



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 07:48 PM UTC

PDB ID : 4QBZ / pdb_00004qbz
Title : Crystal structure of human TLR8 in complex with DS-802
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2014-05-09
Resolution : 2.00 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	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

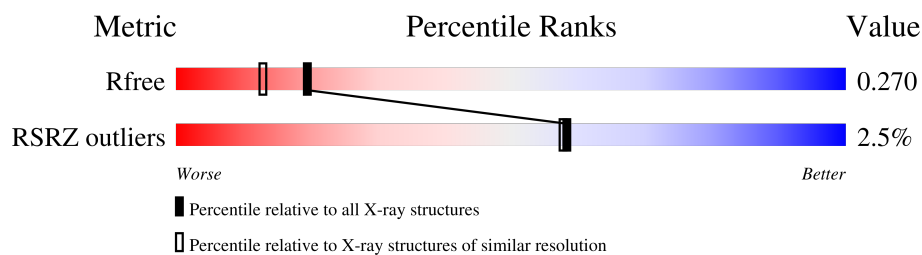
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	754	Total	C	N	O	S	0	0	0
			6071	3882	1029	1141	19			
1	B	751	Total	C	N	O	S	0	1	0
			6062	3878	1031	1134	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

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

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

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

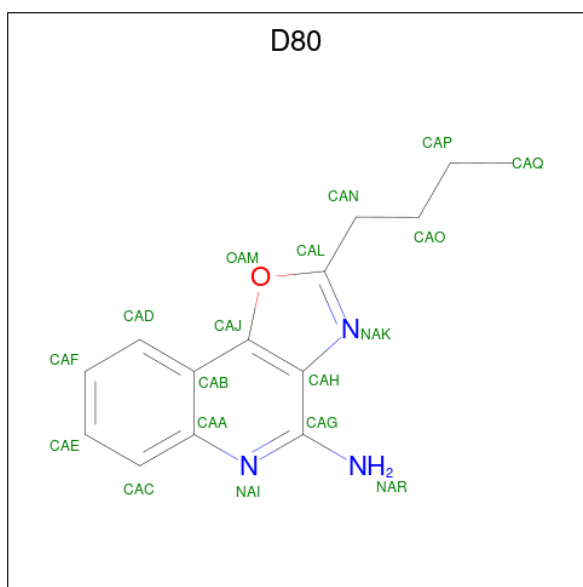
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 7 is 2-butyl[1,3]oxazolo[4,5-c]quinolin-4-amine (CCD ID: D80) (formula: $C_{14}H_{15}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			18	14	3	1		
7	B	1	Total	C	N	O	0	0
			18	14	3	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	277	Total	O	0	0
			277	277		
8	B	229	Total	O	0	0
			229	229		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.15Å 156.72Å 86.16Å 90.00° 77.10° 90.00°	Depositor
Resolution (Å)	26.38 – 2.00 26.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (26.38-2.00) 99.5 (26.38-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.209 , 0.264 0.218 , 0.270	Depositor DCC
R_{free} test set	6273 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13074	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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

4.5 Carbohydrates [i](#)

19 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	0.82	0	17,19,21	1.37	4 (23%)
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	1.57	4 (23%)
2	BMA	C	3	2	11,11,12	0.44	0	15,15,17	1.70	3 (20%)
2	MAN	C	4	2	11,11,12	0.70	0	13,15,17	3.37	7 (53%)
2	BMA	C	5	2	11,11,12	0.29	0	15,15,17	2.37	9 (60%)
3	NAG	D	1	3,1	14,14,15	1.03	1 (7%)	17,19,21	1.88	5 (29%)
3	NAG	D	2	3	14,14,15	0.52	0	17,19,21	1.83	4 (23%)
4	NAG	E	1	4,1	14,14,15	0.60	0	17,19,21	1.56	2 (11%)
4	NAG	E	2	4	14,14,15	0.96	1 (7%)	17,19,21	2.29	6 (35%)
4	BMA	E	3	4	11,11,12	0.43	0	15,15,17	1.93	6 (40%)
5	NAG	F	1	5,1	14,14,15	0.62	0	17,19,21	1.84	7 (41%)
5	NAG	F	2	5	14,14,15	0.92	1 (7%)	17,19,21	1.66	3 (17%)
5	BMA	F	3	5	11,11,12	0.47	0	15,15,17	1.81	4 (26%)
5	MAN	F	4	5	11,11,12	0.53	0	15,15,17	2.51	8 (53%)
3	NAG	G	1	3,1	14,14,15	0.79	1 (7%)	17,19,21	2.01	5 (29%)
3	NAG	G	2	3	14,14,15	0.60	0	17,19,21	2.94	7 (41%)
4	NAG	H	1	4,1	14,14,15	0.79	0	17,19,21	1.53	2 (11%)
4	NAG	H	2	4	14,14,15	0.75	0	17,19,21	1.64	4 (23%)
4	BMA	H	3	4	11,11,12	0.53	0	15,15,17	1.84	4 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	1/2/18/22	0/1/1/1
2	BMA	C	5	2	-	1/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,1	-	0/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	O5-C1	-2.59	1.39	1.43
4	E	2	NAG	C8-C7	-2.33	1.45	1.50
3	G	1	NAG	O5-C1	-2.14	1.40	1.43
5	F	2	NAG	O5-C1	-2.07	1.40	1.43

