



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 05:40 PM BST

PDB ID : 5KXB
Title : Wisteria floribunda lectin in complex with GalNAc
Authors : Evans, S.V.; Haji-Ghassemi, O.
Deposited on : 2016-07-20
Resolution : 2.33 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
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

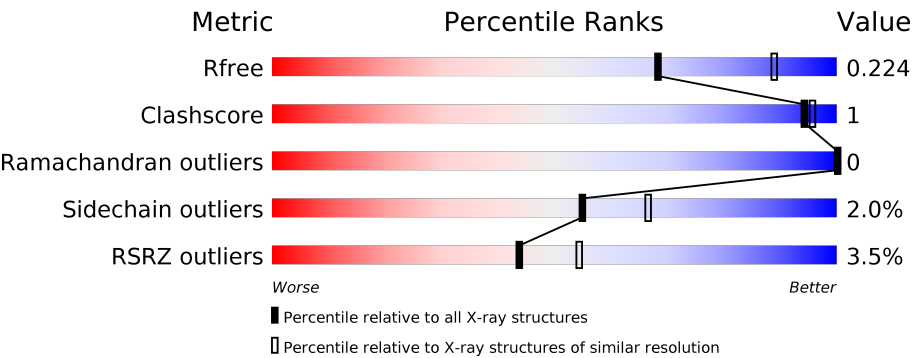
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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.



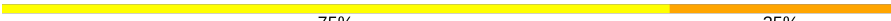
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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>%</div><div><div></div><div>93%</div><div></div></div><div></div></div>
1	B	243	<div><div>6%</div><div><div></div><div>92%</div><div></div></div><div><div></div><div>5%</div><div></div></div></div>
1	C	243	<div><div>%</div><div><div></div><div>93%</div><div></div></div><div><div></div><div>5%</div><div></div></div></div>
1	D	243	<div><div>5%</div><div><div></div><div>93%</div><div></div></div><div><div></div><div>5%</div><div></div></div></div>
2	E	6	<div><div></div><div><div></div><div>17%</div><div></div></div><div><div></div><div>83%</div><div></div></div></div>
3	F	4	<div><div></div><div><div></div><div>25%</div><div></div></div><div><div></div><div>75%</div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
3	G	4	 A horizontal bar chart showing the quality of chain G. The bar is divided into two segments: a yellow segment on the left representing 75% and an orange segment on the right representing 25%. The percentages are labeled below the bar.

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7889 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.

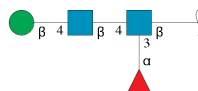
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	0	0	0
			1851	1179	303	369			
1	B	238	Total	C	N	O	0	0	0
			1851	1179	303	369			
1	C	238	Total	C	N	O	0	0	0
			1851	1179	303	369			
1	D	238	Total	C	N	O	0	0	0
			1851	1179	303	369			

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]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
2	E	6	Total	C	N	O	0	0	0
			69	39	2	28			

- Molecule 3 is an oligosaccharide called 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.



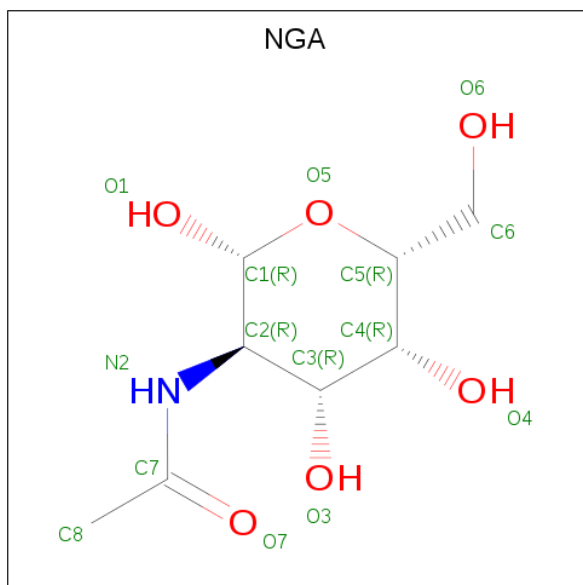
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	4	Total	C	N	O	0	0	0
			49	28	2	19			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		
4	B	1	Total	C	N	O	0	0
			15	8	1	6		
4	C	1	Total	C	N	O	0	0
			15	8	1	6		
4	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

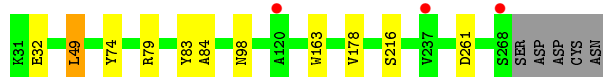
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total 60	O 60	0	0
7	B	55	Total 55	O 55	0	0
7	C	79	Total 79	O 79	0	0
7	D	56	Total 56	O 56	0	0

