



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:06 AM UTC

PDB ID : 6TY5 / pdb_00006ty5
Title : Crystal structure of human TLR8 in complex with Compound 11
Authors : Faller, M.; Zink, F.
Deposited on : 2020-01-15
Resolution : 2.79 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 : 4-5-2 with Phenix2.0
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

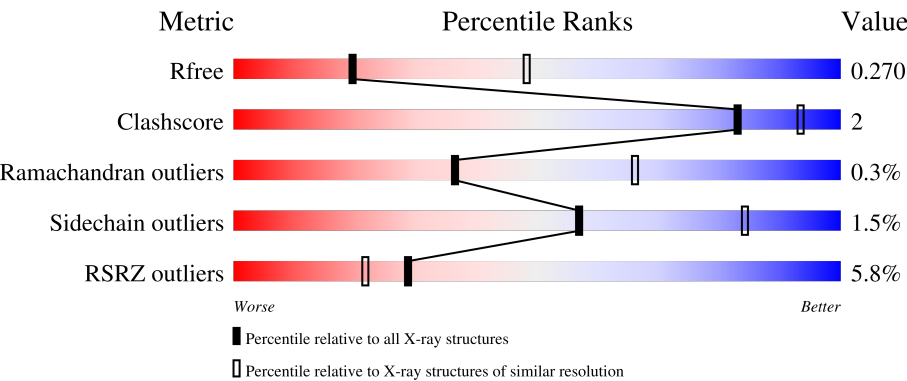
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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.



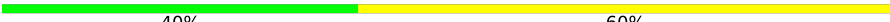
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	5% 84% 8% 9%
1	B	807	6% 84% 8% 8%
2	C	5	40% 60%
2	E	5	40% 60%
2	F	5	40% 60%

Continued on next page...

Continued from previous page...

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

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12526 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.

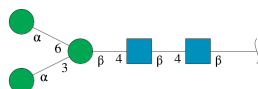
- Molecule 1 is a protein called Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	0	0
			5838	3735	987	1097	19			
1	B	743	Total	C	N	O	S	0	0	0
			5885	3759	1001	1106	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-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



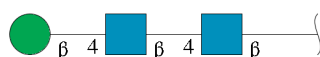
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			61	34	2	25			

Continued on next page...

Continued from previous page...

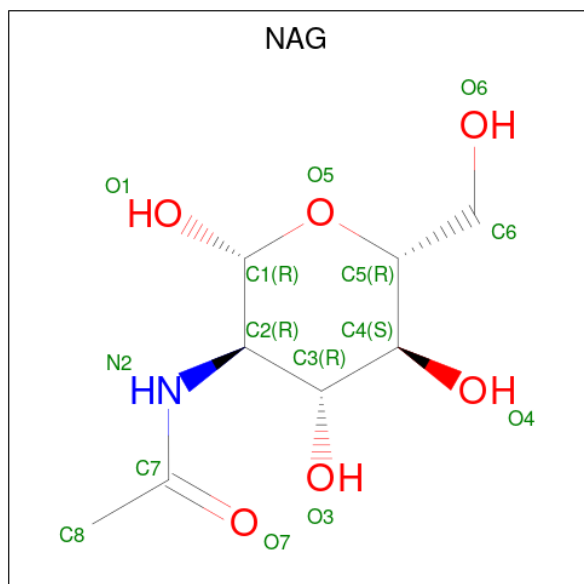
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



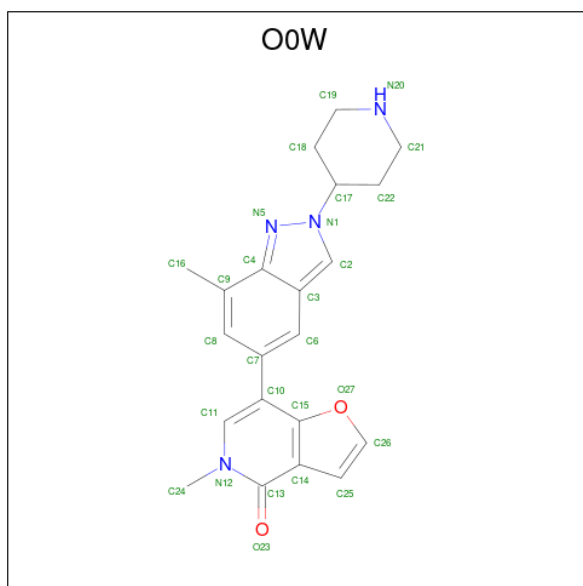
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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		

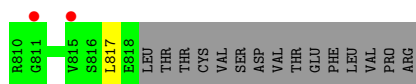
- Molecule 5 is 5-methyl-7-(7-methyl-2-piperidin-4-yl-indazol-5-yl)furo[3,2-c]pyridin-4-one (CCD ID: O0W) (formula: C₂₁H₂₂N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			27	21	4	2		
5	B	1	Total	C	N	O	0	0
			27	21	4	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	122	Total	O	0	0
			122	122		
6	B	137	Total	O	0	0
			137	137		



- 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



- 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



- 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



- 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



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



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.81Å 87.72Å 153.46Å 90.00° 120.46° 90.00°	Depositor
Resolution (Å)	74.64 – 2.79 74.64 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.1 (74.64-2.79) 96.1 (74.64-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.7 (3-OCT-2019)	Depositor
R, R_{free}	0.237 , 0.264 0.240 , 0.270	Depositor DCC
R_{free} test set	2315 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12526	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: NAG, BMA, OOW, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/5955	0.86	0/8089
1	B	0.52	0/6002	0.86	0/8151
All	All	0.52	0/11957	0.86	0/16240

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	5838	0	5726	27	0
1	B	5885	0	5802	30	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	B	54	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	122	0	0	1	0
6	B	137	0	0	0	0
All	All	12526	0	11960	57	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 2.

All (57) 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:373:HIS:HA	1:B:400:ASN:HB3	1.83	0.59
1:A:373:HIS:HA	1:A:400:ASN:HB3	1.84	0.59
1:B:45:VAL:HB	1:B:65:VAL:HA	1.86	0.57
1:A:343:ASP:OD2	1:A:469:HIS:HD2	1.88	0.57
1:B:343:ASP:OD2	1:B:469:HIS:HD2	1.88	0.57
1:B:520:VAL:HA	1:B:543:ASP:HB3	1.90	0.54
1:A:240:GLU:HA	1:A:243:LYS:HD3	1.90	0.54
1:A:541:ARG:HB3	1:A:567:TYR:HB2	1.89	0.53
1:A:520:VAL:HA	1:A:543:ASP:HB3	1.90	0.53
1:B:577:LEU:HD12	1:B:605:LEU:HD11	1.91	0.53
1:B:39:LYS:HD3	1:B:46:ILE:HD11	1.91	0.53
1:A:577:LEU:HD12	1:A:605:LEU:HD11	1.91	0.52
1:B:240:GLU:HA	1:B:243:LYS:HD3	1.91	0.52
1:A:76:THR:HG22	1:A:98:PRO:HG3	1.91	0.51
1:A:670:HIS:HA	1:A:694:ASP:HB3	1.93	0.50
1:B:670:HIS:HA	1:B:694:ASP:HB3	1.93	0.50
1:B:46:ILE:HG22	1:B:67:GLU:HB2	1.93	0.50
1:A:49:CYS:HB3	1:A:70:LEU:HD23	1.95	0.48
1:B:154:ILE:HD12	1:B:464:HIS:CE1	2.48	0.48
1:A:715:ARG:HE	1:A:739:LYS:NZ	2.11	0.48
1:B:715:ARG:HE	1:B:739:LYS:NZ	2.11	0.48
1:B:422:ILE:HG23	1:B:475:ILE:HD12	1.94	0.48
1:A:154:ILE:HD12	1:A:464:HIS:CE1	2.48	0.47
1:A:806:PRO:HD2	1:A:809:GLN:HB2	1.96	0.47
1:A:327:ILE:HG12	1:A:344:LEU:HD13	1.97	0.47
1:B:327:ILE:HG12	1:B:344:LEU:HD13	1.97	0.47
1:A:575:HIS:HD2	6:A:1150:HOH:O	1.99	0.46
1:B:806:PRO:HD2	1:B:809:GLN:HB2	1.96	0.46
1:A:399:ILE:HD12	1:A:420:LEU:HD11	1.98	0.46
1:B:154:ILE:CD1	1:B:464:HIS:CE1	2.99	0.46
1:A:154:ILE:CD1	1:A:464:HIS:CE1	2.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:LEU:HA	1:B:742:ASP:HB3	1.99	0.45
1:B:479:CYS:SG	1:B:534:TYR:CD1	3.10	0.45
1:A:479:CYS:SG	1:A:534:TYR:CD1	3.10	0.45
1:B:192:ILE:HD11	1:B:213:LEU:HD22	1.99	0.45
1:A:336:LEU:HD13	1:A:339:LEU:HD22	1.99	0.44
1:A:239:GLU:HA	1:A:282:ALA:HA	1.99	0.44
1:A:718:LEU:HA	1:A:742:ASP:HB3	1.99	0.44
1:B:240:GLU:HG2	1:B:243:LYS:NZ	2.33	0.44
1:B:399:ILE:HD12	1:B:420:LEU:HD11	1.99	0.44
1:A:192:ILE:HD11	1:A:213:LEU:HD22	1.99	0.44
1:A:240:GLU:HG2	1:A:243:LYS:NZ	2.33	0.44
1:B:207:SER:HA	1:B:228:PHE:HB2	2.00	0.44
1:B:239:GLU:HA	1:B:282:ALA:HA	1.99	0.43
1:A:207:SER:HA	1:A:228:PHE:HB2	2.01	0.43
1:B:76:THR:HG22	1:B:98:PRO:HG3	2.00	0.43
1:B:336:LEU:HD13	1:B:339:LEU:HD22	1.99	0.43
1:B:412:LYS:HB3	1:B:503:ASN:HB3	2.00	0.43
1:A:412:LYS:HB3	1:A:503:ASN:HB3	2.01	0.42
1:B:574:THR:HA	1:B:575:HIS:HA	1.83	0.41
1:A:606:GLU:HG3	1:A:637:GLY:HA3	2.03	0.41
1:A:198:GLU:HG3	1:A:219:LYS:HB3	2.03	0.41
1:B:198:GLU:HG3	1:B:219:LYS:HB3	2.03	0.41
1:B:606:GLU:HG3	1:B:637:GLY:HA3	2.02	0.41
1:A:140:ILE:HD13	1:A:166:ILE:HD11	2.03	0.40
1:B:182:TYR:HE2	1:B:266:PRO:HD2	1.86	0.40
1:B:715:ARG:HE	1:B:739:LYS:HZ3	1.68	0.40

