



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 08:15 PM BST

PDB ID : 3FXI
Title : Crystal structure of the human TLR4-human MD-2-E.coli LPS Ra complex
Authors : Park, B.S.; Song, D.H.; Kim, H.M.; Lee, J.-O.
Deposited on : 2009-01-21
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

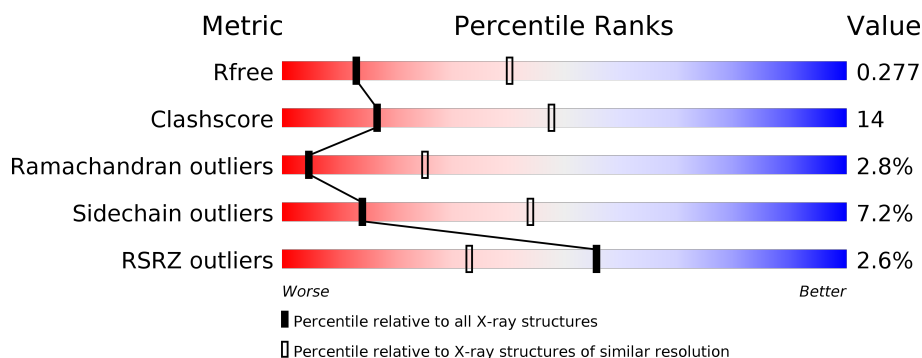
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	605	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>5%</div> </div> </div>
1	B	605	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>5%</div> </div> </div>
2	C	142	<div> <div></div> <div> <div></div> <div>58%</div> <div>34%</div> <div>7%</div> </div> </div>
2	D	142	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>31%</div> <div>7%</div> </div> </div>
3	E	7	<div> <div></div> <div> <div></div> <div>14%</div> <div>86%</div> </div> </div>
4	F	2	<div> <div></div> <div> <div></div> <div>100%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
4	I	2	 50% 50%
4	J	2	 50% 50%
5	H	7	 14% 86%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MG	B	2001	-	-	-	X
3	PA1	E	2	X	-	-	-
6	FTT	B	1003	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 12500 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.

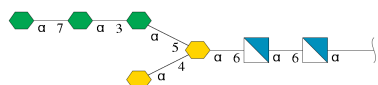
- Molecule 1 is a protein called Toll-like receptor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4803	3075	790	911	27			
1	B	601	Total	C	N	O	S	0	0	0
			4803	3075	790	911	27			

- Molecule 2 is a protein called Lymphocyte antigen 96.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	140	Total	C	N	O	S	0	0	0
			1133	730	186	207	10			
2	D	140	Total	C	N	O	S	0	0	0
			1133	730	186	207	10			

- Molecule 3 is an oligosaccharide called L-glycero-alpha-D-manno-heptopyranose-(1-7)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose.



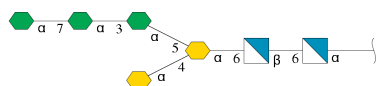
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	0	0	0
			92	49	2	41			

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



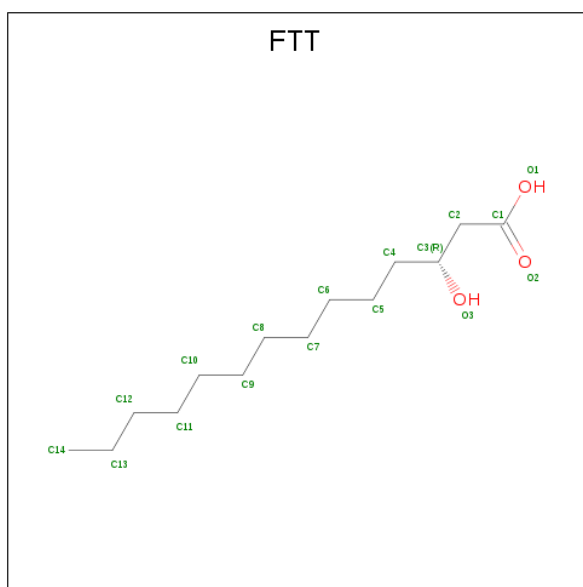
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called L-glycero-alpha-D-manno-heptopyranose-(1-7)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose.



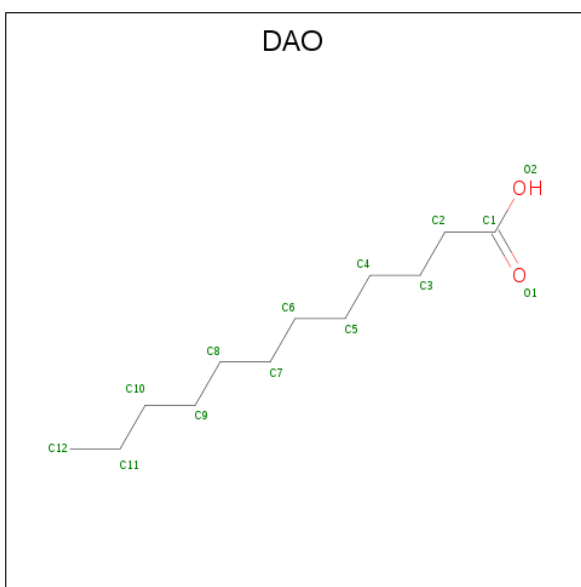
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	7	Total	C	N	O	0	0	0
			92	49	2	41			

- Molecule 6 is 3-HYDROXY-TETRADECANOIC ACID (three-letter code: FTT) (formula: C₁₄H₂₈O₃).