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C1-O5-C5	8.77	123.94	112.19
2	C	4	MAN	C2-C3-C4	-8.17	98.89	110.67
2	C	4	MAN	C3-C4-C5	-5.59	104.38	109.99
5	F	4	MAN	O3-C3-C2	-5.42	99.00	110.05
4	E	2	NAG	O7-C7-C8	-5.10	112.97	122.05
5	F	3	BMA	O3-C3-C2	4.36	118.95	110.05
4	H	3	BMA	C2-C3-C4	-4.30	103.29	110.86
3	G	1	NAG	C4-C3-C2	-4.23	104.82	111.02
4	E	3	BMA	C2-C3-C4	-4.20	103.47	110.86
5	F	2	NAG	O5-C5-C6	-4.20	99.50	107.66
4	E	1	NAG	O4-C4-C3	-4.13	100.64	110.38
3	G	2	NAG	O5-C5-C4	4.02	120.62	110.83
2	C	5	BMA	C2-C3-C4	-3.92	103.97	110.86
3	D	1	NAG	C4-C3-C2	-3.84	105.40	111.02
3	G	1	NAG	C1-O5-C5	-3.79	107.11	112.19
2	C	4	MAN	O3-C3-C2	3.79	119.28	109.86
3	G	2	NAG	C1-C2-N2	3.73	116.31	110.43
3	D	2	NAG	C8-C7-N2	3.67	122.21	116.12
4	H	3	BMA	O3-C3-C4	3.62	118.91	110.38
5	F	4	MAN	O5-C1-C2	-3.60	102.20	110.79
2	C	3	BMA	C2-C3-C4	-3.59	104.54	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C1-C2-N2	3.53	115.99	110.43
4	E	3	BMA	O3-C3-C4	3.42	118.44	110.38
2	C	5	BMA	C3-C4-C5	3.42	116.42	110.23
4	E	2	NAG	C8-C7-N2	3.39	121.73	116.12
2	C	5	BMA	C1-C2-C3	-3.30	104.84	109.64
2	C	4	MAN	C1-C2-C3	-3.28	101.92	111.23
2	C	3	BMA	O3-C3-C2	3.25	116.69	110.05
3	D	1	NAG	C1-C2-N2	-3.20	105.40	110.43
2	C	2	NAG	O7-C7-C8	-3.19	116.37	122.05
3	D	1	NAG	O3-C3-C2	-3.18	102.79	109.40
5	F	4	MAN	O5-C5-C6	3.14	113.78	107.66
2	C	5	BMA	O4-C4-C3	-3.14	102.97	110.38
4	H	1	NAG	O5-C1-C2	-3.09	106.52	111.29
3	G	1	NAG	O3-C3-C4	3.07	117.62	110.38
2	C	2	NAG	C1-C2-N2	3.07	115.28	110.43
3	D	2	NAG	C3-C4-C5	-3.06	104.68	110.23
3	G	2	NAG	C8-C7-N2	3.06	121.19	116.12
4	H	2	NAG	C4-C3-C2	-3.05	106.54	111.02
4	E	2	NAG	C2-N2-C7	3.05	126.99	122.90
5	F	1	NAG	C1-O5-C5	2.95	116.14	112.19
4	H	2	NAG	O5-C5-C6	2.93	113.37	107.66
2	C	4	MAN	O4-C4-C5	2.92	116.52	109.32
2	C	5	BMA	O5-C1-C2	-2.88	103.92	110.79
2	C	4	MAN	O3-C3-C4	2.82	116.00	110.15
3	G	1	NAG	O4-C4-C3	-2.80	103.78	110.38
4	H	2	NAG	O4-C4-C3	-2.80	103.78	110.38
4	H	1	NAG	O5-C5-C4	-2.71	104.23	110.83
4	E	3	BMA	C1-C2-C3	2.69	113.57	109.64
5	F	1	NAG	O4-C4-C3	2.67	116.67	110.38
5	F	4	MAN	O2-C2-C1	-2.65	103.15	109.22
3	G	2	NAG	O6-C6-C5	-2.65	102.31	111.33
4	E	2	NAG	O3-C3-C4	-2.65	104.13	110.38
5	F	1	NAG	C1-C2-N2	-2.63	106.29	110.43
3	G	2	NAG	O7-C7-C8	-2.61	117.41	122.05
2	C	1	NAG	O6-C6-C5	-2.60	102.47	111.33
5	F	3	BMA	O3-C3-C4	-2.59	104.26	110.38
2	C	5	BMA	O5-C5-C6	-2.57	102.65	107.66
2	C	1	NAG	O3-C3-C4	2.56	116.41	110.38
5	F	4	MAN	C1-C2-C3	2.52	113.32	109.64
3	D	1	NAG	C3-C4-C5	2.52	114.80	110.23
3	D	2	NAG	O7-C7-C8	-2.50	117.60	122.05
4	E	2	NAG	O6-C6-C5	-2.48	102.89	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	4	MAN	C2-C3-C4	2.48	115.21	110.86
5	F	1	NAG	O7-C7-N2	2.46	126.33	121.98
3	D	2	NAG	C2-N2-C7	-2.45	119.61	122.90
5	F	3	BMA	C1-O5-C5	2.44	115.46	112.19
2	C	3	BMA	O4-C4-C3	-2.43	104.66	110.38
2	C	2	NAG	O7-C7-N2	2.38	126.19	121.98
2	C	1	NAG	C2-N2-C7	-2.38	119.71	122.90
3	G	2	NAG	O3-C3-C4	-2.38	104.78	110.38
4	E	1	NAG	O5-C1-C2	-2.34	107.67	111.29
5	F	1	NAG	O6-C6-C5	-2.31	103.47	111.33
5	F	2	NAG	O5-C1-C2	-2.29	107.74	111.29
2	C	1	NAG	C6-C5-C4	2.29	118.64	113.02
5	F	1	NAG	O4-C4-C5	-2.29	103.69	109.32
4	E	3	BMA	O4-C4-C5	-2.25	103.79	109.32
4	H	3	BMA	C3-C4-C5	2.23	114.27	110.23
2	C	5	BMA	O3-C3-C4	2.22	115.61	110.38
2	C	5	BMA	O5-C5-C4	2.21	116.21	110.83
3	G	1	NAG	O6-C6-C5	-2.21	103.82	111.33
5	F	4	MAN	O3-C3-C4	2.19	115.53	110.38
4	H	2	NAG	O7-C7-N2	2.17	125.82	121.98
4	E	3	BMA	O2-C2-C3	-2.13	105.74	110.15
3	D	1	NAG	C6-C5-C4	-2.12	107.81	113.02
5	F	2	NAG	C6-C5-C4	2.12	118.23	113.02
4	H	3	BMA	C1-C2-C3	2.12	112.72	109.64
5	F	4	MAN	O4-C4-C3	2.11	115.35	110.38
2	C	2	NAG	C2-N2-C7	-2.09	120.10	122.90
5	F	1	NAG	O5-C1-C2	-2.08	108.07	111.29
5	F	3	BMA	C1-C2-C3	2.07	112.67	109.64
2	C	5	BMA	O2-C2-C1	-2.07	104.48	109.22
2	C	4	MAN	O6-C6-C5	-2.03	104.42	111.33
4	E	3	BMA	O4-C4-C3	-2.01	105.65	110.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2

