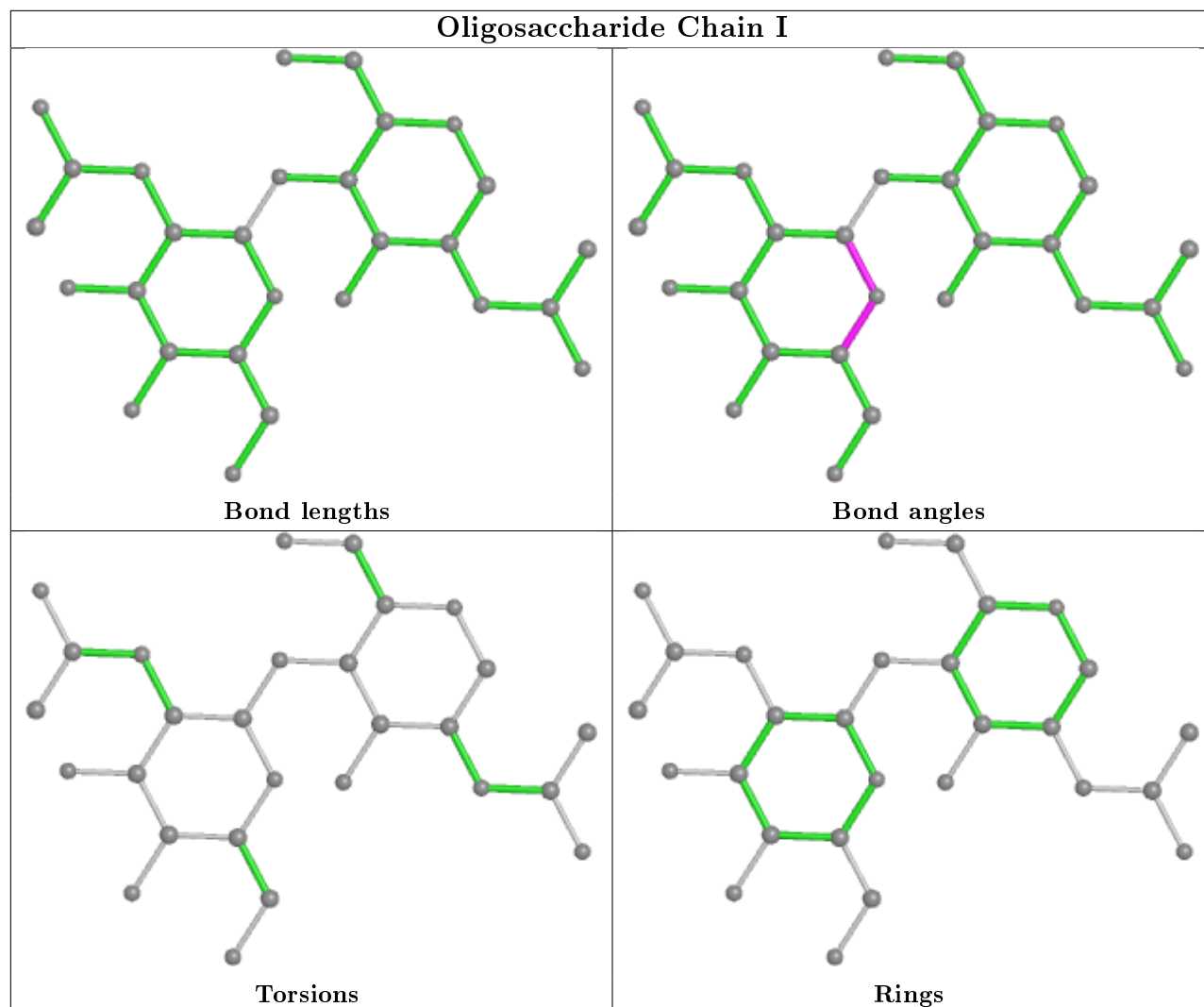
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

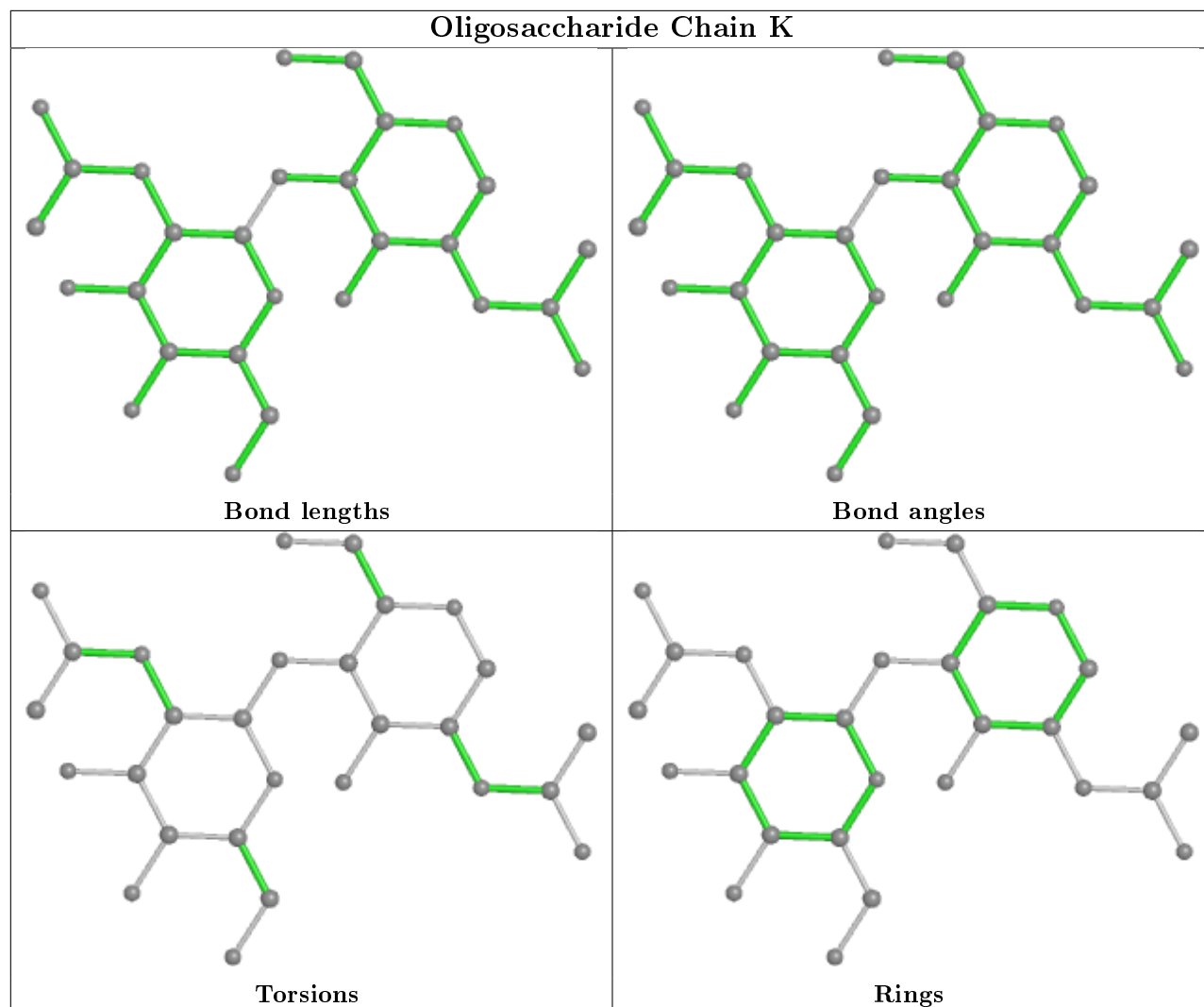
**Oligosaccharide Chain E****Bond lengths****Bond angles****Torsions****Rings**

