



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2022 – 03:11 pm GMT

PDB ID : 7R52
Title : Crystal structure of human TLR8 in complex with Compound 2
Authors : Faller, M.; Zink, F.
Deposited on : 2022-02-10
Resolution : 2.94 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

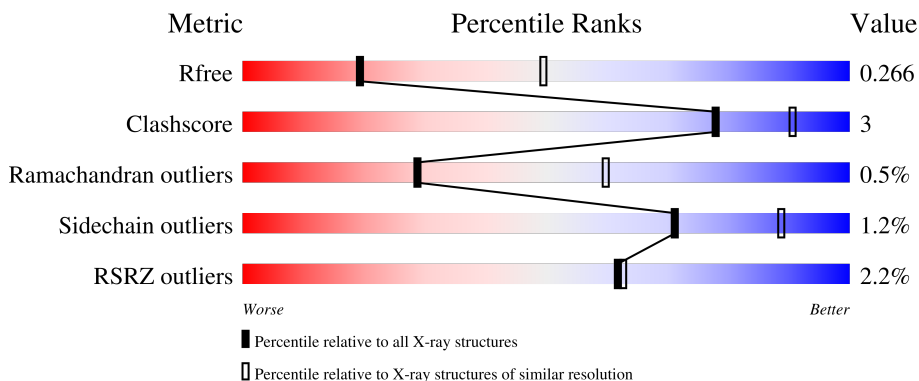
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	807	
1	B	807	
2	C	5	
2	E	5	
2	F	5	

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Mol	Chain	Length	Quality of chain
2	H	5	 60% 40%
3	D	3	 67% 33%
3	G	3	 67% 33%

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
4	NAG	A	906	-	-	-	X
4	NAG	B	903	-	-	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 11900 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.

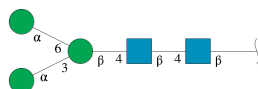
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	733	5619	3579	952	1069	19	0	0	0
1	B	733	5542	3527	926	1070	19	0	0	0

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



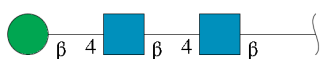
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	5	61	34	2	25	0	0	0

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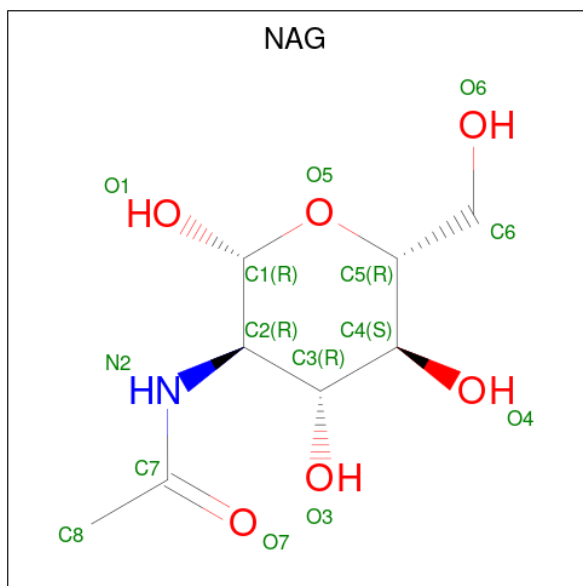
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



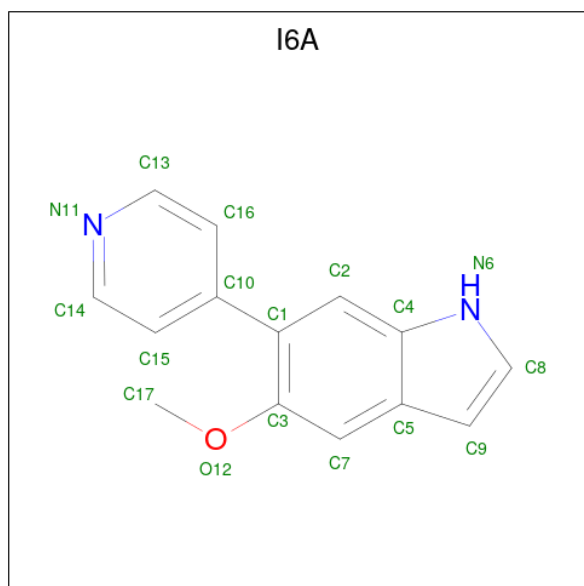
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is 5-methoxy-6-pyridin-4-yl-1 {H}-indole (three-letter code: I6A) (formula: C₁₄H₁₂N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	14	2	1		
5	B	1	Total	C	N	O	0	0
			17	14	2	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	119	Total	O	0	0
			119	119		
6	B	96	Total	O	0	0
			96	96		

nose

Chain C:  40% 60%

• Molecule 2: 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

Chain E:  40% 60%

• Molecule 2: 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

Chain F:  40% 60%

• Molecule 2: 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

Chain H:  60% 40%

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67% 33%

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  67% 33%

4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.54Å 87.23Å 153.05Å 90.00° 120.10° 90.00°	Depositor
Resolution (Å)	132.42 – 2.94 132.41 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.9 (132.42-2.94) 99.0 (132.41-2.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.96Å)	Xtrriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.253 , 0.274 0.246 , 0.266	Depositor DCC
R_{free} test set	2007 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	81.3	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11900	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I6A, NAG, MAN, BMA

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	0.24	0/5731	0.45	0/7817
1	B	0.24	0/5650	0.44	0/7717
All	All	0.24	0/11381	0.44	0/15534

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

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	5619	0	5342	32	0
1	B	5542	0	5191	33	0
2	C	61	0	52	0	0
2	E	61	0	52	0	0
2	F	61	0	52	0	0
2	H	61	0	52	0	0
3	D	39	0	34	0	0
3	G	39	0	34	0	0
4	A	84	0	78	0	0
4	B	84	0	78	0	0
5	A	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	17	0	0	0	0
6	A	119	0	0	0	0
6	B	96	0	0	0	0
All	All	11900	0	10965	65	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 65 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:SER:HA	1:B:755:ALA:HA	1.39	1.01
1:A:729:SER:HA	1:A:755:ALA:HA	1.56	0.88
1:A:385:ASP:HA	1:A:388:GLN:HG3	1.68	0.74
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.81	0.62
1:B:373:HIS:HA	1:B:400:ASN:HB3	1.81	0.62

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	721/807 (89%)	678 (94%)	39 (5%)	4 (1%)	25	56
1	B	721/807 (89%)	676 (94%)	42 (6%)	3 (0%)	34	64
All	All	1442/1614 (89%)	1354 (94%)	81 (6%)	7 (0%)	29	60

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	601	ASP

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Mol	Chain	Res	Type
1	B	601	ASP
1	B	330	GLY
1	A	189	LYS
1	A	330	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	613/751 (82%)	605 (99%)	8 (1%)	69 88
1	B	598/751 (80%)	592 (99%)	6 (1%)	76 91
All	All	1211/1502 (81%)	1197 (99%)	14 (1%)	71 89

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	817	LEU
1	B	49	CYS
1	B	626	ASP
1	B	541	ARG
1	B	581	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	581	GLN
1	B	469	HIS
1	B	84	GLN
1	A	625	ASN
1	B	284	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

