



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2025 – 10:08 AM EDT

PDB ID : 9OMM / pdb\_00009omm  
Title : WrtF fucosyltransferase - tetrasaccharide product  
Authors : Forrester, T.J.B.; Kimber, M.S.  
Deposited on : 2025-05-14  
Resolution : 2.25 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](mailto: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>.

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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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

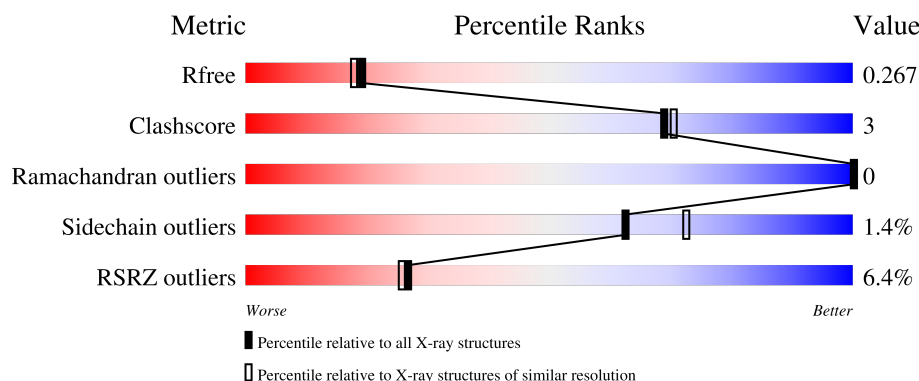
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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  $\geq 3$ , 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	279	<div> <div>9%</div> <div>84%</div> <div>9%</div> <div>8%</div> </div>
1	B	279	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
2	C	2	<div> <div>100%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8316 atoms, of which 4126 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	258	Total	C	H	N	O	S	0	0	0
			3970	1263	1981	335	385	6			
1	B	271	Total	C	H	N	O	S	0	0	0
			4164	1327	2070	358	403	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP A0A6P1C6J0
A	1	GLY	-	expression tag	UNP A0A6P1C6J0
A	199	SER	THR	conflict	UNP A0A6P1C6J0
A	268	ALA	-	expression tag	UNP A0A6P1C6J0
A	269	ALA	-	expression tag	UNP A0A6P1C6J0
A	270	ALA	-	expression tag	UNP A0A6P1C6J0
A	271	LEU	-	expression tag	UNP A0A6P1C6J0
A	272	GLU	-	expression tag	UNP A0A6P1C6J0
A	273	HIS	-	expression tag	UNP A0A6P1C6J0
A	274	HIS	-	expression tag	UNP A0A6P1C6J0
A	275	HIS	-	expression tag	UNP A0A6P1C6J0
A	276	HIS	-	expression tag	UNP A0A6P1C6J0
A	277	HIS	-	expression tag	UNP A0A6P1C6J0
A	278	HIS	-	expression tag	UNP A0A6P1C6J0
B	0	MET	-	expression tag	UNP A0A6P1C6J0
B	1	GLY	-	expression tag	UNP A0A6P1C6J0
B	199	SER	THR	conflict	UNP A0A6P1C6J0
B	268	ALA	-	expression tag	UNP A0A6P1C6J0
B	269	ALA	-	expression tag	UNP A0A6P1C6J0
B	270	ALA	-	expression tag	UNP A0A6P1C6J0
B	271	LEU	-	expression tag	UNP A0A6P1C6J0
B	272	GLU	-	expression tag	UNP A0A6P1C6J0
B	273	HIS	-	expression tag	UNP A0A6P1C6J0
B	274	HIS	-	expression tag	UNP A0A6P1C6J0
B	275	HIS	-	expression tag	UNP A0A6P1C6J0

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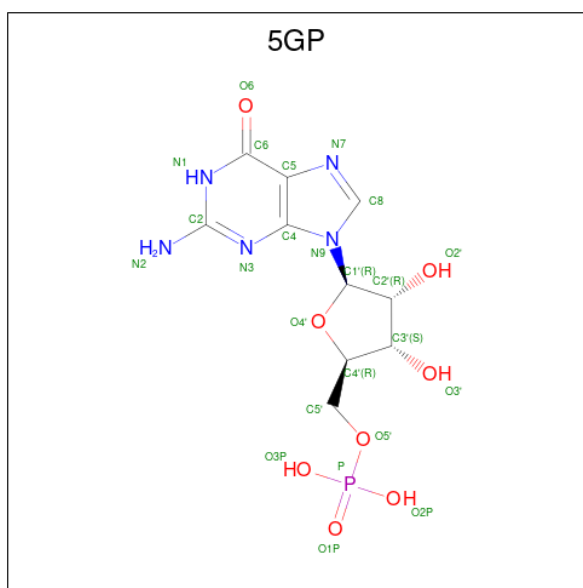
Chain	Residue	Modelled	Actual	Comment	Reference
B	276	HIS	-	expression tag	UNP A0A6P1C6J0
B	277	HIS	-	expression tag	UNP A0A6P1C6J0
B	278	HIS	-	expression tag	UNP A0A6P1C6J0

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-4)-beta-D-glucopyranose.



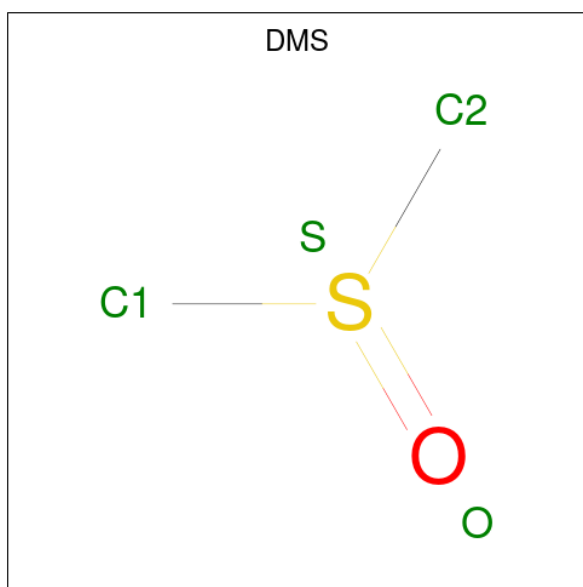
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	O	0	0	0
			42	12	21	9			

