



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2021 – 09:14 AM EDT

PDB ID : 1FAY  
Title : WINGED BEAN ACIDIC LECTIN COMPLEXED WITH METHYL-ALPHA-D-GALACTOSE (MONOCLINIC FORM)  
Authors : Manoj, N.; Srinivas, V.R.; Surolia, A.; Vijayan, M.; Suguna, K.  
Deposited on : 2000-07-14  
Resolution : 3.30 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	:	2.23.2
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)	:	2.23.2

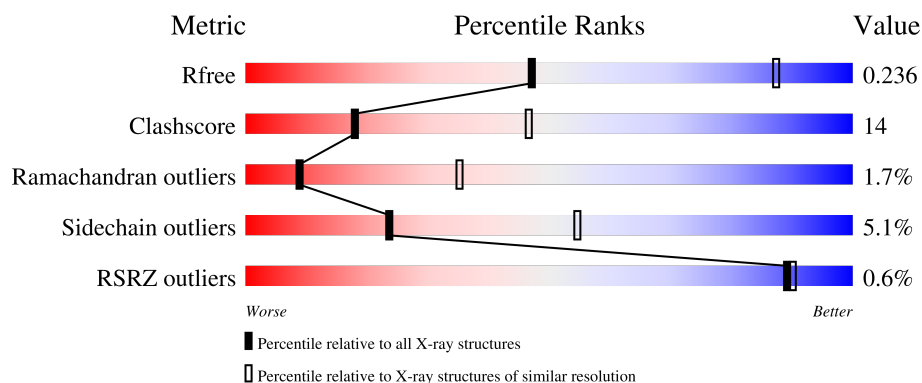
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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.








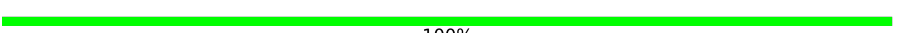



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	238	<div> <div>69%</div> <div>27%</div> <div>..</div> </div>
1	B	238	<div> <div>66%</div> <div>30%</div> <div>..</div> </div>
1	C	238	<div> <div>71%</div> <div>26%</div> <div>..</div> </div>
1	D	238	<div> <div>69%</div> <div>27%</div> <div>..</div> </div>
1	E	238	<div> <div>69%</div> <div>27%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	238	
1	G	238	
1	H	238	
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14293 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 ACIDIC LECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1742	1116	290	335	1			
1	B	236	Total	C	N	O	S	0	0	0
			1762	1131	292	338	1			
1	C	236	Total	C	N	O	S	0	0	0
			1738	1118	287	332	1			
1	D	236	Total	C	N	O	S	0	0	0
			1739	1115	290	333	1			
1	E	236	Total	C	N	O	S	0	0	0
			1744	1121	289	333	1			
1	F	236	Total	C	N	O	S	0	0	0
			1741	1117	291	332	1			
1	G	236	Total	C	N	O	S	0	0	0
			1724	1107	287	329	1			
1	H	236	Total	C	N	O	S	0	0	0
			1735	1116	288	330	1			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASN	SER	engineered mutation	GB 6018681
A	101	GLN	GLY	engineered mutation	GB 6018681
A	?	-	SER	deletion	GB 6018681
A	?	-	ASN	deletion	GB 6018681
A	120	PHE	LEU	engineered mutation	GB 6018681
B	28	ASN	SER	engineered mutation	GB 6018681
B	101	GLN	GLY	engineered mutation	GB 6018681
B	?	-	SER	deletion	GB 6018681
B	?	-	ASN	deletion	GB 6018681
B	120	PHE	LEU	engineered mutation	GB 6018681
C	28	ASN	SER	engineered mutation	GB 6018681
C	101	GLN	GLY	engineered mutation	GB 6018681
C	?	-	SER	deletion	GB 6018681

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ASN	deletion	GB 6018681
C	120	PHE	LEU	engineered mutation	GB 6018681
D	28	ASN	SER	engineered mutation	GB 6018681
D	101	GLN	GLY	engineered mutation	GB 6018681
D	?	-	SER	deletion	GB 6018681
D	?	-	ASN	deletion	GB 6018681
D	120	PHE	LEU	engineered mutation	GB 6018681
E	28	ASN	SER	engineered mutation	GB 6018681
E	101	GLN	GLY	engineered mutation	GB 6018681
E	?	-	SER	deletion	GB 6018681
E	?	-	ASN	deletion	GB 6018681
E	120	PHE	LEU	engineered mutation	GB 6018681
F	28	ASN	SER	engineered mutation	GB 6018681
F	101	GLN	GLY	engineered mutation	GB 6018681
F	?	-	SER	deletion	GB 6018681
F	?	-	ASN	deletion	GB 6018681
F	120	PHE	LEU	engineered mutation	GB 6018681
G	28	ASN	SER	engineered mutation	GB 6018681
G	101	GLN	GLY	engineered mutation	GB 6018681
G	?	-	SER	deletion	GB 6018681
G	?	-	ASN	deletion	GB 6018681
G	120	PHE	LEU	engineered mutation	GB 6018681
H	28	ASN	SER	engineered mutation	GB 6018681
H	101	GLN	GLY	engineered mutation	GB 6018681
H	?	-	SER	deletion	GB 6018681
H	?	-	ASN	deletion	GB 6018681
H	120	PHE	LEU	engineered mutation	GB 6018681

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



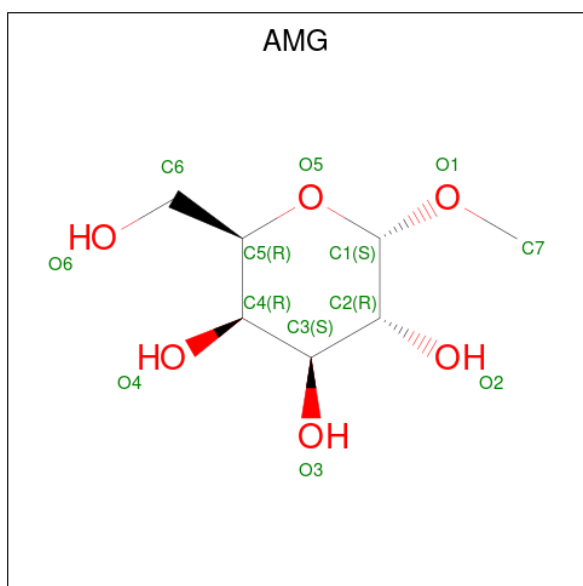
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is methyl alpha-D-galactopyranoside (three-letter code: AMG) (formula:  $C_7H_{14}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	7	6		
3	B	1	Total	C	O	0	0
			13	7	6		
3	C	1	Total	C	O	0	0
			13	7	6		
3	D	1	Total	C	O	0	0
			13	7	6		
3	E	1	Total	C	O	0	0
			13	7	6		
3	F	1	Total	C	O	0	0
			13	7	6		
3	G	1	Total	C	O	0	0
			13	7	6		
3	H	1	Total	C	O	0	0
			13	7	6		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mn 1	0	0
4	B	1	Total 1	Mn 1	0	0
4	C	1	Total 1	Mn 1	0	0
4	D	1	Total 1	Mn 1	0	0
4	E	1	Total 1	Mn 1	0	0
4	F	1	Total 1	Mn 1	0	0
4	G	1	Total 1	Mn 1	0	0
4	H	1	Total 1	Mn 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0
5	B	1	Total 1	Ca 1	0	0
5	C	1	Total 1	Ca 1	0	0
5	D	1	Total 1	Ca 1	0	0
5	E	1	Total 1	Ca 1	0	0
5	F	1	Total 1	Ca 1	0	0
5	G	1	Total 1	Ca 1	0	0
5	H	1	Total 1	Ca 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total 11	O 11	0	0

