



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:05 PM UTC

PDB ID : 8JR3 / pdb_00008jr3
Title : Crystal structure of Hendra Virus attachment(G) glycoprotein mutant S586N
in complex with neutralizing antibody 14F8
Authors : Li, Y.H.; Huang, X.Y.; Xu, J.J.; Chen, W.
Deposited on : 2023-06-16
Resolution : 3.22 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

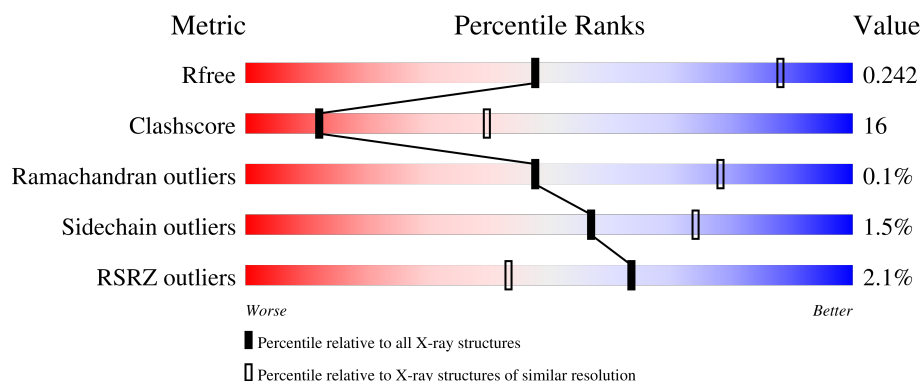
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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.



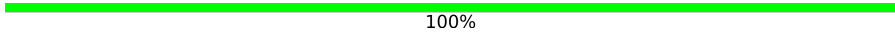
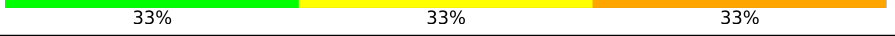
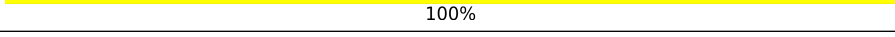
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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 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	E	416	0% 65% 32% ..
1	F	416	0% 66% 31% .
2	A	217	4% 71% 27% ..
2	B	217	2% 75% 25%
3	C	212	0% 63% 34% .

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Mol	Chain	Length	Quality of chain
3	D	212	
4	G	3	
5	H	3	
5	N	3	
5	O	3	
6	I	2	
6	J	2	
6	L	2	
6	M	2	
7	K	4	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13414 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 Glycoprotein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	416	Total	C	N	O	S	0	0	0
			3289	2096	552	622	19			
1	F	416	Total	C	N	O	S	0	0	0
			3289	2096	552	622	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	586	ASN	SER	engineered mutation	UNP O89343
F	586	ASN	SER	engineered mutation	UNP O89343

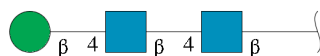
- Molecule 2 is a protein called Heavy chain of neutralizing antibody 14F8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	215	Total	C	N	O	S	0	0	0
			1608	1022	262	319	5			
2	B	217	Total	C	N	O	S	0	0	0
			1624	1033	265	321	5			

- Molecule 3 is a protein called Light chain of neutralizing antibody 14F8.

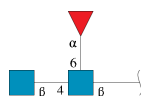
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	212	Total	C	N	O	S	0	0	0
			1638	1031	274	328	5			
3	C	212	Total	C	N	O	S	0	0	0
			1638	1031	274	328	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



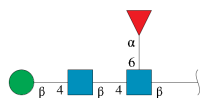
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	N	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	O	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



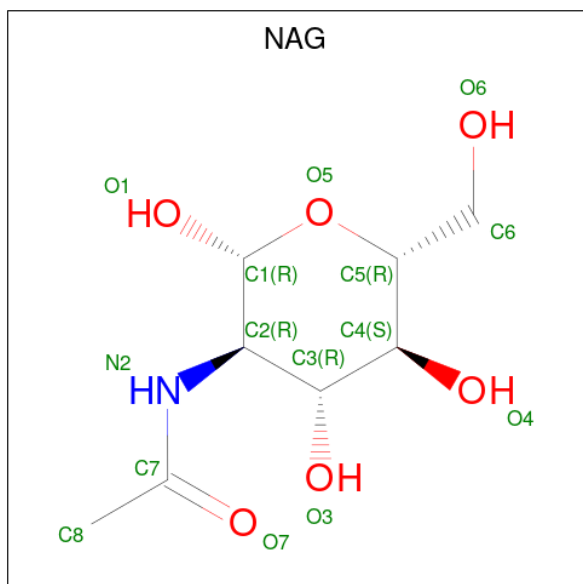
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



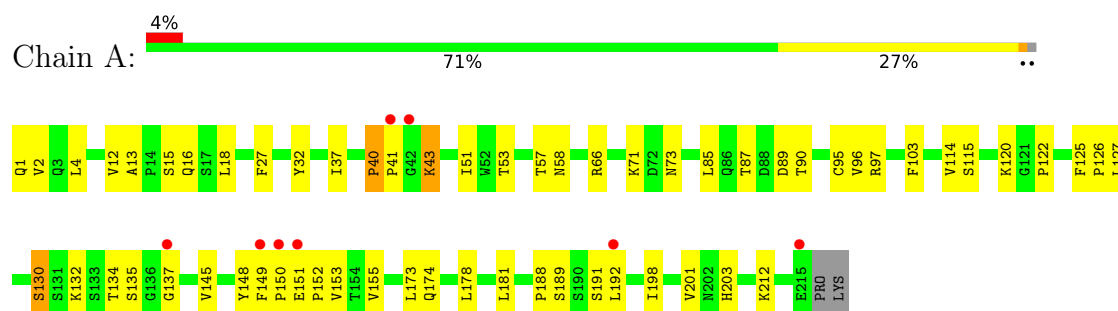
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	4	Total	C	N	O	0	0	0
			49	28	2	19			

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

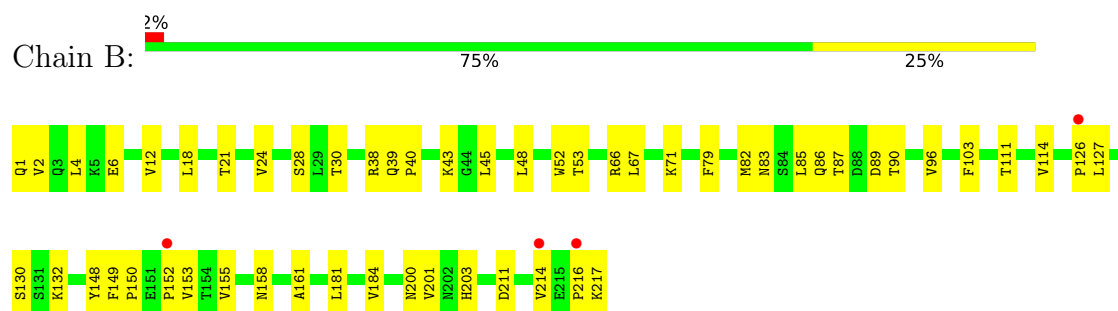


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

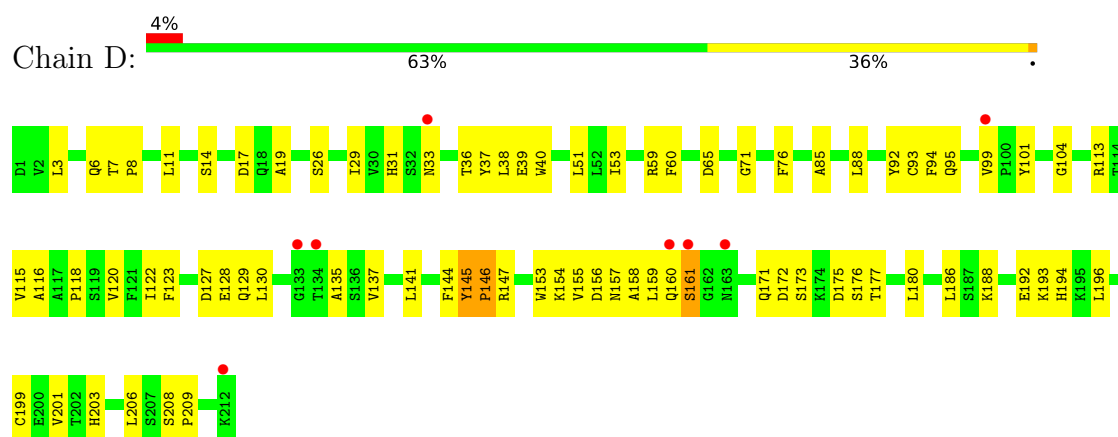
- Molecule 2: Heavy chain of neutralizing antibody 14F8



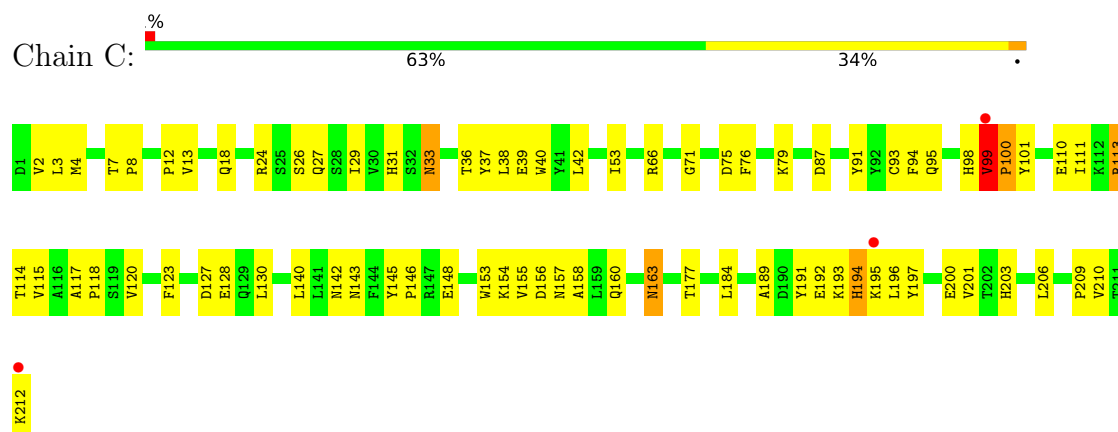
- Molecule 2: Heavy chain of neutralizing antibody 14F8



