



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2026 – 12:40 PM UTC

PDB ID : 9MHY / pdb_00009mhy
Title : Human TLR8 ectodomain with small molecule agonist 1
Authors : Critton, D.A.
Deposited on : 2024-12-12
Resolution : 1.66 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	:	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

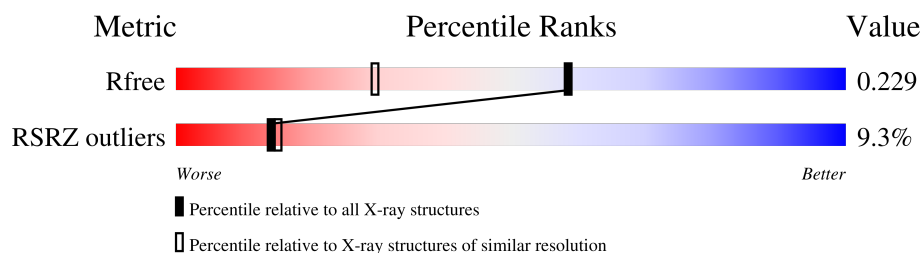
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	2563 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26408 atoms, of which 12624 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	747	Total	C	H	N	O	S	6036	4	0
			12078	3866	6036	1025	1131	20			
1	B	747	Total	C	H	N	O	S	6044	4	0
			12092	3868	6044	1029	1132	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.

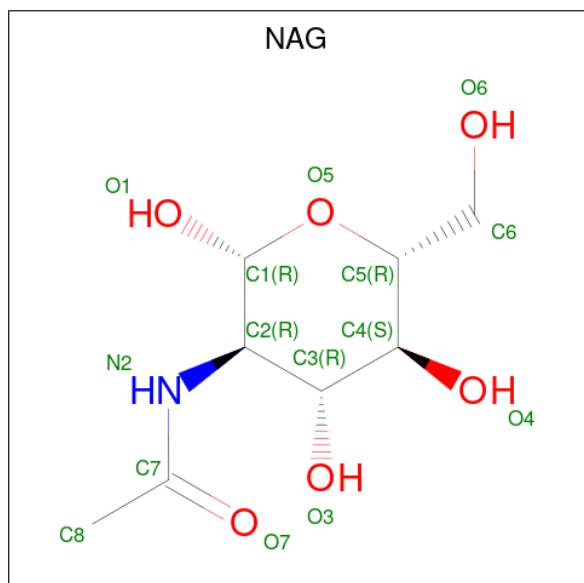
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	H	N	O	52	0	0
			113	34	52	2	25			
2	F	5	Total	C	H	N	O	52	0	0
			113	34	52	2	25			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	3	Total	C	H	N	O	34	0	0
			73	22	34	2	15			
3	E	3	Total	C	H	N	O	34	0	0
			73	22	34	2	15			
3	G	3	Total	C	H	N	O	34	0	0
			73	22	34	2	15			
3	H	3	Total	C	H	N	O	34	0	0
			73	22	34	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



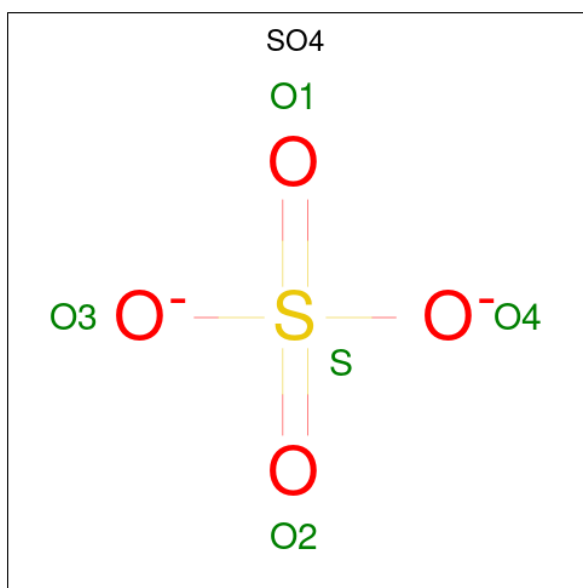
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		

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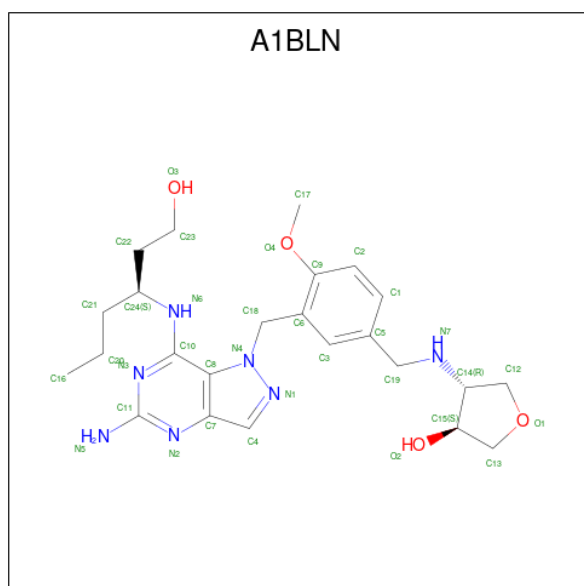
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	A	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	B	1	Total	C	H	N	O	13	0
			27	8	13	1	5		
4	B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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is (3S,4R)-4-[(3-[(5-amino-7-[(3S)-1-hydroxyhexan-3-yl]amino}-1H-pyrazolo[4,3-d]pyrimidin-1-yl)methyl]-4-methoxyphenyl)methyl]amino]oxolan-3-ol (CCD ID: A1BLN) (formula: C₂₄H₃₅N₇O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H N O 70 24 35 7 4	35	0
6	B	1	Total C H N O 70 24 35 7 4	35	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	539	Total O 539 539	0	0
7	B	540	Total O 540 540	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.58Å 82.41Å 83.44Å 116.05° 97.71° 98.68°	Depositor
Resolution (Å)	73.03 – 1.66 73.03 – 1.66	Depositor EDS
% Data completeness (in resolution range)	61.3 (73.03-1.66) 61.3 (73.03-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.66Å)	Xtriage
Refinement program	BUSTER 2.11.7 (20-MAY-2020)	Depositor
R, R_{free}	0.201 , 0.223 0.204 , 0.229	Depositor DCC
R_{free} test set	6152 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.001 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26408	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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](#)

22 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	0.33	0	17,19,21	0.76	1 (5%)
2	NAG	C	2	2	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
2	BMA	C	3	2	11,11,12	0.25	0	15,15,17	0.41	0
2	MAN	C	4	2	11,11,12	0.24	0	15,15,17	0.74	1 (6%)
2	MAN	C	5	2	11,11,12	0.27	0	13,15,17	0.47	0
3	NAG	D	1	3,1	14,14,15	0.27	0	17,19,21	0.75	1 (5%)
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.55	0
3	BMA	D	3	3	11,11,12	0.25	0	15,15,17	0.34	0
3	NAG	E	1	3,1	14,14,15	0.42	0	17,19,21	0.85	1 (5%)
3	NAG	E	2	3	14,14,15	0.26	0	17,19,21	0.38	0
3	BMA	E	3	3	11,11,12	0.22	0	15,15,17	0.38	0
2	NAG	F	1	2,1	14,14,15	0.32	0	17,19,21	0.75	1 (5%)
2	NAG	F	2	2	14,14,15	0.30	0	17,19,21	0.66	1 (5%)
2	BMA	F	3	2	11,11,12	0.28	0	15,15,17	0.40	0
2	MAN	F	4	2	11,11,12	0.20	0	15,15,17	0.73	1 (6%)
2	MAN	F	5	2	11,11,12	0.23	0	13,15,17	0.48	0
3	NAG	G	1	3,1	14,14,15	0.33	0	17,19,21	0.71	0
3	NAG	G	2	3	14,14,15	0.32	0	17,19,21	0.56	0
3	BMA	G	3	3	11,11,12	0.25	0	15,15,17	0.34	0
3	NAG	H	1	3,1	14,14,15	0.44	0	17,19,21	0.54	0
3	NAG	H	2	3	14,14,15	0.26	0	17,19,21	0.39	0
3	BMA	H	3	3	11,11,12	0.23	0	15,15,17	0.40	0