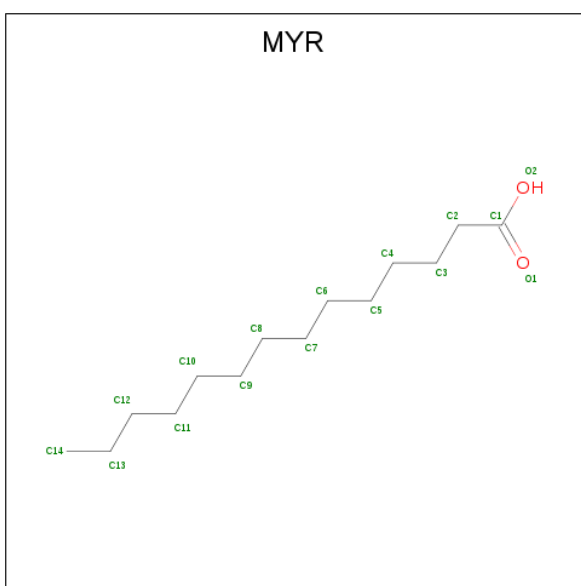
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	14	2		
6	A	1	Total	C	O	0	0
			16	14	2		
6	A	1	Total	C	O	0	0
			16	14	2		
6	A	1	Total	C	O	0	0
			16	14	2		
6	B	1	Total	C	O	0	0
			16	14	2		
6	B	1	Total	C	O	0	0
			16	14	2		
6	B	1	Total	C	O	0	0
			16	14	2		

- Molecule 7 is LAURIC ACID (three-letter code: DAO) (formula: C₁₂H₂₄O₂).



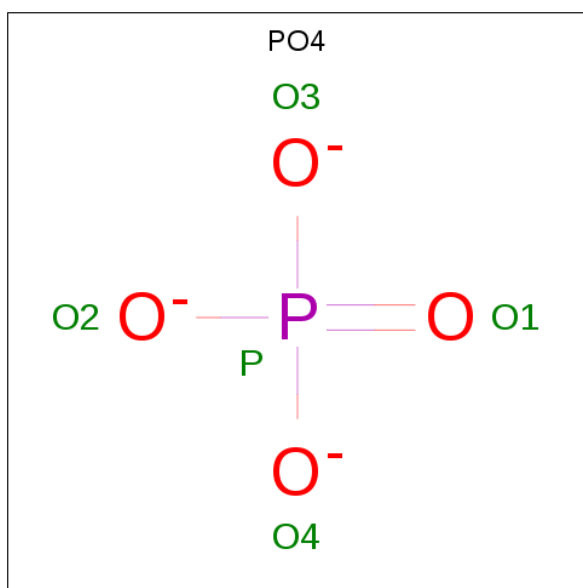
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	12	1		
7	B	1	Total	C	O	0	0
			13	12	1		

- Molecule 8 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



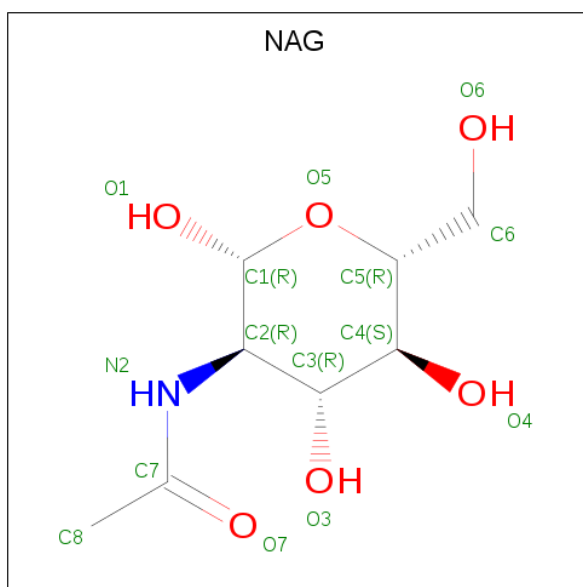
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			15	14	1		
8	B	1	Total	C	O	0	0
			15	14	1		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	P	0	0
			4	3	1		
9	A	1	Total	O	P	0	0
			4	3	1		
9	A	1	Total	O	P	0	0
			4	3	1		
9	A	1	Total	O	P	0	0
			4	3	1		
9	B	1	Total	O	P	0	0
			4	3	1		
9	B	1	Total	O	P	0	0
			4	3	1		
9	B	1	Total	O	P	0	0
			4	3	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



