



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 09:13 PM UTC

PDB ID : 9MHX / pdb_00009mhx
Title : Human TLR8 ectodomain with small molecule agonist 7
Authors : Critton, D.A.
Deposited on : 2024-12-12
Resolution : 2.13 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

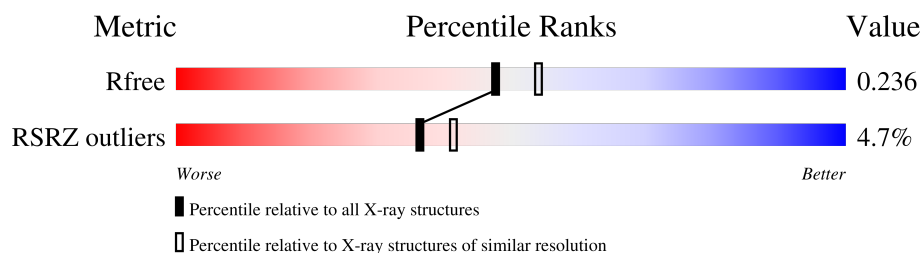
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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	3689 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25530 atoms, of which 12215 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	748	Total	C	H	N	O	S	5811	2	0
			11741	3799	5811	1001	1111	19			
1	B	741	Total	C	H	N	O	S	5737	1	0
			11594	3757	5737	985	1096	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(2-6)]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
2	C	5	Total	C	H	N	O	52	0	0
			113	34	52	2	25			
2	F	5	Total	C	H	N	O	52	0	0
			113	34	52	2	25			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyran

ose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	5	Total	C	H	N	O	53	0	0
			114	34	53	2	25			

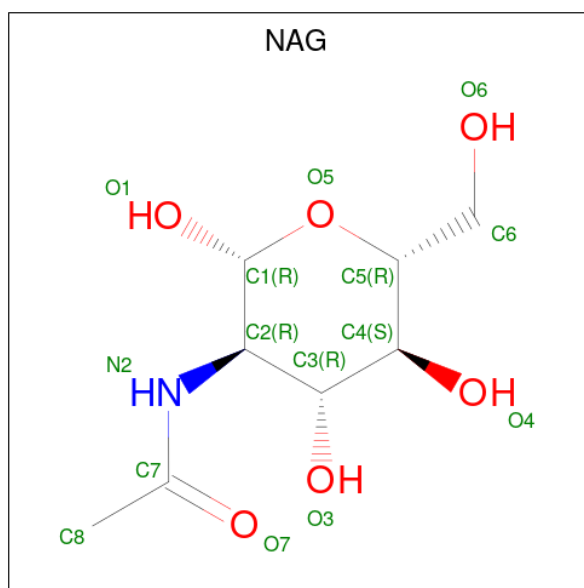
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	5	Total	C	H	N	O	52	0	0
			113	34	52	2	25			
4	G	5	Total	C	H	N	O	52	0	0
			113	34	52	2	25			

- Molecule 5 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.

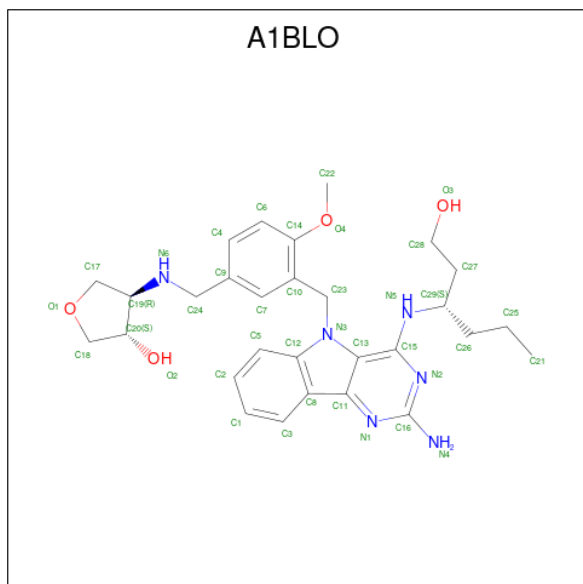
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	4	Total	C	H	N	O	44	0	0
			94	28	44	2	20			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
6	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		

- Molecule 7 is (3S,4R)-4-[(3-[(2-amino-4-[(3S)-1-hydroxyhexan-3-yl]amino}-5H-pyrimido[5,4-b]indol-5-yl)methyl]-4-methoxyphenyl)methyl]amino]oxolan-3-ol (CCD ID: A1BLO) (formula: C₂₉H₃₈N₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	38	0
			77	29	38	6	4		
7	B	1	Total	C	H	N	O	38	0
			77	29	38	6	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	412	Total	O	0	0
			412	412		
8	B	375	Total	O	0	0
			375	375		

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	86.24Å 86.24Å 217.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.92 – 2.13 19.92 – 2.13	Depositor EDS
% Data completeness (in resolution range)	86.8 (19.92-2.13) 86.7 (19.92-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.13Å)	Xtriage
Refinement program	BUSTER 2.11.8 (20-APR-2021)	Depositor
R, R_{free}	0.220 , 0.242 0.212 , 0.236	Depositor DCC
R_{free} test set	4367 reflections (4.33%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,l 0.034 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25530	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

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
2	NAG	C	1	2,1	14,14,15	0.38	0	17,19,21	0.79	0
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	0.69	1 (5%)
2	BMA	C	3	2	11,11,12	0.21	0	15,15,17	0.44	0
2	MAN	C	4	2	11,11,12	0.26	0	15,15,17	0.58	0
2	MAN	C	5	2	11,11,12	0.24	0	13,15,17	0.43	0
3	NAG	D	1	3,1	14,14,15	0.26	0	17,19,21	0.71	0
3	NAG	D	2	3	14,14,15	0.27	0	17,19,21	0.49	0
3	BMA	D	3	3	11,11,12	0.23	0	15,15,17	0.55	0
3	MAN	D	4	3	11,11,12	0.51	0	15,15,17	2.30	3 (20%)
3	MAN	D	5	3	11,11,12	0.23	0	15,15,17	0.63	1 (6%)
4	NAG	E	1	4,1	14,14,15	0.41	0	17,19,21	0.62	0
4	NAG	E	2	4	14,14,15	0.26	0	17,19,21	0.49	0
4	BMA	E	3	4	11,11,12	0.24	0	15,15,17	0.71	0
4	MAN	E	4	4	11,11,12	0.30	0	15,15,17	0.66	1 (6%)
4	MAN	E	5	4	11,11,12	0.47	0	15,15,17	1.66	2 (13%)
2	NAG	F	1	2,1	14,14,15	0.33	0	17,19,21	0.82	1 (5%)
2	NAG	F	2	2	14,14,15	0.32	0	17,19,21	0.73	1 (5%)
2	BMA	F	3	2	11,11,12	0.24	0	15,15,17	0.45	0
2	MAN	F	4	2	11,11,12	0.25	0	15,15,17	0.58	0
2	MAN	F	5	2	11,11,12	0.26	0	13,15,17	0.45	0
4	NAG	G	1	4,1	14,14,15	0.24	0	17,19,21	0.68	0
4	NAG	G	2	4	14,14,15	0.26	0	17,19,21	0.52	0
4	BMA	G	3	4	11,11,12	0.25	0	15,15,17	0.41	0
4	MAN	G	4	4	11,11,12	0.20	0	15,15,17	0.58	1 (6%)
4	MAN	G	5	4	11,11,12	0.71	0	15,15,17	2.05	4 (26%)
5	NAG	H	1	5,1	14,14,15	0.41	0	17,19,21	0.60	0
5	NAG	H	2	5	14,14,15	0.24	0	17,19,21	0.51	0
5	BMA	H	3	5	11,11,12	0.24	0	15,15,17	0.50	0
5	MAN	H	4	5	11,11,12	0.39	0	15,15,17	1.76	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	C	5	2	-	0/2/18/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
2	MAN	F	5	2	-	0/2/18/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	1/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	C1-O5-C5	6.11	120.37	112.19
5	H	4	MAN	O2-C2-C3	5.70	121.96	110.15
4	G	5	MAN	C1-O5-C5	5.56	119.63	112.19
4	E	5	MAN	O2-C2-C3	4.83	120.15	110.15
3	D	4	MAN	O2-C2-C3	4.52	119.51	110.15
4	G	5	MAN	O2-C2-C3	3.50	117.41	110.15
3	D	4	MAN	C1-C2-C3	3.50	114.74	109.64
4	G	5	MAN	C1-C2-C3	3.08	114.14	109.64
4	E	5	MAN	C1-C2-C3	2.69	113.56	109.64
2	F	2	NAG	O5-C1-C2	-2.61	107.26	111.29
2	C	2	NAG	O5-C1-C2	-2.43	107.53	111.29
5	H	4	MAN	O2-C2-C1	2.41	114.74	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5	MAN	O2-C2-C1	2.29	114.46	109.22
5	H	4	MAN	C1-O5-C5	2.22	115.17	112.19
3	D	5	MAN	C1-O5-C5	2.05	114.94	112.19
2	F	1	NAG	O5-C1-C2	-2.04	108.13	111.29
4	G	4	MAN	C1-O5-C5	2.04	114.92	112.19
4	E	4	MAN	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

