



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2022 – 06:07 PM EDT

PDB ID : 7S8H
Title : Structure of Lassa virus glycoprotein bound to Fab 18.5C and Fab 36.1F
Authors : Hastie, K.M.; Enriquez, A.S.
Deposited on : 2021-09-17
Resolution : 2.70 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 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 : 2.28.1
buster-report : 1.1.7 (2018)
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) : 2.28.1

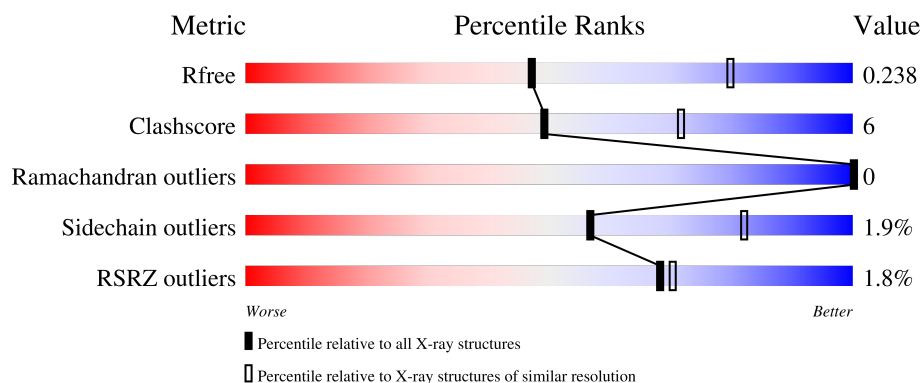
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	201	<div> <div>4%</div> <div>86%</div> <div>6%</div> <div>7%</div> </div>
2	H	228	<div> <div>82%</div> <div>13%</div> <div>...</div> </div>
3	L	217	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
4	B	229	<div> <div>4%</div> <div>76%</div> <div>19%</div> <div>5%</div> </div>
5	C	216	<div> <div>3%</div> <div>81%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
6	a	165	
7	D	4	
8	E	2	
8	G	2	
8	J	2	
8	K	2	
8	M	2	
9	F	3	
10	I	6	
10	N	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MAN	I	5	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 9824 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 G1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1486	938	249	283	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	CYS	GLY	engineered mutation	UNP P08669
A	258	ARG	LEU	engineered mutation	UNP P08669
A	259	ARG	LEU	engineered mutation	UNP P08669

- Molecule 2 is a protein called 18.5C Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1643	1035	285	316	7			

- Molecule 3 is a protein called 18.5C Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1642	1034	275	329	4			

- Molecule 4 is a protein called 36.1F Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	218	Total	C	N	O	S	0	0	0
			1625	1027	278	315	5			

- Molecule 5 is a protein called 36.1F Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	215	Total	C	N	O	S	0	0	0
			1659	1041	280	334	4			

- Molecule 6 is a protein called Glycoprotein G2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	a	163	Total	C	N	O	S	0	0	0
			1321	830	224	253	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	329	PRO	GLU	engineered mutation	UNP P08669
a	332	THR	MET	engineered mutation	UNP P08669
a	350	CYS	ILE	engineered mutation	UNP P08669

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



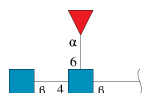
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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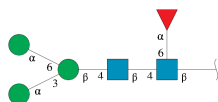
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 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
9	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	6	Total	C	N	O	0	0	0
			71	40	2	29			
10	N	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

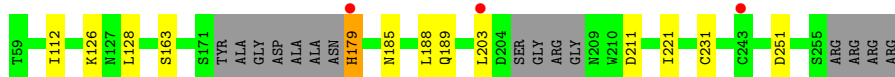
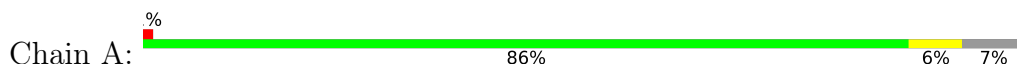
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	13	Total	O	0	0
			13	13		
12	H	13	Total	O	0	0
			13	13		
12	L	12	Total	O	0	0
			12	12		
12	B	6	Total	O	0	0
			6	6		
12	C	8	Total	O	0	0
			8	8		
12	a	12	Total	O	0	0
			12	12		

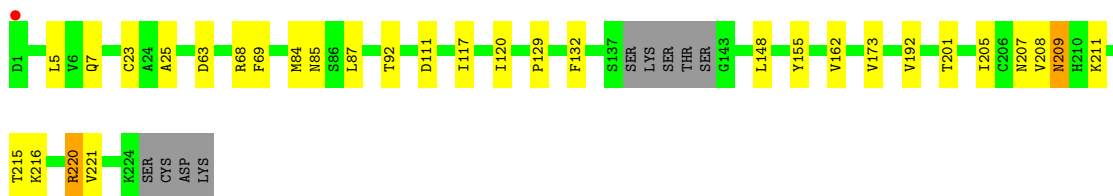
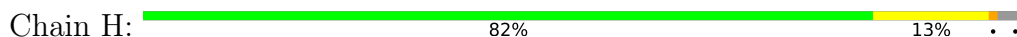
3 Residue-property plots [i](#)

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.

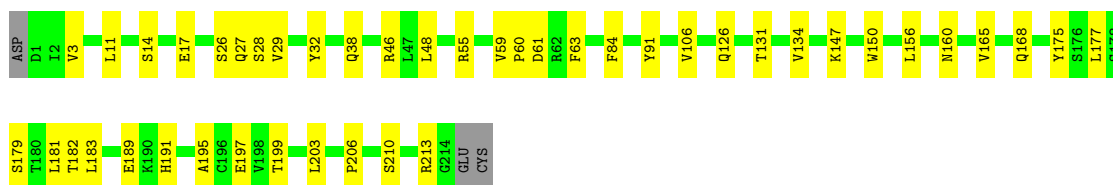
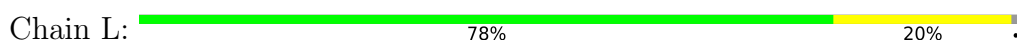
- Molecule 1: Glycoprotein G1



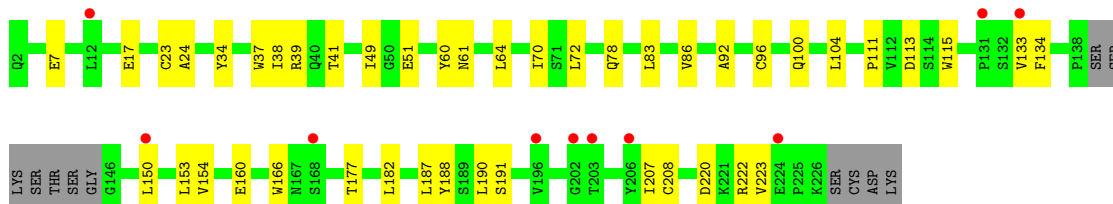
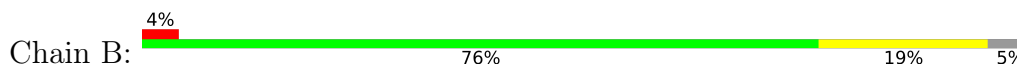
- Molecule 2: 18.5C Fab Heavy Chain



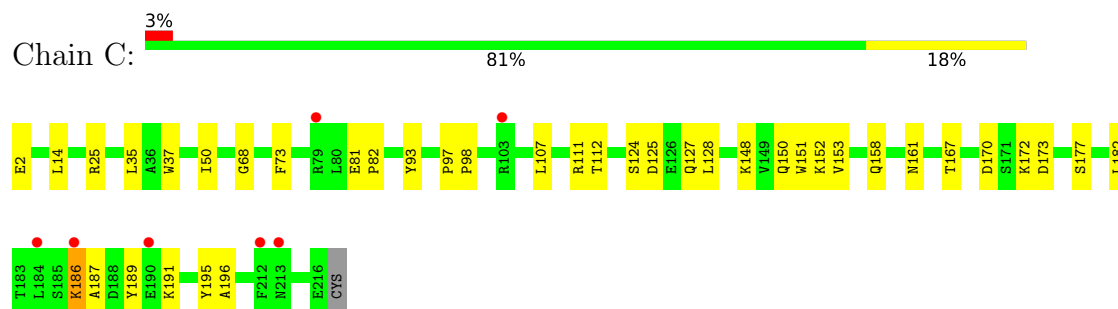
- Molecule 3: 18.5C Fab Light Chain



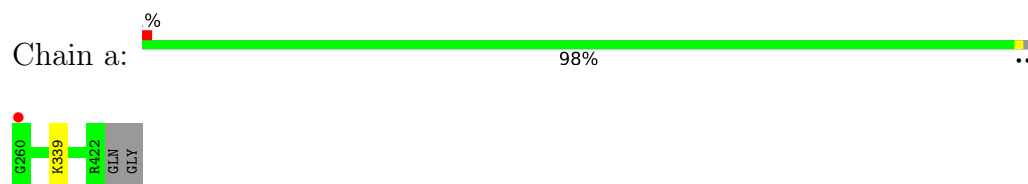
- Molecule 4: 36.1F Fab Heavy Chain



● Molecule 5: 36.1F Fab Light Chain



● Molecule 6: Glycoprotein G2



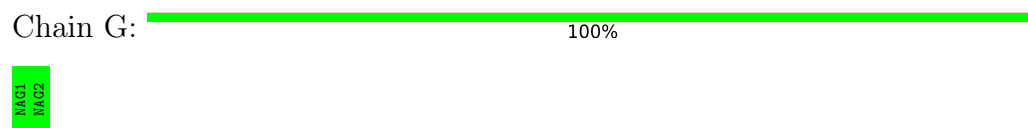
● Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

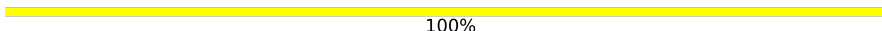


- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

MAG1
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67% 33%


MAG1
MAG2
FUC3

- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  33% 67%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.06Å 163.06Å 173.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.18 – 2.70 47.18 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.18-2.70) 100.0 (47.18-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.217 , 0.251 0.203 , 0.238	Depositor DCC
R_{free} test set	3602 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9824	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, BMA, FUC, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.30	0/1519	0.52	0/2058
2	H	0.31	0/1680	0.57	0/2283
3	L	0.30	0/1681	0.56	0/2285
4	B	0.31	0/1663	0.56	0/2267
5	C	0.31	0/1697	0.55	0/2307
6	a	0.31	0/1349	0.51	0/1822
All	All	0.31	0/9589	0.55	0/13022

There are no bond length outliers.