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	724/807 (90%)	673 (93%)	49 (7%)	2 (0%)	36	66
1	B	733/807 (91%)	683 (93%)	48 (6%)	2 (0%)	36	66
All	All	1457/1614 (90%)	1356 (93%)	97 (7%)	4 (0%)	36	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	GLY
1	B	330	GLY
1	A	378	VAL
1	B	378	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	658/751 (88%)	646 (98%)	12 (2%)	51	82
1	B	665/751 (88%)	657 (99%)	8 (1%)	63	87
All	All	1323/1502 (88%)	1303 (98%)	20 (2%)	57	84

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	CYS
1	A	51	ASN
1	A	215	HIS
1	A	268	VAL
1	A	296	SER
1	A	416	ASN
1	A	430	ILE
1	A	465	SER
1	A	475	ILE
1	A	594	ASN
1	A	701	LEU
1	A	735	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	51	ASN
1	B	268	VAL
1	B	296	SER
1	B	416	ASN
1	B	430	ILE
1	B	465	SER
1	B	594	ASN
1	B	817	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	51	ASN
1	A	171	ASN
1	A	284	GLN
1	A	285	ASN
1	A	312	HIS
1	A	466	ASN
1	A	469	HIS
1	A	575	HIS
1	A	581	GLN
1	A	593	HIS
1	A	594	ASN
1	A	629	ASN
1	B	41	GLN
1	B	51	ASN
1	B	77	HIS
1	B	115	ASN
1	B	174	ASN
1	B	202	ASN
1	B	284	GLN
1	B	285	ASN
1	B	312	HIS
1	B	466	ASN
1	B	469	HIS
1	B	539	ASN
1	B	581	GLN
1	B	593	HIS
1	B	594	ASN
1	B	625	ASN
1	B	629	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	685	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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	2,1	14,14,15	0.31	0	17,19,21	0.48	0
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	0.62	0
2	BMA	C	3	2	11,11,12	0.24	0	15,15,17	0.71	1 (6%)
2	MAN	C	4	2	11,11,12	0.31	0	15,15,17	0.81	1 (6%)
2	MAN	C	5	2	11,11,12	0.31	0	15,15,17	0.82	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
3	NAG	D	2	3	14,14,15	0.31	0	17,19,21	0.41	0
3	BMA	D	3	3	11,11,12	0.29	0	15,15,17	0.52	0
2	NAG	E	1	2,1	14,14,15	0.30	0	17,19,21	0.60	1 (5%)
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.52	0
2	BMA	E	3	2	11,11,12	0.26	0	15,15,17	0.43	0
2	MAN	E	4	2	11,11,12	0.30	0	15,15,17	0.69	1 (6%)
2	MAN	E	5	2	11,11,12	0.30	0	15,15,17	0.74	1 (6%)
2	NAG	F	1	2,1	14,14,15	0.29	0	17,19,21	0.49	0
2	NAG	F	2	2	14,14,15	0.28	0	17,19,21	0.63	0
2	BMA	F	3	2	11,11,12	0.24	0	15,15,17	0.72	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	F	4	2	11,11,12	0.29	0	15,15,17	0.84	1 (6%)
2	MAN	F	5	2	11,11,12	0.31	0	15,15,17	0.81	1 (6%)
3	NAG	G	1	3,1	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
3	NAG	G	2	3	14,14,15	0.30	0	17,19,21	0.42	0
3	BMA	G	3	3	11,11,12	0.28	0	15,15,17	0.50	0
2	NAG	H	1	2,1	14,14,15	0.30	0	17,19,21	0.58	1 (5%)
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.53	0
2	BMA	H	3	2	11,11,12	0.26	0	15,15,17	0.54	0
2	MAN	H	4	2	11,11,12	0.30	0	15,15,17	0.69	1 (6%)
2	MAN	H	5	2	11,11,12	0.32	0	15,15,17	0.75	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	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	-	0/2/19/22	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
2	NAG	E	1	2,1	-	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	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	-	0/2/19/22	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
2	NAG	H	1	2,1	-	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	MAN	C1-O5-C5	3.09	116.33	112.19
2	C	5	MAN	C1-O5-C5	3.07	116.31	112.19
2	F	5	MAN	C1-O5-C5	3.01	116.22	112.19
2	C	4	MAN	C1-O5-C5	3.00	116.21	112.19
2	H	5	MAN	C1-O5-C5	2.75	115.87	112.19
2	E	5	MAN	C1-O5-C5	2.68	115.78	112.19
2	E	4	MAN	C1-O5-C5	2.54	115.59	112.19
2	H	4	MAN	C1-O5-C5	2.54	115.59	112.19
2	C	3	BMA	C1-O5-C5	2.24	115.19	112.19
2	F	3	BMA	C1-O5-C5	2.22	115.16	112.19
2	E	1	NAG	C1-O5-C5	2.14	115.06	112.19
2	H	1	NAG	C1-O5-C5	2.10	115.00	112.19
3	G	1	NAG	C1-C2-N2	-2.09	107.15	110.43
3	D	1	NAG	C1-C2-N2	-2.06	107.19	110.43

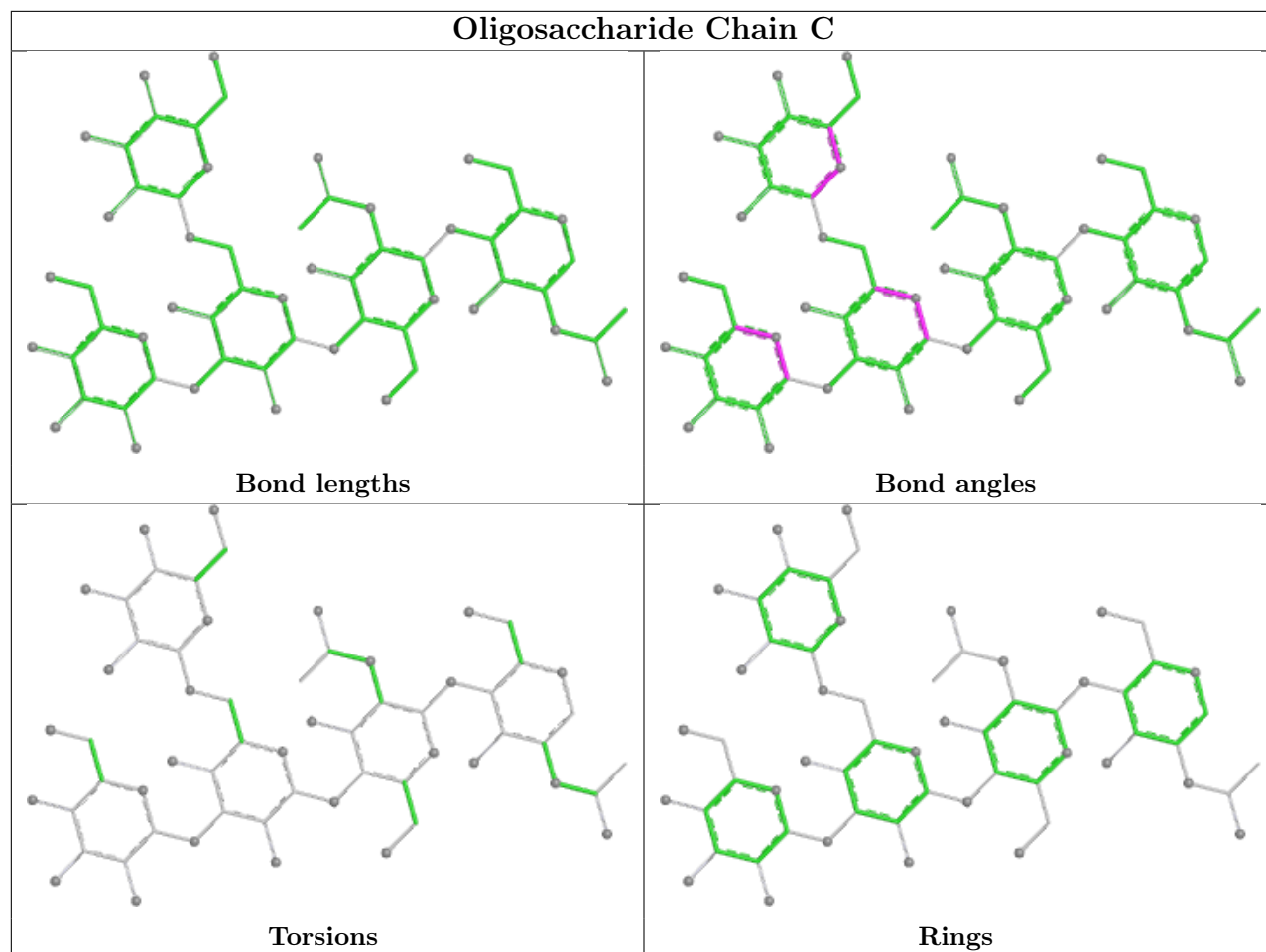
There are no chirality outliers.