- Molecule 3 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



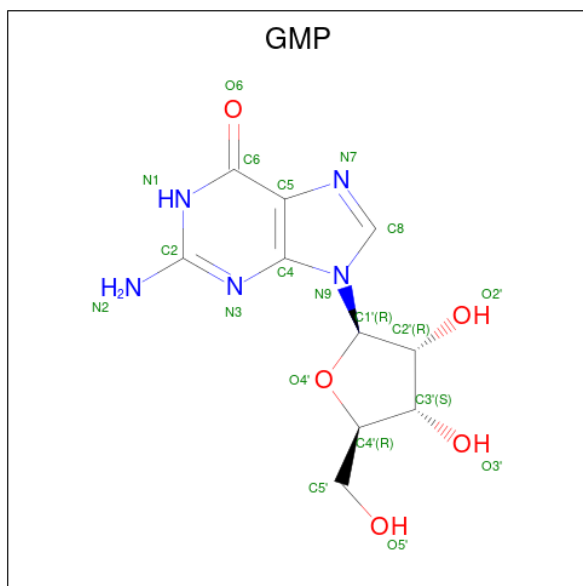
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			36	10	12	5	8		

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



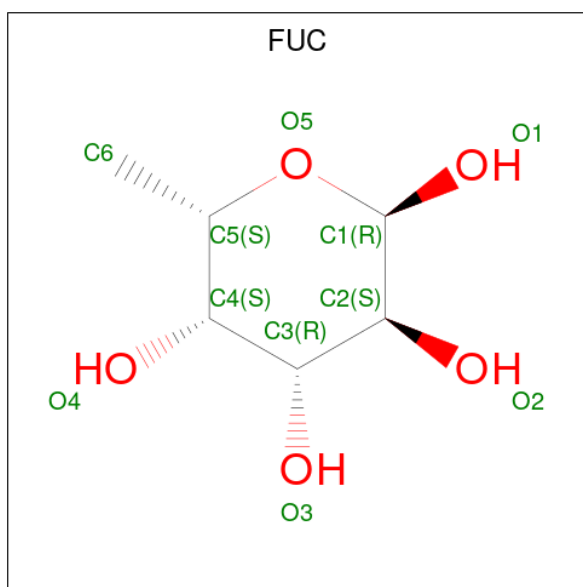
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 5 is GUANOSINE (CCD ID: GMP) (formula:  $C_{10}H_{13}N_5O_5$ ) (labeled as "Ligand of Interest" by depositor).



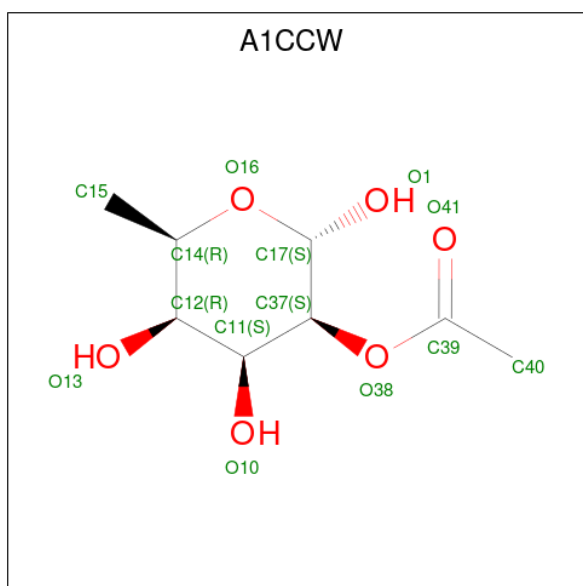
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	0	0
			33	10	13	5	5		

- Molecule 6 is alpha-L-fucopyranose (CCD ID: FUC) (formula:  $C_6H_{12}O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 7 is 2-O-acetyl-6-deoxy-alpha-D-talopyranose (CCD ID: A1CCW) (formula:  $C_8H_{14}O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			25	8	12	5		

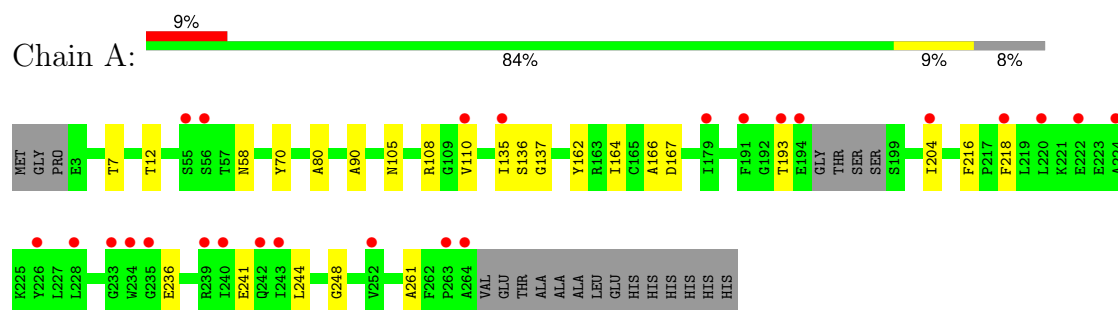
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total 6	O 6	0	0
8	B	8	Total 8	O 8	0	0

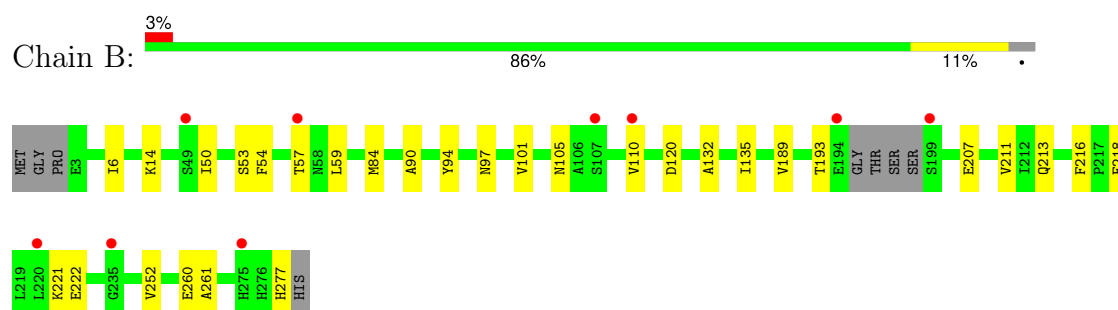
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Glycosyltransferase



#### • Molecule 1: Glycosyltransferase



#### • Molecule 2: alpha-L-fucopyranose-(1-4)-beta-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.64Å 65.67Å 128.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.07 – 2.25 46.07 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.07-2.25) 95.4 (46.07-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.215 , 0.265 0.225 , 0.267	Depositor DCC
$R_{free}$ test set	2011 reflections (8.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.0	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.031 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8316	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8280e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BGC, DMS, FUC, A1CCW, 5GP, GMP

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	0.09	0/2023	0.24	0/2740
1	B	0.09	0/2133	0.25	0/2891
All	All	0.09	0/4156	0.25	0/5631

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	1989	1981	1981	12	0
1	B	2094	2070	2070	16	0
2	C	21	21	19	0	0
3	A	24	12	12	0	0
4	A	4	6	6	0	0
5	B	20	13	13	1	0
6	B	11	11	10	0	0
7	B	13	12	0	0	0
8	A	6	0	0	0	0
8	B	8	0	0	0	0
All	All	4190	4126	4111	28	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.