26 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	1,2	14,14,15	0.28	0	17,19,21	0.42	0
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.94	2 (11%)
2	BMA	C	3	2	11,11,12	0.26	0	15,15,17	0.39	0
2	MAN	C	4	2	11,11,12	0.29	0	15,15,17	0.81	1 (6%)
2	MAN	C	5	2	11,11,12	0.30	0	15,15,17	0.72	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.27	0	17,19,21	0.53	0
3	NAG	D	2	3	14,14,15	0.30	0	17,19,21	0.53	0
3	BMA	D	3	3	11,11,12	0.32	0	15,15,17	0.70	1 (6%)
2	NAG	E	1	1,2	14,14,15	0.27	0	17,19,21	0.58	1 (5%)
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.44	0
2	BMA	E	3	2	11,11,12	0.27	0	15,15,17	0.51	0
2	MAN	E	4	2	11,11,12	0.33	0	15,15,17	0.85	1 (6%)
2	MAN	E	5	2	11,11,12	0.34	0	15,15,17	0.80	1 (6%)
2	NAG	F	1	1,2	14,14,15	0.27	0	17,19,21	0.43	0
2	NAG	F	2	2	14,14,15	0.29	0	17,19,21	0.90	2 (11%)
2	BMA	F	3	2	11,11,12	0.27	0	15,15,17	0.47	0
2	MAN	F	4	2	11,11,12	0.32	0	15,15,17	0.83	1 (6%)
2	MAN	F	5	2	11,11,12	0.33	0	15,15,17	0.75	1 (6%)
3	NAG	G	1	1,3	14,14,15	0.27	0	17,19,21	0.53	0
3	NAG	G	2	3	14,14,15	0.28	0	17,19,21	0.60	1 (5%)
3	BMA	G	3	3	11,11,12	0.31	0	15,15,17	0.51	0
2	NAG	H	1	1,2	14,14,15	0.27	0	17,19,21	0.57	0
2	NAG	H	2	2	14,14,15	0.28	0	17,19,21	0.47	0
2	BMA	H	3	2	11,11,12	0.28	0	15,15,17	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	H	4	2	11,11,12	0.36	0	15,15,17	0.85	1 (6%)
2	MAN	H	5	2	11,11,12	0.36	0	15,15,17	0.78	1 (6%)

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	1,2	-	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	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	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	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	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
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
2	MAN	H	5	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4	MAN	C1-O5-C5	3.08	116.36	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	MAN	C1-O5-C5	3.05	116.32	112.19
2	F	4	MAN	C1-O5-C5	3.00	116.26	112.19
2	C	4	MAN	C1-O5-C5	2.89	116.10	112.19
2	F	5	MAN	C1-O5-C5	2.73	115.89	112.19

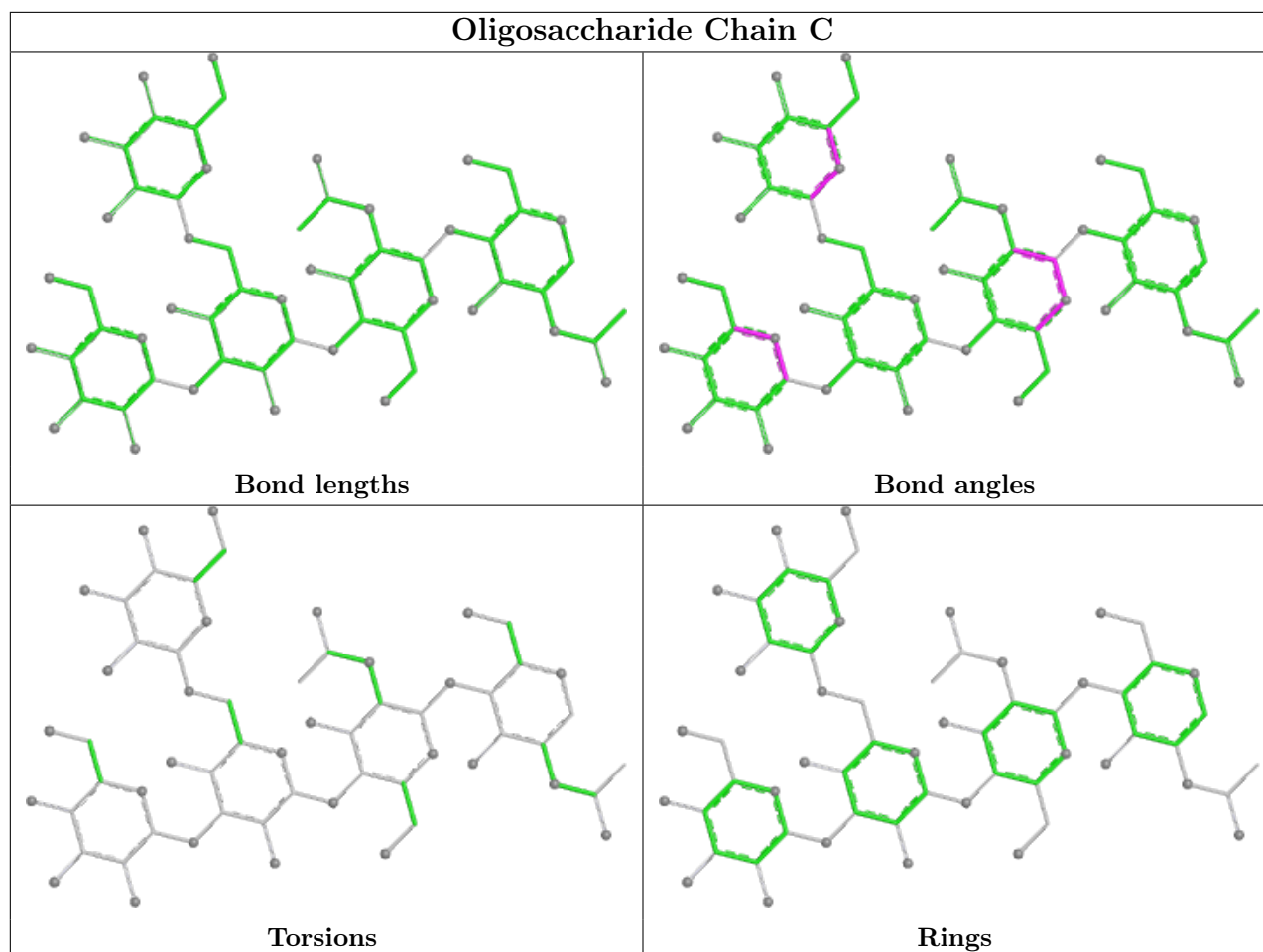
There are no chirality outliers.