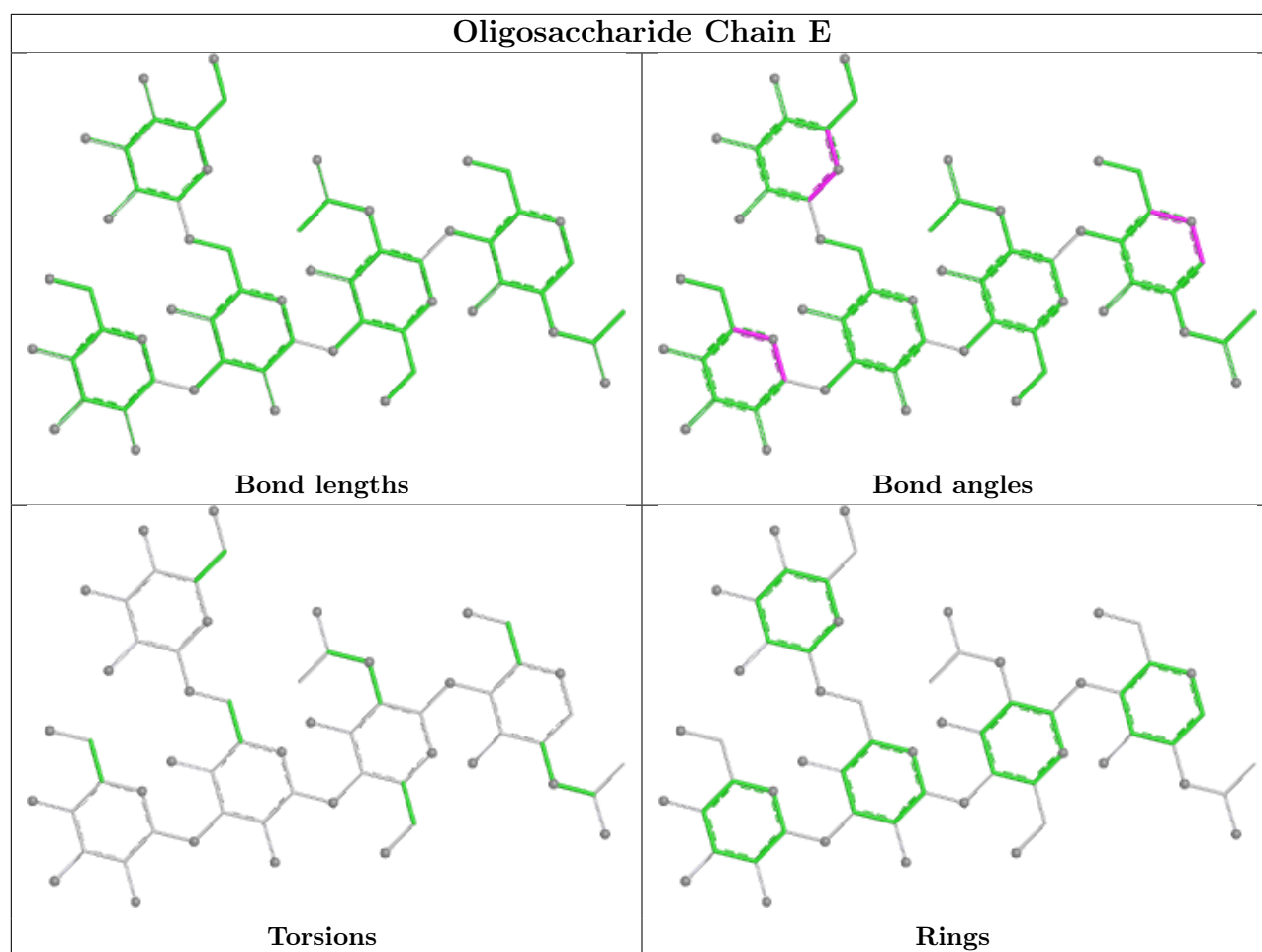
There are no torsion outliers.

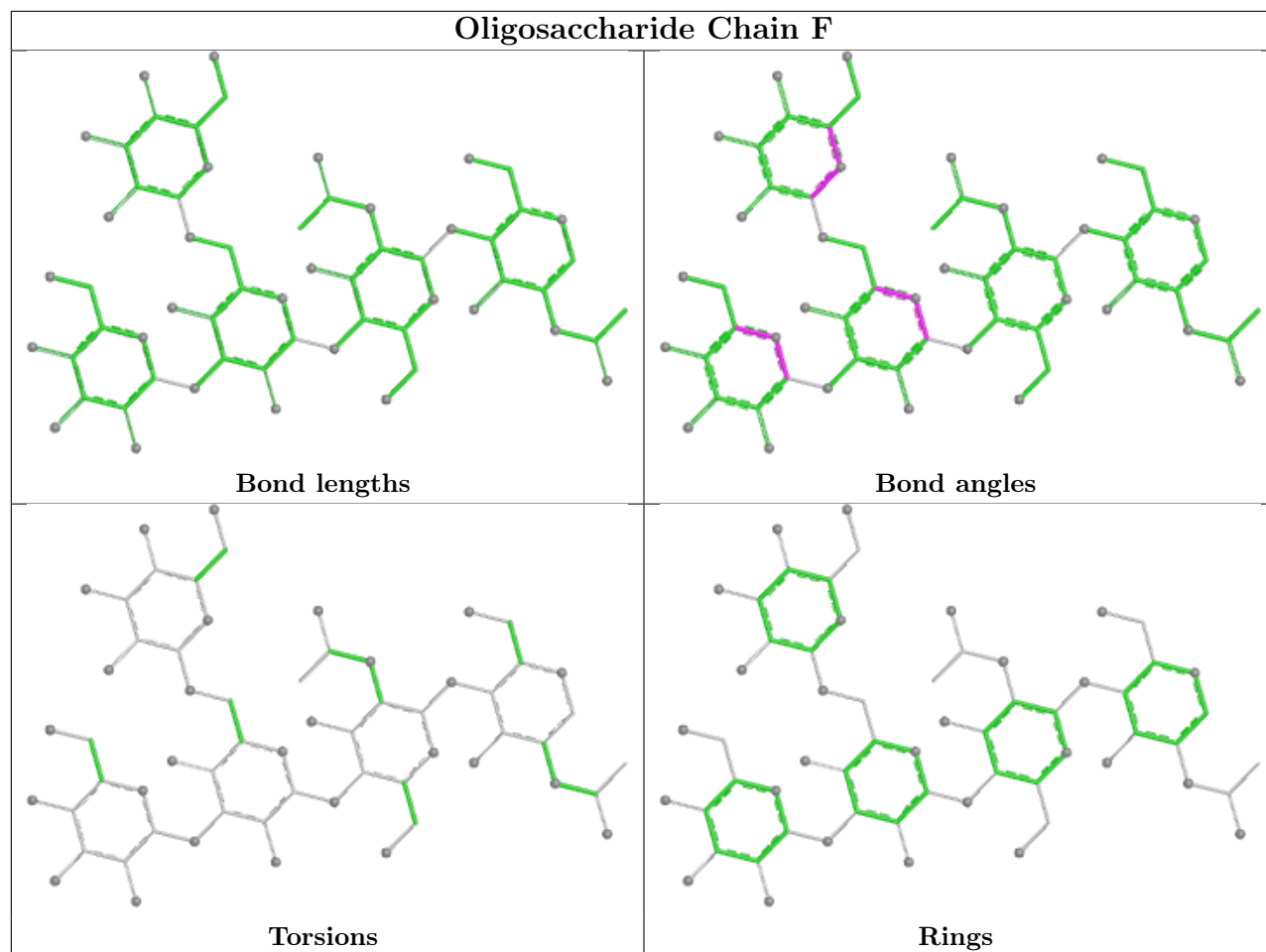
There are no ring outliers.

No monomer is involved in short contacts.