All (28) 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:57:THR:HG23	1:B:59:LEU:HB2	1.63	0.80
1:B:97:ASN:O	1:B:101:VAL:HG23	2.04	0.58
1:A:236:GLU:N	1:A:236:GLU:OE1	2.35	0.57
1:A:7:THR:HG21	1:A:80:ALA:CB	2.35	0.57
1:B:252:VAL:HG12	1:B:277:HIS:CG	2.41	0.56
1:A:12:THR:HG22	1:A:90:ALA:HB2	1.90	0.53
1:A:162:TYR:O	1:A:166:ALA:HB2	2.08	0.53
1:B:54:PHE:O	1:B:57:THR:HG22	2.09	0.53
1:B:207:GLU:O	1:B:211:VAL:HG23	2.10	0.52
1:A:244:LEU:O	1:A:248:GLY:N	2.43	0.51
1:B:120:ASP:CG	1:B:193:THR:HG21	2.35	0.51
1:B:50:ILE:O	1:B:53:SER:OG	2.27	0.48
1:A:167:ASP:OD1	1:A:167:ASP:N	2.47	0.48
1:B:94:TYR:CD1	1:B:189:VAL:HG22	2.49	0.48
1:B:132:ALA:HB2	1:B:260:GLU:HB2	1.98	0.46
1:B:216:PHE:HB3	1:B:218:PHE:CZ	2.52	0.45
1:A:105:ASN:O	1:A:110:VAL:HG12	2.17	0.45
1:B:6:ILE:HD13	1:B:84:MET:HB2	1.98	0.45
1:B:90:ALA:HB3	5:B:301:GMP:O3'	2.17	0.44
1:A:164:ILE:HG21	1:A:204:ILE:HG12	1.99	0.43
1:B:120:ASP:OD2	1:B:193:THR:HG21	2.19	0.42
1:A:136:SER:OG	1:A:137:GLY:N	2.44	0.42
1:A:135:ILE:HD11	1:A:261:ALA:CB	2.50	0.42
1:B:213:GLN:HE22	1:B:221:LYS:HD3	1.84	0.41
1:B:105:ASN:O	1:B:110:VAL:HG12	2.20	0.41
1:A:216:PHE:HB3	1:A:218:PHE:CZ	2.56	0.41
1:A:70:TYR:CZ	1:A:166:ALA:HB3	2.56	0.40
1:B:135:ILE:HD11	1:B:261:ALA:CB	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	254/279 (91%)	247 (97%)	7 (3%)	0	100	100
1	B	267/279 (96%)	259 (97%)	8 (3%)	0	100	100
All	All	521/558 (93%)	506 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	214/230 (93%)	210 (98%)	4 (2%)	52	62
1	B	224/230 (97%)	222 (99%)	2 (1%)	75	83
All	All	438/460 (95%)	432 (99%)	6 (1%)	62	72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	108	ARG
1	A	193	THR
1	A	241	GLU
1	B	14	LYS
1	B	222	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	259	GLN
1	B	105	ASN

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Mol	Chain	Res	Type
1	B	275	HIS

### 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 ⓘ

2 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	BGC	C	1	7,2	11,11,12	1.79	5 (45%)	15,15,17	0.77	0
2	FUC	C	2	2	10,10,11	1.99	3 (30%)	14,14,16	0.91	1 (7%)

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	BGC	C	1	7,2	-	2/2/19/22	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	FUC	C2-C3	-4.61	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	BGC	O5-C1	3.14	1.49	1.43
2	C	1	BGC	C2-C3	-2.44	1.48	1.52
2	C	1	BGC	O5-C5	2.41	1.48	1.43
2	C	2	FUC	O5-C1	2.36	1.47	1.43
2	C	2	FUC	O3-C3	2.25	1.48	1.43
2	C	1	BGC	O4-C4	2.06	1.48	1.43
2	C	1	BGC	O2-C2	2.03	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	FUC	C6-C5-C4	-2.03	109.38	113.08

There are no chirality outliers.

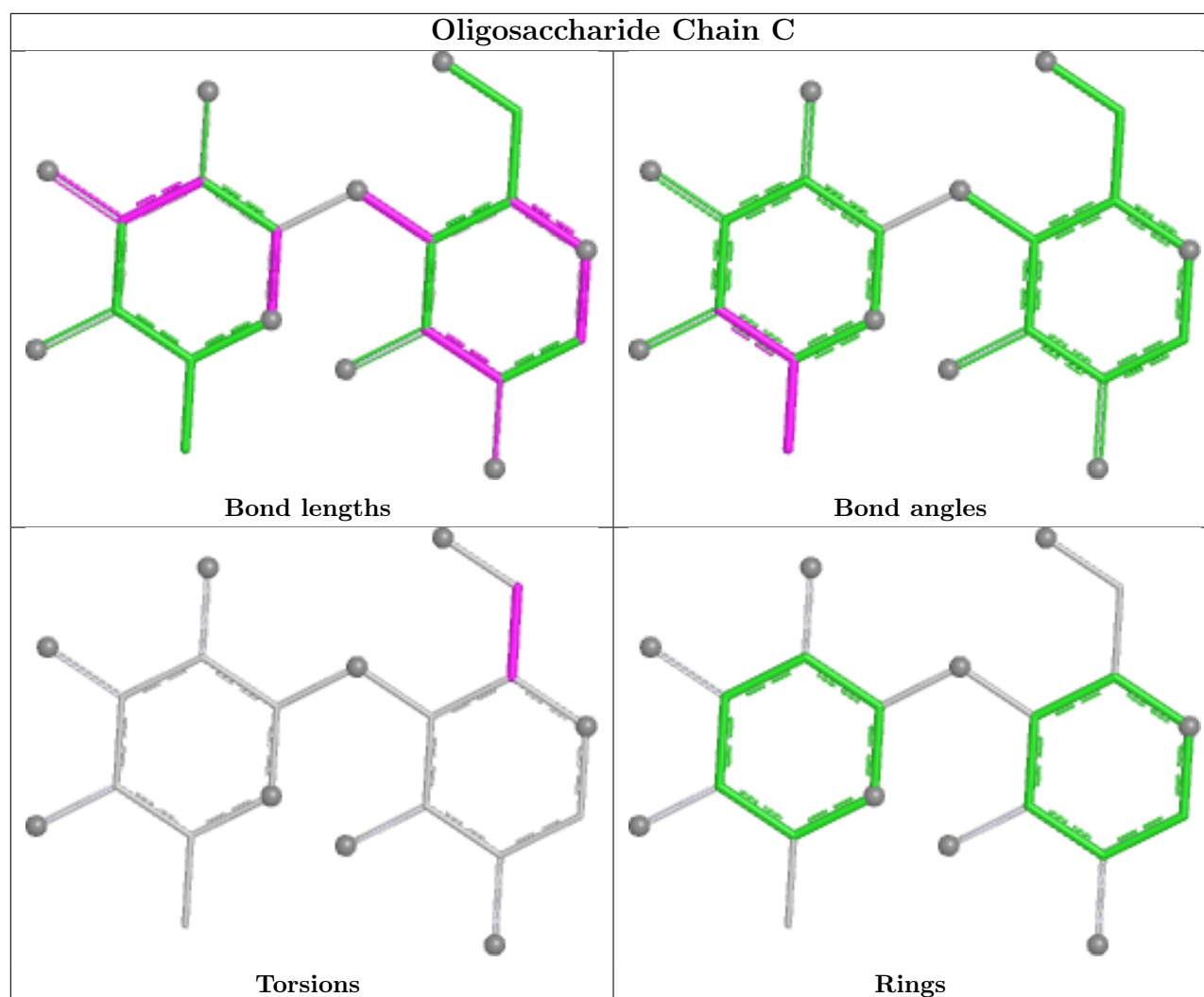
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	BGC	O5-C5-C6-O6
2	C	1	BGC	C4-C5-C6-O6

