



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:02 AM UTC

PDB ID : 6V46 / pdb_00006v46
Title : The crystal structure of hemagglutinin from A/turkey/Ontario/6118/1968 (H8N4)
Authors : Yang, H.; Stevens, J.
Deposited on : 2019-11-27
Resolution : 2.25 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

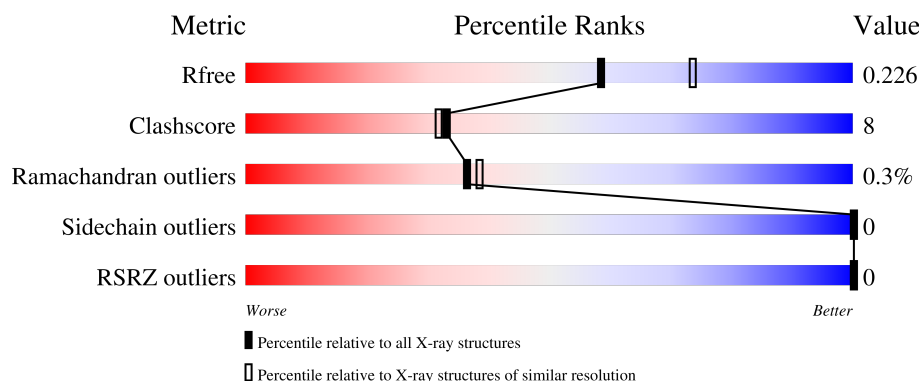
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



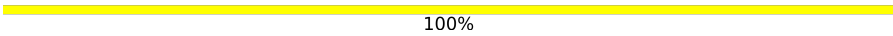
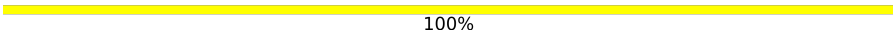
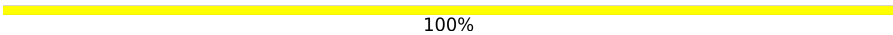
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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 ≥ 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	331	
1	C	331	
1	E	331	
2	B	183	
2	D	183	

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Mol	Chain	Length	Quality of chain
2	F	183	 76% 15% 9%
3	G	3	 100%
3	I	3	 100%
3	K	3	 100%
4	H	2	 50% 50%
4	J	2	 50% 50%
4	L	2	 50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12485 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 HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2562	1605	452	492	13			
1	C	323	Total	C	N	O	S	0	0	0
			2562	1605	452	492	13			
1	E	323	Total	C	N	O	S	0	0	0
			2562	1605	452	492	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP F2P175
A	-2	ASP	-	expression tag	UNP F2P175
A	-1	PRO	-	expression tag	UNP F2P175
A	0	GLY	-	expression tag	UNP F2P175
C	-3	ALA	-	expression tag	UNP F2P175
C	-2	ASP	-	expression tag	UNP F2P175
C	-1	PRO	-	expression tag	UNP F2P175
C	0	GLY	-	expression tag	UNP F2P175
E	-3	ALA	-	expression tag	UNP F2P175
E	-2	ASP	-	expression tag	UNP F2P175
E	-1	PRO	-	expression tag	UNP F2P175
E	0	GLY	-	expression tag	UNP F2P175

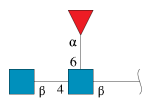
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1334	823	229	274	8			
2	D	166	Total	C	N	O	S	0	0	0
			1334	823	229	274	8			
2	F	166	Total	C	N	O	S	0	0	0
			1334	823	229	274	8			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP F2P175
B	176	GLY	-	expression tag	UNP F2P175
B	177	ARG	-	expression tag	UNP F2P175
B	178	LEU	-	expression tag	UNP F2P175
B	179	VAL	-	expression tag	UNP F2P175
B	180	PRO	-	expression tag	UNP F2P175
B	181	ARG	-	expression tag	UNP F2P175
B	182	GLY	-	expression tag	UNP F2P175
B	183	SER	-	expression tag	UNP F2P175
D	175	SER	-	expression tag	UNP F2P175
D	176	GLY	-	expression tag	UNP F2P175
D	177	ARG	-	expression tag	UNP F2P175
D	178	LEU	-	expression tag	UNP F2P175
D	179	VAL	-	expression tag	UNP F2P175
D	180	PRO	-	expression tag	UNP F2P175
D	181	ARG	-	expression tag	UNP F2P175
D	182	GLY	-	expression tag	UNP F2P175
D	183	SER	-	expression tag	UNP F2P175
F	175	SER	-	expression tag	UNP F2P175
F	176	GLY	-	expression tag	UNP F2P175
F	177	ARG	-	expression tag	UNP F2P175
F	178	LEU	-	expression tag	UNP F2P175
F	179	VAL	-	expression tag	UNP F2P175
F	180	PRO	-	expression tag	UNP F2P175
F	181	ARG	-	expression tag	UNP F2P175
F	182	GLY	-	expression tag	UNP F2P175
F	183	SER	-	expression tag	UNP F2P175

- Molecule 3 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.



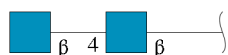
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

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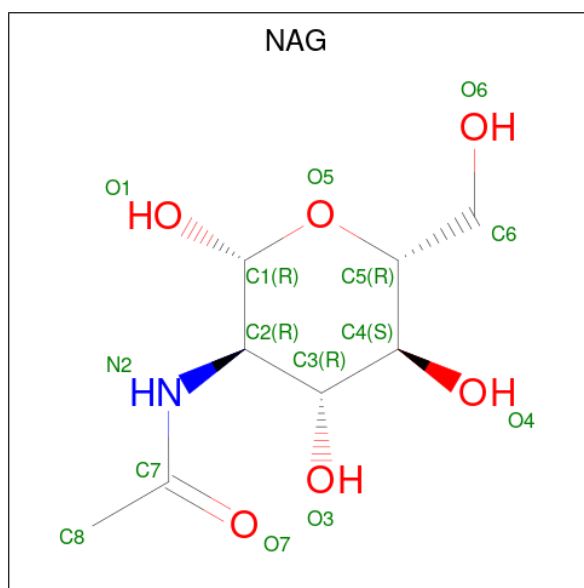
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	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			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

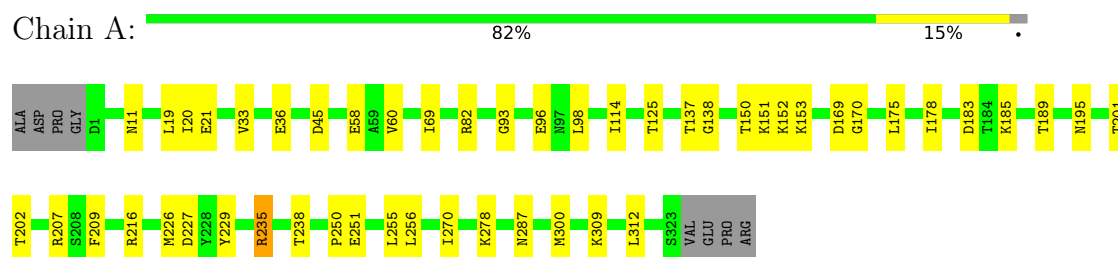
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	136	Total	O	0	0
			136	136		
6	B	50	Total	O	0	0
			50	50		
6	C	127	Total	O	0	0
			127	127		
6	D	55	Total	O	0	0
			55	55		
6	E	131	Total	O	0	0
			131	131		
6	F	58	Total	O	0	0
			58	58		

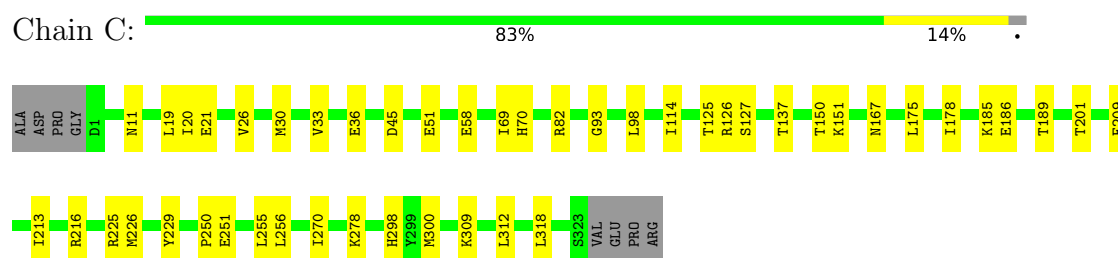
3 Residue-property plots

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.

