



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:28 PM BST

PDB ID : 5KXD
Title : Wisteria floribunda lectin in complex with GalNAc(beta1-4)GlcNAc (LacdiNAc) at pH 6.5
Authors : Evans, S.V.; Haji-Ghassemi, O.
Deposited on : 2016-07-20
Resolution : 1.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

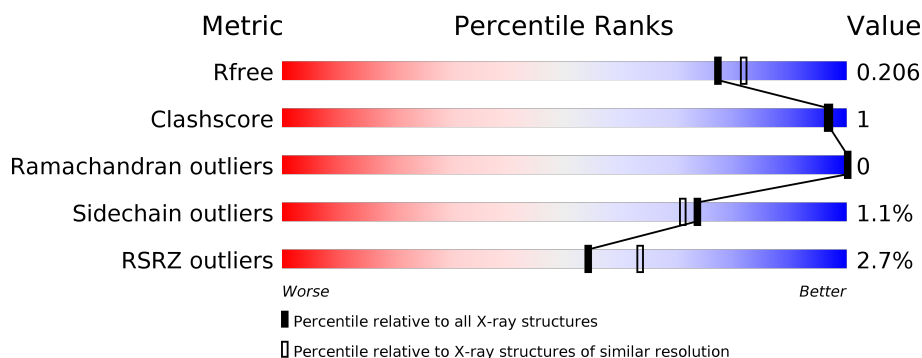
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 on 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	243	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div></div> </div> <div>..</div> </div>
1	B	243	<div> <div>3%</div> <div> <div></div> <div>96%</div> <div>5%</div> <div></div> </div> <div>..</div> </div>
1	C	243	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> <div>..</div> </div>
1	D	243	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> <div></div> </div> <div>..</div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	G	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	7	<div><div></div><div>29%</div><div>71%</div></div>

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
2	FUC	G	2	-	-	-	X
3	MAN	F	5	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8367 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 Wisteria floribunda agglutinin.

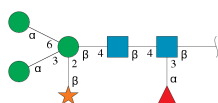
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	0	0	0
			1851	1179	304	368			
1	B	238	Total	C	N	O	0	0	0
			1851	1179	304	368			
1	C	238	Total	C	N	O	0	0	0
			1851	1179	304	368			
1	D	238	Total	C	N	O	0	0	0
			1851	1179	304	368			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	G	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	0	0	0
			80	45	2	33			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

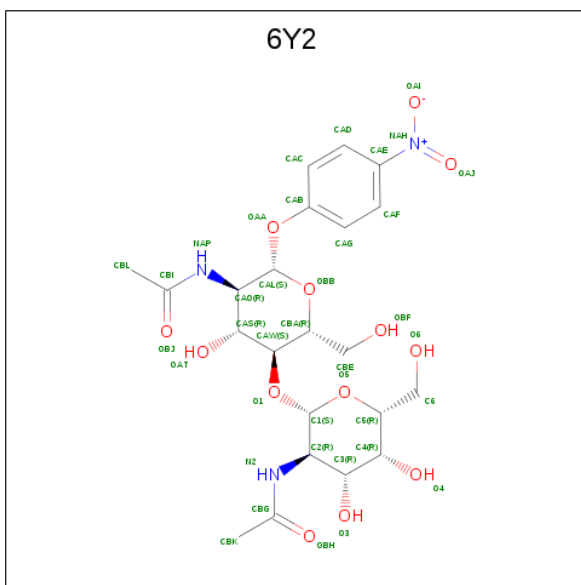
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	A	1	Total	Mn	0	0
			1	1		
5	D	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



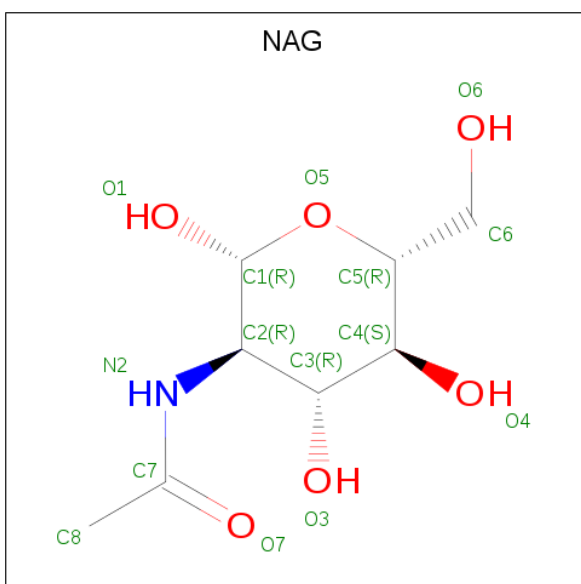
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is {N}-[(2 {S},3 {R},4 {R},5 {R},6 {R})-2-[(2 {R},3 {S},4 {R},5 {R},6 {S})-5-acetamido-2-(hydroxymethyl)-6-(4-nitrophenoxy)-4-oxidanyl-oxan-3-yl]oxy-6-(hydroxymethyl)-4,5-bis(oxidanyl)oxan-3-yl]ethanamide (three-letter code: 6Y2) (formula: C₂₂H₃₁N₃O₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			38	22	3	13		
7	B	1	Total	C	N	O	0	0
			38	22	3	13		
7	C	1	Total	C	N	O	0	0
			38	22	3	13		
7	D	1	Total	C	N	O	0	0
			38	22	3	13		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	179	Total	O	0	0
			179	179		
9	B	165	Total	O	0	0
			165	165		
9	C	163	Total	O	0	0
			163	163		
9	D	130	Total	O	0	0
			130	130		

3 Residue-property plots [i](#)

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.

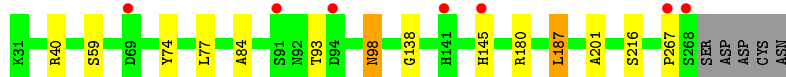
- Molecule 1: *Wisteria floribunda* agglutinin



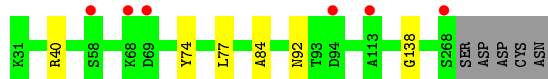
- Molecule 1: *Wisteria floribunda* agglutinin



- Molecule 1: *Wisteria floribunda* agglutinin



- Molecule 1: *Wisteria floribunda* agglutinin



- Molecule 2: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

MAG1
FUC2

- Molecule 3: beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  29% 71%

MAG1
MAG2
BMA3
XYP4
MAN5
MAN6
FUC7

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.10Å 104.27Å 148.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 24.85 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-1.95) 98.2 (24.85-1.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.179 , 0.198 0.188 , 0.206	Depositor DCC
R_{free} test set	4358 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8367	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6Y2, XYP, BMA, NAG, CA, MN, FUC, ACT, 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	0.55	0/1899	0.75	2/2599 (0.1%)
1	B	0.54	0/1899	0.71	0/2599
1	C	0.55	0/1899	0.78	3/2599 (0.1%)
1	D	0.52	0/1899	0.72	1/2599 (0.0%)
All	All	0.54	0/7596	0.74	6/10396 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ARG	CG-CD-NE	-7.58	95.88	111.80
1	C	187	LEU	CB-CG-CD1	-7.26	98.66	111.00
1	C	40	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	C	180	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	D	40	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	180	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1851	0	1781	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1851	0	1781	4	0
1	C	1851	0	1781	7	0
1	D	1851	0	1781	2	0
2	E	24	0	22	0	0
2	G	24	0	22	0	0
3	F	80	0	60	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
6	C	8	0	6	0	0
6	D	8	0	6	1	0
7	A	38	0	0	0	0
7	B	38	0	0	0	0
7	C	38	0	0	0	0
7	D	38	0	0	0	0
8	B	14	0	13	0	0
9	A	179	0	0	1	1
9	B	165	0	0	0	0
9	C	163	0	0	0	2
9	D	130	0	0	1	0
All	All	8367	0	7259	14	2

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 1.