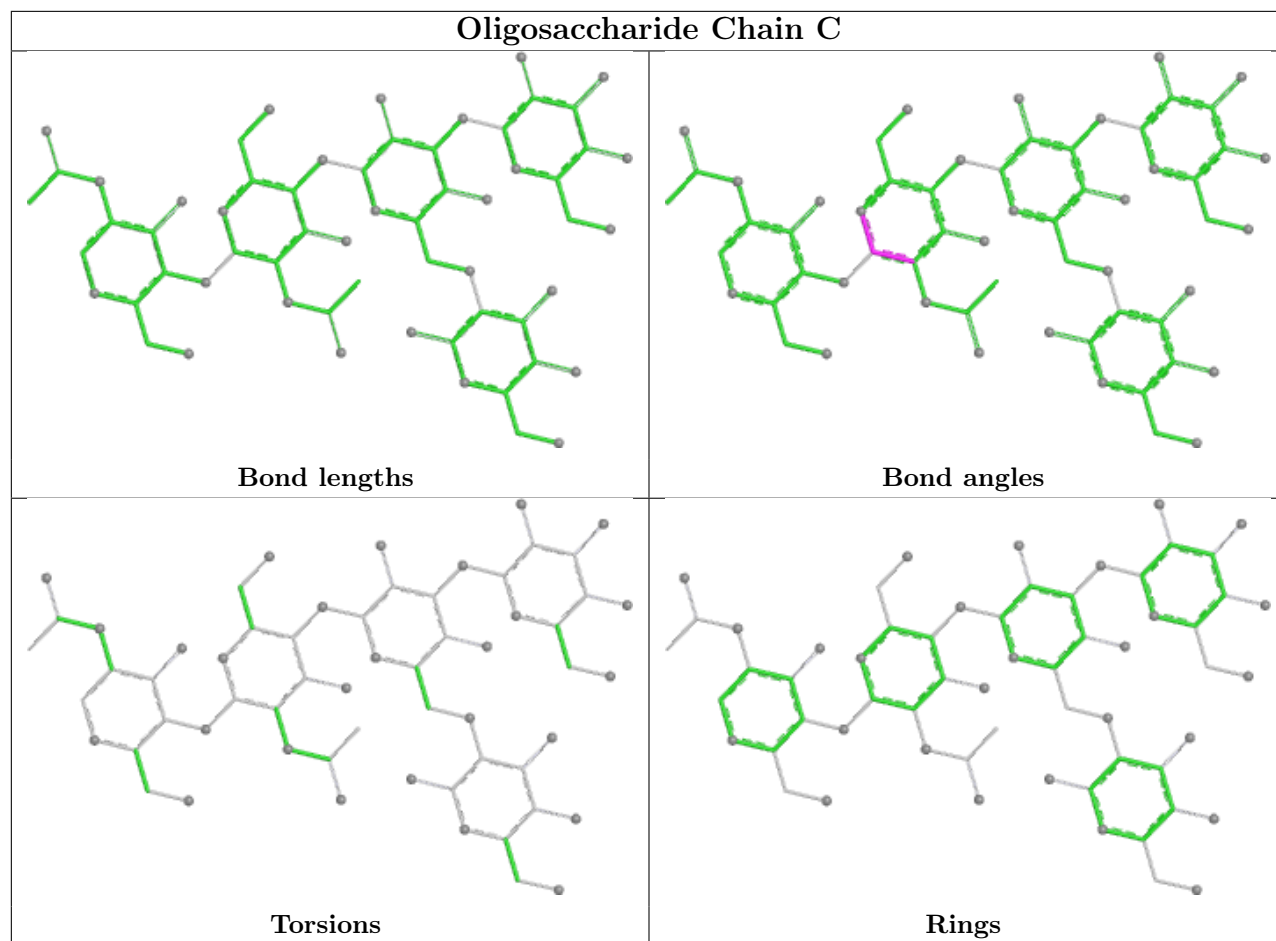
Mol	Chain	Res	Type	Atoms
3	D	3	BMA	C4-C5-C6-O6