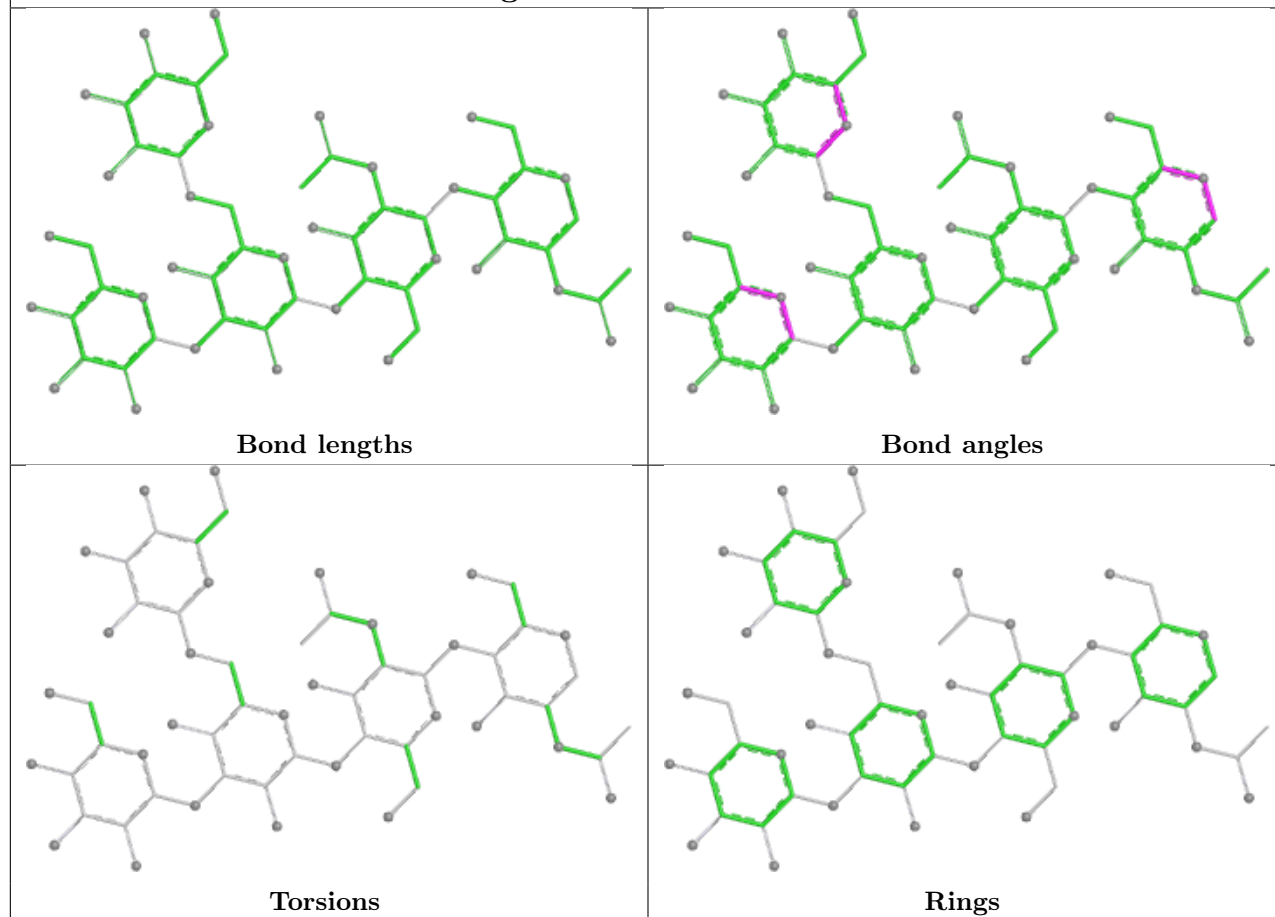
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



