



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 09:07 PM JST

PDB ID : 5Y3J
Title : Crystal structure of horse TLR9 in complex with two DNAs (CpG DNA and TCGCAC DNA)
Authors : Ohto, U.; Ishida, H.; Shimizu, T.
Deposited on : 2017-07-29
Resolution : 1.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

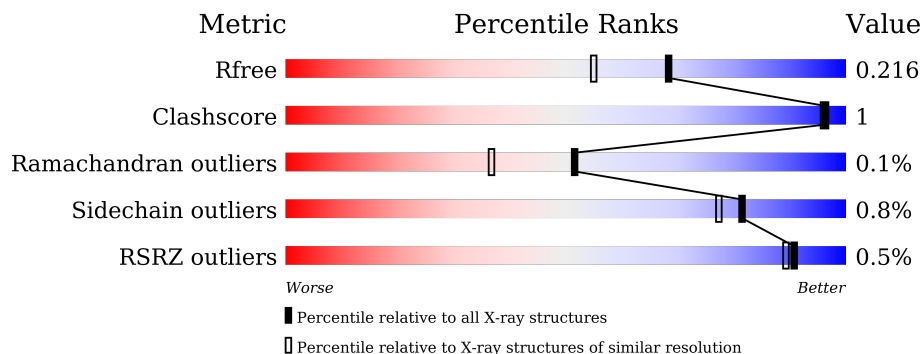
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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.



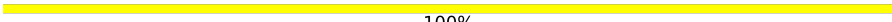
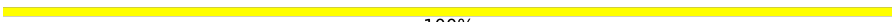
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	802	 89% 6%
1	B	802	 90% 6%
2	C	10	 60% 30% 10%
2	D	10	 60% 40%
3	E	6	 100%
3	F	6	 100%

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
4	H	2	 100%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 15035 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Toll-like receptor 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	750	6039	3845	1071	1094	29	0	17	0
1	B	750	6010	3829	1062	1090	29	0	15	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ARG	-	expression tag	UNP Q2EEY0
A	23	SER	-	expression tag	UNP Q2EEY0
A	24	PRO	-	expression tag	UNP Q2EEY0
A	25	TRP	-	expression tag	UNP Q2EEY0
A	818	GLU	CYS	conflict	UNP Q2EEY0
A	820	LEU	-	expression tag	UNP Q2EEY0
A	821	VAL	-	expression tag	UNP Q2EEY0
A	822	PRO	-	expression tag	UNP Q2EEY0
A	823	ARG	-	expression tag	UNP Q2EEY0
B	22	ARG	-	expression tag	UNP Q2EEY0
B	23	SER	-	expression tag	UNP Q2EEY0
B	24	PRO	-	expression tag	UNP Q2EEY0
B	25	TRP	-	expression tag	UNP Q2EEY0
B	818	GLU	CYS	conflict	UNP Q2EEY0
B	820	LEU	-	expression tag	UNP Q2EEY0
B	821	VAL	-	expression tag	UNP Q2EEY0
B	822	PRO	-	expression tag	UNP Q2EEY0
B	823	ARG	-	expression tag	UNP Q2EEY0

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*GP*CP*GP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	C	10	Total	C	N	O	P	0	0	0
			203	99	33	62	9			
2	D	10	Total	C	N	O	P	0	0	0
			203	99	33	62	9			

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*CP*GP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	E	6	Total	C	N	O	P	0	0	0
			117	57	21	34	5			
3	F	6	Total	C	N	O	P	0	0	0
			117	57	21	34	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	G	2	Total	C	N	O		0	0	0
			28	16	2	10				
4	H	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0
6	B	1	1	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	999	999	999	0	0
7	B	960	960	960	0	0
7	C	34	34	34	0	0
7	E	26	26	26	0	0
7	D	31	31	31	0	0
7	F	28	28	28	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.