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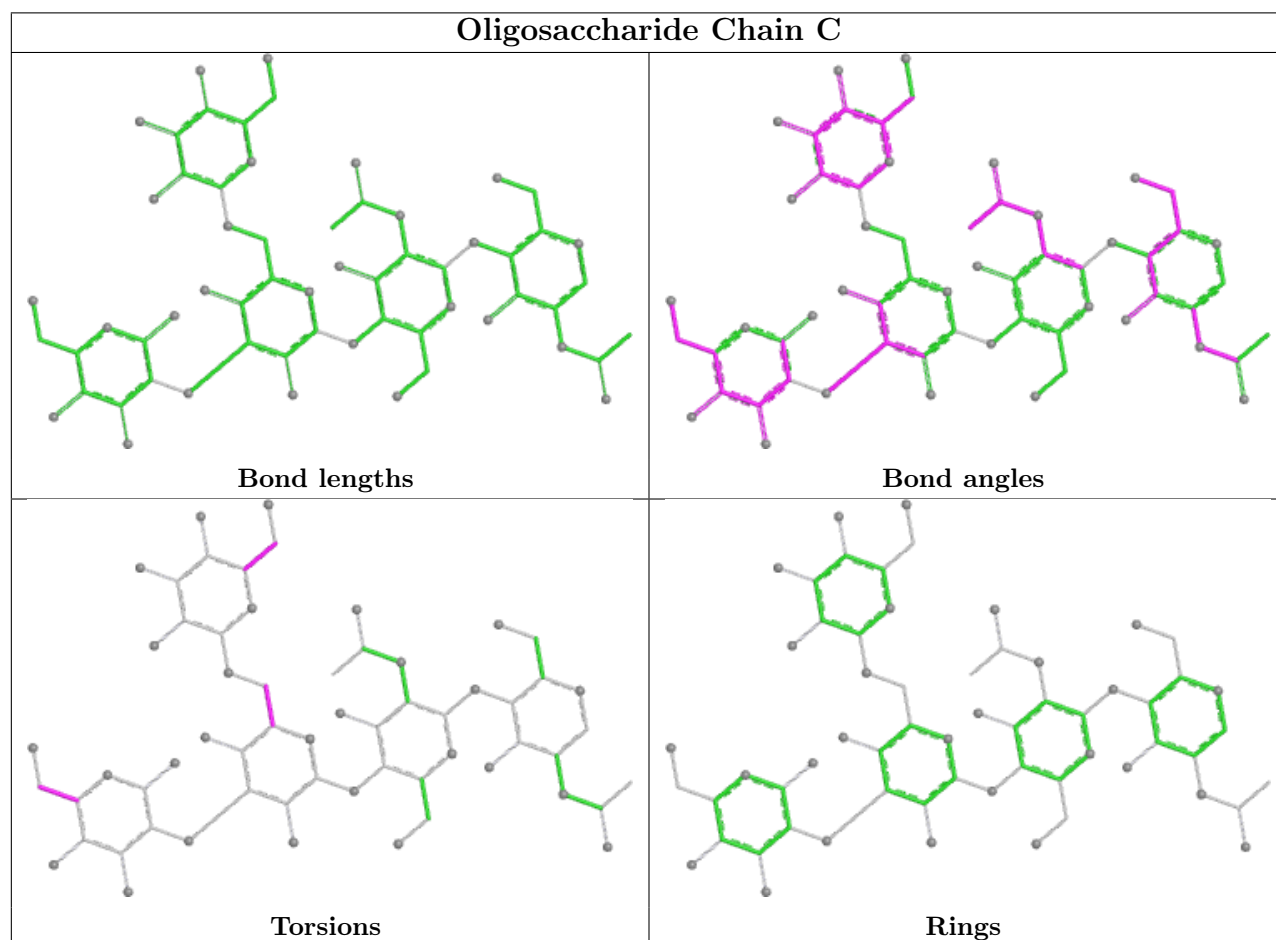
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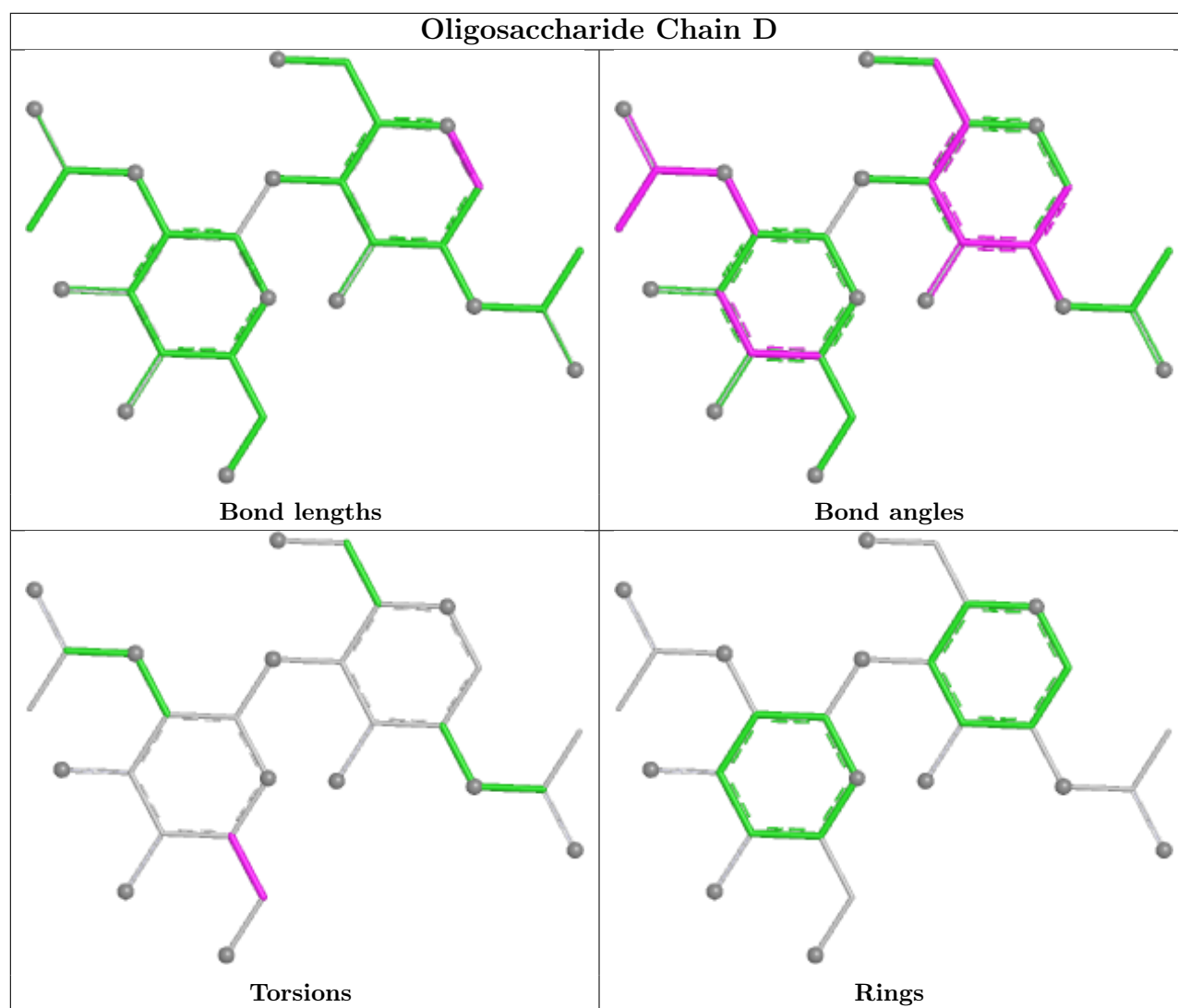
Mol	Chain	Res	Type	Atoms
4	H	3	BMA	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
5	F	4	MAN	O5-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
2	C	5	BMA	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6

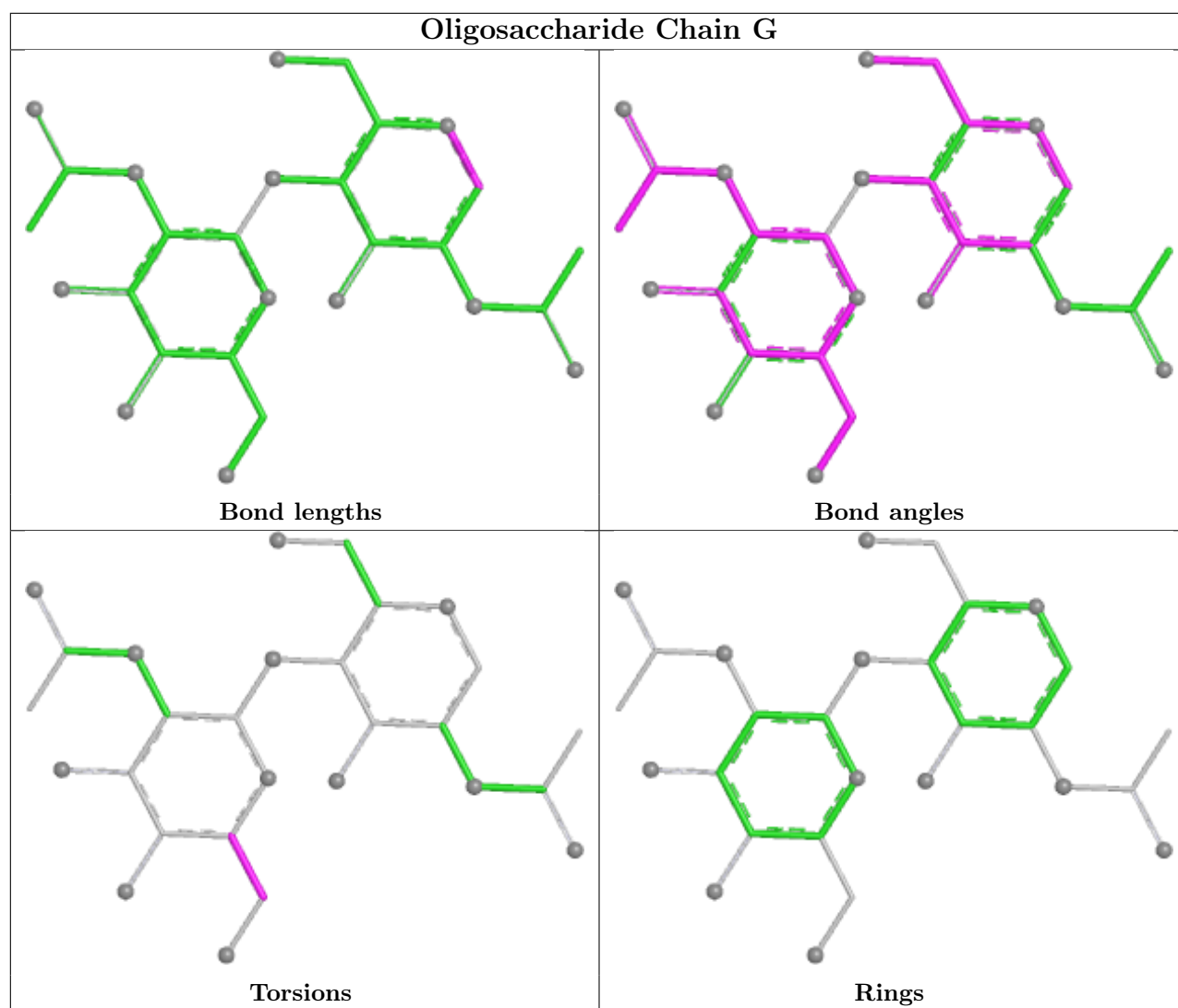
There are no ring outliers.