There are no bond angle outliers.

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	1486	0	1414	6	1
2	H	1643	0	1631	17	0
3	L	1642	0	1589	25	1
4	B	1625	0	1625	31	0
5	C	1659	0	1611	23	1
6	a	1321	0	1265	0	1
7	D	50	0	43	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	28	0	25	0	0
8	G	28	0	25	0	0
8	J	28	0	25	0	0
8	K	28	0	25	0	0
8	M	28	0	25	0	0
9	F	38	0	34	1	0
10	I	71	0	61	0	0
10	N	71	0	61	0	0
11	a	14	0	13	0	0
12	A	13	0	0	0	0
12	B	6	0	0	1	0
12	C	8	0	0	1	0
12	H	13	0	0	0	0
12	L	12	0	0	0	0
12	a	12	0	0	0	0
All	All	9824	0	9472	101	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 101 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)
2:H:205:ILE:HD11	2:H:220:ARG:HG3	1.52	0.92
2:H:205:ILE:CD1	2:H:220:ARG:HG3	2.19	0.73
3:L:55:ARG:NH1	3:L:63:PHE:O	2.22	0.73
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.72	0.72
5:C:167:THR:HG22	5:C:177:SER:H	1.54	0.71

All (2) 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)
3:L:203:LEU:O	5:C:148:LYS:NZ[2_555]	2.11	0.09
1:A:211:ASP:OD2	6:a:339:LYS:NZ[3_455]	2.16	0.04

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	180/201 (90%)	172 (96%)	8 (4%)	0	100	100
2	H	215/228 (94%)	212 (99%)	3 (1%)	0	100	100
3	L	212/217 (98%)	203 (96%)	9 (4%)	0	100	100
4	B	214/229 (93%)	211 (99%)	3 (1%)	0	100	100
5	C	213/216 (99%)	207 (97%)	6 (3%)	0	100	100
6	a	161/165 (98%)	158 (98%)	3 (2%)	0	100	100
All	All	1195/1256 (95%)	1163 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	170/179 (95%)	167 (98%)	3 (2%)	59	83
2	H	184/193 (95%)	178 (97%)	6 (3%)	38	67
3	L	183/186 (98%)	179 (98%)	4 (2%)	52	79
4	B	185/195 (95%)	183 (99%)	2 (1%)	73	90
5	C	187/188 (100%)	182 (97%)	5 (3%)	44	74
6	a	146/147 (99%)	146 (100%)	0	100	100
All	All	1055/1088 (97%)	1035 (98%)	20 (2%)	57	82

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	187	LEU
5	C	150	GLN
5	C	186	LYS
5	C	172	LYS
2	H	209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
2	H	209	ASN
5	C	127	GLN

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 ⓘ

29 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	$\# Z > 2$
7	NAG	D	1	1,7	14,14,15	0.29	0	17,19,21	0.75	1 (5%)
7	NAG	D	2	7	14,14,15	0.39	0	17,19,21	1.05	1 (5%)
7	BMA	D	3	7	11,11,12	2.02	2 (18%)	15,15,17	1.65	3 (20%)
7	MAN	D	4	7	11,11,12	1.29	1 (9%)	15,15,17	1.84	4 (26%)
8	NAG	E	1	1,8	14,14,15	0.22	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	E	2	8	14,14,15	0.31	0	17,19,21	0.63	1 (5%)
9	NAG	F	1	1,9	14,14,15	0.54	0	17,19,21	0.45	0
9	NAG	F	2	9	14,14,15	0.45	0	17,19,21	1.23	1 (5%)
9	FUC	F	3	9	10,10,11	0.80	0	14,14,16	0.79	0
8	NAG	G	1	1,8	14,14,15	0.42	0	17,19,21	0.52	0
8	NAG	G	2	8	14,14,15	0.24	0	17,19,21	0.35	0
10	NAG	I	1	1,10	14,14,15	0.50	0	17,19,21	0.78	0
10	NAG	I	2	10	14,14,15	0.19	0	17,19,21	0.56	0
10	BMA	I	3	10	11,11,12	0.62	0	15,15,17	0.92	0
10	MAN	I	4	10	11,11,12	1.38	2 (18%)	15,15,17	2.50	4 (26%)
10	MAN	I	5	10	11,11,12	1.26	1 (9%)	15,15,17	0.95	0
10	FUC	I	6	10	10,10,11	1.14	1 (10%)	14,14,16	0.82	0
8	NAG	J	1	1,8	14,14,15	0.46	0	17,19,21	0.54	0
8	NAG	J	2	8	14,14,15	0.49	0	17,19,21	1.10	2 (11%)
8	NAG	K	1	1,8	14,14,15	0.39	0	17,19,21	0.68	1 (5%)
8	NAG	K	2	8	14,14,15	0.37	0	17,19,21	0.37	0
8	NAG	M	1	8,6	14,14,15	0.69	1 (7%)	17,19,21	0.78	1 (5%)
8	NAG	M	2	8	14,14,15	0.73	1 (7%)	17,19,21	0.92	1 (5%)
10	NAG	N	1	10,6	14,14,15	0.73	1 (7%)	17,19,21	0.70	0
10	NAG	N	2	10	14,14,15	0.17	0	17,19,21	0.48	0
10	BMA	N	3	10	11,11,12	1.04	1 (9%)	15,15,17	0.95	1 (6%)
10	MAN	N	4	10	11,11,12	1.27	2 (18%)	15,15,17	1.77	2 (13%)
10	MAN	N	5	10	11,11,12	1.27	2 (18%)	15,15,17	1.38	2 (13%)
10	FUC	N	6	10	10,10,11	0.71	0	14,14,16	0.72	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
7	NAG	D	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	2	7	-	0/6/23/26	0/1/1/1
7	BMA	D	3	7	-	2/2/19/22	0/1/1/1
7	MAN	D	4	7	-	0/2/19/22	0/1/1/1
8	NAG	E	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	2	8	-	2/6/23/26	0/1/1/1
9	NAG	F	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	FUC	F	3	9	-	-	0/1/1/1
8	NAG	G	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	G	2	8	-	4/6/23/26	0/1/1/1
10	NAG	I	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
10	BMA	I	3	10	-	1/2/19/22	0/1/1/1
10	MAN	I	4	10	-	1/2/19/22	0/1/1/1
10	MAN	I	5	10	-	0/2/19/22	0/1/1/1
10	FUC	I	6	10	-	-	0/1/1/1
8	NAG	J	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	2/6/23/26	0/1/1/1
8	NAG	K	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	1/6/23/26	0/1/1/1
8	NAG	M	1	8,6	-	2/6/23/26	0/1/1/1
8	NAG	M	2	8	-	4/6/23/26	0/1/1/1
10	NAG	N	1	10,6	-	1/6/23/26	0/1/1/1
10	NAG	N	2	10	-	0/6/23/26	0/1/1/1
10	BMA	N	3	10	-	0/2/19/22	0/1/1/1
10	MAN	N	4	10	-	1/2/19/22	0/1/1/1
10	MAN	N	5	10	-	0/2/19/22	1/1/1/1
10	FUC	N	6	10	-	-	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	3	BMA	C1-C2	6.03	1.66	1.52
7	D	4	MAN	C1-C2	3.13	1.59	1.52
10	N	4	MAN	C1-C2	2.84	1.58	1.52
10	N	5	MAN	C1-C2	2.81	1.58	1.52
10	I	4	MAN	O5-C1	2.73	1.48	1.43

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	4	MAN	C1-O5-C5	7.02	121.71	112.19
10	N	4	MAN	C1-O5-C5	5.73	119.95	112.19
10	I	4	MAN	O5-C1-C2	5.00	118.48	110.77
7	D	4	MAN	C1-O5-C5	4.62	118.45	112.19
9	F	2	NAG	C2-N2-C7	4.33	129.07	122.90

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	2	NAG	O5-C5-C6-O6
7	D	3	BMA	O5-C5-C6-O6
8	J	2	NAG	O5-C5-C6-O6
8	M	2	NAG	C4-C5-C6-O6
8	G	2	NAG	O5-C5-C6-O6

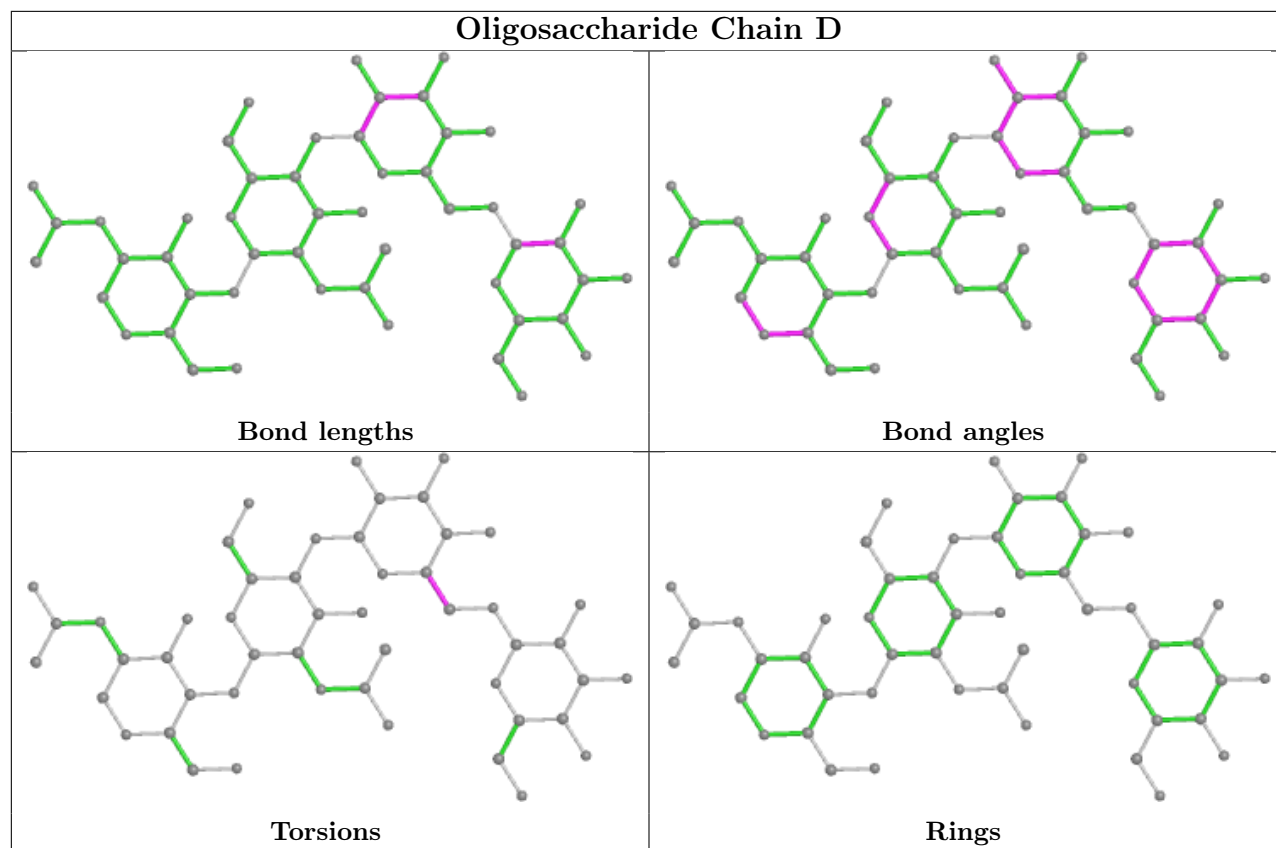
All (1) ring outliers are listed below:

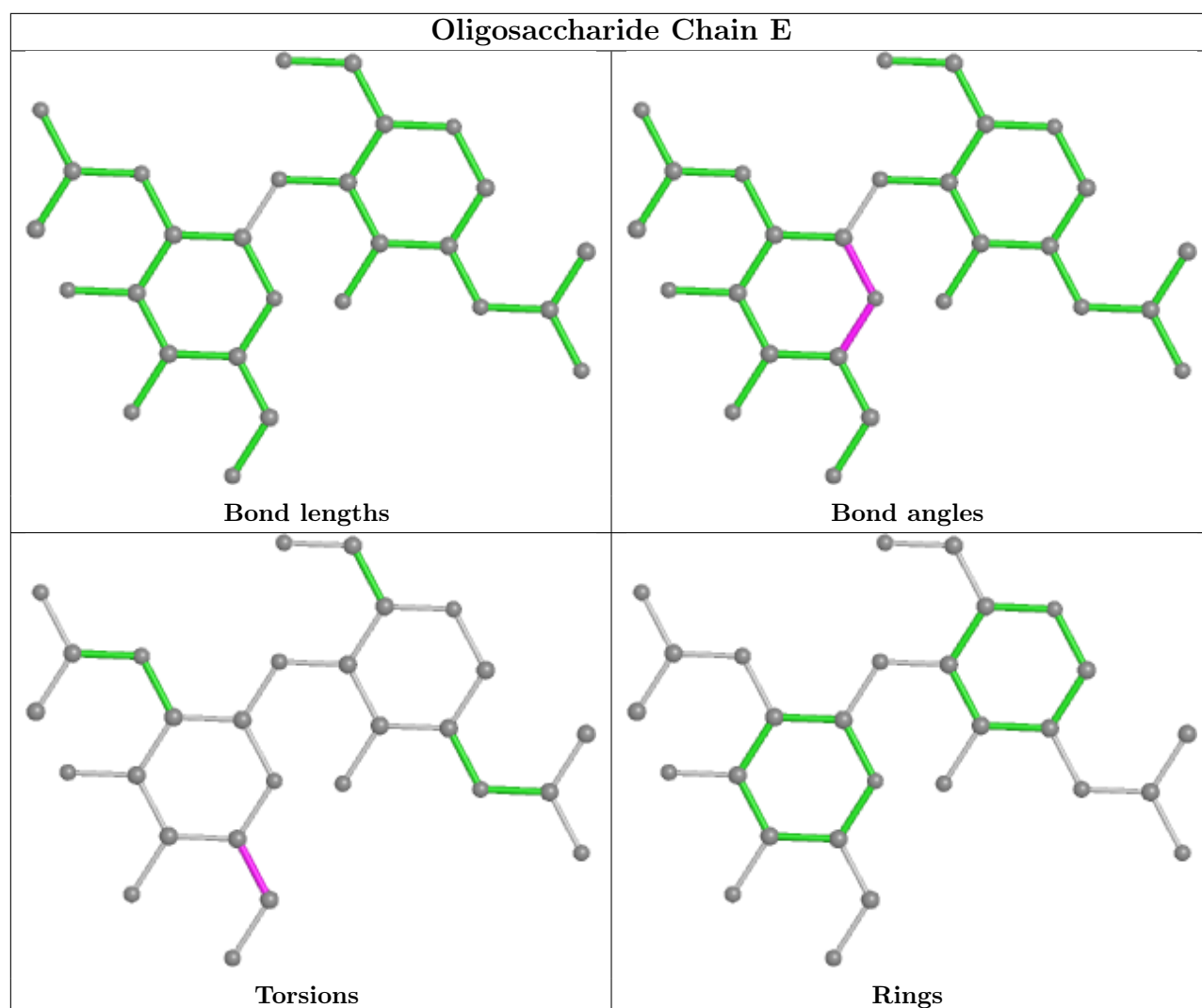
Mol	Chain	Res	Type	Atoms
10	N	5	MAN	C1-C2-C3-C4-C5-O5

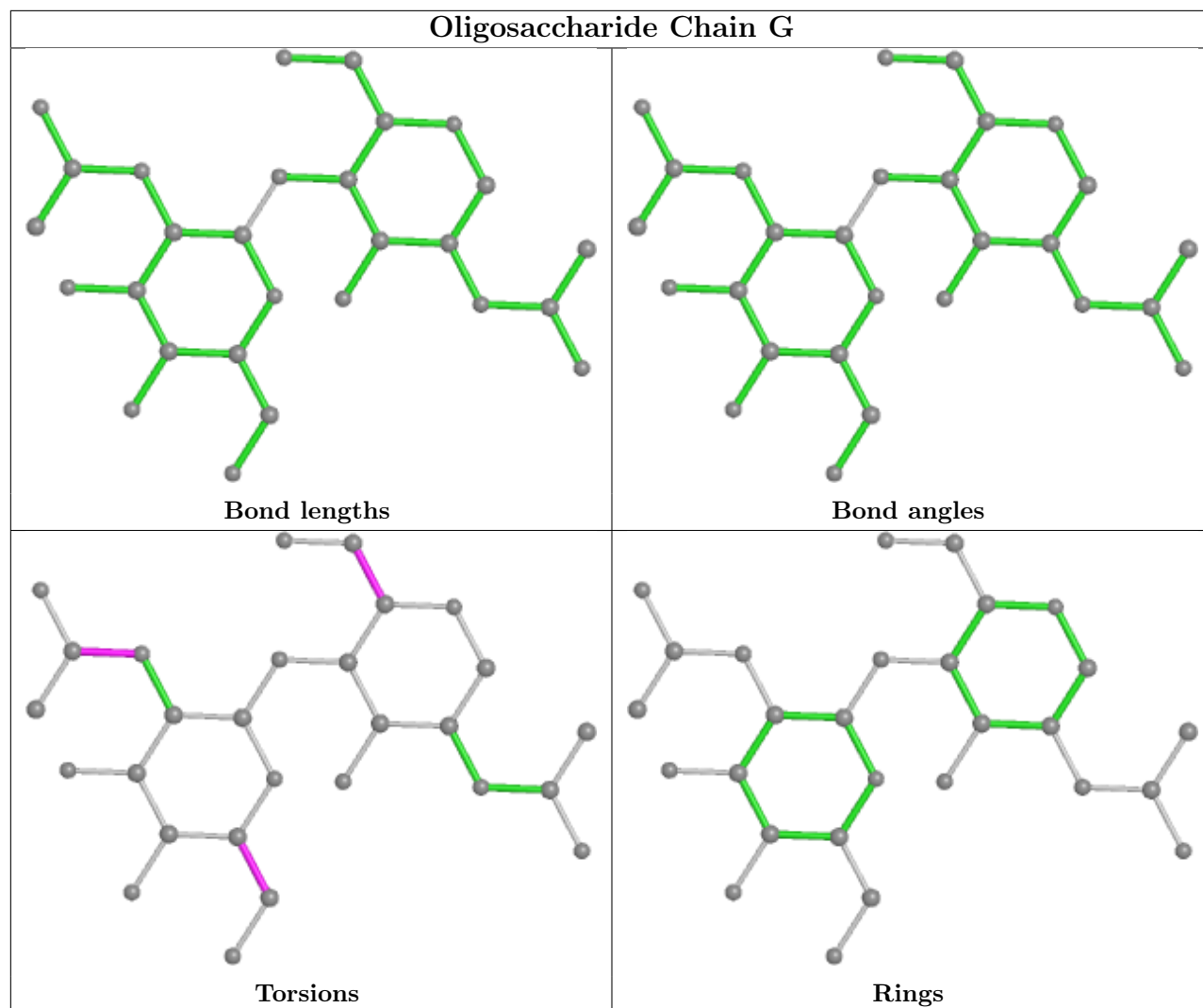
4 monomers are involved in 3 short contacts:

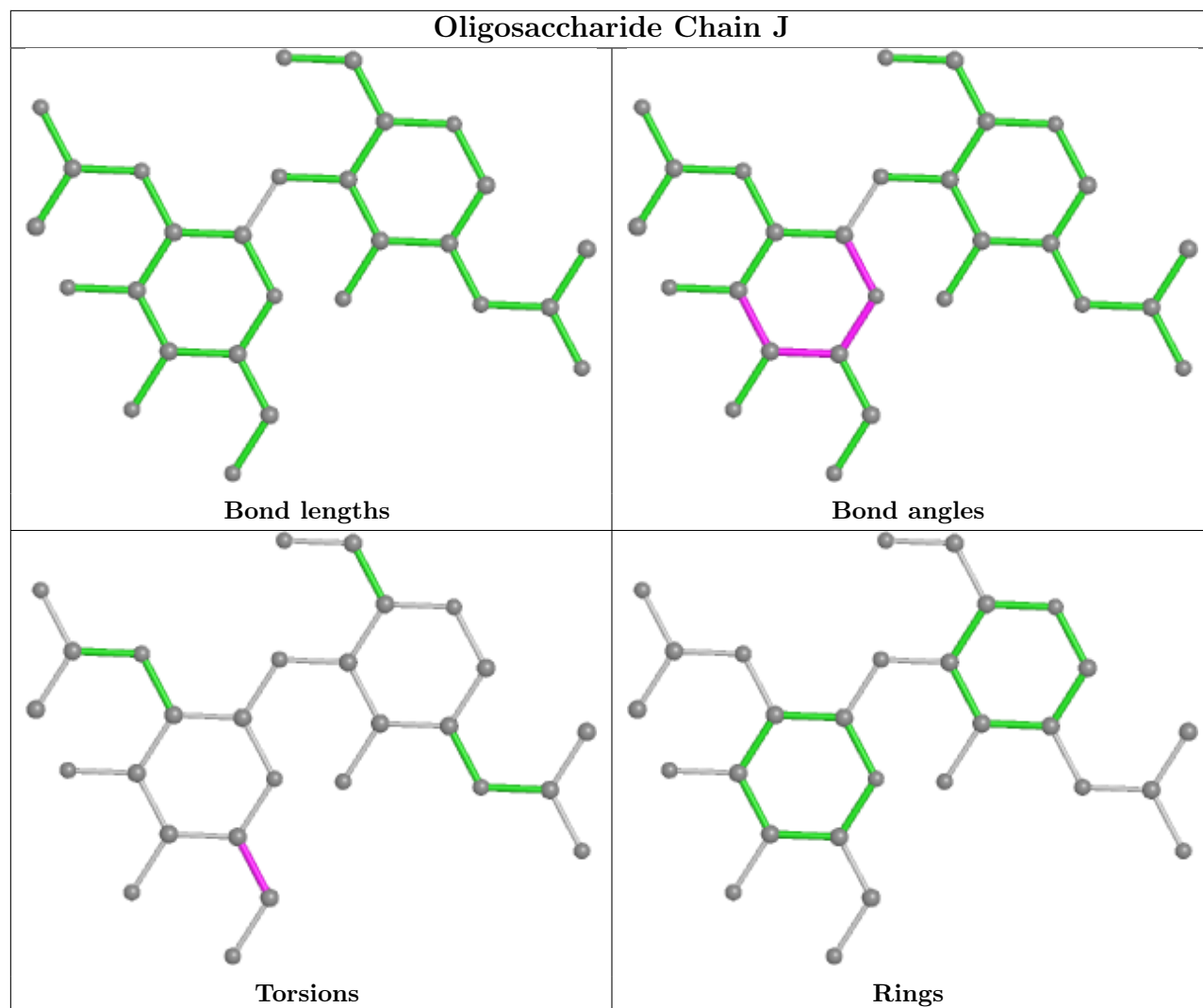
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	2	NAG	1	0
7	D	4	MAN	1	0
7	D	2	NAG	1	0
7	D	3	BMA	2	0

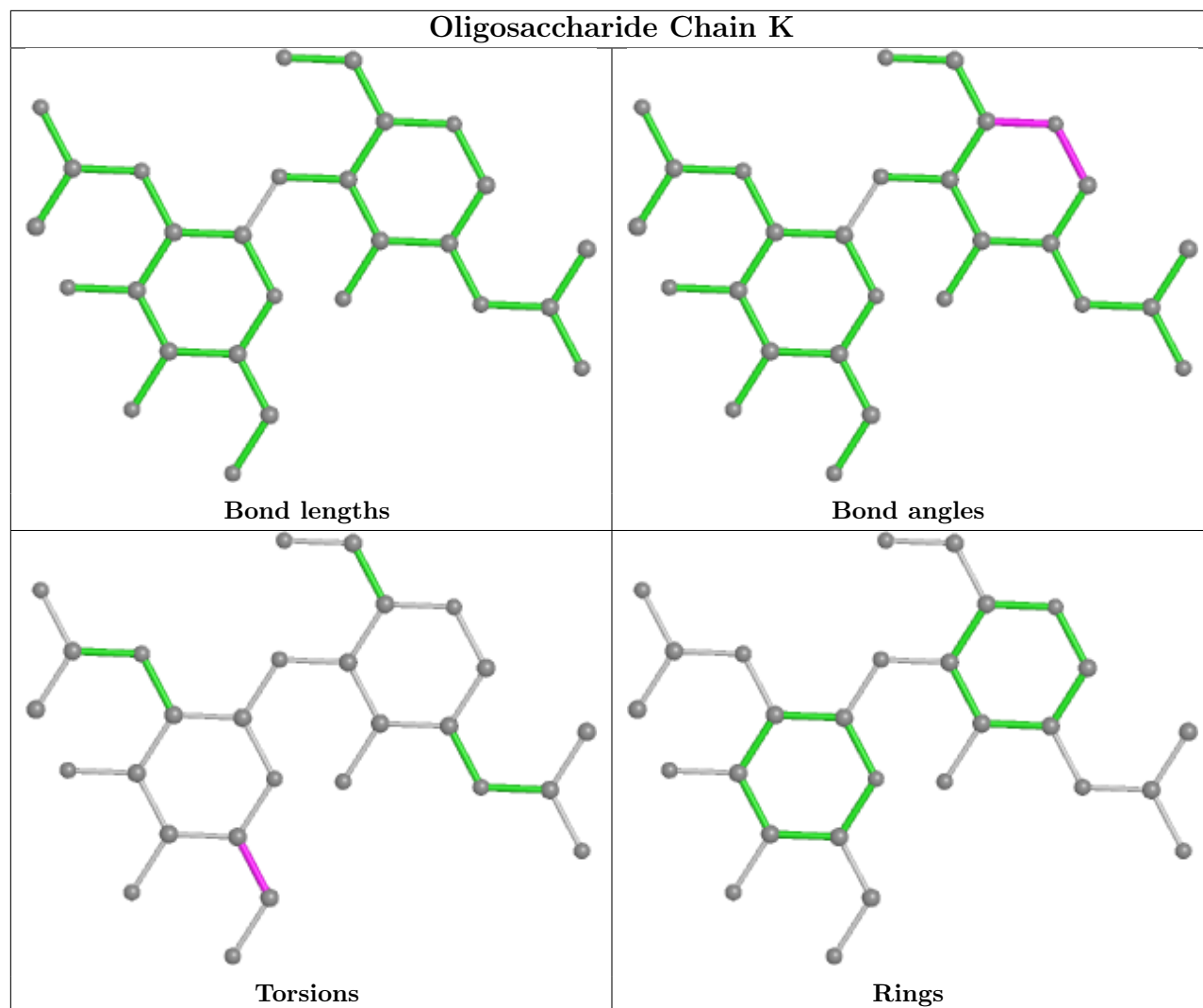
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