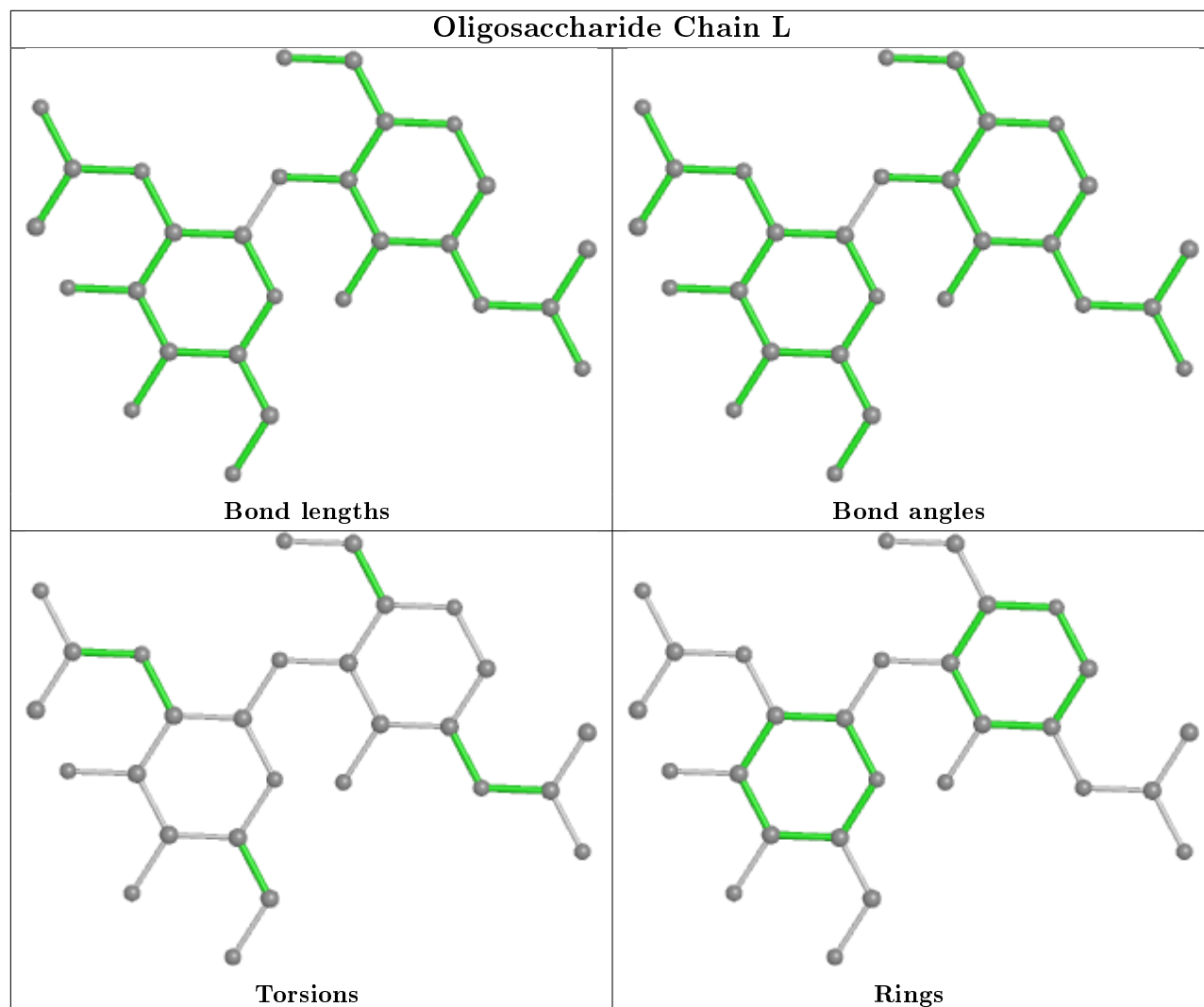


**Oligosaccharide Chain J****Bond lengths****Bond angles****Torsions****Rings**

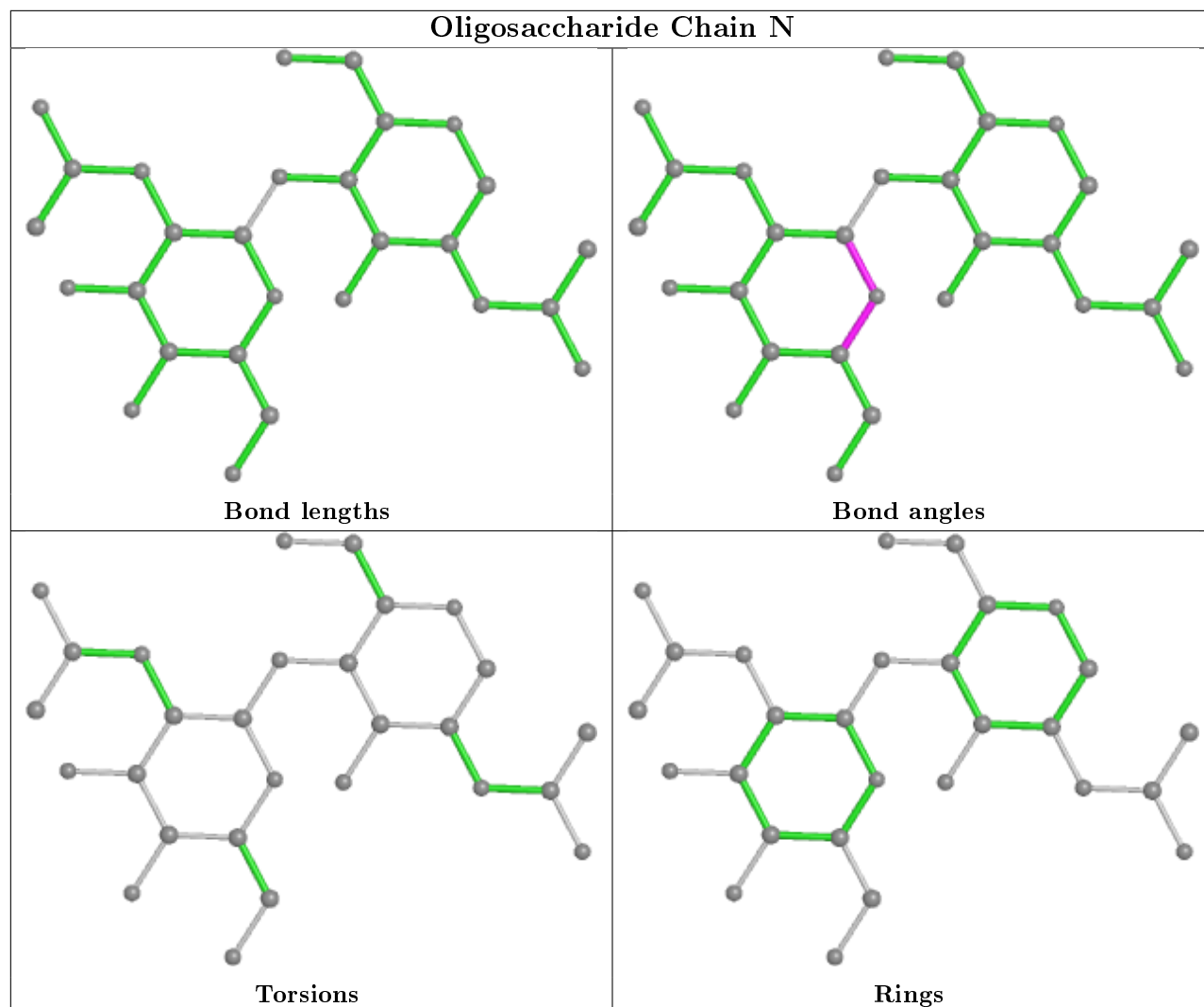




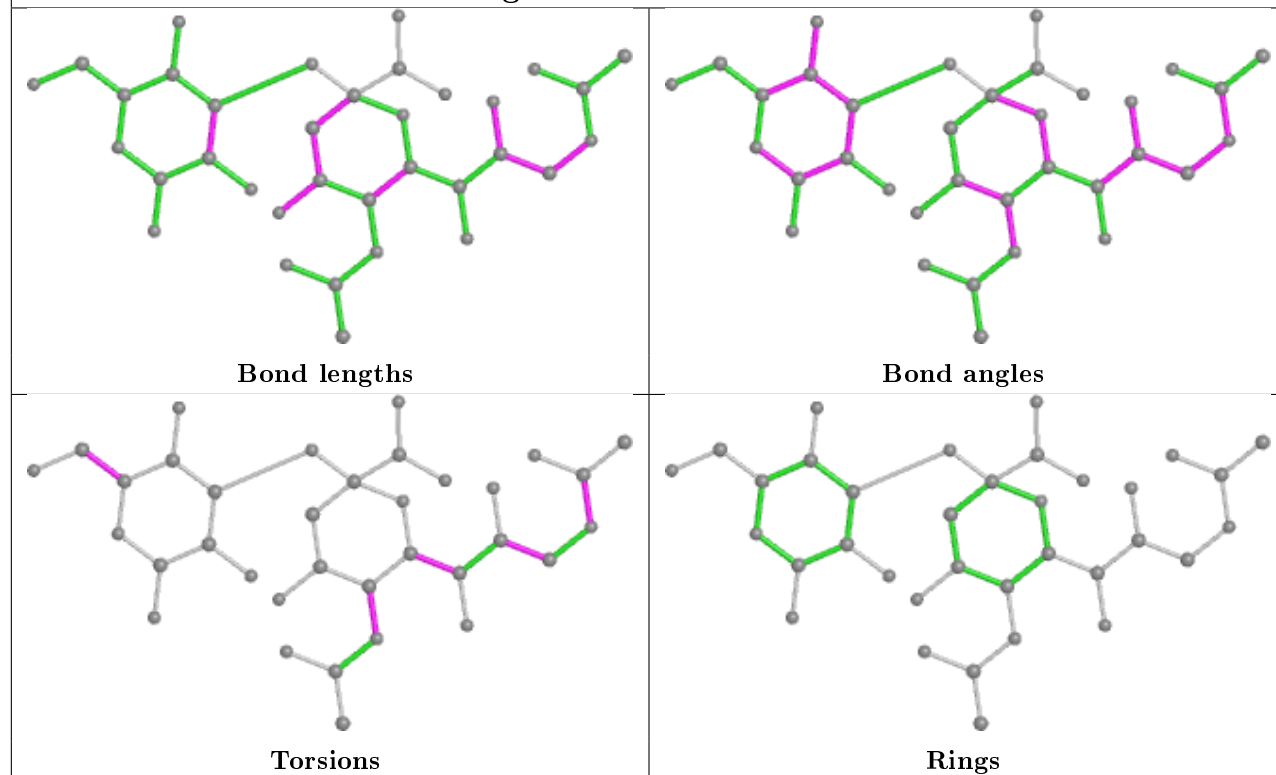




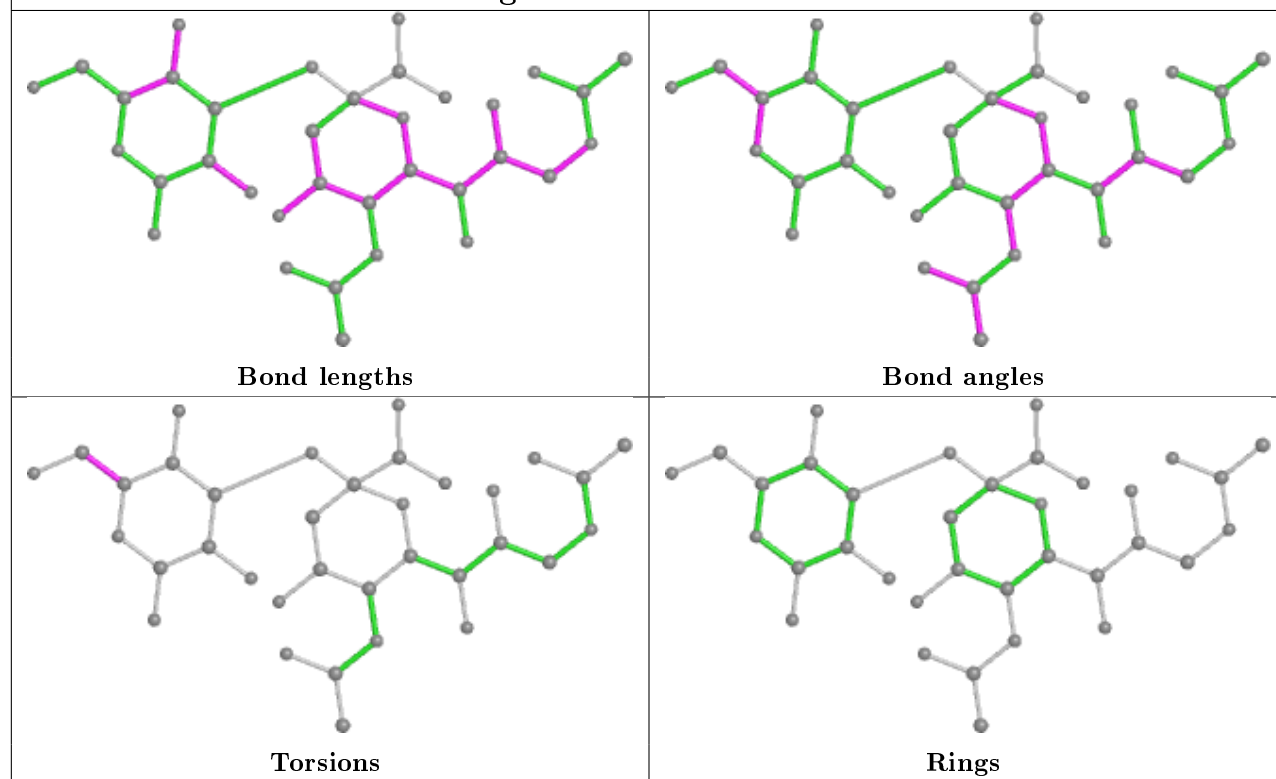




## Oligosaccharide Chain H



## Oligosaccharide Chain M



## 5.6 Ligand geometry

2 ligands 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	$\# Z  > 2$
6	NAG	D	703	2	14,14,15	0.52	0	17,19,21	1.23	2 (11%)