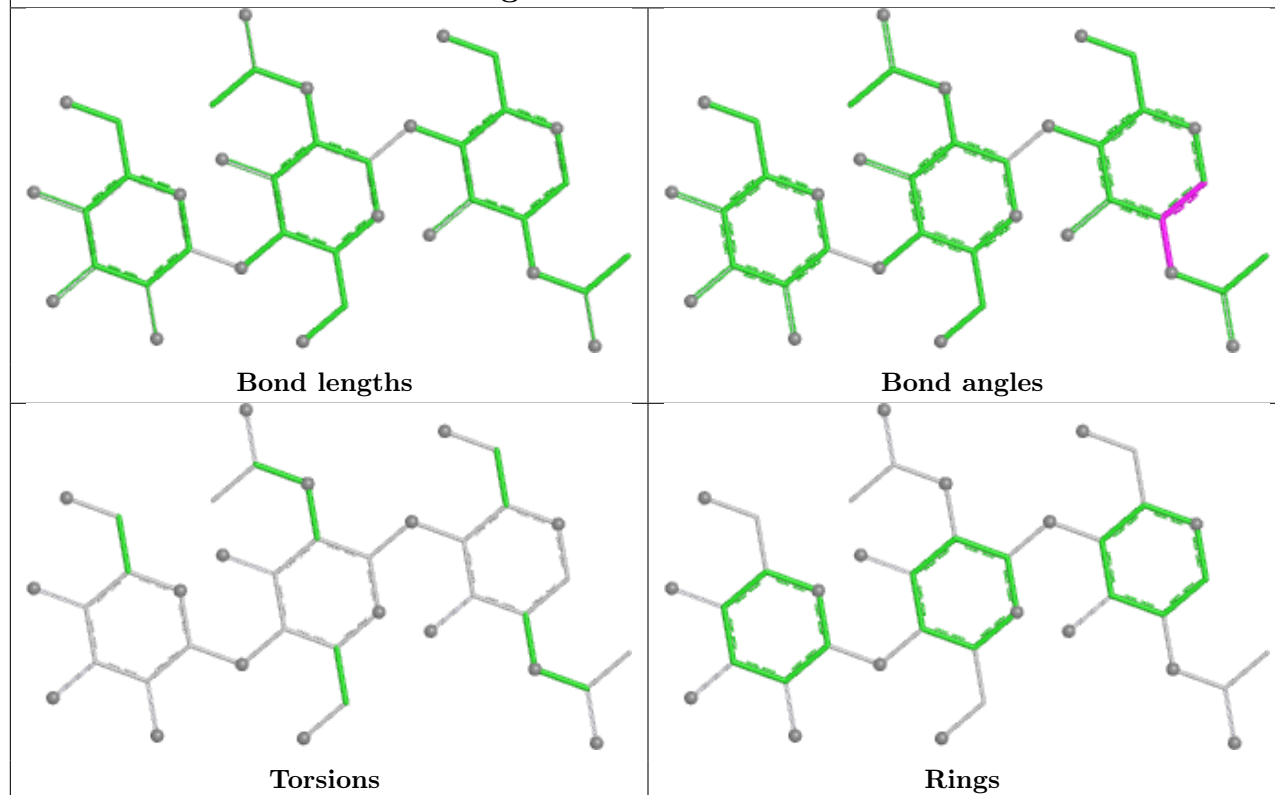


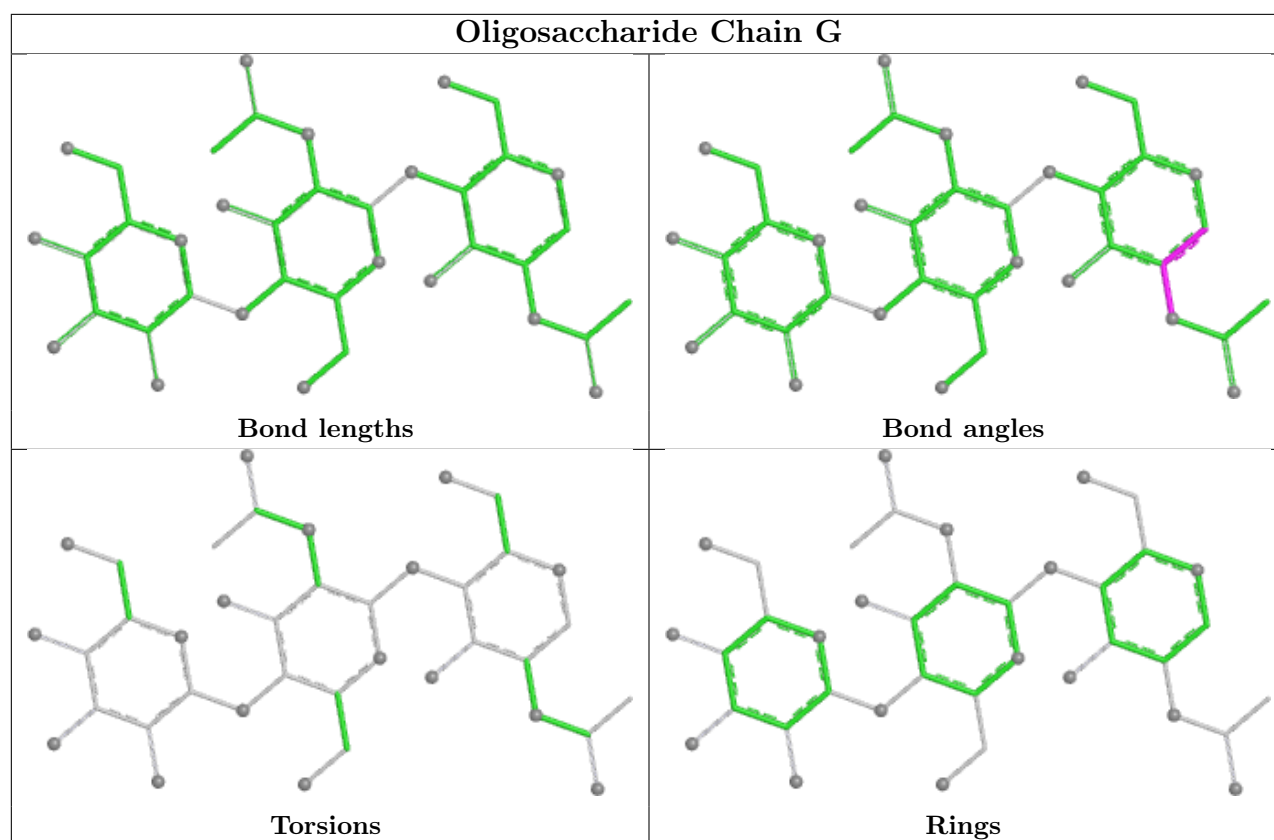


Oligosaccharide Chain H



Oligosaccharide Chain D





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	$\# Z > 2$
5	O0W	B	1121	-	29,31,31	2.27	8 (27%)	34,46,46	2.89	15 (44%)
4	NAG	B	1110	1	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	A	1009	1	14,14,15	0.29	0	17,19,21	0.43	0
4	NAG	B	1119	1	14,14,15	0.30	0	17,19,21	0.98	2 (11%)
4	NAG	B	1120	1	14,14,15	0.29	0	17,19,21	0.51	0
4	NAG	A	1018	1	14,14,15	0.32	0	17,19,21	1.00	2 (11%)
4	NAG	A	1017	1	14,14,15	0.31	0	17,19,21	0.64	1 (5%)
4	NAG	A	1019	1	14,14,15	0.30	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1016	1	14,14,15	0.31	0	17,19,21	0.60	1 (5%)
5	O0W	B	1101	-	29,31,31	2.22	8 (27%)	34,46,46	2.77	14 (41%)
4	NAG	B	1117	1	14,14,15	0.29	0	17,19,21	0.59	1 (5%)
4	NAG	A	1015	1	14,14,15	0.30	0	17,19,21	0.66	1 (5%)
4	NAG	B	1118	1	14,14,15	0.30	0	17,19,21	0.61	1 (5%)
4	NAG	B	1116	1	14,14,15	0.28	0	17,19,21	0.65	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
5	O0W	B	1121	-	-	1/8/16/16	0/5/5/5
4	NAG	B	1110	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1119	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1120	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1018	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1017	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1019	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1016	1	-	0/6/23/26	0/1/1/1
5	O0W	B	1101	-	-	0/8/16/16	0/5/5/5
4	NAG	B	1117	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1015	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1118	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1116	1	-	0/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1121	O0W	C8-C7	6.95	1.49	1.39
5	B	1101	O0W	C8-C7	6.39	1.49	1.39
5	B	1101	O0W	C4-N5	-5.21	1.26	1.33
5	B	1101	O0W	C10-C15	4.81	1.48	1.43
5	B	1121	O0W	C4-N5	-4.76	1.27	1.33
5	B	1121	O0W	C10-C15	4.67	1.48	1.43
5	B	1121	O0W	C2-N1	-4.23	1.31	1.35
5	B	1101	O0W	C2-N1	-3.67	1.31	1.35
5	B	1121	O0W	C9-C4	2.73	1.47	1.43
5	B	1121	O0W	O27-C15	-2.62	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1101	O0W	C13-N12	-2.51	1.36	1.39
5	B	1101	O0W	C9-C4	2.43	1.46	1.43
5	B	1101	O0W	O27-C15	-2.38	1.34	1.38
5	B	1121	O0W	C13-N12	-2.31	1.36	1.39
5	B	1101	O0W	C14-C15	-2.19	1.33	1.37
5	B	1121	O0W	C14-C15	-2.17	1.33	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1121	O0W	O27-C15-C14	9.04	116.70	110.47
5	B	1101	O0W	O27-C15-C14	8.42	116.28	110.47
5	B	1121	O0W	C4-N5-N1	6.54	109.49	104.17
5	B	1101	O0W	C4-N5-N1	6.34	109.33	104.17
5	B	1121	O0W	C26-C25-C14	-4.74	102.39	106.24
5	B	1101	O0W	C7-C6-C3	-4.46	118.31	121.92
5	B	1101	O0W	C26-C25-C14	-4.35	102.71	106.24
5	B	1121	O0W	O27-C26-C25	4.24	117.04	111.21
5	B	1121	O0W	C17-N1-N5	4.24	124.73	119.76
5	B	1101	O0W	O27-C26-C25	3.89	116.57	111.21
5	B	1121	O0W	C25-C14-C15	-3.72	103.70	105.96
5	B	1121	O0W	C26-O27-C15	-3.72	100.16	105.58
5	B	1101	O0W	C25-C14-C15	-3.69	103.73	105.96
5	B	1121	O0W	C7-C6-C3	-3.62	118.99	121.92
5	B	1101	O0W	C26-O27-C15	-3.34	100.72	105.58
4	A	1018	NAG	C1-O5-C5	3.31	116.63	112.19
4	B	1119	NAG	C1-O5-C5	3.30	116.61	112.19
5	B	1101	O0W	C8-C9-C4	-3.08	115.83	118.64
5	B	1121	O0W	C8-C9-C4	-2.91	115.98	118.64
5	B	1121	O0W	C2-N1-N5	-2.88	110.05	113.14
5	B	1121	O0W	O23-C13-C14	-2.75	119.13	124.96
5	B	1101	O0W	O23-C13-C14	-2.73	119.17	124.96
5	B	1121	O0W	C6-C7-C10	-2.62	117.33	120.74
5	B	1101	O0W	C2-N1-N5	-2.58	110.38	113.14
4	A	1015	NAG	C1-O5-C5	2.58	115.64	112.19
4	B	1116	NAG	C1-O5-C5	2.53	115.58	112.19
5	B	1101	O0W	C18-C17-N1	2.39	114.22	110.95
5	B	1101	O0W	C22-C17-N1	2.26	114.04	110.95
4	A	1016	NAG	C1-O5-C5	2.20	115.14	112.19
4	A	1017	NAG	C1-O5-C5	2.19	115.13	112.19
4	A	1018	NAG	O5-C1-C2	2.19	114.68	111.29
5	B	1121	O0W	C17-N1-C2	-2.15	125.21	128.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1118	NAG	C1-O5-C5	2.12	115.03	112.19
4	B	1117	NAG	C1-O5-C5	2.12	115.03	112.19
5	B	1121	O0W	O23-C13-N12	2.11	123.93	119.97
4	B	1119	NAG	O5-C1-C2	2.07	114.49	111.29
5	B	1101	O0W	O23-C13-N12	2.04	123.80	119.97
5	B	1101	O0W	C11-C10-C15	-2.03	117.21	121.53
5	B	1121	O0W	C11-C10-C15	-2.02	117.24	121.53

There are no chirality outliers.