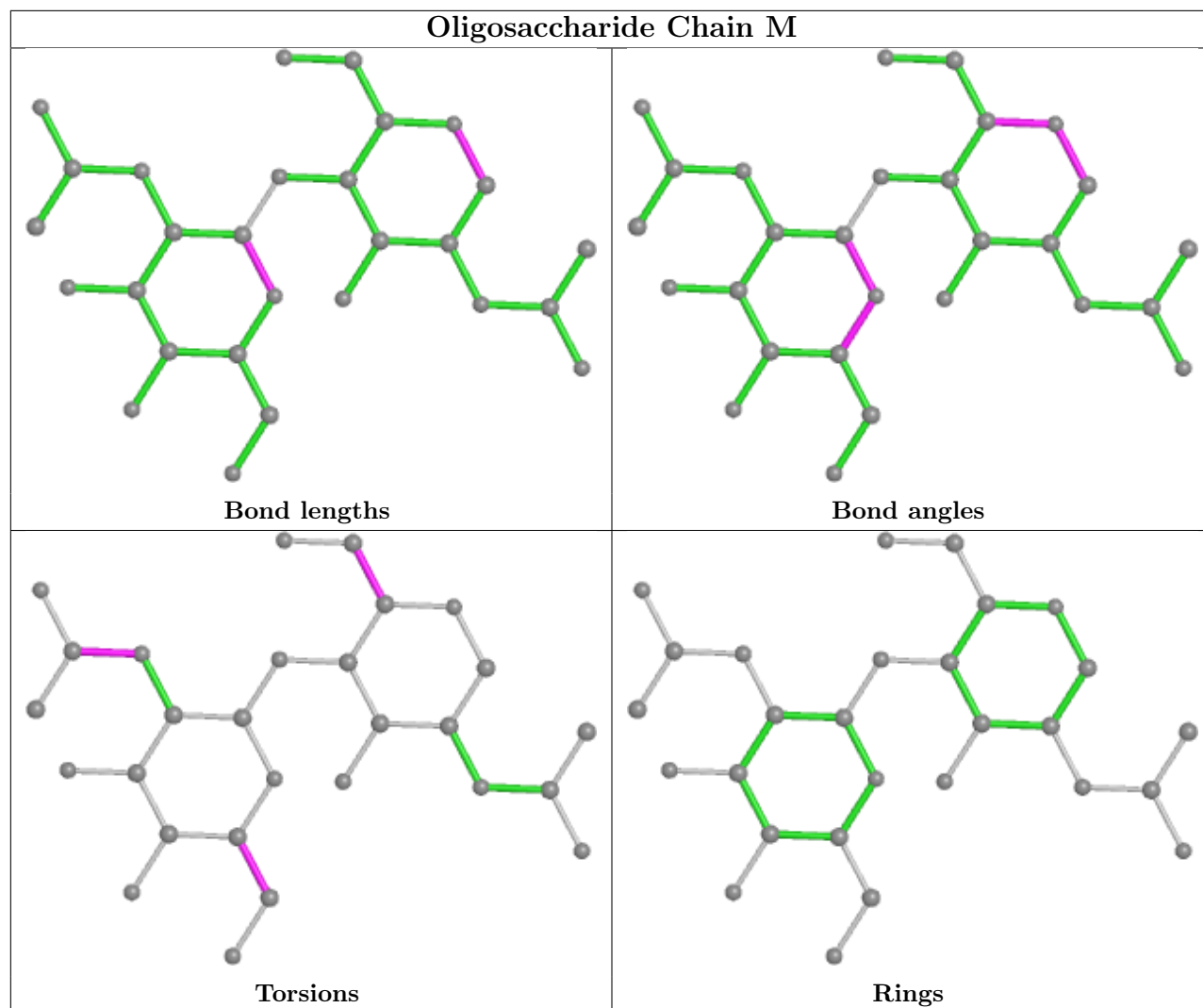


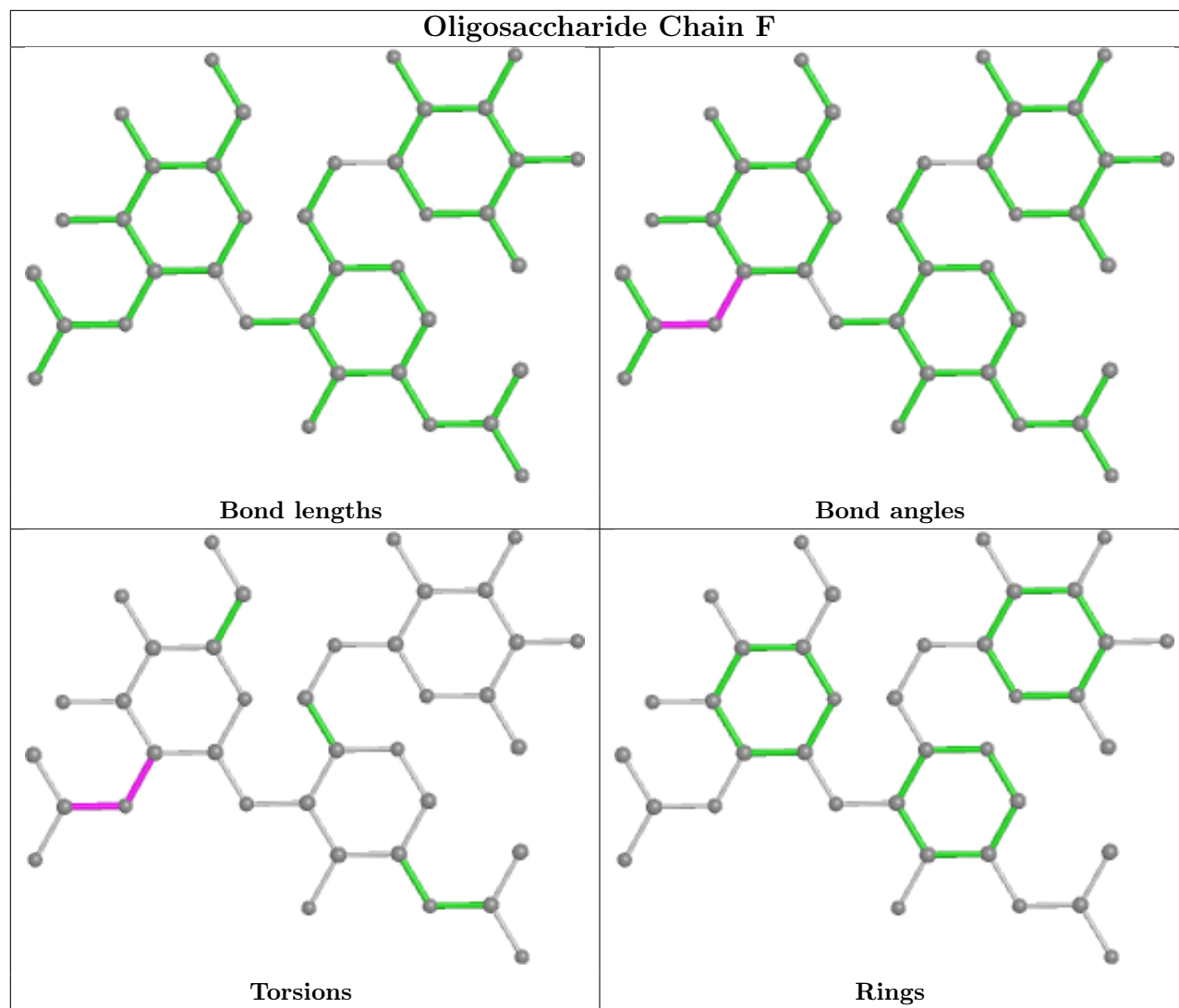


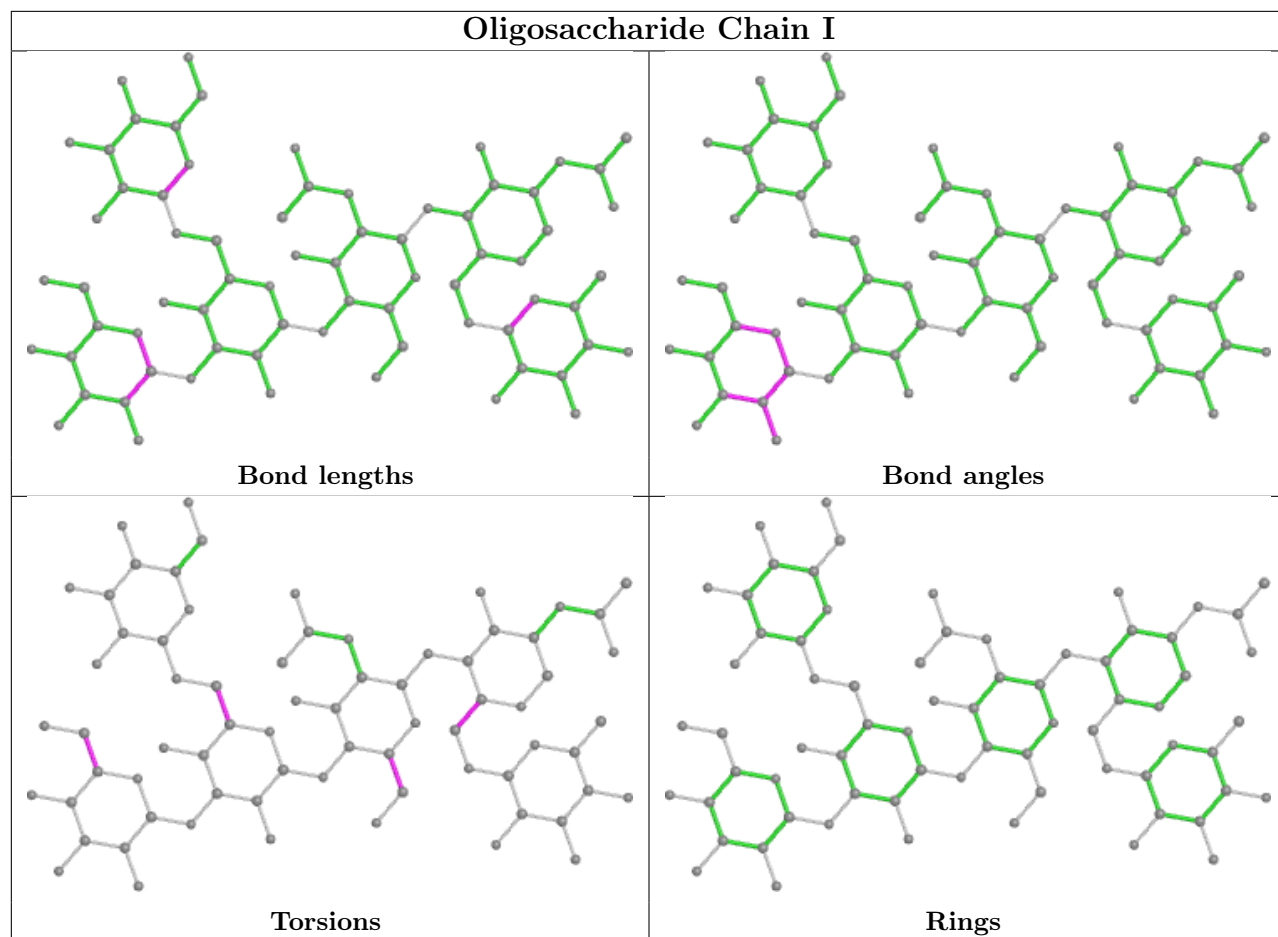


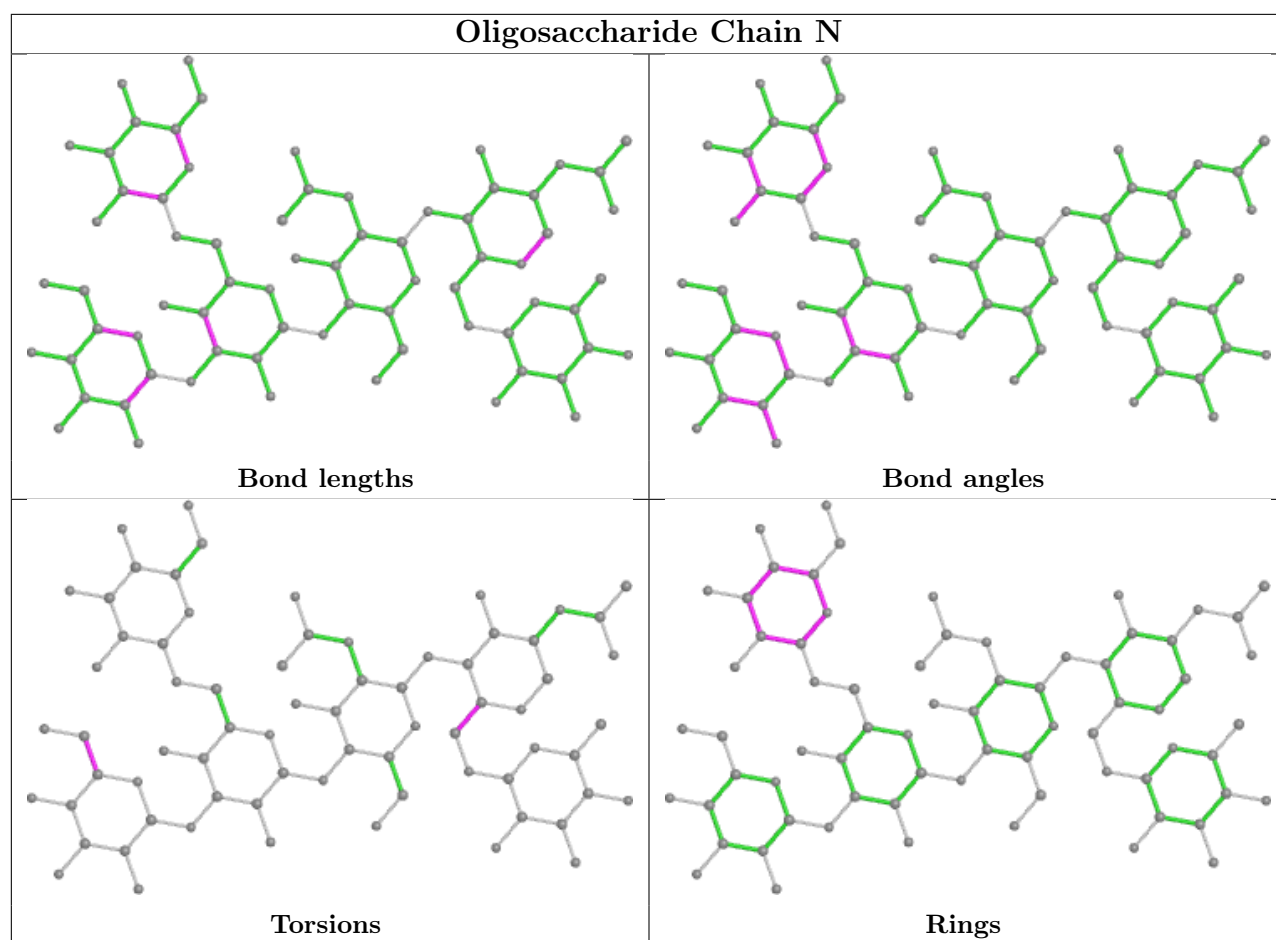












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
11	NAG	a	501	6	14,14,15	0.41	0	17,19,21	1.28	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
11	NAG	a	501	6	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	501	NAG	C2-N2-C7	4.44	129.23	122.90
11	a	501	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

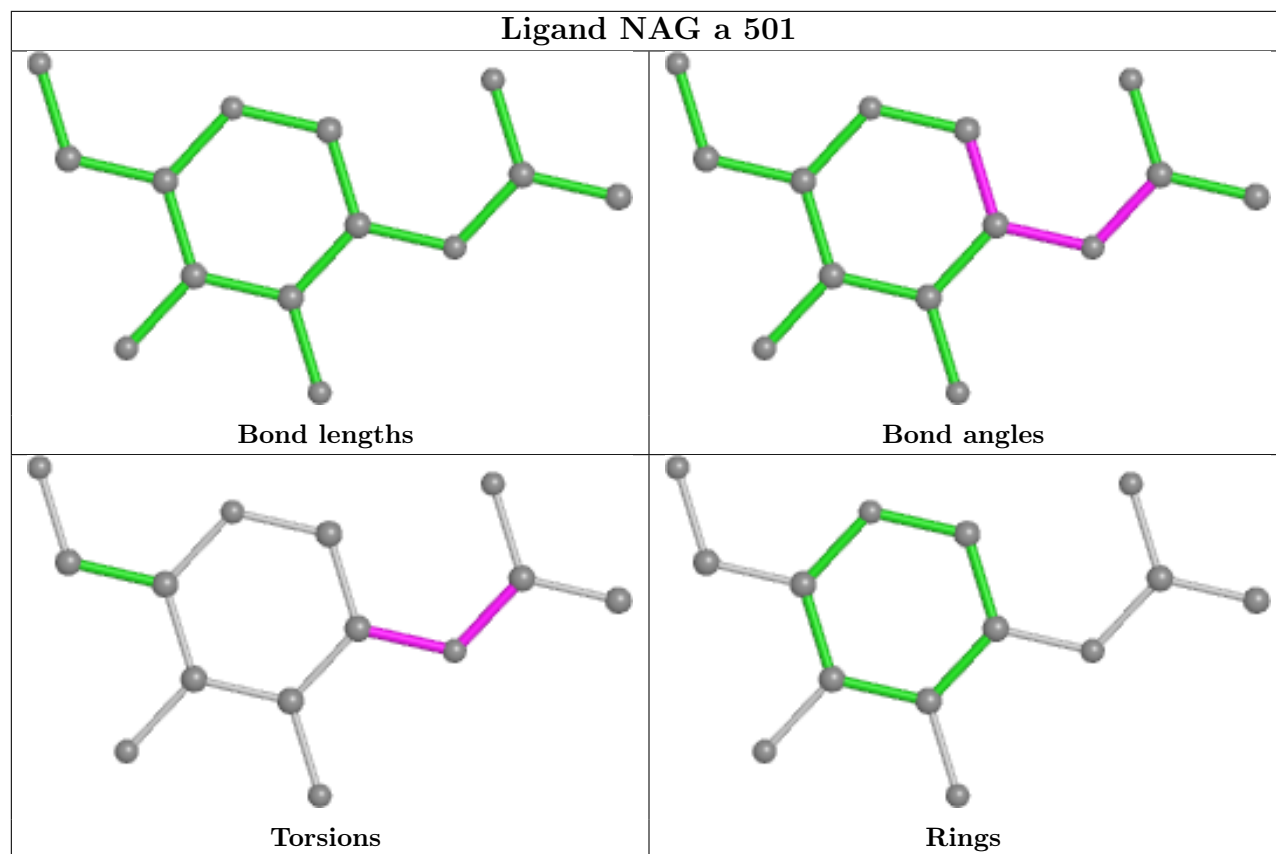
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	a	501	NAG	C8-C7-N2-C2
11	a	501	NAG	O7-C7-N2-C2
11	a	501	NAG	C3-C2-N2-C7

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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	186/201 (92%)	0.05	3 (1%) 72 74	41, 60, 99, 140	0
2	H	219/228 (96%)	-0.26	1 (0%) 91 92	42, 63, 112, 141	0
3	L	214/217 (98%)	-0.17	0 100 100	46, 77, 113, 131	0
4	B	218/229 (95%)	0.24	10 (4%) 32 31	52, 98, 143, 183	0
5	C	215/216 (99%)	0.08	7 (3%) 46 46	64, 91, 135, 167	0
6	a	163/165 (98%)	0.13	1 (0%) 89 91	37, 54, 100, 141	0
All	All	1215/1256 (96%)	0.01	22 (1%) 68 70	37, 74, 129, 183	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	203	THR	3.5
6	a	260	GLY	3.3
4	B	150	LEU	3.2
4	B	224	GLU	3.1
5	C	212	PHE	3.0

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](#)

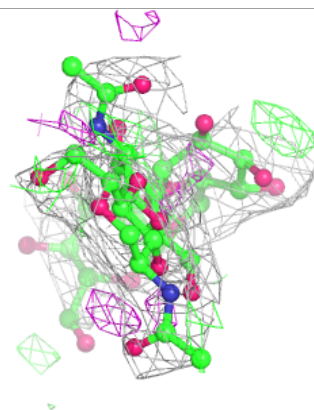