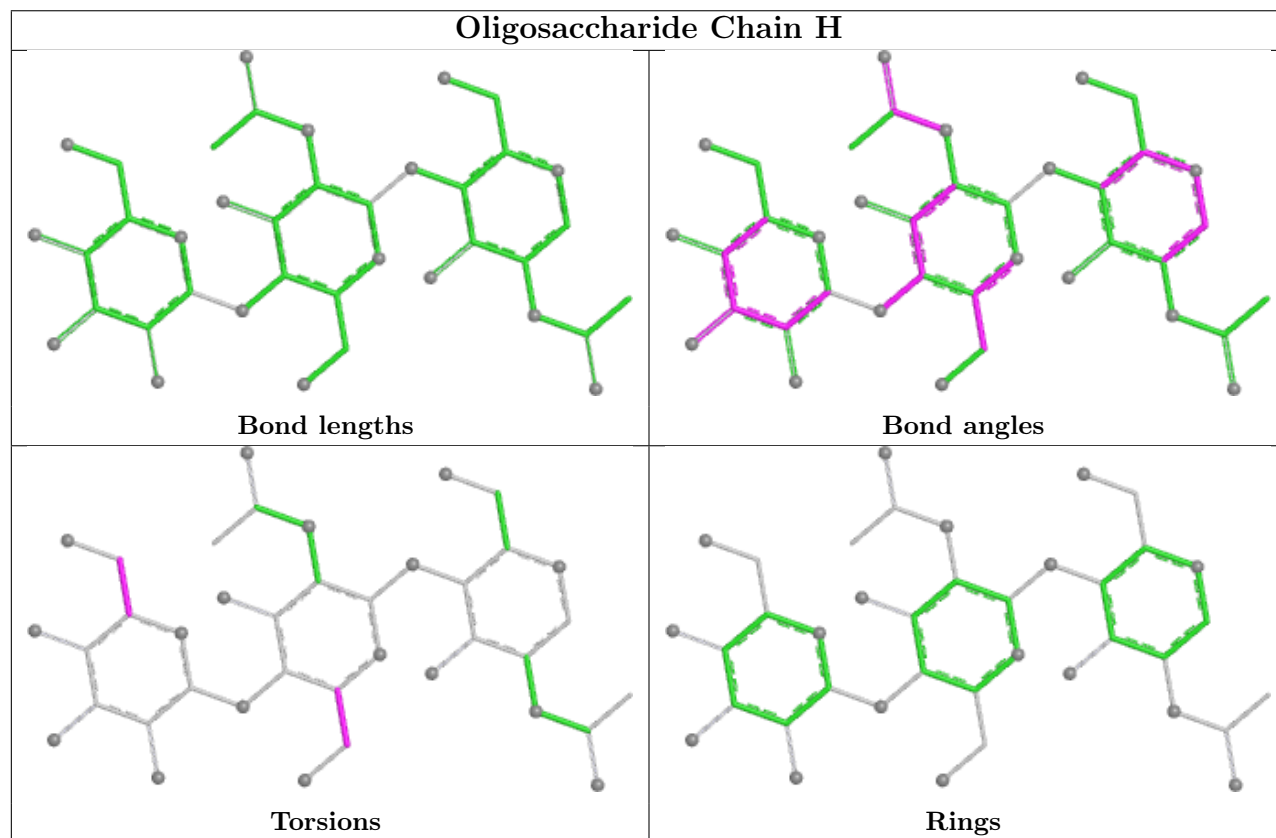
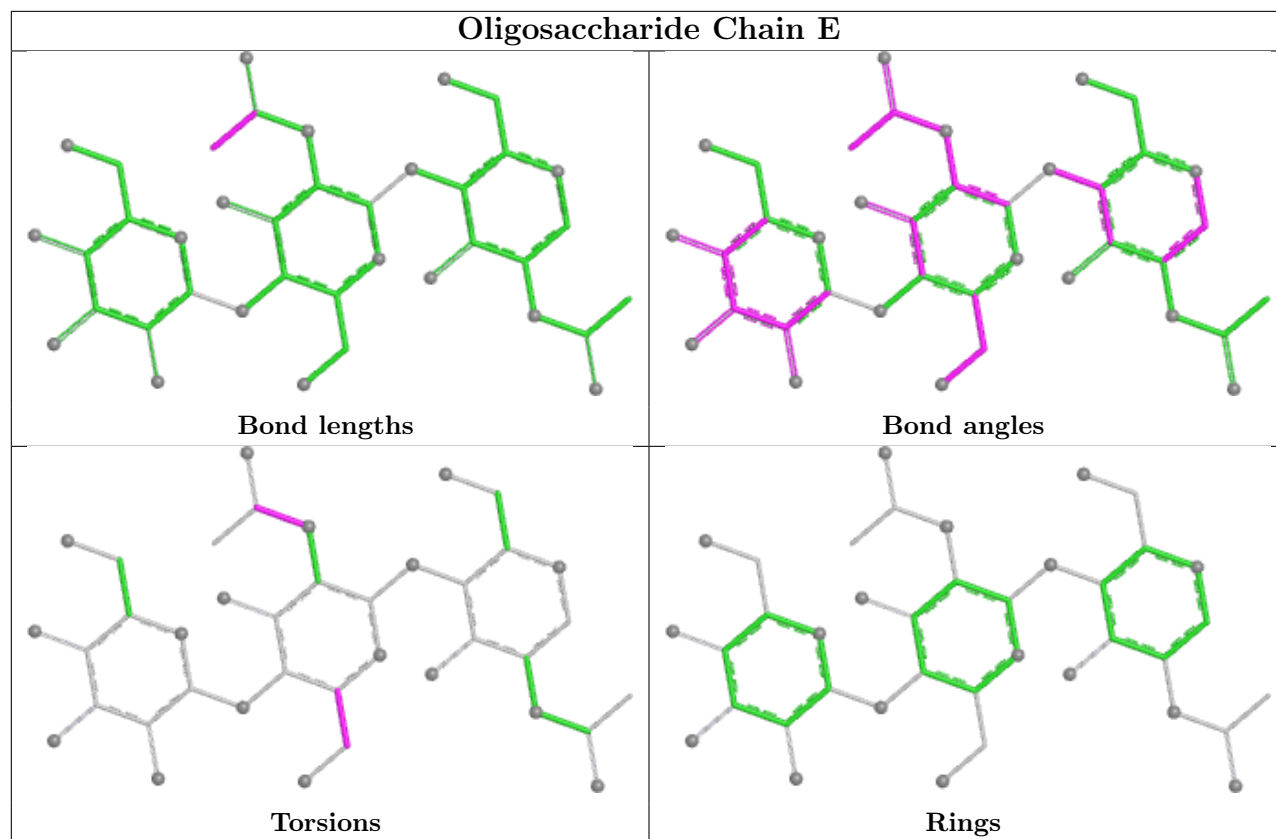
No monomer is involved in short contacts.