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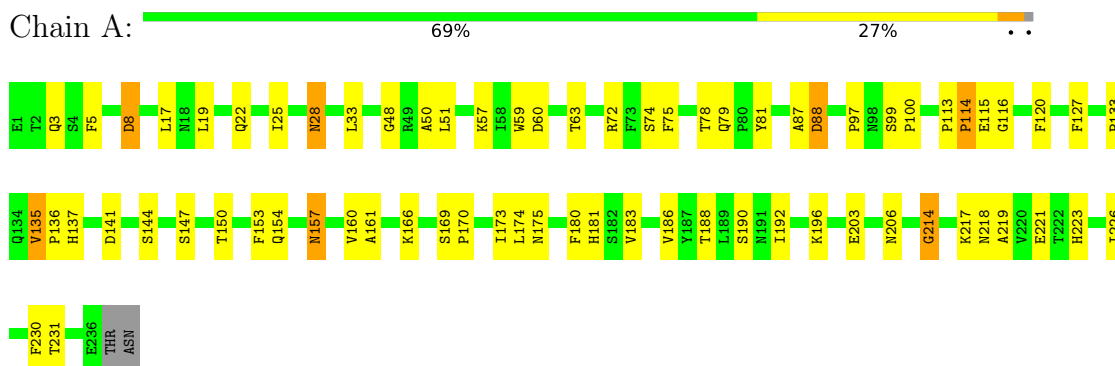
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	17	Total 17	O 17	0	0
6	C	8	Total 8	O 8	0	0
6	D	8	Total 8	O 8	0	0
6	E	10	Total 10	O 10	0	0
6	F	14	Total 14	O 14	0	0
6	G	6	Total 6	O 6	0	0
6	H	6	Total 6	O 6	0	0



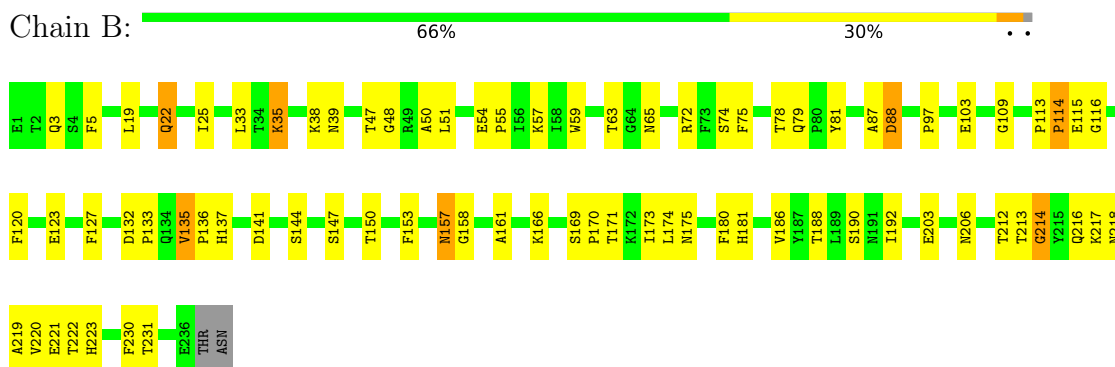
### 3 Residue-property plots

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.

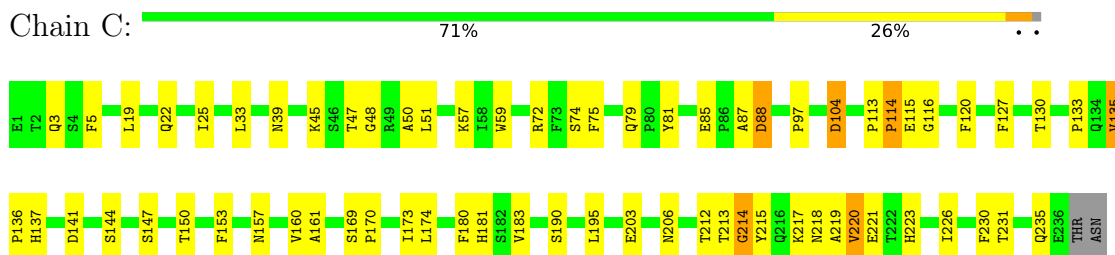
#### • Molecule 1: ACIDIC LECTIN



#### • Molecule 1: ACIDIC LECTIN

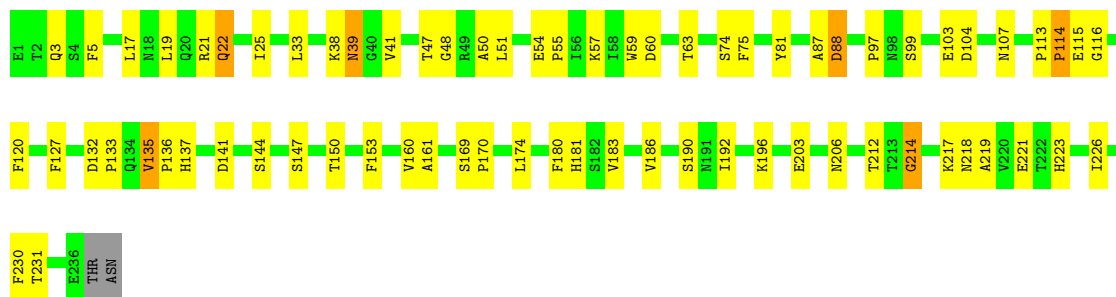


#### • Molecule 1: ACIDIC LECTIN



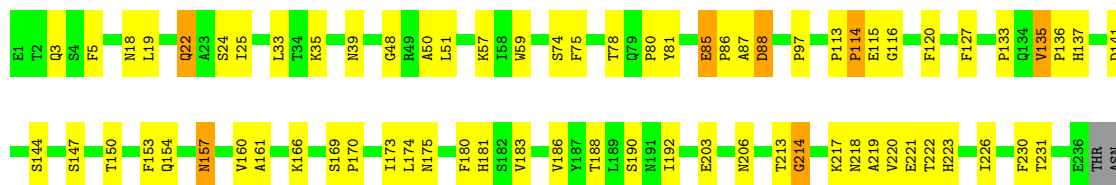
#### • Molecule 1: ACIDIC LECTIN

Chain D:  69% 27% ..



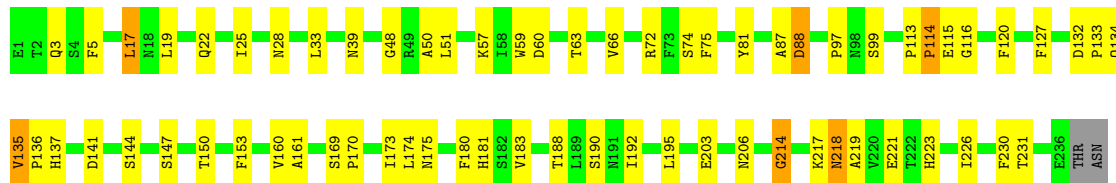
• Molecule 1: ACIDIC LECTIN

Chain E:  69% 27% ..



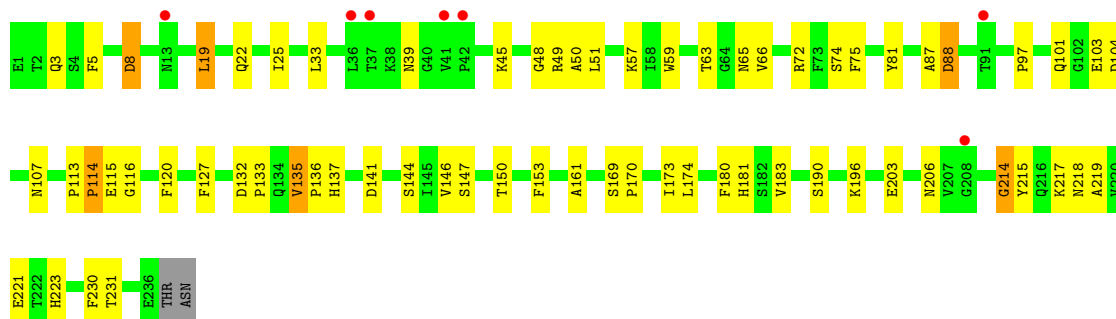
• Molecule 1: ACIDIC LECTIN

Chain F:  71% 26% ..