All (14) 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:C:93:THR:HB	1:C:267:PRO:HG3	1.82	0.61
6:D:305:ACT:H1	9:D:509:HOH:O	2.06	0.55
1:A:186:ASP:OD2	9:A:401:HOH:O	2.19	0.52
1:A:84:ALA:HB2	1:B:84:ALA:HB2	1.92	0.52
1:A:98:ASN:ND2	1:A:201:ALA:H	2.09	0.50
1:C:84:ALA:HB2	1:D:84:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ASN:ND2	1:C:201:ALA:H	2.11	0.48
1:B:77:LEU:HD11	1:B:138:GLY:HA3	1.97	0.47
1:C:77:LEU:HD11	1:C:138:GLY:HA3	1.97	0.47
1:B:222:ASN:HD21	1:C:216:SER:HA	1.79	0.47
1:A:77:LEU:HD11	1:A:138:GLY:HA3	1.97	0.46
1:B:222:ASN:ND2	1:C:216:SER:HA	2.33	0.43
1:D:77:LEU:HD11	1:D:138:GLY:HA3	2.00	0.43
1:C:145:HIS:O	1:C:145:HIS:ND1	2.54	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:496:HOH:O	9:C:535:HOH:O[4_555]	2.04	0.16
9:A:420:HOH:O	9:C:409:HOH:O[3_544]	2.13	0.07

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	236/243 (97%)	232 (98%)	4 (2%)	0	100	100
1	B	236/243 (97%)	232 (98%)	4 (2%)	0	100	100
1	C	236/243 (97%)	231 (98%)	5 (2%)	0	100	100
1	D	236/243 (97%)	232 (98%)	4 (2%)	0	100	100
All	All	944/972 (97%)	927 (98%)	17 (2%)	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	210/215 (98%)	208 (99%)	2 (1%)	76	74
1	B	210/215 (98%)	209 (100%)	1 (0%)	88	88
1	C	210/215 (98%)	206 (98%)	4 (2%)	57	50
1	D	210/215 (98%)	208 (99%)	2 (1%)	76	74
All	All	840/860 (98%)	831 (99%)	9 (1%)	73	71

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	TYR
1	A	222	ASN
1	B	74	TYR
1	C	59	SER
1	C	74	TYR
1	C	98	ASN
1	C	187	LEU
1	D	74	TYR
1	D	92	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	145	HIS
1	A	222	ASN
1	B	175	ASN
1	B	222	ASN
1	C	61	HIS
1	C	98	ASN
1	D	173	ASN
1	D	175	ASN

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 ⓘ

11 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	E	1	1,2	14,14,15	0.49	0	17,19,21	1.33	1 (5%)
2	FUC	E	2	2	10,10,11	0.30	0	14,14,16	0.62	0
3	NAG	F	1	1,3	14,14,15	0.44	0	17,19,21	1.16	1 (5%)
3	NAG	F	2	3	14,14,15	0.47	0	17,19,21	1.08	2 (11%)
3	BMA	F	3	3	11,11,12	0.63	0	15,15,17	1.60	3 (20%)
3	XYP	F	4	3	9,9,10	0.38	0	10,12,14	0.90	0
3	MAN	F	5	3	11,11,12	0.50	0	15,15,17	0.86	0
3	MAN	F	6	3	11,11,12	0.61	0	15,15,17	1.40	2 (13%)
3	FUC	F	7	3	10,10,11	1.29	2 (20%)	14,14,16	1.28	1 (7%)
2	NAG	G	1	1,2	14,14,15	0.31	0	17,19,21	1.23	3 (17%)
2	FUC	G	2	2	10,10,11	0.29	0	14,14,16	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	XYP	F	4	3	-	-	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	FUC	F	7	3	-	-	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	7	FUC	O5-C1	-2.57	1.39	1.43
3	F	7	FUC	O2-C2	-2.08	1.38	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	BMA	O5-C5-C6	3.86	113.25	107.20
3	F	6	MAN	C1-C2-C3	3.38	113.82	109.67
2	E	1	NAG	C1-O5-C5	3.28	116.64	112.19
3	F	3	BMA	C6-C5-C4	-2.86	106.30	113.00
2	G	1	NAG	O5-C5-C6	2.74	111.50	107.20
3	F	1	NAG	C1-O5-C5	2.59	115.70	112.19
3	F	3	BMA	C1-O5-C5	2.32	115.34	112.19
2	G	1	NAG	O3-C3-C2	-2.29	104.73	109.47
2	G	1	NAG	C1-O5-C5	2.25	115.24	112.19
3	F	7	FUC	O5-C1-C2	-2.24	107.31	110.77
3	F	6	MAN	O5-C5-C6	2.11	110.52	107.20
3	F	2	NAG	O4-C4-C3	-2.08	105.53	110.35
3	F	2	NAG	O4-C4-C5	2.07	114.44	109.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	3	BMA	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6