6	NAG	B	703	2	14,14,15	0.27	0	17,19,21	0.57	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
6	NAG	D	703	2	-	2/6/23/26	0/1/1/1
6	NAG	B	703	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	D	703	NAG	C1-O5-C5	3.64	117.12	112.19
6	D	703	NAG	O5-C5-C6	-2.37	103.49	107.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	703	NAG	C4-C5-C6-O6
6	D	703	NAG	O5-C5-C6-O6
6	B	703	NAG	O5-C5-C6-O6
6	D	703	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	703	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	424/427 (99%)	-0.17	20 (4%) 31 30	24, 35, 85, 131	0
1	C	424/427 (99%)	-0.44	4 (0%) 84 83	20, 33, 58, 89	0
2	B	149/166 (89%)	0.72	19 (12%) 3 3	22, 48, 128, 201	0
2	D	149/166 (89%)	0.68	19 (12%) 3 3	26, 49, 141, 173	0
All	All	1146/1186 (96%)	-0.04	62 (5%) 25 24	20, 37, 91, 201	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	34	GLY	23.5
2	B	32	GLY	18.8
2	D	33	GLY	15.4
2	B	37	ALA	14.1
2	D	32	GLY	12.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GAL	H	1	12/12	0.69	0.30	96,109,121,131	0
5	GAL	M	1	12/12	0.79	0.25	68,88,102,113	0