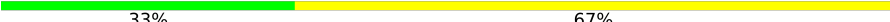
- Molecule 3: Light chain of neutralizing antibody 14F8



- Molecule 3: Light chain of neutralizing antibody 14F8

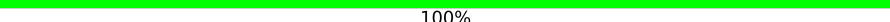


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%


MAG1
MAG2
BMA3

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

Chain H:  100%

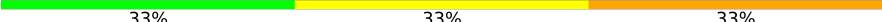

MAG1
MAG2
FUC3

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

Chain N:  67% 33%


MAG1
MAG2
FUC3

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

Chain O:  33% 33% 33%


MAG1
MAG2
FUC3

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

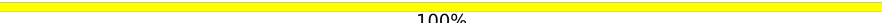

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%


MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	110.84Å 257.01Å 193.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.79 – 3.22 37.79 – 3.22	Depositor EDS
% Data completeness (in resolution range)	98.9 (37.79-3.22) 99.0 (37.79-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.215 , 0.241 0.215 , 0.242	Depositor DCC
R_{free} test set	2000 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13414	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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

5.1 Standard geometry

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

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	E	0.55	1/3369 (0.0%)	0.95	8/4588 (0.2%)
1	F	0.54	0/3369	0.97	8/4588 (0.2%)
2	A	0.49	0/1648	0.86	2/2251 (0.1%)
2	B	0.36	0/1665	0.72	0/2274
3	C	0.51	0/1674	0.96	5/2273 (0.2%)
3	D	0.64	0/1674	1.08	4/2273 (0.2%)
All	All	0.53	1/13399 (0.0%)	0.94	27/18247 (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
1	E	0	4
1	F	0	4
3	C	0	1
3	D	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	434	ASN	CG-ND2	5.78	1.45	1.33

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	100	PRO	N-CA-C	-10.89	94.09	111.19
1	F	318	ARG	CD-NE-CZ	8.24	135.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	323	PRO	N-CA-C	7.40	122.11	110.50
1	E	490	GLN	CA-C-O	-7.31	113.36	121.84
3	D	145	TYR	CB-CA-C	-7.26	101.21	113.04

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	258	ARG	Sidechain
1	E	291	TYR	Sidechain
1	E	487	ARG	Sidechain
1	E	495	ARG	Sidechain
1	F	212	ARG	Sidechain

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	E	3289	0	3229	103	1
1	F	3289	0	3227	106	0
2	A	1608	0	1584	45	0
2	B	1624	0	1604	36	0
3	C	1638	0	1601	63	0
3	D	1638	0	1601	67	1
4	G	39	0	34	0	0
5	H	38	0	34	0	0
5	N	38	0	34	3	0
5	O	38	0	34	1	0
6	I	28	0	25	0	0
6	J	28	0	25	2	0
6	L	28	0	25	1	0
6	M	28	0	25	1	0
7	K	49	0	43	0	0
8	F	14	0	13	0	0
All	All	13414	0	13138	415	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 16.

The worst 5 of 415 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:F:201:ARG:HE	1:F:262:VAL:HG21	1.34	0.91
1:F:448:LEU:HB2	1:F:516:ARG:HH12	1.37	0.88
1:F:318:ARG:HH11	1:F:333:LYS:HD2	1.41	0.84
1:F:290:PHE:HE2	1:F:318:ARG:NH2	1.78	0.82
1:F:290:PHE:CE2	1:F:318:ARG:NH2	2.47	0.81

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:PRO:O	3:D:161:SER:OG[8_555]	1.93	0.27

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	E	414/416 (100%)	401 (97%)	12 (3%)	1 (0%)	43	73
1	F	414/416 (100%)	400 (97%)	14 (3%)	0	100	100
2	A	213/217 (98%)	212 (100%)	1 (0%)	0	100	100
2	B	215/217 (99%)	211 (98%)	4 (2%)	0	100	100
3	C	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
3	D	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
All	All	1676/1690 (99%)	1627 (97%)	48 (3%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	491	SER

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	E	373/373 (100%)	364 (98%)	9 (2%)	43	68
1	F	373/373 (100%)	367 (98%)	6 (2%)	55	73
2	A	186/188 (99%)	183 (98%)	3 (2%)	55	73
2	B	188/188 (100%)	187 (100%)	1 (0%)	81	84
3	C	188/188 (100%)	185 (98%)	3 (2%)	55	73
3	D	188/188 (100%)	187 (100%)	1 (0%)	81	84
All	All	1496/1498 (100%)	1473 (98%)	23 (2%)	57	74

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	588	ILE
2	A	132	LYS
2	A	130	SER
3	D	113	ARG
1	E	587	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	39	GLN
3	D	194	HIS
2	A	58	ASN
2	B	167	HIS
3	D	143	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 ⓘ

24 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	$\# Z > 2$
4	NAG	G	1	4,1	14,14,15	0.40	0	17,19,21	1.15	2 (11%)
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	1.18	2 (11%)
4	BMA	G	3	4	11,11,12	0.58	0	15,15,17	0.69	0
5	NAG	H	1	5,1	14,14,15	0.19	0	17,19,21	0.51	0
5	NAG	H	2	5	14,14,15	0.23	0	17,19,21	0.50	0
5	FUC	H	3	5	10,10,11	0.84	0	14,14,16	0.61	0
6	NAG	I	1	1,6	14,14,15	0.33	0	17,19,21	0.67	0
6	NAG	I	2	6	14,14,15	0.75	1 (7%)	17,19,21	0.61	0
6	NAG	J	1	1,6	14,14,15	0.48	0	17,19,21	2.72	3 (17%)
6	NAG	J	2	6	14,14,15	1.29	1 (7%)	17,19,21	1.90	3 (17%)
7	NAG	K	1	7,1	14,14,15	0.28	0	17,19,21	0.60	0
7	NAG	K	2	7	14,14,15	0.44	0	17,19,21	0.72	1 (5%)
7	BMA	K	3	7	11,11,12	0.68	0	15,15,17	0.57	0
7	FUC	K	4	7	10,10,11	0.79	1 (10%)	14,14,16	0.54	0
6	NAG	L	1	1,6	14,14,15	0.56	0	17,19,21	0.70	0
6	NAG	L	2	6	14,14,15	0.45	0	17,19,21	0.64	0
6	NAG	M	1	1,6	14,14,15	0.51	0	17,19,21	0.83	1 (5%)
6	NAG	M	2	6	14,14,15	0.20	0	17,19,21	0.56	0
5	NAG	N	1	5,1	14,14,15	0.34	0	17,19,21	0.58	0
5	NAG	N	2	5	14,14,15	0.23	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUC	N	3	5	10,10,11	1.94	2 (20%)	14,14,16	1.99	4 (28%)
5	NAG	O	1	5,1	14,14,15	0.32	0	17,19,21	0.70	0
5	NAG	O	2	5	14,14,15	0.21	0	17,19,21	0.84	1 (5%)
5	FUC	O	3	5	10,10,11	0.85	0	14,14,16	0.64	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
4	NAG	G	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1
5	FUC	H	3	5	-	-	0/1/1/1
6	NAG	I	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	J	2	6	-	3/6/23/26	0/1/1/1
7	NAG	K	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	0/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	FUC	K	4	7	-	-	0/1/1/1
6	NAG	L	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	NAG	M	1	1,6	-	5/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	0/6/23/26	0/1/1/1
5	FUC	N	3	5	-	-	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
5	FUC	O	3	5	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	3	FUC	C1-C2	4.57	1.63	1.52
6	J	2	NAG	O5-C1	4.41	1.51	1.43
5	N	3	FUC	O5-C5	3.30	1.50	1.43
6	I	2	NAG	C1-C2	2.08	1.55	1.52
7	K	4	FUC	O5-C1	-2.04	1.40	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1	NAG	C2-N2-C7	10.04	136.35	122.90
6	J	2	NAG	C1-O5-C5	5.51	119.57	112.19
6	J	2	NAG	C2-N2-C7	4.25	128.59	122.90
5	N	3	FUC	C1-C2-C3	3.93	115.36	109.64
5	N	3	FUC	O2-C2-C1	3.57	117.40	109.22