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

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

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

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	MAN	C1-O5-C5	2.55	115.60	112.19
2	C	2	NAG	O5-C1-C2	-2.51	107.41	111.29
2	F	4	MAN	C1-O5-C5	2.50	115.54	112.19
2	F	2	NAG	O5-C1-C2	-2.36	107.64	111.29
3	D	1	NAG	O5-C1-C2	-2.05	108.13	111.29

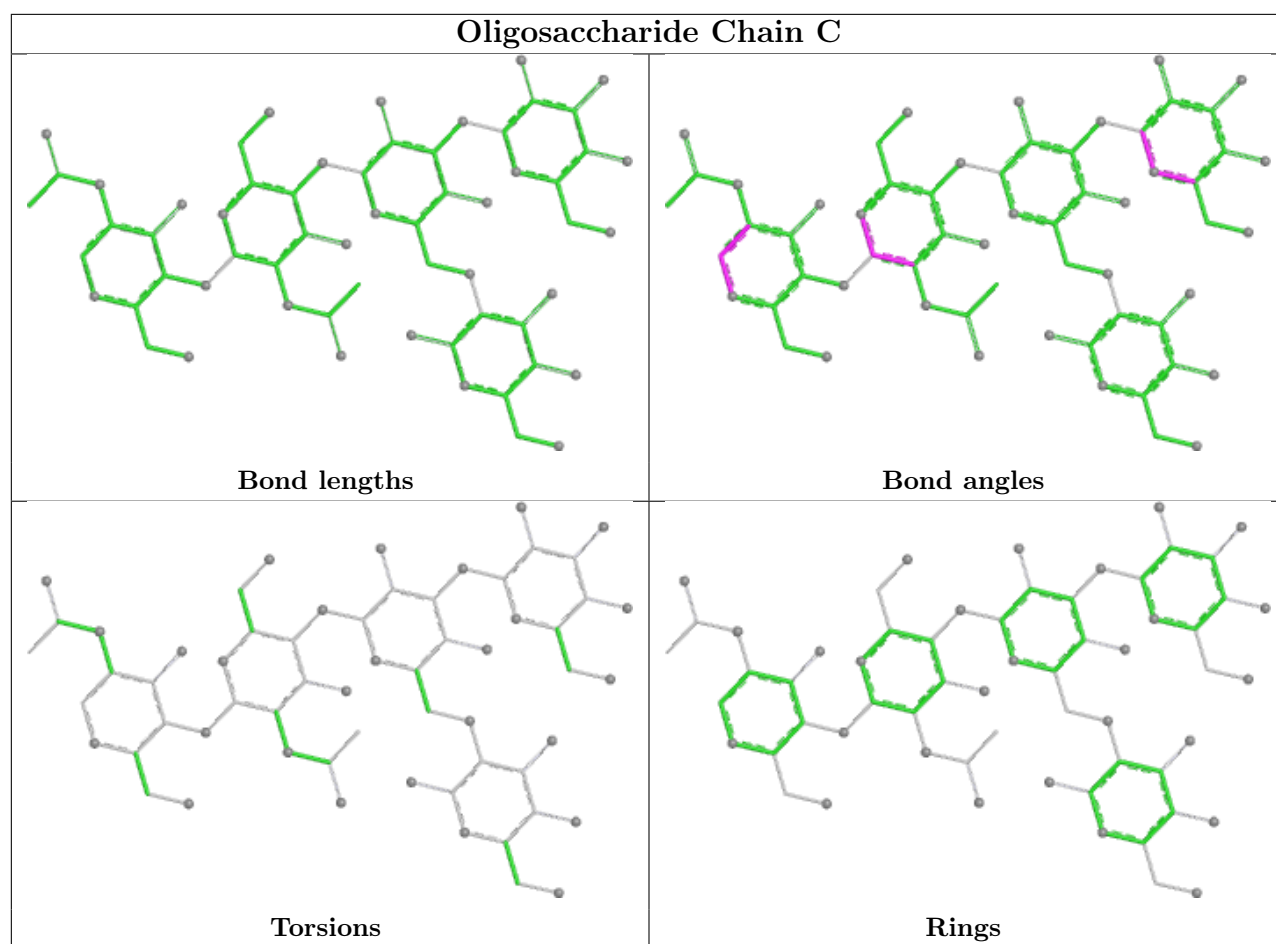
There are no chirality outliers.