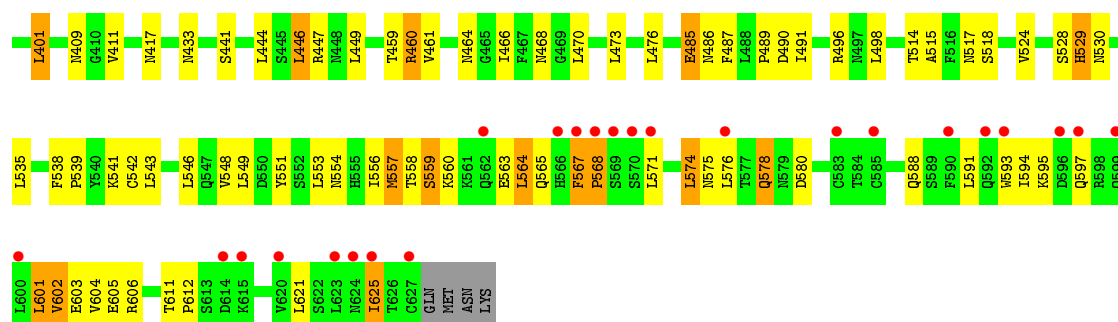
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

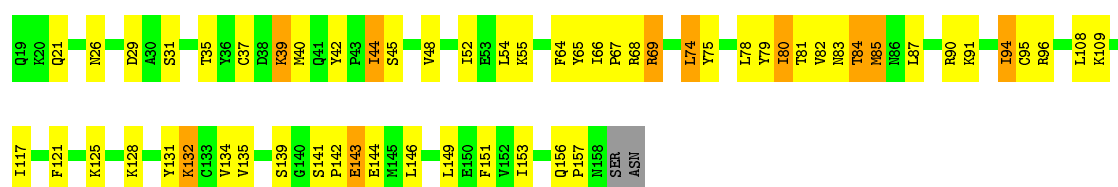
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total 1	O 1	0	0
12	B	1	Total 1	O 1	0	0



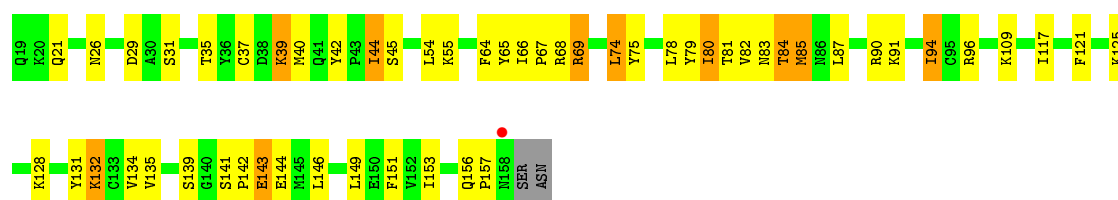
• Molecule 2: Lymphocyte antigen 96

Chain C: 58% 34% 7%



• Molecule 2: Lymphocyte antigen 96

Chain D: 61% 31% 7%



• Molecule 3: L-glycero-alpha-D-manno-heptopyranose-(1-7)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-alpha-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose

Chain E: 14% 86%



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

Chain F: 100%



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

Chain G:  100%

HA01
HA02

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

Chain I:  50% 50%

HA01
HA02

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

Chain J:  50% 50%

HA01
HA02

- Molecule 5: L-glycero-alpha-D-manno-heptopyranose-(1-7)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-L-glycero-alpha-D-manno-heptopyranose-(1-5)-[3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)]3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-6)-2-amino-2-deoxy-beta-D-glucopyranose-(1-6)-2-amino-2-deoxy-alpha-D-glucopyranose

Chain H:  14% 86%

PA11
GCS2
K003
GMH4
GMH5
GMH6
K007

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.16Å 103.50Å 251.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.87 – 3.10 47.86 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (47.87-3.10) 93.9 (47.86-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.281 0.236 , 0.277	Depositor DCC
R_{free} test set	2204 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12500	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: PA1, MG, KDO, NAG, PO4, MYR, DAO, GCS, GMH, FTT

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	0.43	0/4903	0.70	4/6639 (0.1%)
1	B	0.45	0/4903	0.70	5/6639 (0.1%)
2	C	0.45	0/1159	0.75	1/1562 (0.1%)
2	D	0.47	0/1159	0.75	1/1562 (0.1%)
All	All	0.45	0/12124	0.71	11/16402 (0.1%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	CB-CA-C	-6.93	96.54	110.40
1	A	67	ARG	CB-CA-C	-6.91	96.57	110.40
1	B	68	HIS	N-CA-CB	6.24	121.84	110.60
1	A	68	HIS	N-CA-CB	6.12	121.61	110.60
1	B	66	LEU	CB-CA-C	5.80	121.21	110.20

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	4803	0	4743	130	0
1	B	4803	0	4743	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1133	0	1129	48	0
2	D	1133	0	1129	45	0
3	E	92	0	68	0	0
4	F	28	0	25	0	0
4	G	28	0	25	2	0
4	I	28	0	25	1	0
4	J	28	0	25	1	0
5	H	92	0	68	0	0
6	A	64	0	106	5	0
6	B	64	0	106	4	0
7	A	13	0	23	1	0
7	B	13	0	23	1	0
8	A	15	0	27	0	0
8	B	15	0	27	0	0
9	A	16	0	0	0	0
9	B	16	0	0	0	0
10	A	42	0	39	1	0
10	B	42	0	39	0	0
10	C	14	0	13	1	0
10	D	14	0	13	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
All	All	12500	0	12396	351	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 14.