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](#)

5 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	GMP	B	301	-	18,22,22	2.62	7 (38%)	18,33,33	1.57	4 (22%)
7	A1CCW	B	303	2,6	13,13,14	1.97	5 (38%)	16,18,20	1.94	3 (18%)
3	5GP	A	301	-	22,26,26	1.28	3 (13%)	24,40,40	1.43	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DMS	A	302	-	3,3,3	0.67	0	3,3,3	0.46	0
6	FUC	B	302	7	11,11,11	1.63	3 (27%)	16,16,16	1.10	2 (12%)

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	GMP	B	301	-	-	2/2/22/22	0/3/3/3
7	A1CCW	B	303	2,6	-	2/4/21/24	0/1/1/1
6	FUC	B	302	7	-	-	0/1/1/1
3	5GP	A	301	-	-	4/6/26/26	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	GMP	C2-N3	5.34	1.46	1.33
5	B	301	GMP	C4-N3	4.99	1.49	1.37
5	B	301	GMP	C2-N2	4.89	1.45	1.34
3	A	301	5GP	C5-C6	-4.22	1.39	1.47
5	B	301	GMP	C6-N1	3.82	1.43	1.37
7	B	303	A1CCW	O38-C39	3.39	1.42	1.35
6	B	302	FUC	O5-C1	3.34	1.51	1.42
5	B	301	GMP	C5-C6	3.28	1.53	1.47
6	B	302	FUC	C3-C2	-2.96	1.44	1.52
5	B	301	GMP	C2-N1	2.85	1.44	1.37
7	B	303	A1CCW	O10-C11	2.69	1.49	1.43
5	B	301	GMP	C5-C4	-2.63	1.36	1.43
7	B	303	A1CCW	O16-C14	2.61	1.48	1.43
7	B	303	A1CCW	C11-C37	-2.38	1.48	1.53
6	B	302	FUC	O3-C3	2.21	1.48	1.43
7	B	303	A1CCW	C40-C39	2.07	1.56	1.49
3	A	301	5GP	C6-N1	-2.07	1.34	1.37
3	A	301	5GP	C5-C4	-2.04	1.38	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	303	A1CCW	O38-C39-C40	6.11	121.98	111.09
5	B	301	GMP	C8-N7-C5	3.21	108.01	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	GMP	C5-C6-N1	3.05	119.89	114.07
3	A	301	5GP	C8-N7-C5	3.00	107.66	102.55
3	A	301	5GP	C5-C6-N1	2.96	119.72	114.07
5	B	301	GMP	C2-N1-C6	-2.83	119.93	125.11
3	A	301	5GP	N2-C2-N1	2.49	122.02	116.76
3	A	301	5GP	C2-N1-C6	-2.39	120.74	125.11
6	B	302	FUC	C1-O5-C5	-2.32	110.76	114.37
3	A	301	5GP	O6-C6-C5	-2.27	119.82	124.32
6	B	302	FUC	C6-C5-C4	-2.19	109.07	113.08
7	B	303	A1CCW	O38-C39-O41	-2.13	118.88	122.99
5	B	301	GMP	O6-C6-C5	-2.09	120.18	124.32
7	B	303	A1CCW	C15-C14-C12	-2.03	109.36	113.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	5GP	C5'-O5'-P-O2P
3	A	301	5GP	C5'-O5'-P-O3P
7	B	303	A1CCW	O41-C39-O38-C37
7	B	303	A1CCW	C40-C39-O38-C37
5	B	301	GMP	O4'-C4'-C5'-O5'
5	B	301	GMP	C3'-C4'-C5'-O5'
3	A	301	5GP	C5'-O5'-P-O1P
3	A	301	5GP	O4'-C4'-C5'-O5'