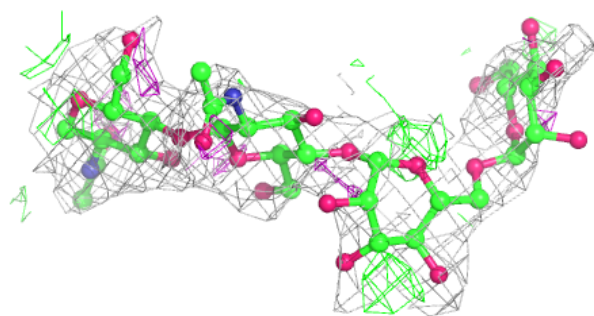
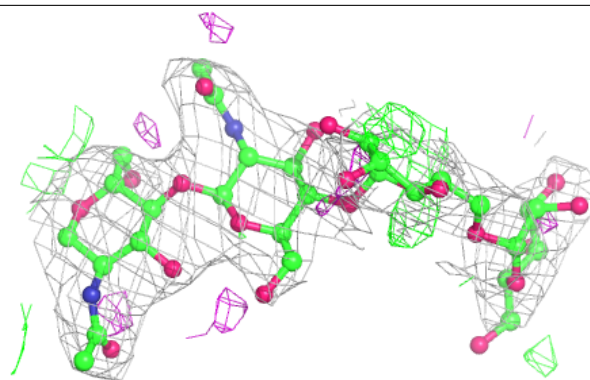
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	MAN	N	5	11/12	0.34	0.37	97,131,160,164	0
10	MAN	N	4	11/12	0.65	0.39	108,152,162,165	0
10	BMA	N	3	11/12	0.72	0.33	132,146,162,168	0
7	BMA	D	3	11/12	0.73	0.23	110,133,143,145	0
10	MAN	I	4	11/12	0.78	0.34	126,146,156,159	0
10	MAN	I	5	11/12	0.79	0.52	128,152,166,171	0
7	MAN	D	4	11/12	0.81	0.34	137,150,159,160	0
9	NAG	F	2	14/15	0.83	0.16	114,136,148,148	0
8	NAG	K	2	14/15	0.87	0.23	72,117,123,124	0
8	NAG	M	2	14/15	0.87	0.21	98,129,134,135	0
10	BMA	I	3	11/12	0.88	0.18	127,134,151,154	0
8	NAG	G	2	14/15	0.89	0.33	107,114,135,137	0
7	NAG	D	2	14/15	0.89	0.20	81,109,138,141	0
10	FUC	I	6	10/11	0.90	0.26	98,122,142,144	0
8	NAG	J	2	14/15	0.91	0.21	102,120,126,135	0
10	NAG	I	2	14/15	0.91	0.18	89,108,127,145	0
10	NAG	N	2	14/15	0.91	0.18	81,109,125,137	0
8	NAG	E	2	14/15	0.92	0.14	75,94,116,123	0
9	NAG	F	1	14/15	0.92	0.13	70,92,125,137	0
9	FUC	F	3	10/11	0.93	0.16	112,139,143,144	0
8	NAG	K	1	14/15	0.93	0.12	68,79,101,115	0
10	FUC	N	6	10/11	0.93	0.13	65,103,110,110	0
8	NAG	J	1	14/15	0.94	0.14	59,79,97,109	0
7	NAG	D	1	14/15	0.94	0.18	53,68,86,91	0
8	NAG	M	1	14/15	0.95	0.15	58,76,103,113	0
10	NAG	I	1	14/15	0.95	0.12	66,92,107,118	0
10	NAG	N	1	14/15	0.96	0.14	51,69,89,96	0
8	NAG	G	1	14/15	0.97	0.18	67,82,101,109	0
8	NAG	E	1	14/15	0.98	0.11	64,74,89,91	0