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

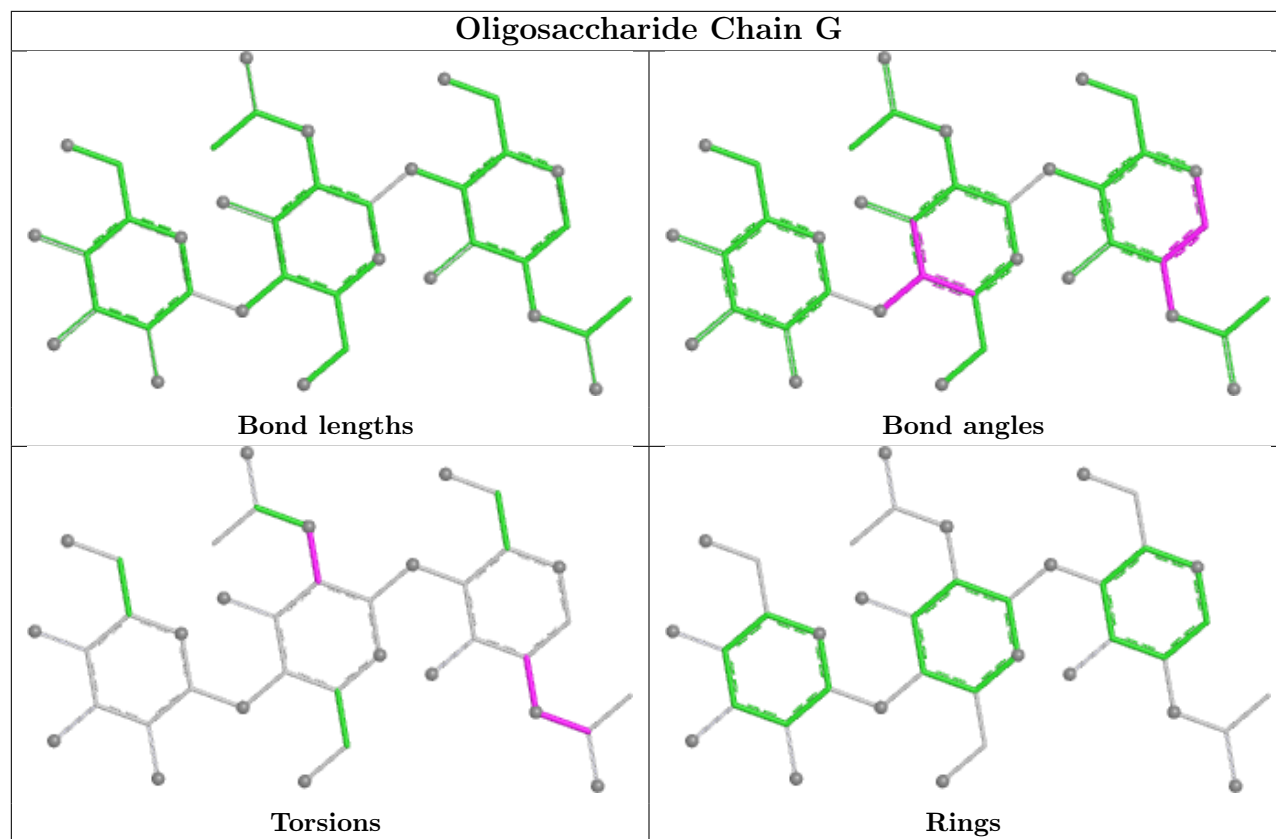
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C1-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7
5	O	2	NAG	C1-C2-N2-C7
6	J	1	NAG	C3-C2-N2-C7
6	J	2	NAG	C1-C2-N2-C7

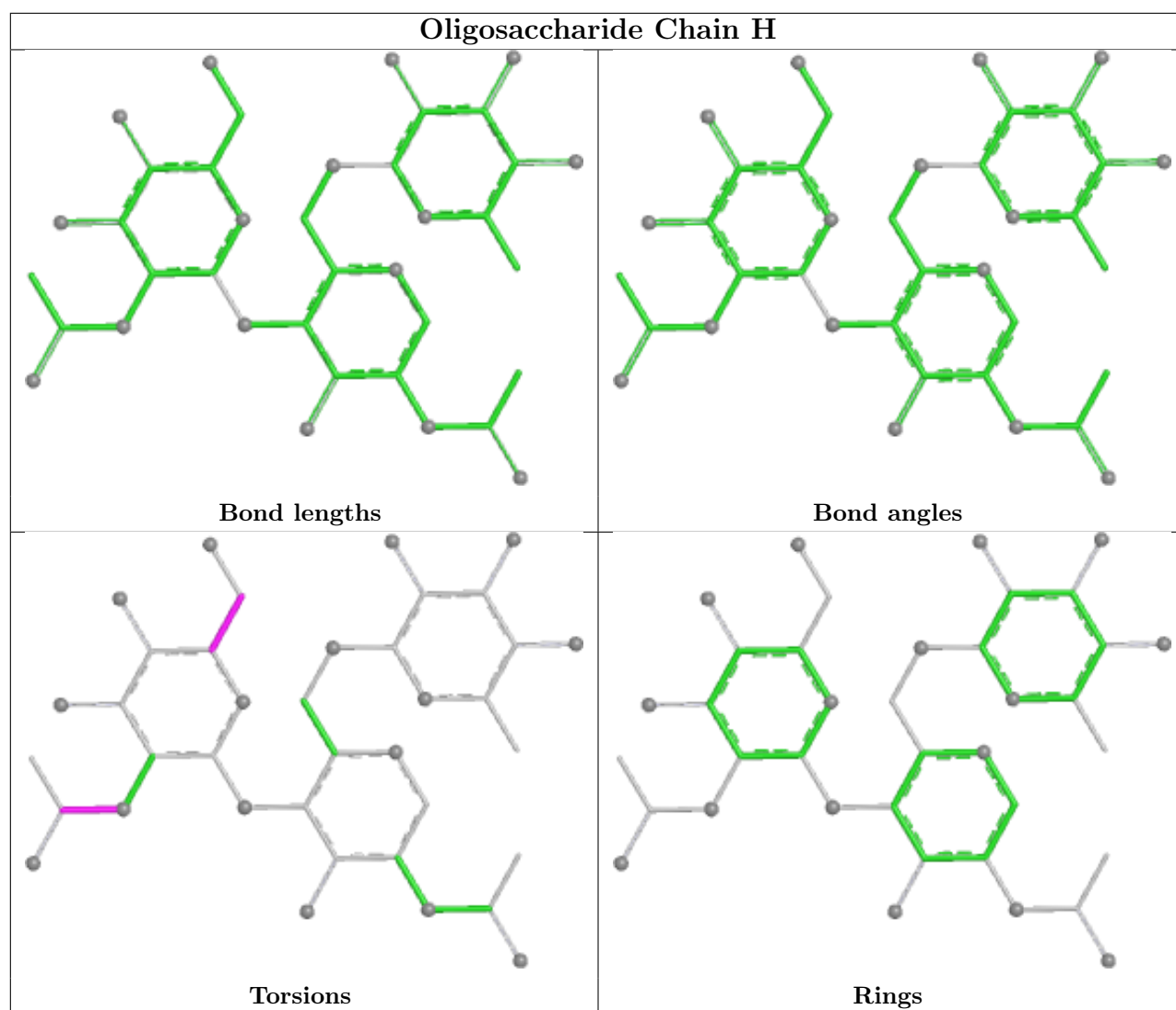
There are no ring outliers.

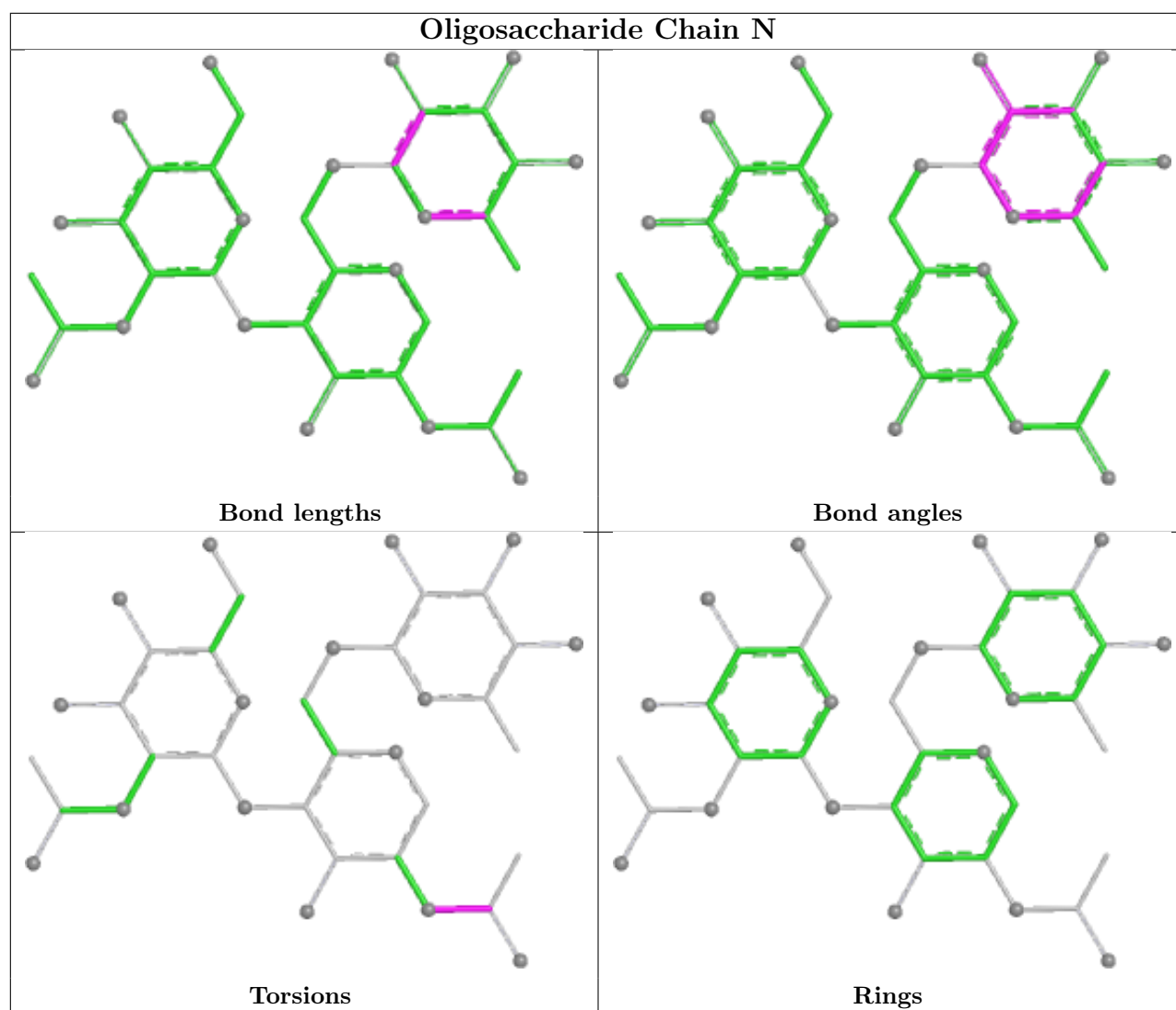
9 monomers are involved in 8 short contacts:

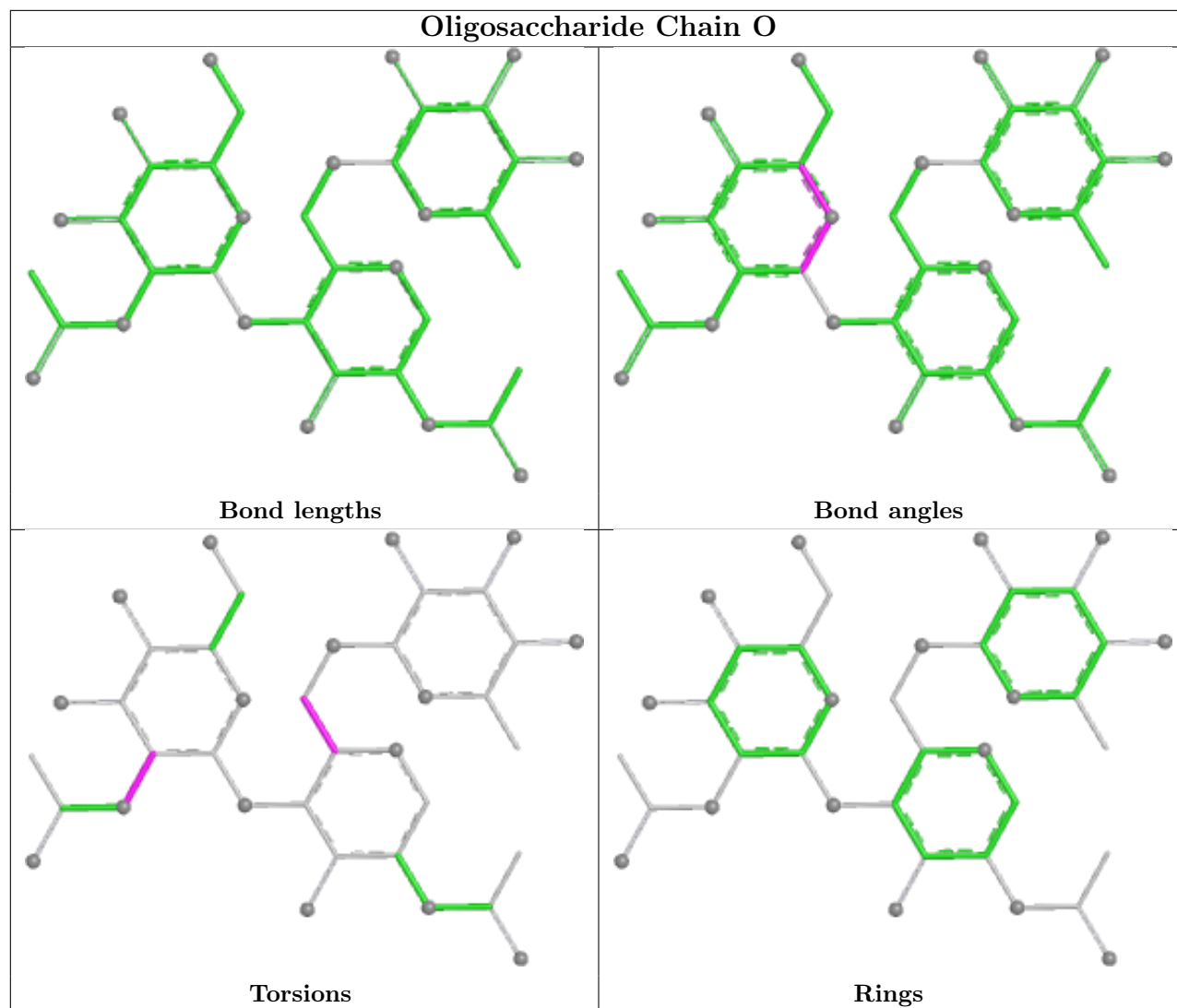
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	1	NAG	2	0
5	N	3	FUC	2	0
5	O	1	NAG	1	0
6	L	1	NAG	1	0
6	L	2	NAG	1	0
5	O	2	NAG	1	0
5	N	2	NAG	1	0
6	M	1	NAG	1	0
6	J	1	NAG	2	0

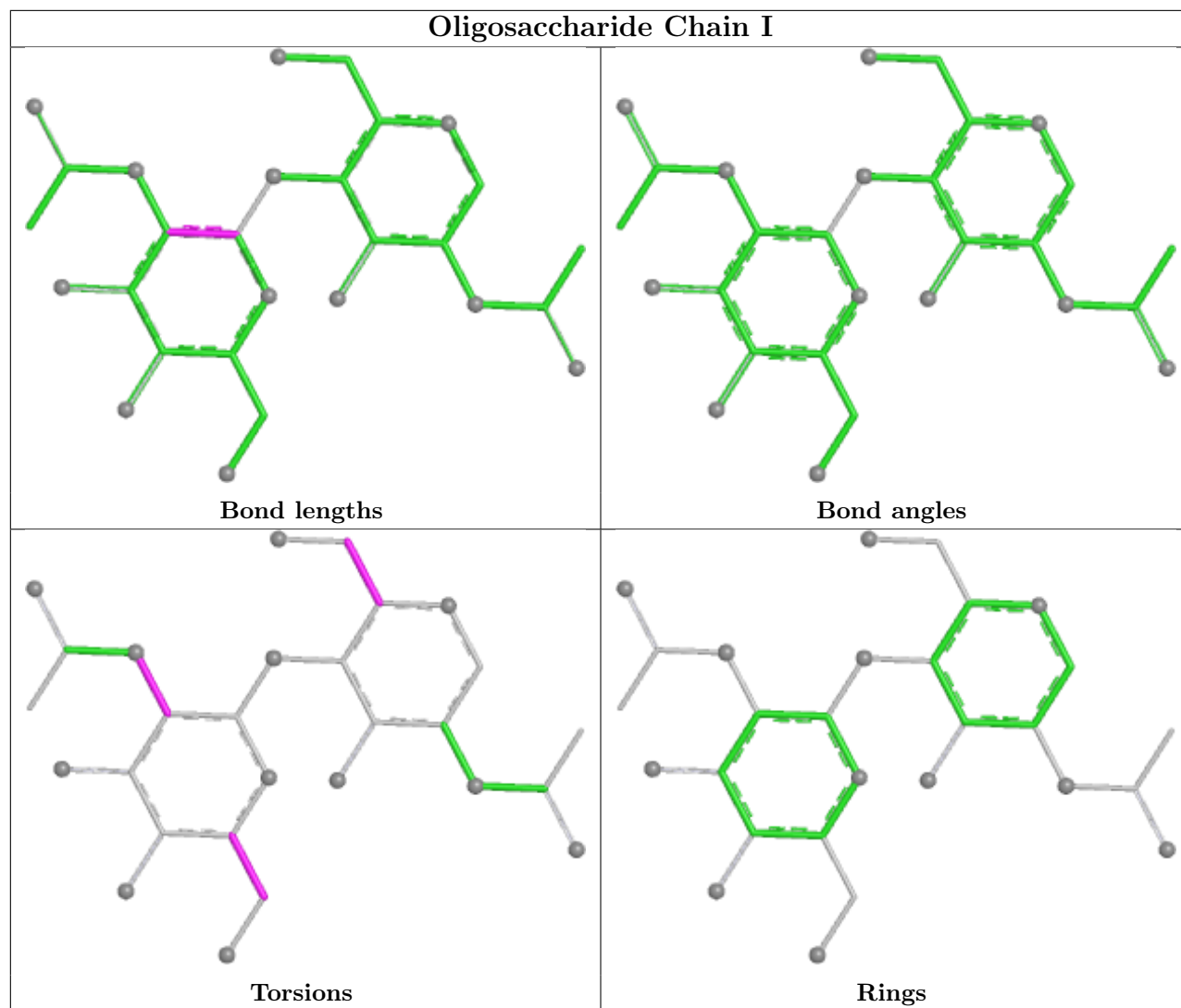
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