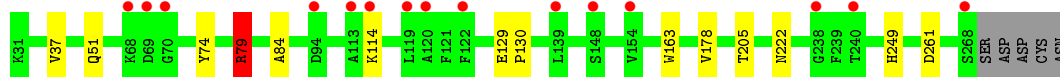
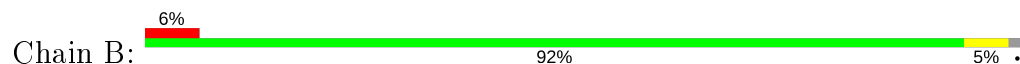
3 Residue-property plots [i](#)

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.

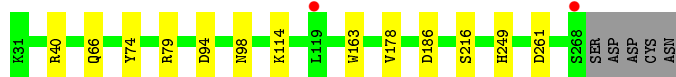
- Molecule 1: *Wisteria floribunda* agglutinin



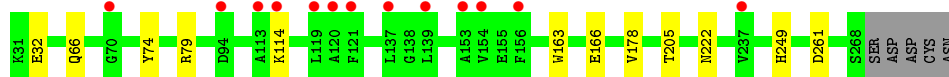
- Molecule 1: *Wisteria floribunda* agglutinin



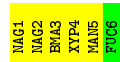
- Molecule 1: *Wisteria floribunda* agglutinin



- Molecule 1: *Wisteria floribunda* agglutinin



- Molecule 2: beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)]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




- Molecule 3: 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:  25% 75%

MAG1
MAG2
BMA3
FUC4

- Molecule 3: 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 G:  75% 25%

MAG1
MAG2
BMA3
FUC4

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	121.19 Å 157.27 Å 55.73 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.33 30.20 – 2.33	Depositor EDS
% Data completeness (in resolution range)	88.9 (30.00-2.33) 89.0 (30.20-2.33)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.34 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.184 , 0.224 0.190 , 0.224	Depositor DCC
R_{free} test set	2065 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7889	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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: XYP, BMA, NAG, CA, MN, NGA, FUC, 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	0.56	0/1899	0.74	2/2599 (0.1%)
1	B	0.55	0/1899	0.99	3/2599 (0.1%)
1	C	0.57	0/1899	0.75	3/2599 (0.1%)
1	D	0.56	0/1899	0.74	2/2599 (0.1%)
All	All	0.56	0/7596	0.81	10/10396 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	ARG	NE-CZ-NH2	24.79	132.70	120.30
1	B	79	ARG	NE-CZ-NH1	-24.38	108.11	120.30
1	A	79	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	D	79	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	C	79	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	B	79	ARG	CB-CG-CD	-6.46	94.81	111.60
1	C	79	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	186	ASP	CB-CG-OD1	5.93	123.63	118.30
1	D	79	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	79	ARG	NE-CZ-NH1	5.81	123.20	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	1779	5	0
1	B	1851	0	1779	9	0
1	C	1851	0	1779	3	0
1	D	1851	0	1780	5	0
2	E	69	0	51	0	0
3	F	49	0	43	0	0
3	G	49	0	43	1	0
4	A	15	0	15	0	0
4	B	15	0	15	0	0
4	C	15	0	15	0	0
4	D	15	0	15	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	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	60	0	0	0	0
7	B	55	0	0	0	0
7	C	79	0	0	0	0
7	D	56	0	0	1	0
All	All	7889	0	7314	19	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 1.