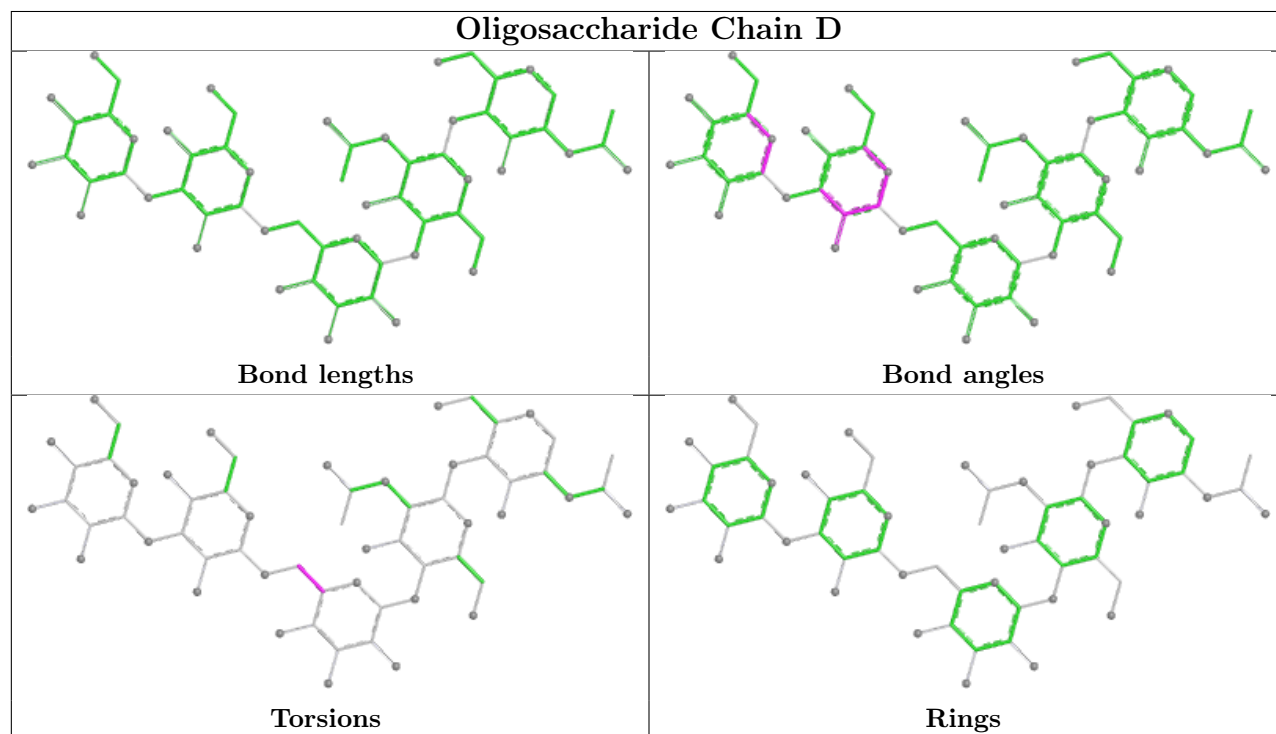
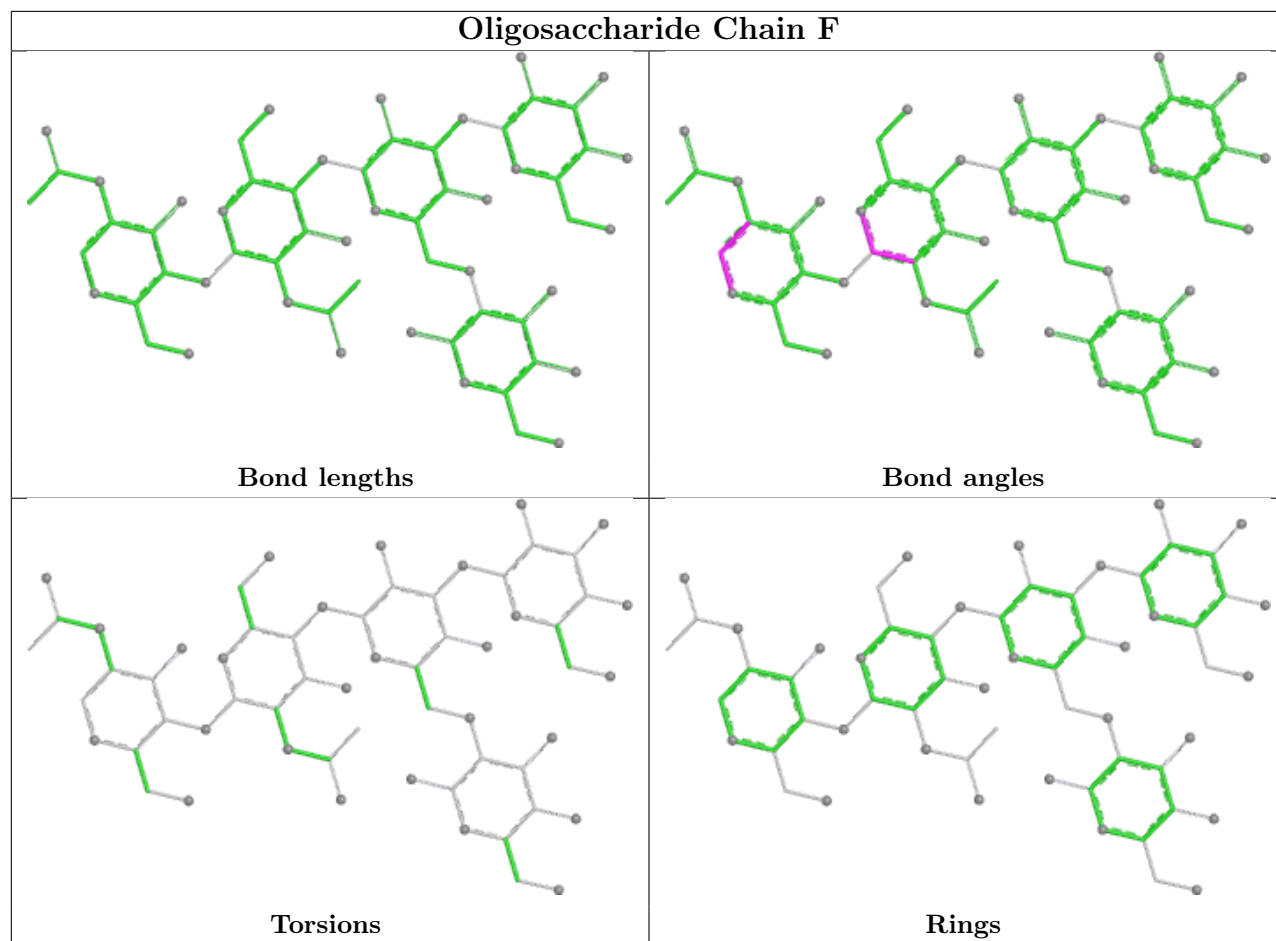
All (1) ring outliers are listed below:

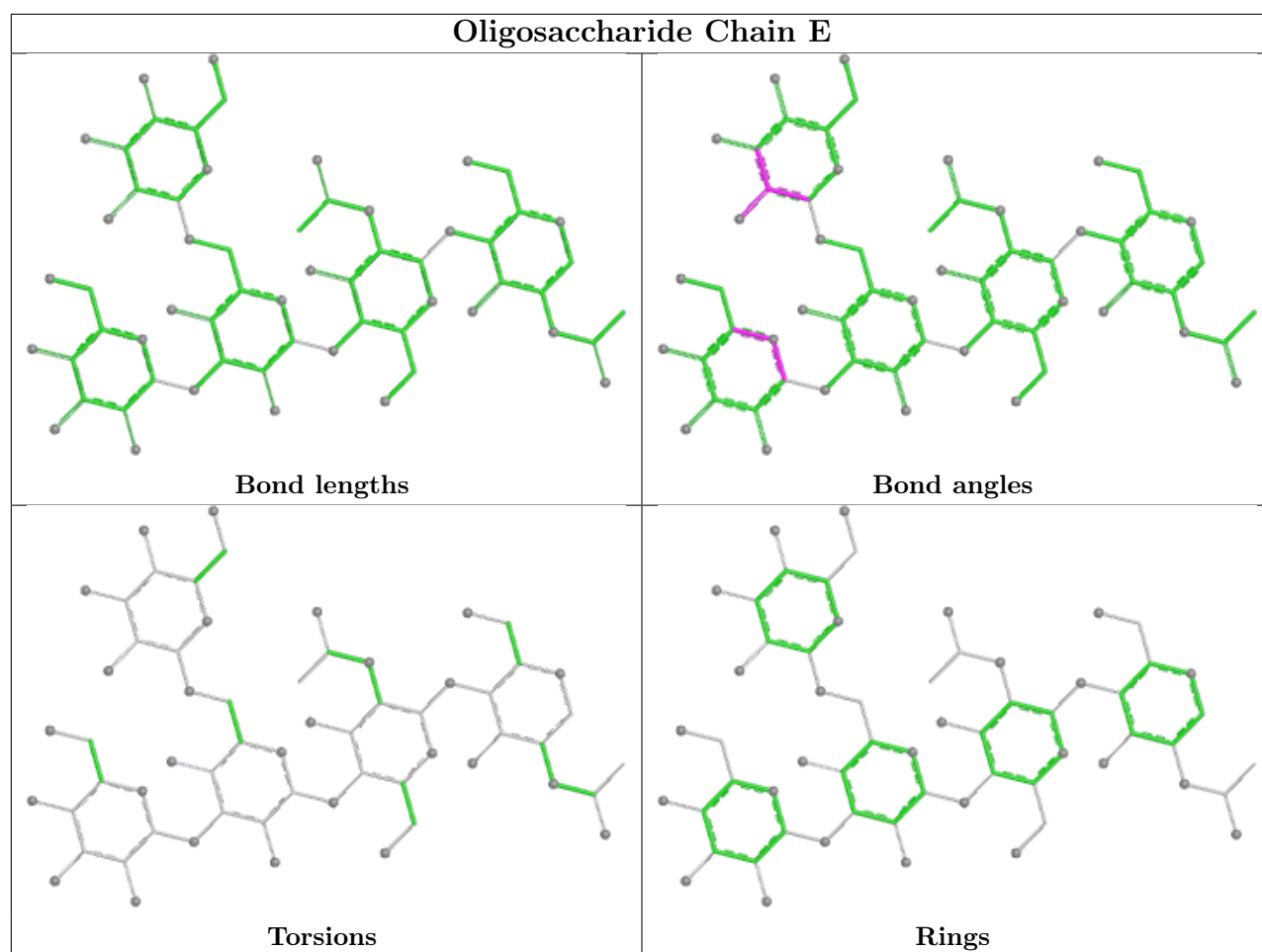
Mol	Chain	Res	Type	Atoms
4	G	5	MAN	C1-C2-C3-C4-C5-O5