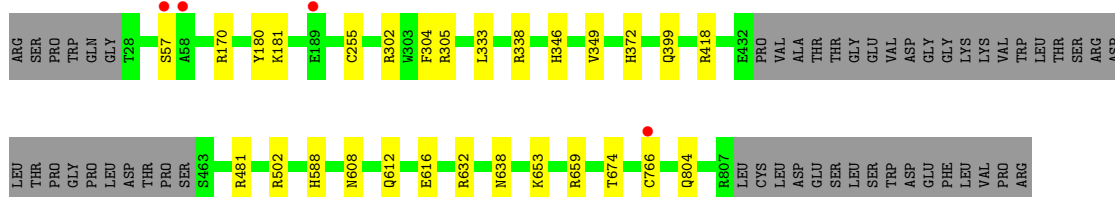
- Molecule 1: Toll-like receptor 9

Chain A:  89% 6%



- Molecule 1: Toll-like receptor 9

Chain B:  90% 6%



- Molecule 2: DNA (5'-D(*AP*GP*GP*CP*GP*TP*TP*TP*TP*T)-3')

Chain C:  60% 30% 10%



- Molecule 2: DNA (5'-D(*AP*GP*GP*CP*GP*TP*TP*TP*TP*T)-3')

Chain D:  60% 40%



- Molecule 3: DNA (5'-D(*TP*CP*GP*CP*AP*C)-3')

Chain E:  100%


There are no outlier residues recorded for this chain.

- Molecule 3: DNA (5'-D(*TP*CP*GP*CP*AP*C)-3')

Chain F:  100%

There are no outlier residues recorded for this chain.

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

Chain G:  100%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.49Å 125.20Å 139.29Å 90.00° 94.78° 90.00°	Depositor
Resolution (Å)	49.40 – 1.81 49.39 – 1.81	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.40-1.81) 98.8 (49.39-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.178 , 0.206 0.187 , 0.216	Depositor DCC
R_{free} test set	8576 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15035	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.16 % 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 2.1310e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG, NAG

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	0.70	0/6179	0.87	13/8401 (0.2%)
1	B	0.71	0/6151	0.86	13/8366 (0.2%)
2	C	0.71	1/226 (0.4%)	0.85	0/348
2	D	0.73	1/226 (0.4%)	0.81	0/348
3	E	0.72	0/130	0.76	0/198
3	F	0.79	0/130	0.84	0/198
All	All	0.71	2/13042 (0.0%)	0.86	26/17859 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	DG	O3'-P	-6.64	1.53	1.61
2	C	5	DG	O3'-P	-5.12	1.55	1.61

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	632	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	B	170	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	502	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	561[A]	MET	CG-SD-CE	6.62	110.80	100.20
1	A	561[B]	MET	CG-SD-CE	6.62	110.80	100.20
1	A	302	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	502	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	302	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	481	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	302	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	659	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	632	ARG	NE-CZ-NH2	5.80	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	502	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	502	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	302	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	170	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	80	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	632	ARG	CG-CD-NE	-5.30	100.67	111.80
1	B	338	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	590	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	659	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	418	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	338	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	481	ARG	NE-CZ-NH1	5.13	122.87	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	6039	0	6032	13	0
1	B	6010	0	6001	9	0
2	C	203	0	117	2	0
2	D	203	0	117	2	0
3	E	117	0	69	0	0
3	F	117	0	69	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
5	A	112	0	104	0	0
5	B	98	0	91	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	999	0	0	2	0
7	B	960	0	0	2	1
7	C	34	0	0	0	0
7	D	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	26	0	0	0	0
7	F	28	0	0	0	0
All	All	15035	0	12650	26	1

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 (26) 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:A:381:GLN:HE21	1:A:385[B]:GLN:HE21	1.31	0.78
1:B:346:HIS:HB3	1:B:349:VAL:HG22	1.80	0.62
1:A:346:HIS:HB3	1:A:349:VAL:HG22	1.89	0.54
1:B:304:PHE:HB3	1:B:333:LEU:HD21	1.88	0.54
2:C:2:DG:H2''	2:C:3:DG:C8	2.44	0.53
1:B:653:LYS:HG2	7:B:1657:HOH:O	2.11	0.49
1:B:674[B]:THR:HG22	7:B:1281:HOH:O	2.12	0.49
2:C:4:DC:H2''	2:C:5:DG:H5'	1.95	0.48
1:A:674:THR:HG22	7:A:1125:HOH:O	2.13	0.47
1:A:546[A]:ARG:HG2	1:A:546[A]:ARG:HH21	1.80	0.46
1:A:653:LYS:HD3	7:A:1272:HOH:O	2.16	0.46
2:D:2:DG:H2''	2:D:3:DG:C8	2.50	0.46
1:B:372:HIS:HB2	1:B:399:GLN:O	2.16	0.45
1:A:372:HIS:HB2	1:A:399:GLN:O	2.18	0.44
1:A:588:HIS:ND1	1:A:612:GLN:NE2	2.66	0.44
1:A:608:ASN:O	1:A:638:ASN:HA	2.19	0.43
1:B:588:HIS:ND1	1:B:612:GLN:NE2	2.66	0.43
1:B:608:ASN:O	1:B:638:ASN:HA	2.18	0.43
1:A:644:LEU:O	1:A:647[B]:THR:OG1	2.31	0.43
1:A:804:GLN:N	1:A:804:GLN:CD	2.73	0.42
1:B:804:GLN:N	1:B:804:GLN:CD	2.73	0.41
1:A:101:ALA:O	1:A:107:HIS:HA	2.20	0.41
1:B:180:TYR:CE2	1:B:181:LYS:HG3	2.56	0.41
1:A:343:PHE:HA	1:A:373:GLY:O	2.21	0.41
2:D:7:DT:H3'	2:D:7:DT:O2	2.21	0.41
1:A:180:TYR:CE2	1:A:181:LYS:HG3	2.56	0.40