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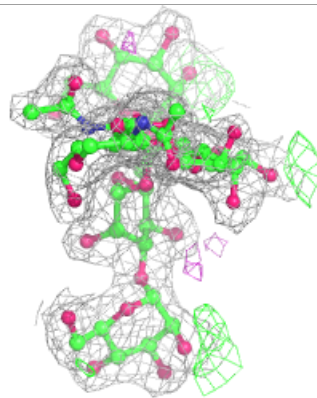
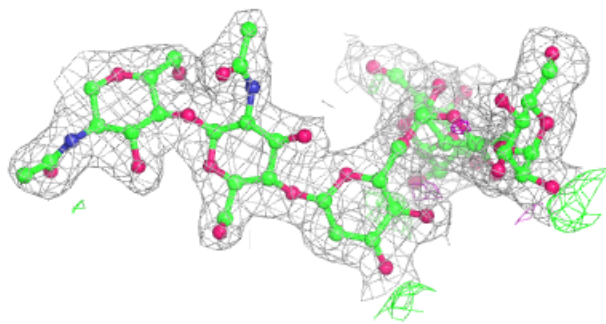
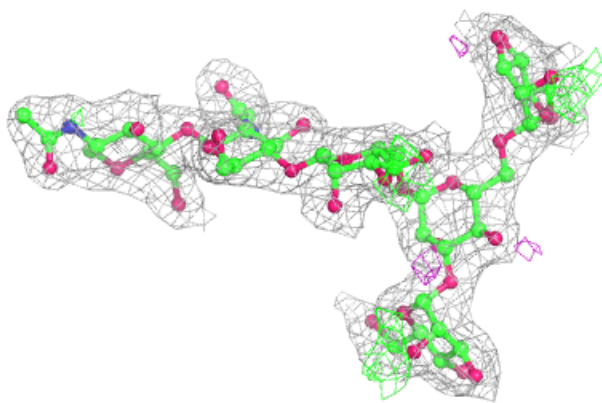
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	F	3	11/12	0.83	0.23	39,43,52,56	0
4	NAG	G	2	14/15	0.86	0.16	56,63,76,85	0
4	NAG	K	2	14/15	0.86	0.16	39,47,57,57	0
3	MAN	E	6	11/12	0.87	0.10	31,36,39,47	0
5	5N6	H	2	23/24	0.88	0.19	71,81,85,87	0
4	NAG	G	1	14/15	0.89	0.13	53,56,62,63	0
4	NAG	L	2	14/15	0.89	0.13	45,50,60,72	0
3	MAN	J	5	11/12	0.91	0.10	31,34,38,41	0
3	NAG	F	2	14/15	0.93	0.12	29,35,40,44	0
3	MAN	F	5	11/12	0.93	0.19	43,47,54,57	0
3	MAN	J	6	11/12	0.93	0.11	36,40,45,52	0
5	5N6	M	2	23/24	0.93	0.14	43,52,60,62	0
3	MAN	E	5	11/12	0.93	0.10	30,34,37,40	0
3	BMA	E	3	11/12	0.94	0.10	29,32,35,38	0
4	NAG	N	2	14/15	0.94	0.12	34,40,45,47	0
3	NAG	E	2	14/15	0.94	0.12	28,35,38,40	0
3	MAN	F	4	11/12	0.94	0.09	38,41,47,49	0
3	BMA	J	3	11/12	0.94	0.09	29,33,36,41	0
4	NAG	L	1	14/15	0.94	0.13	43,48,63,65	0
3	NAG	J	1	14/15	0.95	0.09	30,34,36,39	0
4	NAG	I	1	14/15	0.95	0.13	27,33,35,37	0
4	NAG	I	2	14/15	0.95	0.12	36,40,47,53	0
3	NAG	F	1	14/15	0.95	0.09	27,33,36,36	0
3	NAG	J	2	14/15	0.95	0.10	24,29,35,37	0
4	NAG	K	1	14/15	0.96	0.10	23,30,34,40	0
4	NAG	N	1	14/15	0.96	0.10	27,30,34,35	0
3	MAN	F	6	11/12	0.96	0.10	36,39,44,47	0
3	MAN	J	4	11/12	0.97	0.07	23,30,35,40	0
3	NAG	E	1	14/15	0.97	0.08	33,36,44,49	0
3	MAN	E	4	11/12	0.98	0.10	26,30,33,38	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.

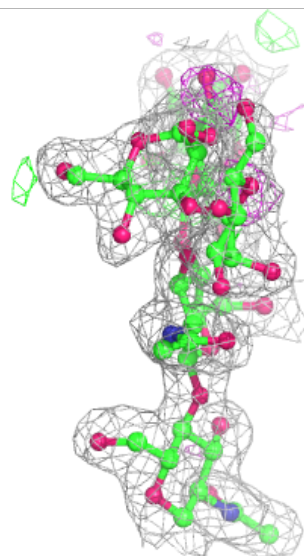
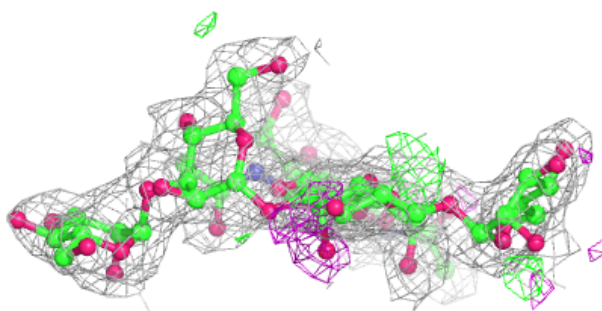
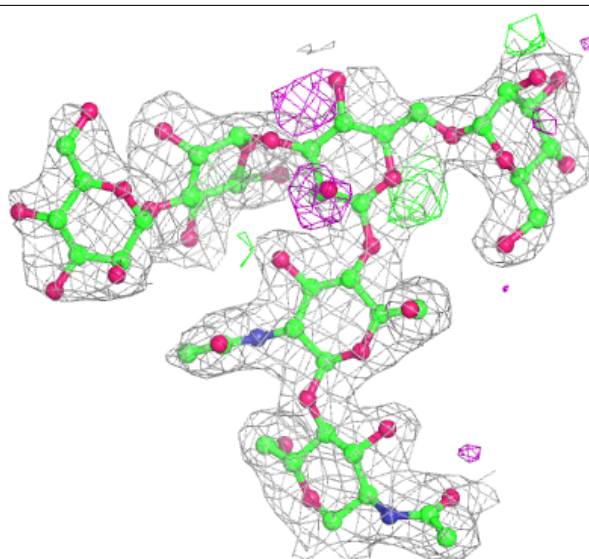
**Electron density around Chain E:**