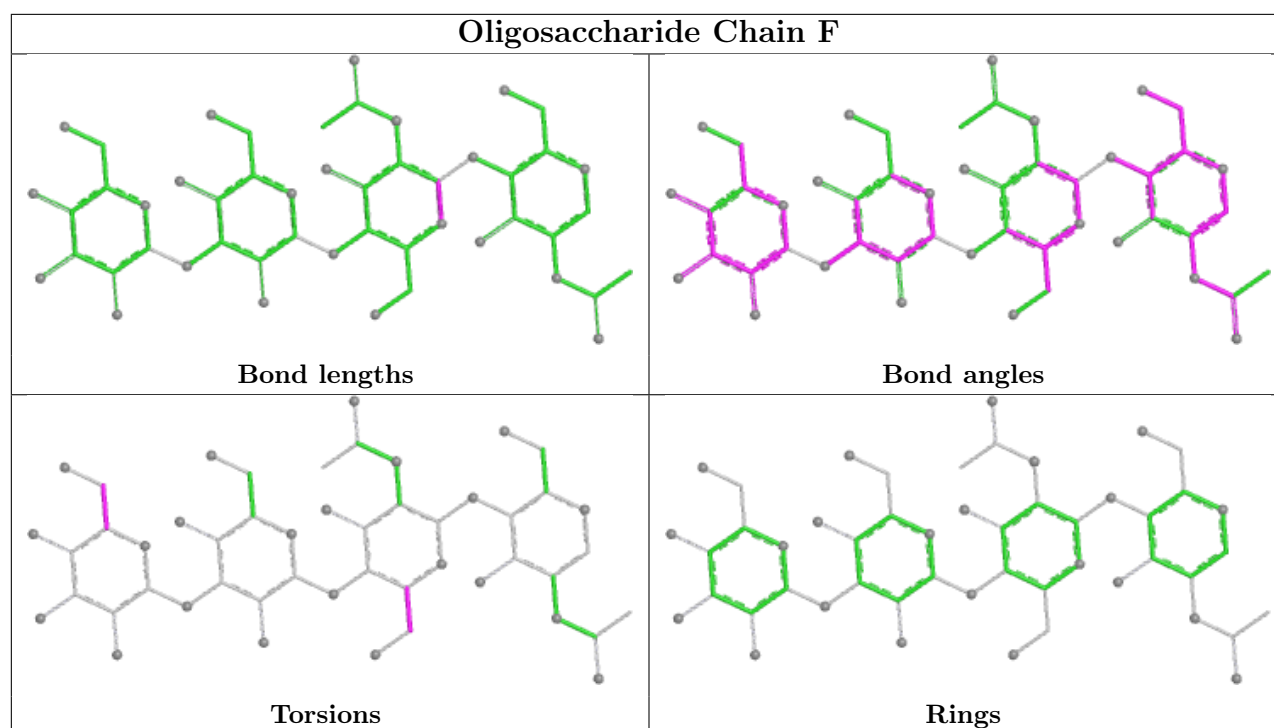
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











4.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	B	914	1	14,14,15	0.73	0	17,19,21	2.28	8 (47%)
6	NAG	A	907	1	14,14,15	0.47	0	17,19,21	1.13	2 (11%)
6	NAG	B	909	1	14,14,15	0.55	0	17,19,21	2.07	6 (35%)
6	NAG	A	911	1	14,14,15	0.41	0	17,19,21	2.70	4 (23%)
6	NAG	B	915	1	14,14,15	0.50	0	17,19,21	3.43	8 (47%)
7	D80	A	917	-	20,20,20	2.62	6 (30%)	25,28,28	2.63	9 (36%)
6	NAG	A	901	1	14,14,15	0.65	0	17,19,21	1.58	4 (23%)
6	NAG	B	906	1	14,14,15	0.43	0	17,19,21	2.31	9 (52%)
6	NAG	A	910	1	14,14,15	0.76	0	17,19,21	1.69	3 (17%)
6	NAG	B	910	1	14,14,15	0.37	0	17,19,21	2.12	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	915	1	14,14,15	0.89	1 (7%)	17,19,21	2.80	6 (35%)
6	NAG	A	916	1	14,14,15	0.62	0	17,19,21	2.97	7 (41%)
7	D80	B	901	-	20,20,20	2.70	7 (35%)	25,28,28	3.04	9 (36%)

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
6	NAG	B	914	1	-	0/6/23/26	0/1/1/1
6	NAG	A	907	1	-	0/6/23/26	0/1/1/1
6	NAG	B	909	1	-	0/6/23/26	0/1/1/1
6	NAG	A	911	1	-	2/6/23/26	0/1/1/1
6	NAG	B	915	1	-	0/6/23/26	0/1/1/1
7	D80	A	917	-	-	0/4/4/4	0/3/3/3
6	NAG	A	901	1	-	2/6/23/26	0/1/1/1
6	NAG	B	906	1	-	2/6/23/26	0/1/1/1
6	NAG	A	910	1	-	2/6/23/26	0/1/1/1
6	NAG	B	910	1	-	3/6/23/26	0/1/1/1
6	NAG	A	915	1	-	2/6/23/26	0/1/1/1
6	NAG	A	916	1	-	2/6/23/26	0/1/1/1
7	D80	B	901	-	-	1/4/4/4	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	901	D80	CAJ-CAH	8.72	1.47	1.36
7	A	917	D80	CAJ-CAH	8.48	1.47	1.36
7	A	917	D80	CAL-NAK	4.87	1.35	1.29
7	B	901	D80	OAM-CAJ	-4.52	1.32	1.38
7	B	901	D80	CAL-NAK	3.94	1.34	1.29
7	A	917	D80	OAM-CAJ	-3.89	1.33	1.38
7	B	901	D80	CAH-CAG	2.69	1.48	1.41
7	A	917	D80	CAJ-CAB	-2.49	1.38	1.43
7	B	901	D80	CAD-CAB	-2.33	1.37	1.42
7	A	917	D80	CAH-CAG	2.25	1.47	1.41
7	B	901	D80	CAB-CAA	-2.20	1.39	1.42
7	B	901	D80	CAC-CAA	-2.16	1.38	1.41
7	A	917	D80	OAM-CAL	2.09	1.39	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	915	NAG	O5-C1	-2.04	1.40	1.43