All (1) 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)
7:B:1881:HOH:O	7:B:1881:HOH:O[2_555]	1.02	1.18

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	763/802 (95%)	732 (96%)	30 (4%)	1 (0%)	51	37
1	B	761/802 (95%)	729 (96%)	32 (4%)	0	100	100
All	All	1524/1604 (95%)	1461 (96%)	62 (4%)	1 (0%)	51	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	PHE

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	683/712 (96%)	677 (99%)	6 (1%)	78	74
1	B	681/712 (96%)	676 (99%)	5 (1%)	84	80
All	All	1364/1424 (96%)	1353 (99%)	11 (1%)	81	77

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	255	CYS
1	A	385[A]	GLN
1	A	385[B]	GLN
1	A	616	GLU
1	A	766	CYS
1	B	57	SER
1	B	255	CYS
1	B	305	ARG
1	B	616	GLU
1	B	766	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	335	GLN
1	A	367	GLN
1	A	612	GLN
1	A	637	GLN
1	A	641	HIS
1	A	650	ASN
1	B	335	GLN
1	B	367	GLN
1	B	385	GLN
1	B	394	GLN
1	B	612	GLN
1	B	637	GLN
1	B	650	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 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
4	NAG	G	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	1.20	3 (17%)
4	NAG	G	2	4	14,14,15	0.97	0	17,19,21	2.16	3 (17%)
4	NAG	H	1	1,4	14,14,15	1.00	1 (7%)	17,19,21	1.08	1 (5%)
4	NAG	H	2	4	14,14,15	0.75	0	17,19,21	1.90	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	-3.09	1.38	1.43
4	G	1	NAG	O5-C1	-2.41	1.39	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2	NAG	C1-O5-C5	5.57	119.74	112.19
4	H	2	NAG	C1-O5-C5	4.71	118.57	112.19
4	G	2	NAG	O3-C3-C2	4.64	119.07	109.47
4	H	2	NAG	C8-C7-N2	-3.32	110.48	116.10
4	G	1	NAG	C1-O5-C5	2.76	115.93	112.19
4	H	2	NAG	C2-N2-C7	2.51	126.48	122.90
4	H	2	NAG	O3-C3-C2	2.50	114.63	109.47
4	G	2	NAG	O3-C3-C4	-2.21	105.24	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C1-O5-C5	2.21	115.18	112.19
4	G	1	NAG	C3-C4-C5	-2.11	106.48	110.24
4	G	1	NAG	O5-C5-C4	-2.07	105.79	110.83

There are no chirality outliers.