The worst 5 of 351 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:473:LEU:HD21	1:B:476:LEU:HD23	1.52	0.90
1:A:473:LEU:HD21	1:A:476:LEU:HD23	1.52	0.90
2:D:80:ILE:H	2:D:80:ILE:HD12	1.42	0.85
1:B:48:ILE:H	1:B:48:ILE:HD12	1.42	0.85
1:A:375:LEU:HD21	1:A:378:LEU:HG	1.58	0.84

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/605 (99%)	482 (80%)	98 (16%)	19 (3%)	4	22
1	B	599/605 (99%)	484 (81%)	96 (16%)	19 (3%)	4	22
2	C	138/142 (97%)	126 (91%)	10 (7%)	2 (1%)	11	40
2	D	138/142 (97%)	125 (91%)	11 (8%)	2 (1%)	11	40
All	All	1474/1494 (99%)	1217 (83%)	215 (15%)	42 (3%)	5	25

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	ALA
1	A	529	HIS
1	B	515	ALA
1	B	529	HIS
2	C	143	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/563 (99%)	525 (94%)	34 (6%)	18	49
1	B	559/563 (99%)	522 (93%)	37 (7%)	16	47
2	C	130/132 (98%)	116 (89%)	14 (11%)	6	25
2	D	130/132 (98%)	116 (89%)	14 (11%)	6	25
All	All	1378/1390 (99%)	1279 (93%)	99 (7%)	14	44

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	271	LYS
1	B	387	PHE
2	D	69	ARG
1	B	293	LEU
1	B	310	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	592	GLN
1	B	200	GLN
1	B	597	GLN
1	B	51	ASN
1	B	129	GLN

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 ⓘ

22 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$
3	PA1	E	1	3	12,12,12	1.09	1 (8%)	16,17,17	2.30	6 (37%)
3	PA1	E	2	3	11,11,12	0.75	0	12,15,17	2.48	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	KDO	E	3	3	12,15,16	1.40	2 (16%)	16,21,24	1.36	2 (12%)
3	GMH	E	4	9,3	13,13,14	0.75	0	17,18,20	1.74	2 (11%)
3	GMH	E	5	9,3	13,13,14	1.08	1 (7%)	17,18,20	2.04	3 (17%)
3	GMH	E	6	3	13,13,14	0.89	1 (7%)	17,18,20	2.05	2 (11%)
3	KDO	E	7	3	12,15,16	0.78	0	16,21,24	0.99	0
4	NAG	F	1	1,4	14,14,15	0.81	0	17,19,21	0.81	1 (5%)
4	NAG	F	2	4	14,14,15	1.14	1 (7%)	17,19,21	0.80	0
4	NAG	G	1	1,4	14,14,15	0.93	0	17,19,21	0.80	1 (5%)
4	NAG	G	2	4	14,14,15	0.89	1 (7%)	17,19,21	0.84	0
5	PA1	H	1	5	12,12,12	0.92	1 (8%)	16,17,17	2.26	6 (37%)
5	GCS	H	2	5	11,11,12	0.77	0	12,15,17	2.43	3 (25%)
5	KDO	H	3	5	12,15,16	1.40	2 (16%)	16,21,24	1.36	2 (12%)
5	GMH	H	4	9,5	13,13,14	0.80	0	17,18,20	1.78	1 (5%)
5	GMH	H	5	9,5	13,13,14	1.02	0	17,18,20	2.07	3 (17%)
5	GMH	H	6	5	13,13,14	0.81	1 (7%)	17,18,20	2.07	3 (17%)
5	KDO	H	7	5	12,15,16	0.84	0	16,21,24	0.94	0
4	NAG	I	1	1,4	14,14,15	0.60	0	17,19,21	0.85	1 (5%)
4	NAG	I	2	4	14,14,15	0.71	0	17,19,21	0.98	1 (5%)
4	NAG	J	1	1,4	14,14,15	0.72	0	17,19,21	0.98	1 (5%)
4	NAG	J	2	4	14,14,15	0.79	0	17,19,21	0.77	1 (5%)

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
3	PA1	E	1	3	-	0/2/22/22	0/1/1/1
3	PA1	E	2	3	1/1/4/5	0/2/19/22	0/1/1/1
3	KDO	E	3	3	-	1/6/26/30	0/1/1/1
3	GMH	E	4	9,3	-	0/6/23/26	0/1/1/1
3	GMH	E	5	9,3	-	0/6/23/26	0/1/1/1
3	GMH	E	6	3	-	0/6/23/26	0/1/1/1
3	KDO	E	7	3	-	0/6/26/30	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	5/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PA1	H	1	5	-	0/2/22/22	0/1/1/1
5	GCS	H	2	5	-	0/2/19/22	0/1/1/1
5	KDO	H	3	5	-	1/6/26/30	0/1/1/1
5	GMH	H	4	9,5	-	0/6/23/26	0/1/1/1
5	GMH	H	5	9,5	-	0/6/23/26	0/1/1/1
5	GMH	H	6	5	-	0/6/23/26	0/1/1/1
5	KDO	H	7	5	-	0/6/26/30	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2	NAG	C1-C2	3.44	1.57	1.52
3	E	3	KDO	C4-C5	3.05	1.57	1.52
5	H	3	KDO	C4-C5	2.96	1.56	1.52
5	H	1	PA1	C1-C2	2.38	1.55	1.52
3	E	1	PA1	C1-C2	2.32	1.55	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	6	GMH	C1-O5-C5	6.77	122.58	111.48
5	H	6	GMH	C1-O5-C5	6.75	122.53	111.48
5	H	5	GMH	C1-O5-C5	6.59	122.28	111.48
3	E	5	GMH	C1-O5-C5	6.51	122.14	111.48
3	E	2	PA1	C1-O5-C5	6.29	120.71	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	2	PA1	C1