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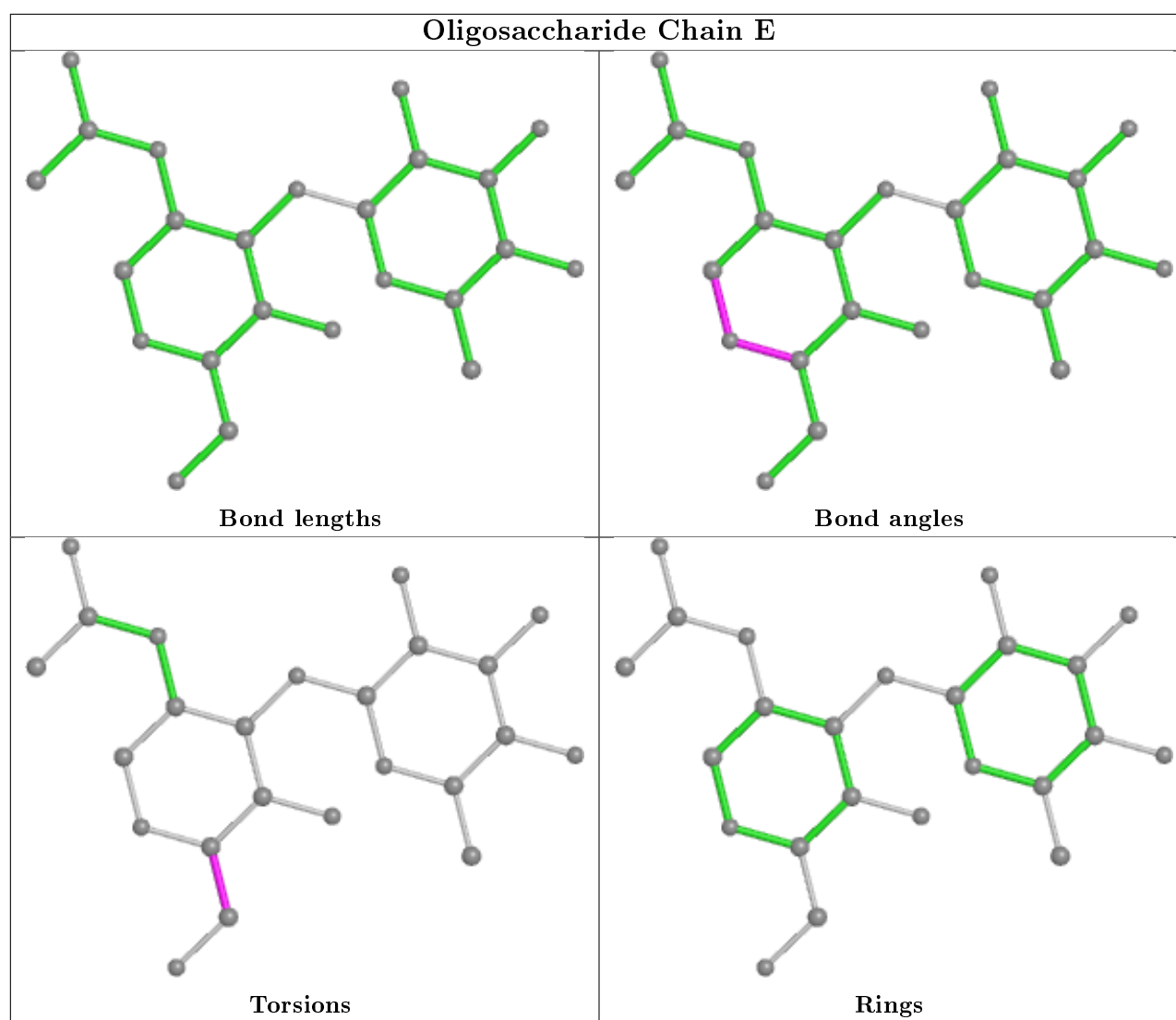
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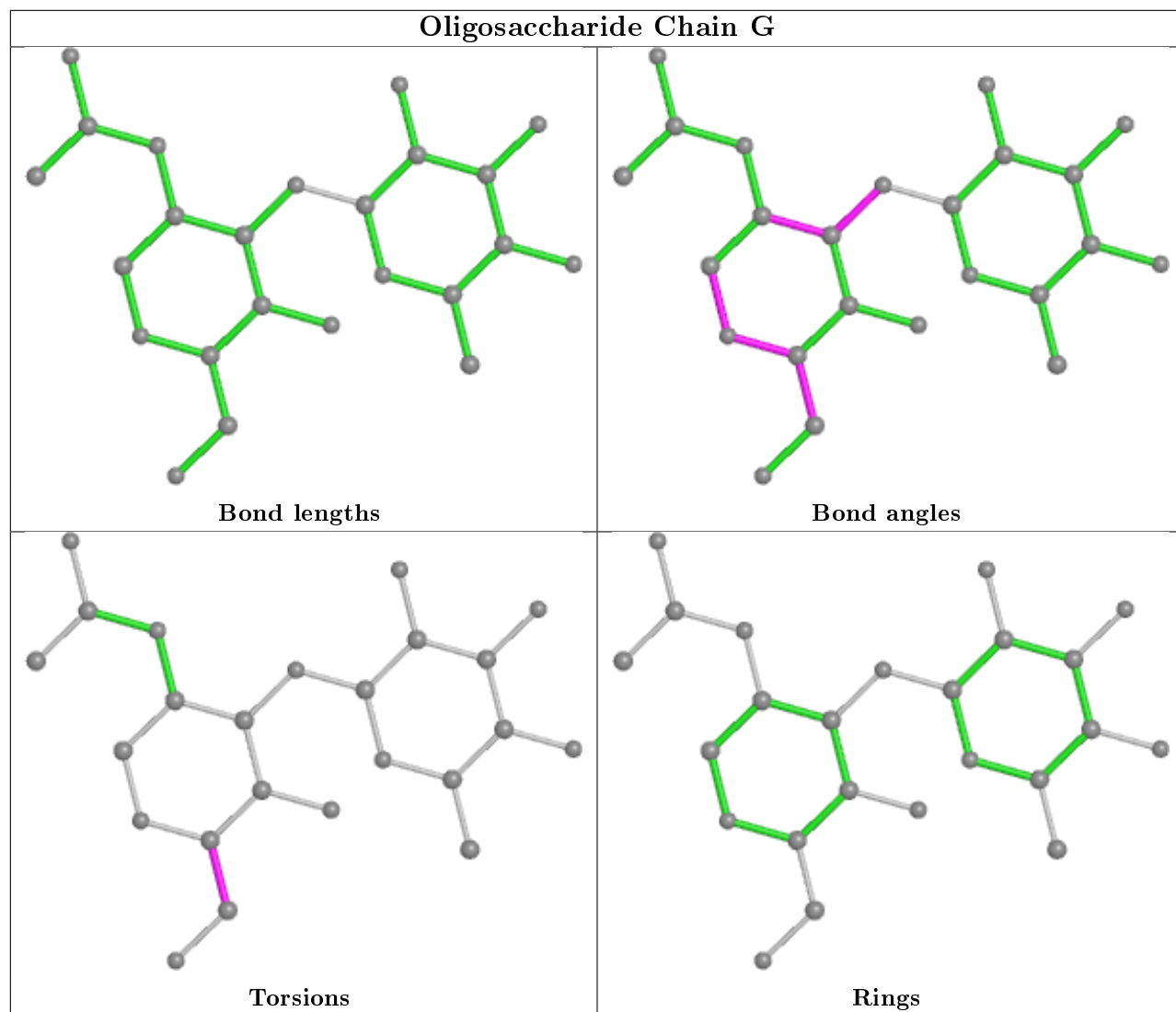
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	F	5	MAN	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6