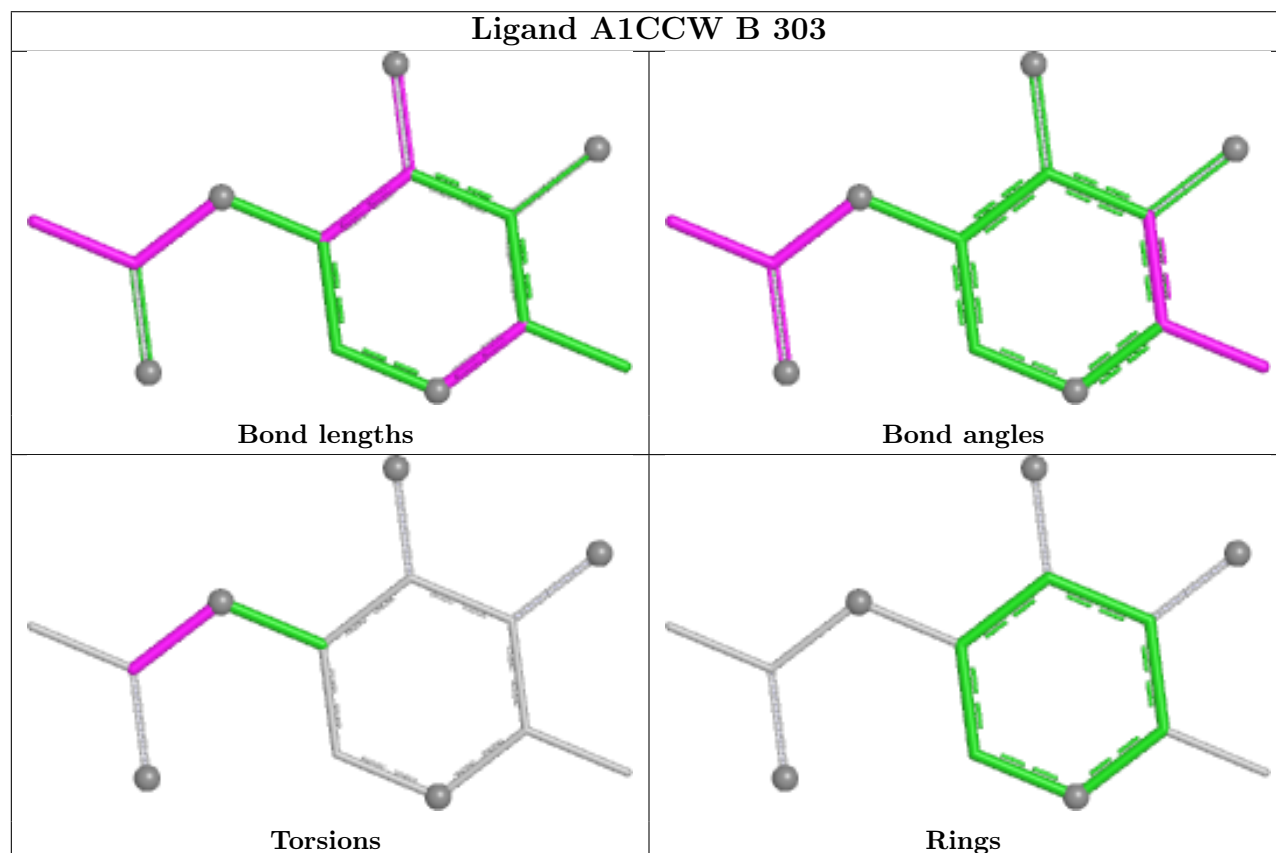
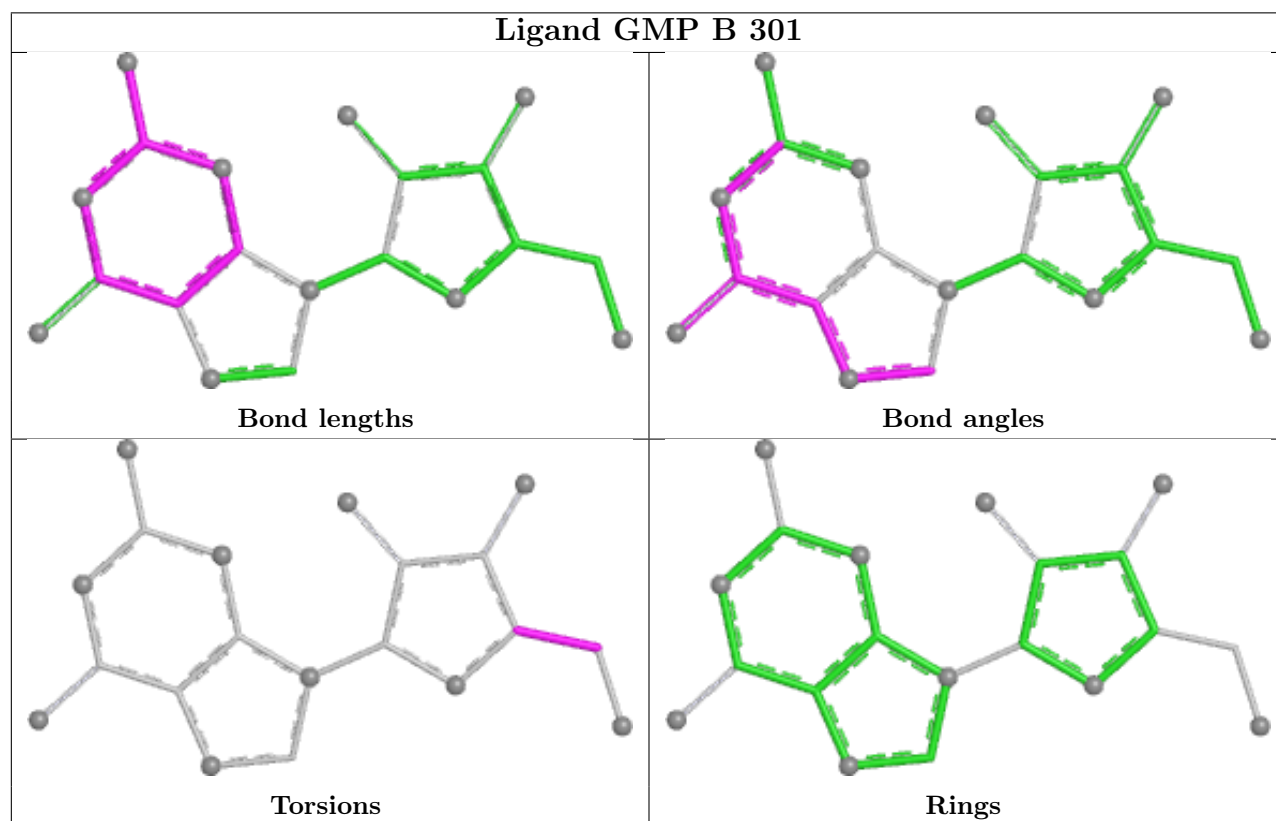
There are no ring outliers.