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2

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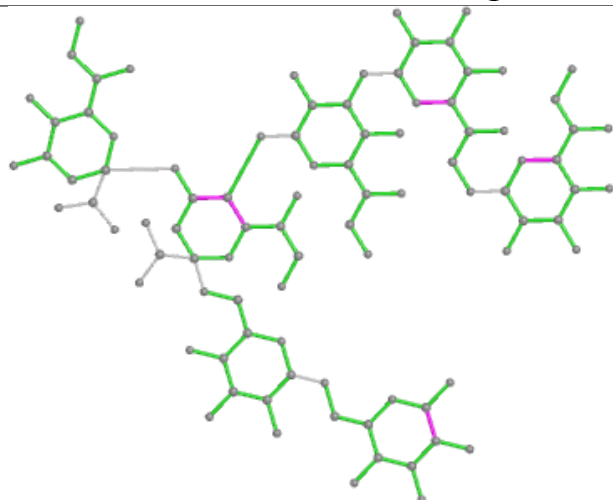
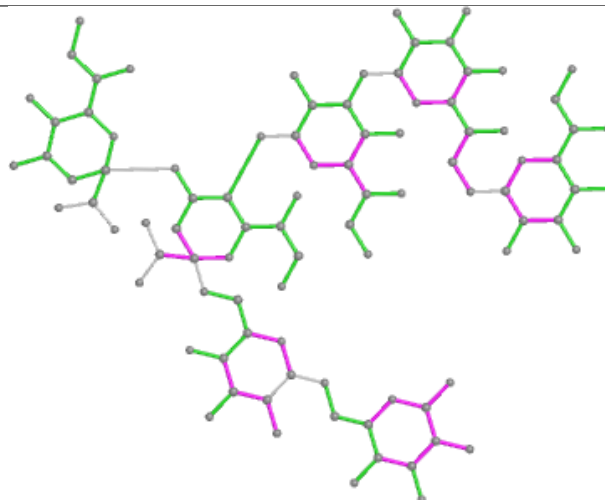
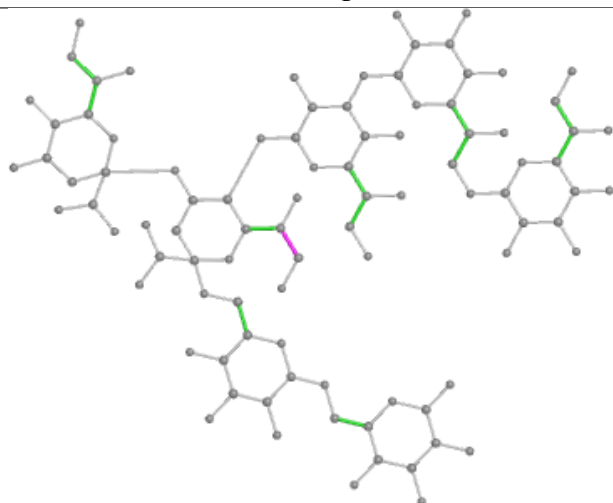
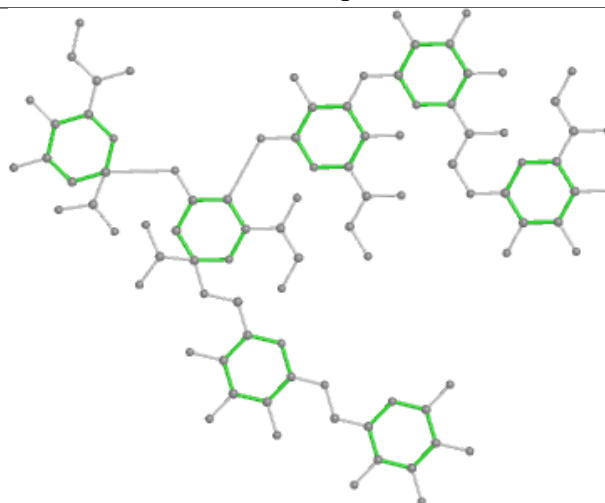
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2