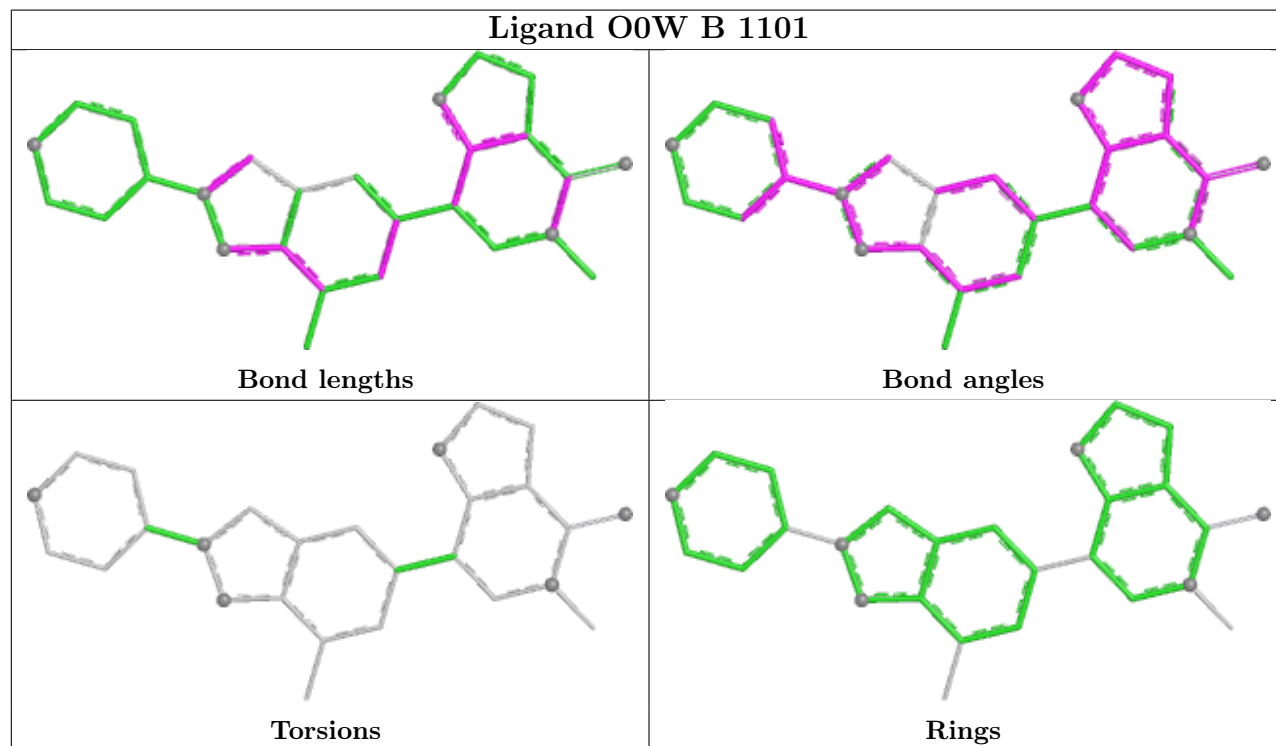
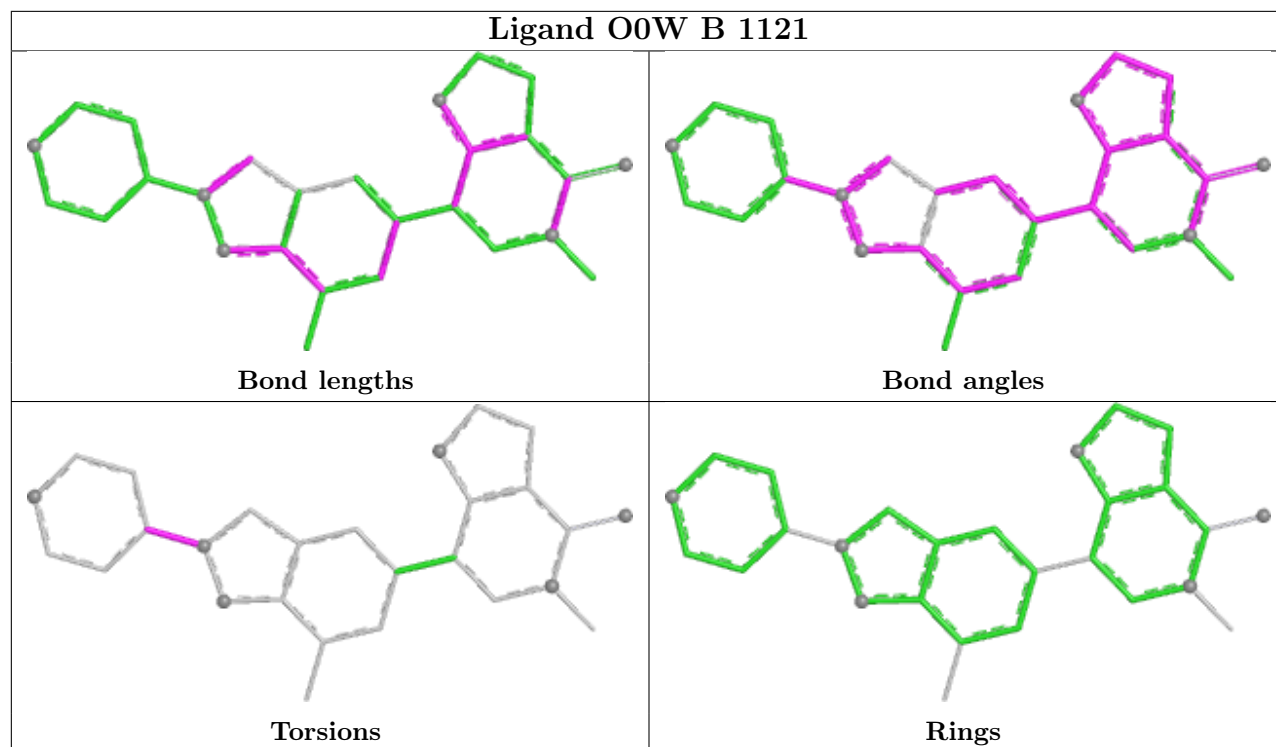
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1121	O0W	C18-C17-N1-C2
4	A	1017	NAG	C1-C2-N2-C7
4	B	1118	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 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	738/807 (91%)	0.59	41 (5%)	30 23	48, 77, 101, 118	0
1	B	743/807 (92%)	0.64	45 (6%)	27 20	46, 78, 124, 141	0
All	All	1481/1614 (91%)	0.61	86 (5%)	29 22	46, 77, 115, 141	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	732	LEU	4.3
1	A	707	LEU	4.1
1	A	733	SER	3.5
1	B	654	ILE	3.4
1	A	58	PRO	3.4
1	B	653	HIS	3.3
1	B	762	THR	3.2
1	B	571	ALA	3.2
1	B	182	TYR	3.1
1	B	735	VAL	3.1
1	A	31	SER	3.0
1	A	818	GLU	2.9
1	A	467	PHE	2.9
1	A	811	GLY	2.9
1	B	626	ASP	2.8
1	A	732	LEU	2.8
1	A	702	PHE	2.8
1	A	574	THR	2.7
1	B	286	LEU	2.7
1	B	605	LEU	2.7
1	A	602	LYS	2.7
1	B	733	SER	2.7
1	A	678	PHE	2.7
1	B	568	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	603	TYR	2.7
1	A	346	PHE	2.6
1	B	628	ASP	2.6
1	B	808	ASP	2.6
1	B	200	LEU	2.6
1	B	283	PHE	2.6
1	B	659	PHE	2.6
1	A	710	PHE	2.6
1	B	731	PHE	2.5
1	B	625	ASN	2.5
1	B	679	PHE	2.5
1	A	260	CYS	2.5
1	B	566	HIS	2.5
1	B	755	ALA	2.5
1	A	433	LEU	2.4
1	A	261	PHE	2.4
1	A	94	LEU	2.4
1	B	201	THR	2.4
1	B	580	ILE	2.4
1	A	703	LEU	2.3
1	A	808	ASP	2.3
1	A	735	VAL	2.3
1	B	806	PRO	2.3
1	B	61	VAL	2.3
1	B	683	LEU	2.3
1	B	783	PHE	2.3
1	A	758	THR	2.3
1	A	572	GLY	2.3
1	A	817	LEU	2.3
1	A	414	PHE	2.3
1	A	183	PHE	2.2
1	A	731	PHE	2.2
1	A	607	SER	2.2
1	B	113	GLY	2.2
1	B	701	LEU	2.2
1	B	769	LEU	2.2
1	A	769	LEU	2.2
1	B	57	VAL	2.2
1	B	780	ILE	2.2
1	A	609	SER	2.2
1	B	702	PHE	2.2
1	B	758	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	236	TYR	2.1
1	A	113	GLY	2.1
1	A	815	VAL	2.1
1	B	46	ILE	2.1
1	B	634	ILE	2.1
1	B	518	ALA	2.1
1	B	660	LEU	2.1
1	B	730	GLY	2.1
1	A	570	ILE	2.1
1	B	815	VAL	2.1
1	B	48	GLU	2.1
1	A	35	PRO	2.1
1	A	382	LEU	2.1
1	A	165	GLY	2.1
1	A	801	VAL	2.1
1	B	31	SER	2.0
1	A	54	LEU	2.0
1	A	70	LEU	2.0
1	B	811	GLY	2.0
1	A	760	THR	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	F	5	11/12	0.39	0.17	95,96,96,96	0
2	MAN	H	5	11/12	0.42	0.16	87,87,88,88	0
3	BMA	G	3	11/12	0.44	0.18	80,81,81,81	0
2	MAN	C	5	11/12	0.52	0.15	95,96,96,96	0
2	MAN	F	4	11/12	0.56	0.20	95,96,96,96	0
2	MAN	E	5	11/12	0.56	0.14	85,86,86,86	0
3	BMA	D	3	11/12	0.60	0.16	71,72,72,72	0
2	MAN	C	4	11/12	0.60	0.18	95,95,96,96	0

Continued on next page...