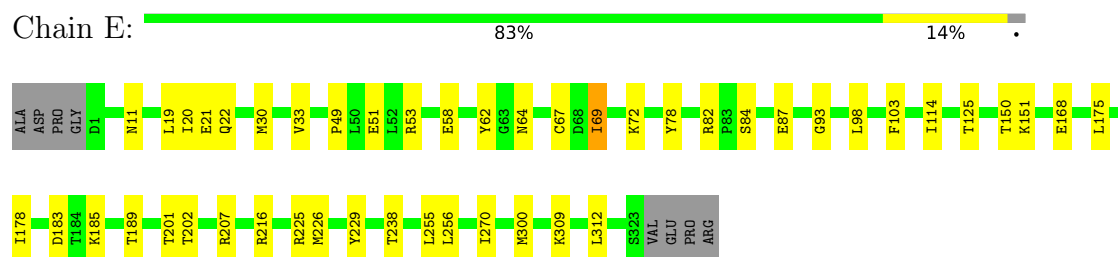
- Molecule 1: Hemagglutinin HA1 chain



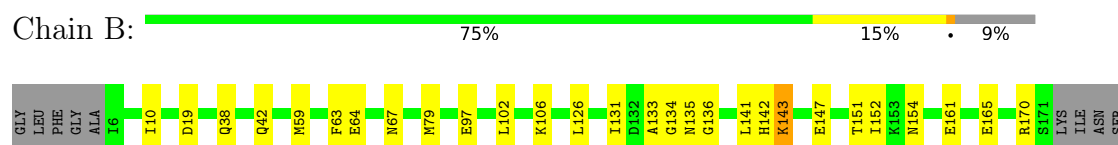
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



- Molecule 2: Hemagglutinin HA2 chain



GLY
ARG
LEU
VAL
PRO
ARG
GLY
SER

• Molecule 2: Hemagglutinin HA2 chain

Chain D:  77% 13% 9%

GLY I6 I10 G16 D19 K39 E64 M67 K75 M79 E97 L102 K106 R125 I131 D132 A133 G134 N135 G136 E147 T151 M154 G155 T156 H159 K160 E161 Y162 E163 S171 LYS ILE ASN SER GLY ARG LEU

VAL
PRO
ARG
GLY
SER

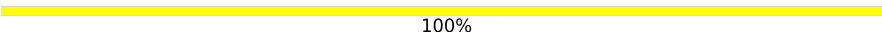
• Molecule 2: Hemagglutinin HA2 chain

Chain F:  76% 15% 9%

GLY I6 F9 I10 K39 E64 M79 D86 E97 L102 K116 V122 R125 L126 N129 A130 I131 D132 A133 G134 N135 G136 H142 E147 T151 M154 G155 T156 H159 E165 R170 S171 LYS ILE ASN SER GLY ARG

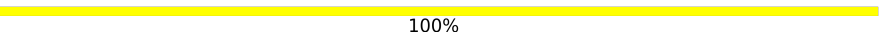
LEU
VAL
PRO
ARG
GLY
SER

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

Chain G:  100%

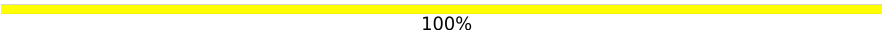
NAG1
NAG2
FUC3

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

Chain I:  100%

NAG1
NAG2
FUC3

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

Chain K:  100%

NAG1
NAG2
FUC3

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

Chain H:  50% 50%



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

Chain J:  50%  50%



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

Chain L:  50%  50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.05Å 98.09Å 132.74Å 90.00° 115.20° 90.00°	Depositor
Resolution (Å)	45.41 – 2.25 45.41 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.9 (45.41-2.25) 96.9 (45.41-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.187 , 0.225 0.188 , 0.226	Depositor DCC
R_{free} test set	4565 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.398 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.448 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12485	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.51	1/2621 (0.0%)	0.69	1/3555 (0.0%)
1	C	0.51	0/2621	0.69	1/3555 (0.0%)
1	E	0.48	0/2621	0.66	0/3555
2	B	0.46	0/1355	0.73	2/1822 (0.1%)
2	D	0.53	0/1355	0.79	3/1822 (0.2%)
2	F	0.50	0/1355	0.80	5/1822 (0.3%)
All	All	0.50	1/11928 (0.0%)	0.71	12/16131 (0.1%)

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
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	ARG	CB-CG	-5.44	1.36	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	39	LYS	CA-CB-CG	8.80	131.70	114.10
2	B	143	LYS	CA-C-N	-8.08	110.36	122.47
2	B	143	LYS	C-N-CA	-8.08	110.36	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	HIS	CB-CA-C	-7.02	99.05	110.77
2	D	39	LYS	CB-CG-CD	6.85	127.05	111.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	134	GLY	Peptide
2	D	134	GLY	Peptide
2	F	134	GLY	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	2562	0	2488	51	0
1	C	2562	0	2487	41	0
1	E	2562	0	2487	48	0
2	B	1334	0	1250	25	0
2	D	1334	0	1250	20	0
2	F	1334	0	1250	20	0
3	G	38	0	34	0	0
3	I	38	0	34	0	0
3	K	38	0	34	0	0
4	H	28	0	25	0	0
4	J	28	0	25	0	0
4	L	28	0	25	0	0
5	A	14	0	13	0	0
5	C	14	0	13	0	0
5	E	14	0	13	0	0
6	A	136	0	0	12	0
6	B	50	0	0	2	0
6	C	127	0	0	11	0
6	D	55	0	0	2	0
6	E	131	0	0	9	0
6	F	58	0	0	2	0
All	All	12485	0	11428	181	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 8.