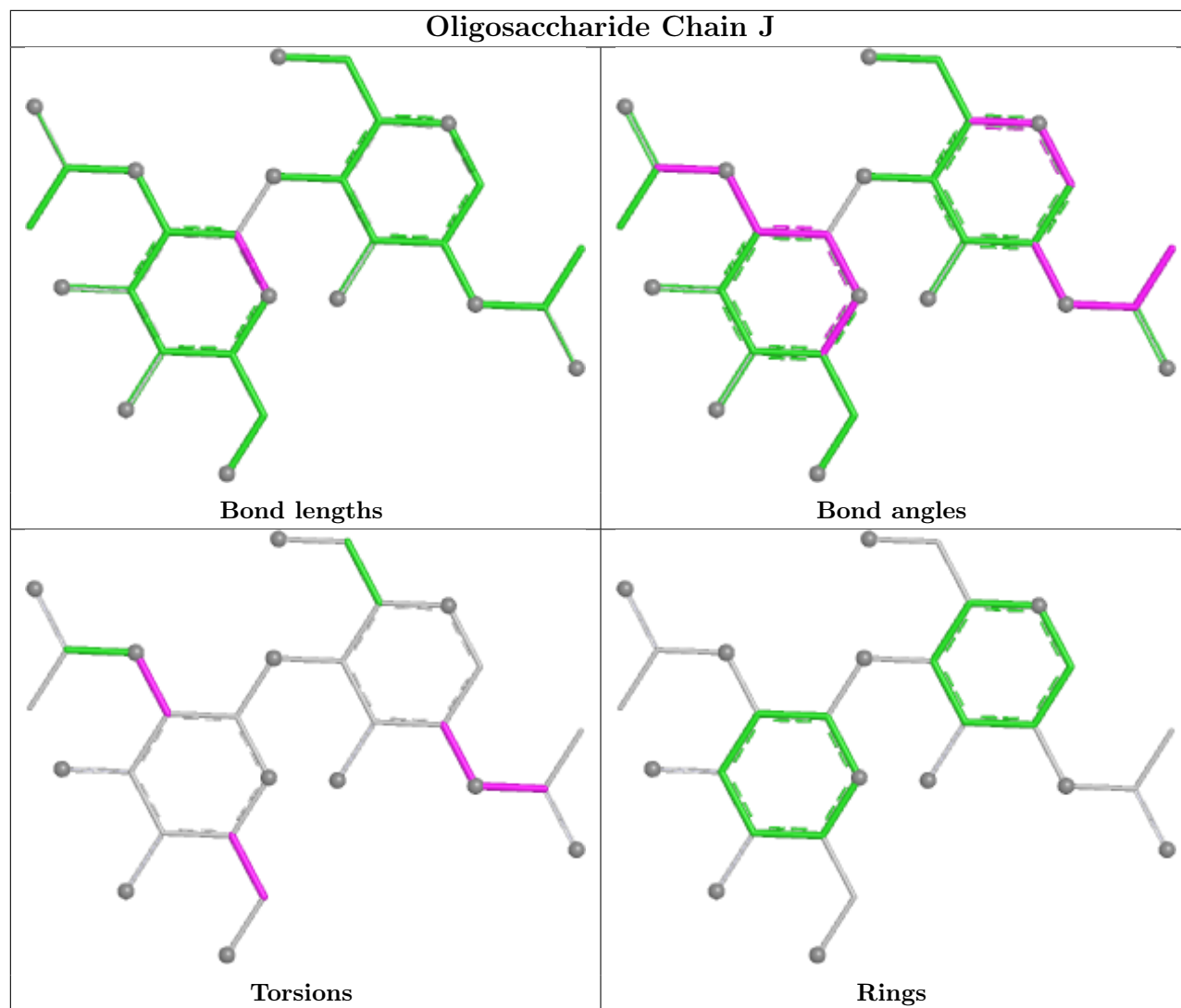


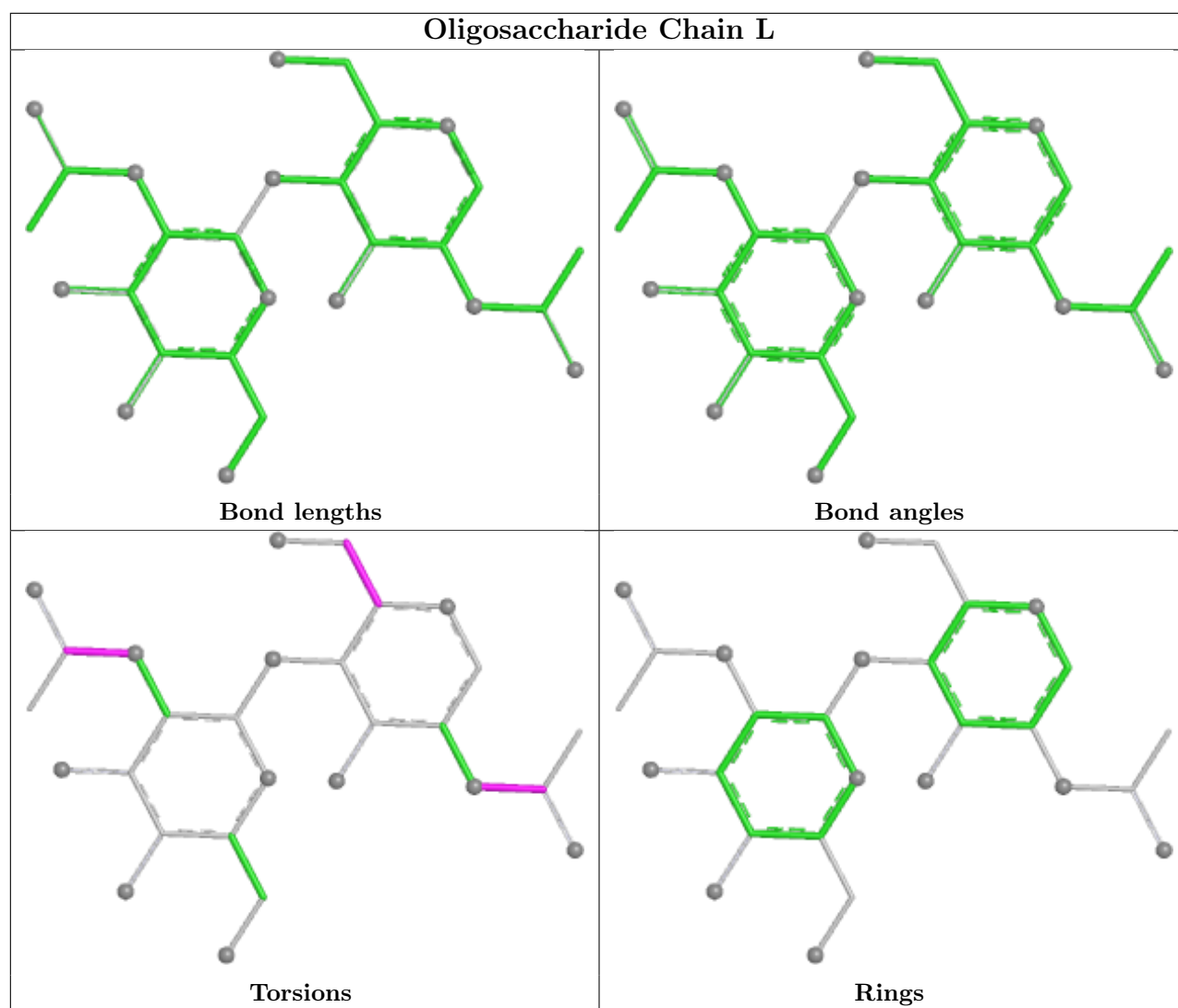


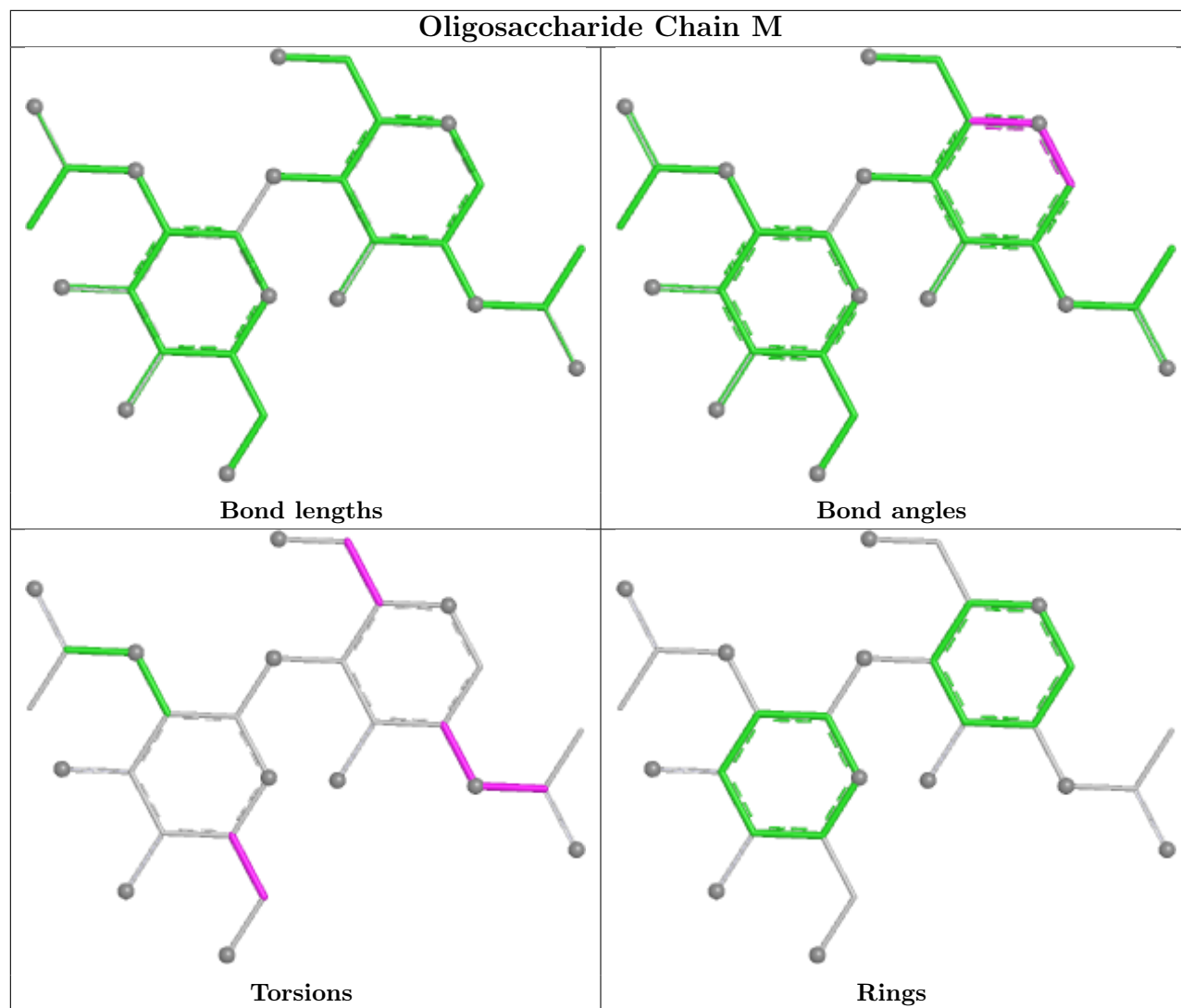


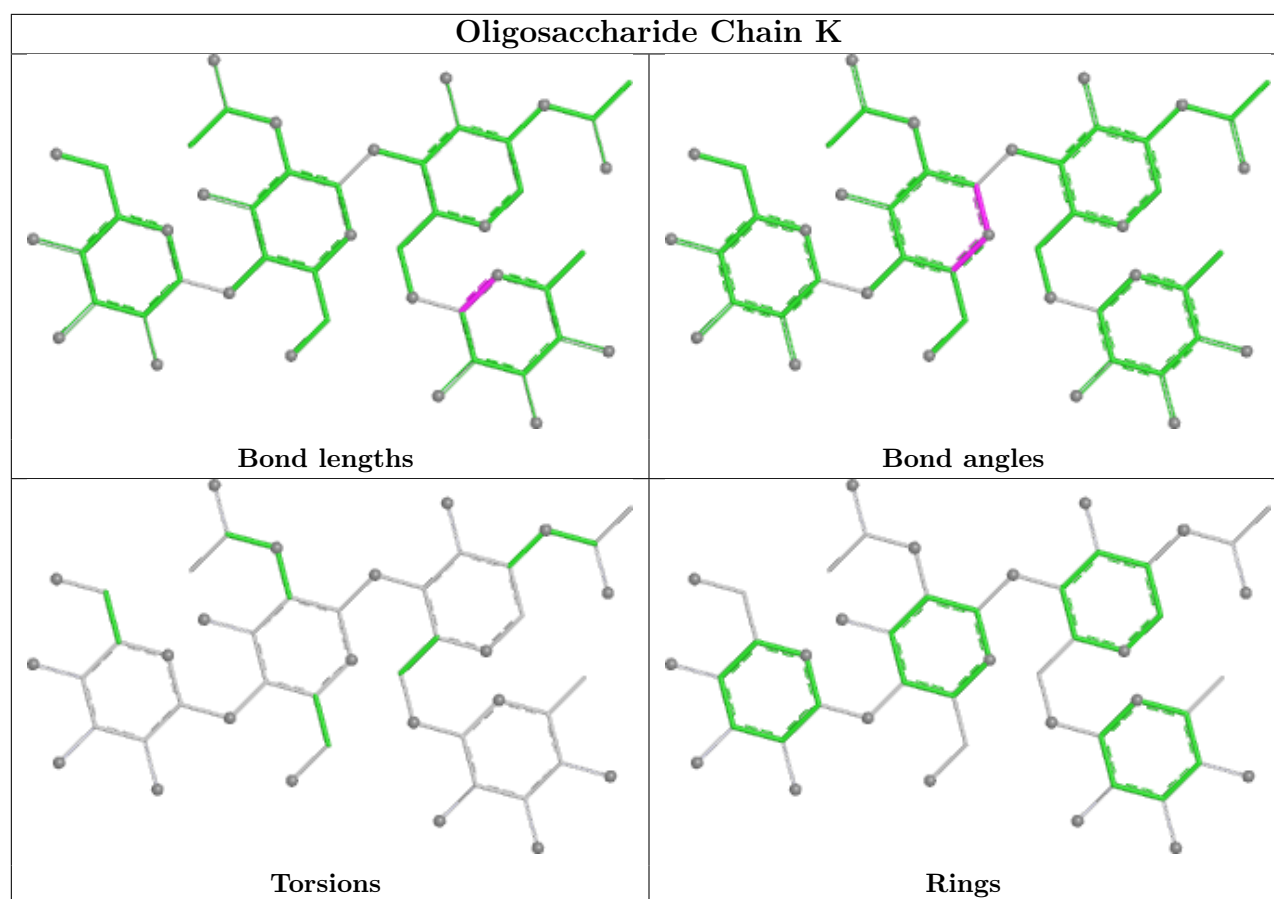












5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
8	NAG	F	701	1	14,14,15	0.28	0	17,19,21	0.59	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
8	NAG	F	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	E	416/416 (100%)	-0.01	6 (1%) 73 54	30, 51, 90, 171	0
1	F	416/416 (100%)	-0.01	6 (1%) 73 54	29, 52, 89, 132	0
2	A	215/217 (99%)	0.27	8 (3%) 45 28	28, 66, 160, 212	0
2	B	217/217 (100%)	0.11	4 (1%) 67 48	33, 60, 129, 162	0
3	C	212/212 (100%)	0.15	3 (1%) 73 54	35, 63, 106, 132	0
3	D	212/212 (100%)	0.31	8 (3%) 44 28	34, 63, 116, 156	0
All	All	1688/1690 (99%)	0.10	35 (2%) 63 43	28, 57, 109, 212	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	42	GLY	4.3
1	E	259	GLY	4.0
2	B	214	VAL	3.6
3	D	99	VAL	3.6
2	B	152	PRO	3.5

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](#)

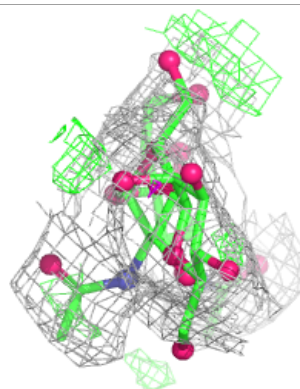
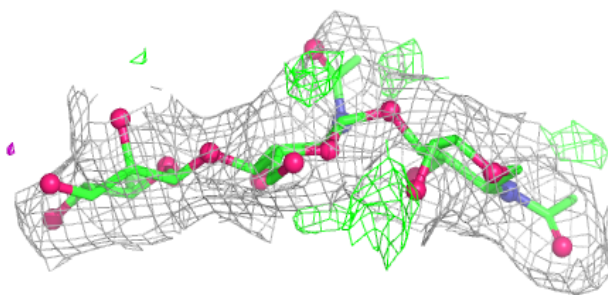
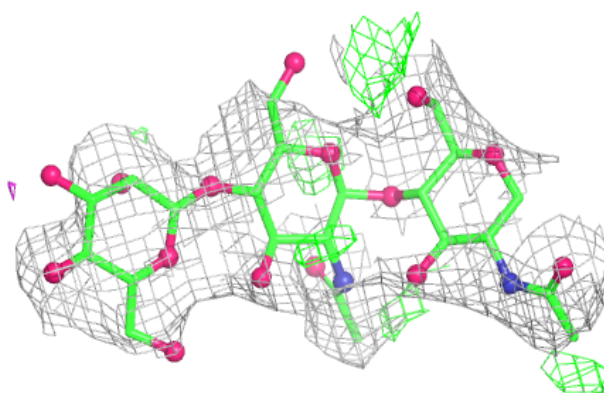