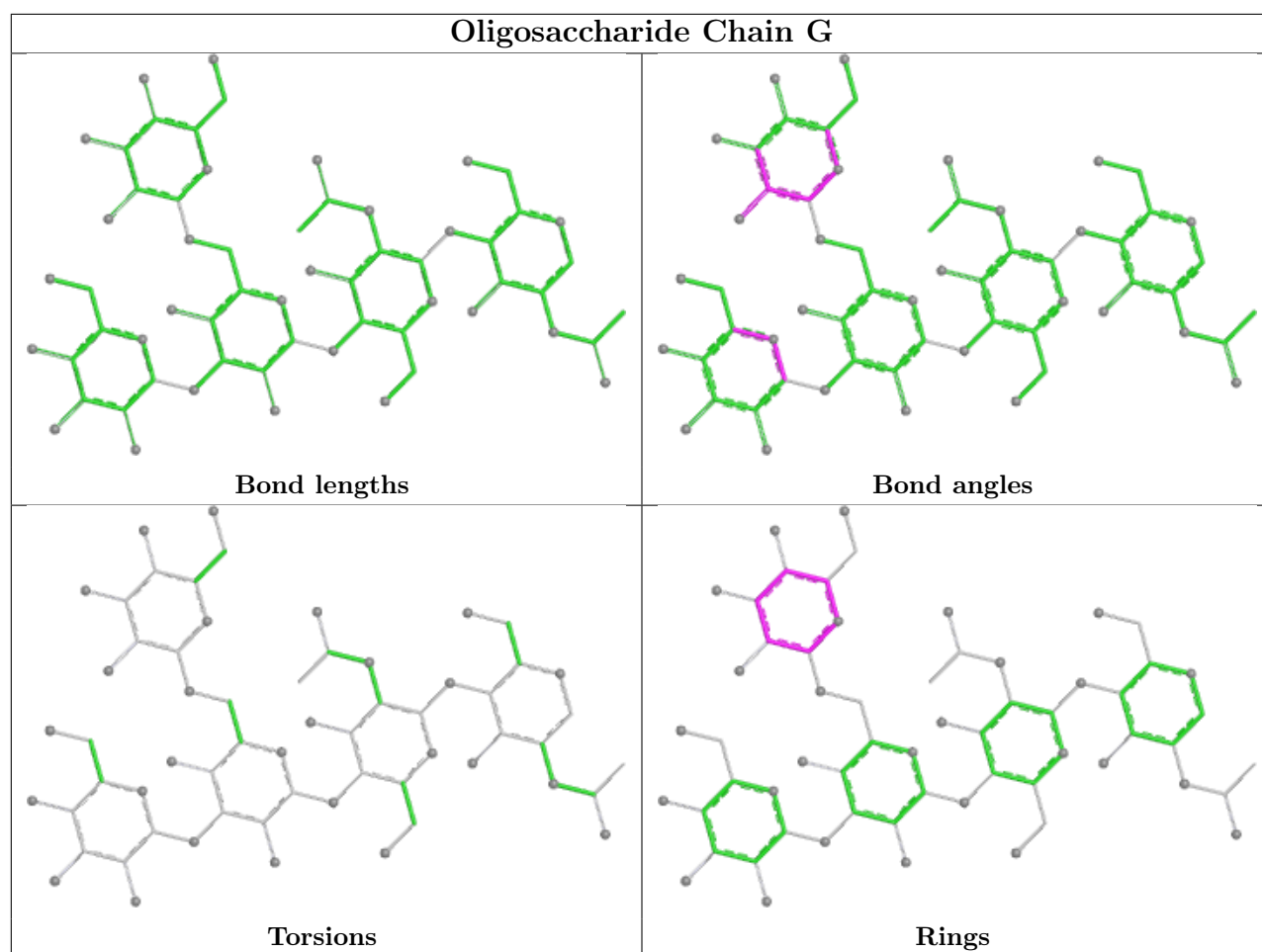
No monomer is involved in short contacts.

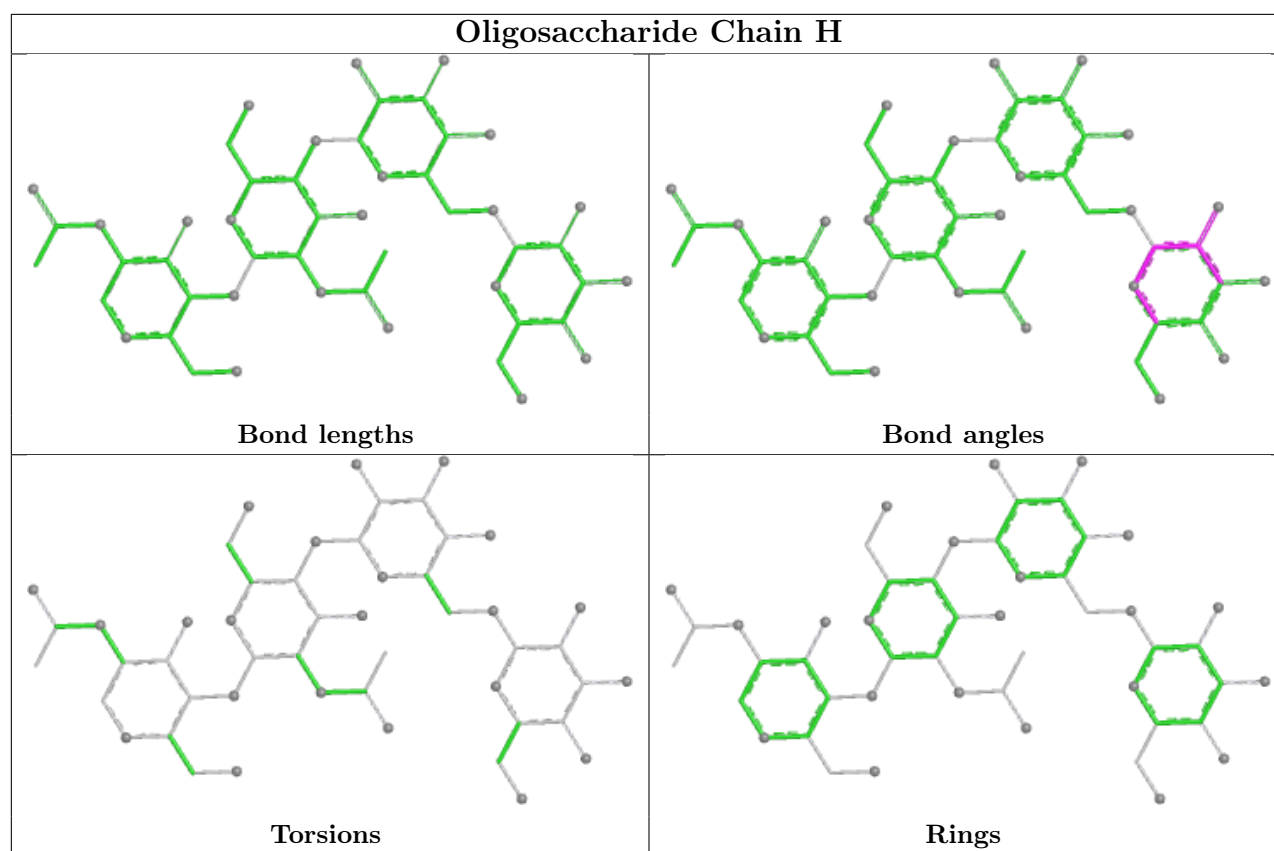
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