All (19) 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:205:THR:HG23	1:B:222:ASN:HD22	1.72	0.53
1:D:205:THR:HG23	1:D:222:ASN:HD22	1.74	0.53
1:B:79:ARG:HD2	1:B:130:PRO:HG3	1.93	0.51
1:D:32:GLU:OE2	7:D:401:HOH:O	2.19	0.50
1:A:84:ALA:HB2	1:B:84:ALA:HB2	1.95	0.48
1:B:129:GLU:HG3	1:B:130:PRO:HD2	1.96	0.47
1:C:163:TRP:HB2	1:C:178:VAL:HG22	1.96	0.46
1:D:163:TRP:HB2	1:D:178:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:TRP:HB2	1:A:178:VAL:HG22	2.00	0.44
3:G:2:NAG:O7	3:G:4:FUC:H61	2.17	0.44
1:B:163:TRP:HB2	1:B:178:VAL:HG22	1.98	0.44
1:B:222:ASN:HD21	1:C:216:SER:HA	1.83	0.43
1:A:216:SER:HA	1:D:222:ASN:HD21	1.85	0.42
1:A:32:GLU:HA	1:B:37:VAL:O	2.21	0.41
1:B:51:GLN:OE1	1:B:79:ARG:HD3	2.20	0.41
1:A:49:LEU:HD12	1:A:83:TYR:CD2	2.56	0.41
1:B:114:LYS:O	1:B:249:HIS:HA	2.21	0.41
1:C:114:LYS:O	1:C:249:HIS:HA	2.20	0.41
1:D:114:LYS:O	1:D:249:HIS:HA	2.20	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	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%)	232 (98%)	4 (2%)	0	100	100
1	D	236/243 (97%)	232 (98%)	4 (2%)	0	100	100
All	All	944/972 (97%)	928 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/215 (98%)	206 (98%)	4 (2%)	57	68
1	B	210/215 (98%)	207 (99%)	3 (1%)	67	78
1	C	210/215 (98%)	204 (97%)	6 (3%)	42	52
1	D	210/215 (98%)	206 (98%)	4 (2%)	57	68
All	All	840/860 (98%)	823 (98%)	17 (2%)	55	66

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	74	TYR
1	A	98	ASN
1	A	261	ASP
1	B	74	TYR
1	B	79	ARG
1	B	261	ASP
1	C	40	ARG
1	C	66	GLN
1	C	74	TYR
1	C	94	ASP
1	C	98	ASN
1	C	261	ASP
1	D	66	GLN
1	D	74	TYR
1	D	166	GLU
1	D	261	ASP

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	B	46	GLN
1	B	175	ASN
1	B	222	ASN
1	C	92	ASN
1	C	98	ASN
1	D	92	ASN
1	D	173	ASN

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Mol	Chain	Res	Type
1	D	222	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 ⓘ

14 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	0.69	0	17,19,21	1.23	1 (5%)
2	NAG	E	2	2	14,14,15	0.44	0	17,19,21	0.93	1 (5%)
2	BMA	E	3	2	11,11,12	1.18	1 (9%)	15,15,17	1.46	3 (20%)
2	XYP	E	4	2	9,9,10	1.15	1 (11%)	10,12,14	1.56	2 (20%)
2	MAN	E	5	2	11,11,12	0.89	0	15,15,17	1.56	1 (6%)
2	FUC	E	6	2	10,10,11	0.29	0	14,14,16	0.63	0
3	NAG	F	1	1,3	14,14,15	0.58	0	17,19,21	1.27	3 (17%)
3	NAG	F	2	3	14,14,15	0.66	0	17,19,21	1.22	2 (11%)
3	BMA	F	3	3	11,11,12	1.10	1 (9%)	15,15,17	1.43	3 (20%)
3	FUC	F	4	3	10,10,11	0.29	0	14,14,16	0.63	0
3	NAG	G	1	1,3	14,14,15	0.61	0	17,19,21	1.42	5 (29%)
3	NAG	G	2	3	14,14,15	0.71	0	17,19,21	1.43	3 (17%)
3	BMA	G	3	3	11,11,12	1.11	0	15,15,17	1.45	1 (6%)
3	FUC	G	4	3	10,10,11	0.31	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	-	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	XYP	E	4	2	-	-	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	FUC	E	6	2	-	-	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	FUC	G	4	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	XYP	C4-C3	2.54	1.56	1.52
2	E	3	BMA	C4-C5	2.18	1.57	1.53
3	F	3	BMA	C2-C3	2.14	1.55	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	MAN	C1-O5-C5	4.77	118.66	112.19
3	G	3	BMA	O5-C5-C6	4.74	114.64	107.20
3	G	2	NAG	O4-C4-C5	3.06	116.91	109.30
3	F	3	BMA	O5-C5-C6	3.02	111.94	107.20
3	F	2	NAG	C1-O5-C5	3.00	116.25	112.19
3	G	1	NAG	O5-C1-C2	-2.96	106.61	111.29
3	G	2	NAG	C1-O5-C5	2.92	116.14	112.19
3	G	1	NAG	O3-C3-C4	-2.67	104.18	110.35
2	E	3	BMA	O4-C4-C3	-2.65	104.22	110.35
3	G	1	NAG	C1-O5-C5	2.50	115.58	112.19
3	G	2	NAG	O5-C1-C2	-2.48	107.37	111.29
3	F	3	BMA	O2-C2-C1	2.47	114.20	109.15
3	F	1	NAG	C4-C3-C2	2.40	114.54	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	BMA	C3-C4-C5	2.40	114.51	110.24
2	E	4	XYP	O3-C3-C4	2.40	114.58	109.99
3	G	1	NAG	O4-C4-C5	2.37	115.18	109.30
2	E	1	NAG	O3-C3-C2	-2.33	104.64	109.47
2	E	4	XYP	C5-O5-C1	2.26	115.00	111.52
2	E	2	NAG	C1-O5-C5	2.26	115.25	112.19
3	F	2	NAG	O5-C1-C2	-2.23	107.77	111.29
3	F	3	BMA	C2-C3-C4	2.20	114.70	110.89
3	G	1	NAG	O4-C4-C3	-2.18	105.31	110.35
3	F	1	NAG	O4-C4-C5	2.07	114.44	109.30
2	E	3	BMA	O5-C5-C6	2.03	110.39	107.20
3	F	1	NAG	C3-C4-C5	-2.02	106.63	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