The worst 5 of 181 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:HG21	1:E:216:ARG:HD2	1.20	1.20
1:A:216:ARG:HD2	1:C:201:THR:HG21	1.20	1.15
1:C:216:ARG:HD2	1:E:201:THR:HG21	1.26	1.10
2:F:6:ILE:N	6:F:201:HOH:O	1.94	0.98
1:A:201:THR:HG21	1:E:216:ARG:CD	1.94	0.96

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	321/331 (97%)	311 (97%)	10 (3%)	0	100	100
1	C	321/331 (97%)	310 (97%)	10 (3%)	1 (0%)	36	38
1	E	321/331 (97%)	311 (97%)	9 (3%)	1 (0%)	36	38
2	B	164/183 (90%)	155 (94%)	8 (5%)	1 (1%)	21	20
2	D	164/183 (90%)	156 (95%)	7 (4%)	1 (1%)	21	20
2	F	164/183 (90%)	155 (94%)	9 (6%)	0	100	100
All	All	1455/1542 (94%)	1398 (96%)	53 (4%)	4 (0%)	36	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	143	LYS
2	D	162	TYR
1	E	69	ILE

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Mol	Chain	Res	Type
1	C	69	ILE

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	282/288 (98%)	282 (100%)	0	100	100
1	C	282/288 (98%)	282 (100%)	0	100	100
1	E	282/288 (98%)	282 (100%)	0	100	100
2	B	145/157 (92%)	145 (100%)	0	100	100
2	D	145/157 (92%)	145 (100%)	0	100	100
2	F	145/157 (92%)	145 (100%)	0	100	100
All	All	1281/1335 (96%)	1281 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
2	D	67	ASN
2	D	68	HIS
2	F	68	HIS
2	F	67	ASN
2	B	68	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

15 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	G	1	1,3	14,14,15	1.01	1 (7%)	17,19,21	0.83	0
3	NAG	G	2	3	14,14,15	0.89	2 (14%)	17,19,21	0.74	1 (5%)
3	FUC	G	3	3	10,10,11	1.47	2 (20%)	14,14,16	1.37	2 (14%)
4	NAG	H	1	4,1	14,14,15	0.49	0	17,19,21	0.64	0
4	NAG	H	2	4	14,14,15	1.28	2 (14%)	17,19,21	1.28	2 (11%)
3	NAG	I	1	1,3	14,14,15	1.20	1 (7%)	17,19,21	0.79	0
3	NAG	I	2	3	14,14,15	0.87	1 (7%)	17,19,21	0.73	1 (5%)
3	FUC	I	3	3	10,10,11	1.88	2 (20%)	14,14,16	1.41	2 (14%)
4	NAG	J	1	4,1	14,14,15	0.47	0	17,19,21	0.63	0
4	NAG	J	2	4	14,14,15	1.26	1 (7%)	17,19,21	1.25	3 (17%)
3	NAG	K	1	1,3	14,14,15	1.00	1 (7%)	17,19,21	0.87	2 (11%)
3	NAG	K	2	3	14,14,15	0.92	2 (14%)	17,19,21	0.68	1 (5%)
3	FUC	K	3	3	10,10,11	1.24	2 (20%)	14,14,16	1.40	2 (14%)
4	NAG	L	1	4,1	14,14,15	0.38	0	17,19,21	0.65	0
4	NAG	L	2	4	14,14,15	1.29	2 (14%)	17,19,21	1.33	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	FUC	G	3	3	-	-	0/1/1/1
4	NAG	H	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	O5-C1	-4.40	1.36	1.43
3	I	3	FUC	O5-C5	4.22	1.51	1.43
4	L	2	NAG	O5-C1	-4.00	1.37	1.43
4	J	2	NAG	O5-C1	-3.99	1.37	1.43
3	K	1	NAG	O5-C1	-3.64	1.37	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2	NAG	C4-C3-C2	3.91	116.75	111.02
4	J	2	NAG	C4-C3-C2	3.79	116.58	111.02
3	G	3	FUC	O5-C5-C4	3.74	116.29	109.55
4	H	2	NAG	C4-C3-C2	3.71	116.45	111.02
3	K	3	FUC	O5-C5-C4	3.55	115.94	109.55

There are no chirality outliers.

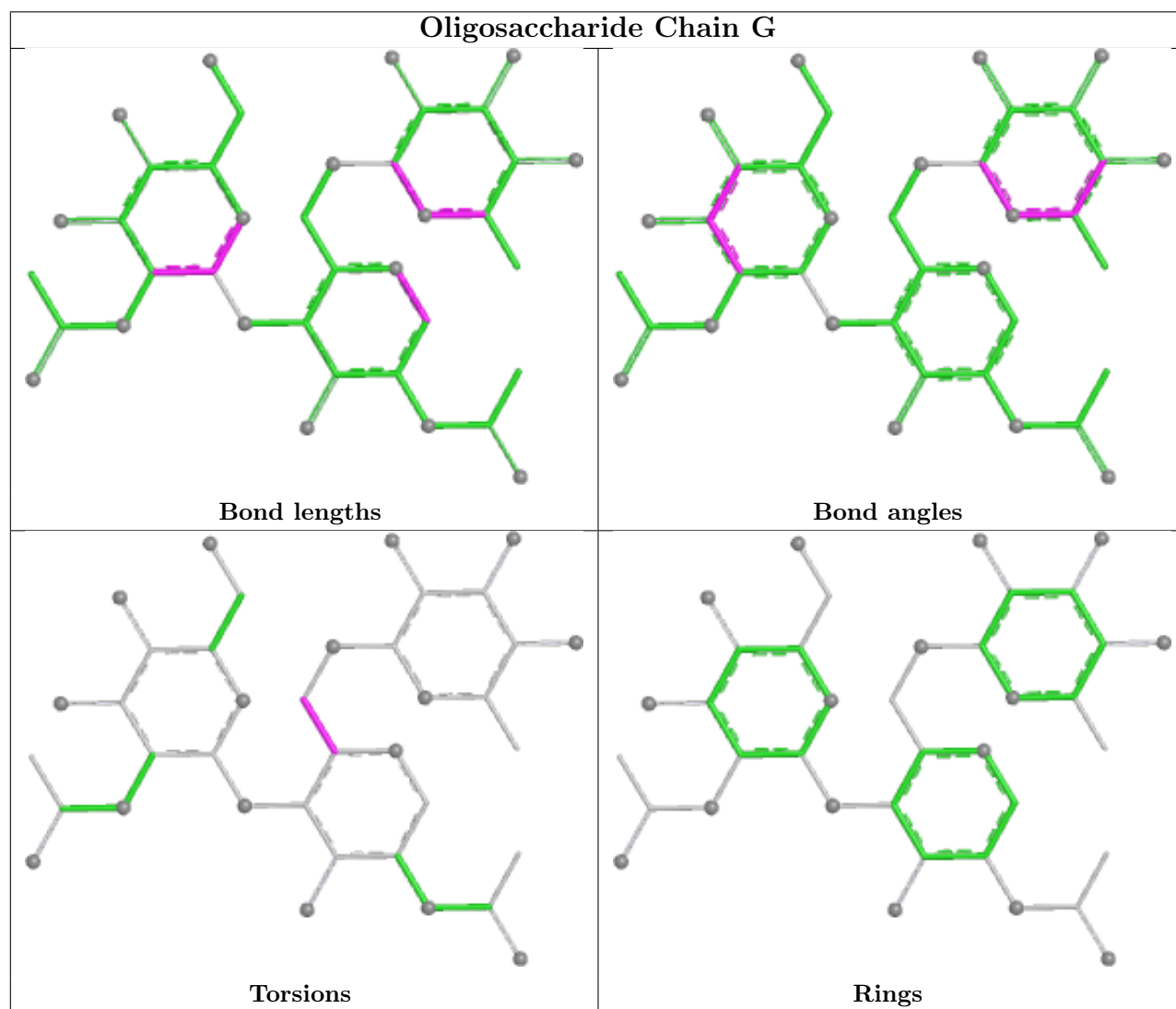
5 of 9 torsion outliers are listed below:

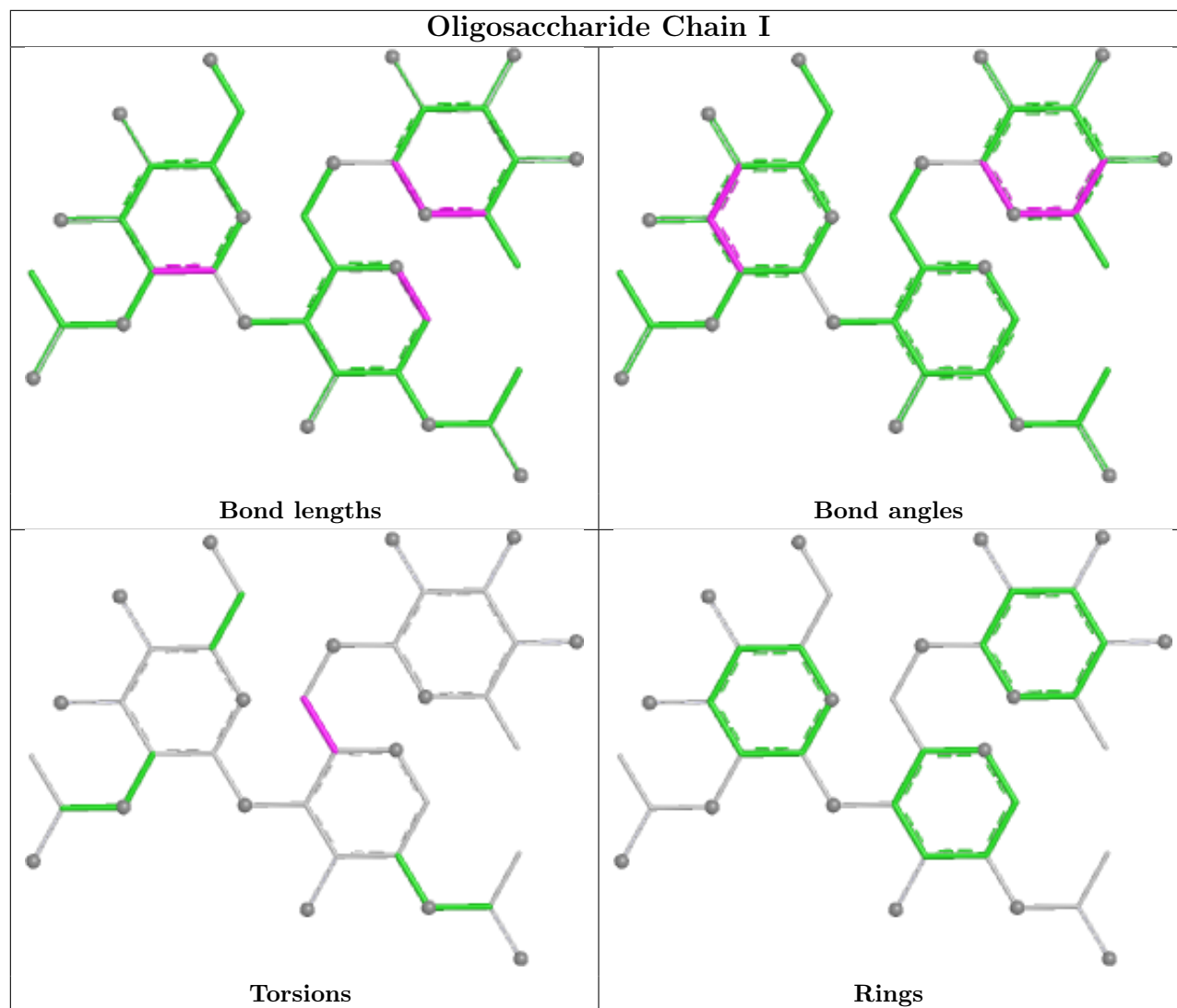
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6

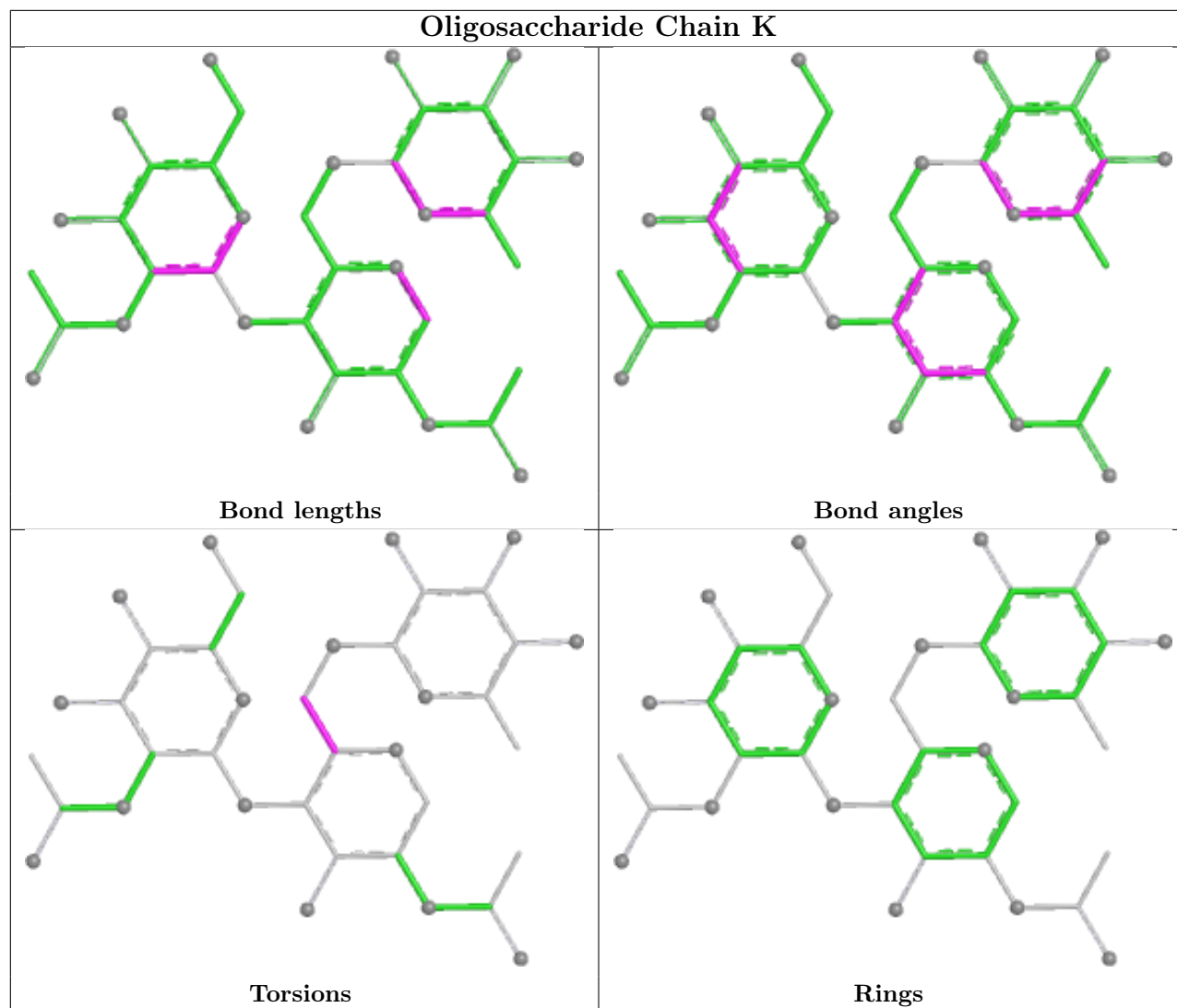
There are no ring outliers.