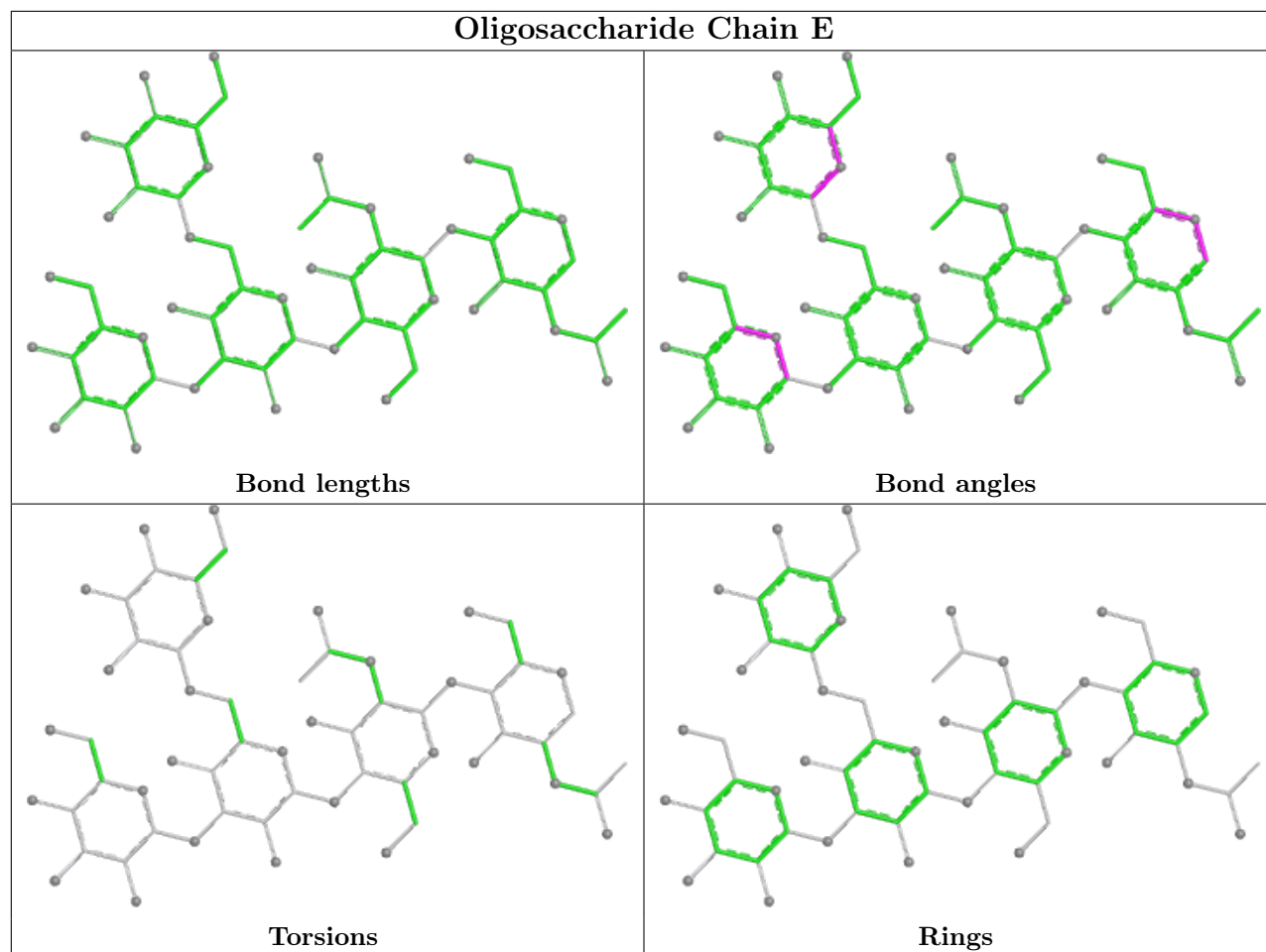
There are no torsion outliers.

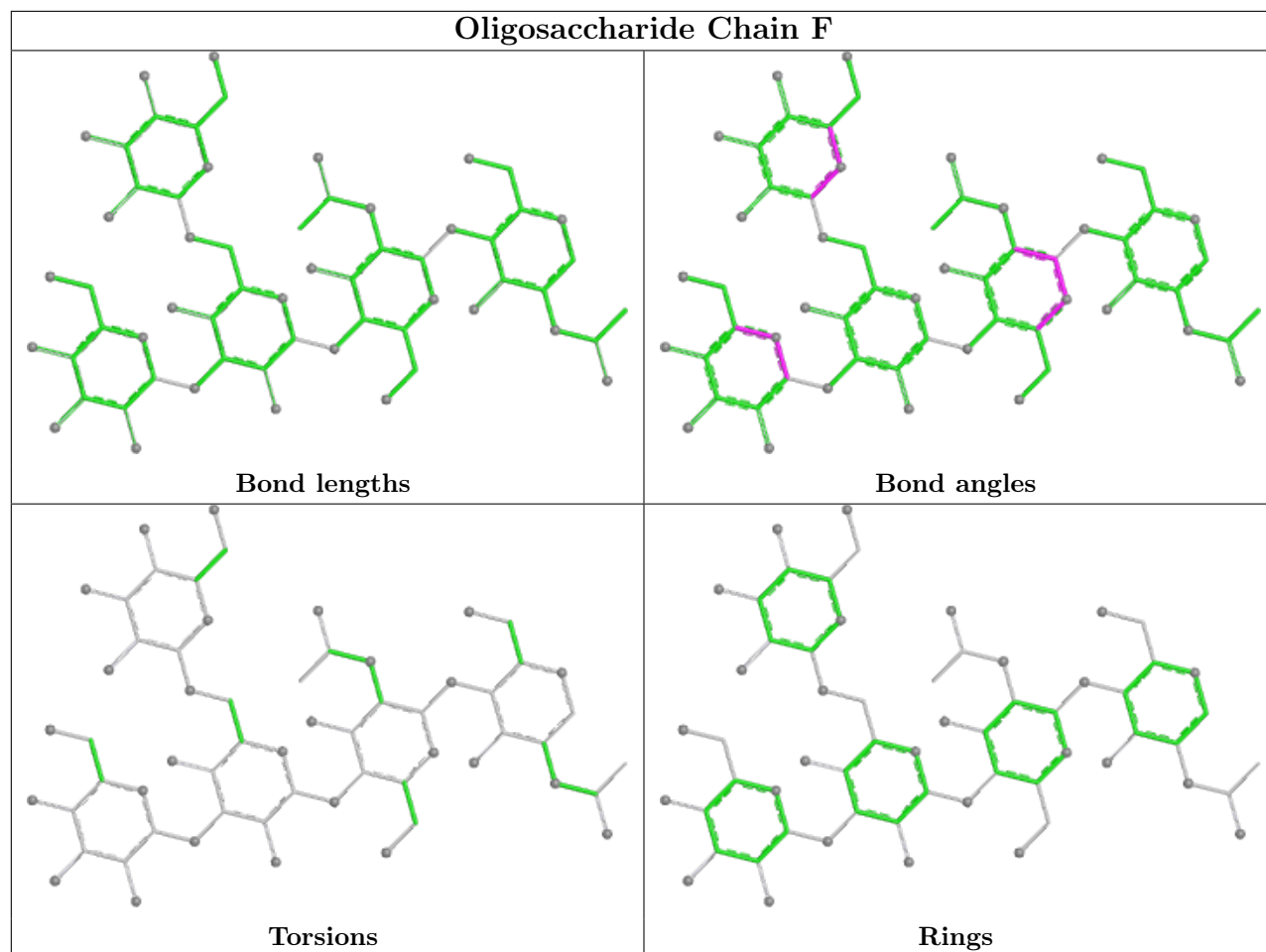
There are no ring outliers.