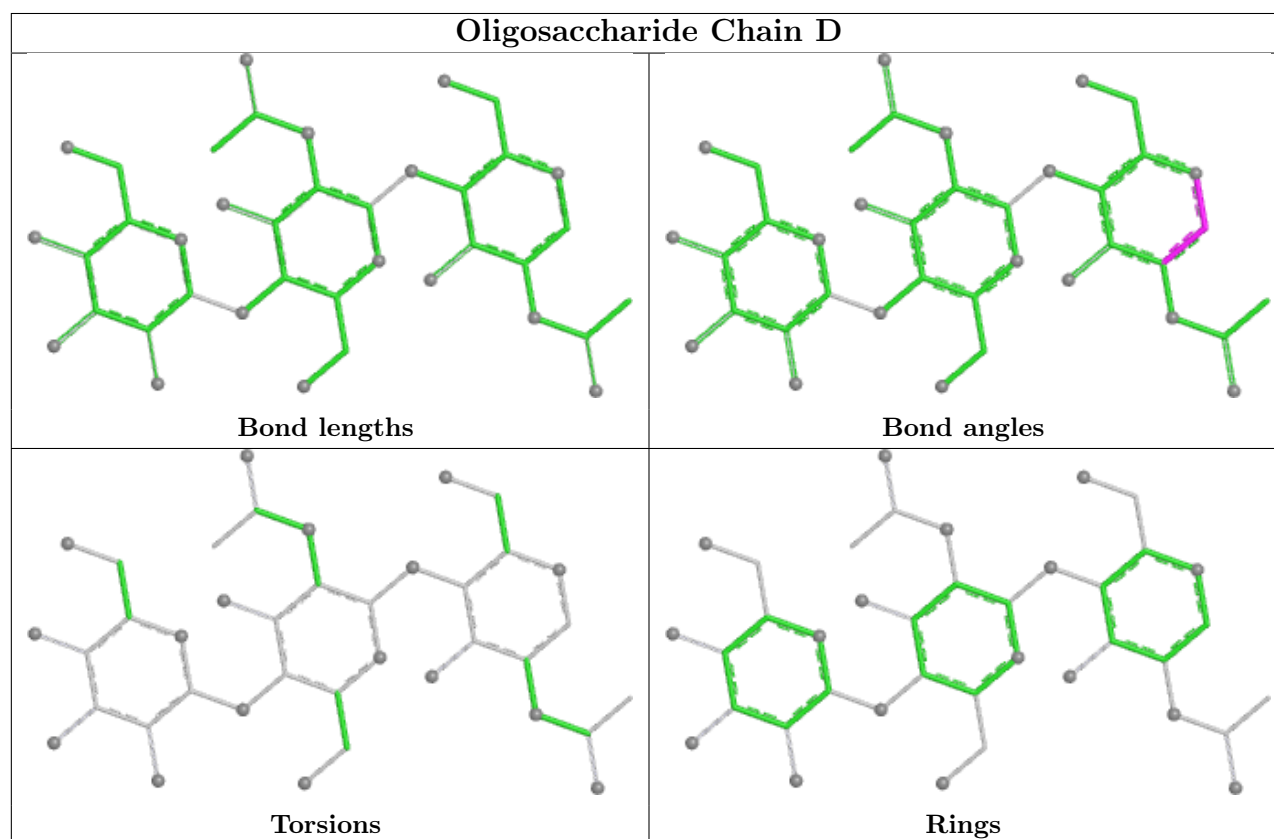
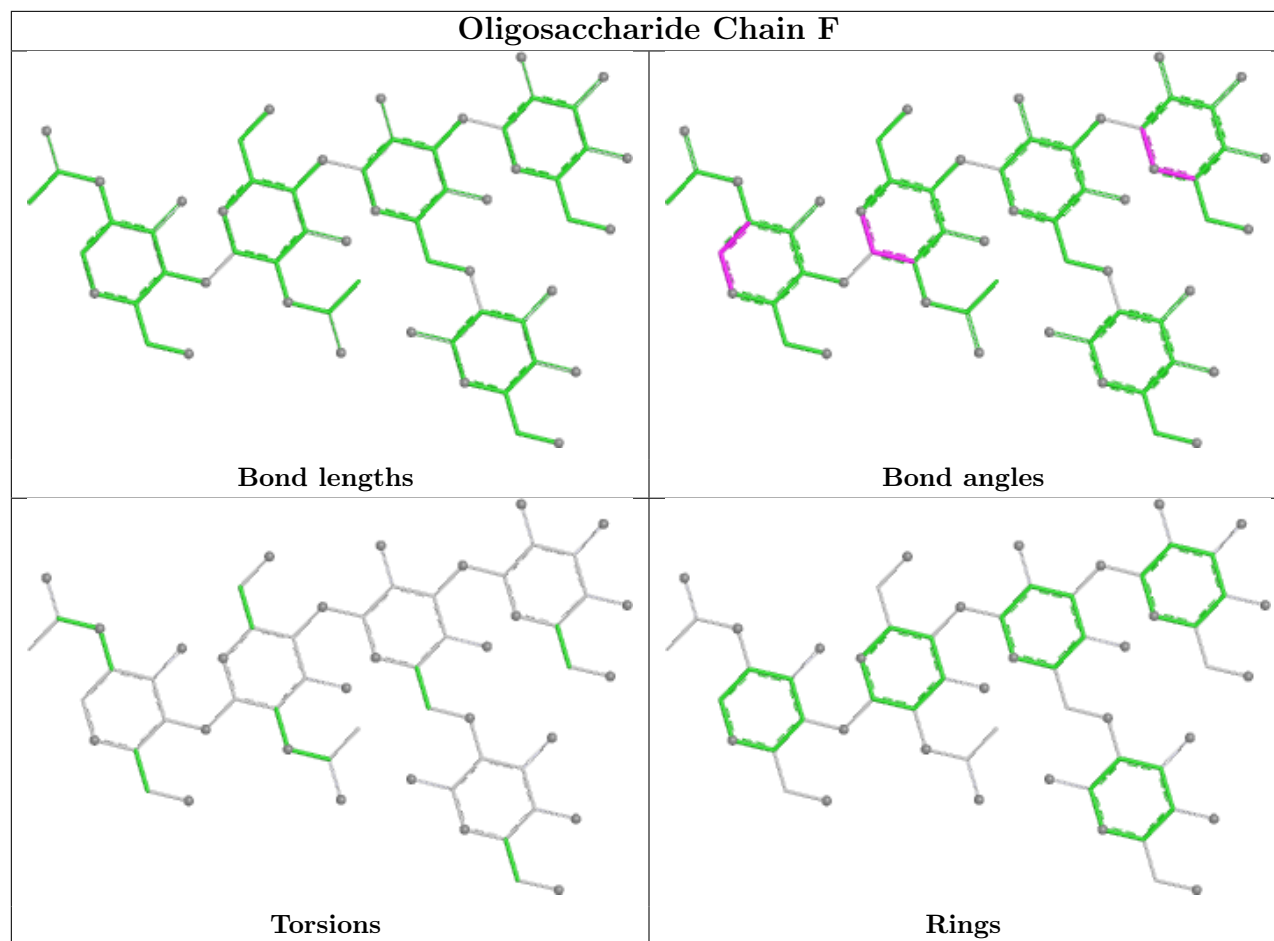
There are no torsion outliers.

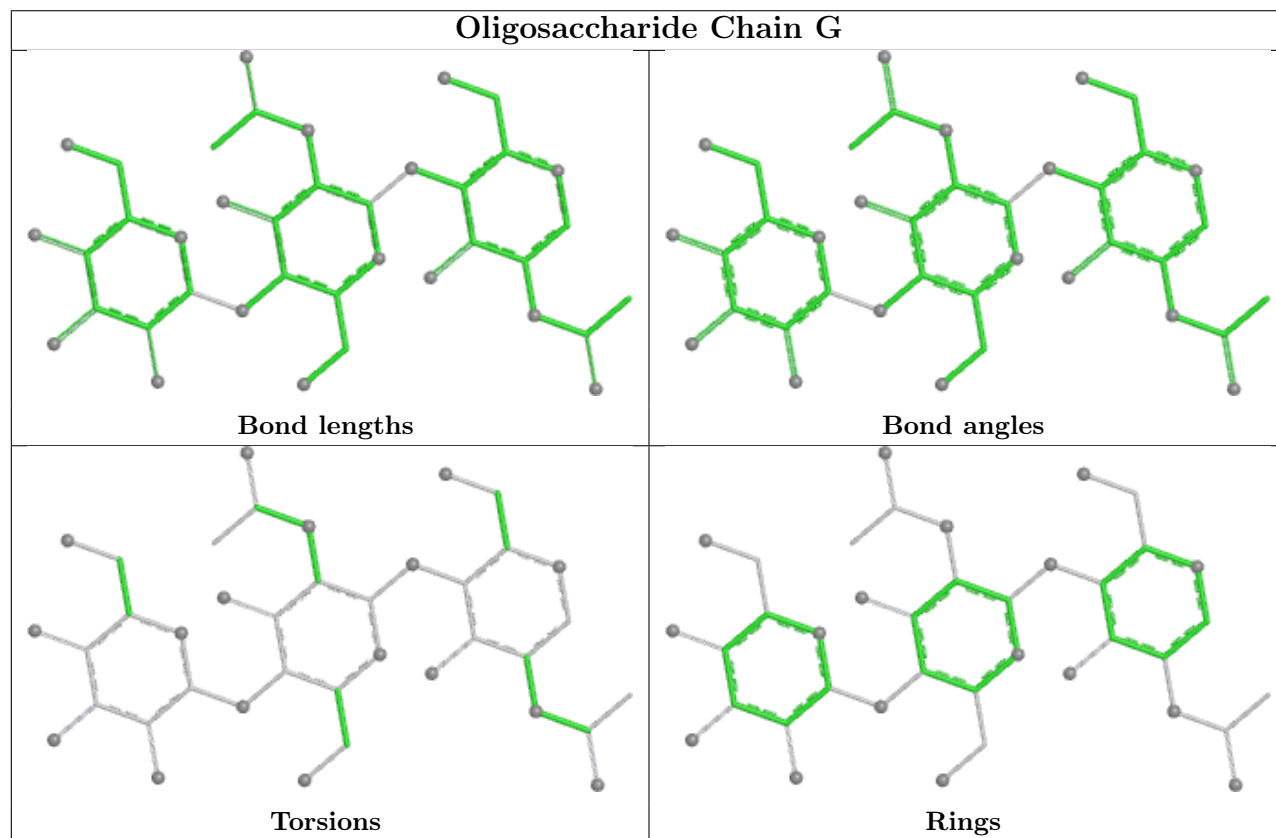
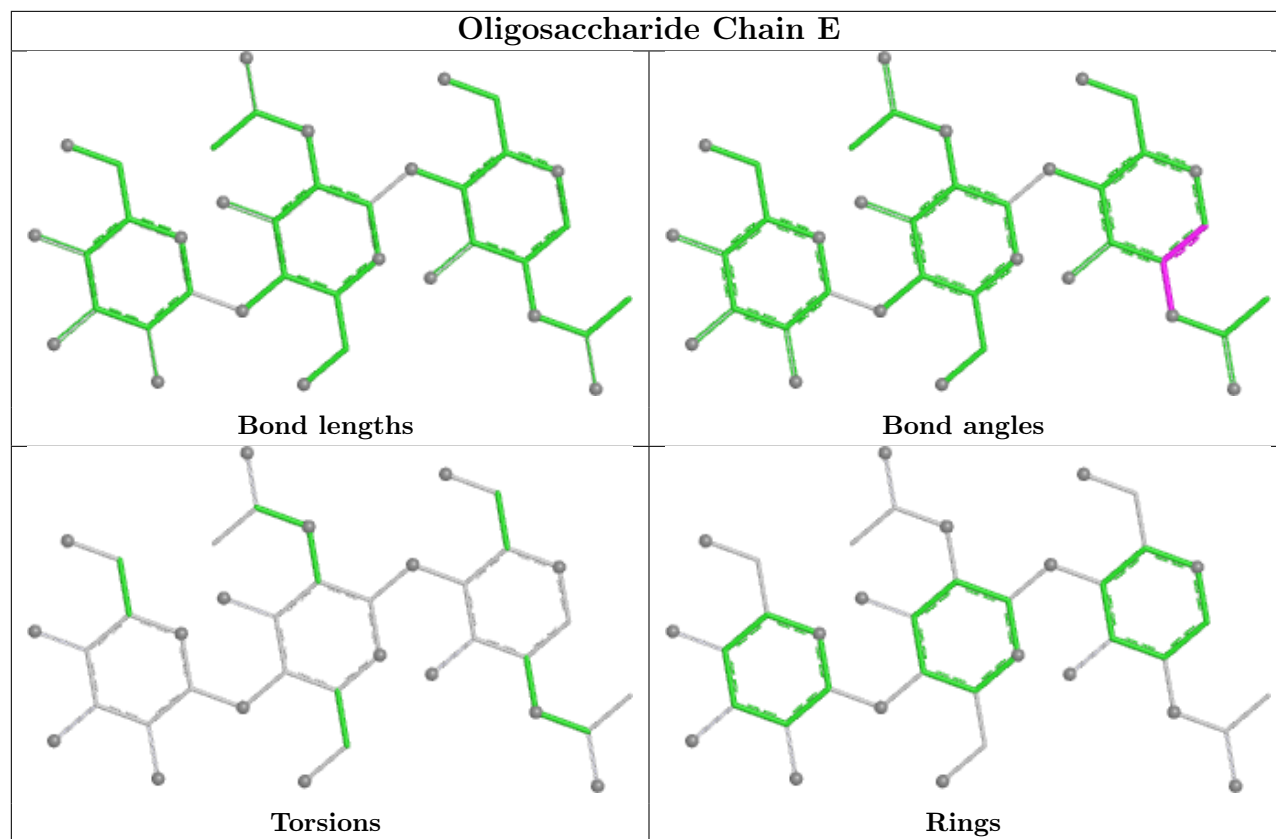
There are no ring outliers.