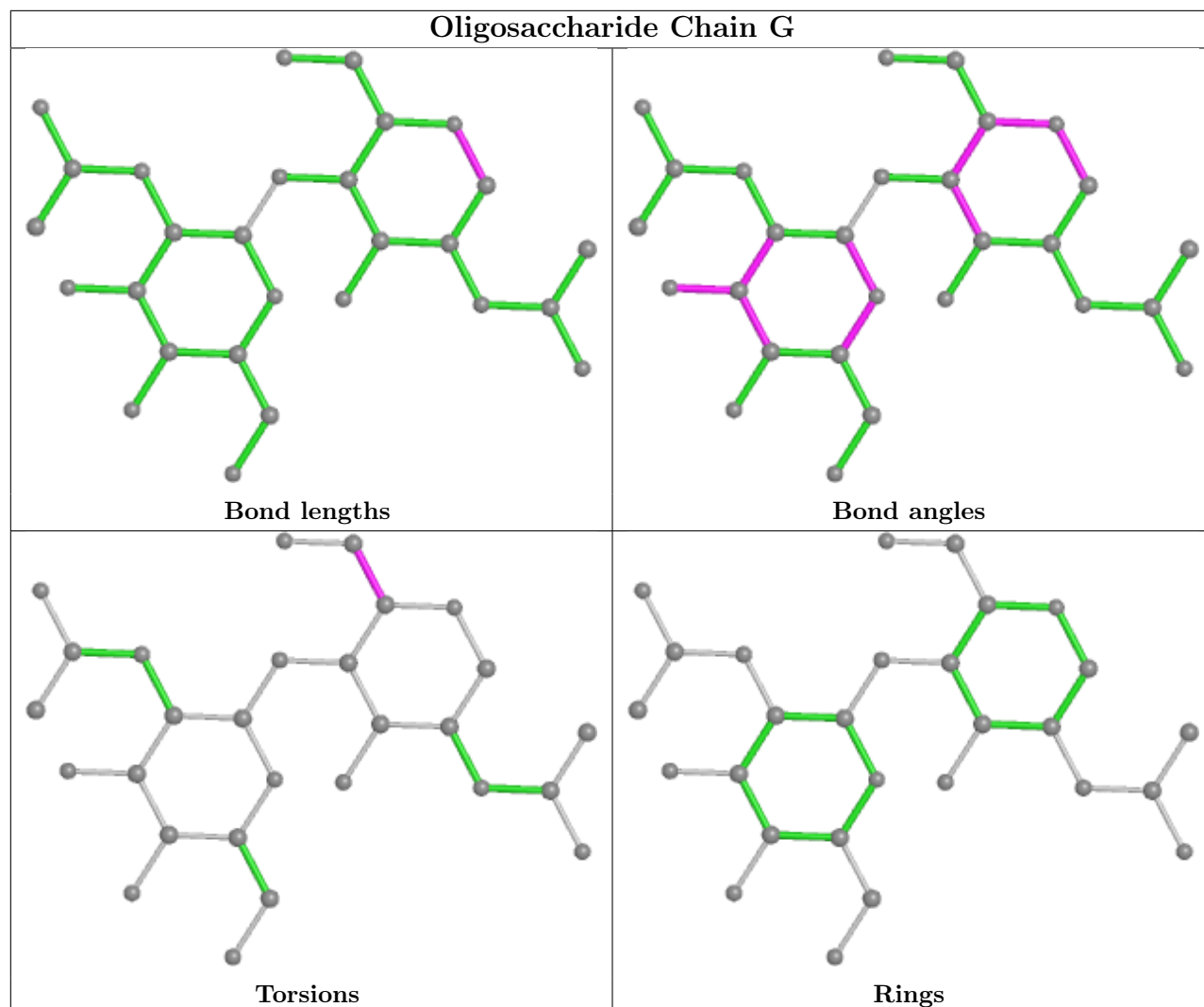
All (5) torsion outliers are listed below:

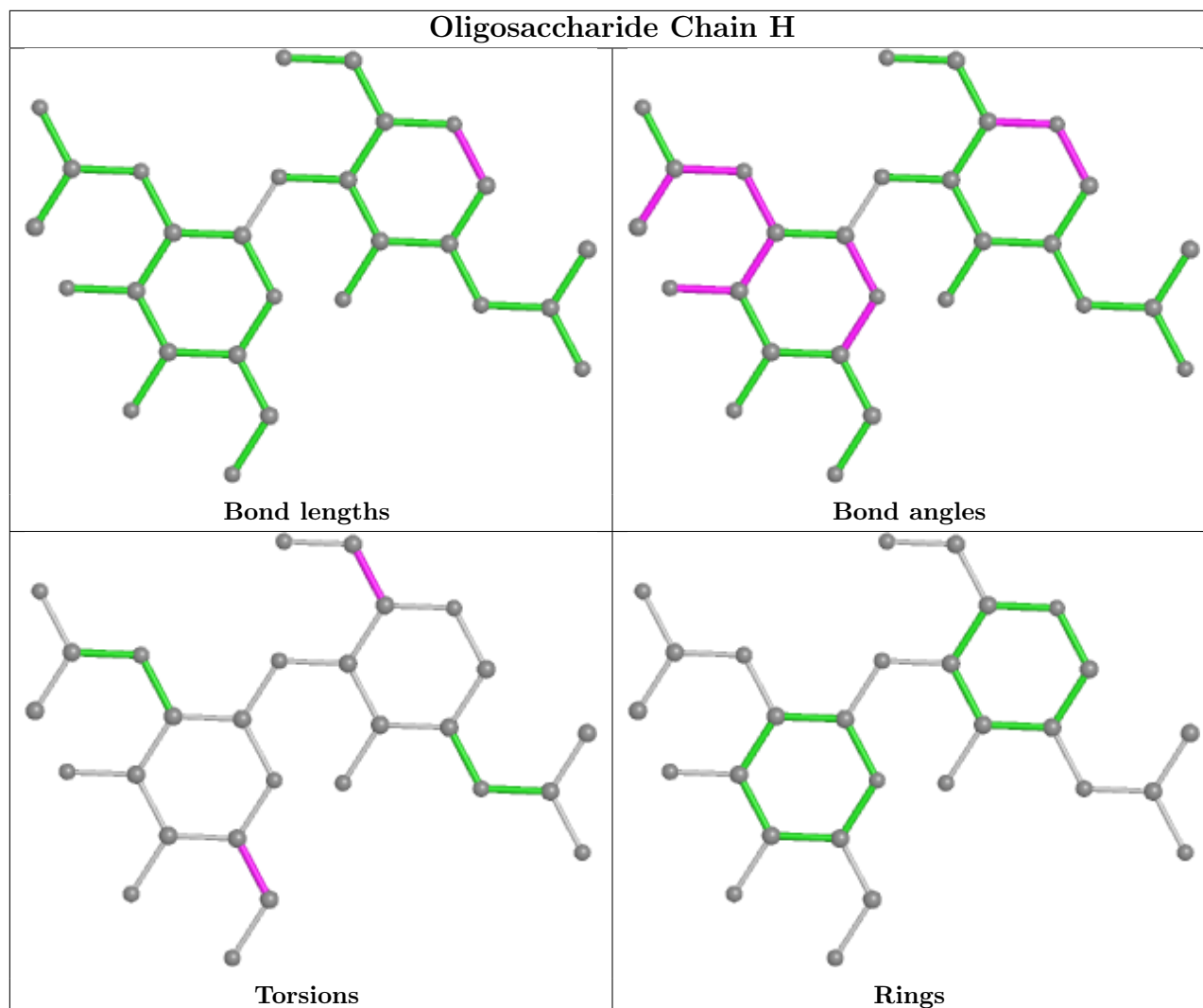
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6