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	915	NAG	C1-O5-C5	11.06	127.00	112.19
6	A	911	NAG	C1-O5-C5	9.56	125.00	112.19
7	B	901	D80	OAM-CAL-NAK	-7.85	108.94	115.47
7	A	917	D80	CAG-CAH-NAK	7.68	139.34	131.72
7	B	901	D80	CAG-CAH-NAK	7.45	139.10	131.72
6	A	916	NAG	C1-O5-C5	-6.91	102.93	112.19
6	A	916	NAG	C1-C2-N2	6.27	120.32	110.43
6	B	910	NAG	C1-C2-N2	5.64	119.33	110.43
6	A	915	NAG	O3-C3-C4	-5.60	97.17	110.38
7	B	901	D80	CAJ-CAH-NAK	-5.28	105.06	109.02
6	A	915	NAG	O5-C1-C2	-4.66	104.08	111.29
7	A	917	D80	OAM-CAL-NAK	-4.61	111.63	115.47
6	A	916	NAG	O5-C1-C2	-4.55	104.25	111.29
6	A	915	NAG	C1-O5-C5	4.54	118.28	112.19
7	B	901	D80	OAM-CAL-CAN	4.51	127.73	117.83
6	B	914	NAG	C2-N2-C7	4.44	128.85	122.90
6	B	914	NAG	C1-O5-C5	4.36	118.03	112.19
6	A	915	NAG	O6-C6-C5	-4.26	96.83	111.33
7	A	917	D80	CAJ-CAH-NAK	-4.20	105.86	109.02
6	B	909	NAG	C6-C5-C4	-4.16	102.81	113.02
7	B	901	D80	OAM-CAJ-CAB	4.12	133.64	124.69
6	B	915	NAG	C2-N2-C7	-4.02	117.52	122.90
6	B	906	NAG	C3-C4-C5	4.00	117.49	110.23
6	B	910	NAG	O5-C5-C6	3.95	115.36	107.66
6	B	910	NAG	C2-N2-C7	3.89	128.12	122.90
6	B	906	NAG	C6-C5-C4	-3.84	103.58	113.02
6	A	910	NAG	C1-O5-C5	3.79	117.27	112.19
7	A	917	D80	OAM-CAL-CAN	3.78	126.12	117.83
6	A	910	NAG	O5-C1-C2	-3.75	105.49	111.29
6	B	909	NAG	C1-C2-N2	3.71	116.28	110.43
6	B	906	NAG	O4-C4-C5	3.61	118.22	109.32
6	A	915	NAG	O4-C4-C3	-3.61	101.88	110.38
6	B	915	NAG	O5-C1-C2	-3.60	105.72	111.29
7	A	917	D80	CAN-CAL-NAK	-3.58	122.24	128.81
6	A	916	NAG	O5-C5-C6	3.42	114.32	107.66
6	B	909	NAG	C2-N2-C7	-3.34	118.43	122.90
7	B	901	D80	CAH-CAJ-CAB	-3.31	120.06	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	915	NAG	C4-C3-C2	-3.30	106.18	111.02
6	B	914	NAG	C1-C2-N2	-3.20	105.38	110.43
6	B	909	NAG	O6-C6-C5	-3.20	100.43	111.33
6	B	915	NAG	O5-C5-C4	3.16	118.53	110.83
6	B	914	NAG	O4-C4-C3	-3.10	103.06	110.38
7	B	901	D80	CAN-CAL-NAK	-3.08	123.16	128.81
7	A	917	D80	CAO-CAN-CAL	-3.00	106.74	113.27
6	B	906	NAG	C1-O5-C5	2.98	116.18	112.19
6	A	901	NAG	O6-C6-C5	-2.91	101.42	111.33
6	A	911	NAG	O5-C1-C2	2.87	115.73	111.29
6	A	916	NAG	O7-C7-C8	-2.81	117.05	122.05
6	B	906	NAG	C8-C7-N2	-2.75	111.56	116.12
7	A	917	D80	CAH-CAJ-CAB	-2.72	120.84	124.42
6	B	915	NAG	C6-C5-C4	-2.71	106.37	113.02
6	B	914	NAG	O7-C7-C8	-2.70	117.24	122.05
7	B	901	D80	OAM-CAJ-CAH	-2.69	106.29	108.25
6	A	915	NAG	C1-C2-N2	-2.66	106.25	110.43
6	A	910	NAG	O6-C6-C5	-2.63	102.37	111.33
6	B	906	NAG	C1-C2-N2	-2.58	106.37	110.43
6	A	916	NAG	O3-C3-C4	-2.58	104.30	110.38
6	A	907	NAG	O7-C7-C8	-2.57	117.47	122.05
7	A	917	D80	CAD-CAB-CAA	2.56	121.20	118.36
7	A	917	D80	OAM-CAJ-CAB	2.55	130.22	124.69
6	B	915	NAG	O3-C3-C4	-2.47	104.56	110.38
6	A	907	NAG	C1-C2-N2	-2.44	106.58	110.43
6	B	906	NAG	C4-C3-C2	-2.43	107.46	111.02
6	A	911	NAG	O4-C4-C3	-2.42	104.67	110.38
6	A	901	NAG	C6-C5-C4	-2.39	107.14	113.02
6	B	914	NAG	O5-C1-C2	-2.39	107.60	111.29
6	B	914	NAG	O7-C7-N2	2.36	126.16	121.98
6	A	901	NAG	C1-O5-C5	2.36	115.35	112.19
6	B	909	NAG	C4-C3-C2	-2.34	107.59	111.02
6	B	914	NAG	O3-C3-C4	-2.22	105.14	110.38
6	B	906	NAG	O3-C3-C4	-2.19	105.21	110.38
6	A	901	NAG	O5-C5-C4	2.18	116.13	110.83
6	B	915	NAG	O5-C5-C6	2.18	111.90	107.66
6	B	906	NAG	O7-C7-N2	2.15	125.78	121.98
6	A	911	NAG	C3-C4-C5	2.06	113.96	110.23
6	A	916	NAG	O6-C6-C5	-2.04	104.40	111.33
7	B	901	D80	CAC-CAA-CAB	2.03	121.33	119.13
6	B	909	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	911	NAG	O5-C5-C6-O6
6	A	915	NAG	C4-C5-C6-O6
6	A	915	NAG	O5-C5-C6-O6
6	A	916	NAG	O5-C5-C6-O6
6	A	910	NAG	O5-C5-C6-O6
6	B	910	NAG	C4-C5-C6-O6
6	A	910	NAG	C4-C5-C6-O6
6	A	916	NAG	C4-C5-C6-O6
6	B	910	NAG	O5-C5-C6-O6
6	A	911	NAG	C4-C5-C6-O6
6	B	906	NAG	O5-C5-C6-O6
6	A	901	NAG	C4-C5-C6-O6
7	B	901	D80	CAL-CAN-CAO-CAP
6	B	906	NAG	C4-C5-C6-O6
6	A	901	NAG	O5-C5-C6-O6
6	B	910	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	754/811 (92%)	0.06	17 (2%) 61 60	20, 34, 59, 90	0
1	B	751/811 (92%)	0.28	21 (2%) 55 54	16, 38, 68, 96	1 (0%)
All	All	1505/1622 (92%)	0.17	38 (2%) 58 58	16, 36, 63, 96	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	817	LEU	5.5
1	B	434	VAL	4.7
1	B	762	THR	4.4
1	B	459	PHE	4.4
1	B	760	THR	4.2
1	B	761	THR	3.8
1	A	818	GLU	3.7
1	B	678	PHE	3.5
1	B	702	PHE	3.4
1	B	61	VAL	3.3
1	B	778	CYS	3.1
1	A	64	TYR	3.0
1	A	434	VAL	3.0
1	B	470	PHE	3.0
1	B	388	GLN	2.9
1	B	85	GLY	2.8
1	A	457	THR	2.7
1	B	100	VAL	2.7
1	B	45	VAL	2.6
1	A	470	PHE	2.6
1	A	31	SER	2.6
1	B	86	LEU	2.4
1	A	100	VAL	2.4
1	A	762	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	732	LEU	2.3
1	B	764	LEU	2.3
1	A	812	LYS	2.3
1	B	433	LEU	2.3
1	A	96	HIS	2.3
1	A	759	LYS	2.3
1	B	31	SER	2.2
1	B	726	HIS	2.2
1	B	246	ILE	2.1
1	A	459	PHE	2.1
1	B	40	LYS	2.1
1	A	815	VAL	2.1
1	A	761	THR	2.0
1	A	99	ASN	2.0

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

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

5.3 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.