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
4	NAG	G	2	14/15	0.51	0.16	81,104,117,117	0
6	NAG	M	2	14/15	0.51	0.15	103,115,125,127	0
5	NAG	O	2	14/15	0.54	0.18	93,102,109,110	0
6	NAG	I	1	14/15	0.55	0.15	58,109,114,115	0
6	NAG	J	2	14/15	0.56	0.13	97,132,140,140	0
4	BMA	G	3	11/12	0.59	0.14	80,103,116,117	0
6	NAG	L	2	14/15	0.60	0.14	94,109,115,116	0
5	FUC	O	3	10/11	0.60	0.19	79,110,117,121	0
5	NAG	H	2	14/15	0.62	0.12	71,90,115,117	0
5	NAG	N	2	14/15	0.63	0.12	94,103,109,110	0
7	BMA	K	3	11/12	0.65	0.10	92,103,110,113	0
5	FUC	N	3	10/11	0.67	0.17	89,113,120,126	0
6	NAG	I	2	14/15	0.68	0.12	96,120,130,131	0
6	NAG	M	1	14/15	0.69	0.12	56,92,107,109	0
6	NAG	J	1	14/15	0.73	0.15	77,103,124,124	0
5	FUC	H	3	10/11	0.76	0.11	67,87,102,102	0
6	NAG	L	1	14/15	0.76	0.12	62,75,93,98	0
7	NAG	K	2	14/15	0.80	0.11	77,92,103,106	0
4	NAG	G	1	14/15	0.81	0.12	43,66,79,98	0
5	NAG	N	1	14/15	0.82	0.10	67,89,101,103	0
7	NAG	K	1	14/15	0.83	0.11	55,80,88,89	0
7	FUC	K	4	10/11	0.86	0.12	65,87,105,108	0
5	NAG	O	1	14/15	0.87	0.10	71,85,91,93	0
5	NAG	H	1	14/15	0.91	0.08	53,72,80,94	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