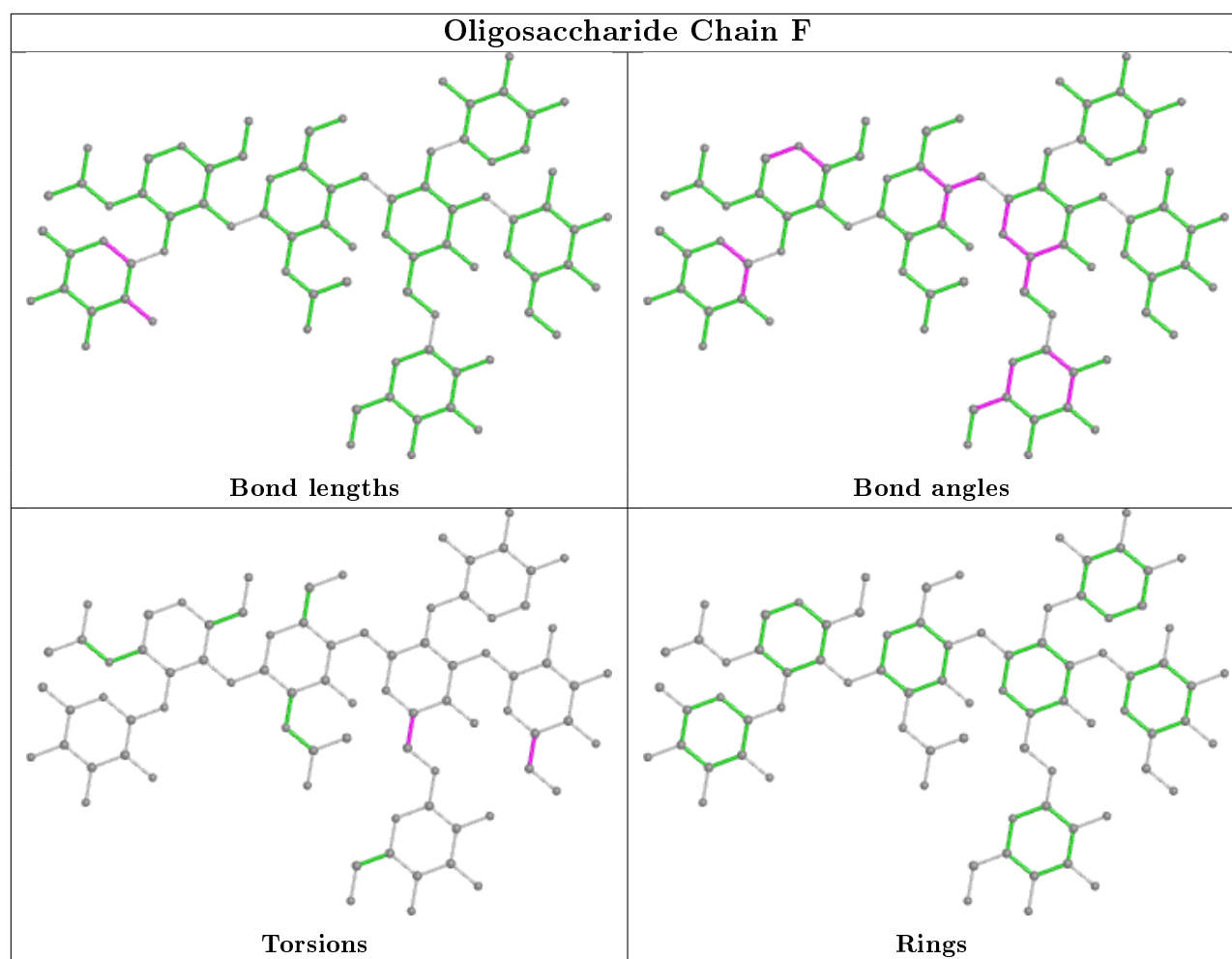
There are no ring outliers.

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](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 for Mogul analysis.

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	$\# Z > 2$
7	6Y2	B	305	-	39,40,40	2.23	2 (5%)	55,57,57	1.18	3 (5%)
6	ACT	D	305	-	1,3,3	0.04	0	0,3,3	0.00	-
6	ACT	A	305	-	1,3,3	1.65	0	0,3,3	0.00	-
6	ACT	B	304	-	1,3,3	0.48	0	0,3,3	0.00	-
6	ACT	D	306	-	1,3,3	1.82	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	B	301	1	14,14,15	0.80	1 (7%)	17,19,21	2.40	7 (41%)
7	6Y2	C	312	-	39,40,40	3.05	6 (15%)	55,57,57	1.08	3 (5%)
7	6Y2	D	307	-	39,40,40	2.97	5 (12%)	55,57,57	1.17	5 (9%)
6	ACT	C	310	-	1,3,3	2.75	1 (100%)	0,3,3	0.00	-
7	6Y2	A	306	-	39,40,40	2.68	4 (10%)	55,57,57	1.10	6 (10%)
6	ACT	C	311	-	1,3,3	1.26	0	0,3,3	0.00	-

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
7	6Y2	B	305	-	-	4/22/64/64	0/3/3/3
8	NAG	B	301	1	-	3/6/23/26	0/1/1/1
7	6Y2	C	312	-	-	4/22/64/64	0/3/3/3
7	6Y2	D	307	-	-	2/22/64/64	0/3/3/3
7	6Y2	A	306	-	-	2/22/64/64	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	312	6Y2	OAJ-NAH	17.20	1.52	1.22
7	D	307	6Y2	OAJ-NAH	16.72	1.51	1.22
7	A	306	6Y2	OAJ-NAH	14.43	1.47	1.22
7	B	305	6Y2	OAJ-NAH	12.02	1.43	1.22
7	D	307	6Y2	CAE-NAH	-4.80	1.33	1.45
7	C	312	6Y2	CAE-NAH	-4.75	1.33	1.45
7	A	306	6Y2	CAE-NAH	-4.65	1.34	1.45
7	B	305	6Y2	CAE-NAH	-3.63	1.36	1.45
7	A	306	6Y2	OAA-CAL	3.34	1.46	1.41
7	A	306	6Y2	CAL-CAO	-3.19	1.47	1.53
7	C	312	6Y2	OAA-CAL	3.05	1.45	1.41
7	D	307	6Y2	CAL-CAO	-3.03	1.48	1.53
6	C	310	ACT	CH3-C	2.75	1.52	1.48
7	D	307	6Y2	C4-C5	2.38	1.58	1.53
7	C	312	6Y2	CBL-CBI	2.25	1.55	1.50
7	C	312	6Y2	CAO-NAP	2.13	1.49	1.45
7	C	312	6Y2	CBK-CBG	2.08	1.54	1.50
8	B	301	NAG	C1-C2	2.07	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	307	6Y2	OAT-CAS	-2.01	1.38	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	301	NAG	C2-N2-C7	5.28	130.42	122.90
8	B	301	NAG	C8-C7-N2	4.84	124.29	116.10
7	B	305	6Y2	CAL-CAO-NAP	-3.30	105.31	111.00
8	B	301	NAG	C1-O5-C5	3.15	116.46	112.19
7	A	306	6Y2	CAL-OB-BA	-3.05	107.69	113.69
7	D	307	6Y2	O1-C1-C2	-2.99	103.07	108.24
7	B	305	6Y2	O1-C1-O5	-2.78	102.91	110.67
7	B	305	6Y2	C1-O5-C5	-2.68	108.43	113.69
8	B	301	NAG	C4-C3-C2	-2.67	107.11	111.02
7	A	306	6Y2	CAS-CAO-NAP	-2.65	105.61	110.62
7	C	312	6Y2	C1-C2-N2	-2.63	106.48	111.00
7	D	307	6Y2	C1-O5-C5	-2.49	108.80	113.69
8	B	301	NAG	C3-C4-C5	-2.44	105.89	110.24
7	C	312	6Y2	CAD-CAE-NAH	2.38	121.16	119.38
7	A	306	6Y2	CAD-CAE-NAH	2.34	121.14	119.38
7	D	307	6Y2	OB-BA	-2.31	103.35	111.29
7	A	306	6Y2	O5-C5-C6	2.30	112.16	106.44
8	B	301	NAG	O7-C7-N2	-2.29	117.73	121.95
7	D	307	6Y2	OB-BA-CAO	-2.21	106.26	110.58
7	A	306	6Y2	CAL-CAO-NAP	-2.21	107.20	111.00
8	B	301	NAG	O7-C7-C8	-2.20	117.98	122.06
7	C	312	6Y2	OAA-CAL-CAO	2.10	109.94	107.09
7	A	306	6Y2	CAB-OAA-CAL	-2.05	114.79	117.79
7	D	307	6Y2	C6-C5-C4	-2.03	108.24	113.00

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	312	6Y2	CAD-CAE-NAH-OAJ
7	C	312	6Y2	CAF-CAE-NAH-OAJ
7	A	306	6Y2	CAD-CAE-NAH-OAJ
7	A	306	6Y2	CAF-CAE-NAH-OAJ
8	B	301	NAG	C8-C7-N2-C2
8	B	301	NAG	O7-C7-N2-C2
7	B	305	6Y2	OB-CBI-NAP-CAO
7	B	305	6Y2	CBL-CBI-NAP-CAO