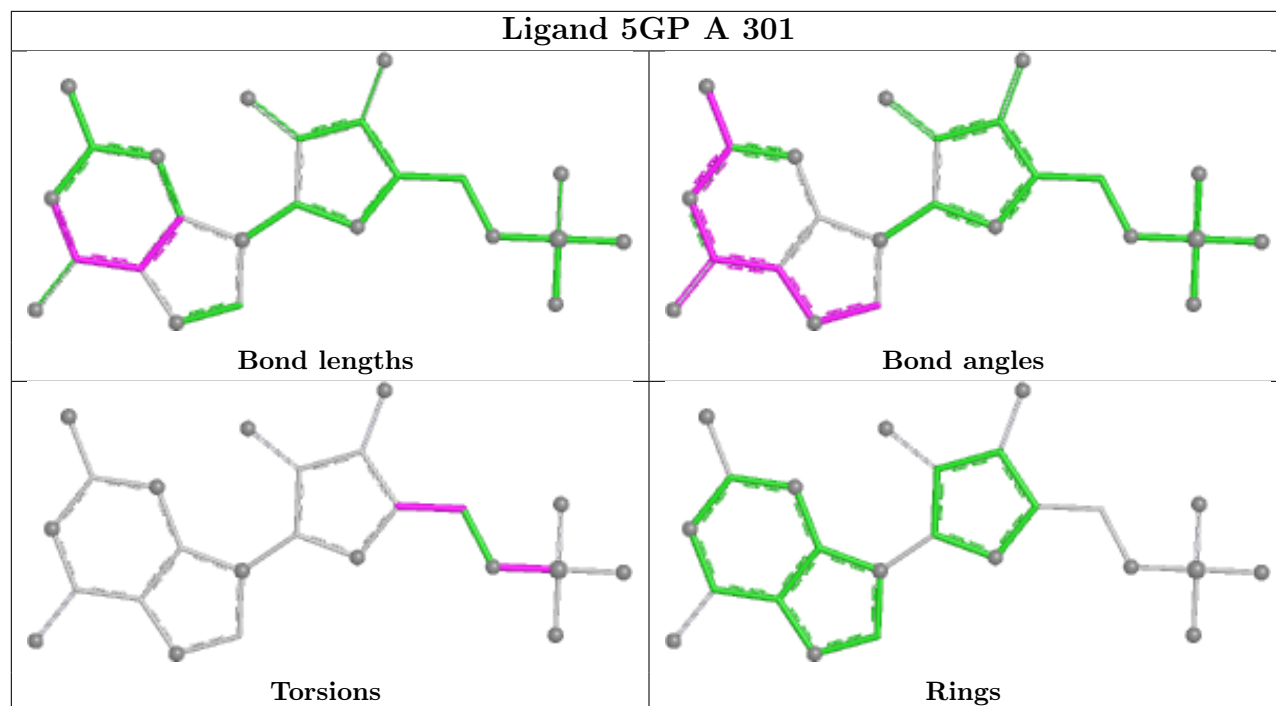
1 monomer is involved in 1 short contact:

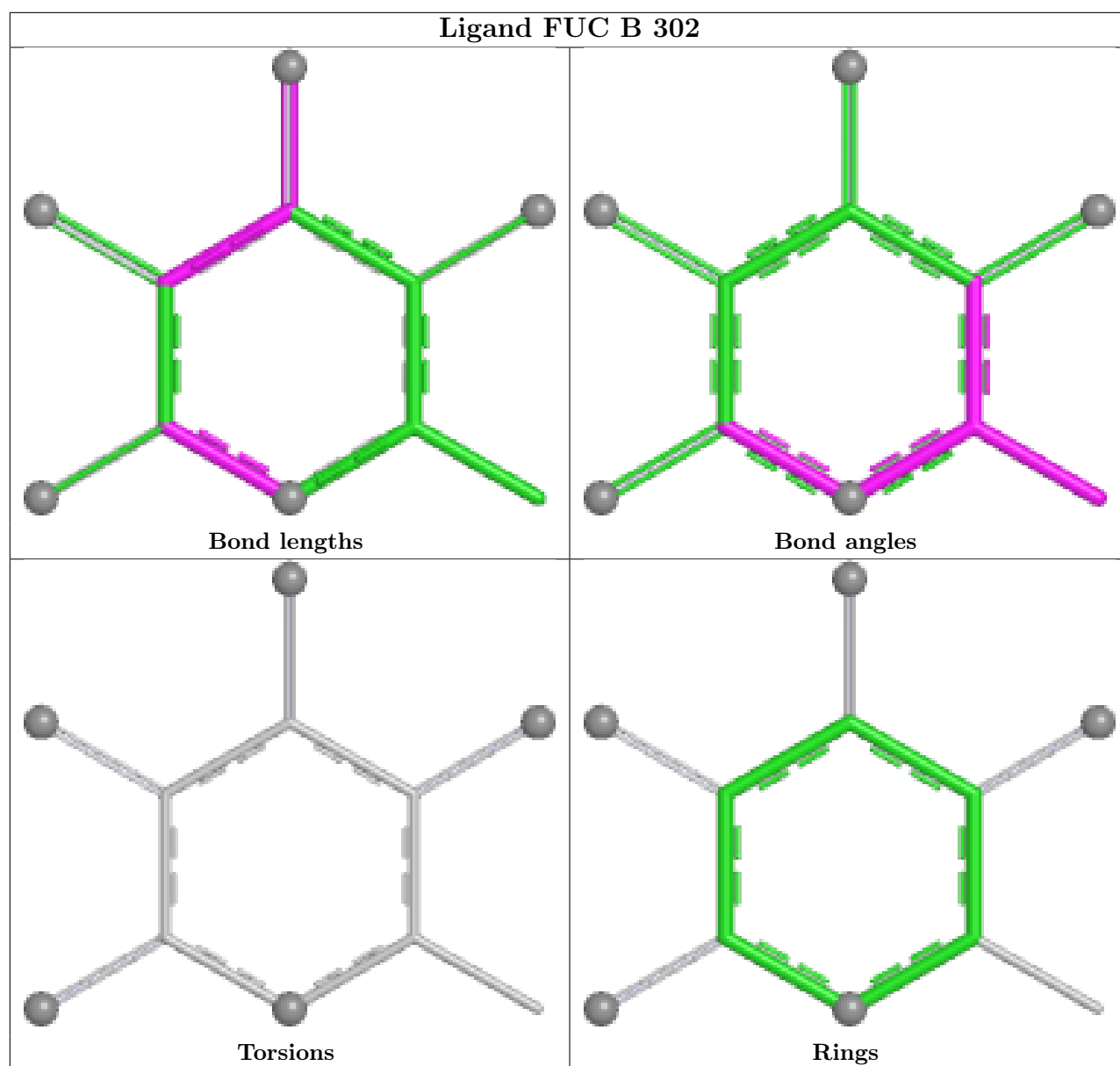
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	GMP	1	0