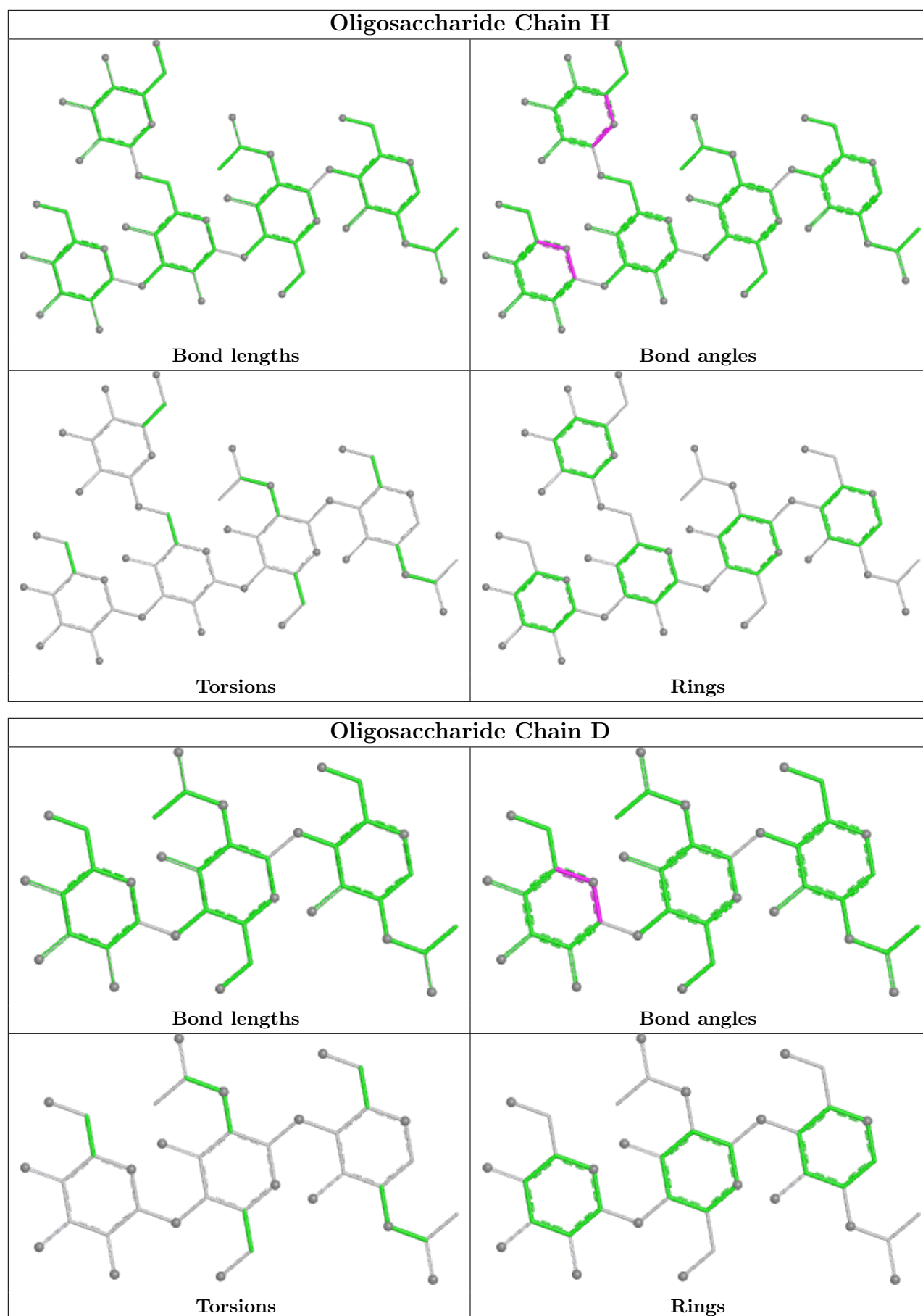
No monomer is involved in short contacts.

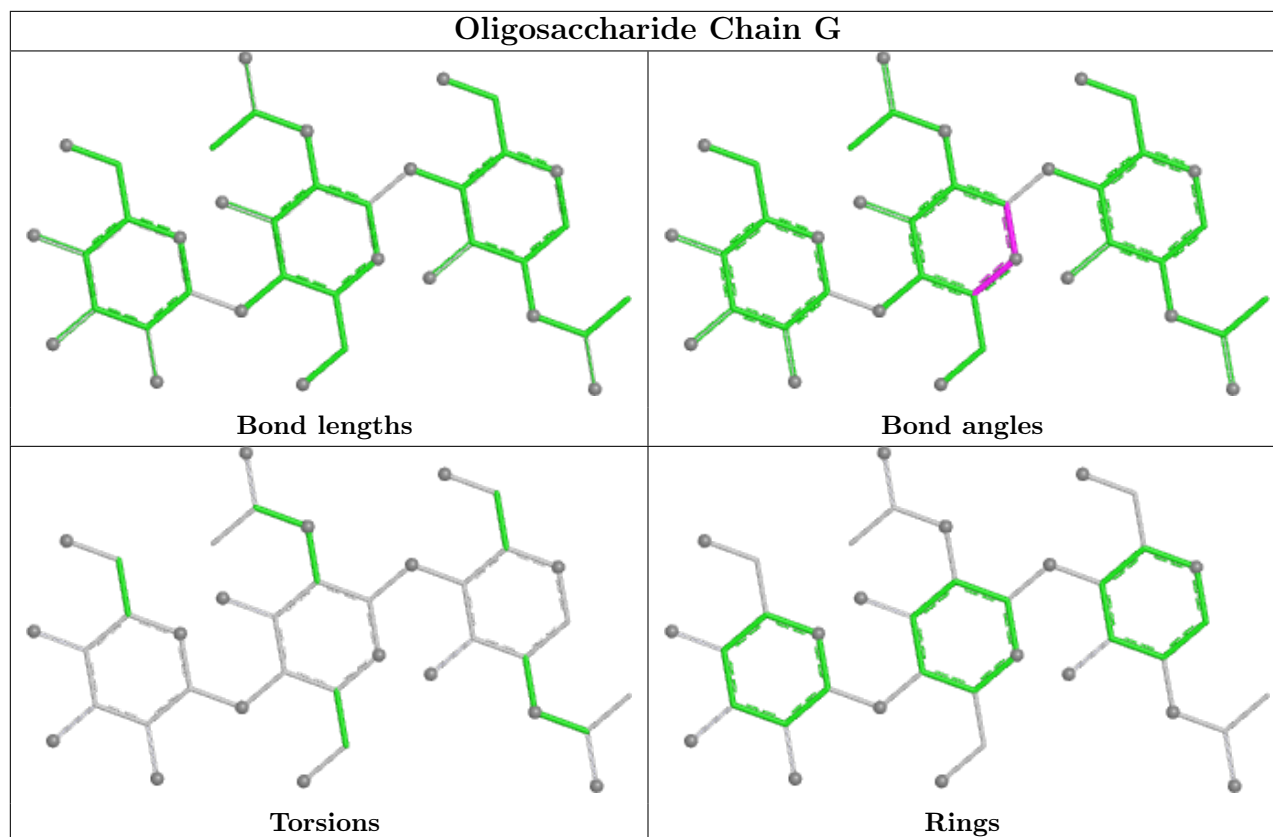
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

14 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	0.27	0	17,19,21	0.64	1 (5%)
4	NAG	A	903	1	14,14,15	0.32	0	17,19,21	0.60	1 (5%)
4	NAG	A	905	1	14,14,15	0.30	0	17,19,21	0.76	1 (5%)
4	NAG	A	906	1	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	A	904	1	14,14,15	0.34	0	17,19,21	0.78	0
5	I6A	A	907	-	17,19,19	1.12	2 (11%)	21,26,26	1.73	4 (19%)
4	NAG	B	904	1	14,14,15	0.33	0	17,19,21	0.84	1 (5%)
4	NAG	B	905	1	14,14,15	0.29	0	17,19,21	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	906	1	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	B	903	1	14,14,15	0.32	0	17,19,21	0.63	1 (5%)
4	NAG	B	902	1	14,14,15	0.27	0	17,19,21	0.61	1 (5%)
4	NAG	B	901	1	14,14,15	0.28	0	17,19,21	0.82	1 (5%)
5	I6A	B	907	-	17,19,19	1.23	2 (11%)	21,26,26	1.78	5 (23%)
4	NAG	A	901	1	14,14,15	0.25	0	17,19,21	0.90	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	902	1	-	0/6/23/26	0/1/1/1
4	NAG	A	903	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	906	1	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1	-	1/6/23/26	0/1/1/1
5	I6A	A	907	-	-	0/6/6/6	0/3/3/3
4	NAG	B	904	1	-	1/6/23/26	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	B	903	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	901	1	-	0/6/23/26	0/1/1/1
5	I6A	B	907	-	-	0/6/6/6	0/3/3/3
4	NAG	A	901	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	907	I6A	C7-C3	2.61	1.41	1.36
5	B	907	I6A	O12-C3	2.37	1.40	1.37
5	A	907	I6A	C7-C3	2.29	1.40	1.36
5	A	907	I6A	O12-C3	2.07	1.40	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	907	I6A	C9-C5-C4	-4.10	102.69	106.20
5	A	907	I6A	C9-C5-C4	-4.01	102.78	106.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	907	I6A	C17-O12-C3	3.37	122.61	117.53
5	B	907	I6A	O12-C3-C7	-3.29	120.98	125.24
4	A	901	NAG	C1-C2-N2	-3.12	105.16	110.49

There are no chirality outliers.