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Mol	Chain	Res	Type	Atoms
7	D	307	6Y2	CAD-CAE-NAH-OAJ
7	B	305	6Y2	CBA-CAW-O1-C1
7	C	312	6Y2	CBA-CAW-O1-C1
8	B	301	NAG	C3-C2-N2-C7
7	D	307	6Y2	CAF-CAE-NAH-OAJ
7	C	312	6Y2	CAS-CAW-O1-C1
7	B	305	6Y2	CAS-CAW-O1-C1

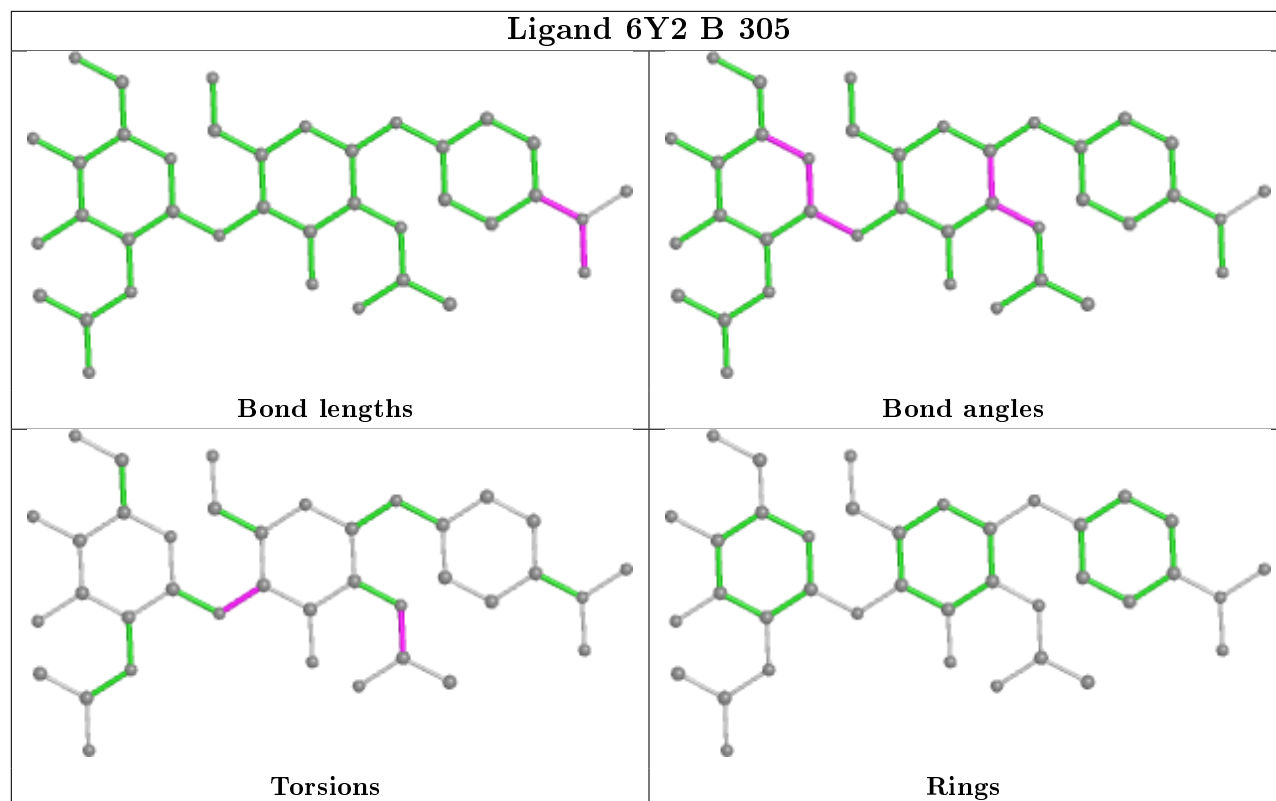
There are no ring outliers.

1 monomer is involved in 1 short contact:

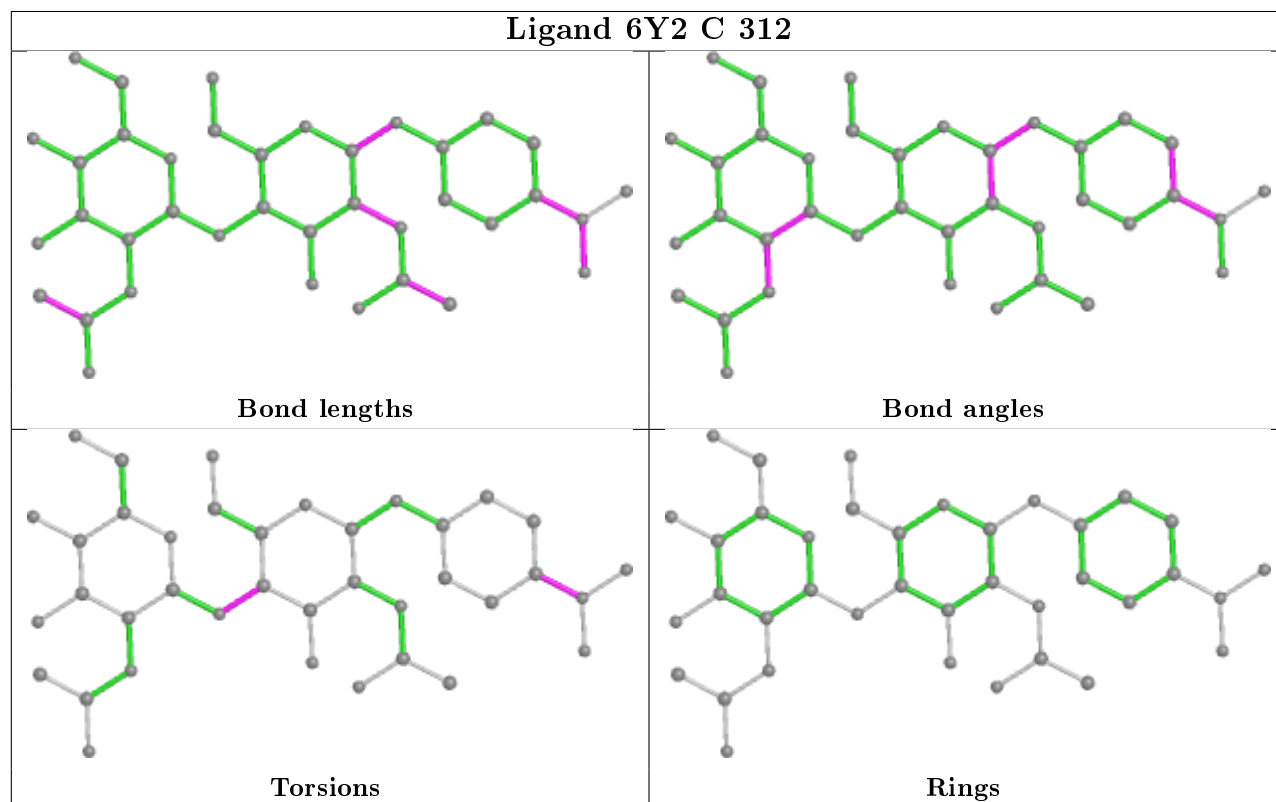
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	305	ACT	1	0