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	258/279 (92%)	0.68	25 (9%)	15 14	49, 75, 122, 144	0
1	B	271/279 (97%)	0.48	9 (3%)	49 50	48, 72, 102, 134	0
All	All	529/558 (94%)	0.58	34 (6%)	27 26	48, 74, 112, 144	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	ILE	3.9
1	A	264	ALA	3.7
1	A	235	GLY	3.5
1	B	110	VAL	3.4
1	A	220	LEU	3.3
1	B	235	GLY	2.8
1	A	191	PHE	2.8
1	A	234	TRP	2.6
1	B	199	SER	2.6
1	B	194	GLU	2.5
1	A	135	ILE	2.5
1	A	204	ILE	2.5
1	B	57	THR	2.5
1	A	193	THR	2.4
1	A	55	SER	2.4
1	A	194	GLU	2.4
1	A	224	ALA	2.4
1	A	222	GLU	2.3
1	A	228	LEU	2.3
1	B	275	HIS	2.3
1	A	226	TYR	2.2
1	A	242	GLN	2.2
1	B	220	LEU	2.2
1	B	49	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	179	ILE	2.2
1	A	56	SER	2.2
1	B	107	SER	2.2
1	A	218	PHE	2.1
1	A	239	ARG	2.1
1	A	263	PRO	2.1
1	A	110	VAL	2.1
1	A	252	VAL	2.1
1	A	233	GLY	2.0
1	A	243	ILE	2.0

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

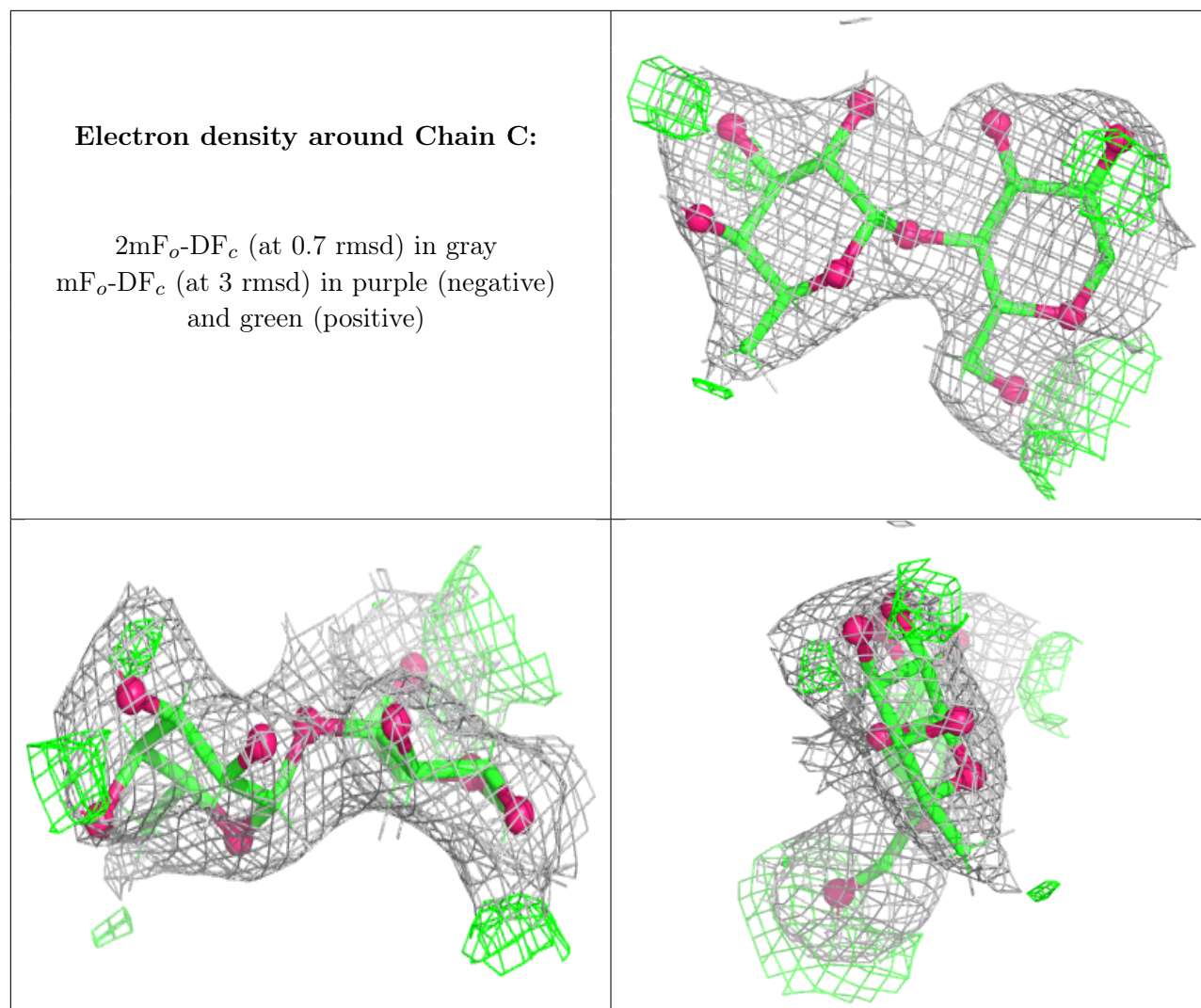
There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 95<sup>th</sup> 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	BGC	C	1	11/12	0.80	0.13	51,62,72,76	21
2	FUC	C	2	10/11	0.83	0.14	51,62,71,82	21

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.



## 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, 95<sup>th</sup> 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.