4.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	911	1	14,14,15	0.30	0	17,19,21	0.63	0
6	NAG	A	912	1	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
6	NAG	A	906	1	14,14,15	0.26	0	17,19,21	0.90	1 (5%)
6	NAG	A	905	1	14,14,15	0.30	0	17,19,21	0.62	0
6	NAG	B	910	1	14,14,15	0.30	0	17,19,21	0.82	1 (5%)
6	NAG	B	908	1	14,14,15	0.35	0	17,19,21	0.79	1 (5%)
6	NAG	B	903	1	14,14,15	0.30	0	17,19,21	0.60	1 (5%)
6	NAG	B	905	1	14,14,15	0.30	0	17,19,21	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	909	1	14,14,15	0.28	0	17,19,21	0.88	1 (5%)
7	A1BLO	A	913	-	43,43,43	0.68	2 (4%)	54,60,60	1.29	2 (3%)
7	A1BLO	B	911	-	43,43,43	0.81	2 (4%)	54,60,60	1.26	2 (3%)
6	NAG	B	907	1	14,14,15	0.27	0	17,19,21	0.91	1 (5%)
6	NAG	B	904	1	14,14,15	0.30	0	17,19,21	0.62	0
6	NAG	A	904	1	14,14,15	0.32	0	17,19,21	1.33	2 (11%)
6	NAG	A	903	1	14,14,15	0.30	0	17,19,21	0.62	0
6	NAG	B	906	1	14,14,15	0.31	0	17,19,21	0.62	0
6	NAG	A	908	1	14,14,15	0.29	0	17,19,21	0.85	1 (5%)
6	NAG	A	901	1	14,14,15	0.29	0	17,19,21	0.77	1 (5%)
6	NAG	A	910	1	14,14,15	0.60	0	17,19,21	0.84	1 (5%)
6	NAG	A	902	1	14,14,15	0.44	0	17,19,21	1.48	2 (11%)
6	NAG	A	907	1	14,14,15	0.28	0	17,19,21	0.79	1 (5%)
6	NAG	B	902	1	14,14,15	0.43	0	17,19,21	1.47	2 (11%)
6	NAG	B	901	1	14,14,15	0.33	0	17,19,21	1.12	1 (5%)
6	NAG	A	909	1	14,14,15	0.27	0	17,19,21	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	911	1	-	1/6/23/26	0/1/1/1
6	NAG	A	912	1	-	0/6/23/26	0/1/1/1
6	NAG	A	906	1	-	0/6/23/26	0/1/1/1
6	NAG	A	905	1	-	0/6/23/26	0/1/1/1
6	NAG	B	910	1	-	0/6/23/26	0/1/1/1
6	NAG	B	908	1	-	0/6/23/26	0/1/1/1
6	NAG	B	903	1	-	0/6/23/26	0/1/1/1
6	NAG	B	905	1	-	1/6/23/26	0/1/1/1
6	NAG	B	909	1	-	0/6/23/26	0/1/1/1
7	A1BLO	A	913	-	-	3/21/31/31	0/5/5/5
7	A1BLO	B	911	-	-	5/21/31/31	0/5/5/5
6	NAG	B	907	1	-	0/6/23/26	0/1/1/1
6	NAG	B	904	1	-	0/6/23/26	0/1/1/1
6	NAG	A	904	1	-	1/6/23/26	0/1/1/1
6	NAG	A	903	1	-	0/6/23/26	0/1/1/1
6	NAG	B	906	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	908	1	-	0/6/23/26	0/1/1/1
6	NAG	A	901	1	-	0/6/23/26	0/1/1/1
6	NAG	A	910	1	-	0/6/23/26	0/1/1/1
6	NAG	A	902	1	-	0/6/23/26	0/1/1/1
6	NAG	A	907	1	-	0/6/23/26	0/1/1/1
6	NAG	B	902	1	-	0/6/23/26	0/1/1/1
6	NAG	B	901	1	-	0/6/23/26	0/1/1/1
6	NAG	A	909	1	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	911	A1BLO	C20-C19	4.31	1.58	1.54
7	A	913	A1BLO	C13-C15	3.05	1.47	1.41
7	A	913	A1BLO	C20-C19	2.71	1.56	1.54
7	B	911	A1BLO	C13-C15	2.55	1.46	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	913	A1BLO	C25-C26-C29	8.14	122.28	114.95
7	B	911	A1BLO	C25-C26-C29	8.02	122.17	114.95
6	A	902	NAG	O5-C1-C2	-5.58	102.66	111.29
6	B	902	NAG	O5-C1-C2	-5.54	102.72	111.29
6	A	904	NAG	O5-C1-C2	-4.61	104.16	111.29
6	B	905	NAG	O5-C1-C2	-4.55	104.26	111.29
6	B	901	NAG	O5-C1-C2	-3.98	105.13	111.29
6	A	906	NAG	O5-C1-C2	-3.07	106.53	111.29
6	B	907	NAG	O5-C1-C2	-3.07	106.54	111.29
6	A	901	NAG	O5-C1-C2	-2.94	106.73	111.29
6	A	904	NAG	C1-C2-N2	2.58	114.50	110.43
6	A	910	NAG	O5-C1-C2	-2.56	107.33	111.29
6	B	905	NAG	C1-C2-N2	2.56	114.46	110.43
6	B	909	NAG	C1-O5-C5	2.50	115.53	112.19
6	A	908	NAG	C1-O5-C5	2.44	115.45	112.19
6	B	910	NAG	C1-O5-C5	2.39	115.38	112.19
6	A	907	NAG	C1-C2-N2	-2.38	106.68	110.43
6	B	908	NAG	O5-C1-C2	-2.22	107.85	111.29
6	B	902	NAG	C1-C2-N2	2.18	113.87	110.43
6	A	902	NAG	C1-C2-N2	2.16	113.84	110.43
7	A	913	A1BLO	C11-C13-N3	2.10	108.46	105.73
6	B	903	NAG	O5-C1-C2	-2.05	108.13	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	912	NAG	C1-O5-C5	2.04	114.91	112.19
7	B	911	A1BLO	C11-C13-N3	2.03	108.38	105.73

There are no chirality outliers.

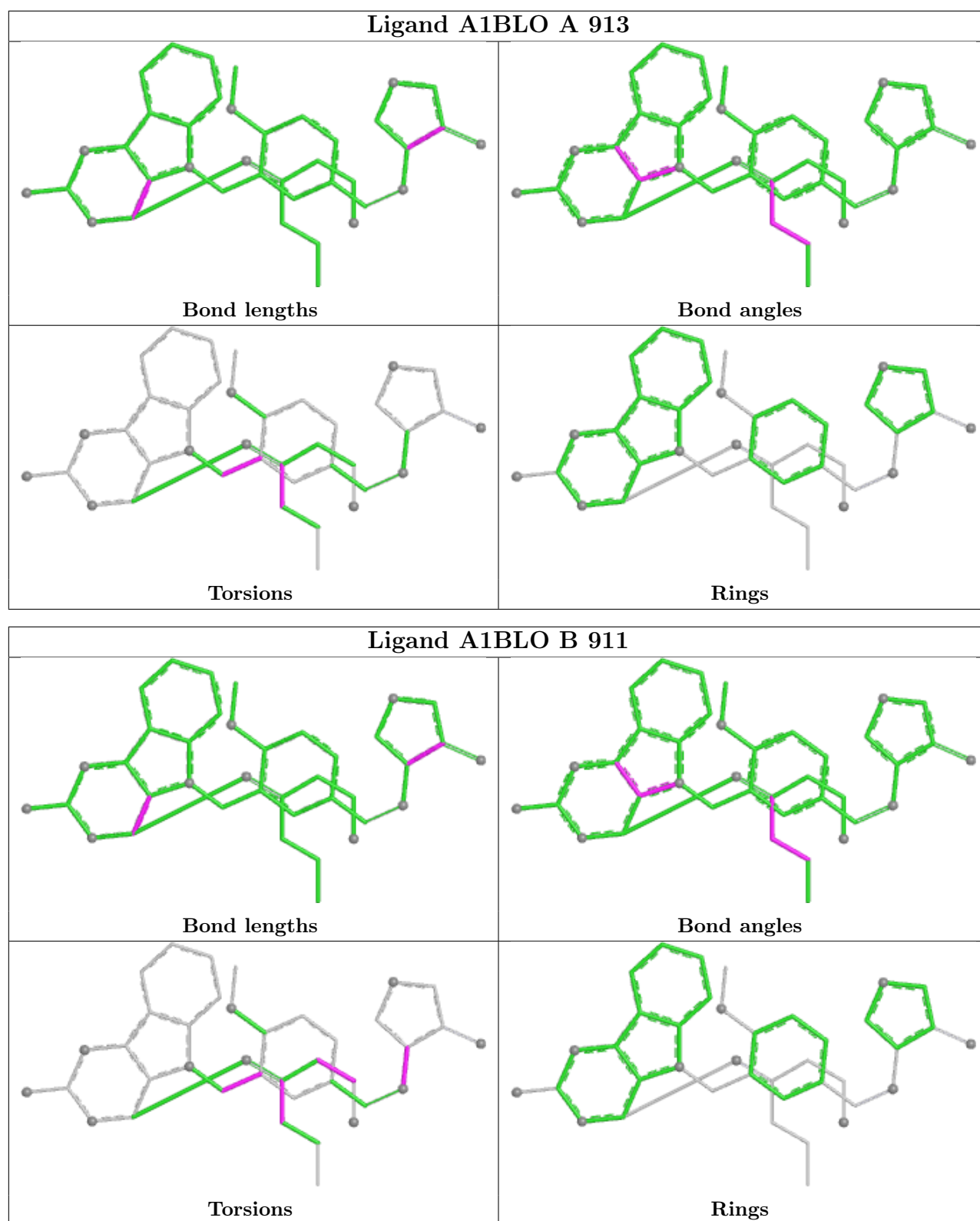
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	913	A1BLO	C25-C26-C29-C27
7	B	911	A1BLO	C25-C26-C29-C27
7	B	911	A1BLO	C25-C26-C29-N5
7	B	911	A1BLO	C29-C27-C28-O3
7	A	913	A1BLO	C25-C26-C29-N5
7	B	911	A1BLO	C17-C19-N6-C24
6	A	909	NAG	C1-C2-N2-C7
6	A	911	NAG	C1-C2-N2-C7
7	B	911	A1BLO	C14-C10-C23-N3
6	B	905	NAG	C8-C7-N2-C2
6	A	904	NAG	C8-C7-N2-C2
7	A	913	A1BLO	C14-C10-C23-N3