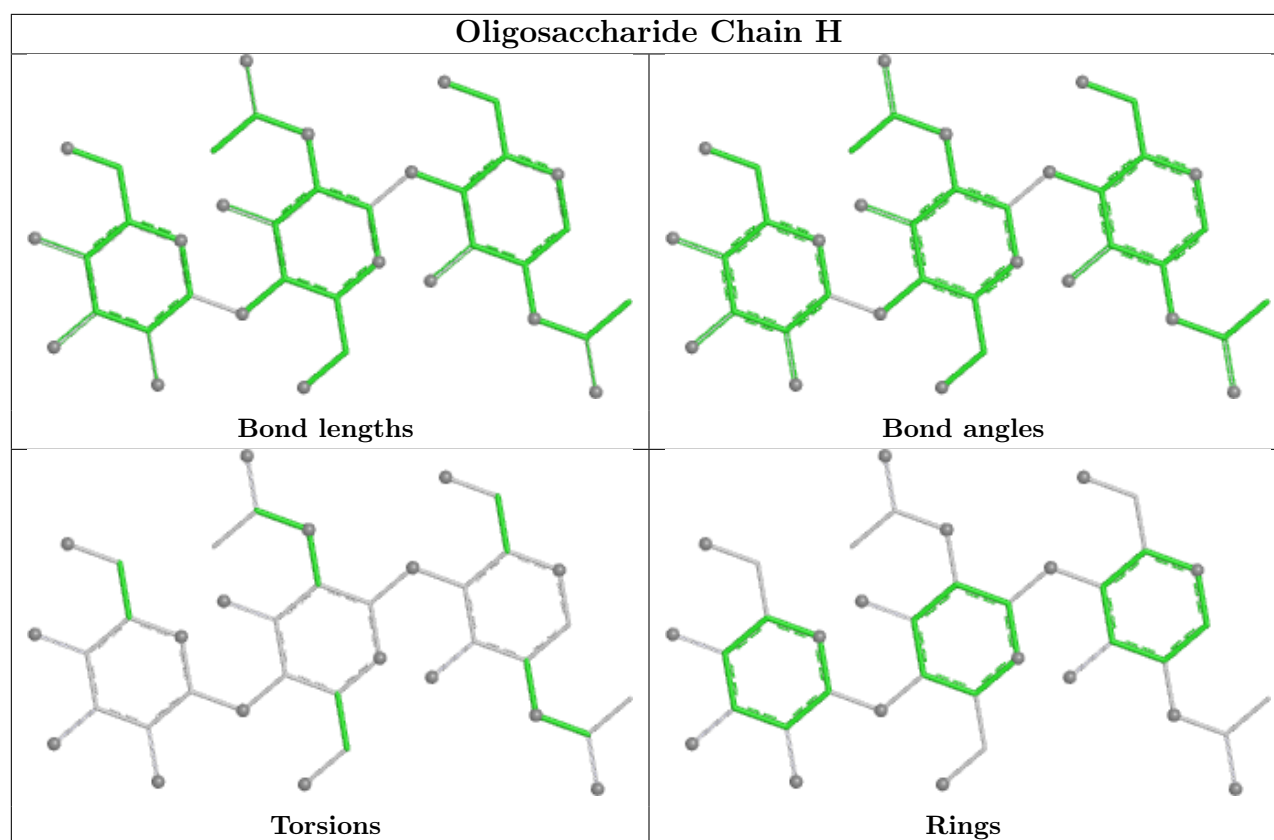
No monomer is involved in short contacts.