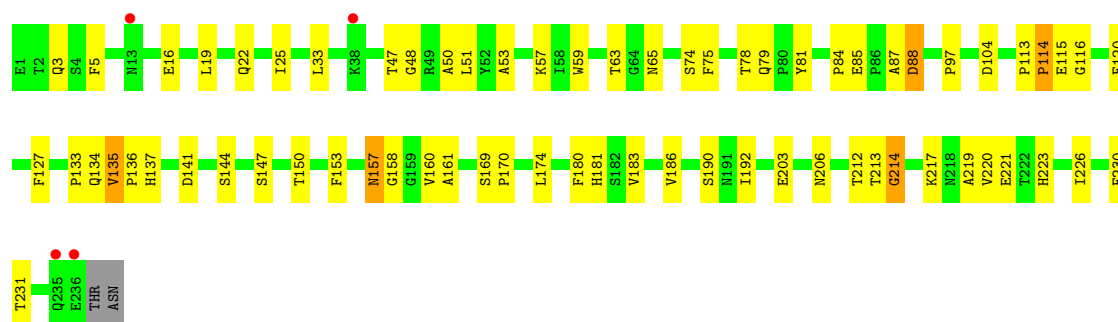
• Molecule 1: ACIDIC LECTIN

Chain G:  71% 26% ..



• Molecule 1: ACIDIC LECTIN

Chain H:  70% 27% ..



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

Chain I: 50% 50%



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

Chain J: 50% 50%



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

Chain K: 100%



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

Chain L: 50% 50%



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

Chain M: 50% 50%



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

Chain N:  100%

MOL  
MOL2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.53Å 125.91Å 138.79Å 90.00° 95.89° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 29.76 – 3.27	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-3.30) 90.8 (29.76-3.27)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 3.24Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, $R_{free}$	0.204 , 0.242 0.197 , 0.236	Depositor DCC
$R_{free}$ test set	1635 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: AMG, MN, NAG, CA

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	0.44	0/1789	0.71	1/2454 (0.0%)
1	B	0.45	0/1809	0.72	1/2479 (0.0%)
1	C	0.45	0/1785	0.72	1/2450 (0.0%)
1	D	0.44	0/1786	0.73	1/2451 (0.0%)
1	E	0.44	0/1791	0.71	1/2456 (0.0%)
1	F	0.44	0/1788	0.72	2/2450 (0.1%)
1	G	0.43	0/1771	0.71	1/2428 (0.0%)
1	H	0.41	0/1782	0.70	1/2444 (0.0%)
All	All	0.44	0/14301	0.72	9/19612 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	114	PRO	N-CA-CB	5.96	110.46	103.30
1	G	114	PRO	N-CA-CB	5.92	110.41	103.30
1	D	114	PRO	N-CA-CB	5.90	110.38	103.30
1	E	114	PRO	N-CA-CB	5.90	110.38	103.30
1	F	114	PRO	N-CA-CB	5.90	110.38	103.30

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	1742	0	1562	52	0
1	B	1762	0	1603	63	0
1	C	1738	0	1559	47	0
1	D	1739	0	1559	46	0
1	E	1744	0	1573	52	0
1	F	1741	0	1573	46	0
1	G	1724	0	1544	42	0
1	H	1735	0	1563	48	0
2	I	28	0	25	0	0
2	J	28	0	25	1	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	5	0
2	N	28	0	25	0	0
3	A	13	0	14	1	0
3	B	13	0	14	2	0
3	C	13	0	14	3	0
3	D	13	0	14	2	0
3	E	13	0	14	2	0
3	F	13	0	14	2	0
3	G	13	0	14	2	0
3	H	13	0	14	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	11	0	0	2	0
6	B	17	0	0	1	0
6	C	8	0	0	2	0
6	D	8	0	0	0	0
6	E	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	14	0	0	1	0
6	G	6	0	0	1	0
6	H	6	0	0	0	0
All	All	14293	0	12798	365	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 14.

The worst 5 of 365 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:H:213:THR:HB	1:H:220:VAL:HG12	1.36	1.06
1:C:213:THR:HB	1:C:220:VAL:HG12	1.41	1.01
1:E:181:HIS:HD2	1:F:181:HIS:HD2	1.01	1.01
1:C:181:HIS:HD2	1:D:181:HIS:HD2	1.04	1.00
1:F:3:GLN:HE22	1:F:57:LYS:H	1.09	1.00

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	234/238 (98%)	215 (92%)	16 (7%)	3 (1%)	12	40
1	B	234/238 (98%)	217 (93%)	14 (6%)	3 (1%)	12	40
1	C	234/238 (98%)	216 (92%)	14 (6%)	4 (2%)	9	35
1	D	234/238 (98%)	213 (91%)	16 (7%)	5 (2%)	7	31
1	E	234/238 (98%)	215 (92%)	15 (6%)	4 (2%)	9	35
1	F	234/238 (98%)	214 (92%)	16 (7%)	4 (2%)	9	35
1	G	234/238 (98%)	213 (91%)	15 (6%)	6 (3%)	5	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	234/238 (98%)	214 (92%)	17 (7%)	3 (1%)	12	40
All	All	1872/1904 (98%)	1717 (92%)	123 (7%)	32 (2%)	9	35

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	104	ASP
1	A	22	GLN
1	A	115	GLU
1	A	214	GLY
1	B	22	GLN

### 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	172/210 (82%)	163 (95%)	9 (5%)	23	54
1	B	176/210 (84%)	168 (96%)	8 (4%)	27	58
1	C	169/210 (80%)	160 (95%)	9 (5%)	22	53
1	D	171/210 (81%)	163 (95%)	8 (5%)	26	57
1	E	171/210 (81%)	161 (94%)	10 (6%)	20	50
1	F	172/210 (82%)	162 (94%)	10 (6%)	20	50
1	G	168/210 (80%)	161 (96%)	7 (4%)	30	60
1	H	169/210 (80%)	160 (95%)	9 (5%)	22	53
All	All	1368/1680 (81%)	1298 (95%)	70 (5%)	24	54

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	113	PRO
1	G	190	SER
1	H	113	PRO
1	C	220	VAL

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Mol	Chain	Res	Type
1	C	190	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	206	ASN
1	H	162	ASN
1	E	181	HIS
1	H	157	ASN
1	G	206	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 ⓘ

12 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	I	1	2,1	14,14,15	0.72	0	17,19,21	0.91	1 (5%)
2	NAG	I	2	2	14,14,15	0.46	0	17,19,21	0.65	0
2	NAG	J	1	2,1	14,14,15	0.77	0	17,19,21	1.16	2 (11%)
2	NAG	J	2	2	14,14,15	0.66	0	17,19,21	0.75	0
2	NAG	K	1	2,1	14,14,15	0.63	0	17,19,21	0.77	0
2	NAG	K	2	2	14,14,15	0.65	0	17,19,21	0.67	0
2	NAG	L	1	2,1	14,14,15	0.49	0	17,19,21	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	L	2	2	14,14,15	0.58	0	17,19,21	0.69	0
2	NAG	M	1	2,1	14,14,15	0.44	0	17,19,21	0.81	1 (5%)
2	NAG	M	2	2	14,14,15	0.56	0	17,19,21	0.65	0
2	NAG	N	1	2,1	14,14,15	0.59	0	17,19,21	0.79	0
2	NAG	N	2	2	14,14,15	0.55	0	17,19,21	0.69	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	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	NAG	C2-N2-C7	-2.89	118.79	122.90
2	I	1	NAG	C1-O5-C5	-2.42	108.91	112.19
2	J	1	NAG	C1-O5-C5	2.42	115.47	112.19
2	M	1	NAG	C2-N2-C7	-2.40	119.48	122.90
2	L	1	NAG	C2-N2-C7	-2.36	119.55	122.90