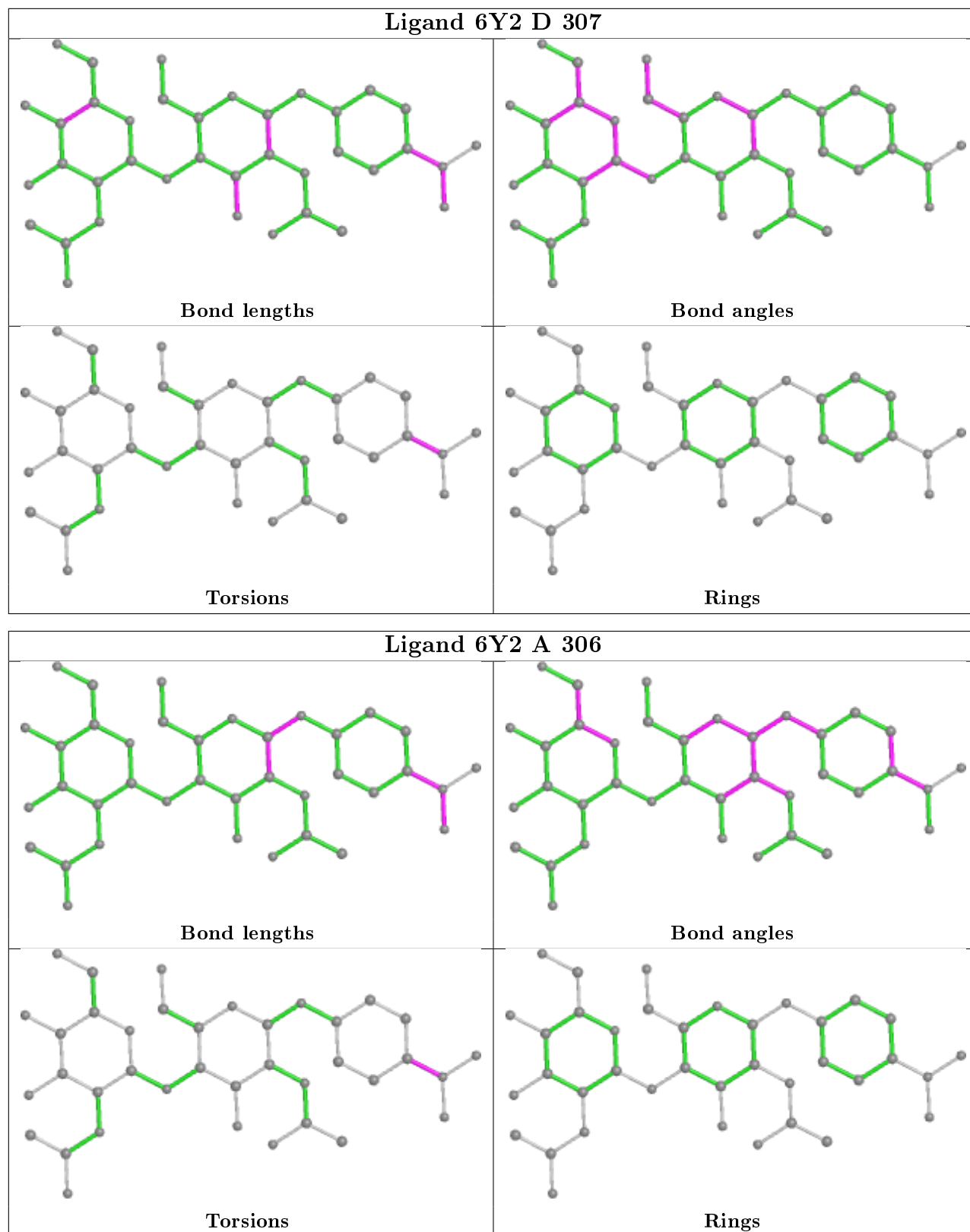
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 6Y2 B 305



Ligand 6Y2 C 312





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	238/243 (97%)	0.07	6 (2%) 57 66	13, 20, 35, 53	0
1	B	238/243 (97%)	0.09	7 (2%) 51 60	12, 20, 39, 57	0
1	C	238/243 (97%)	0.08	7 (2%) 51 60	12, 19, 37, 60	0
1	D	238/243 (97%)	0.08	6 (2%) 57 66	12, 20, 37, 61	0
All	All	952/972 (97%)	0.08	26 (2%) 54 63	12, 20, 37, 61	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	SER	6.2
1	B	268	SER	5.2
1	A	268	SER	4.0
1	D	268	SER	3.6
1	D	69	ASP	3.0
1	C	94	ASP	2.9
1	B	69	ASP	2.9
1	C	145	HIS	2.8
1	A	120	ALA	2.7
1	B	94	ASP	2.6
1	A	69	ASP	2.6
1	D	113	ALA	2.5
1	A	119	LEU	2.5
1	D	68	LYS	2.4
1	B	144	ARG	2.4
1	C	267	PRO	2.3
1	D	94	ASP	2.2
1	C	69	ASP	2.1
1	B	141	HIS	2.1
1	B	44	ASP	2.1
1	D	58	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	141	HIS	2.0
1	A	141	HIS	2.0
1	B	71	GLU	2.0
1	C	91	SER	2.0
1	A	144	ARG	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](#)

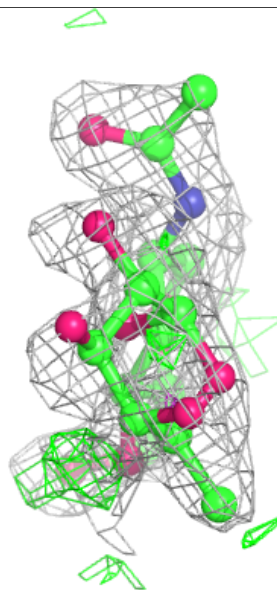
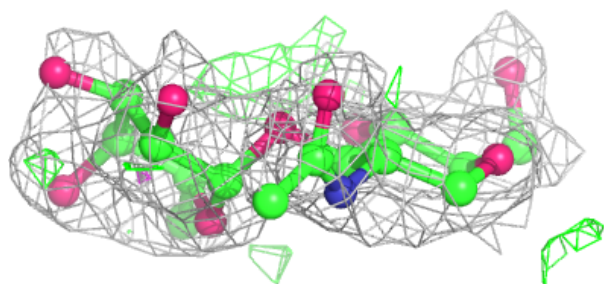
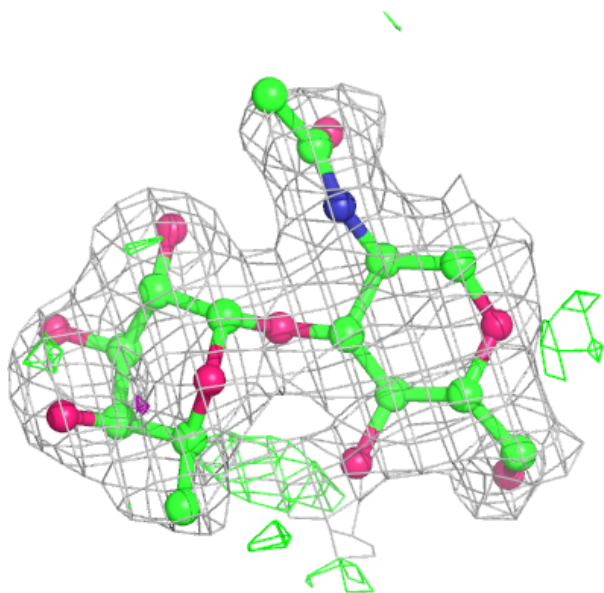
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	F	6	11/12	0.67	0.35	69,74,76,76	0
3	BMA	F	3	11/12	0.72	0.23	53,59,65,67	0
3	MAN	F	5	11/12	0.75	0.45	70,74,81,83	0
2	FUC	E	2	10/11	0.77	0.28	53,56,59,61	0
3	XYP	F	4	9/10	0.77	0.38	61,66,70,74	0
2	FUC	G	2	10/11	0.79	0.45	68,71,72,73	0
2	NAG	E	1	14/15	0.88	0.25	37,44,53,53	0
2	NAG	G	1	14/15	0.88	0.26	44,49,52,58	0
3	NAG	F	2	14/15	0.93	0.15	27,33,39,45	0
3	FUC	F	7	10/11	0.95	0.08	20,22,23,23	0
3	NAG	F	1	14/15	0.97	0.07	19,21,23,23	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.