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



**Electron density around Chain F:**

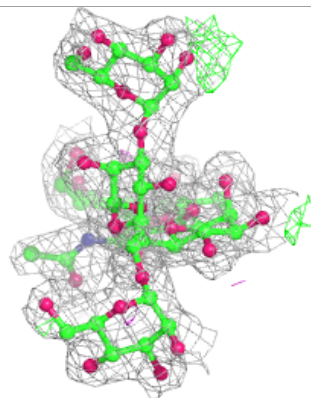
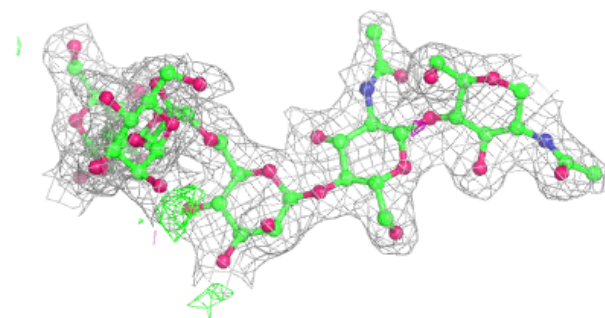
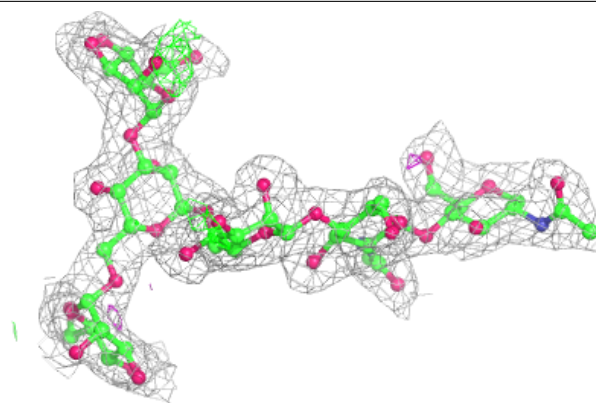
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



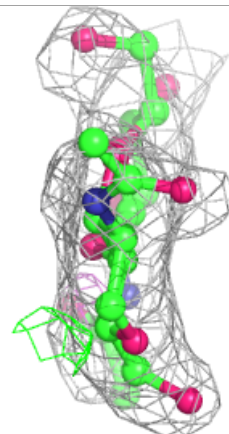
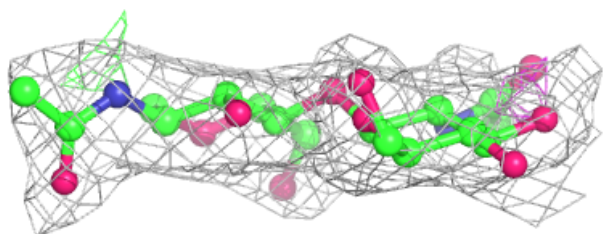
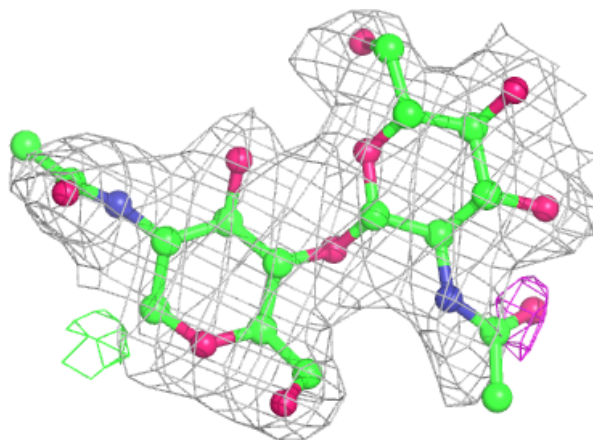


**Electron density around Chain J:**

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

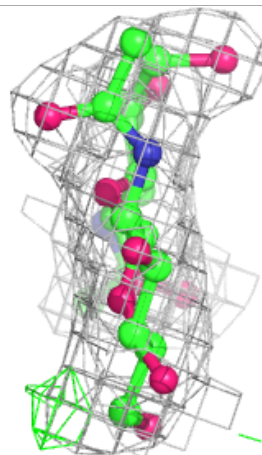
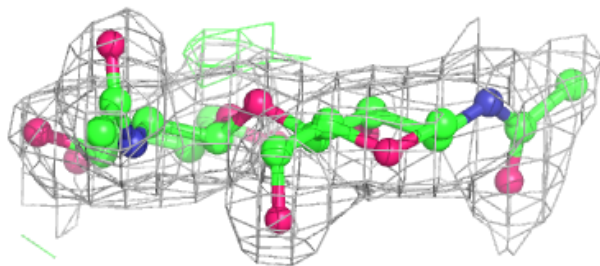
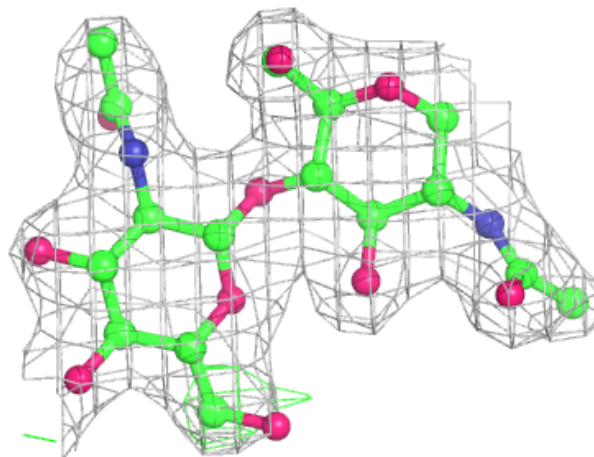
**Electron density around Chain G:**