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](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\# Z > 2$
5	NAG	A	1004	1	14,14,15	0.77	0	17,19,21	1.30	2 (11%)
5	NAG	B	1006	1	14,14,15	0.70	0	17,19,21	0.97	1 (5%)
5	NAG	A	1005	1	14,14,15	0.57	0	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1004	1	14,14,15	0.83	1 (7%)	17,19,21	1.22	1 (5%)
5	NAG	B	1009	1	14,14,15	0.57	0	17,19,21	1.61	4 (23%)
5	NAG	A	1006	1	14,14,15	0.87	0	17,19,21	0.84	0
5	NAG	B	1008	1	14,14,15	0.86	1 (7%)	17,19,21	1.81	4 (23%)
5	NAG	A	1007	1	14,14,15	0.63	0	17,19,21	0.80	0
5	NAG	A	1010	1	14,14,15	0.88	0	17,19,21	1.58	4 (23%)
5	NAG	B	1003	1	14,14,15	0.53	0	17,19,21	1.26	3 (17%)
5	NAG	B	1007	1	14,14,15	0.60	0	17,19,21	1.85	6 (35%)
5	NAG	A	1009	1	14,14,15	0.70	0	17,19,21	1.47	3 (17%)
5	NAG	A	1008	1	14,14,15	0.63	0	17,19,21	1.55	4 (23%)
5	NAG	A	1003	1	14,14,15	0.49	0	17,19,21	1.60	3 (17%)
5	NAG	B	1005	1	14,14,15	0.50	0	17,19,21	0.86	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
5	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1006	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1009	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1008	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1007	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1010	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1003	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1007	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1003	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1005	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1004	NAG	C2-N2	-2.25	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1008	NAG	C2-N2	-2.16	1.42	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1008	NAG	C1-C2-N2	-4.46	102.87	110.49
5	B	1007	NAG	C2-N2-C7	4.09	128.73	122.90
5	B	1009	NAG	C1-O5-C5	3.81	117.36	112.19
5	A	1003	NAG	O5-C5-C6	3.70	113.00	107.20
5	B	1007	NAG	O5-C1-C2	-3.61	105.59	111.29
5	A	1009	NAG	O4-C4-C3	-3.54	102.17	110.35
5	A	1008	NAG	O5-C5-C6	3.31	112.39	107.20
5	A	1008	NAG	O5-C1-C2	-3.05	106.47	111.29
5	A	1003	NAG	O5-C5-C4	-2.99	103.55	110.83
5	A	1004	NAG	C6-C5-C4	-2.96	106.06	113.00
5	A	1003	NAG	C1-C2-N2	-2.93	105.48	110.49
5	A	1004	NAG	O6-C6-C5	-2.88	101.43	111.29
5	B	1008	NAG	O5-C1-C2	-2.84	106.80	111.29
5	A	1009	NAG	O5-C1-C2	-2.83	106.81	111.29
5	A	1010	NAG	C4-C3-C2	2.81	115.13	111.02
5	B	1003	NAG	O5-C5-C6	2.76	111.53	107.20
5	B	1008	NAG	O5-C5-C6	2.69	111.41	107.20
5	A	1010	NAG	C2-N2-C7	2.59	126.60	122.90
5	B	1003	NAG	C1-C2-N2	-2.55	106.13	110.49
5	A	1008	NAG	C1-C2-N2	-2.54	106.14	110.49
5	B	1007	NAG	C1-C2-N2	-2.51	106.20	110.49
5	B	1009	NAG	O6-C6-C5	-2.50	102.71	111.29
5	A	1010	NAG	C6-C5-C4	2.50	118.85	113.00
5	B	1003	NAG	O5-C5-C4	-2.33	105.15	110.83
5	B	1007	NAG	C3-C4-C5	-2.24	106.24	110.24
5	A	1010	NAG	C1-O5-C5	-2.24	109.15	112.19
5	A	1009	NAG	C6-C5-C4	2.18	118.11	113.00
5	B	1007	NAG	C6-C5-C4	2.18	118.11	113.00
5	B	1009	NAG	C6-C5-C4	-2.17	107.92	113.00
5	B	1008	NAG	O3-C3-C4	-2.15	105.39	110.35
5	B	1009	NAG	O4-C4-C3	-2.11	105.47	110.35
5	A	1008	NAG	C6-C5-C4	-2.08	108.14	113.00
5	B	1007	NAG	C8-C7-N2	2.03	119.54	116.10
5	B	1006	NAG	O3-C3-C2	2.02	113.64	109.47
5	B	1004	NAG	O5-C1-C2	-2.00	108.12	111.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1003	NAG	O5-C5-C6-O6
5	A	1003	NAG	C4-C5-C6-O6
5	B	1003	NAG	O5-C5-C6-O6
5	B	1003	NAG	C4-C5-C6-O6
5	B	1007	NAG	C4-C5-C6-O6
5	B	1009	NAG	C4-C5-C6-O6
5	B	1005	NAG	C4-C5-C6-O6
5	B	1005	NAG	O5-C5-C6-O6
5	A	1005	NAG	C4-C5-C6-O6
5	B	1007	NAG	O5-C5-C6-O6
5	B	1009	NAG	O5-C5-C6-O6
5	A	1005	NAG	O5-C5-C6-O6
5	A	1007	NAG	C4-C5-C6-O6
5	A	1010	NAG	C3-C2-N2-C7
5	A	1010	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	750/802 (93%)	-0.37	3 (0%) 92 91	13, 24, 40, 54	0
1	B	750/802 (93%)	-0.36	4 (0%) 91 89	12, 24, 40, 66	0
2	C	10/10 (100%)	-0.25	0 100 100	33, 37, 51, 63	0
2	D	10/10 (100%)	-0.20	0 100 100	34, 39, 52, 64	0
3	E	6/6 (100%)	-0.17	0 100 100	16, 21, 35, 85	0
3	F	6/6 (100%)	-0.20	0 100 100	15, 19, 36, 82	0
All	All	1532/1636 (93%)	-0.36	7 (0%) 91 89	12, 24, 41, 85	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	ALA	2.6
1	B	58	ALA	2.4
1	B	57	SER	2.3
1	A	804	GLN	2.1
1	A	646	CYS	2.1
1	B	766	CYS	2.1
1	B	189	GLU	2.1