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	2	NAG	C4-C5-C6-O6

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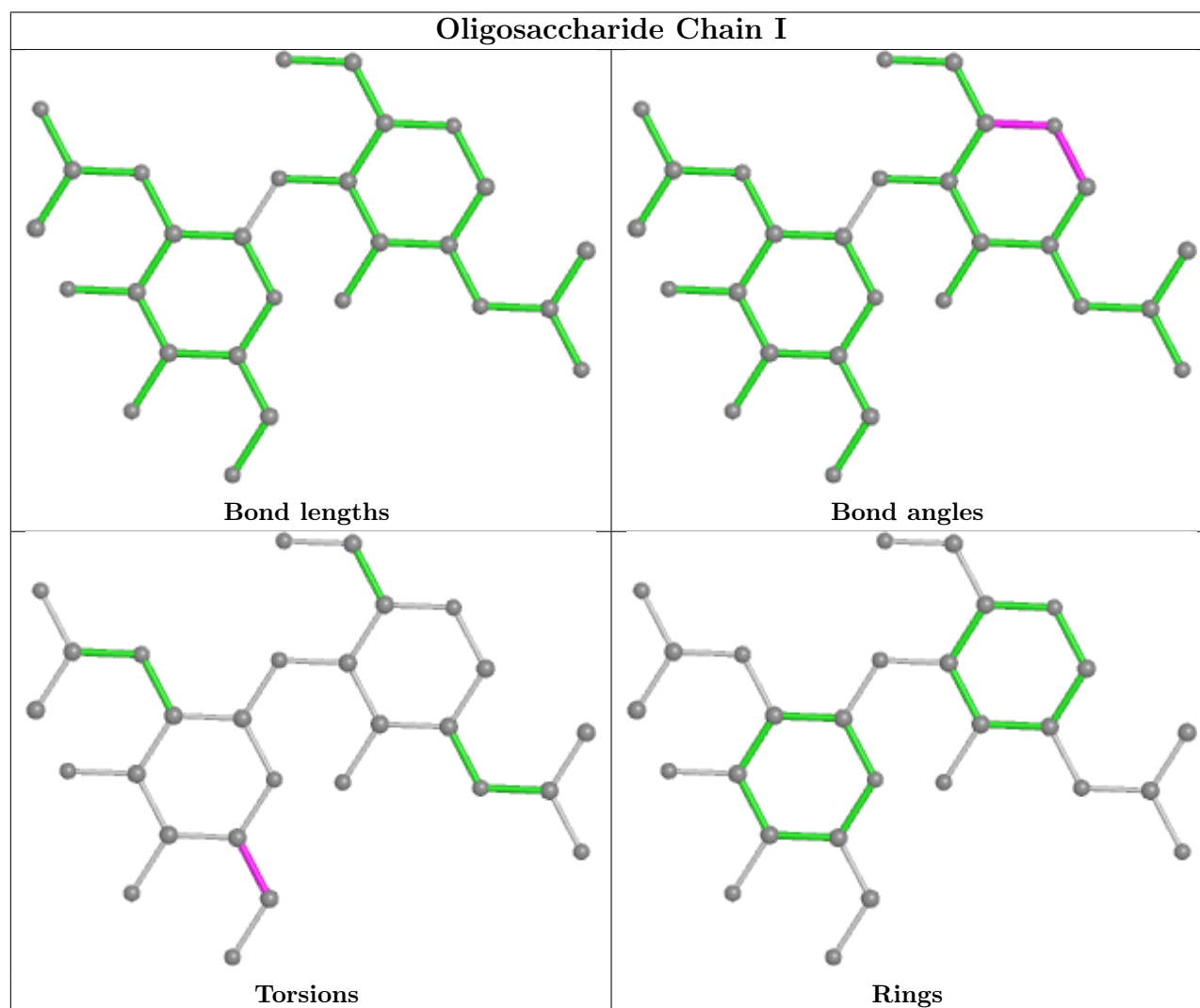
Mol	Chain	Res	Type	Atoms
2	M	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6

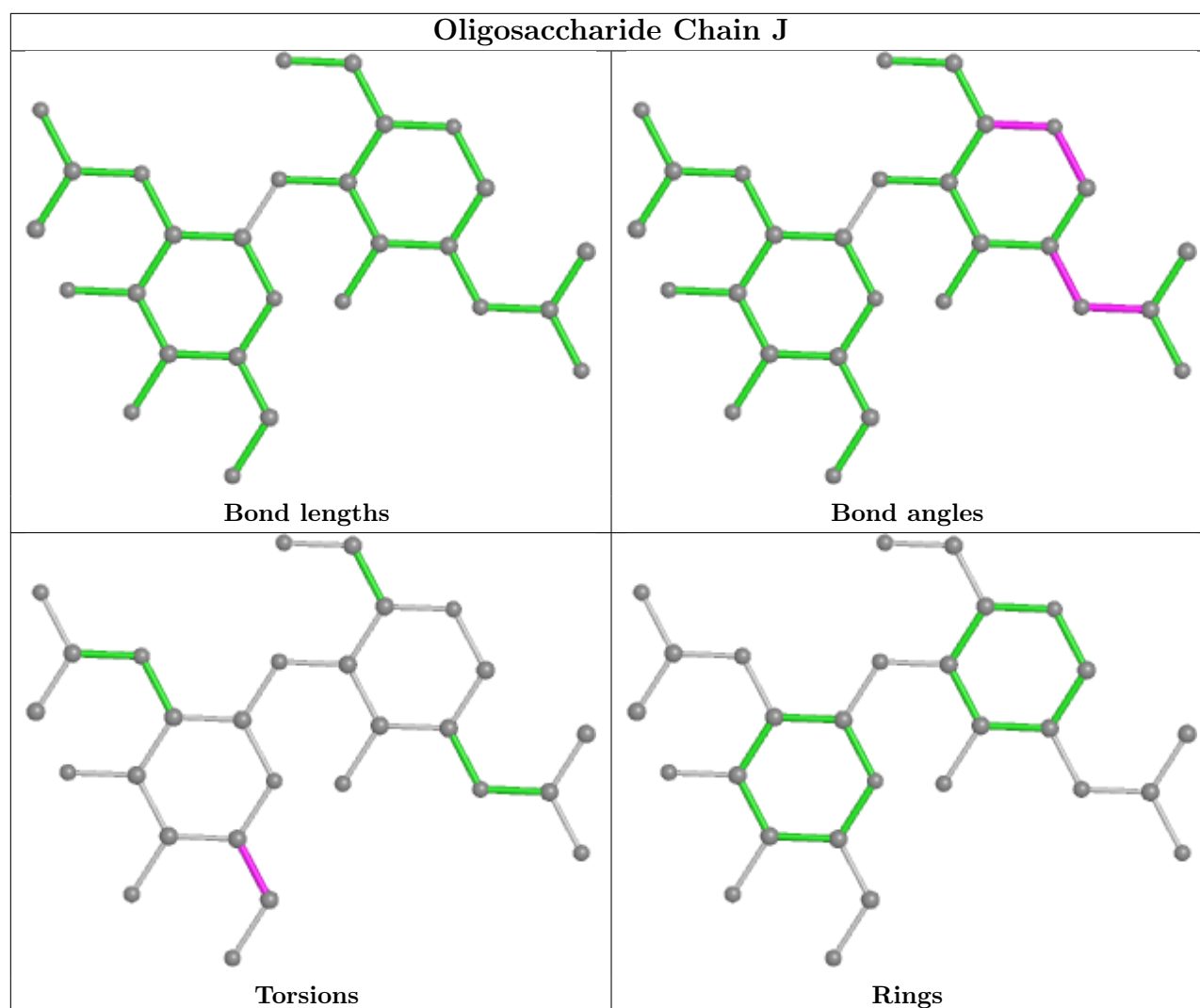
There are no ring outliers.