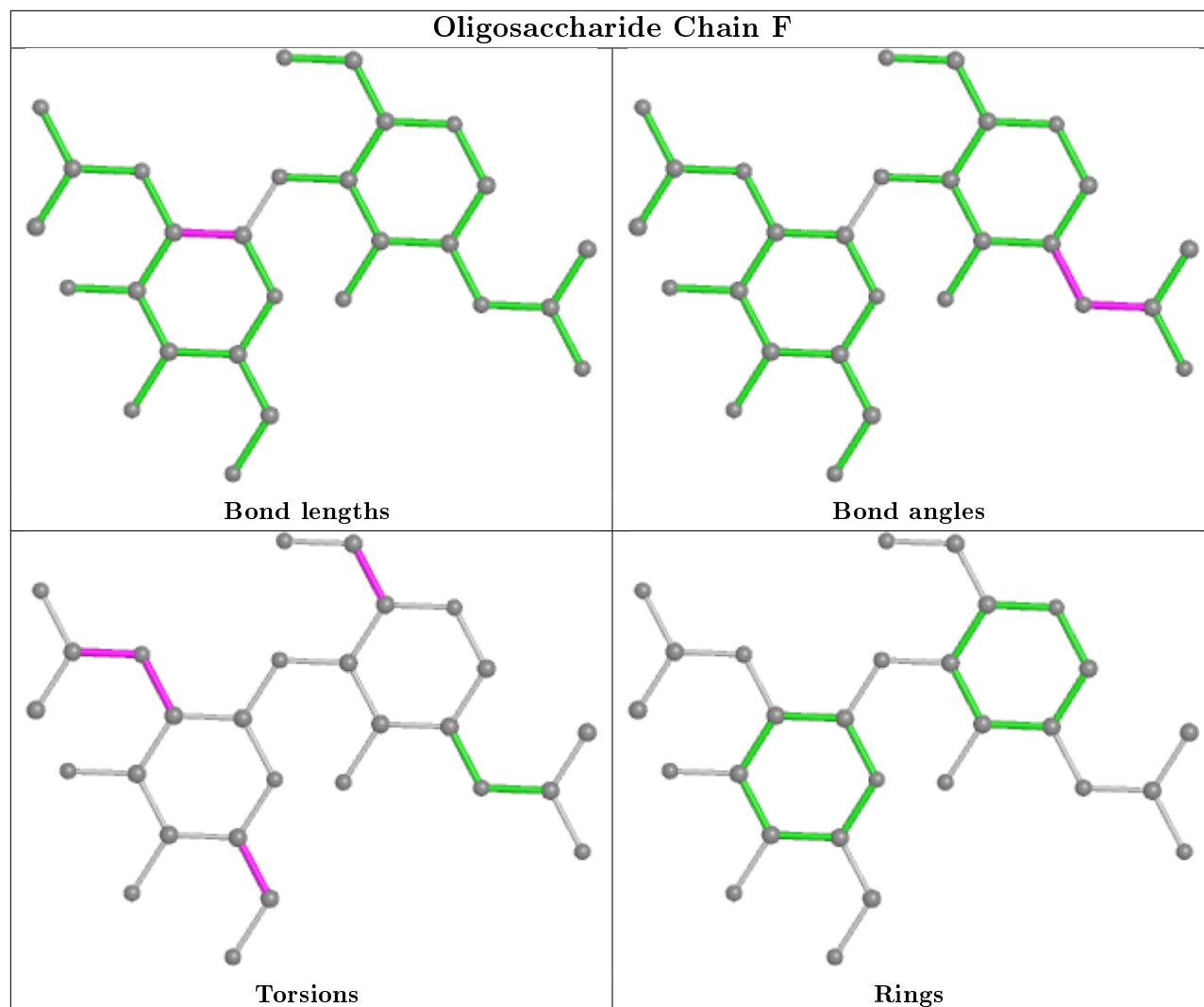
There are no ring outliers.