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

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

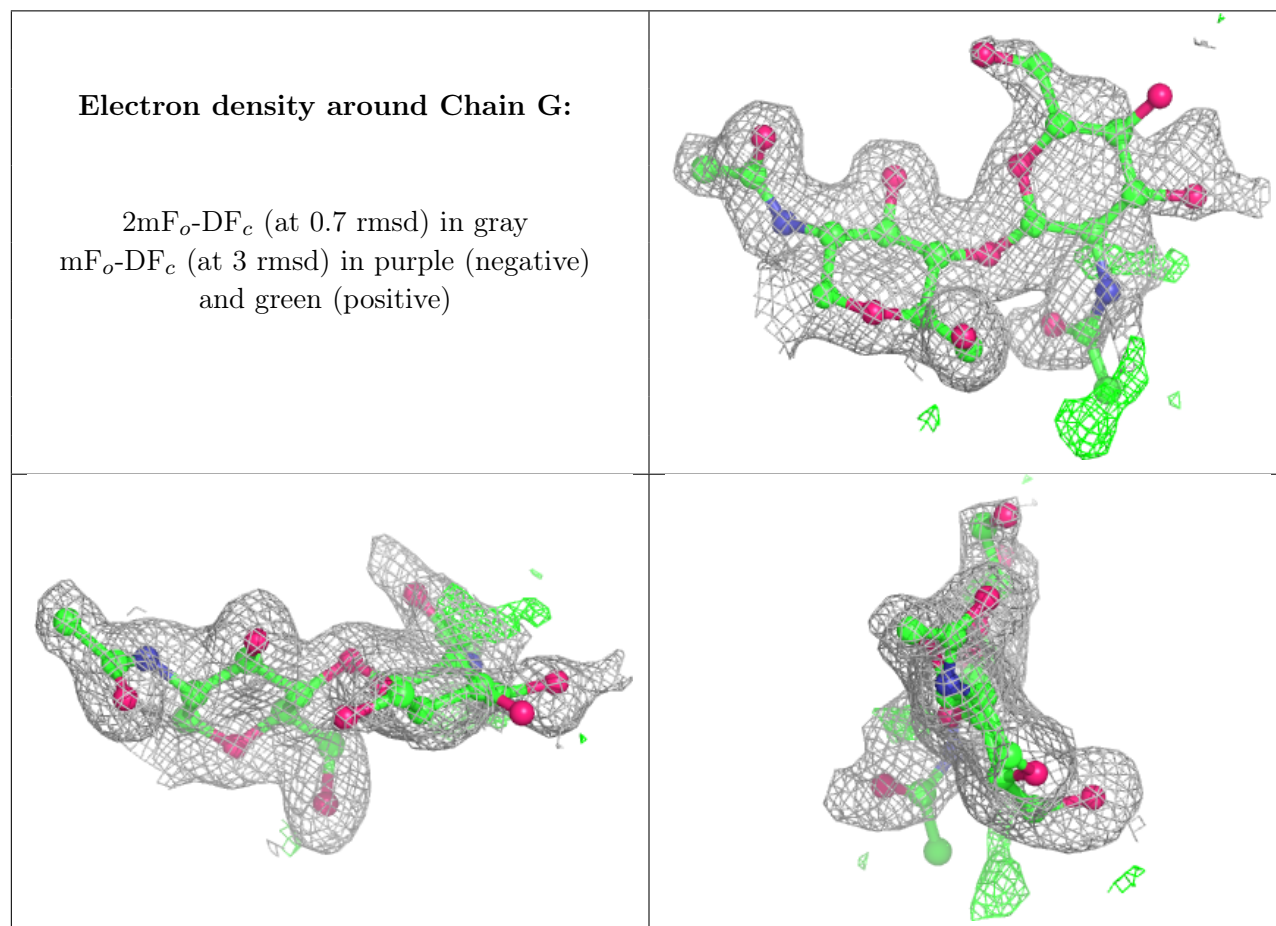
6.3 Carbohydrates [i](#)