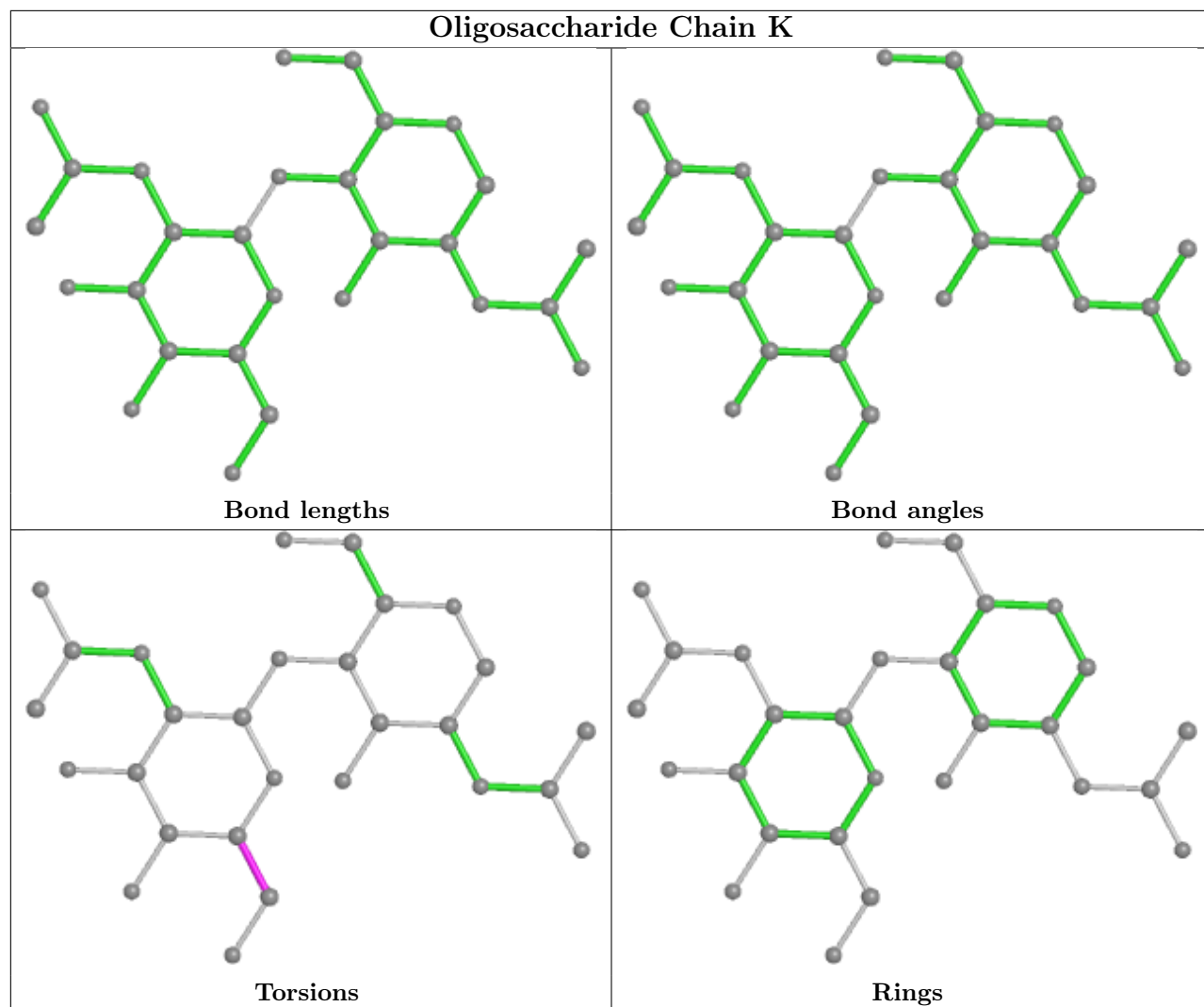
3 monomers are involved in 6 short contacts:

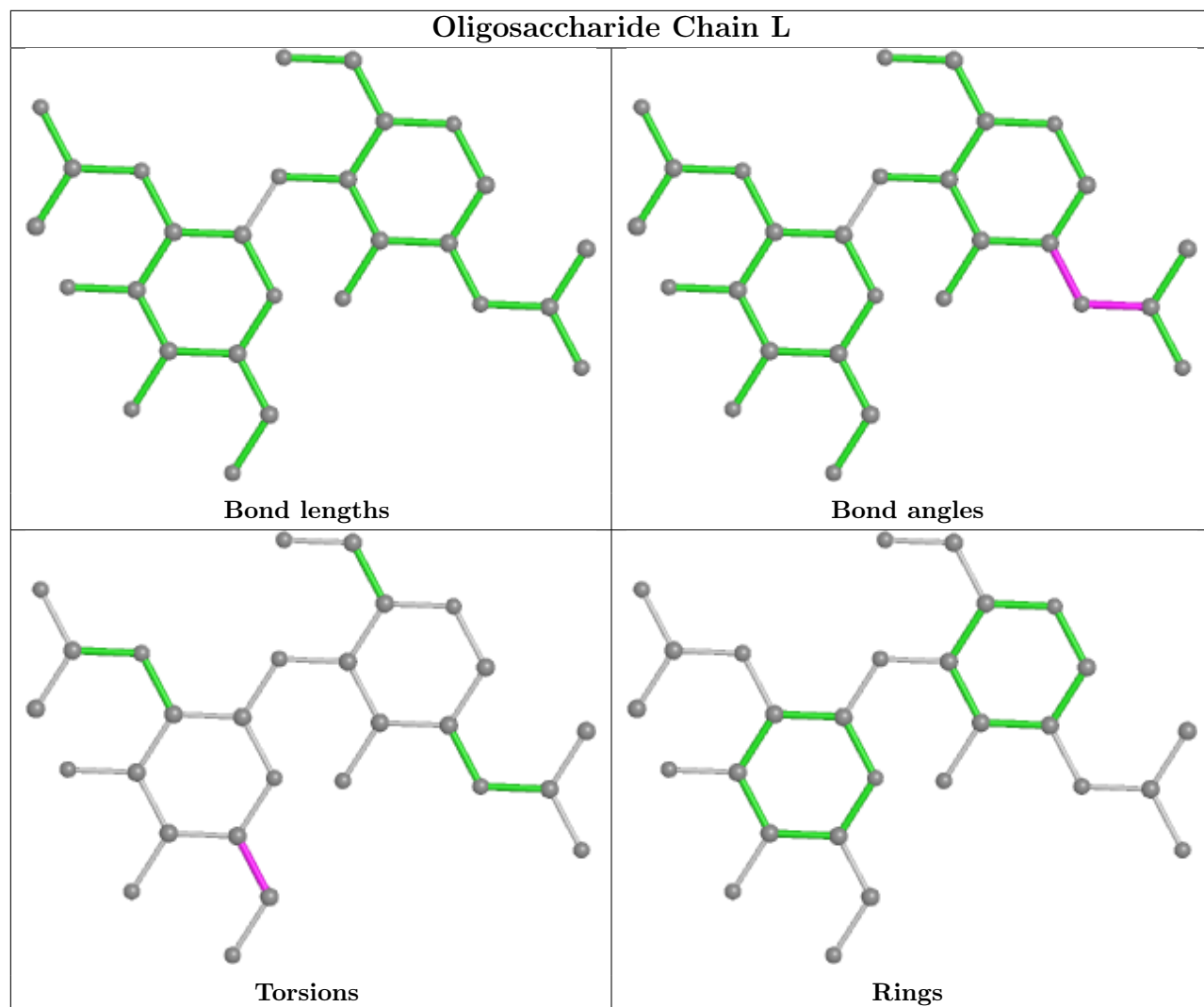
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	1	0
2	M	2	NAG	2	0
2	M	1	NAG	3	0

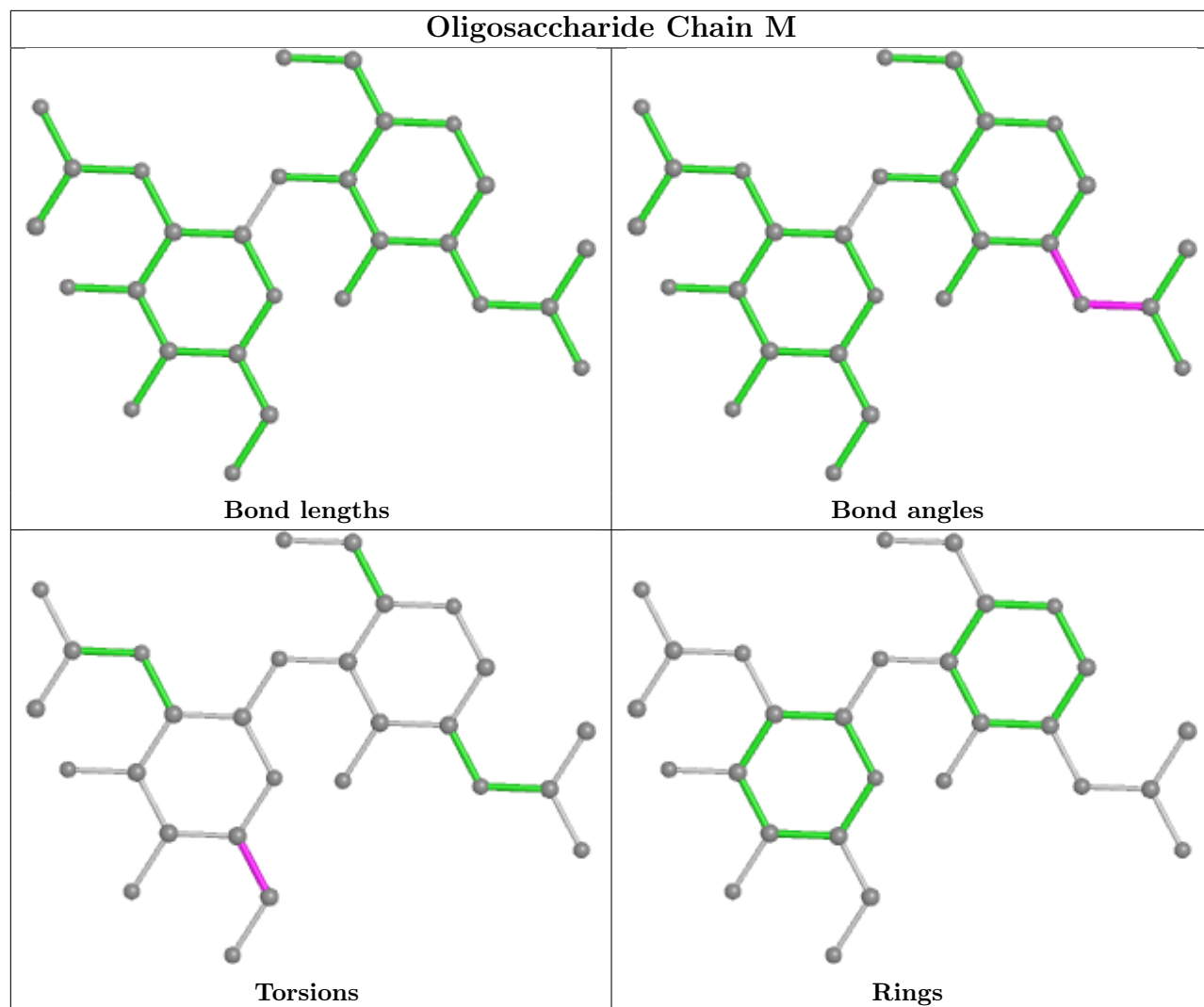
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