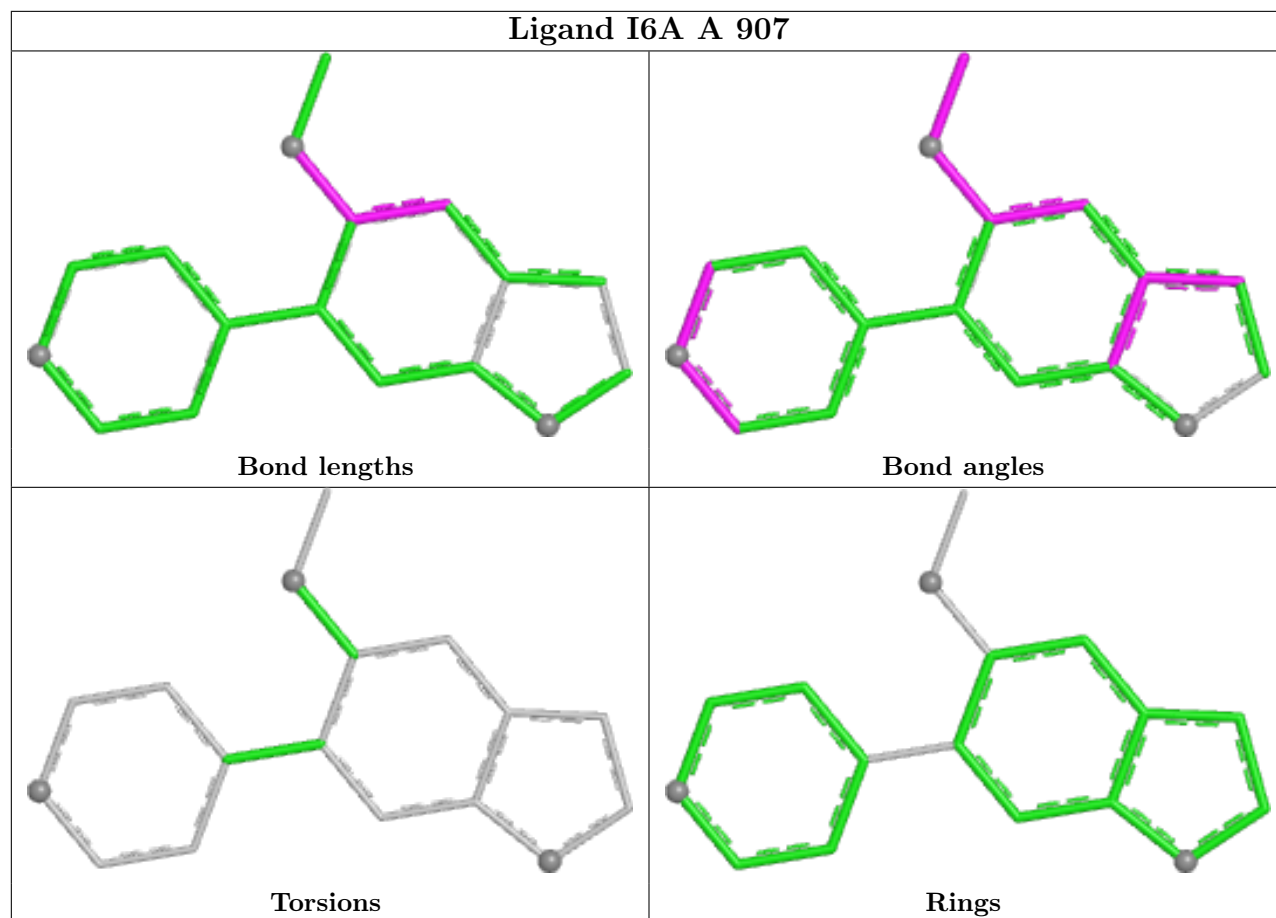
All (2) torsion outliers are listed below:

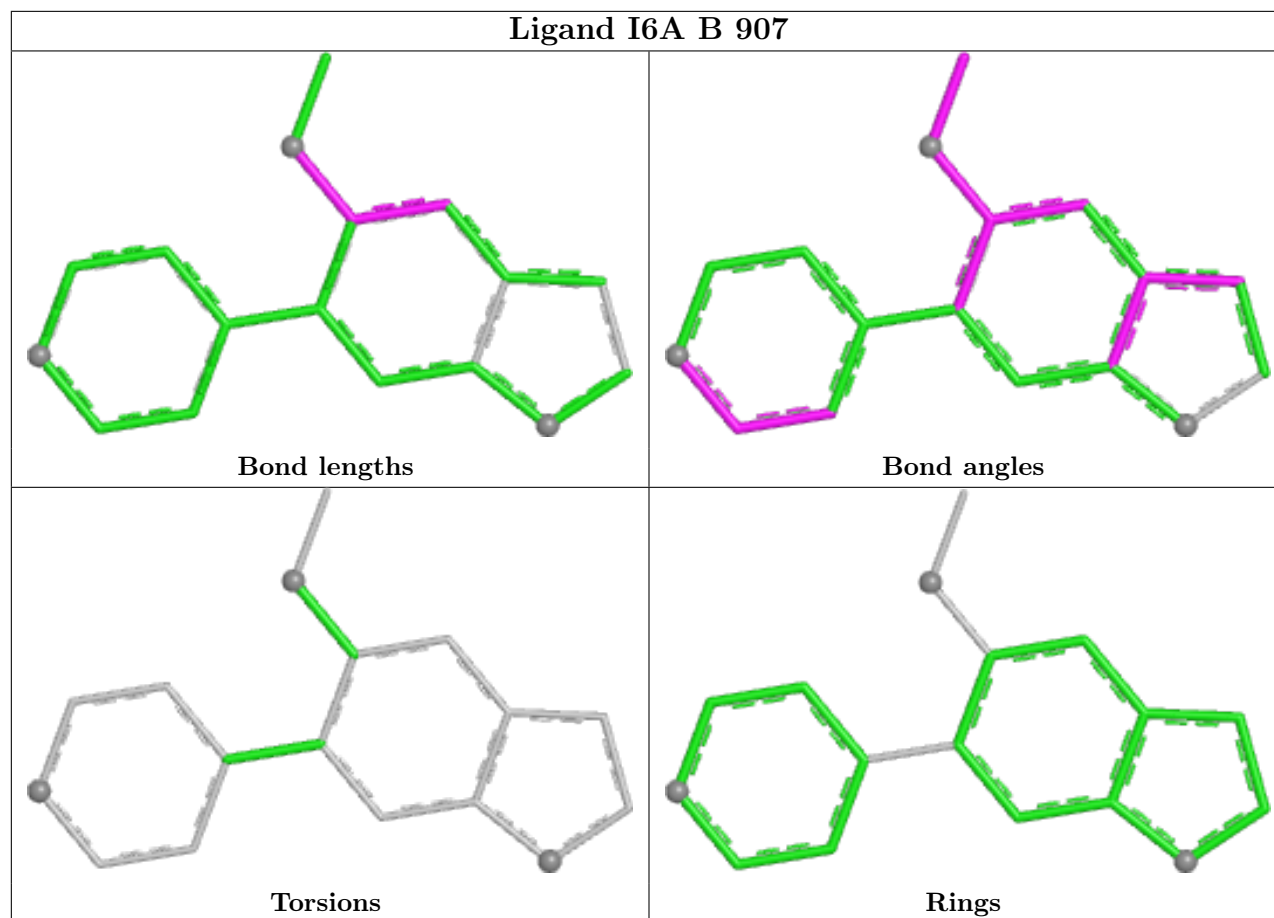
Mol	Chain	Res	Type	Atoms
4	A	904	NAG	C1-C2-N2-C7
4	B	904	NAG	C1-C2-N2-C7