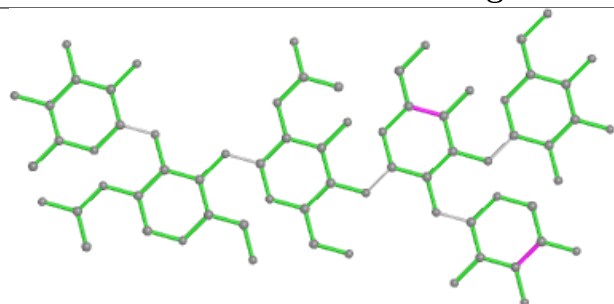
There are no ring outliers.

2 monomers are involved in 1 short contact:

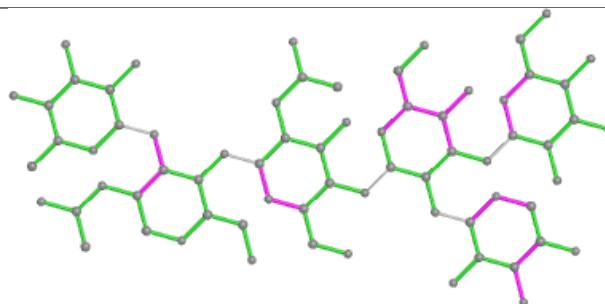
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0
3	G	4	FUC	1	0