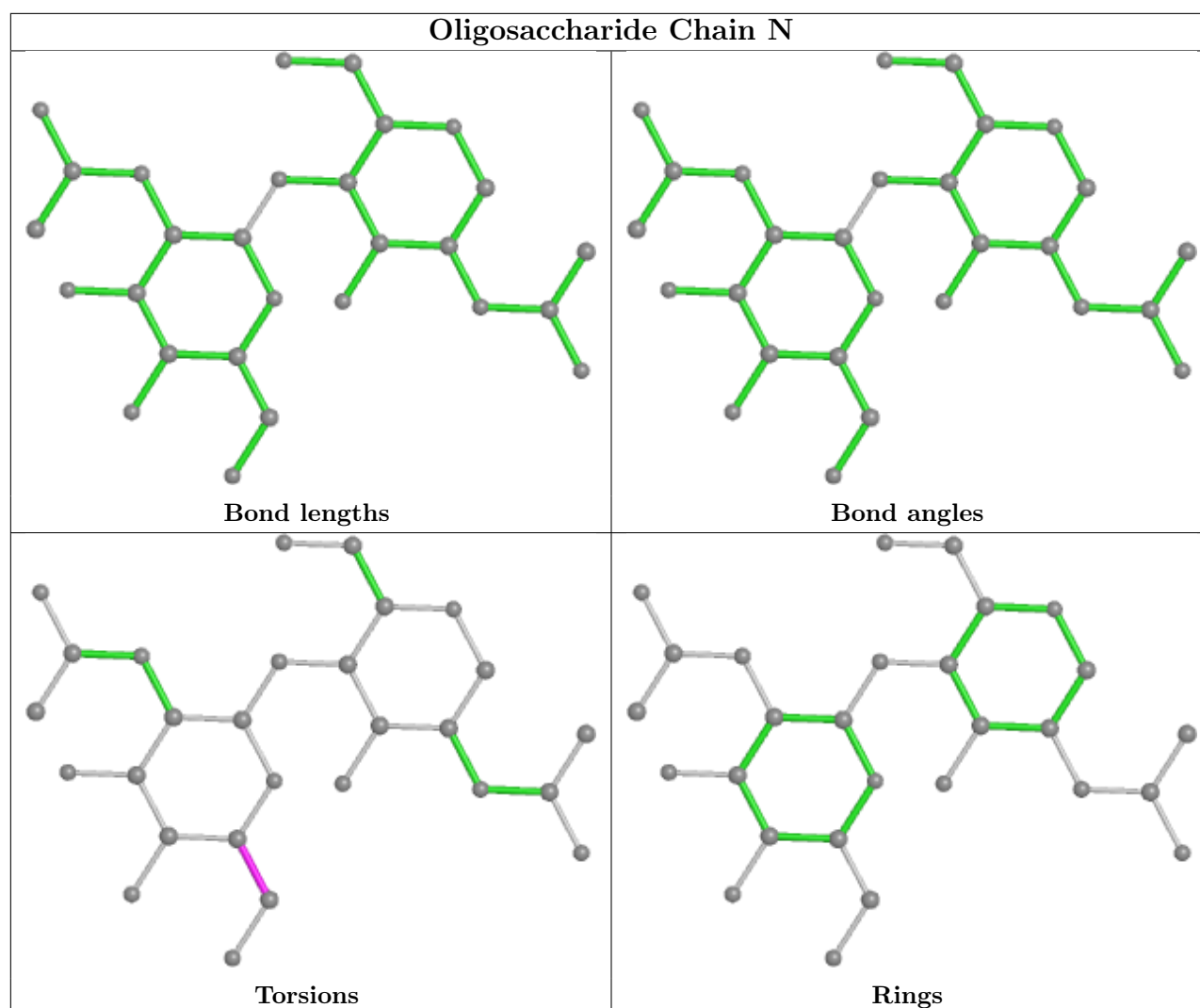












## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	$\# Z  > 2$
3	AMG	D	403	-	13,13,13	0.58	0	18,18,18	0.66	0
3	AMG	H	407	-	13,13,13	0.46	0	18,18,18	0.66	0
3	AMG	C	402	-	13,13,13	0.44	0	18,18,18	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AMG	B	401	-	13,13,13	0.56	0	18,18,18	0.78	1 (5%)
3	AMG	F	405	-	13,13,13	0.45	0	18,18,18	0.66	0
3	AMG	A	400	-	13,13,13	0.51	0	18,18,18	0.72	0
3	AMG	G	406	-	13,13,13	0.48	0	18,18,18	0.67	0
3	AMG	E	404	-	13,13,13	0.47	0	18,18,18	0.62	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
3	AMG	D	403	-	-	0/4/24/24	0/1/1/1
3	AMG	H	407	-	-	0/4/24/24	0/1/1/1
3	AMG	C	402	-	-	0/4/24/24	0/1/1/1
3	AMG	B	401	-	-	0/4/24/24	0/1/1/1
3	AMG	F	405	-	-	0/4/24/24	0/1/1/1
3	AMG	A	400	-	-	0/4/24/24	0/1/1/1
3	AMG	G	406	-	-	0/4/24/24	0/1/1/1
3	AMG	E	404	-	-	0/4/24/24	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	AMG	C7-O1-C1	2.13	116.56	113.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	AMG	2	0
3	H	407	AMG	2	0
3	C	402	AMG	3	0
3	B	401	AMG	2	0
3	F	405	AMG	2	0
3	A	400	AMG	1	0
3	G	406	AMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	404	AMG	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	236/238 (99%)	-0.58	0	100	100	2, 33, 85, 100	0
1	B	236/238 (99%)	-0.77	0	100	100	2, 22, 71, 100	0
1	C	236/238 (99%)	-0.52	0	100	100	3, 41, 91, 100	0
1	D	236/238 (99%)	-0.65	0	100	100	6, 35, 88, 100	0
1	E	236/238 (99%)	-0.49	0	100	100	4, 44, 93, 100	0
1	F	236/238 (99%)	-0.53	0	100	100	3, 39, 90, 100	0
1	G	236/238 (99%)	-0.09	7 (2%)	50	49	10, 70, 100, 100	0
1	H	236/238 (99%)	-0.09	4 (1%)	70	68	11, 76, 100, 100	0
All	All	1888/1904 (99%)	-0.47	11 (0%)	89	90	2, 44, 96, 100	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	36	LEU	3.4
1	G	37	THR	2.7
1	G	91	THR	2.6
1	G	13	ASN	2.5
1	G	42	PRO	2.5