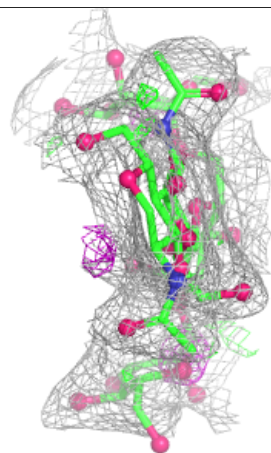
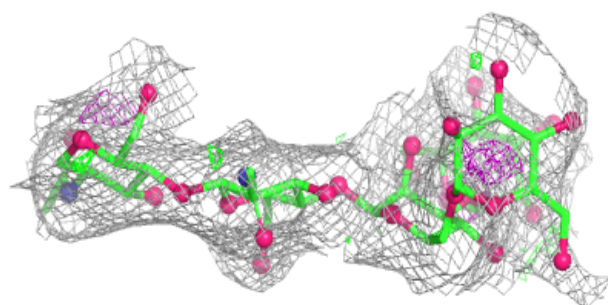
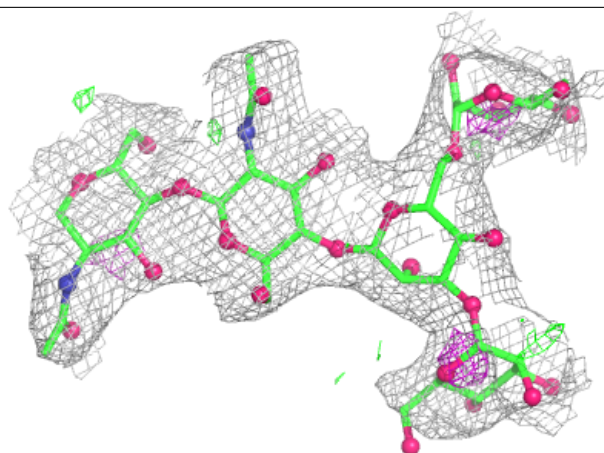
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	E	4	11/12	0.62	0.13	84,85,85,85	0
2	MAN	H	4	11/12	0.65	0.12	86,87,87,87	0
2	BMA	C	3	11/12	0.78	0.11	91,93,94,94	0
2	BMA	F	3	11/12	0.78	0.12	90,92,94,94	0
3	NAG	G	2	14/15	0.80	0.11	73,75,77,78	0
3	NAG	D	2	14/15	0.80	0.11	65,66,68,69	0
2	BMA	E	3	11/12	0.81	0.12	80,82,83,84	0
2	BMA	H	3	11/12	0.83	0.09	82,84,85,86	0
2	NAG	C	2	14/15	0.90	0.12	84,85,87,89	0
2	NAG	F	1	14/15	0.90	0.15	77,78,79,81	0
2	NAG	C	1	14/15	0.90	0.14	78,80,81,82	0
2	NAG	F	2	14/15	0.92	0.12	82,83,85,88	0
2	NAG	H	2	14/15	0.93	0.11	74,75,77,80	0
2	NAG	E	2	14/15	0.93	0.09	70,72,74,77	0
2	NAG	H	1	14/15	0.94	0.10	69,70,71,73	0
3	NAG	D	1	14/15	0.94	0.09	59,60,61,63	0
2	NAG	E	1	14/15	0.95	0.10	63,64,66,68	0
3	NAG	G	1	14/15	0.95	0.09	66,67,69,71	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.

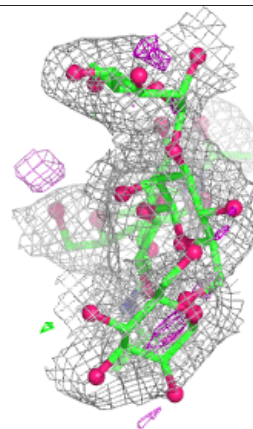
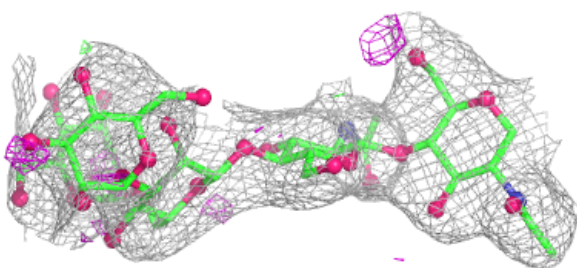
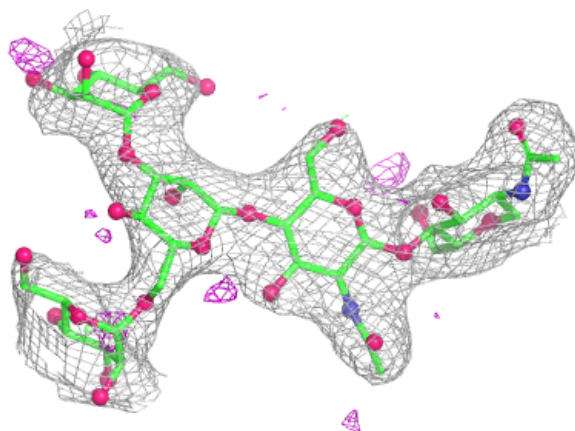
Electron density around Chain C:

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



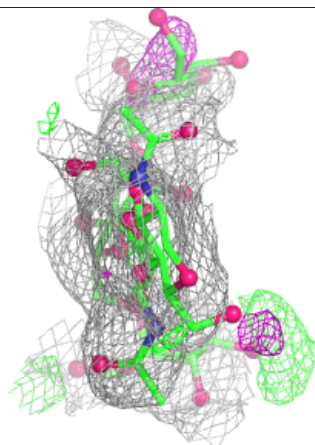
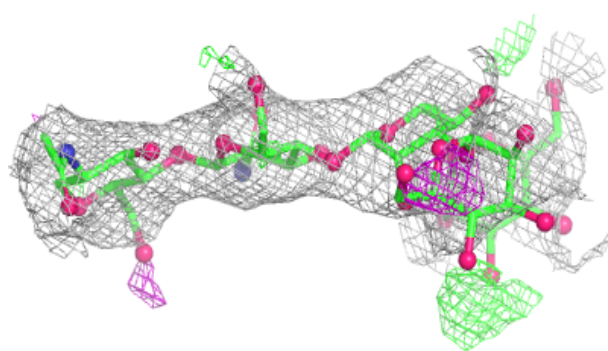
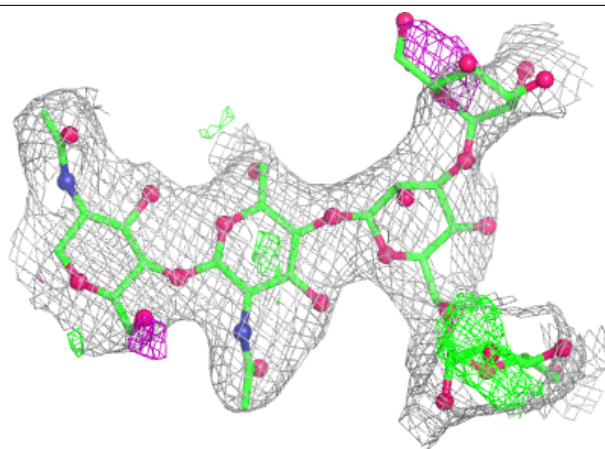
Electron density around Chain E:

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



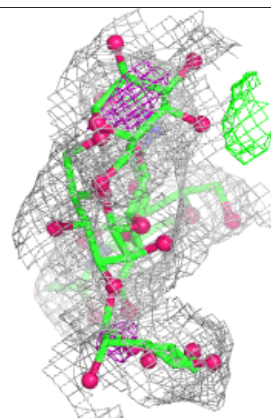
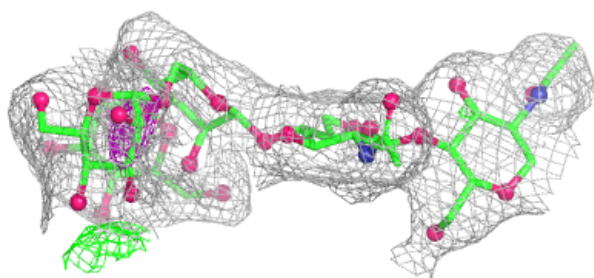
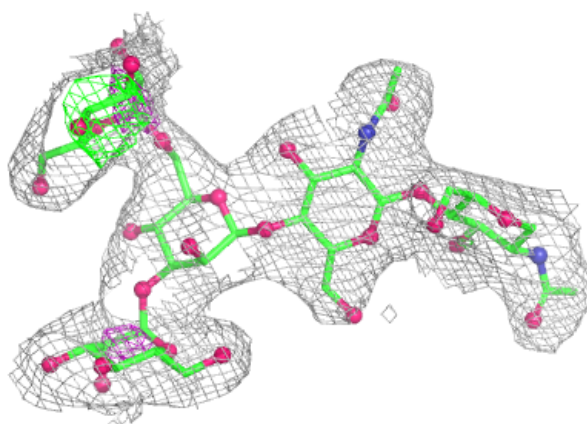
Electron density around Chain F:

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

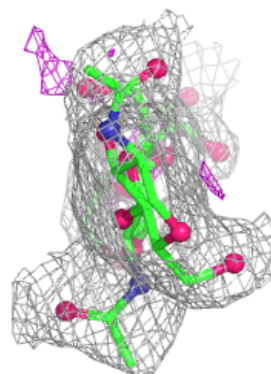
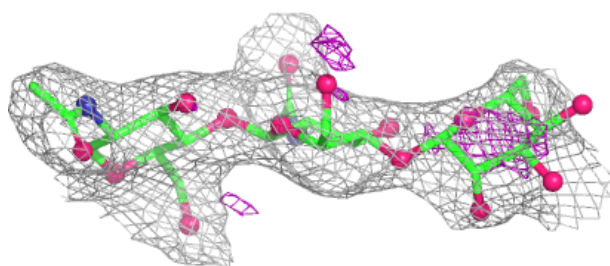
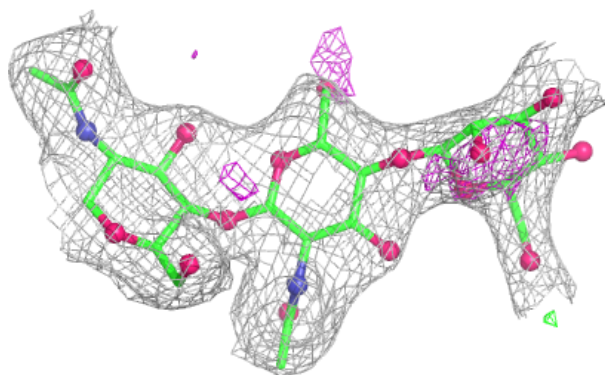