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









4.6 Ligand geometry [i](#)

23 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	$\# Z > 2$
4	NAG	A	902	1	14,14,15	0.32	0	17,19,21	0.81	1 (5%)
4	NAG	B	901	1	14,14,15	0.29	0	17,19,21	0.66	0
4	NAG	B	902	1	14,14,15	0.30	0	17,19,21	0.82	1 (5%)
4	NAG	B	909	1	14,14,15	0.26	0	17,19,21	0.73	1 (5%)
4	NAG	A	908	1	14,14,15	0.33	0	17,19,21	0.67	0
4	NAG	A	905	1	14,14,15	0.31	0	17,19,21	0.58	0
5	SO4	A	911	-	4,4,4	0.50	0	6,6,6	0.35	0
4	NAG	A	903	1	14,14,15	0.29	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	907	1	14,14,15	0.30	0	17,19,21	0.90	1 (5%)
6	A1BLN	B	911	-	38,38,38	0.51	1 (2%)	46,52,52	0.84	3 (6%)
4	NAG	A	909	1	14,14,15	0.26	0	17,19,21	0.73	1 (5%)
4	NAG	B	905	1	14,14,15	0.32	0	17,19,21	0.59	0
4	NAG	B	906	1	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	A	904	1	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	A	901	1	14,14,15	0.28	0	17,19,21	0.66	0
4	NAG	B	903	1	14,14,15	0.29	0	17,19,21	0.95	1 (5%)
4	NAG	B	904	1	14,14,15	0.29	0	17,19,21	0.56	0
5	SO4	A	910	-	4,4,4	0.25	0	6,6,6	0.08	0
5	SO4	B	910	-	4,4,4	0.24	0	6,6,6	0.27	0
4	NAG	A	907	1	14,14,15	0.30	0	17,19,21	0.90	1 (5%)
6	A1BLN	A	912	-	38,38,38	0.80	2 (5%)	46,52,52	0.80	1 (2%)
4	NAG	B	908	1	14,14,15	0.33	0	17,19,21	0.71	0
4	NAG	A	906	1	14,14,15	0.30	0	17,19,21	0.54	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	A	902	1	-	0/6/23/26	0/1/1/1
4	NAG	B	901	1	-	0/6/23/26	0/1/1/1
4	NAG	B	902	1	-	0/6/23/26	0/1/1/1
4	NAG	B	909	1	-	0/6/23/26	0/1/1/1
4	NAG	A	908	1	-	0/6/23/26	0/1/1/1
4	NAG	A	905	1	-	0/6/23/26	0/1/1/1
4	NAG	A	903	1	-	0/6/23/26	0/1/1/1
4	NAG	B	907	1	-	0/6/23/26	0/1/1/1
6	A1BLN	B	911	-	-	1/21/31/31	0/4/4/4
4	NAG	A	909	1	-	0/6/23/26	0/1/1/1
4	NAG	B	905	1	-	0/6/23/26	0/1/1/1
4	NAG	B	906	1	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1	-	0/6/23/26	0/1/1/1
4	NAG	A	901	1	-	0/6/23/26	0/1/1/1
4	NAG	B	903	1	-	0/6/23/26	0/1/1/1
4	NAG	B	904	1	-	0/6/23/26	0/1/1/1
4	NAG	A	907	1	-	0/6/23/26	0/1/1/1
6	A1BLN	A	912	-	-	1/21/31/31	0/4/4/4
4	NAG	B	908	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	906	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	912	A1BLN	C15-C14	3.86	1.57	1.54
6	A	912	A1BLN	C7-C4	2.43	1.46	1.42
6	B	911	A1BLN	C15-C14	2.10	1.56	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	NAG	O5-C1-C2	-3.55	105.80	111.29
4	B	903	NAG	O5-C1-C2	-3.54	105.82	111.29
6	A	912	A1BLN	C7-C8-C10	-3.24	115.81	119.59
6	B	911	A1BLN	C7-C8-C10	-2.93	116.16	119.59
4	B	902	NAG	O5-C1-C2	-2.80	106.96	111.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	911	A1BLN	C5-C19-N7-C14
6	A	912	A1BLN	C5-C19-N7-C14

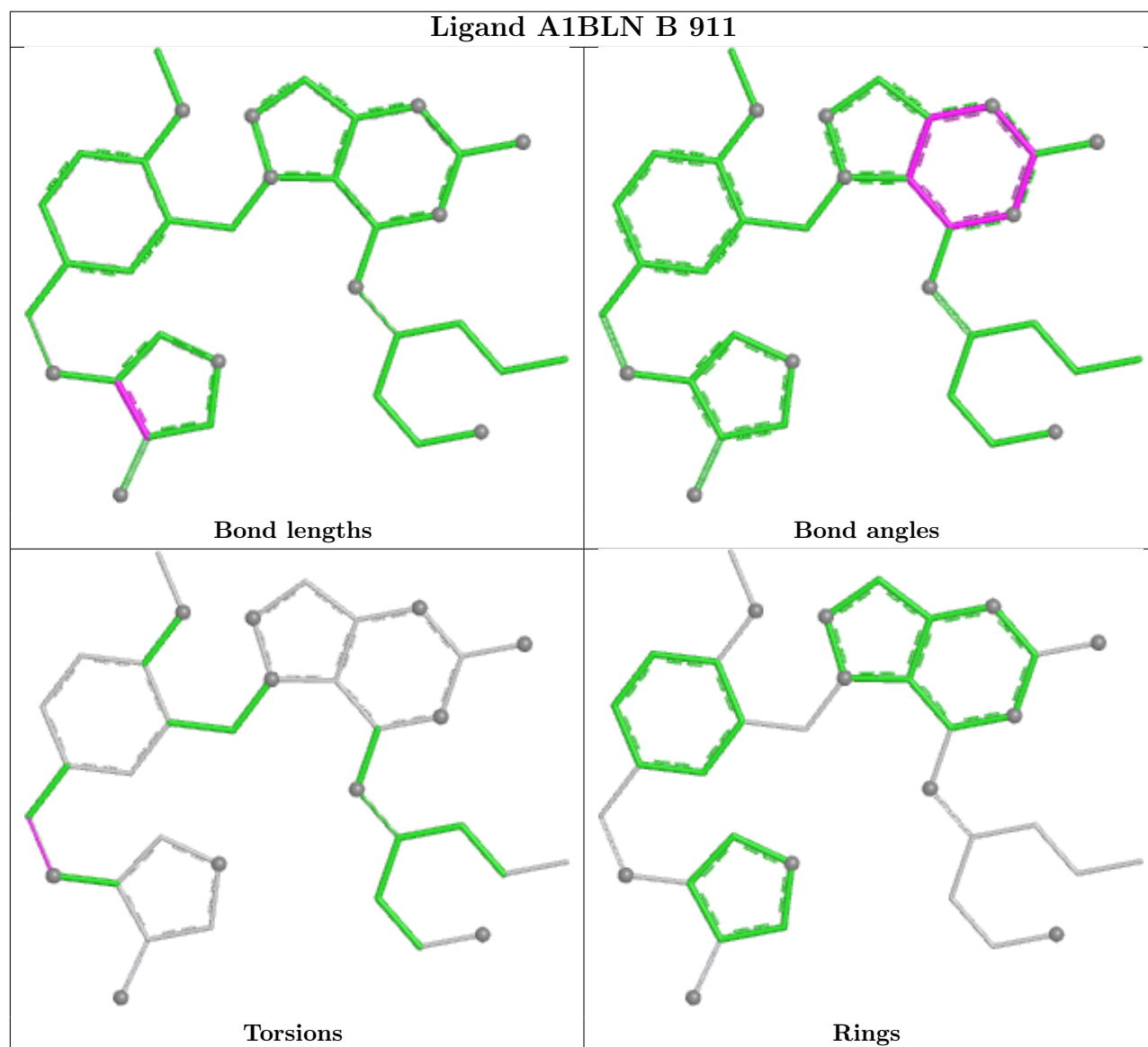
There are no ring outliers.