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	733/807 (90%)	0.13	14 (1%) 66 67	53, 87, 110, 127	0
1	B	733/807 (90%)	0.19	18 (2%) 57 58	57, 90, 164, 175	0
All	All	1466/1614 (90%)	0.16	32 (2%) 62 63	53, 88, 137, 175	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	40	LYS	4.8
1	A	626	ASP	3.9
1	B	604	ASN	3.5
1	B	236	TYR	3.3
1	A	216	VAL	3.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	E	4	11/12	0.68	0.28	96,97,97,97	0
2	MAN	H	4	11/12	0.68	0.19	98,98,99,99	0
2	MAN	C	5	11/12	0.71	0.26	99,100,100,100	0
2	MAN	H	5	11/12	0.72	0.17	99,99,99,99	0
2	MAN	E	5	11/12	0.76	0.17	97,98,98,98	0

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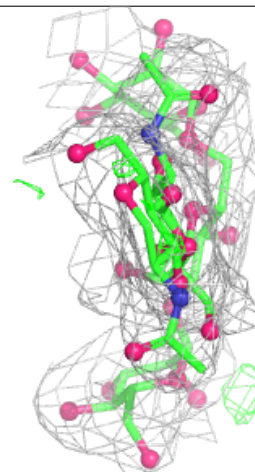
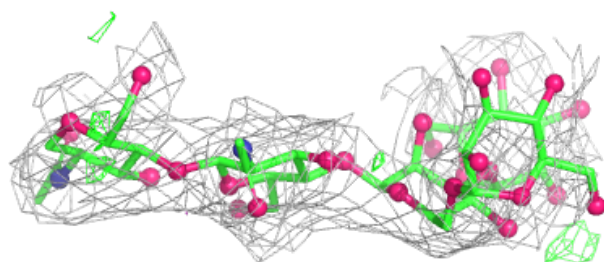
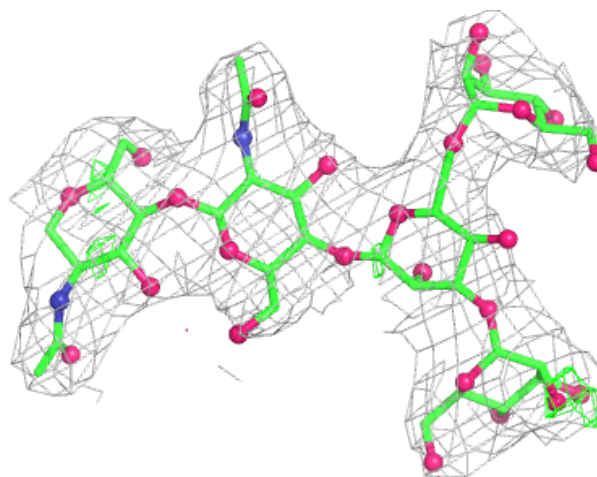
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	C	4	11/12	0.78	0.20	98,99,99,99	0
2	MAN	F	5	11/12	0.78	0.18	98,98,98,98	0
2	BMA	C	3	11/12	0.82	0.19	95,97,98,99	0
3	BMA	D	3	11/12	0.82	0.31	90,91,91,91	0
2	BMA	H	3	11/12	0.84	0.16	94,96,97,98	0
2	MAN	F	4	11/12	0.84	0.21	97,98,98,98	0
3	BMA	G	3	11/12	0.85	0.27	94,95,95,95	0
2	BMA	E	3	11/12	0.87	0.23	90,93,95,96	0
2	BMA	F	3	11/12	0.88	0.12	93,95,96,97	0
3	NAG	G	2	14/15	0.89	0.16	88,90,91,93	0
3	NAG	D	2	14/15	0.90	0.29	84,85,87,89	0
2	NAG	F	1	14/15	0.94	0.24	81,82,83,85	0
2	NAG	C	2	14/15	0.95	0.18	89,90,92,94	0
2	NAG	H	2	14/15	0.95	0.16	86,87,89,91	0
2	NAG	C	1	14/15	0.95	0.22	85,86,87,88	0
2	NAG	E	2	14/15	0.96	0.16	80,81,84,87	0
3	NAG	D	1	14/15	0.96	0.21	76,77,79,81	0
2	NAG	F	2	14/15	0.97	0.19	86,87,89,91	0
3	NAG	G	1	14/15	0.97	0.18	82,82,84,86	0
2	NAG	E	1	14/15	0.97	0.21	73,74,75,78	0
2	NAG	H	1	14/15	0.97	0.19	80,81,82,84	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.

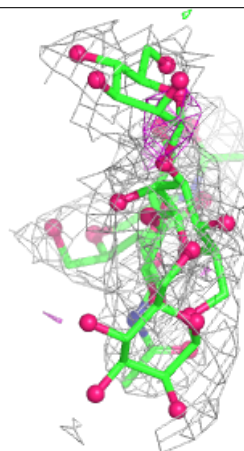
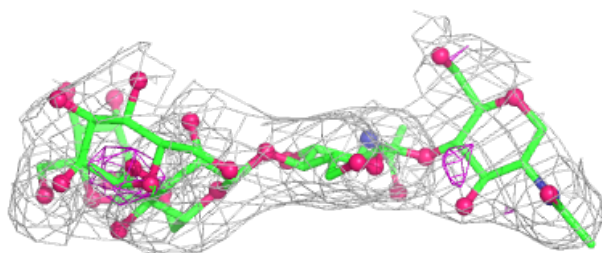
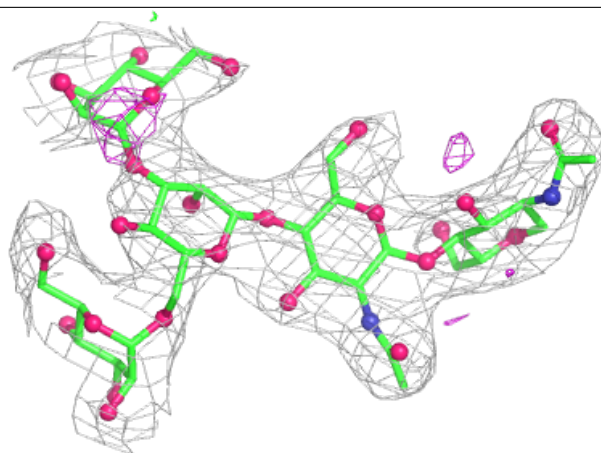
Electron density around Chain C:

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



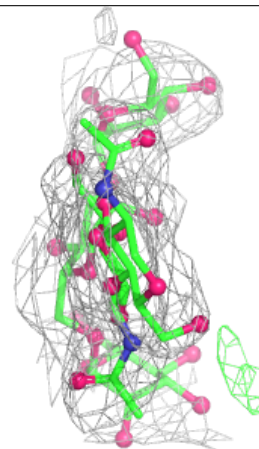
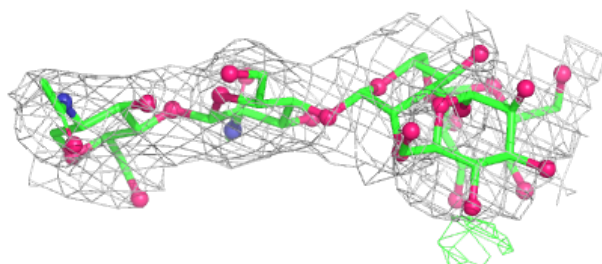
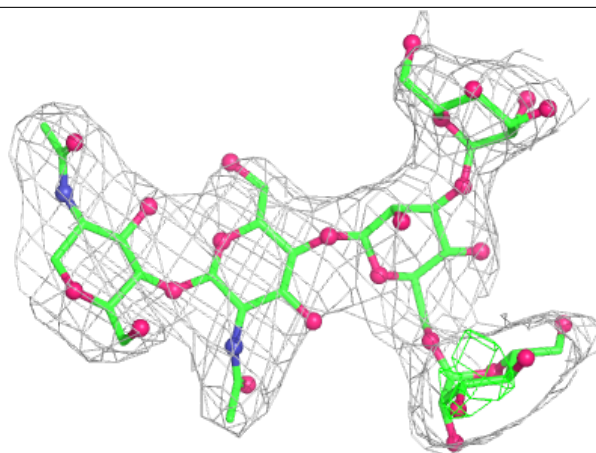
Electron density around Chain E:

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



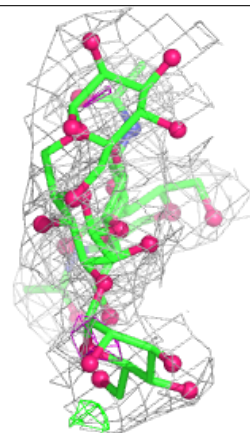
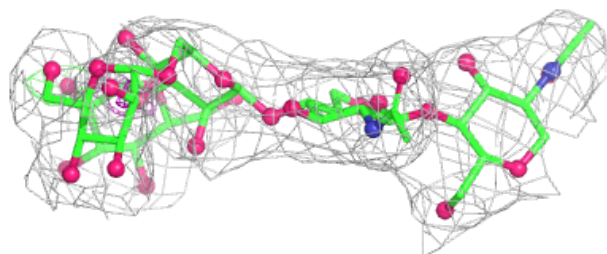
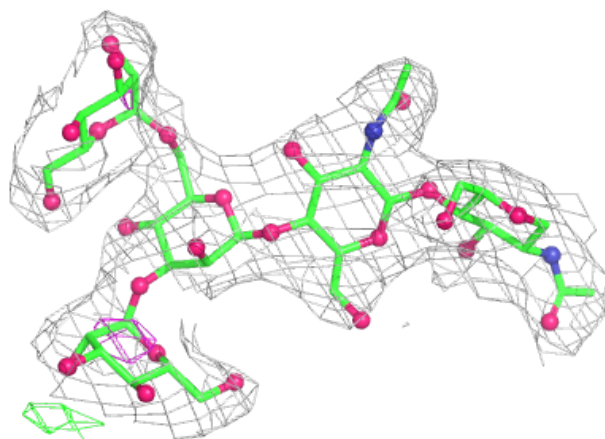
Electron density around Chain F:

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

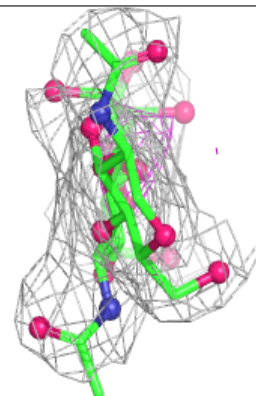
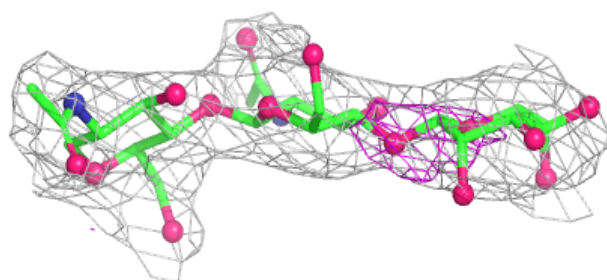
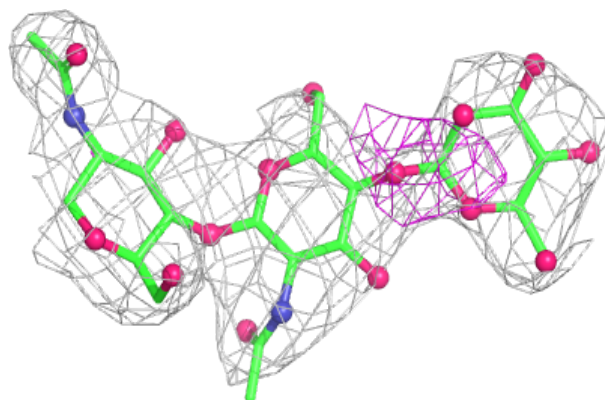


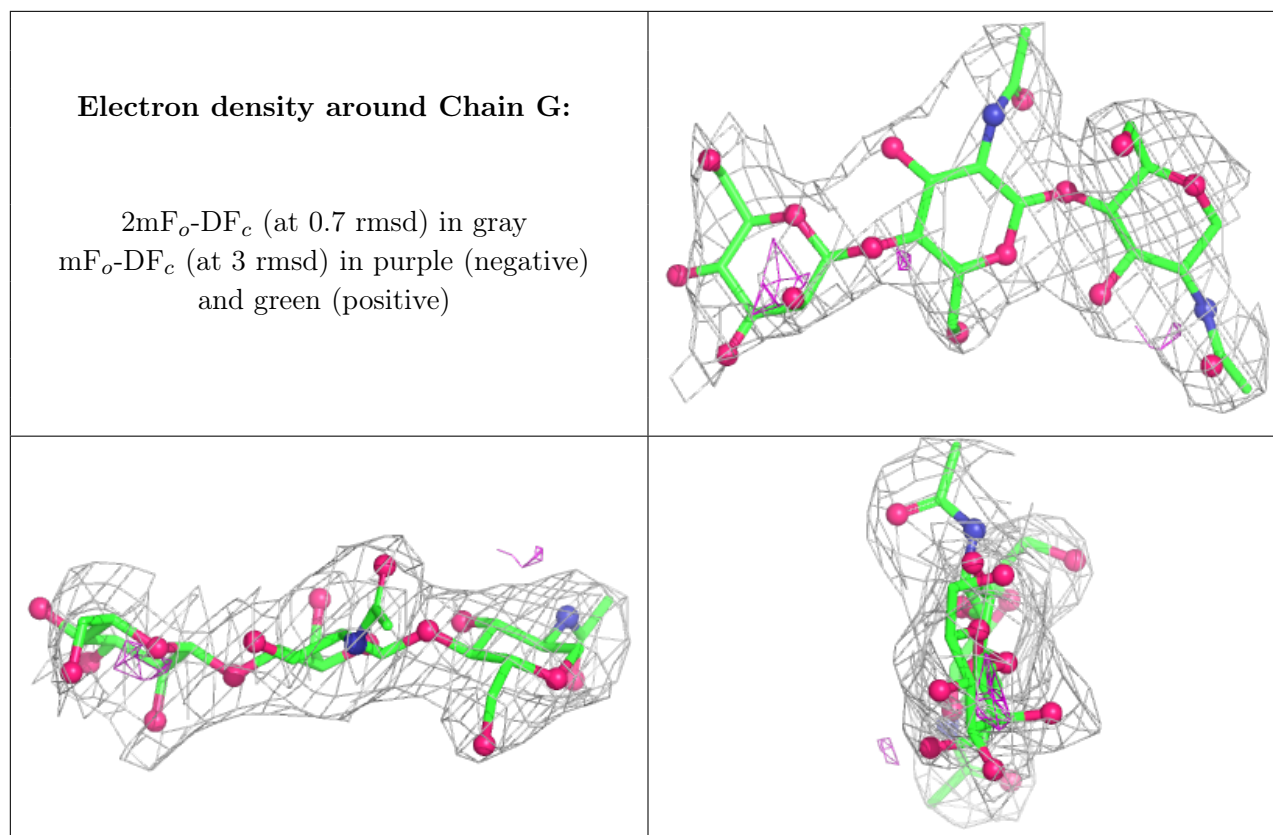
Electron density around Chain H:

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

**Electron density around Chain D:**

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



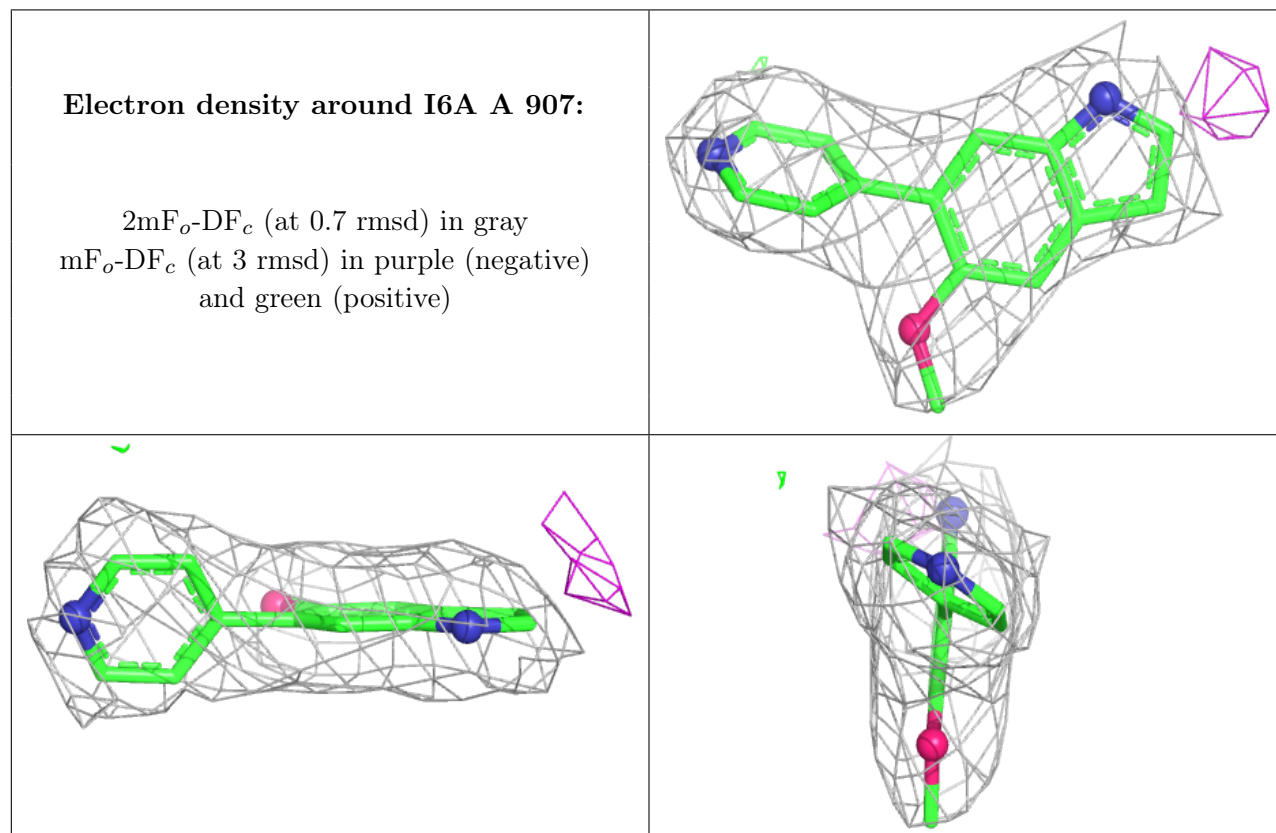


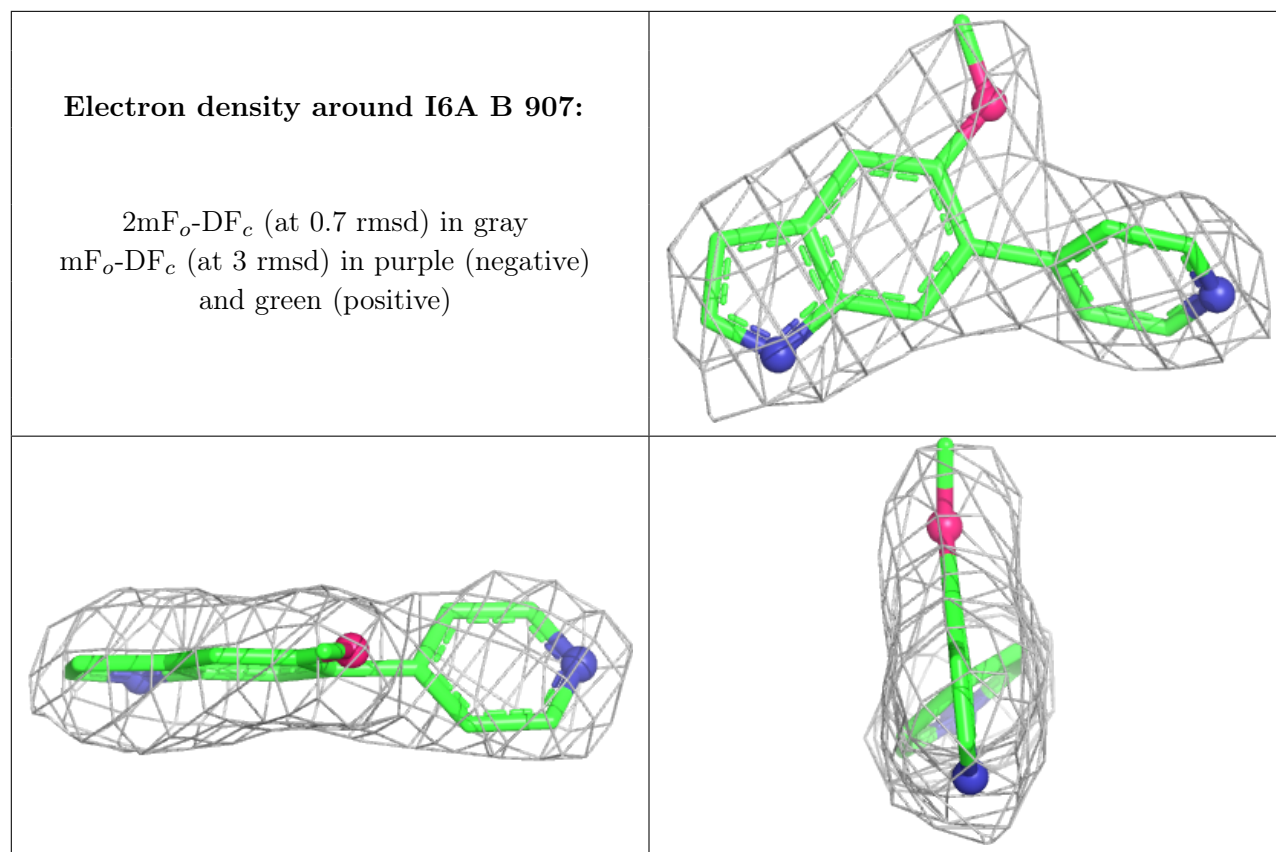
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
4	NAG	A	905	14/15	0.70	0.40	96,97,98,98	0
4	NAG	B	904	14/15	0.70	0.34	94,94,94,95	0
4	NAG	B	903	14/15	0.71	0.44	94,95,95,95	0
4	NAG	A	904	14/15	0.72	0.28	103,104,105,105	0
4	NAG	B	905	14/15	0.75	0.34	102,102,103,104	0
4	NAG	A	906	14/15	0.77	0.41	120,121,121,121	0
4	NAG	B	906	14/15	0.77	0.28	142,142,142,142	0
4	NAG	A	901	14/15	0.81	0.30	81,81,82,83	0
4	NAG	B	901	14/15	0.81	0.22	88,89,89,89	0
4	NAG	A	903	14/15	0.81	0.35	99,99,100,100	0
4	NAG	A	902	14/15	0.83	0.18	98,99,99,99	0
4	NAG	B	902	14/15	0.83	0.20	110,110,110,110	0
5	I6A	A	907	17/17	0.96	0.24	57,57,57,57	0
5	I6A	B	907	17/17	0.97	0.30	58,58,59,59	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.