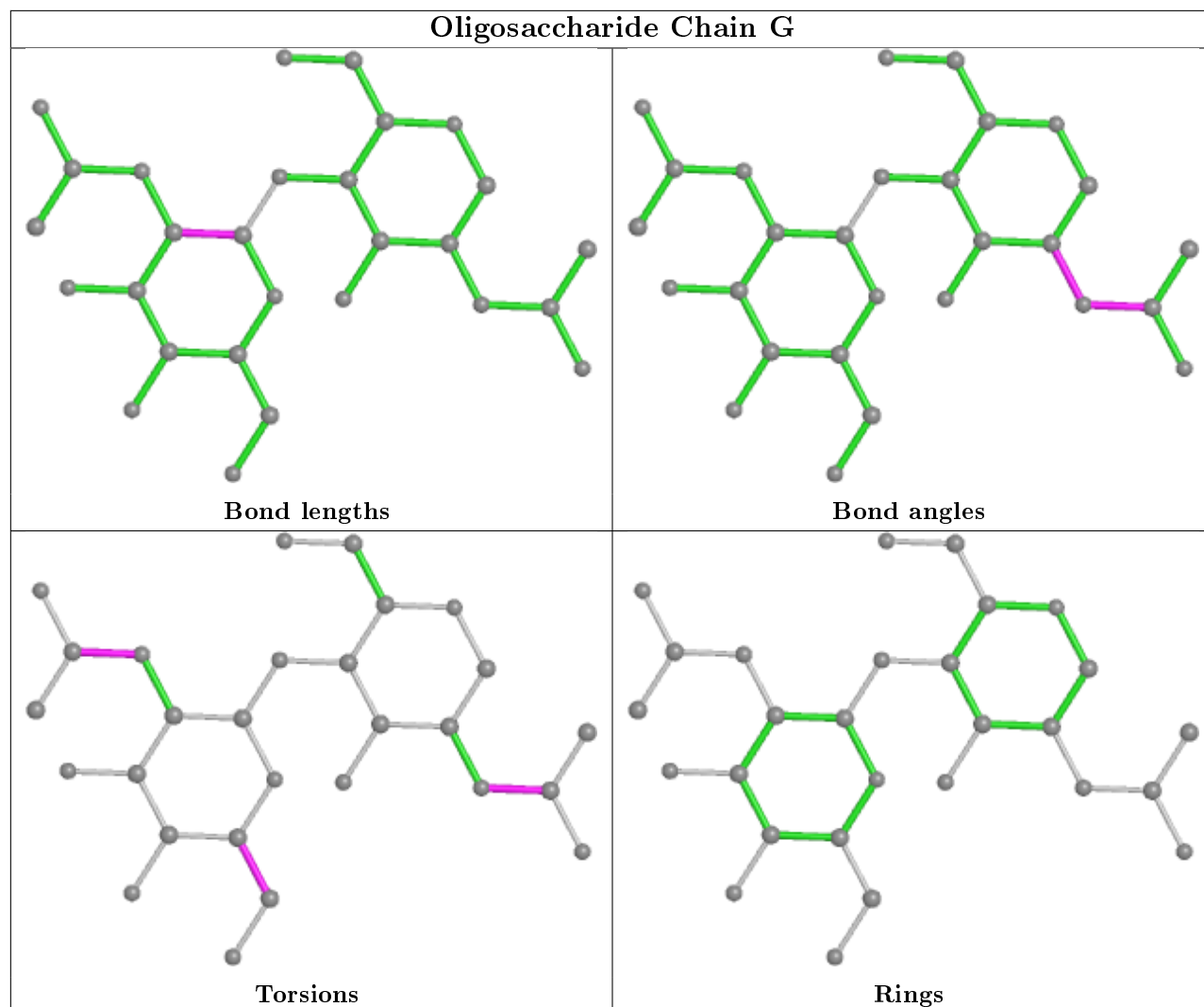
4 monomers are involved in 3 short contacts:

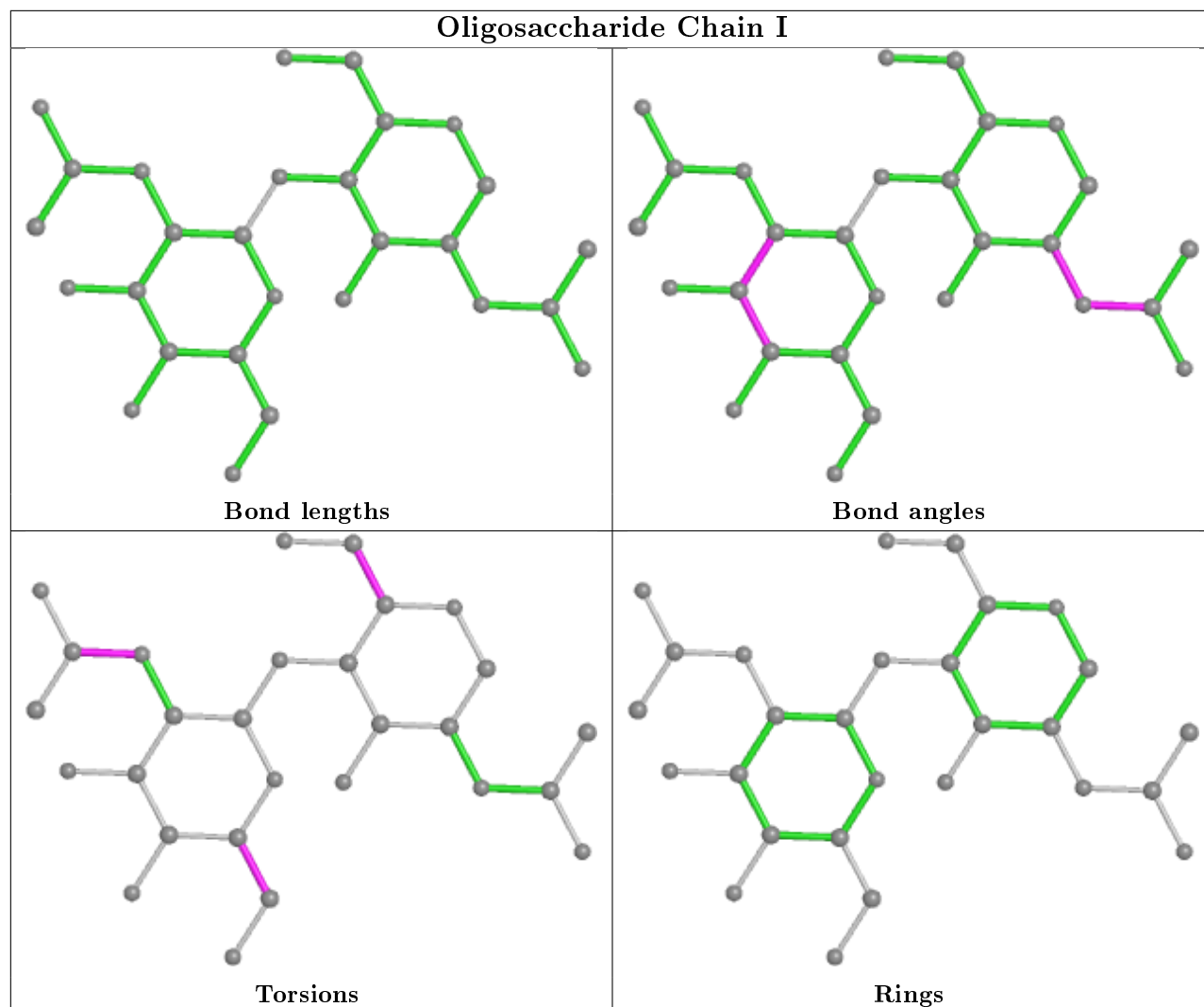
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	2	NAG	1	0
4	G	1	NAG	2	0
4	J	2	NAG	1	0
4	G	2	NAG	1	0