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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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	748/807 (92%)	0.32	30 (4%)	42 48	14, 25, 45, 66	2 (0%)
1	B	741/807 (91%)	0.45	40 (5%)	31 36	12, 26, 49, 73	1 (0%)
All	All	1489/1614 (92%)	0.39	70 (4%)	36 41	12, 26, 47, 73	3 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472	ARG	4.8
1	A	815	VAL	4.1
1	B	762	THR	4.1
1	A	470	PHE	4.0
1	B	471	THR	4.0
1	B	735	VAL	3.9
1	B	49	CYS	3.9
1	B	473	PRO	3.6
1	B	434	VAL	3.6
1	B	780	ILE	3.6
1	A	367	LEU	3.5
1	A	49	CYS	3.5
1	A	759	LYS	3.3
1	A	814	ILE	3.3
1	A	505	PRO	3.2
1	B	433	LEU	3.2
1	B	779	ASP	3.2
1	B	65	VAL	3.2
1	A	758	THR	3.1
1	B	778	CYS	3.1
1	A	702	PHE	3.0
1	B	470	PHE	3.0
1	B	653	HIS	3.0
1	B	244	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	678	PHE	3.0
1	B	89	LEU	3.0
1	B	309	ASN	2.9
1	A	809	GLN	2.9
1	B	236	TYR	2.9
1	A	85	GLY	2.9
1	B	701	LEU	2.8
1	A	100	VAL	2.8
1	A	506	ASP	2.7
1	A	761	THR	2.7
1	B	32	ARG	2.7
1	B	809	GLN	2.7
1	B	100	VAL	2.7
1	B	469	HIS	2.6
1	B	39	LYS	2.5
1	B	643	ARG	2.5
1	A	113	GLY	2.5
1	A	167	SER	2.4
1	B	777	THR	2.4
1	A	461	PHE	2.4
1	B	625	ASN	2.4
1	A	87	GLN	2.4
1	A	643	ARG	2.4
1	B	274	ALA	2.4
1	A	735	VAL	2.2
1	B	811	GLY	2.2
1	B	702	PHE	2.2
1	B	272	GLY	2.2
1	B	474	LEU	2.2
1	A	39	LYS	2.2
1	A	83	PHE	2.2
1	A	762	THR	2.2
1	B	334	THR	2.1
1	B	807	GLY	2.1
1	A	41	GLN	2.1
1	B	802	ILE	2.1
1	B	494	PHE	2.1
1	B	45	VAL	2.1
1	B	40	LYS	2.1
1	A	751	ILE	2.1
1	B	798	LEU	2.0
1	A	186	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	731	PHE	2.0
1	A	810	ARG	2.0
1	A	181	CYS	2.0
1	A	189	LYS	2.0

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

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

5.3 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.

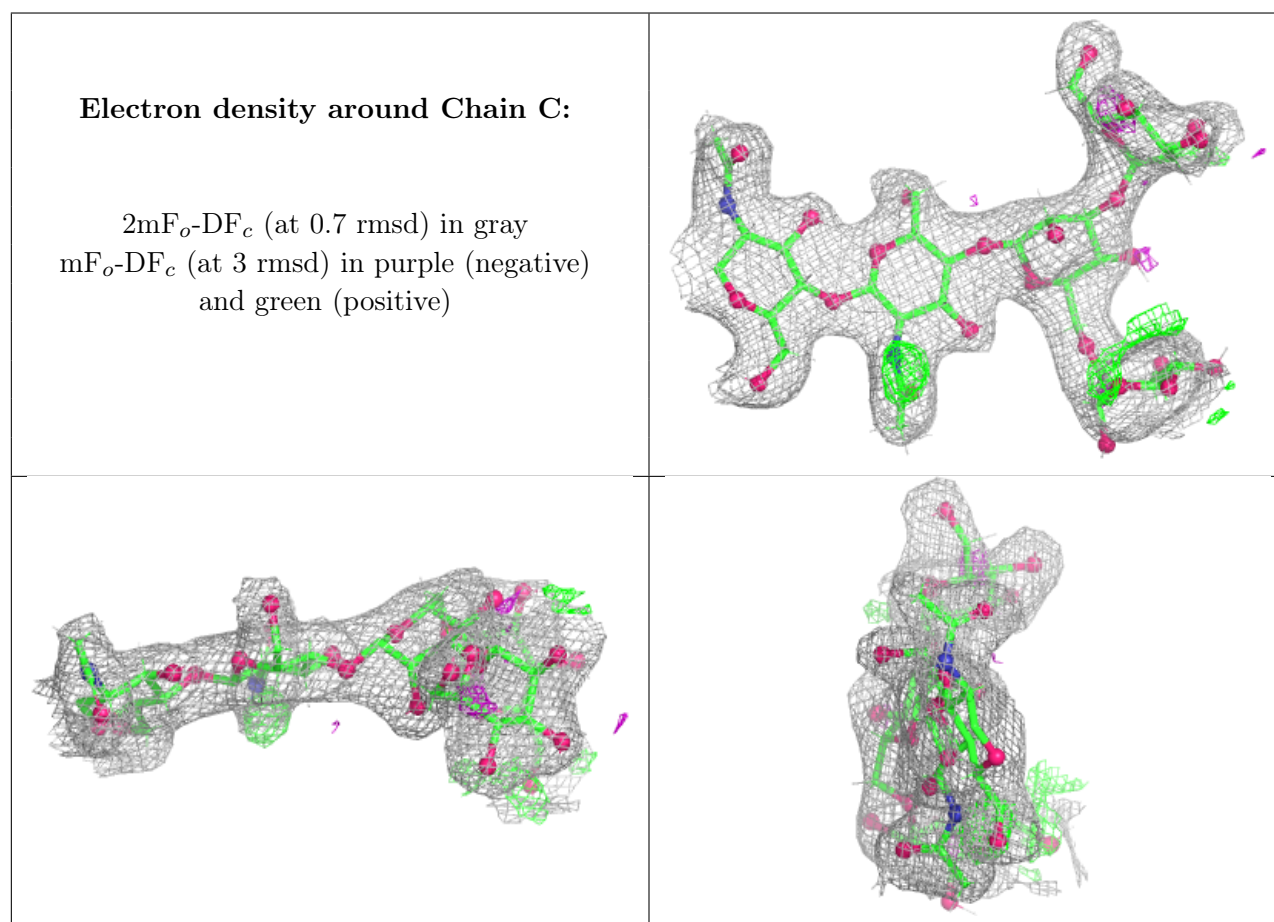
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	E	4	11/12	0.36	0.18	70,74,77,77	10
4	MAN	G	5	11/12	0.48	0.14	70,79,80,80	9
2	MAN	C	5	11/12	0.49	0.14	68,71,73,74	10
5	MAN	H	4	11/12	0.53	0.16	65,68,72,73	10
3	MAN	D	5	11/12	0.55	0.13	73,75,82,82	10
4	MAN	G	4	11/12	0.55	0.12	69,71,78,79	10
4	MAN	E	5	11/12	0.56	0.12	70,74,77,77	10
2	MAN	F	5	11/12	0.56	0.14	67,69,74,75	10
4	BMA	G	3	11/12	0.69	0.11	62,72,76,78	8
3	MAN	D	4	11/12	0.70	0.10	68,76,79,80	9
2	MAN	F	4	11/12	0.70	0.14	61,63,69,69	10
3	BMA	D	3	11/12	0.75	0.10	58,64,71,74	10
5	BMA	H	3	11/12	0.77	0.11	54,60,64,68	10
2	MAN	C	4	11/12	0.77	0.11	57,60,64,64	10
3	NAG	D	2	14/15	0.79	0.12	44,55,61,64	12
4	NAG	G	2	14/15	0.80	0.12	47,56,63,68	13
2	BMA	F	3	11/12	0.80	0.11	56,63,68,70	8
4	BMA	E	3	11/12	0.81	0.10	61,65,72,74	8
2	BMA	C	3	11/12	0.83	0.09	54,60,66,68	8
5	NAG	H	2	14/15	0.84	0.12	39,48,53,56	12
4	NAG	E	2	14/15	0.87	0.11	43,51,56,61	12
2	NAG	C	2	14/15	0.89	0.09	38,45,51,55	12
4	NAG	G	1	14/15	0.94	0.09	35,47,51,55	12
2	NAG	F	2	14/15	0.94	0.09	41,47,51,57	12