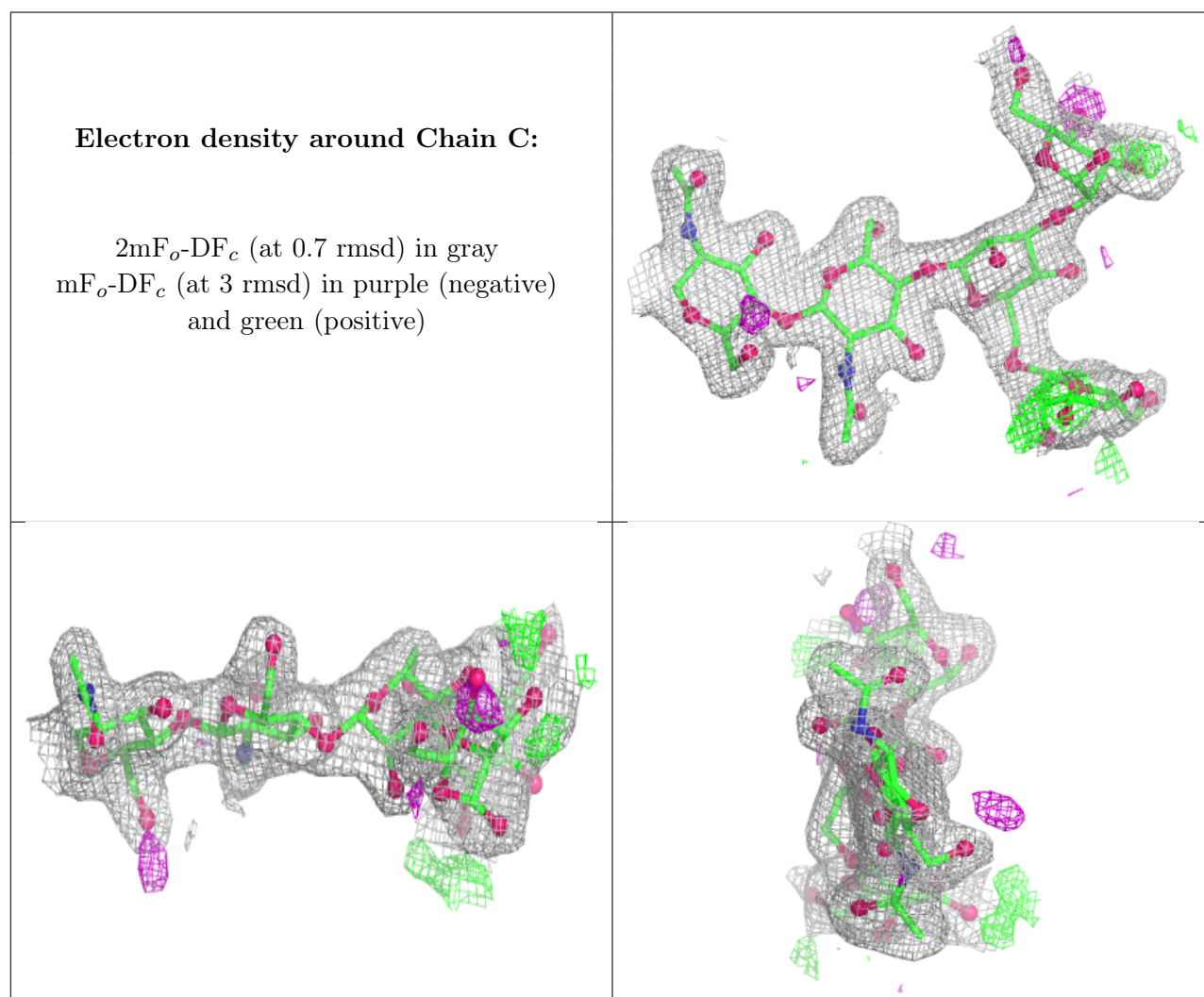
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	F	4	11/12	0.68	0.19	58,67,77,79	0
2	MAN	C	4	11/12	0.76	0.19	44,63,72,94	0
2	BMA	C	5	11/12	0.77	0.14	59,65,68,70	0
4	BMA	H	3	11/12	0.81	0.11	44,51,61,63	0
4	BMA	E	3	11/12	0.84	0.09	42,47,50,61	0
3	NAG	G	2	14/15	0.85	0.12	40,51,56,56	0
5	BMA	F	3	11/12	0.88	0.09	41,46,48,52	0
3	NAG	D	2	14/15	0.91	0.08	36,44,54,55	0
5	NAG	F	2	14/15	0.91	0.08	29,35,42,44	0
2	NAG	C	2	14/15	0.93	0.07	27,33,39,48	0
2	BMA	C	3	11/12	0.93	0.08	42,46,51,55	0
5	NAG	F	1	14/15	0.93	0.09	28,31,37,47	0
4	NAG	H	2	14/15	0.94	0.08	31,33,39,45	0
4	NAG	E	2	14/15	0.94	0.07	25,30,38,38	0

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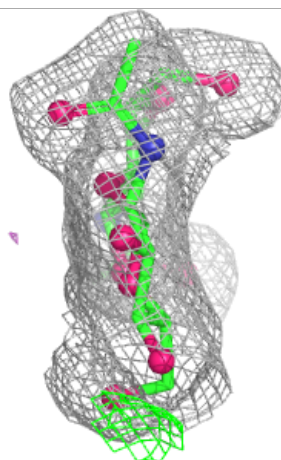
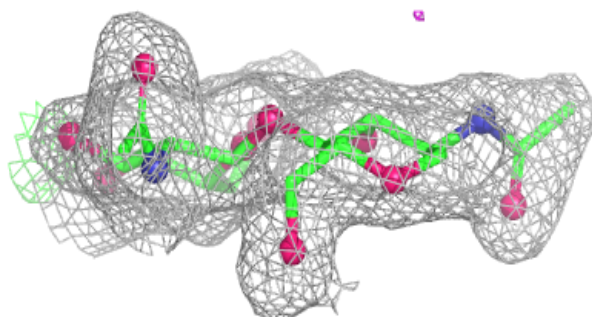
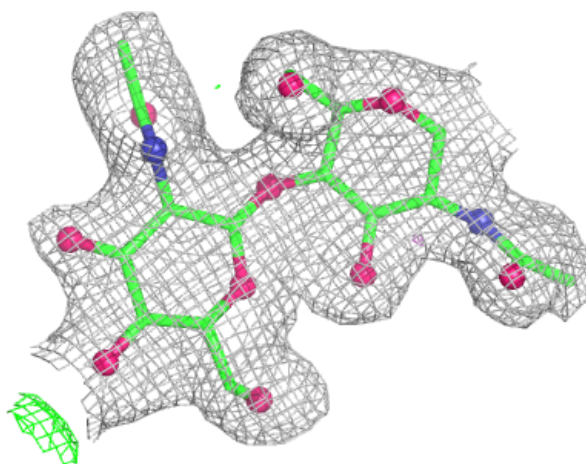
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	G	1	14/15	0.95	0.06	24,26,30,32	0
2	NAG	C	1	14/15	0.95	0.07	23,26,30,38	0
4	NAG	E	1	14/15	0.97	0.05	20,23,27,27	0
4	NAG	H	1	14/15	0.97	0.05	24,28,29,30	0
3	NAG	D	1	14/15	0.98	0.05	22,25,30,32	0

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.



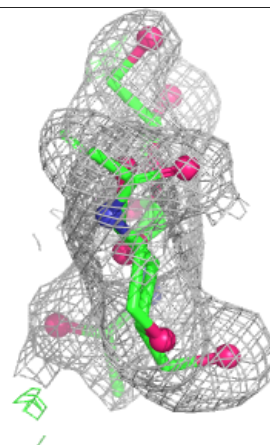
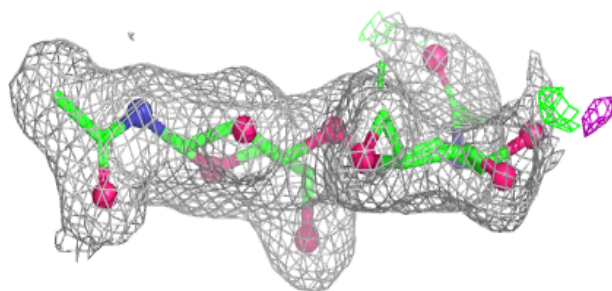
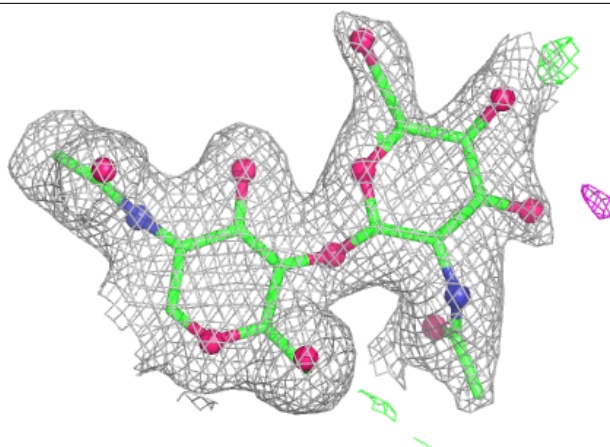
Electron density around Chain D:

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



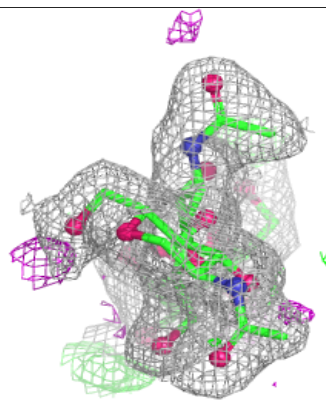
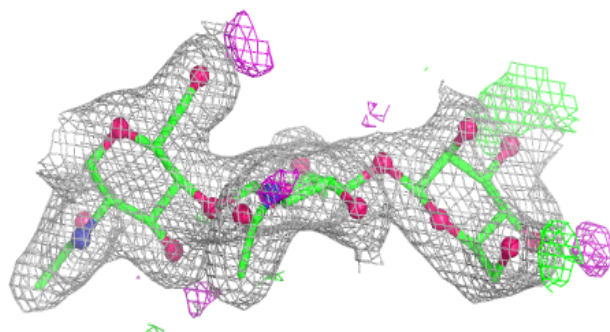
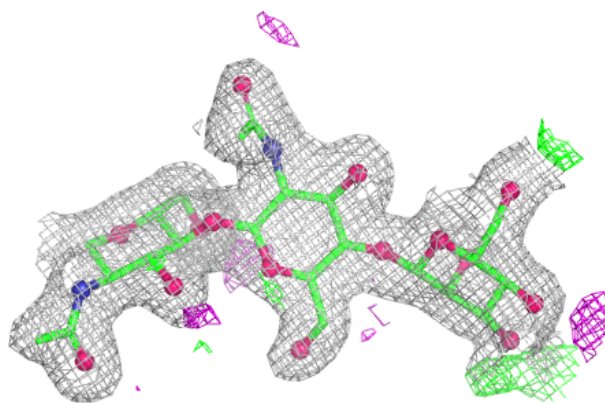
Electron density around Chain G:

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

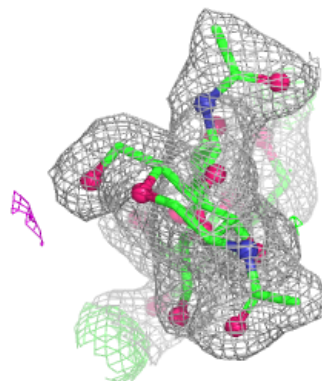
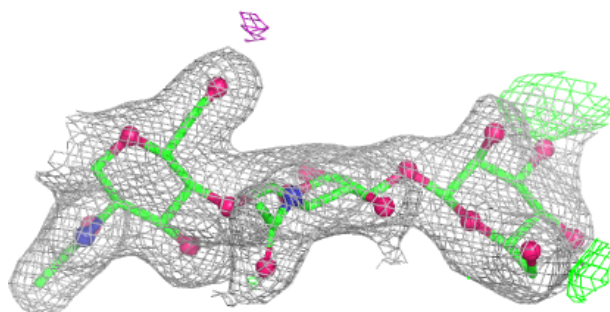
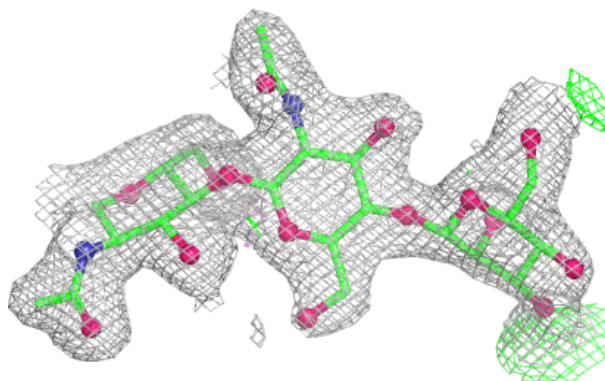


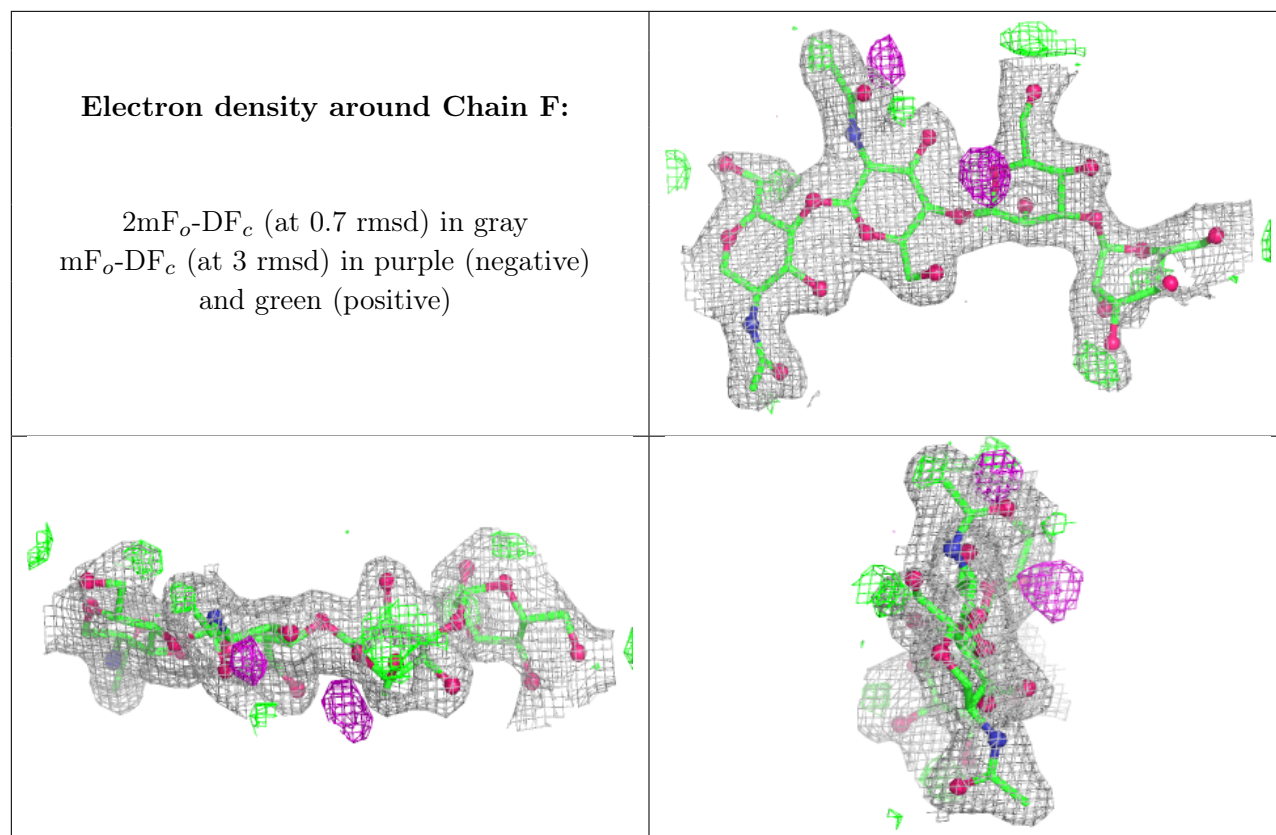
Electron density around Chain E:

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

**Electron density around Chain H:**

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





5.4 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($\text{\AA}^2$)	Q<0.9
6	NAG	A	901	14/15	0.72	0.12	48,57,63,66	0
6	NAG	A	911	14/15	0.78	0.13	57,62,68,71	0
6	NAG	B	910	14/15	0.81	0.12	55,62,65,66	0
6	NAG	B	906	14/15	0.85	0.11	33,43,46,57	0
6	NAG	B	915	14/15	0.86	0.12	48,54,64,65	0
6	NAG	A	910	14/15	0.88	0.09	45,56,60,67	0
6	NAG	B	909	14/15	0.88	0.12	41,54,64,67	0
6	NAG	A	915	14/15	0.88	0.10	33,43,48,50	0
6	NAG	A	916	14/15	0.88	0.11	45,51,63,67	0
6	NAG	B	914	14/15	0.91	0.09	27,40,53,55	0
6	NAG	A	907	14/15	0.92	0.09	33,39,44,47	0
7	D80	A	917	18/18	0.96	0.05	21,25,28,28	0
7	D80	B	901	18/18	0.96	0.06	21,24,28,30	0

5.5 Other polymers [i](#)

There are no such residues in this entry.