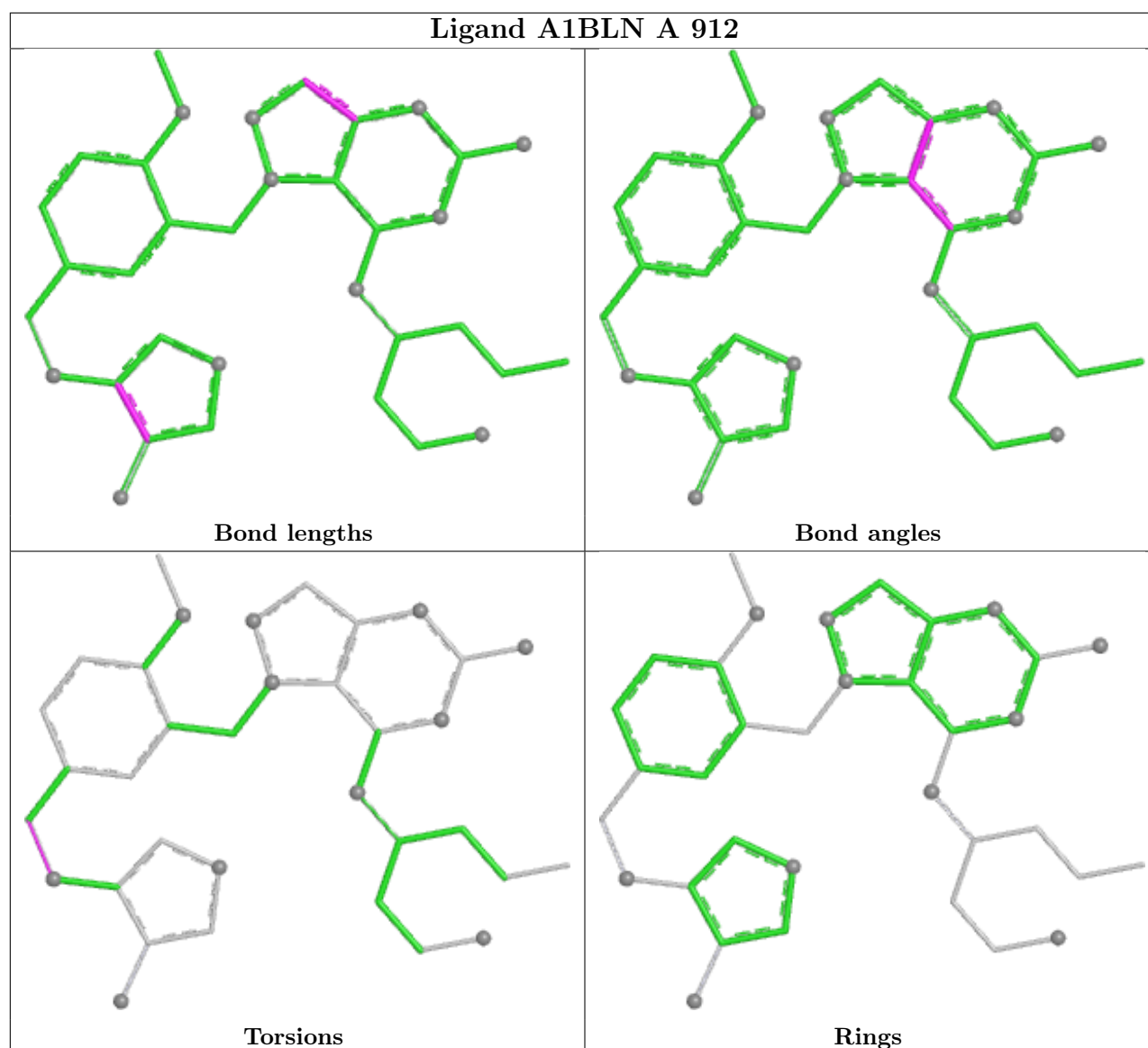
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	904	NAG	0	1

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 [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	747/807 (92%)	0.61	74 (9%) 13 13	6, 15, 29, 51	4 (0%)
1	B	747/807 (92%)	0.62	65 (8%) 16 17	6, 15, 28, 49	4 (0%)
All	All	1494/1614 (92%)	0.62	139 (9%) 14 15	6, 15, 29, 51	8 (0%)

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	732	LEU	12.2
1	A	732	LEU	8.5
1	B	735	VAL	7.8
1	B	733	SER	7.8
1	B	731	PHE	7.3

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.

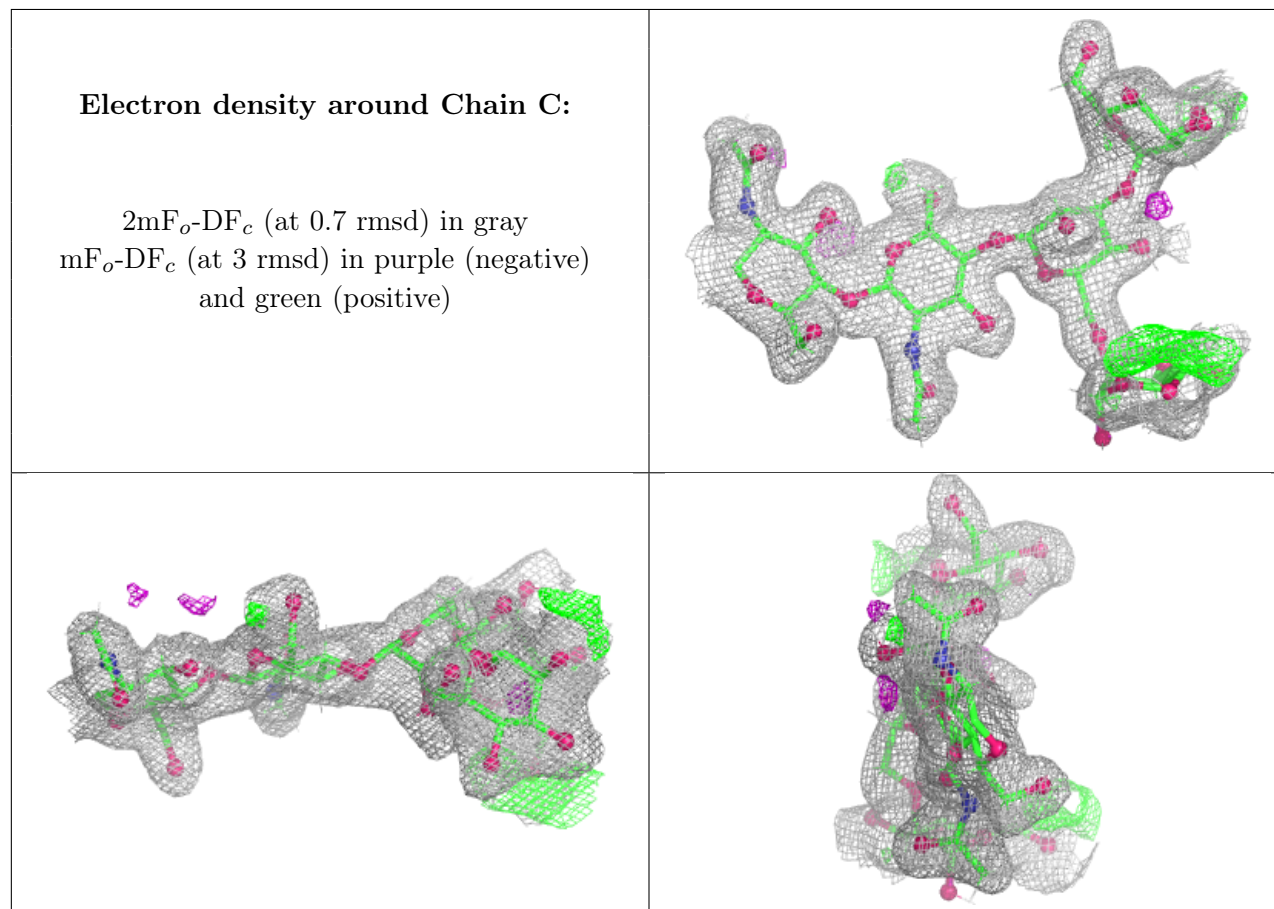
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	G	3	11/12	0.51	0.17	49,53,58,59	10
3	BMA	D	3	11/12	0.58	0.17	49,52,57,58	10
2	MAN	C	5	11/12	0.65	0.16	48,51,61,61	10
2	MAN	F	5	11/12	0.75	0.14	49,53,62,63	10
3	NAG	D	2	14/15	0.77	0.14	36,42,46,47	12