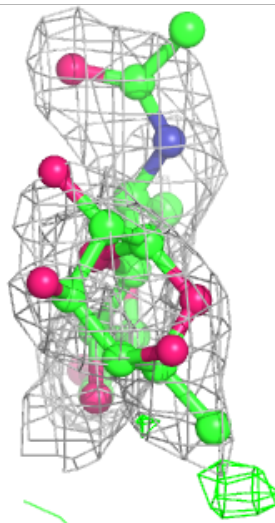
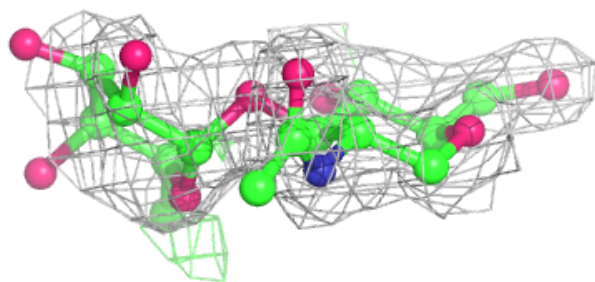
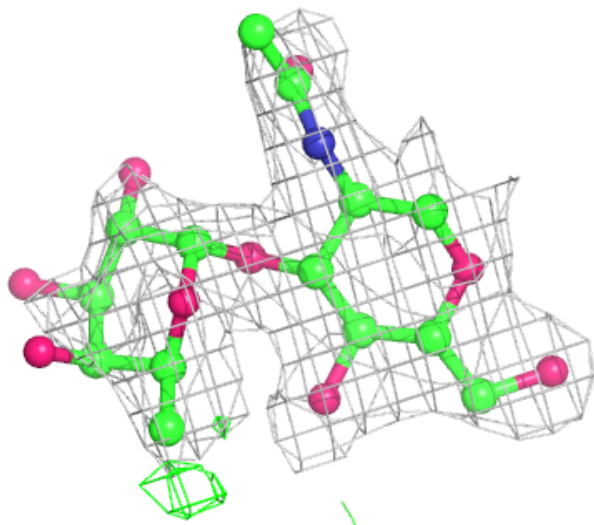
Electron density around Chain E:

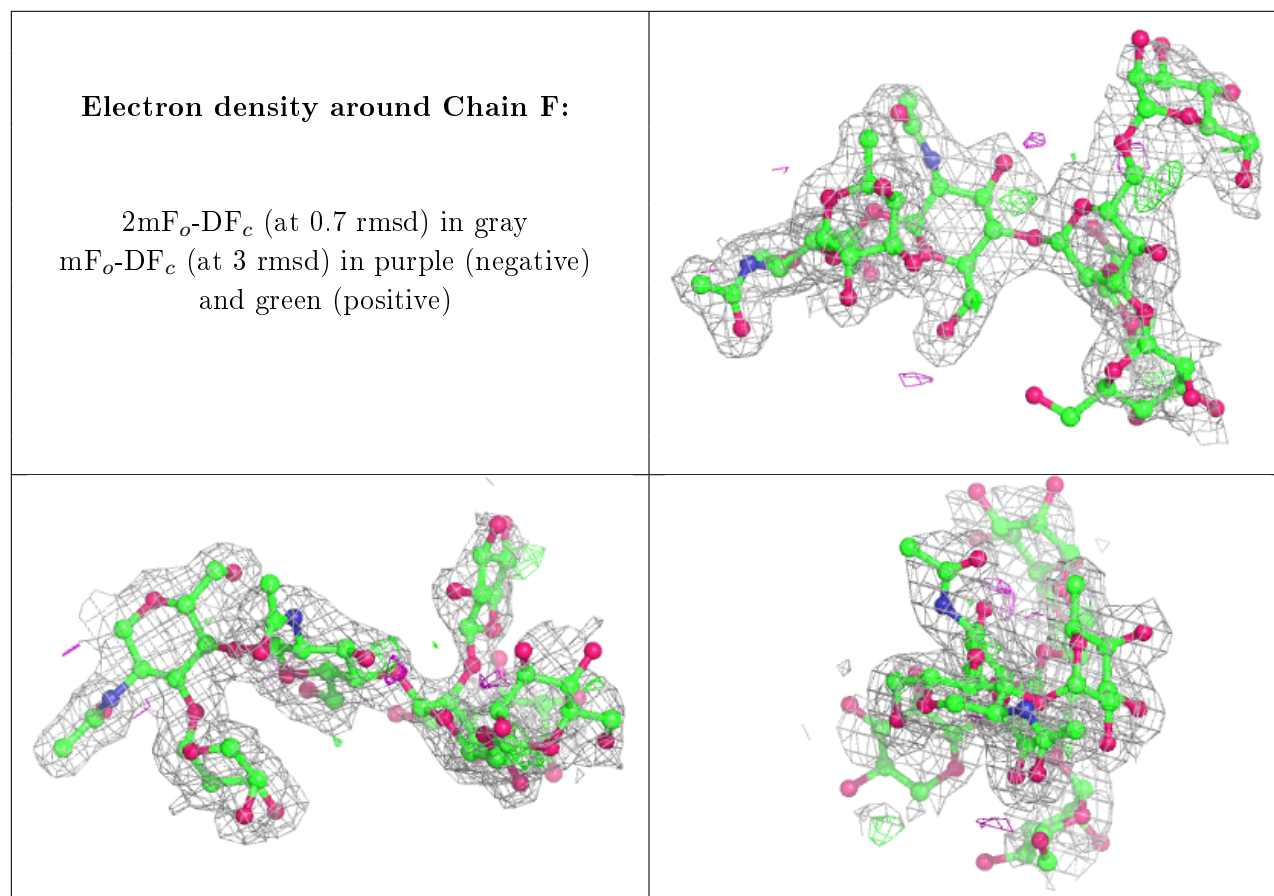
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	NAG	B	301	14/15	0.75	0.28	53,61,66,66	0
6	ACT	A	305	4/4	0.80	0.17	31,34,37,40	0
6	ACT	C	310	4/4	0.81	0.25	32,40,41,41	0
7	6Y2	A	306	38/38	0.87	0.20	20,39,92,98	0
7	6Y2	C	312	38/38	0.88	0.19	18,35,76,80	0
6	ACT	B	304	4/4	0.89	0.14	29,35,36,37	0
7	6Y2	D	307	38/38	0.94	0.12	17,28,43,46	0
7	6Y2	B	305	38/38	0.94	0.10	16,19,38,42	0
6	ACT	D	306	4/4	0.94	0.16	33,39,40,40	0
6	ACT	D	305	4/4	0.95	0.11	32,35,36,39	0
6	ACT	C	311	4/4	0.96	0.14	22,24,25,27	0
4	CA	B	302	1/1	0.99	0.07	14,14,14,14	0
4	CA	D	303	1/1	1.00	0.06	15,15,15,15	0