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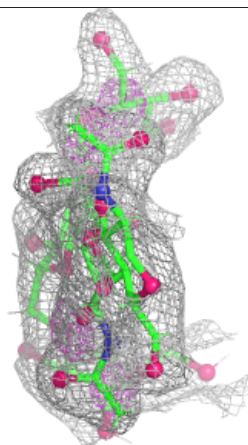
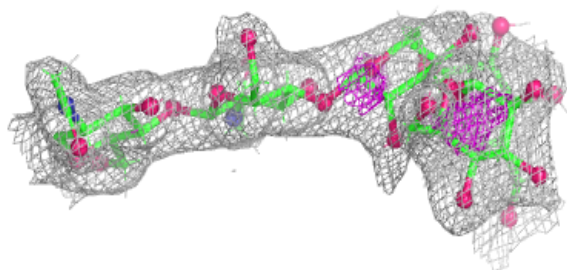
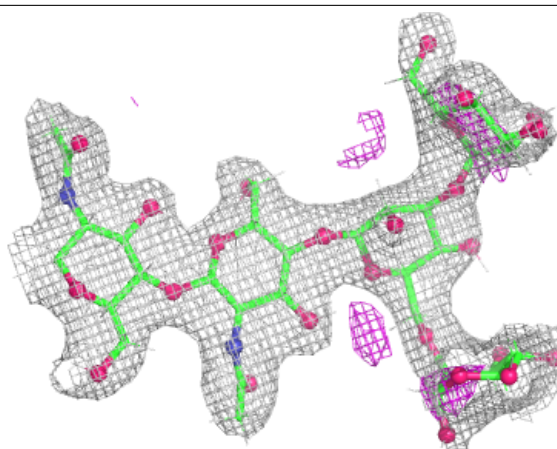
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	1	14/15	0.94	0.07	30,36,40,42	12
2	NAG	F	1	14/15	0.94	0.09	29,36,41,44	12
4	NAG	E	1	14/15	0.95	0.07	30,41,43,48	12
5	NAG	H	1	14/15	0.96	0.07	29,41,43,46	12
3	NAG	D	1	14/15	0.96	0.09	31,42,46,51	12

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.



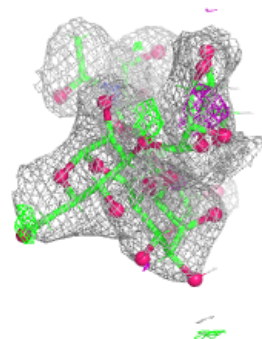
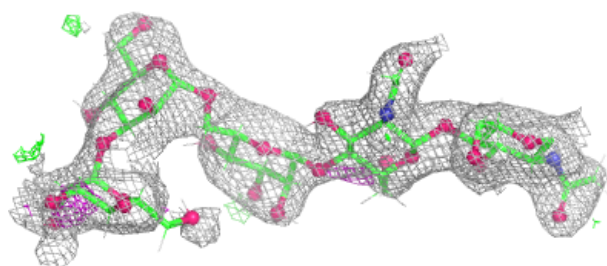
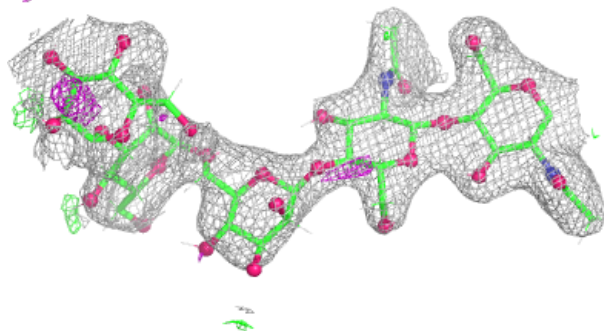
Electron density around Chain F:

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

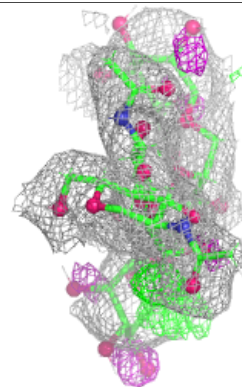
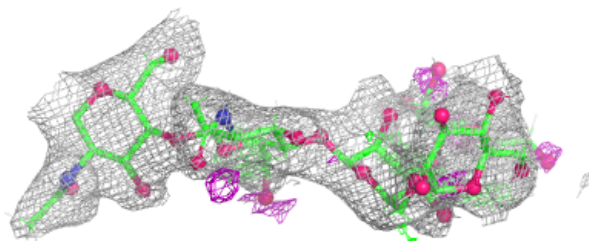
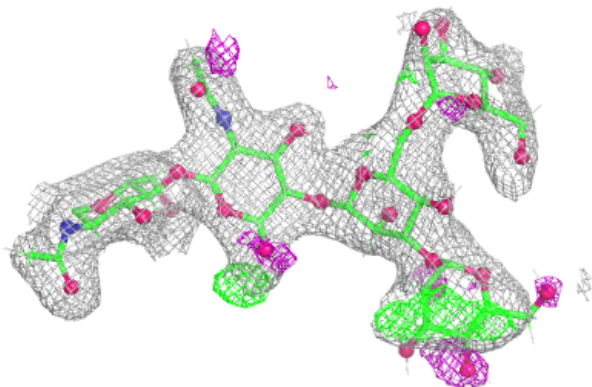


Electron density around Chain D:

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

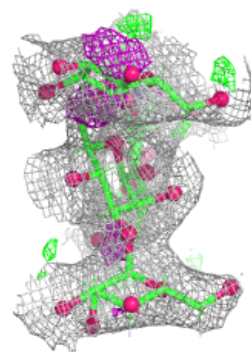
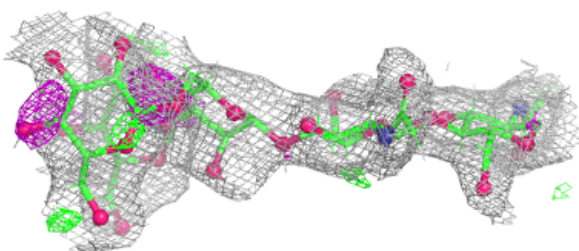
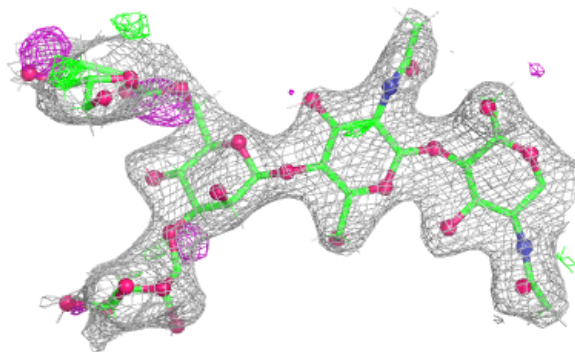
**Electron density around Chain E:**