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



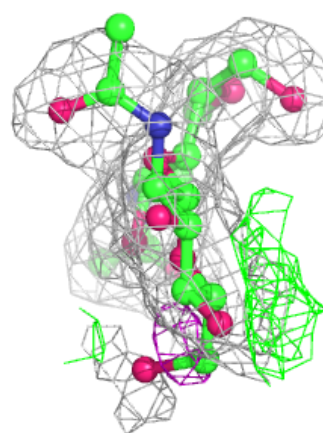
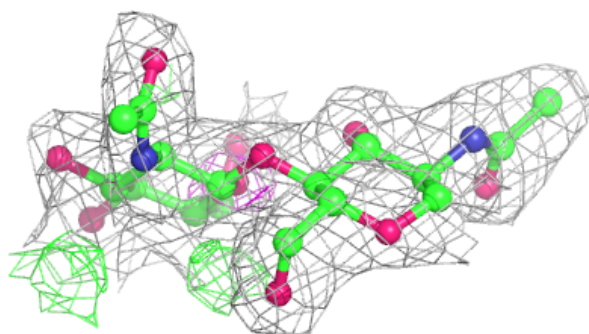
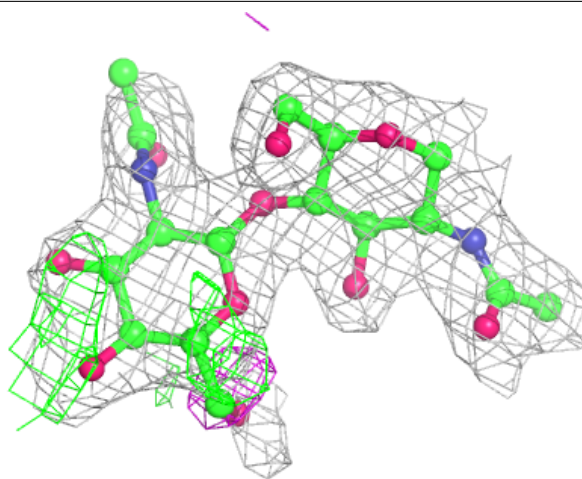
**Electron density around Chain I:**

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and green (positive)



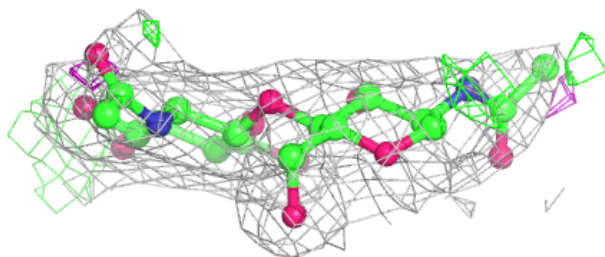
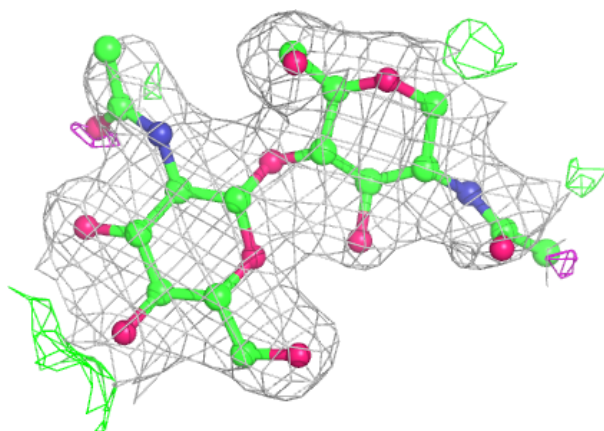
**Electron density around Chain K:**

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



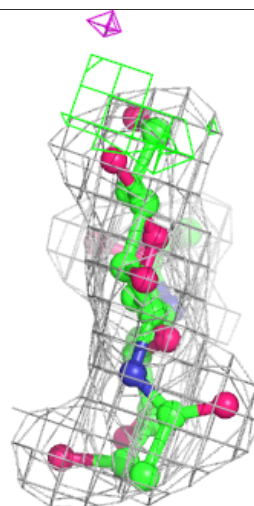
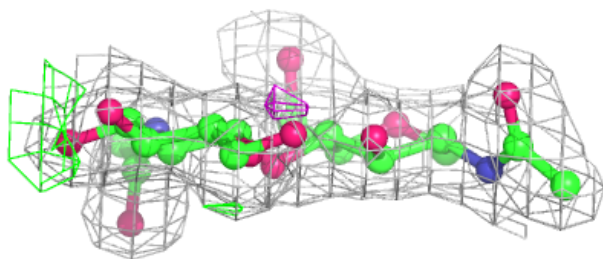
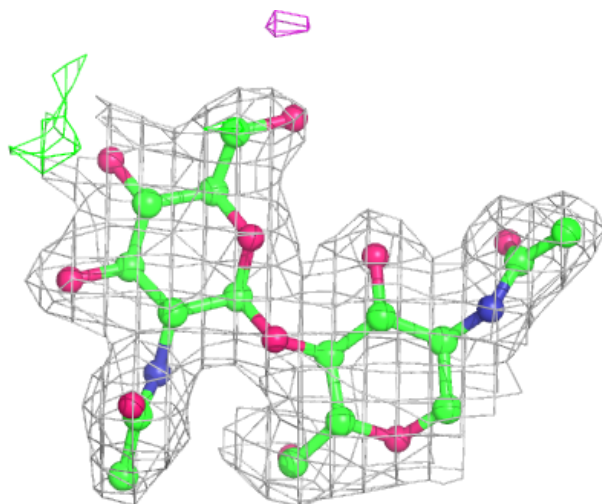
**Electron density around Chain L:**