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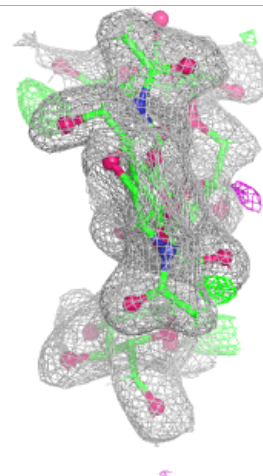
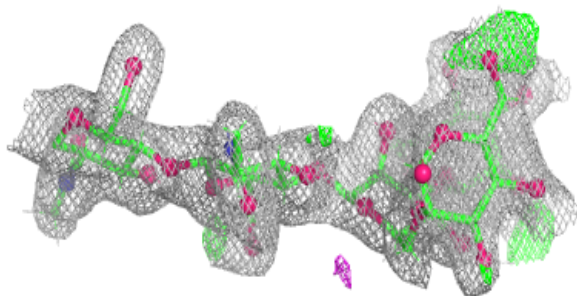
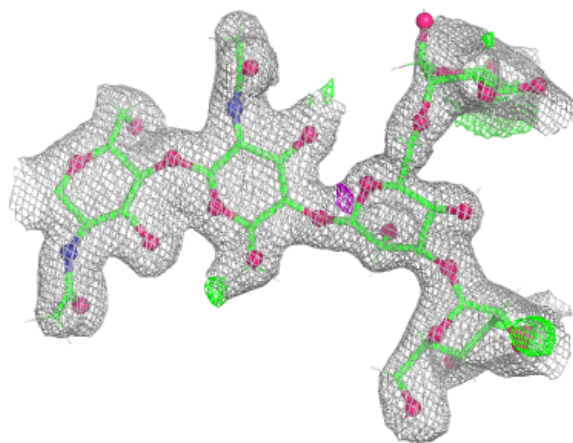
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	H	3	11/12	0.78	0.13	38,43,49,50	10
3	NAG	G	2	14/15	0.82	0.12	36,42,46,47	12
3	BMA	E	3	11/12	0.87	0.11	37,41,47,47	10
2	MAN	F	4	11/12	0.89	0.09	37,39,43,44	10
2	MAN	C	4	11/12	0.90	0.10	38,40,45,46	10
2	BMA	C	3	11/12	0.91	0.09	36,40,50,50	8
3	NAG	E	2	14/15	0.91	0.09	25,28,32,33	12
2	BMA	F	3	11/12	0.92	0.09	35,39,50,50	8
2	NAG	F	2	14/15	0.93	0.08	25,29,35,36	12
2	NAG	C	1	14/15	0.95	0.06	20,22,26,26	12
3	NAG	H	2	14/15	0.95	0.08	25,29,34,35	12
2	NAG	C	2	14/15	0.95	0.07	24,29,34,35	12
3	NAG	H	1	14/15	0.96	0.06	21,22,23,24	12
3	NAG	D	1	14/15	0.96	0.08	21,23,26,31	12
3	NAG	G	1	14/15	0.96	0.07	23,25,27,31	12
2	NAG	F	1	14/15	0.97	0.05	21,23,27,28	12
3	NAG	E	1	14/15	0.97	0.05	19,20,22,23	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.



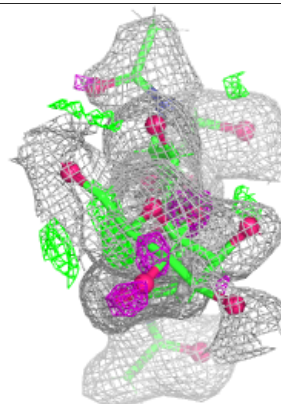
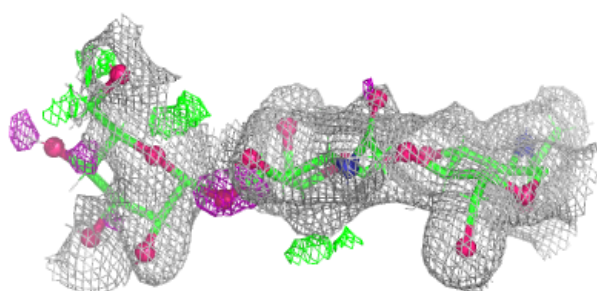
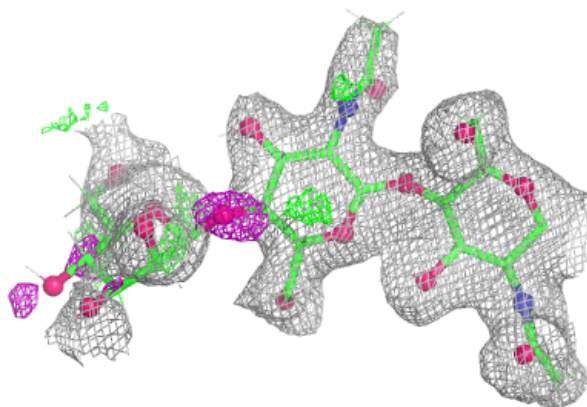
Electron density around Chain F:

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

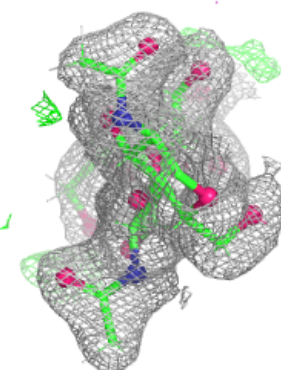
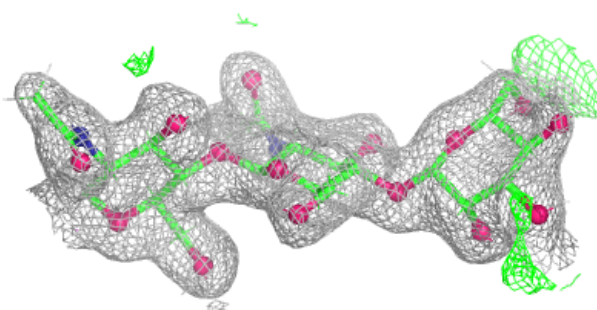
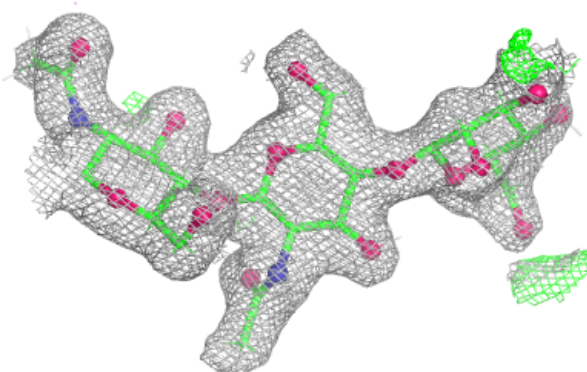


Electron density around Chain D:

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

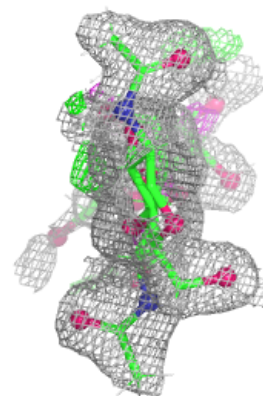
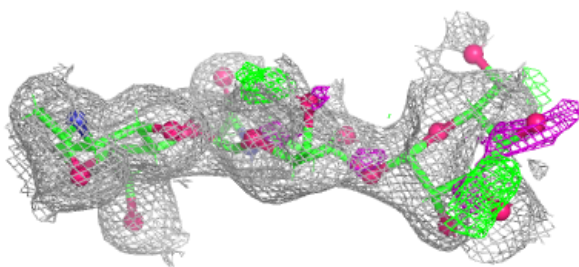
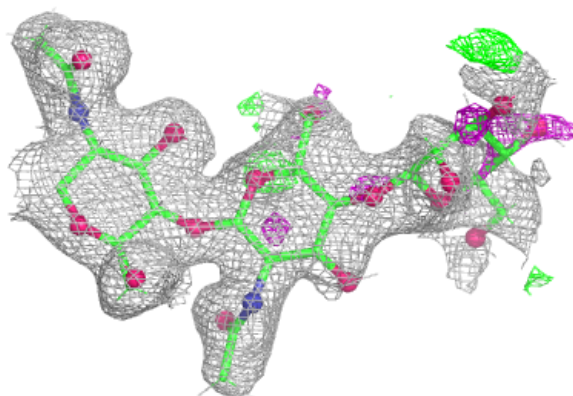
**Electron density around Chain E:**