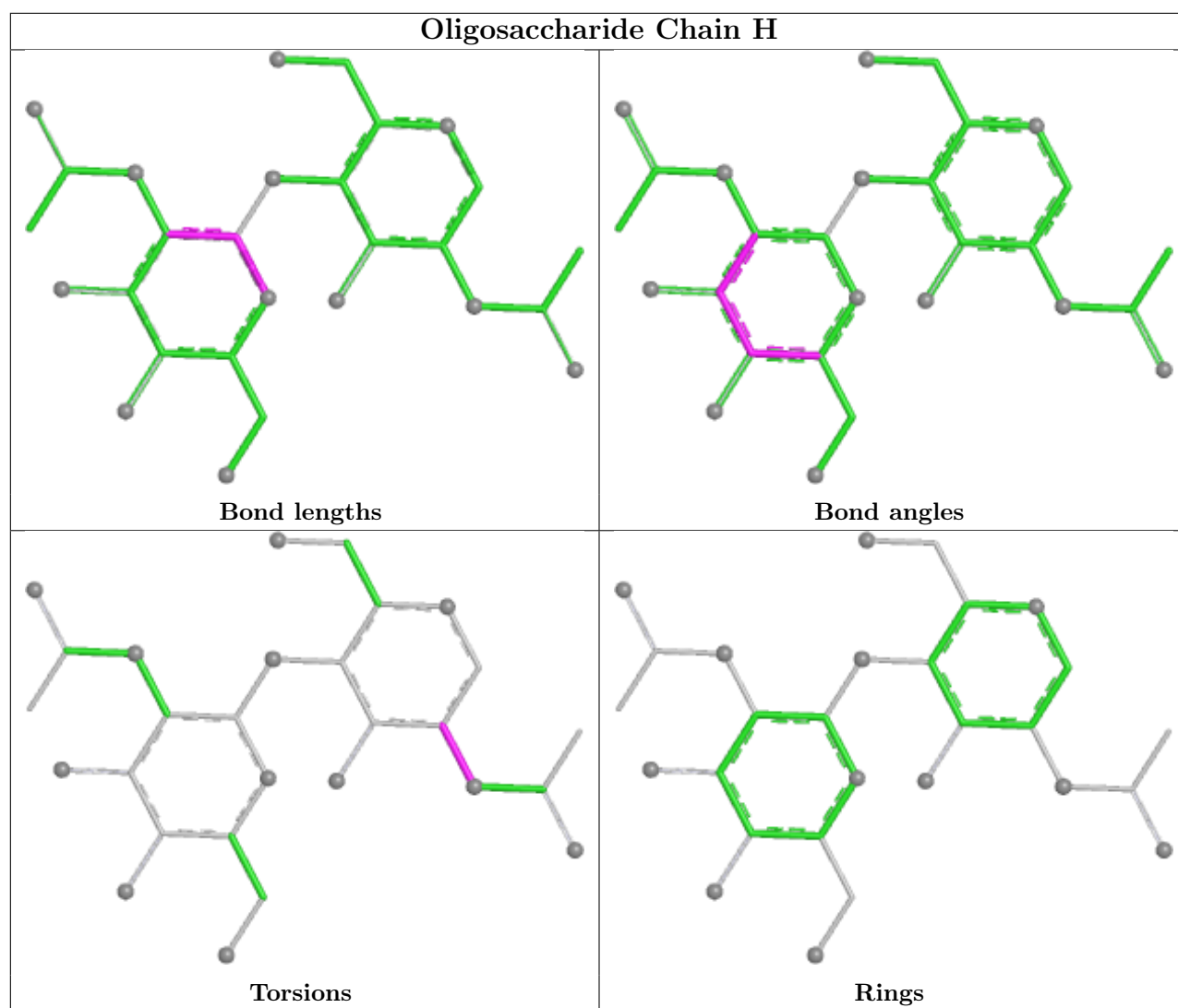
No monomer is involved in short contacts.

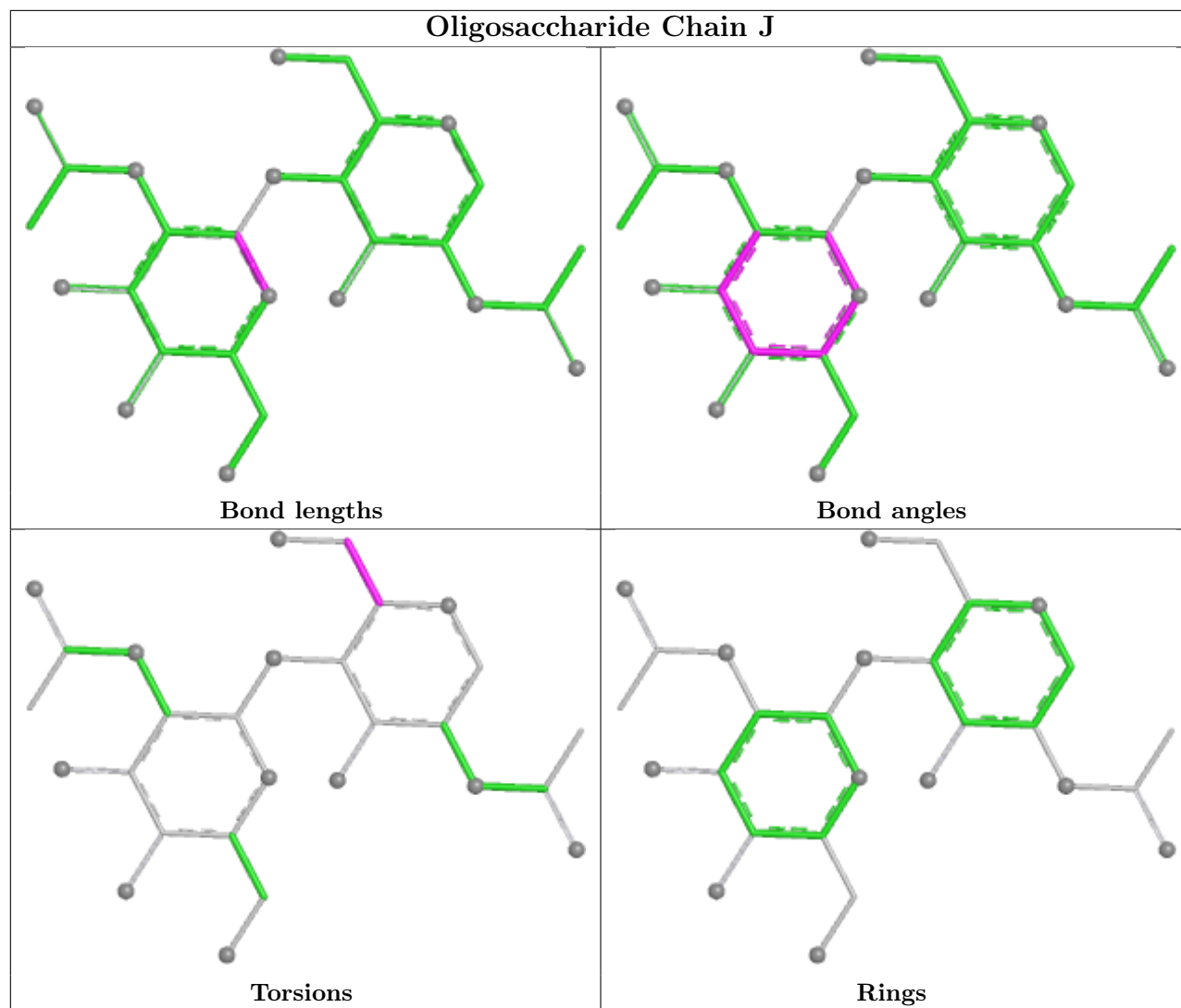
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