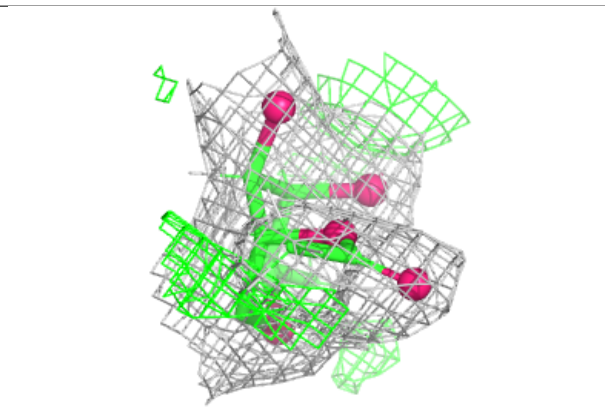
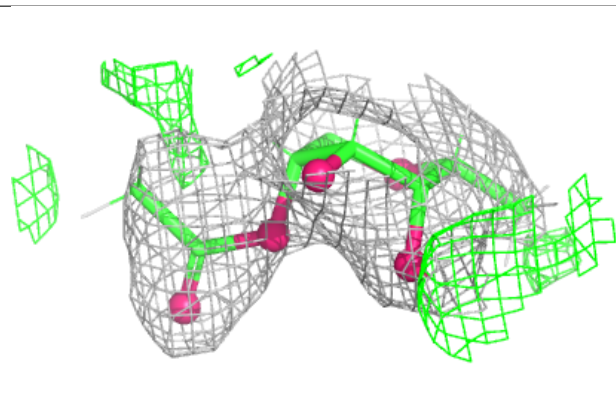
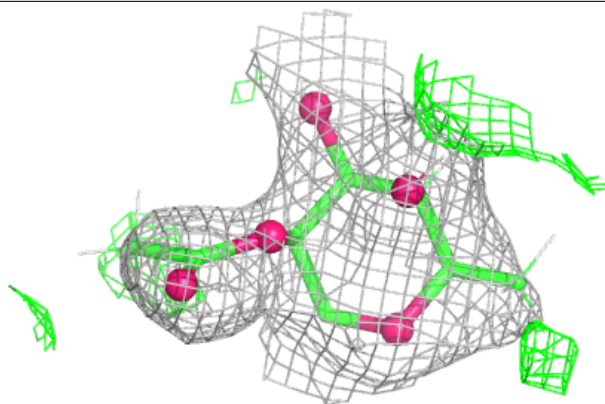
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	A1CCW	B	303	13/14	0.85	0.15	61,72,93,93	25
6	FUC	B	302	11/11	0.87	0.15	73,87,111,111	22
4	DMS	A	302	4/4	0.88	0.17	57,69,83,83	0
5	GMP	B	301	20/20	0.90	0.13	56,65,79,94	0
3	5GP	A	301	24/24	0.91	0.13	49,61,98,112	0

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 A1CCW B 303:**

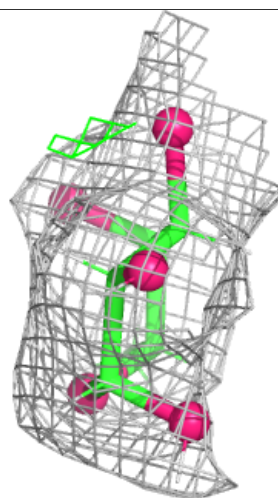
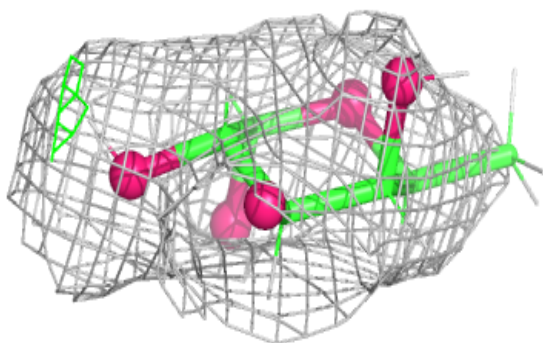
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





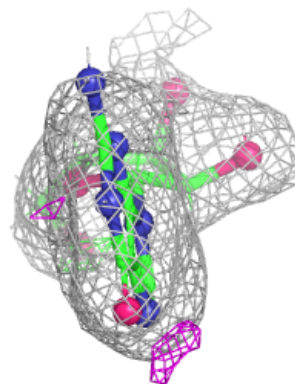
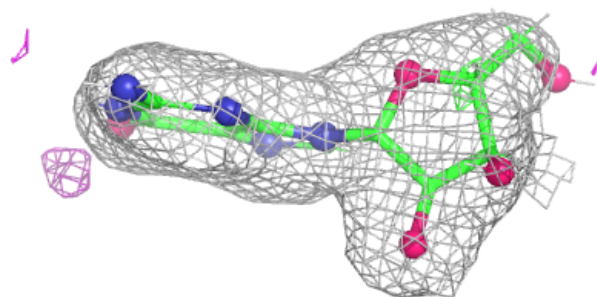
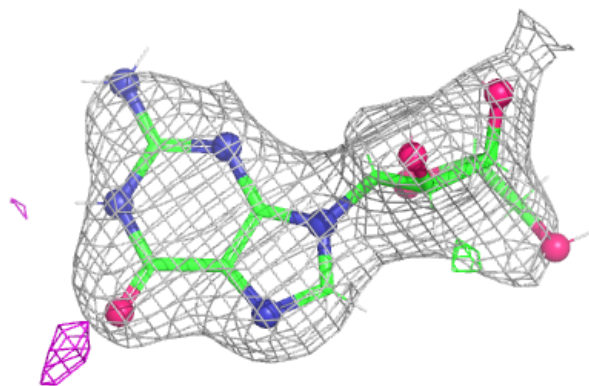
**Electron density around FUC B 302:**

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

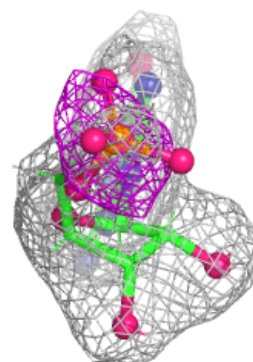
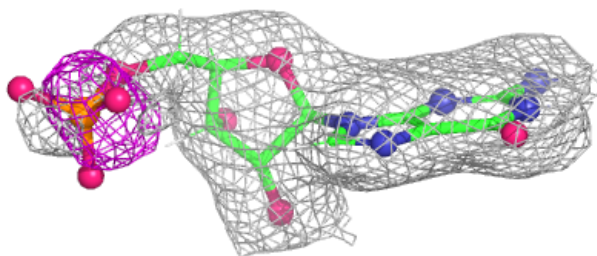
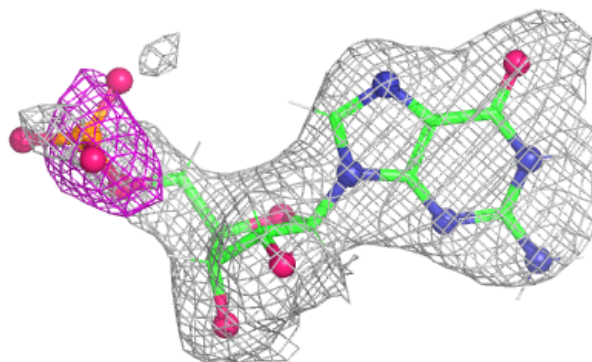


**Electron density around GMP B 301:**

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

**Electron density around 5GP A 301:**

$2mF_o-DF_c$  (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.