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

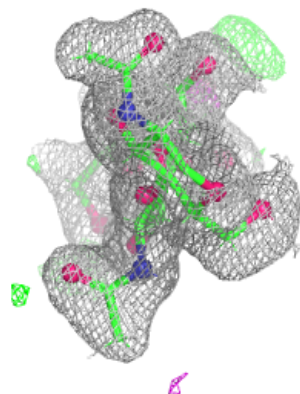
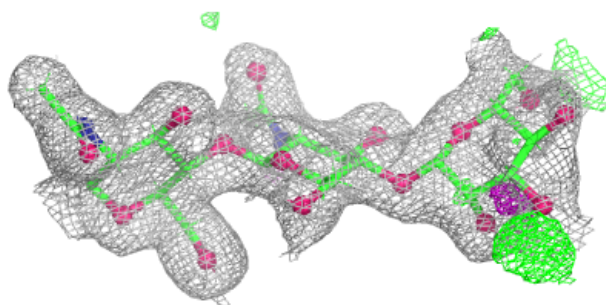
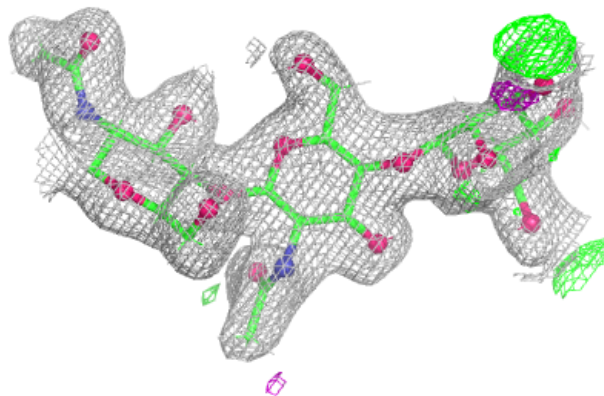


Electron density around Chain G:

$2mF_o-DF_c$ (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 ⓘ

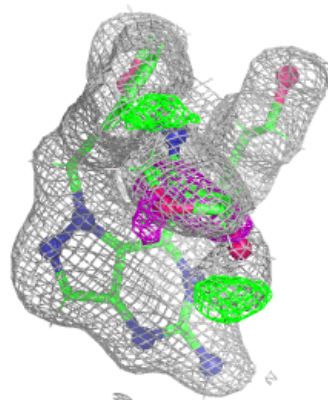
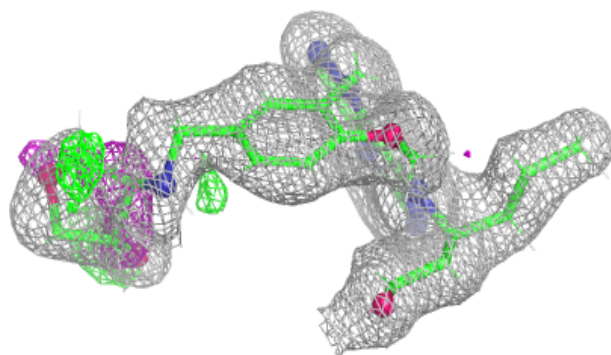
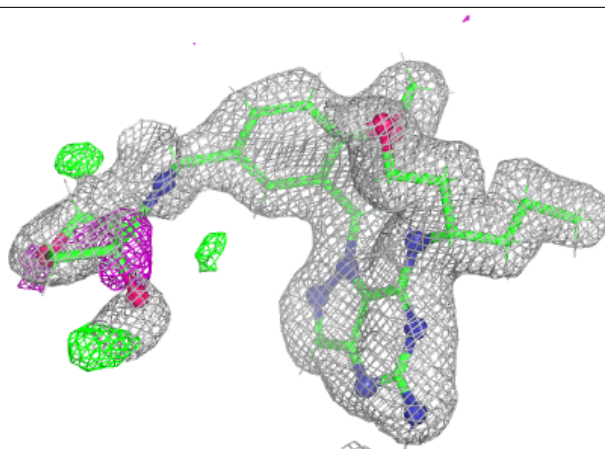
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	NAG	A	905	14/15	0.52	0.17	61,62,82,82	13
4	NAG	B	905	14/15	0.56	0.19	60,62,83,83	13
4	NAG	B	903	14/15	0.64	0.17	48,49,65,65	13
4	NAG	B	902	14/15	0.65	0.17	60,63,83,84	13
5	SO4	A	910	5/5	0.66	0.16	99,99,99,99	0
4	NAG	A	901	14/15	0.70	0.15	62,64,92,93	13
4	NAG	B	907	14/15	0.71	0.14	49,52,67,68	13
4	NAG	B	901	14/15	0.77	0.14	55,56,79,80	13
4	NAG	A	907	14/15	0.77	0.13	45,48,60,61	13
4	NAG	B	906	14/15	0.80	0.13	43,46,59,59	13
4	NAG	A	906	14/15	0.82	0.13	38,42,53,53	13
4	NAG	A	903	14/15	0.83	0.12	45,47,64,65	13
4	NAG	B	909	14/15	0.86	0.11	42,45,62,63	13
4	NAG	B	904	14/15	0.86	0.10	37,40,51,52	13
4	NAG	A	909	14/15	0.88	0.10	37,41,55,56	13
4	NAG	A	908	14/15	0.88	0.09	27,31,40,41	13
4	NAG	A	902	14/15	0.89	0.11	36,39,59,60	13
4	NAG	B	908	14/15	0.89	0.10	33,36,48,48	13
4	NAG	A	904	14/15	0.90	0.09	33,35,46,47	13
5	SO4	A	911	5/5	0.91	0.10	41,41,42,42	0
6	A1BLN	A	912	35/35	0.91	0.09	19,26,47,48	35
5	SO4	B	910	5/5	0.92	0.09	41,41,42,42	0
6	A1BLN	B	911	35/35	0.93	0.09	18,27,48,48	35

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.

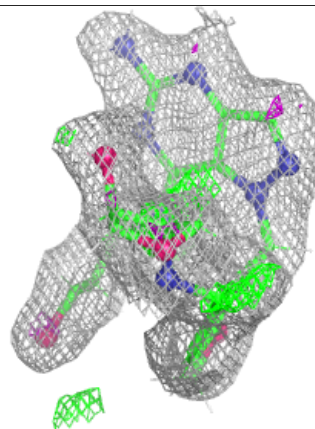
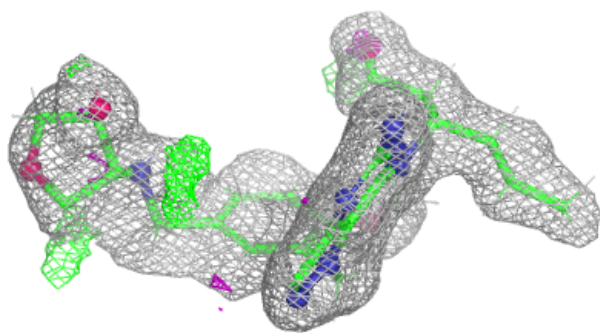
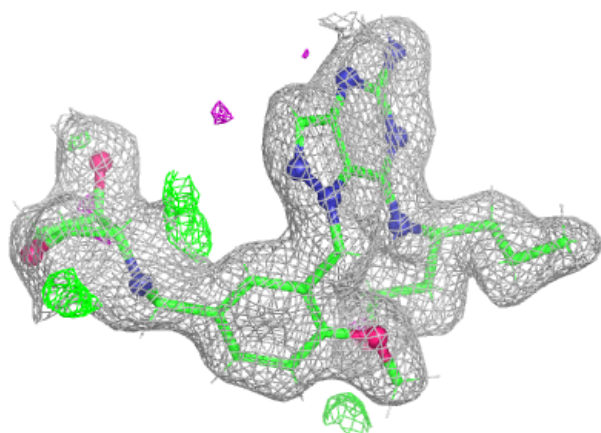
Electron density around A1BLN A 912:

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



Electron density around A1BLN 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 ⓘ

There are no such residues in this entry.