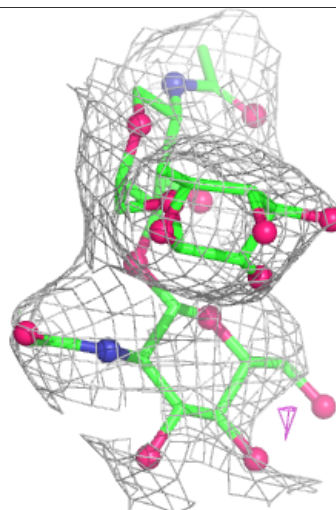
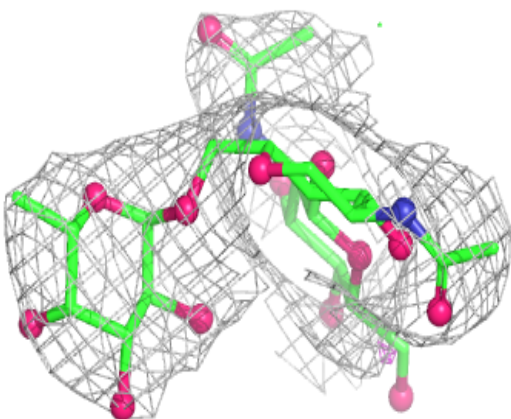
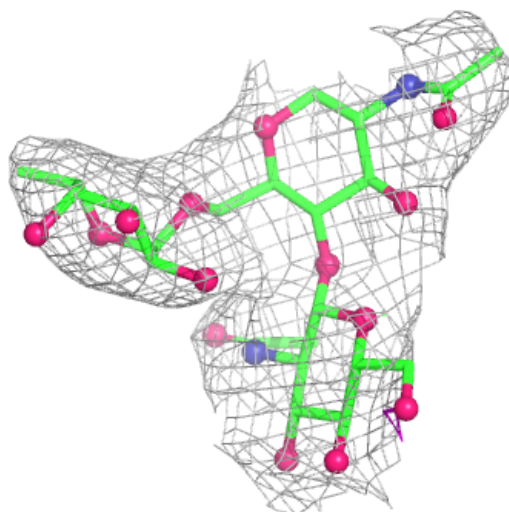
Electron density around Chain G:

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



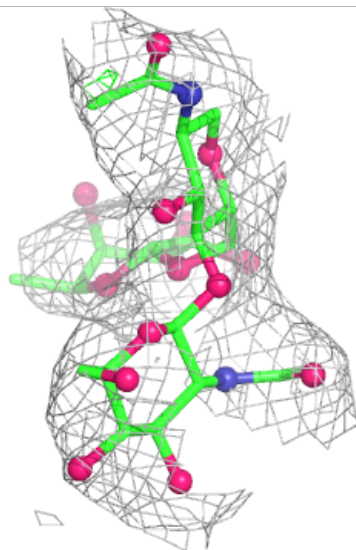
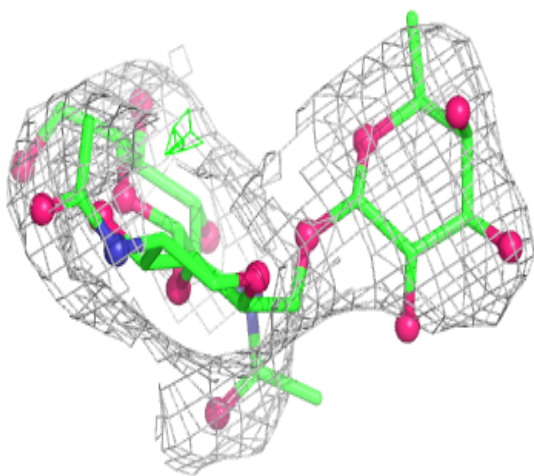
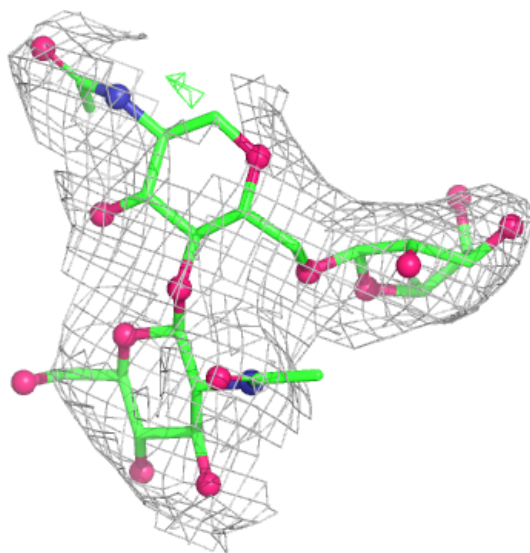
Electron density around Chain H:

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



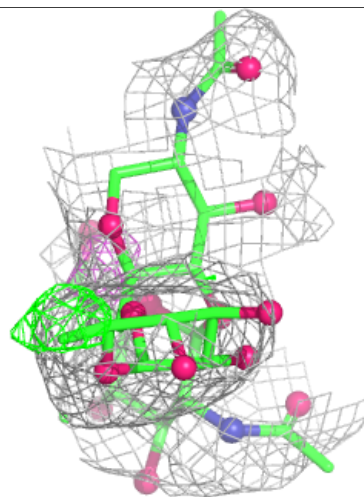
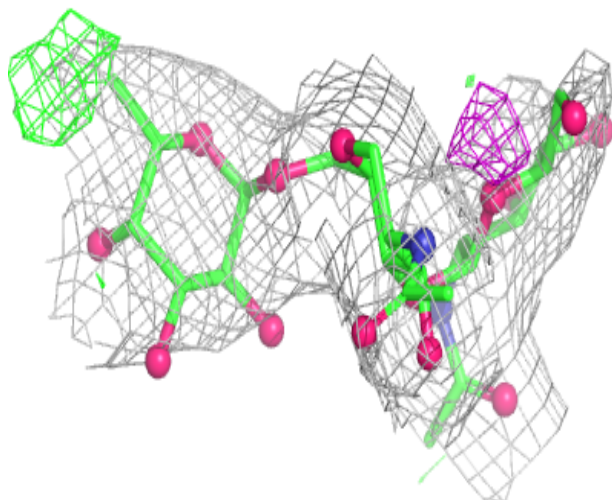
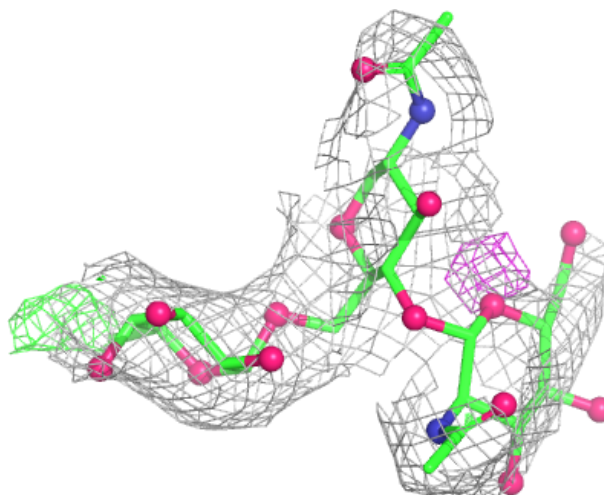
Electron density around Chain N:

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



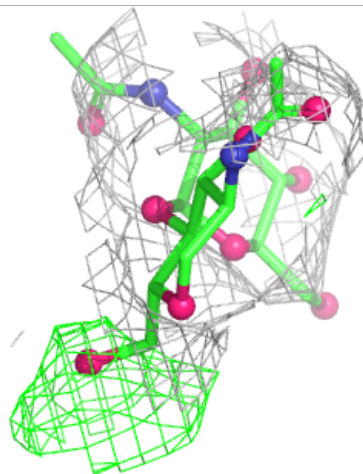
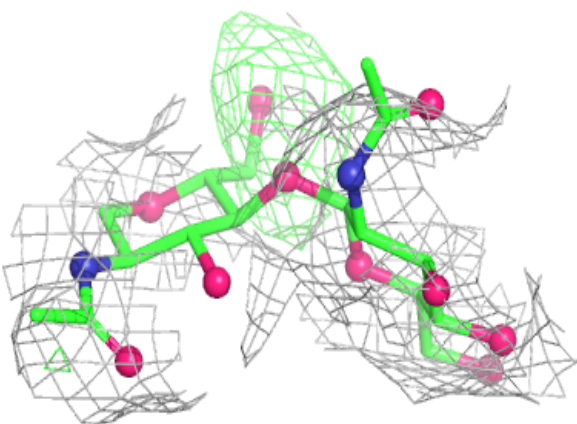
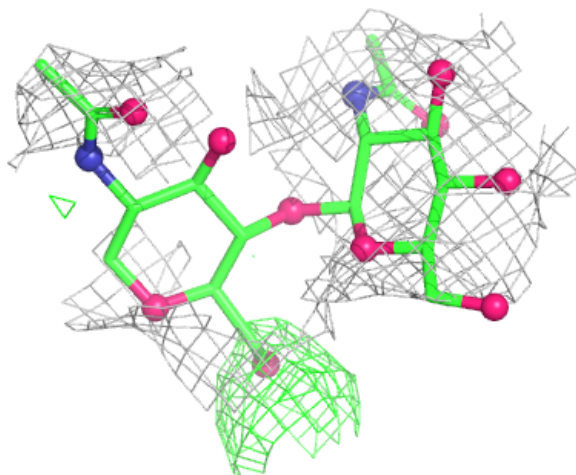
Electron density around Chain O:

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



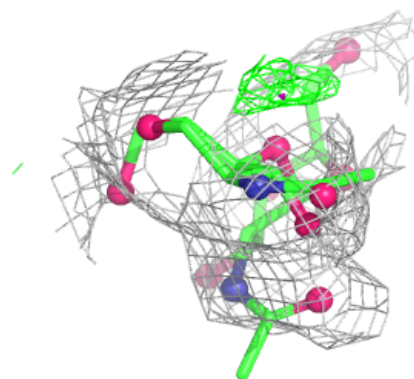
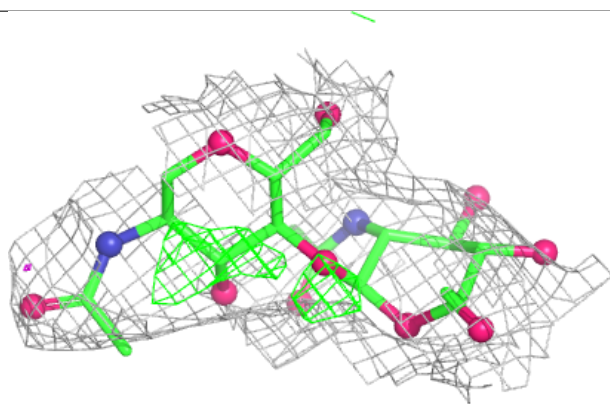
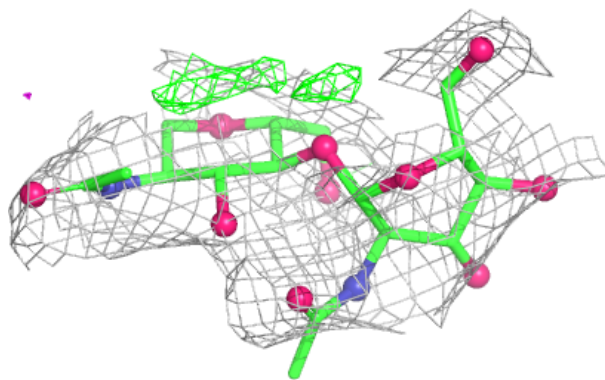
Electron density around Chain I:

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

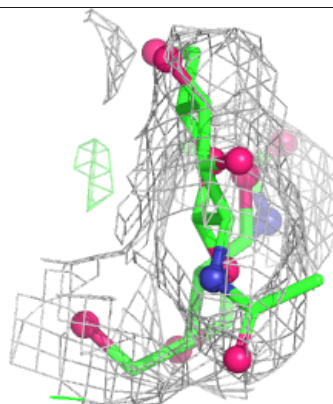
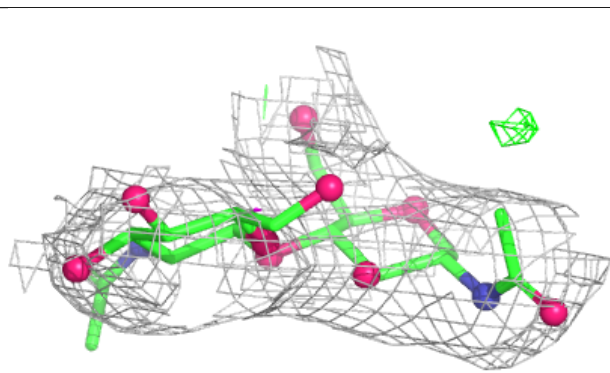
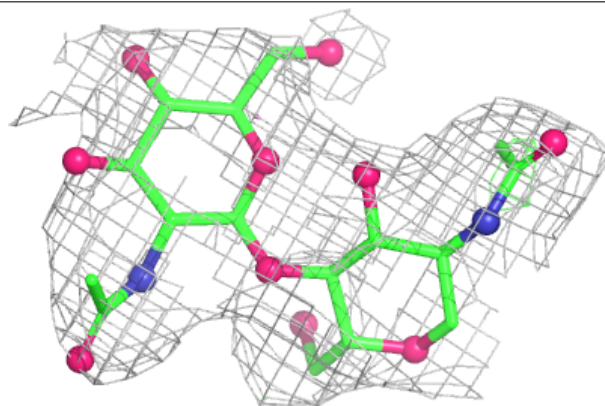


Electron density around Chain J:

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

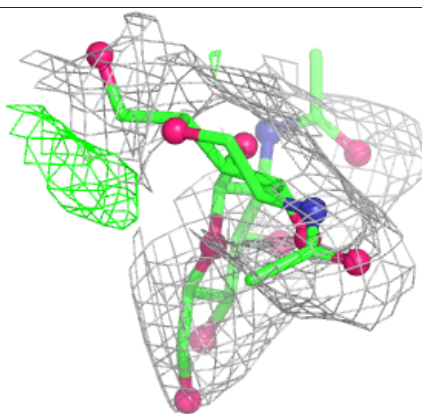
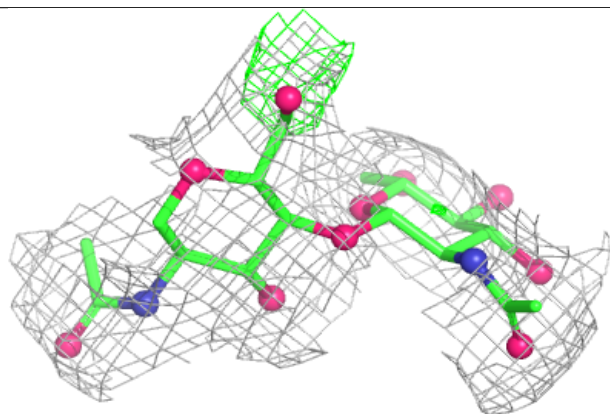
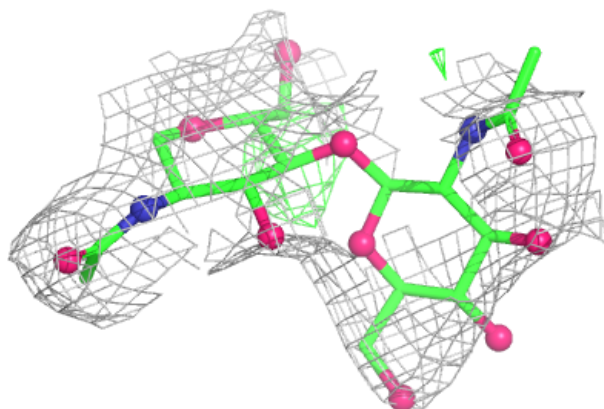
**Electron density around Chain L:**

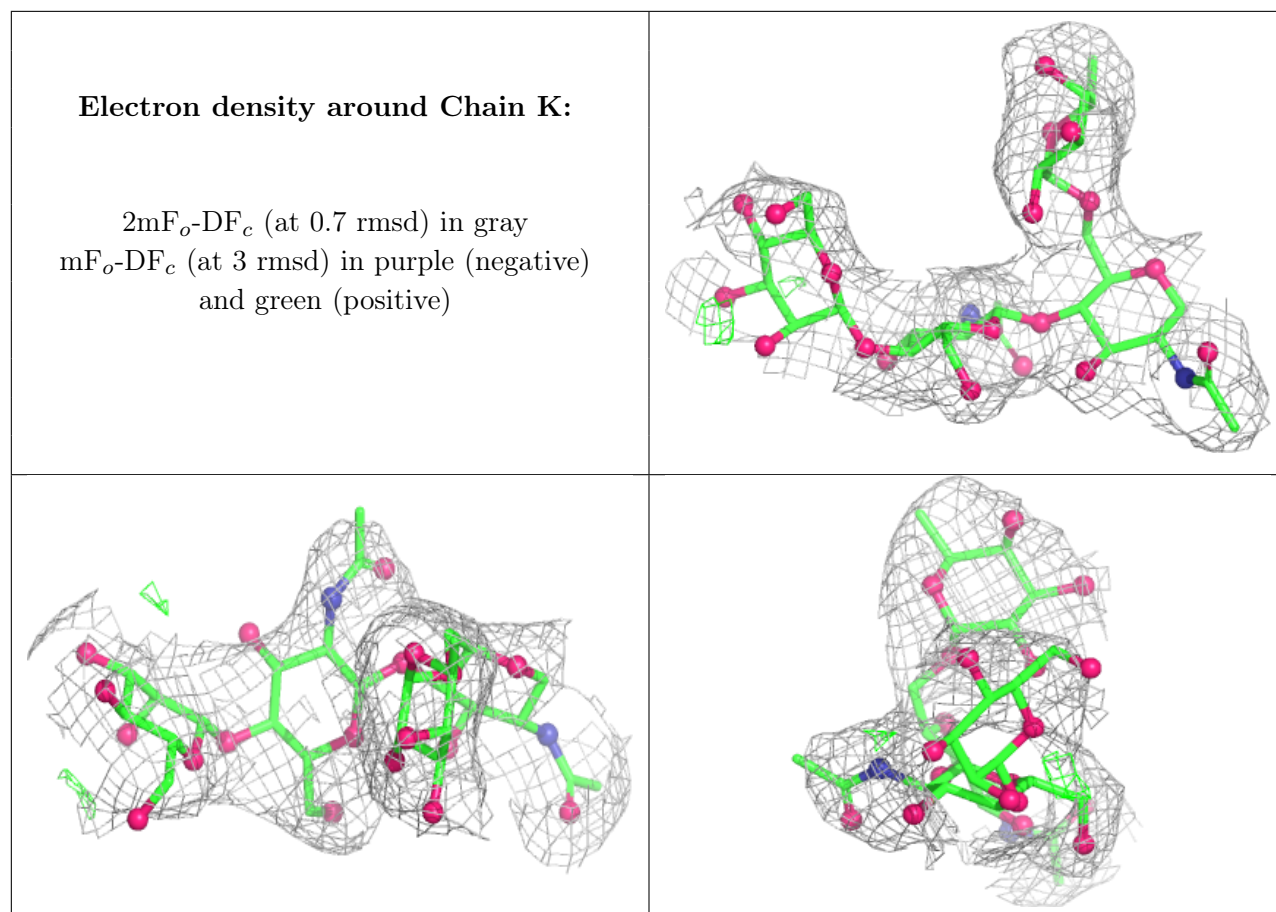
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
8	NAG	F	701	14/15	0.57	0.15	77,106,124,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.