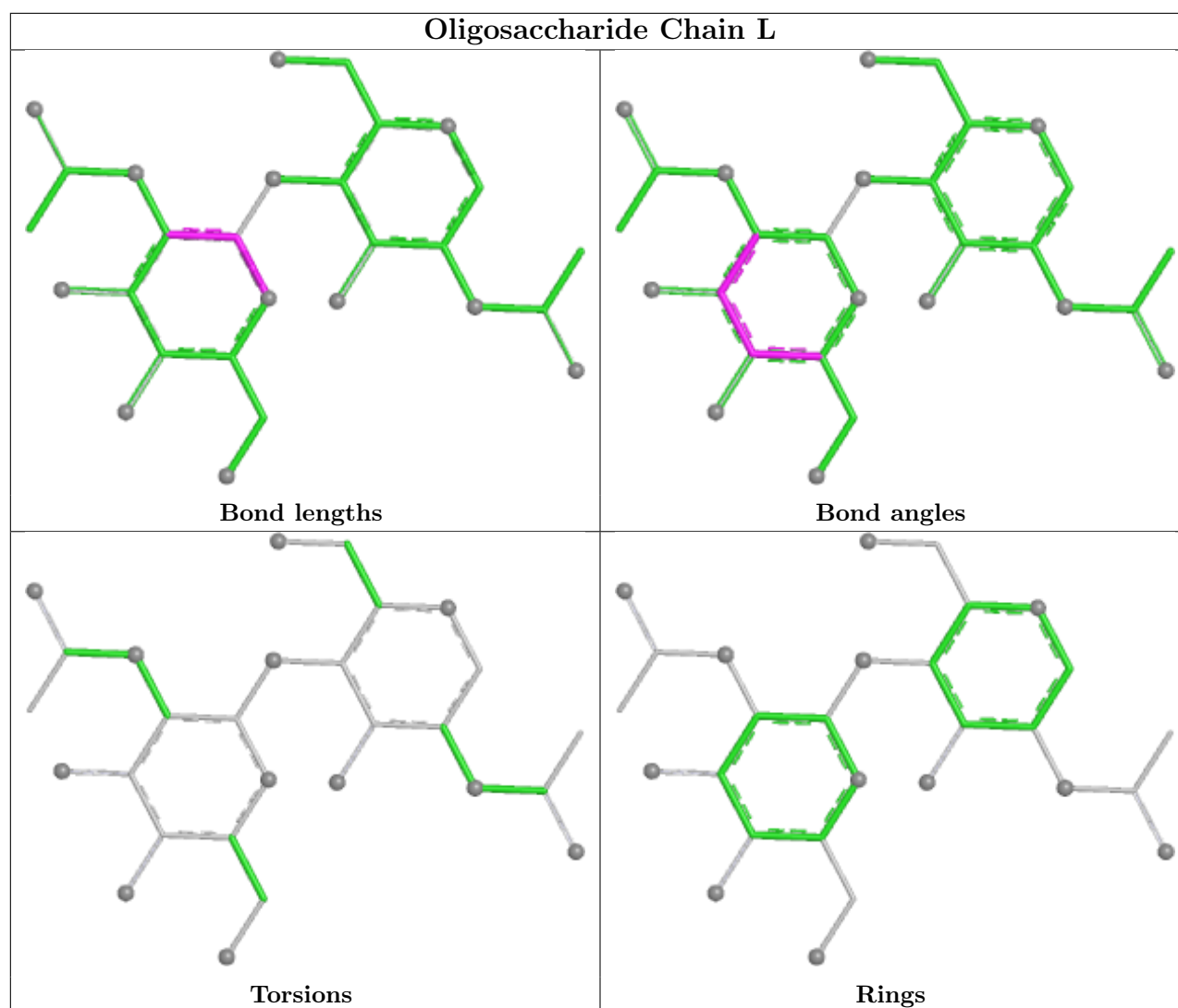












5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
5	NAG	C	501	1	14,14,15	0.86	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	A	501	1	14,14,15	1.05	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	E	501	1	14,14,15	0.99	1 (7%)	17,19,21	1.15	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
5	NAG	C	501	1	-	1/6/23/26	0/1/1/1
5	NAG	A	501	1	-	1/6/23/26	0/1/1/1
5	NAG	E	501	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	NAG	O5-C1	-3.71	1.37	1.43
5	E	501	NAG	O5-C1	-3.51	1.37	1.43
5	C	501	NAG	O5-C1	-2.94	1.38	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	501	NAG	C1-O5-C5	3.77	117.24	112.19
5	A	501	NAG	C1-O5-C5	3.51	116.90	112.19
5	C	501	NAG	C1-O5-C5	3.43	116.79	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	NAG	O5-C5-C6-O6
5	E	501	NAG	O5-C5-C6-O6
5	C	501	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, 95th 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 ²)	Q<0.9
1	A	323/331 (97%)	-1.33	0 100 100	23, 38, 65, 103	0
1	C	323/331 (97%)	-1.30	0 100 100	25, 38, 66, 104	0
1	E	323/331 (97%)	-1.29	0 100 100	24, 38, 65, 103	0
2	B	166/183 (90%)	-1.10	0 100 100	23, 51, 115, 150	0
2	D	166/183 (90%)	-1.14	0 100 100	24, 50, 115, 159	0
2	F	166/183 (90%)	-1.08	0 100 100	24, 50, 117, 164	0
All	All	1467/1542 (95%)	-1.24	0 100 100	23, 40, 89, 164	0

There are no RSRZ outliers to report.

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, 95th 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.