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



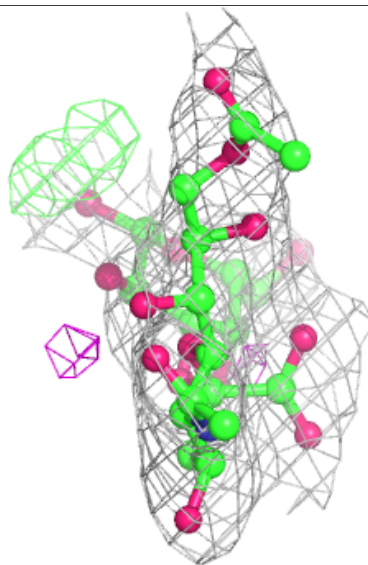
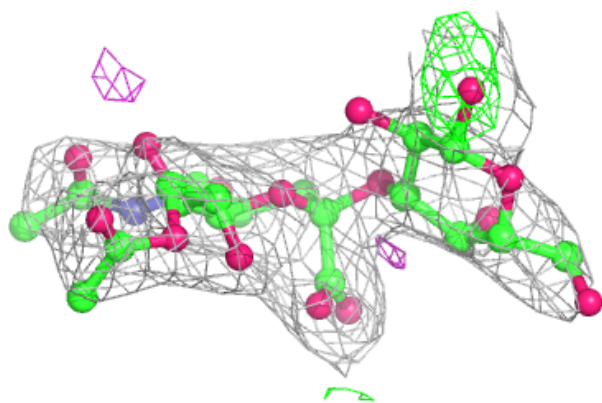
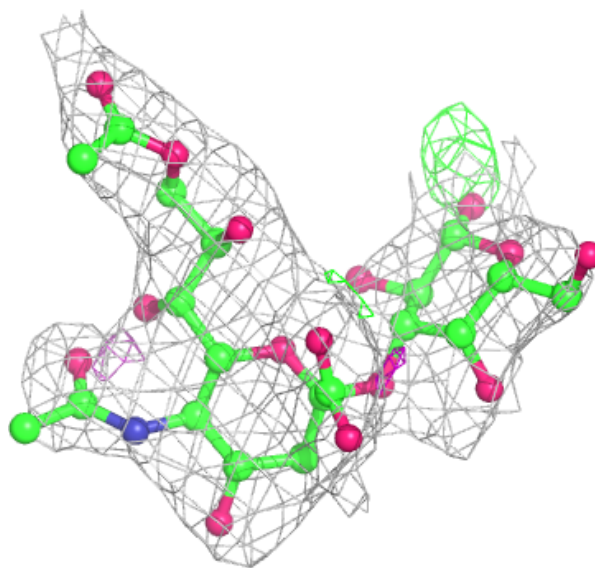
**Electron density around Chain N:**

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

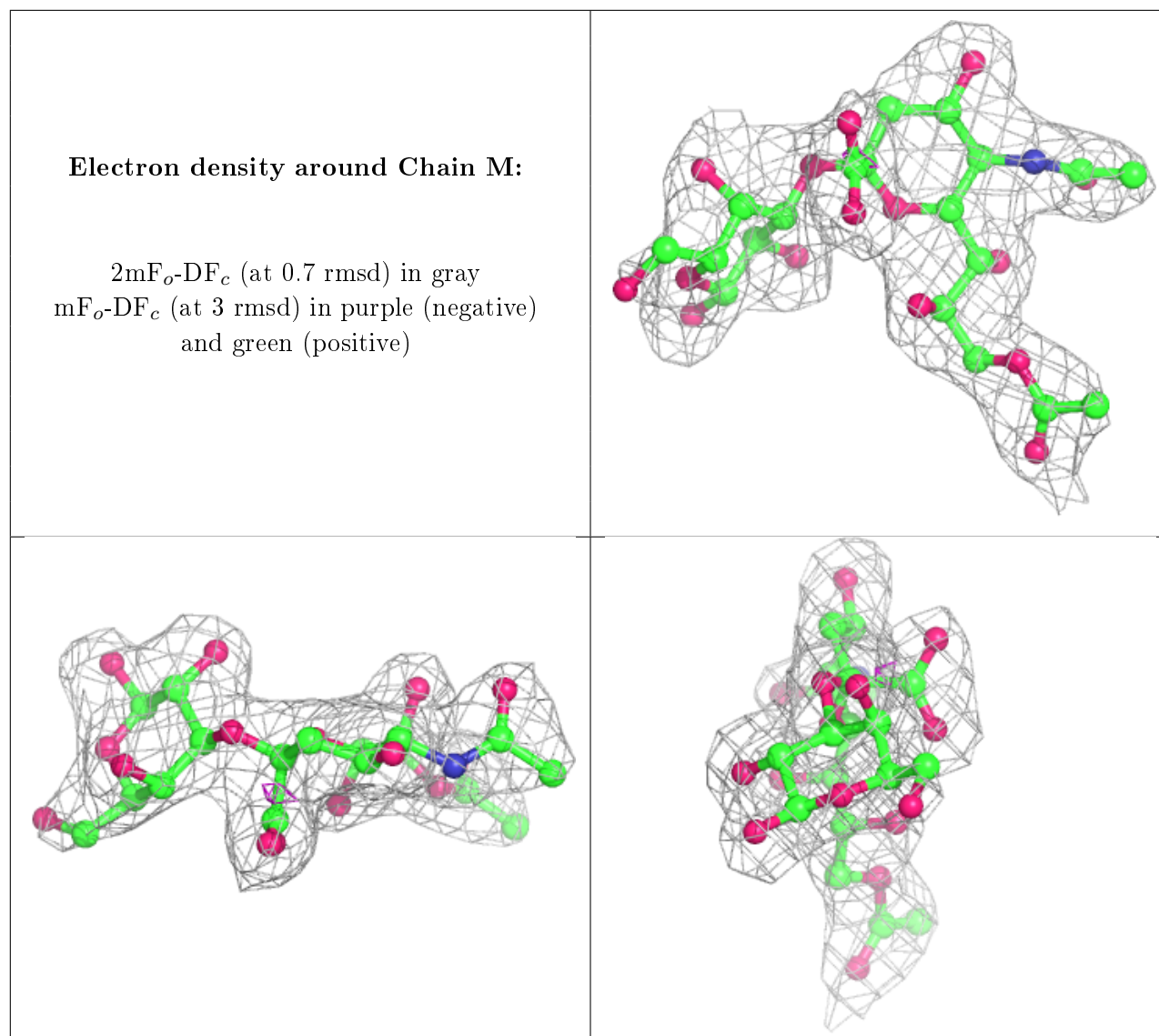


**Electron density around Chain H:**

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







## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	D	703	14/15	0.61	0.44	71,79,82,83	0
6	NAG	B	703	14/15	0.81	0.26	51,59,65,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.