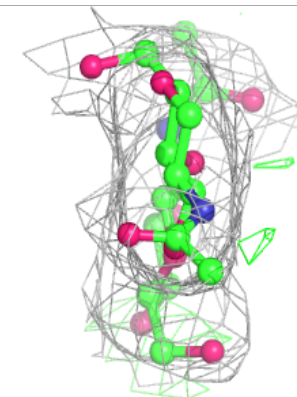
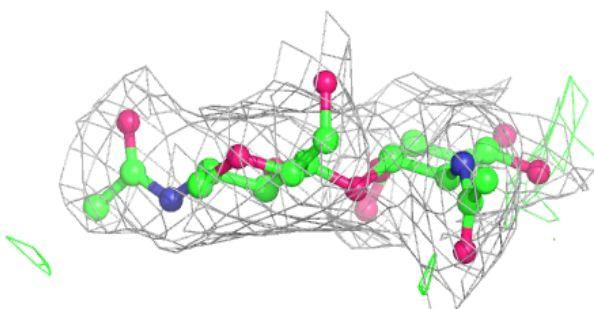
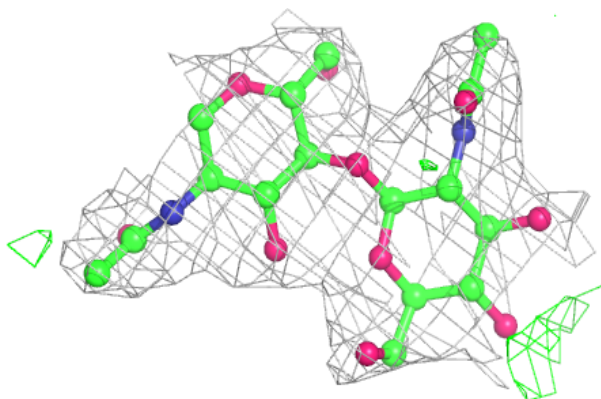
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

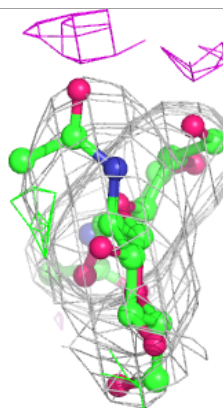
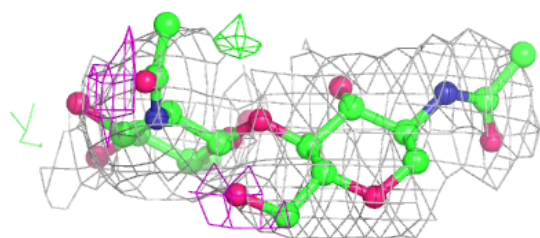
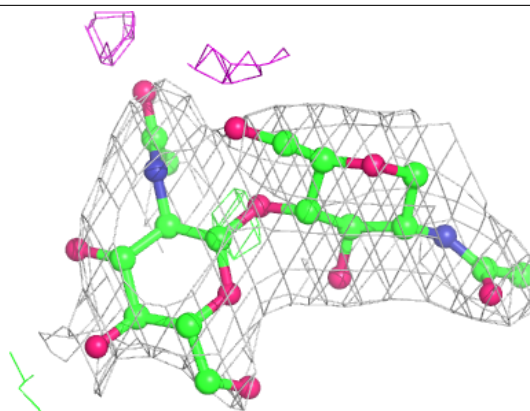
**Electron density around Chain E:**

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and green (positive)

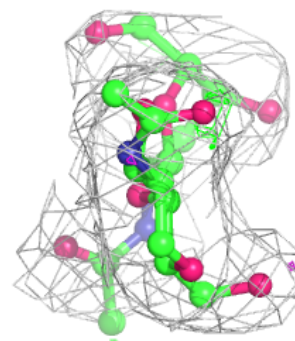
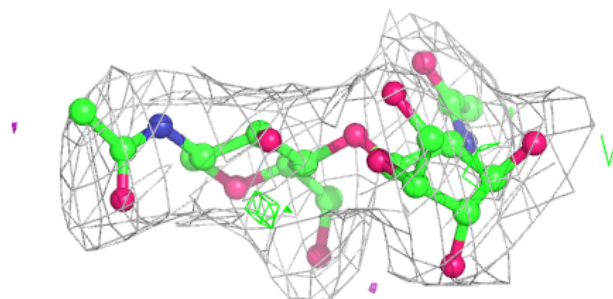
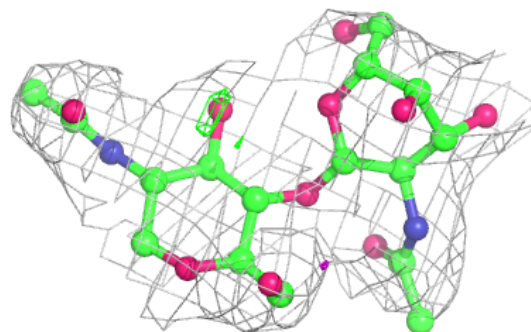


Electron density around Chain G:

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

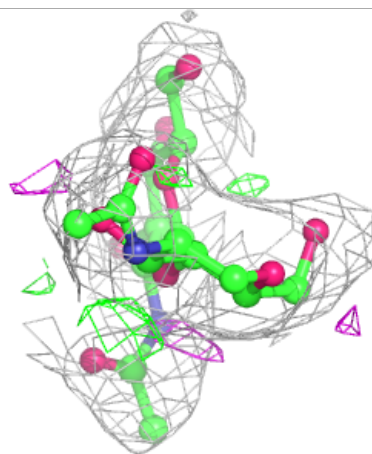
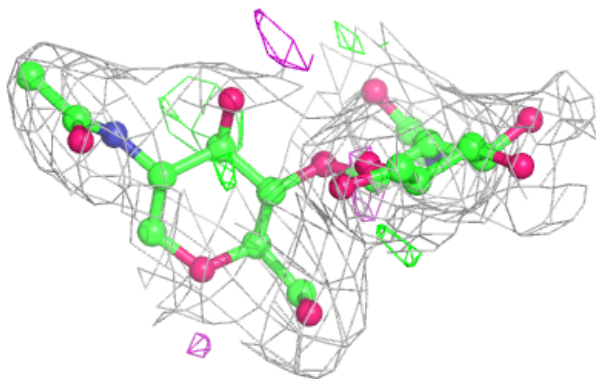
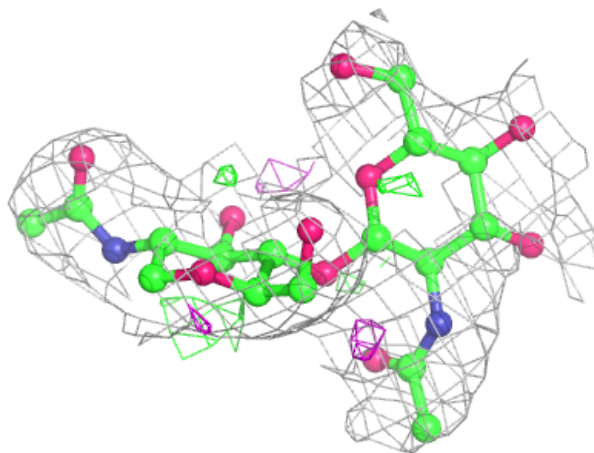
**Electron density around Chain J:**

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and green (positive)



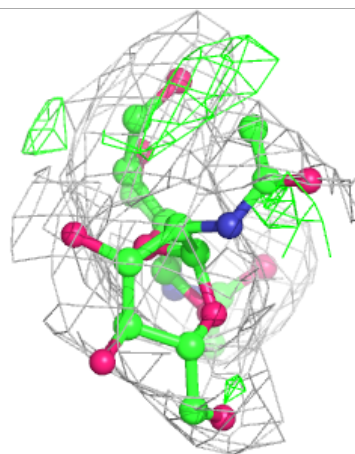
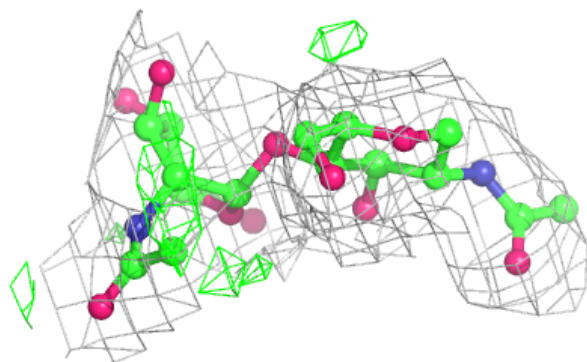
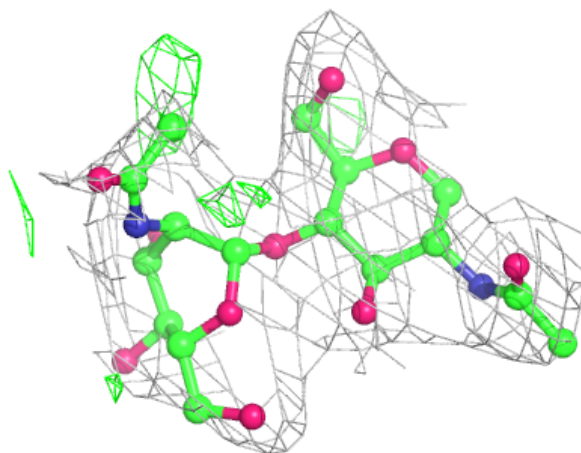
Electron density around Chain K:

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and green (positive)