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

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

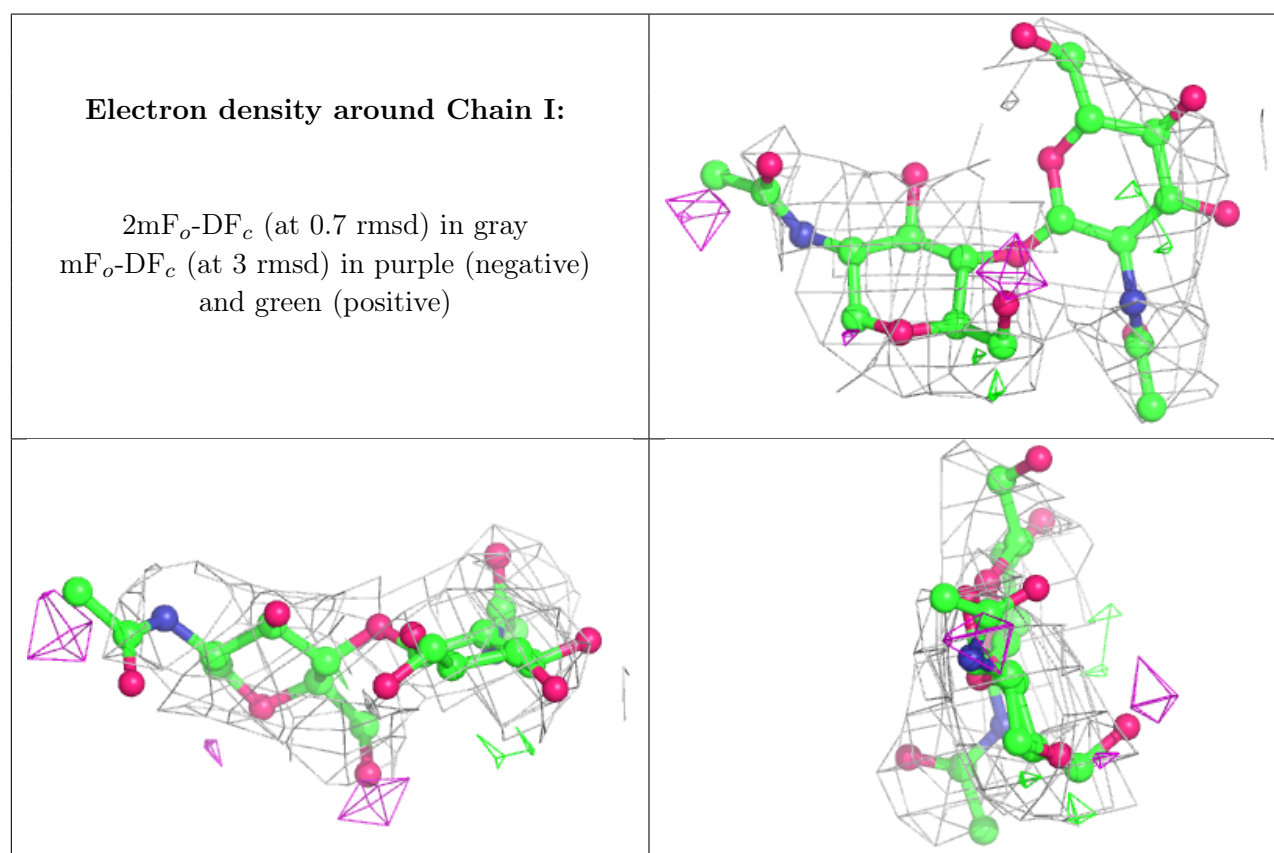
### 6.3 Carbohydrates [i](#)

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.

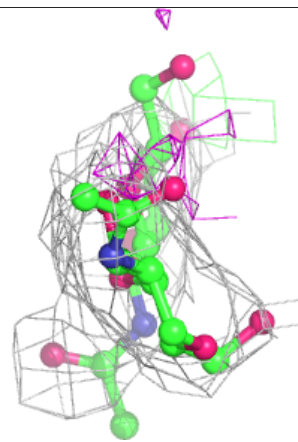
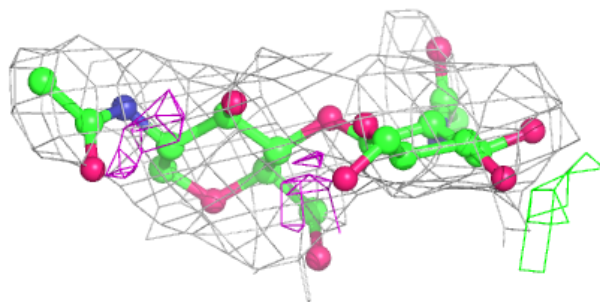
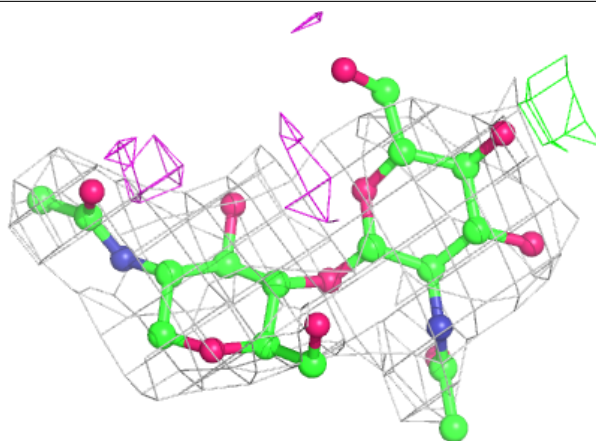
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	N	2	14/15	0.79	0.27	99,99,99,99	0
2	NAG	L	2	14/15	0.83	0.23	97,98,98,98	0
2	NAG	J	2	14/15	0.83	0.30	89,91,93,98	0
2	NAG	M	1	14/15	0.84	0.20	77,77,77,77	0
2	NAG	I	2	14/15	0.85	0.28	99,99,99,99	0
2	NAG	I	1	14/15	0.87	0.35	86,86,86,86	0
2	NAG	M	2	14/15	0.88	0.38	99,99,99,99	0
2	NAG	K	2	14/15	0.88	0.36	99,99,99,99	0
2	NAG	N	1	14/15	0.90	0.19	65,65,65,65	0
2	NAG	K	1	14/15	0.91	0.18	98,98,98,98	0
2	NAG	J	1	14/15	0.92	0.22	48,48,48,48	0
2	NAG	L	1	14/15	0.94	0.15	58,58,58,58	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.



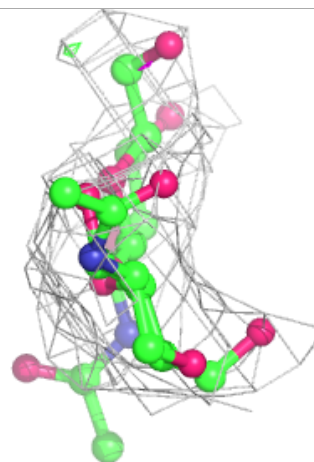
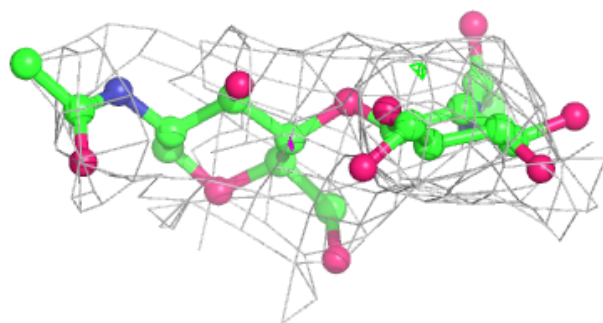
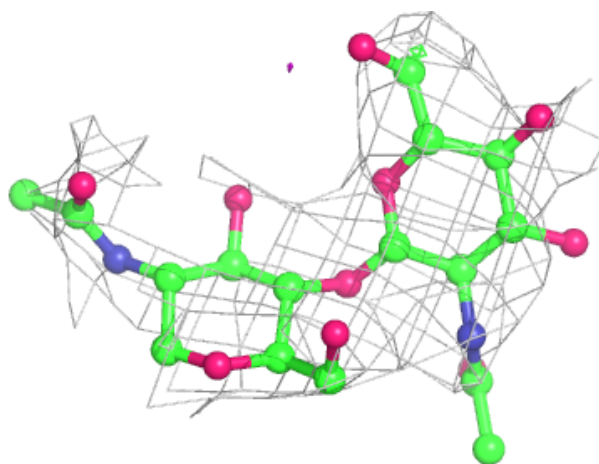
**Electron density around Chain J:**