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

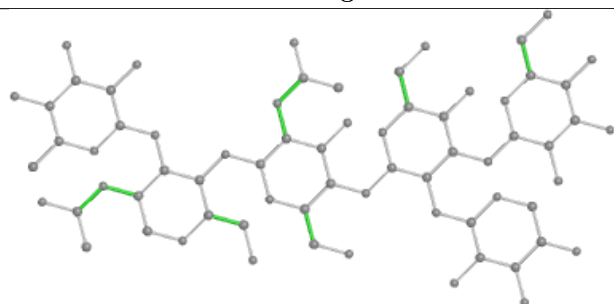
Oligosaccharide Chain E



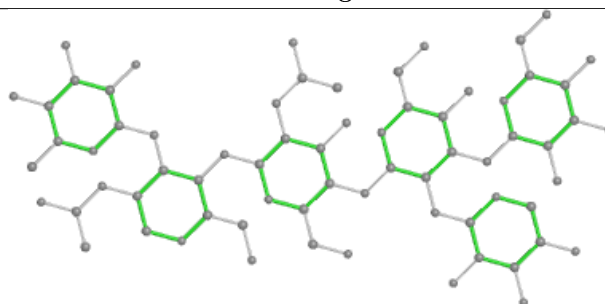
Bond lengths



Bond angles

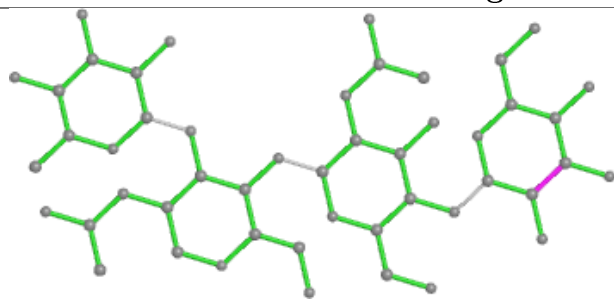


Torsions

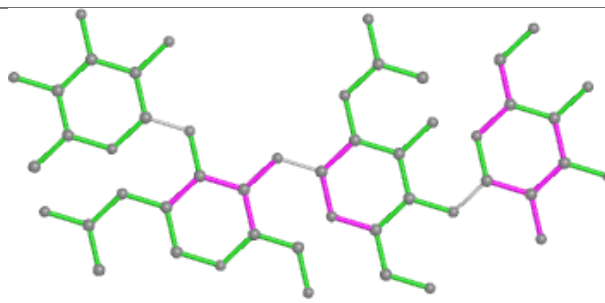


Rings

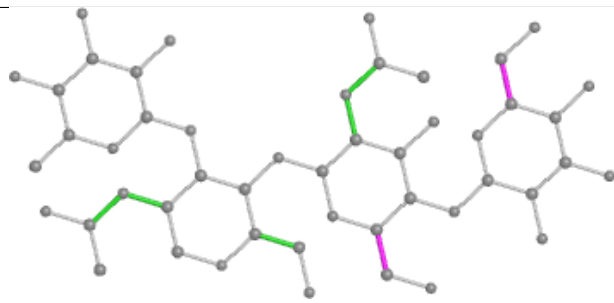
Oligosaccharide Chain F



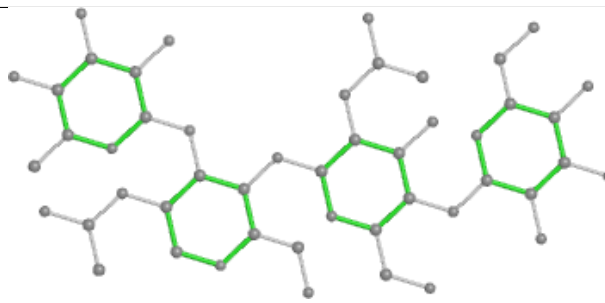
Bond lengths



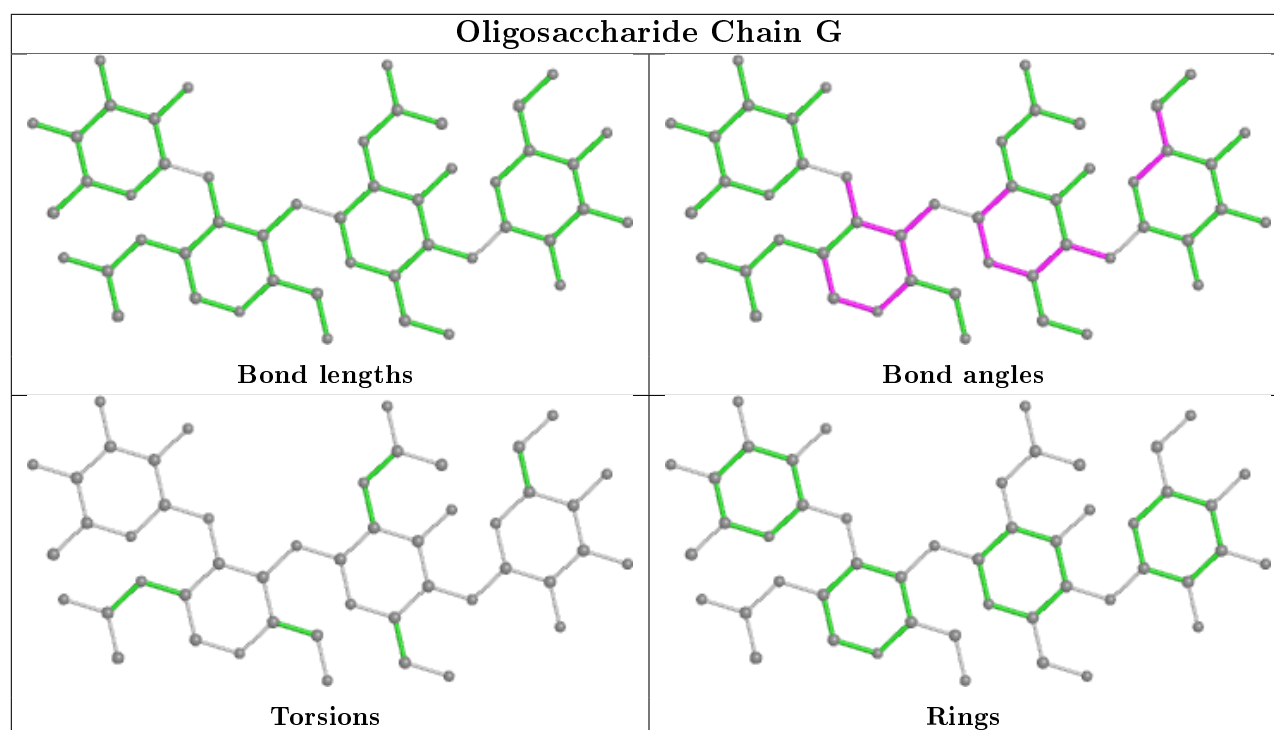
Bond angles



Torsions



Rings



5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
4	NGA	B	305	-	15,15,15	0.52	0	21,21,21	2.57	5 (23%)
4	NGA	D	301	-	15,15,15	0.49	0	21,21,21	1.04	1 (4%)
4	NGA	C	305	-	15,15,15	0.69	0	21,21,21	1.57	4 (19%)
4	NGA	A	307	-	15,15,15	0.63	0	21,21,21	1.39	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NGA	B	305	-	-	2/6/26/26	0/1/1/1
4	NGA	D	301	-	-	2/6/26/26	0/1/1/1
4	NGA	C	305	-	-	0/6/26/26	0/1/1/1
4	NGA	A	307	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	305	NGA	O5-C1-C2	-7.67	101.81	109.52
4	B	305	NGA	C1-C2-C3	-5.69	102.79	110.54
4	C	305	NGA	O5-C1-C2	4.41	113.95	109.52
4	B	305	NGA	C1-C2-N2	4.18	115.57	110.73
4	A	307	NGA	O5-C1-C2	3.83	113.37	109.52
4	B	305	NGA	O1-C1-C2	3.67	116.83	109.22
4	D	301	NGA	C1-C2-C3	-3.46	105.82	110.54
4	C	305	NGA	O1-C1-C2	-3.11	102.75	109.22
4	A	307	NGA	O1-C1-O5	-2.49	102.90	110.38
4	B	305	NGA	C1-O5-C5	-2.39	109.15	113.66