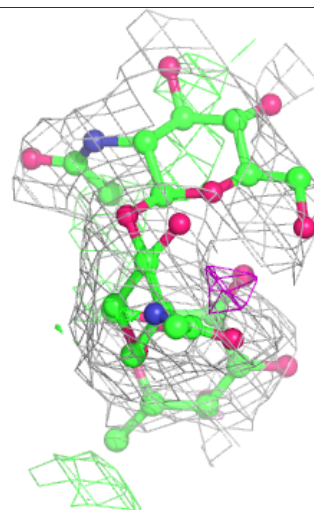
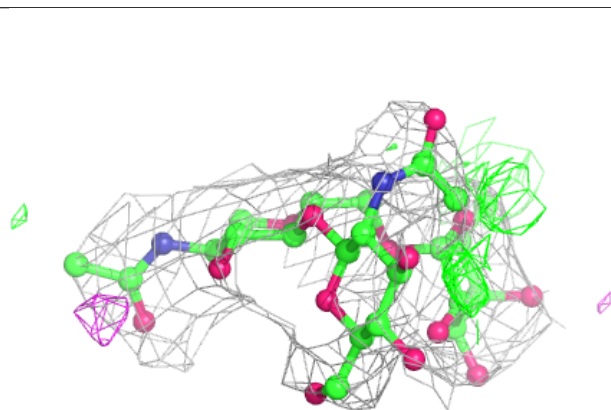
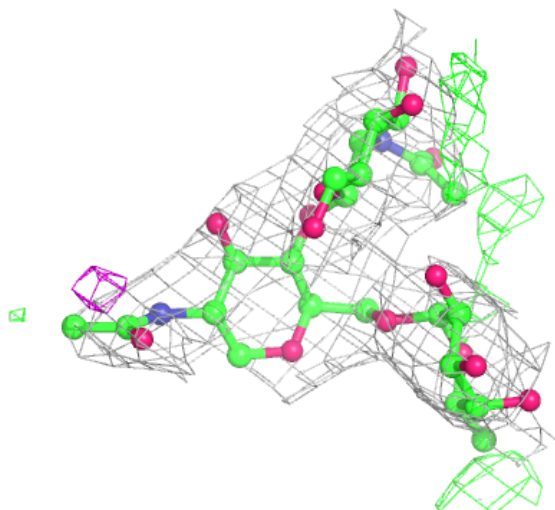
Electron density around Chain M:

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



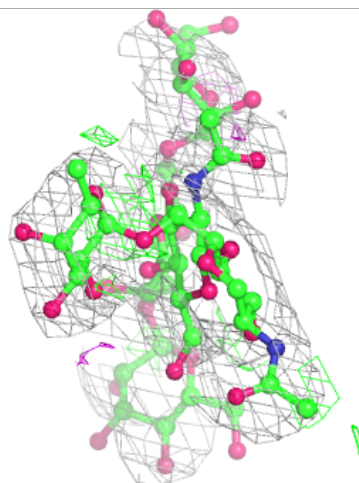
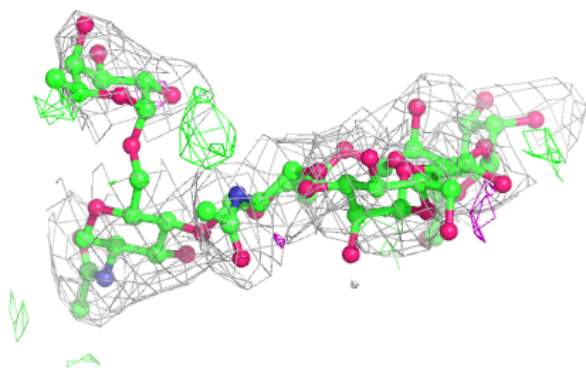
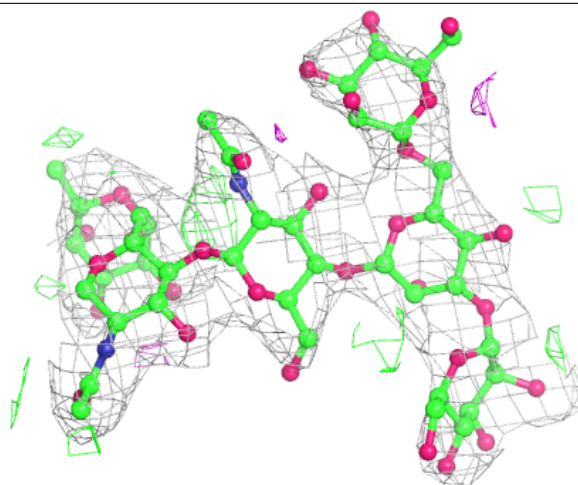
Electron density around Chain F:

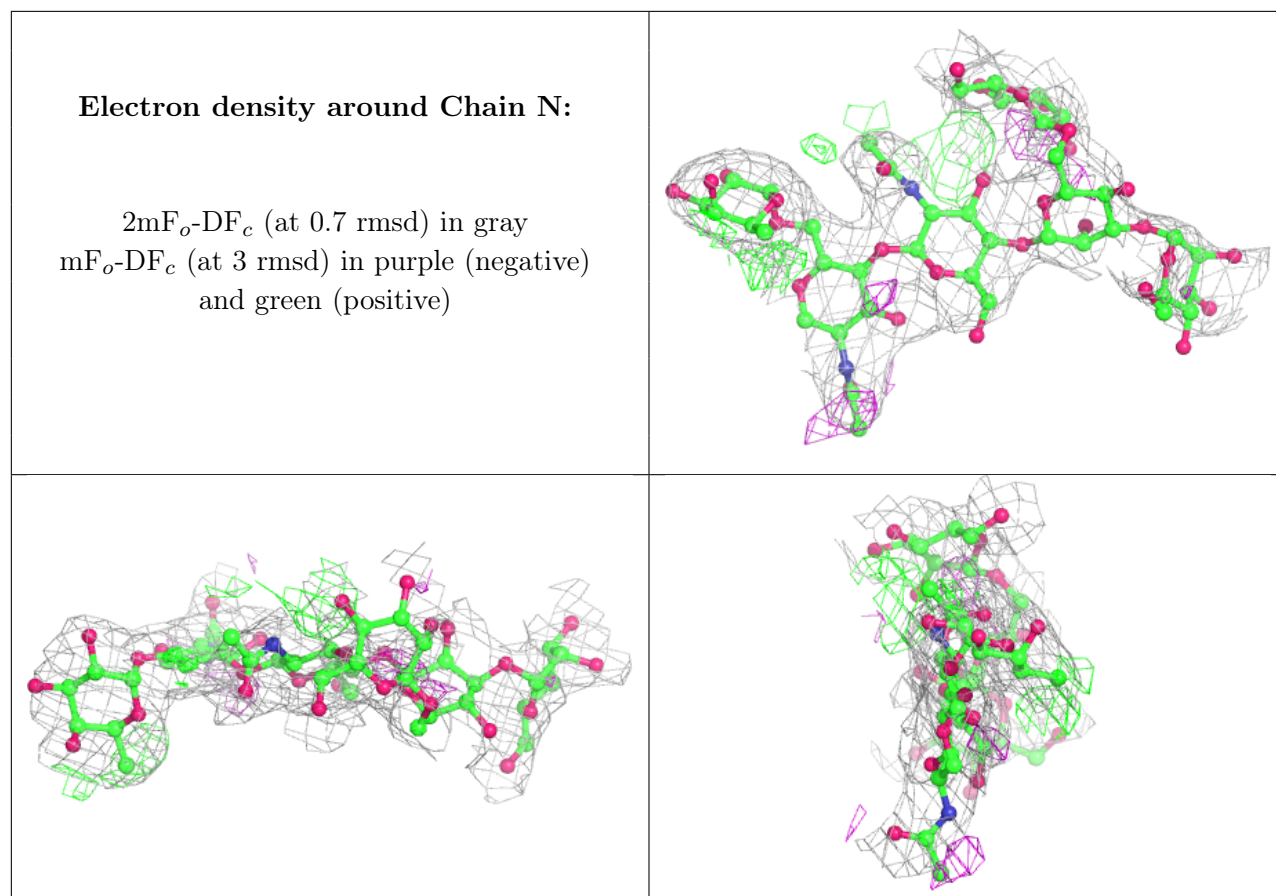
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain I:

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





6.4 Ligands [i](#)

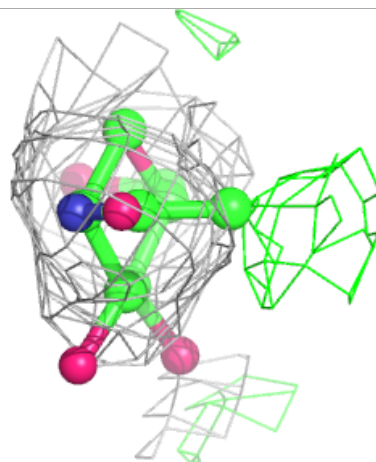
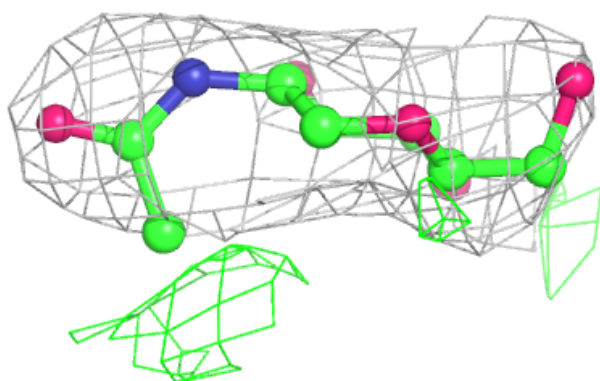
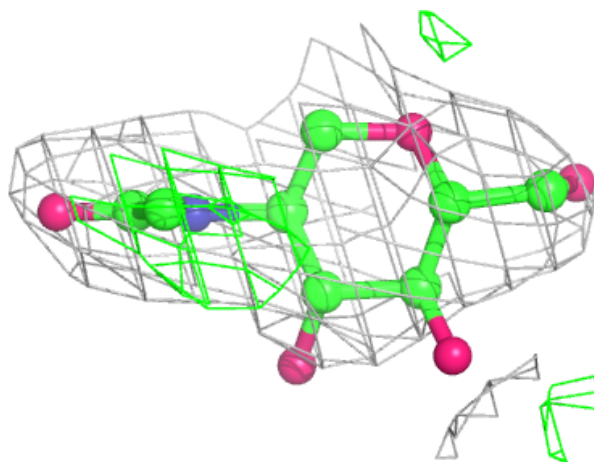
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	NAG	a	501	14/15	0.87	0.20	88,119,138,140	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG a 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.