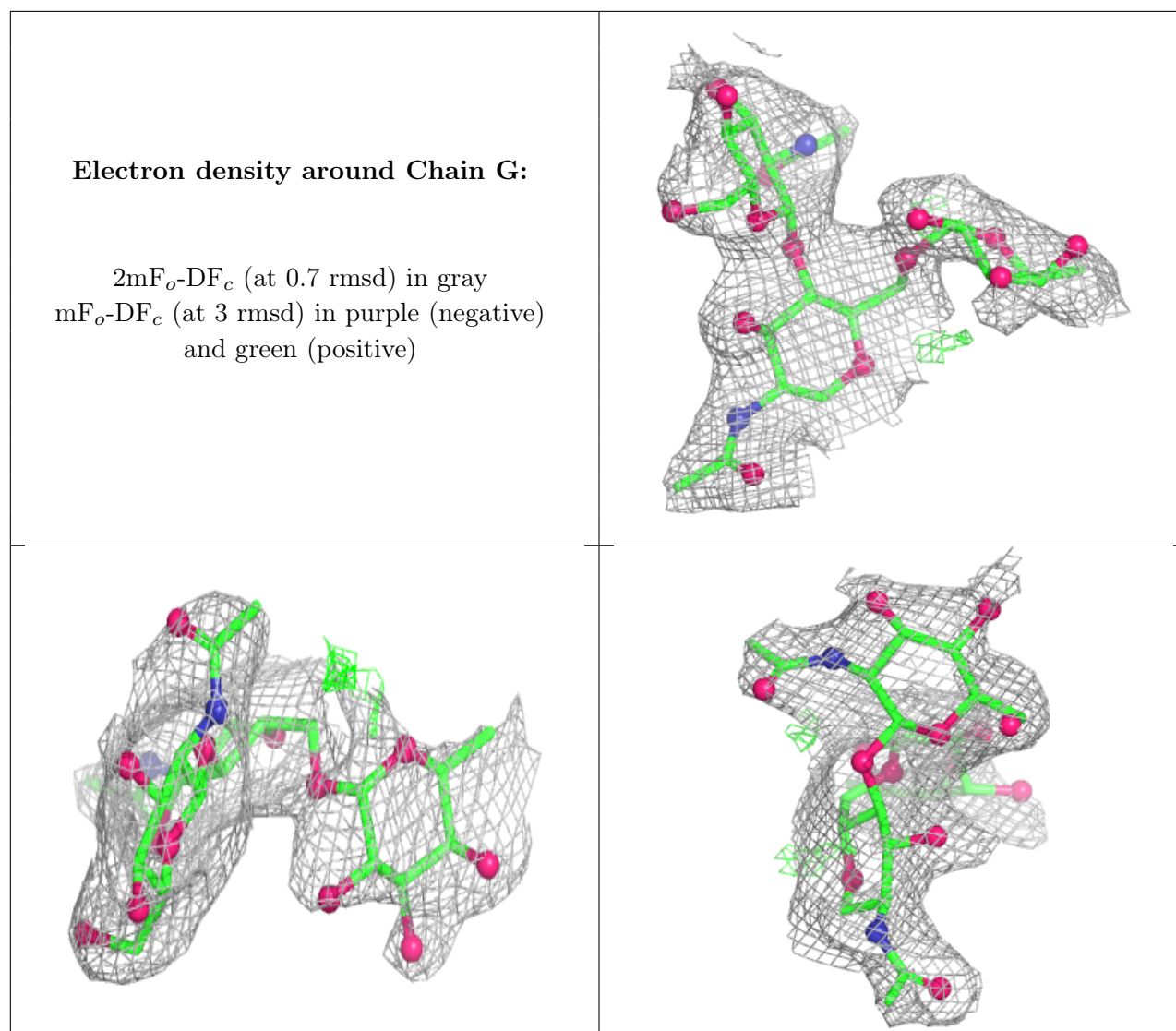
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FUC	G	3	10/11	0.96	0.07	110,111,112,113	0
4	NAG	H	2	14/15	0.96	0.06	72,81,86,88	0
4	NAG	J	2	14/15	0.96	0.05	71,80,84,87	0
3	NAG	K	2	14/15	0.97	0.05	89,99,102,103	0
3	FUC	K	3	10/11	0.97	0.08	107,109,111,112	0
3	NAG	I	2	14/15	0.97	0.05	82,93,97,97	0

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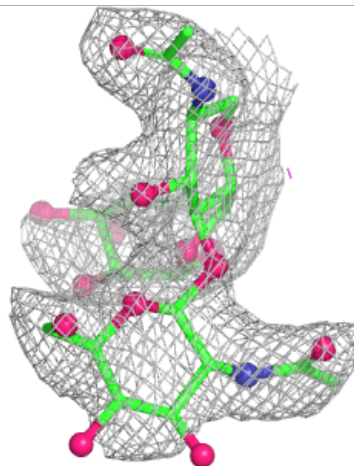
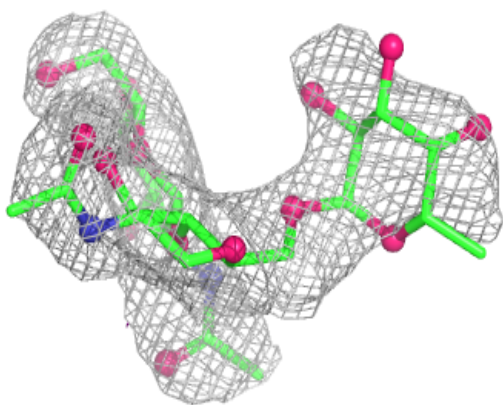
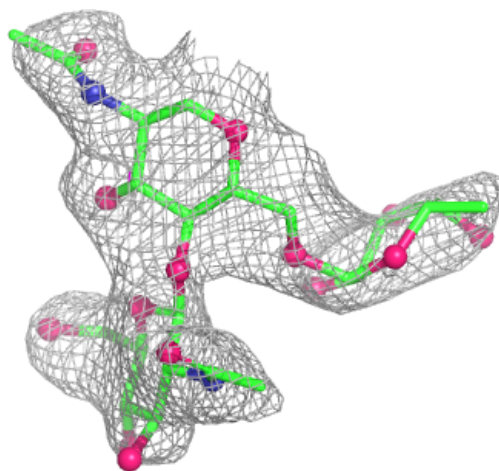
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FUC	I	3	10/11	0.97	0.07	104,107,108,108	0
4	NAG	L	2	14/15	0.97	0.05	69,80,85,86	0
3	NAG	I	1	14/15	0.98	0.04	69,72,89,96	0
3	NAG	G	2	14/15	0.98	0.04	91,97,98,99	0
3	NAG	G	1	14/15	0.99	0.04	69,77,94,102	0
4	NAG	J	1	14/15	0.99	0.03	42,50,58,70	0
3	NAG	K	1	14/15	0.99	0.04	80,84,98,102	0
4	NAG	L	1	14/15	0.99	0.03	41,53,64,65	0
4	NAG	H	1	14/15	0.99	0.03	40,52,62,70	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.



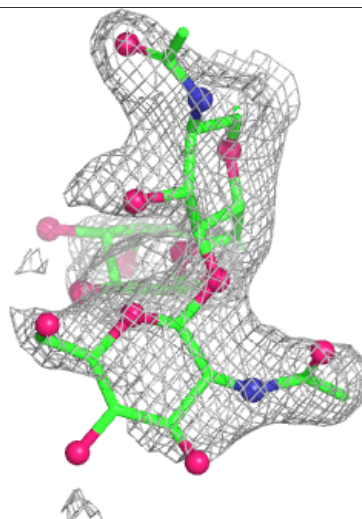
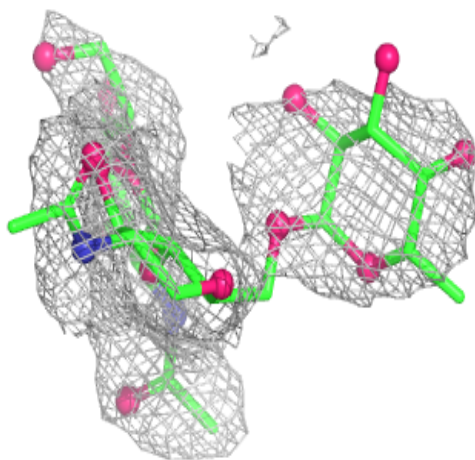
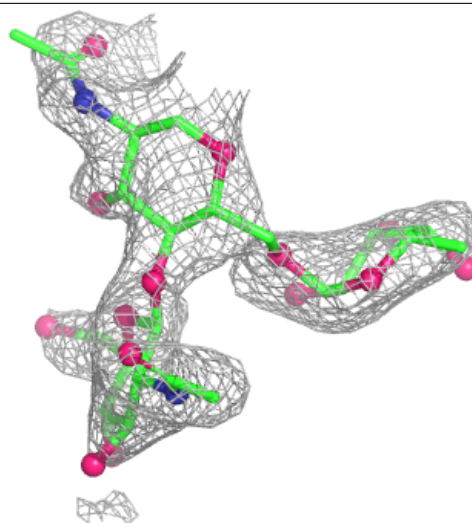
Electron density around Chain I:

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



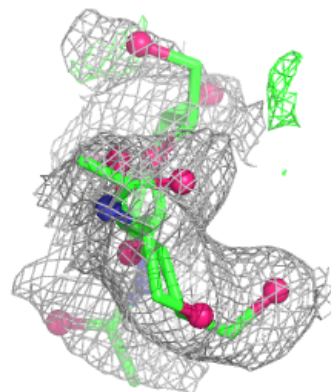
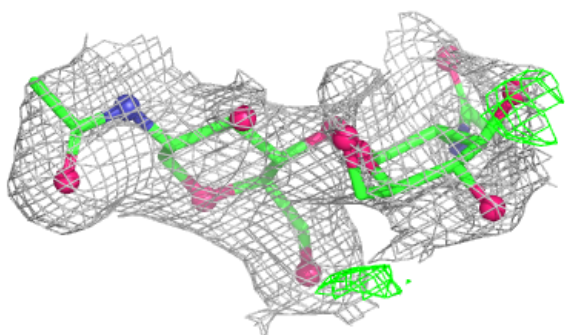
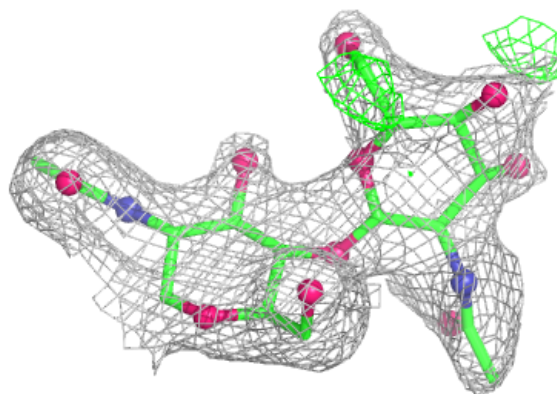
Electron density around Chain K:

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

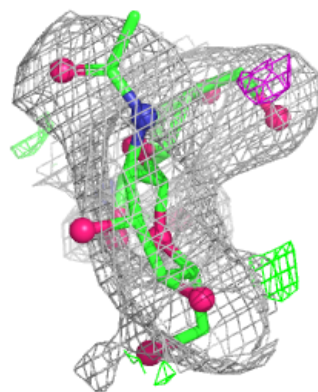
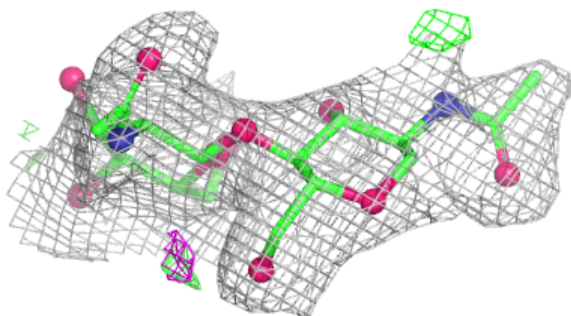
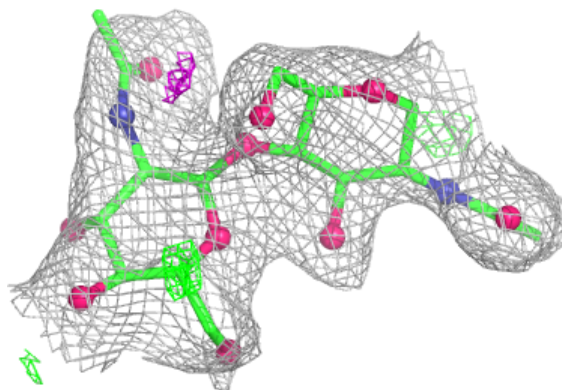


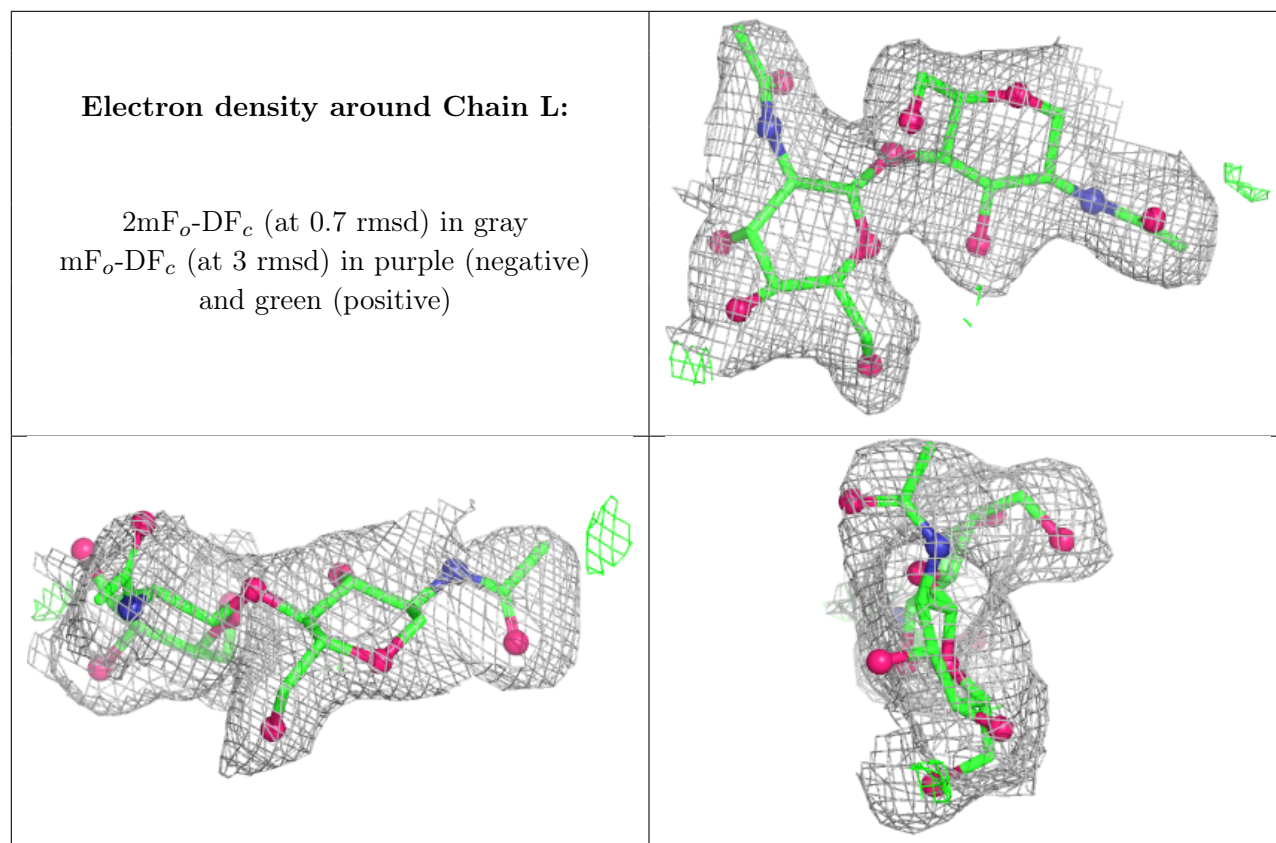
Electron density around Chain H:

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

**Electron density around Chain 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 [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	A	501	14/15	0.98	0.04	46,60,69,74	0
5	NAG	E	501	14/15	0.98	0.04	45,56,67,73	0
5	NAG	C	501	14/15	0.99	0.03	43,56,63,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.