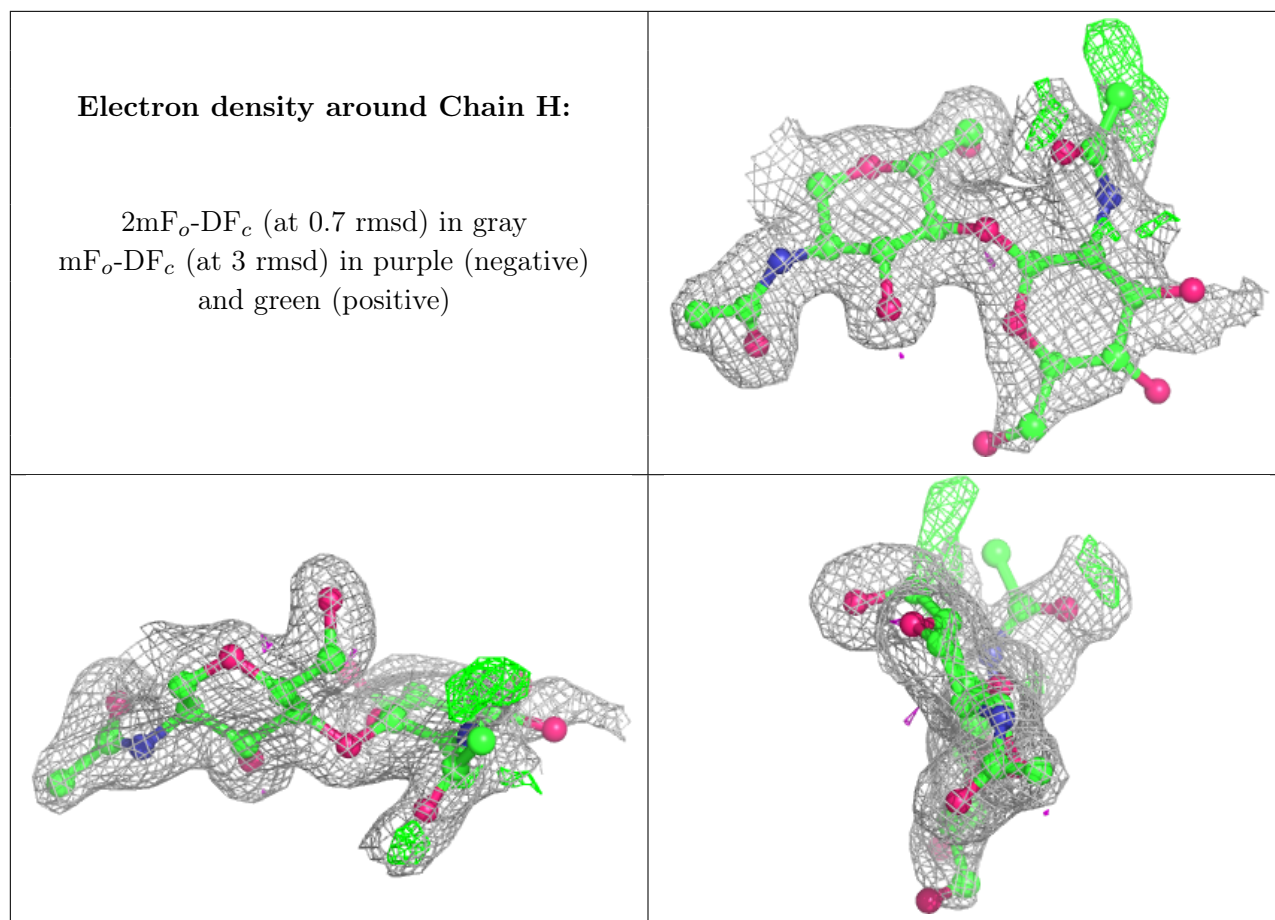
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	G	2	14/15	0.79	0.22	44,55,60,63	0
4	NAG	H	2	14/15	0.82	0.23	45,58,63,65	0
4	NAG	G	1	14/15	0.94	0.10	24,28,29,35	0
4	NAG	H	1	14/15	0.95	0.10	25,28,30,36	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.





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	1005	14/15	0.80	0.31	47,53,57,59	0
5	NAG	B	1005	14/15	0.84	0.29	51,56,62,63	0
5	NAG	A	1010	14/15	0.86	0.33	51,58,70,73	0
5	NAG	B	1007	14/15	0.86	0.14	31,37,43,45	0
5	NAG	A	1007	14/15	0.87	0.12	30,34,41,44	0
5	NAG	A	1003	14/15	0.87	0.19	45,49,57,57	0
5	NAG	A	1006	14/15	0.88	0.16	36,38,41,42	0
5	NAG	B	1003	14/15	0.88	0.17	46,50,55,59	0
5	NAG	B	1006	14/15	0.89	0.15	34,36,39,40	0
5	NAG	A	1008	14/15	0.92	0.10	26,30,35,36	0
5	NAG	B	1008	14/15	0.92	0.10	25,28,31,33	0
5	NAG	A	1009	14/15	0.95	0.10	25,26,30,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	B	1004	14/15	0.95	0.14	28,29,34,35	0
5	NAG	A	1004	14/15	0.95	0.11	28,30,34,37	0
5	NAG	B	1009	14/15	0.97	0.08	26,27,30,32	0
6	MG	A	1011	1/1	0.98	0.16	18,18,18,18	0
6	MG	B	1010	1/1	0.98	0.16	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.