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



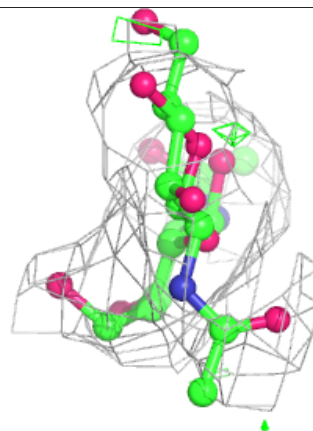
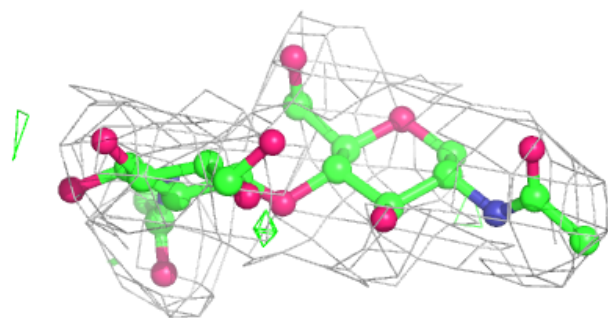
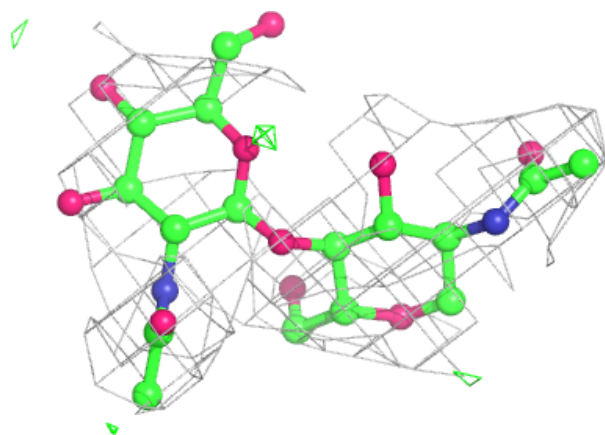
**Electron density around Chain K:**

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



**Electron density around Chain L:**

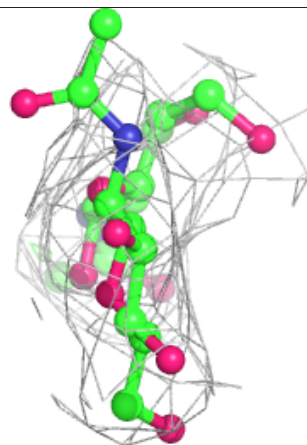
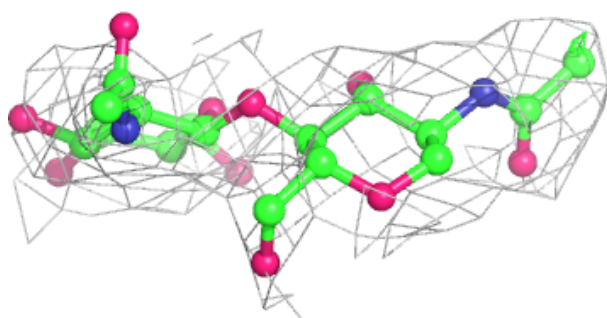
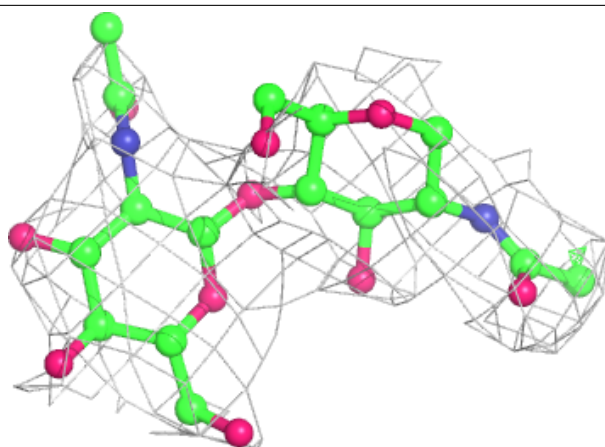
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



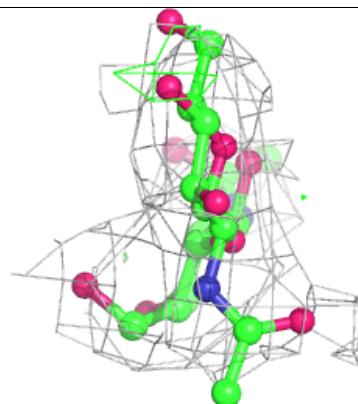
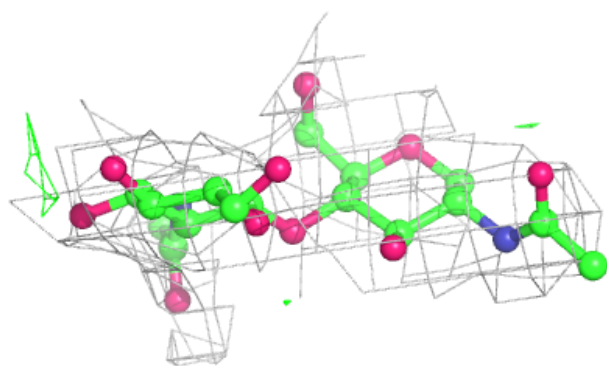
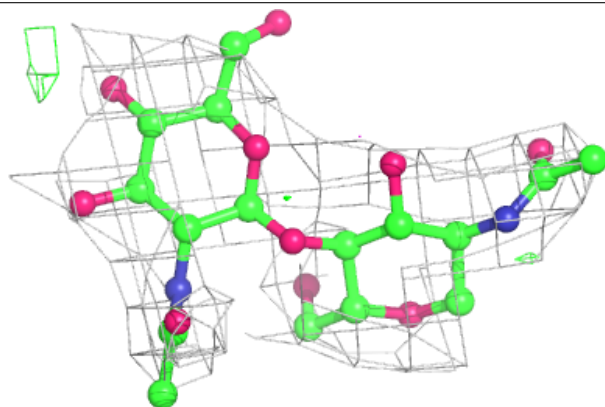


**Electron density around Chain M:**

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

**Electron density around Chain N:**

$2mF_o - DF_c$  (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
3	AMG	G	406	13/13	0.89	0.34	99,99,99,99	0
3	AMG	H	407	13/13	0.89	0.26	99,99,99,99	0
3	AMG	E	404	13/13	0.90	0.27	74,74,74,74	0
3	AMG	F	405	13/13	0.91	0.34	72,72,72,72	0
3	AMG	A	400	13/13	0.92	0.25	55,55,55,55	0
5	CA	E	303	1/1	0.95	0.04	35,35,35,35	0
3	AMG	D	403	13/13	0.96	0.20	37,37,37,37	0
4	MN	E	300	1/1	0.96	0.05	35,35,35,35	0
5	CA	C	303	1/1	0.96	0.07	35,35,35,35	0
3	AMG	C	402	13/13	0.96	0.19	30,30,30,30	0
5	CA	D	303	1/1	0.97	0.07	35,35,35,35	0
3	AMG	B	401	13/13	0.97	0.12	26,26,26,26	0
5	CA	F	303	1/1	0.97	0.05	35,35,35,35	0
5	CA	H	303	1/1	0.97	0.08	35,35,35,35	0
4	MN	C	300	1/1	0.98	0.08	35,35,35,35	0
4	MN	D	300	1/1	0.98	0.07	35,35,35,35	0
4	MN	B	300	1/1	0.98	0.15	35,35,35,35	0
4	MN	H	300	1/1	0.98	0.04	35,35,35,35	0
5	CA	G	303	1/1	0.98	0.03	35,35,35,35	0
5	CA	B	303	1/1	0.98	0.09	35,35,35,35	0
5	CA	A	303	1/1	0.99	0.10	35,35,35,35	0
4	MN	F	300	1/1	0.99	0.12	35,35,35,35	0
4	MN	G	300	1/1	0.99	0.06	35,35,35,35	0
4	MN	A	300	1/1	0.99	0.08	35,35,35,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.