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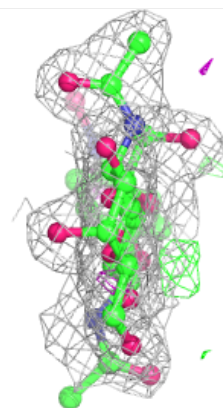
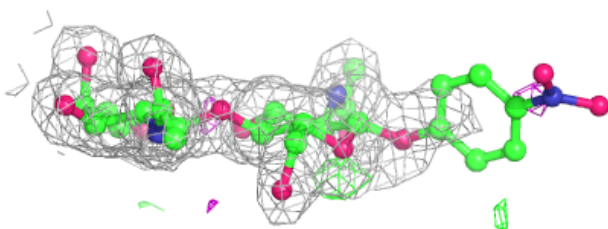
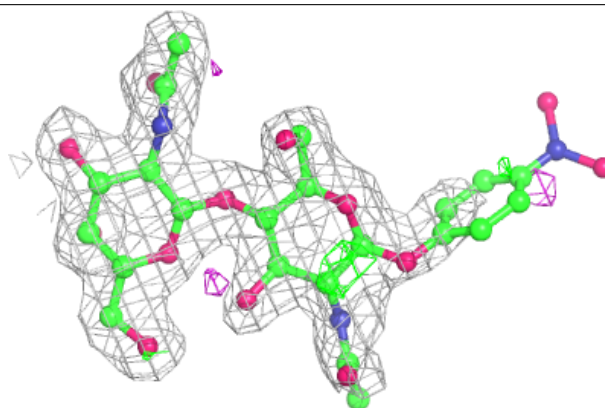
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MN	A	304	1/1	1.00	0.02	19,19,19,19	0
4	CA	C	308	1/1	1.00	0.06	15,15,15,15	0
5	MN	C	309	1/1	1.00	0.02	19,19,19,19	0
5	MN	D	304	1/1	1.00	0.04	19,19,19,19	0
5	MN	B	303	1/1	1.00	0.02	19,19,19,19	0
4	CA	A	303	1/1	1.00	0.07	15,15,15,15	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.

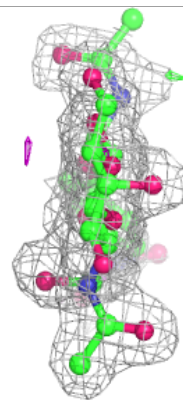
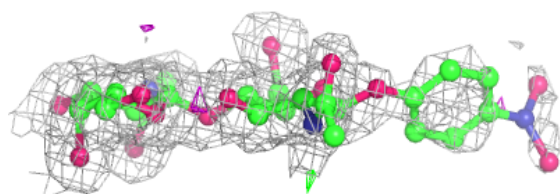
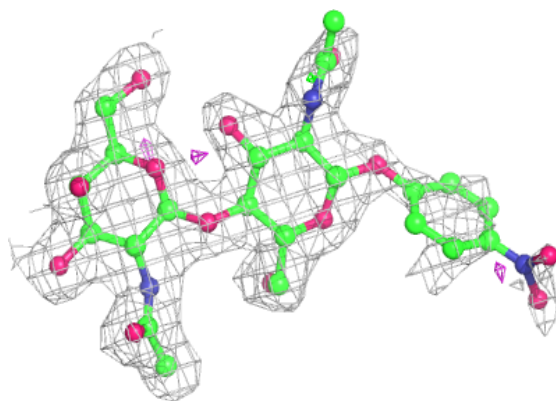
Electron density around 6Y2 A 306:

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

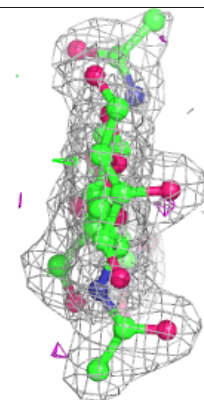
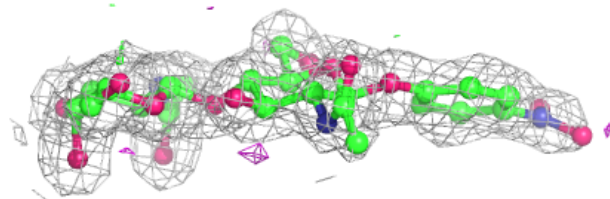
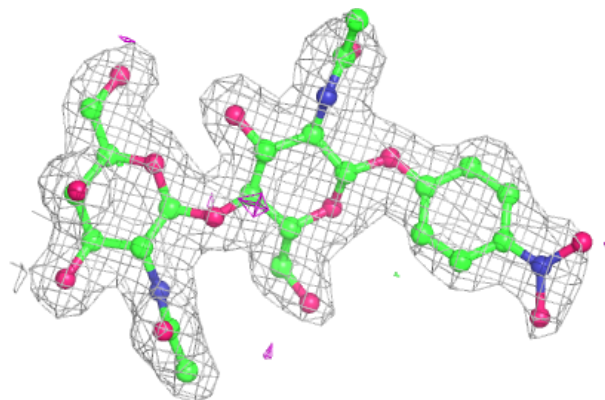


Electron density around 6Y2 C 312:

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

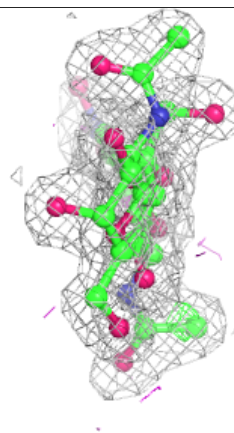
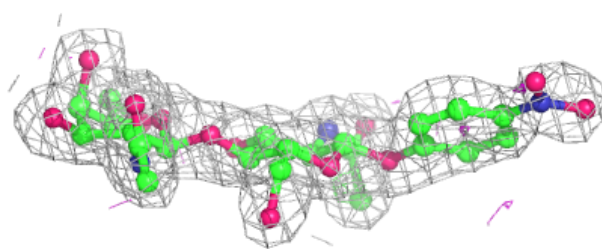
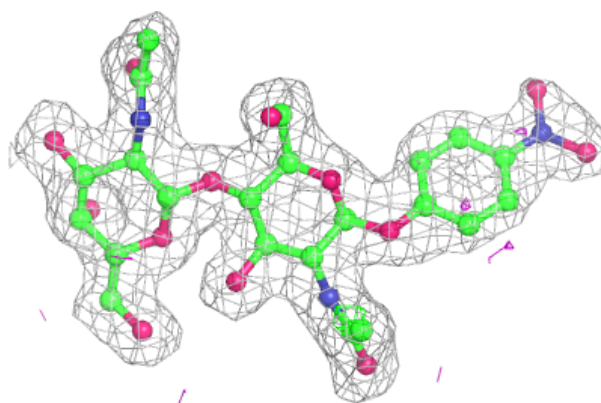
**Electron density around 6Y2 D 307:**

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



Electron density around 6Y2 B 305:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.