4	C	305	NGA	O1-C1-O5	-2.38	103.25	110.38
4	A	307	NGA	O5-C5-C6	2.23	111.98	106.44
4	C	305	NGA	C4-C3-C2	-2.04	107.35	110.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	305	NGA	C1-C2-N2-C7
4	D	301	NGA	C4-C5-C6-O6
4	D	301	NGA	O5-C5-C6-O6
4	A	307	NGA	O5-C5-C6-O6
4	B	305	NGA	O5-C5-C6-O6
4	A	307	NGA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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%)	-0.12	3 (1%) 77 83	23, 34, 52, 73	0
1	B	238/243 (97%)	0.21	15 (6%) 20 28	22, 40, 70, 93	0
1	C	238/243 (97%)	-0.17	2 (0%) 86 90	19, 30, 59, 84	0
1	D	238/243 (97%)	0.19	13 (5%) 25 34	23, 37, 63, 82	0
All	All	952/972 (97%)	0.03	33 (3%) 44 54	19, 35, 63, 93	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	268	SER	4.3
1	B	120	ALA	3.7
1	D	120	ALA	3.5
1	D	119	LEU	3.5
1	D	94	ASP	3.3
1	B	122	PHE	3.2
1	B	268	SER	3.2
1	B	69	ASP	3.1
1	D	121	PHE	3.1
1	D	114	LYS	3.1
1	D	113	ALA	3.1
1	D	137	LEU	3.0
1	B	119	LEU	3.0
1	B	68	LYS	2.8
1	D	70	GLY	2.8
1	B	238	GLY	2.7
1	B	113	ALA	2.7
1	B	154	VAL	2.6
1	A	268	SER	2.6
1	D	153	ALA	2.6
1	D	154	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	120	ALA	2.6
1	B	70	GLY	2.5
1	B	148	SER	2.5
1	C	119	LEU	2.5
1	B	139	LEU	2.4
1	D	156	PHE	2.4
1	B	94	ASP	2.4
1	D	237	VAL	2.4
1	B	114	LYS	2.3
1	B	240	THR	2.3
1	D	139	LEU	2.1
1	A	237	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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