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

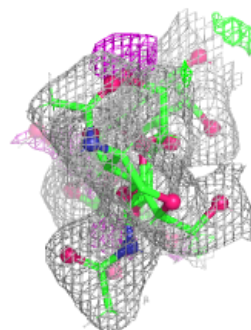
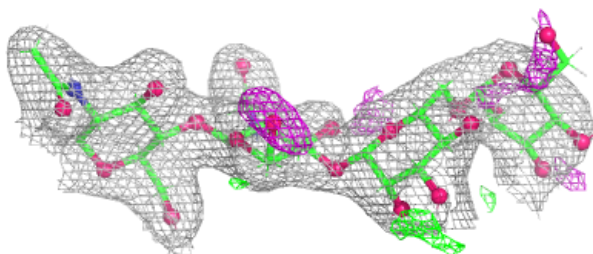
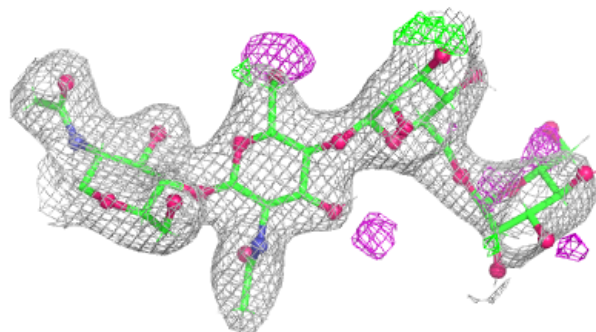


Electron density around Chain G:

$2mF_o-DF_c$ (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)



5.4 Ligands ⓘ

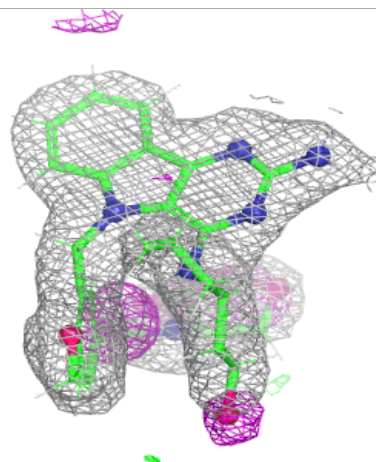
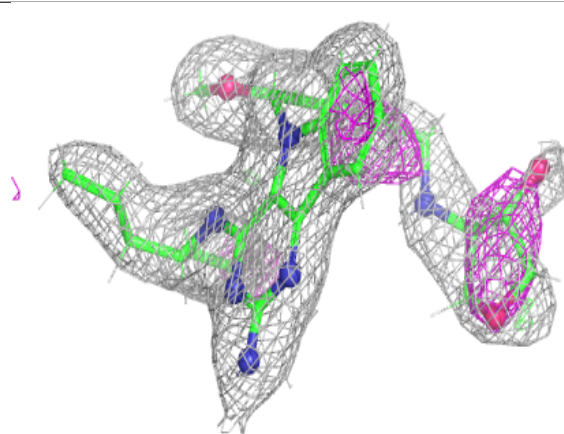
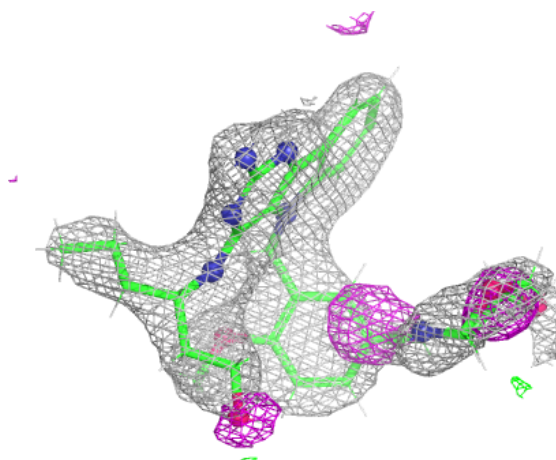
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	NAG	A	902	14/15	0.33	0.21	89,90,117,118	13
6	NAG	A	903	14/15	0.36	0.18	72,74,80,81	13
6	NAG	A	910	14/15	0.36	0.20	83,85,104,105	13
6	NAG	B	908	14/15	0.36	0.19	70,73,77,78	13
6	NAG	A	907	14/15	0.43	0.19	72,75,79,79	13
6	NAG	A	912	14/15	0.46	0.16	69,72,75,75	13
6	NAG	B	902	14/15	0.48	0.18	85,87,106,106	13
6	NAG	A	911	14/15	0.48	0.16	65,68,72,73	13
6	NAG	A	901	14/15	0.50	0.15	91,92,125,127	13
6	NAG	B	904	14/15	0.54	0.15	72,74,79,79	13
6	NAG	B	903	14/15	0.63	0.12	71,72,85,87	13
6	NAG	B	906	14/15	0.70	0.14	67,68,69,70	13
6	NAG	B	909	14/15	0.70	0.13	72,74,82,82	13
6	NAG	B	901	14/15	0.71	0.13	85,87,111,113	13
6	NAG	A	909	14/15	0.75	0.13	86,87,111,113	13
6	NAG	A	904	14/15	0.78	0.11	56,59,60,61	13
6	NAG	A	905	14/15	0.78	0.12	65,66,68,68	13
6	NAG	B	905	14/15	0.80	0.13	51,54,62,62	13
6	NAG	A	906	14/15	0.82	0.13	66,68,77,77	13
6	NAG	A	908	14/15	0.85	0.11	59,61,66,66	13
6	NAG	B	907	14/15	0.85	0.10	72,74,90,92	13
6	NAG	B	910	14/15	0.88	0.09	50,53,57,57	13
7	A1BLO	A	913	39/39	0.88	0.12	37,42,57,57	38
7	A1BLO	B	911	39/39	0.88	0.11	36,41,51,52	38

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.

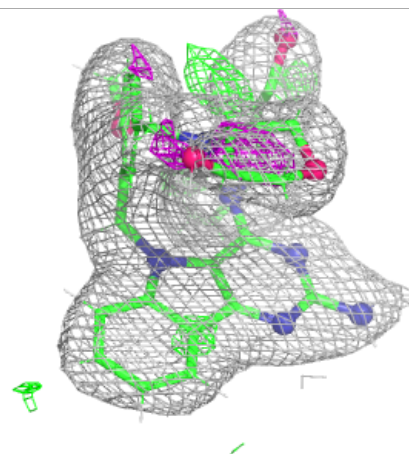
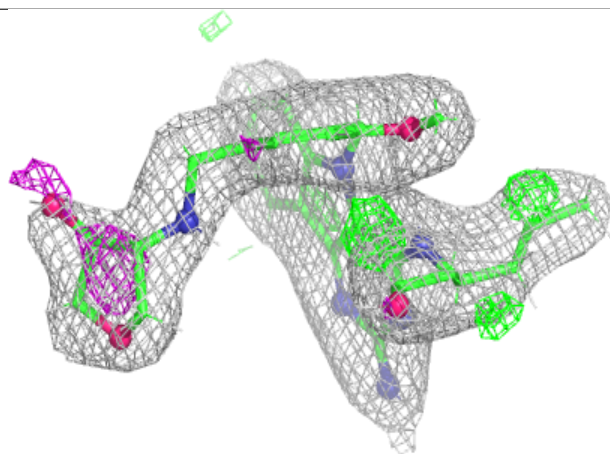
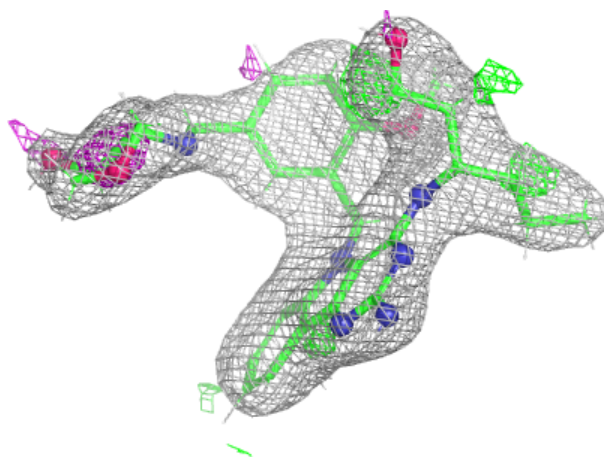
Electron density around A1BLO A 913:

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



Electron density around A1BLO B 911:

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



5.5 Other polymers [i](#)

There are no such residues in this entry.