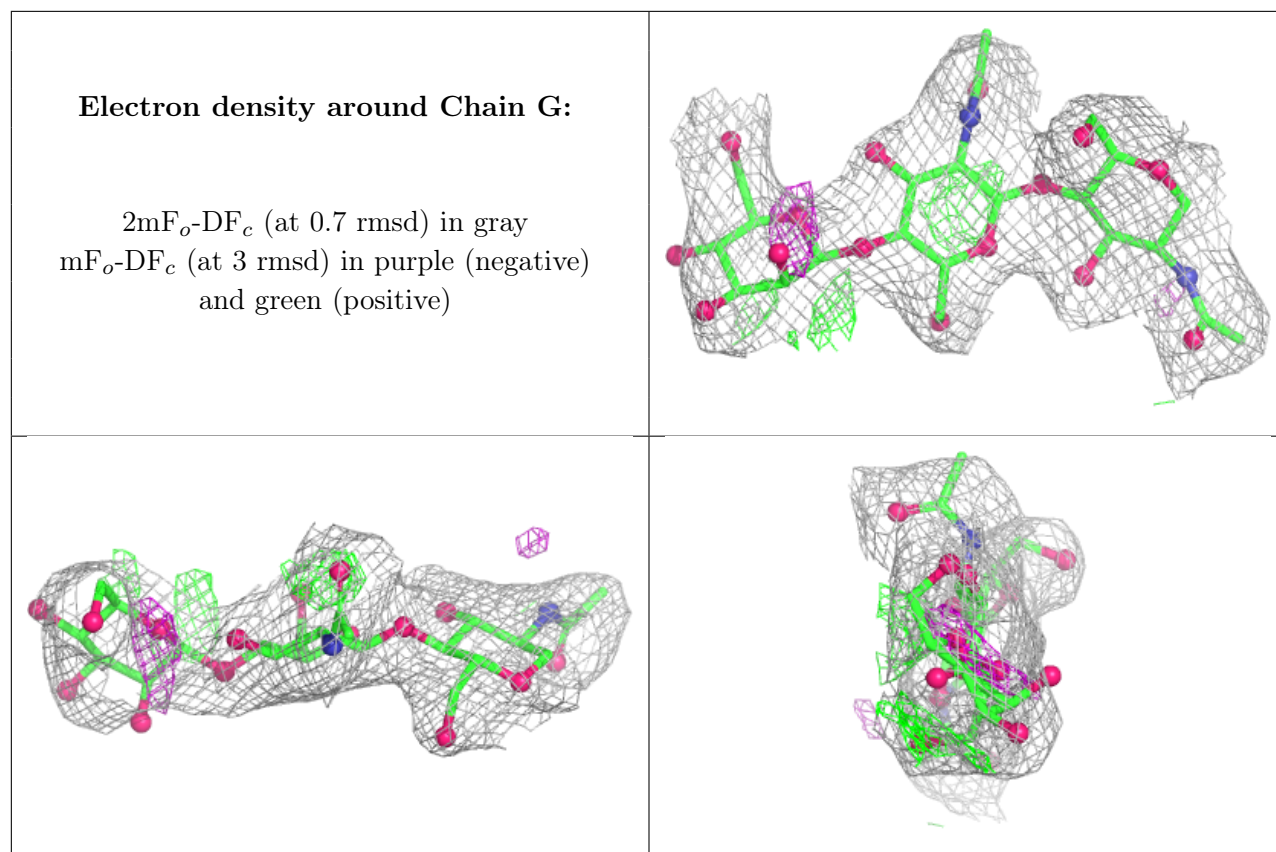
Electron density around Chain H:

$2mF_o-DF_c$ (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](#)

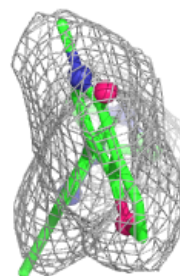
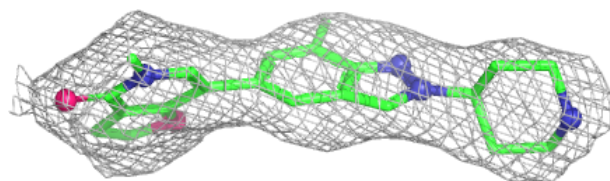
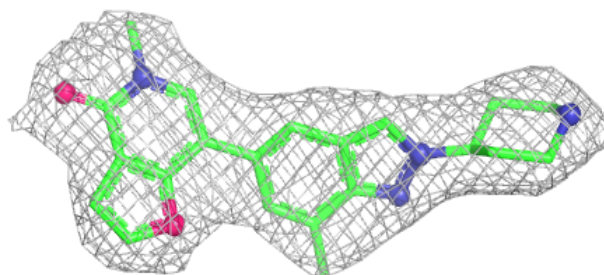
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

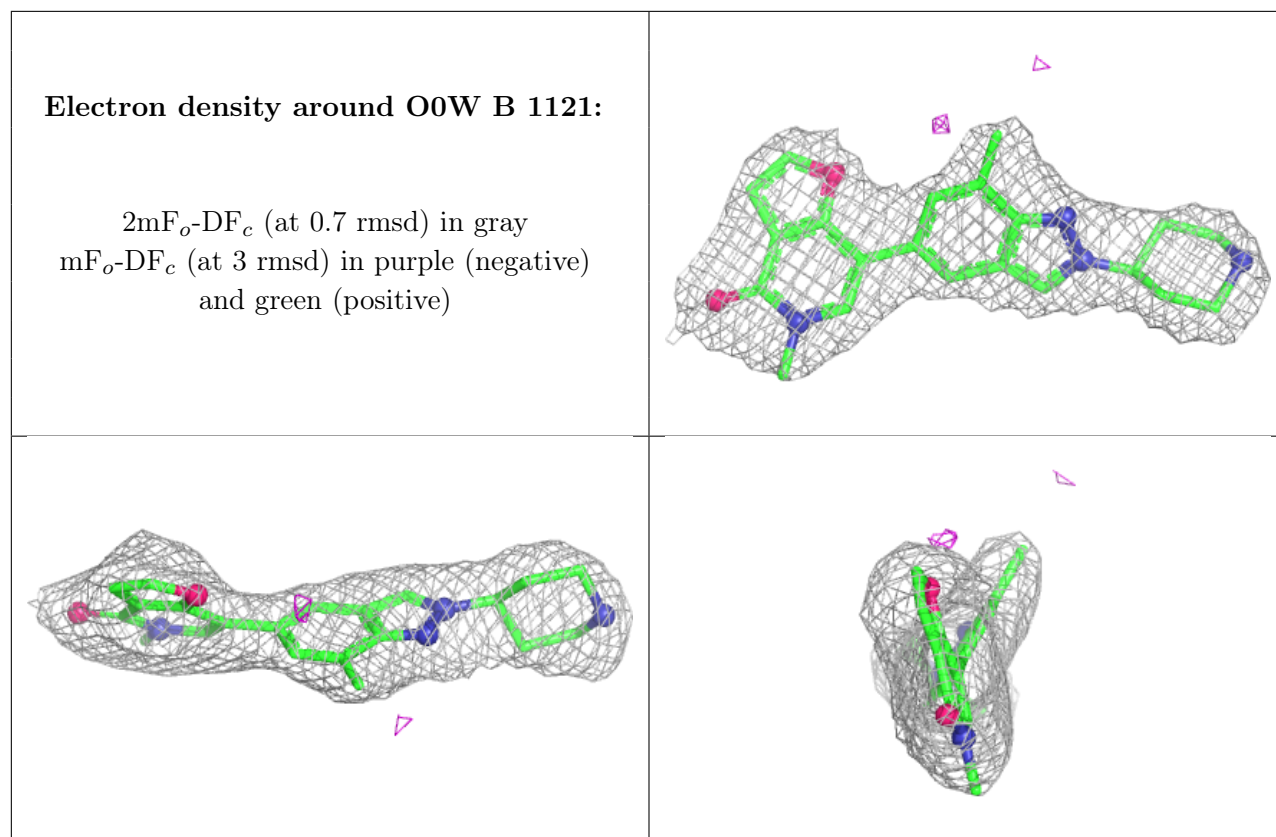
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	1119	14/15	0.33	0.19	93,94,94,94	0
4	NAG	A	1019	14/15	0.39	0.14	108,109,109,109	0
4	NAG	A	1018	14/15	0.46	0.17	85,86,86,86	0
4	NAG	A	1016	14/15	0.47	0.17	86,86,87,87	0
4	NAG	B	1118	14/15	0.52	0.17	85,86,87,87	0
4	NAG	A	1017	14/15	0.53	0.16	94,94,95,95	0
4	NAG	B	1117	14/15	0.53	0.17	79,80,80,80	0
4	NAG	B	1120	14/15	0.58	0.12	115,115,115,115	0
4	NAG	B	1110	14/15	0.72	0.13	78,78,79,79	0
4	NAG	A	1015	14/15	0.75	0.13	91,91,92,92	0
4	NAG	B	1116	14/15	0.84	0.10	84,85,85,85	0
4	NAG	A	1009	14/15	0.89	0.10	67,67,68,68	0
5	O0W	B	1101	27/27	0.94	0.10	56,57,57,57	0
5	O0W	B	1121	27/27	0.94	0.09	58,59,60,60	0

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

Electron density around O0W B 1101:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.