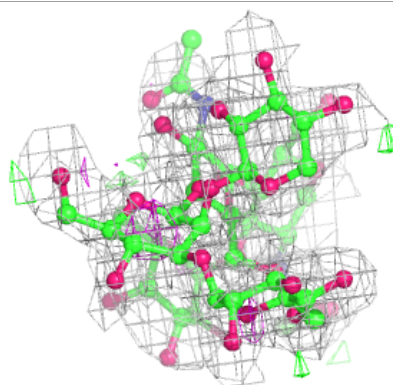
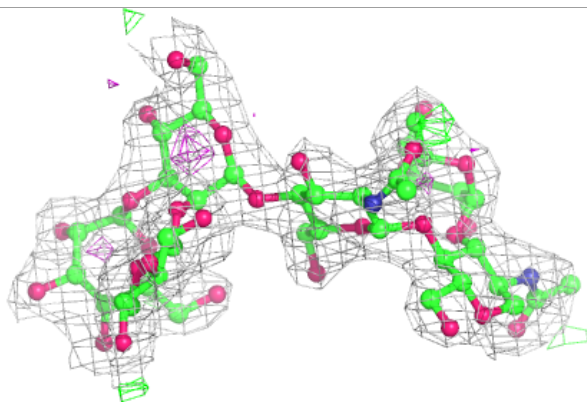
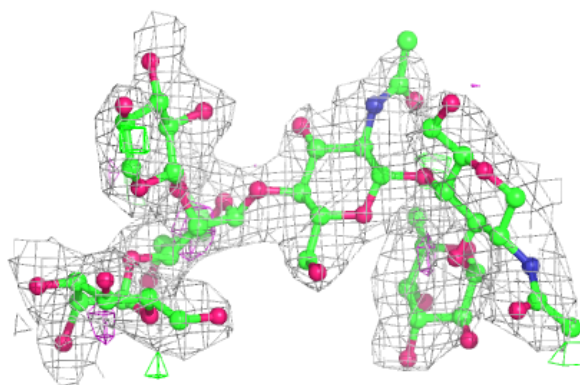
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	F	3	11/12	0.66	0.27	78,90,94,96	0
3	BMA	G	3	11/12	0.71	0.22	75,85,89,89	0
3	FUC	F	4	10/11	0.82	0.31	71,79,82,83	0
2	XYP	E	4	9/10	0.83	0.22	54,59,62,65	0
2	FUC	E	6	10/11	0.84	0.34	61,68,73,74	0
3	FUC	G	4	10/11	0.85	0.18	58,63,68,68	0
2	BMA	E	3	11/12	0.88	0.26	43,48,52,53	0
3	NAG	F	2	14/15	0.89	0.30	66,78,87,90	0
3	NAG	G	2	14/15	0.90	0.21	69,77,90,93	0
3	NAG	G	1	14/15	0.92	0.11	44,51,56,65	0
2	NAG	E	2	14/15	0.92	0.31	53,60,69,69	0
3	NAG	F	1	14/15	0.92	0.27	47,63,69,74	0
2	NAG	E	1	14/15	0.93	0.20	50,55,68,68	0
2	MAN	E	5	11/12	0.95	0.15	28,34,39,44	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

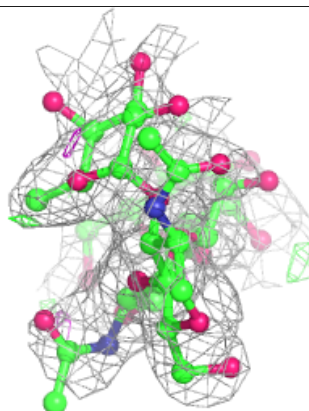
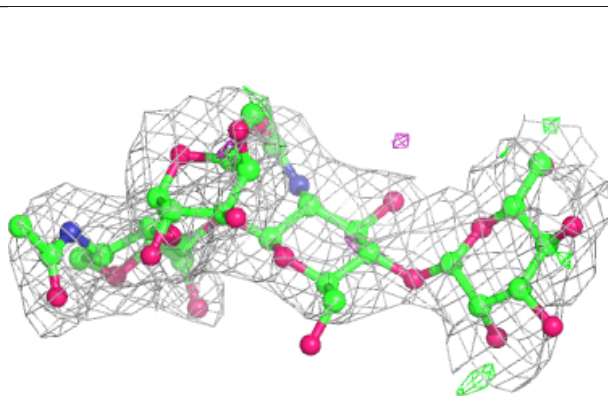
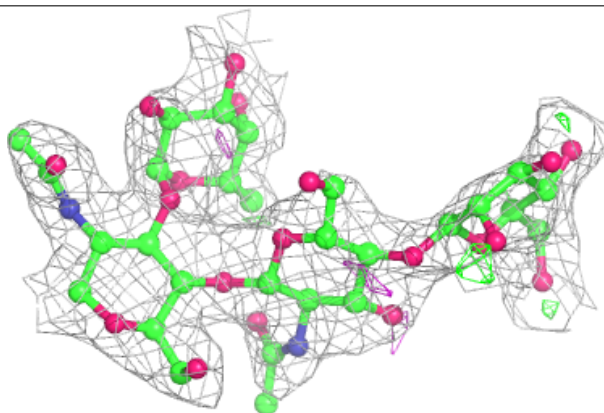
Electron density around Chain E:

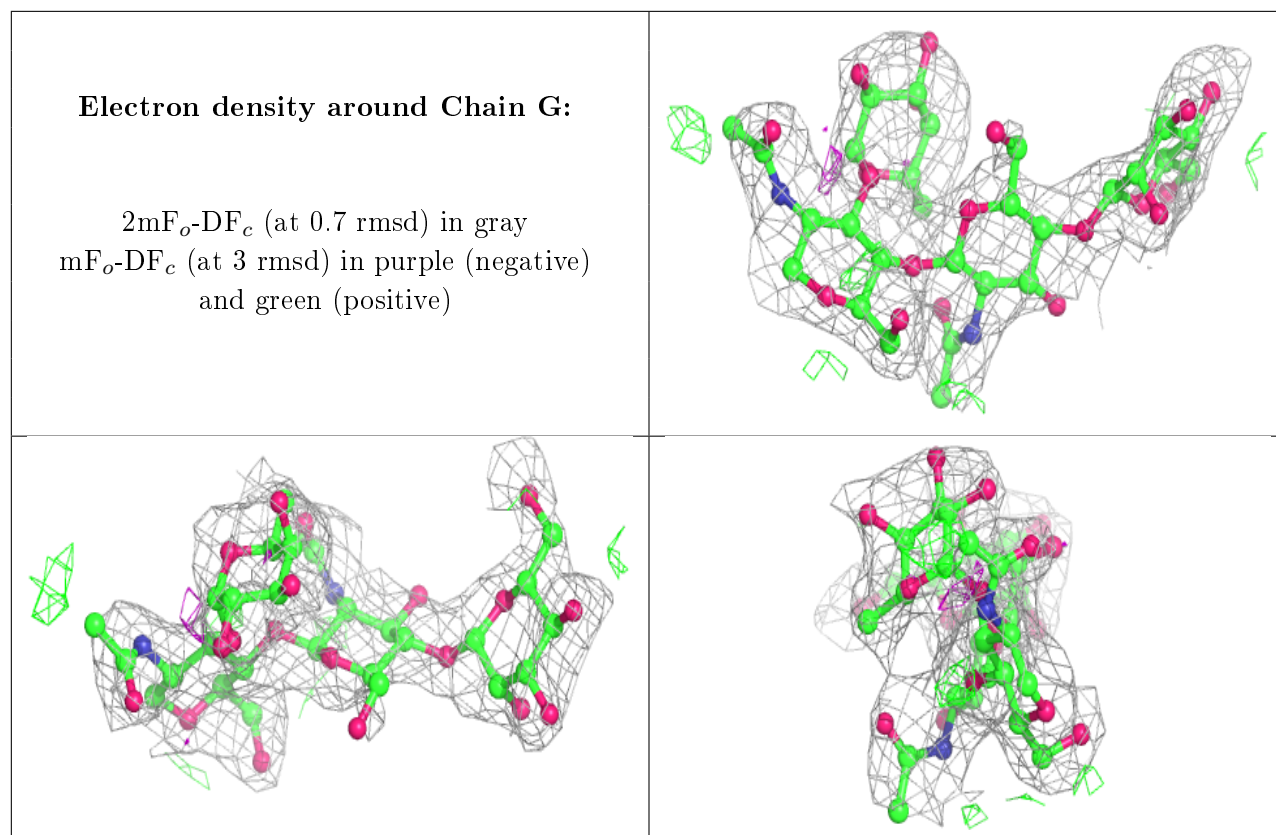
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
4	NGA	B	305	15/15	0.88	0.14	42,57,62,68	0
4	NGA	C	305	15/15	0.94	0.14	32,36,38,48	0
4	NGA	D	301	15/15	0.94	0.13	42,48,49,58	0
4	NGA	A	307	15/15	0.94	0.13	30,37,40,49	0
5	CA	D	302	1/1	0.97	0.07	40,40,40,40	0
5	CA	B	306	1/1	0.98	0.09	38,38,38,38	0
6	MN	B	307	1/1	0.99	0.06	43,43,43,43	0
6	MN	A	309	1/1	0.99	0.04	37,37,37,37	0
6	MN	D	303	1/1	0.99	0.07	40,40,40,40	0
5	CA	A	308	1/1	0.99	0.07	31,31,31,31	0
5	CA	C	306	1/1	1.00	0.07	26,26,26,26	0
6	MN	C	307	1/1	1.00	0.08	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.