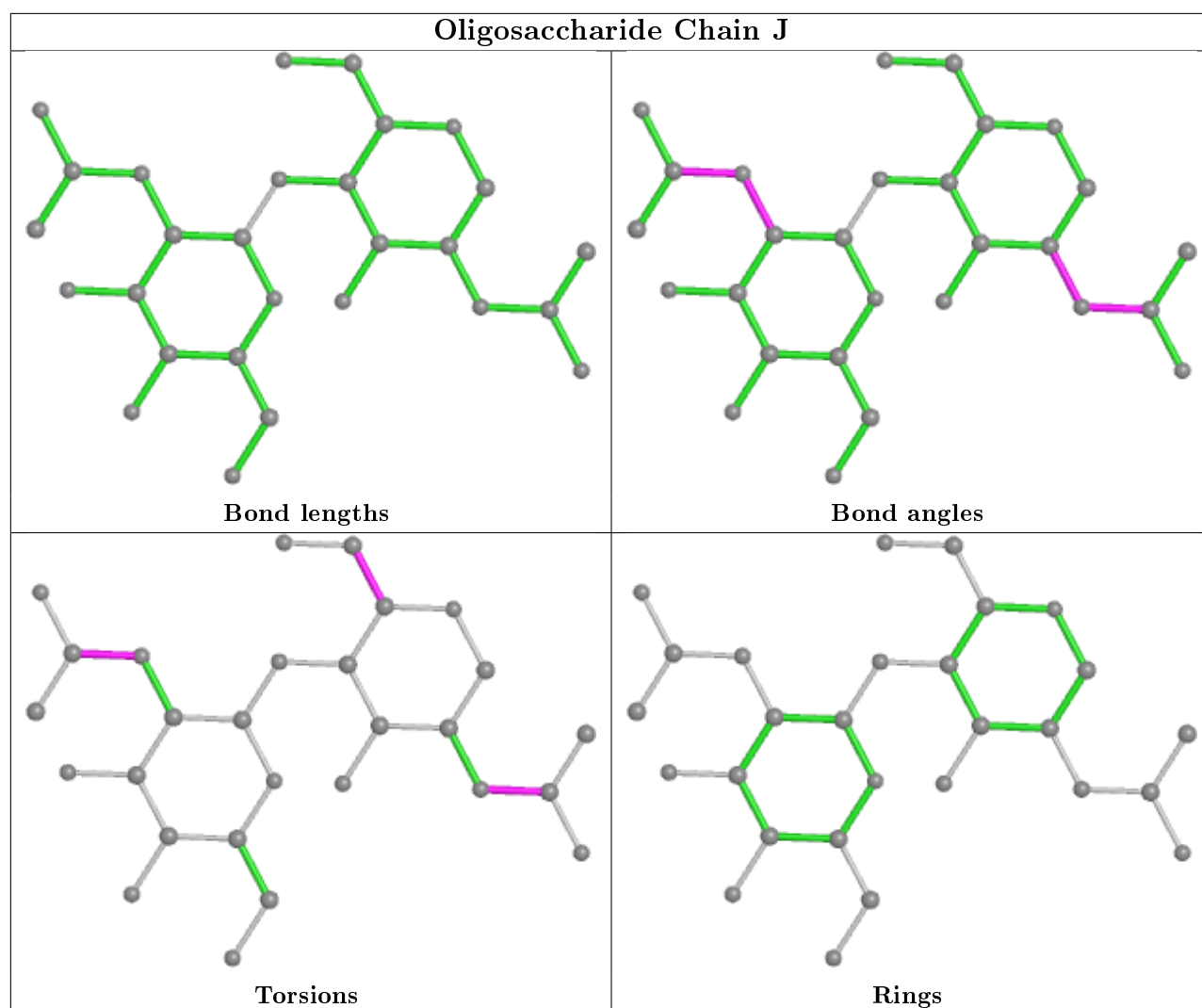
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

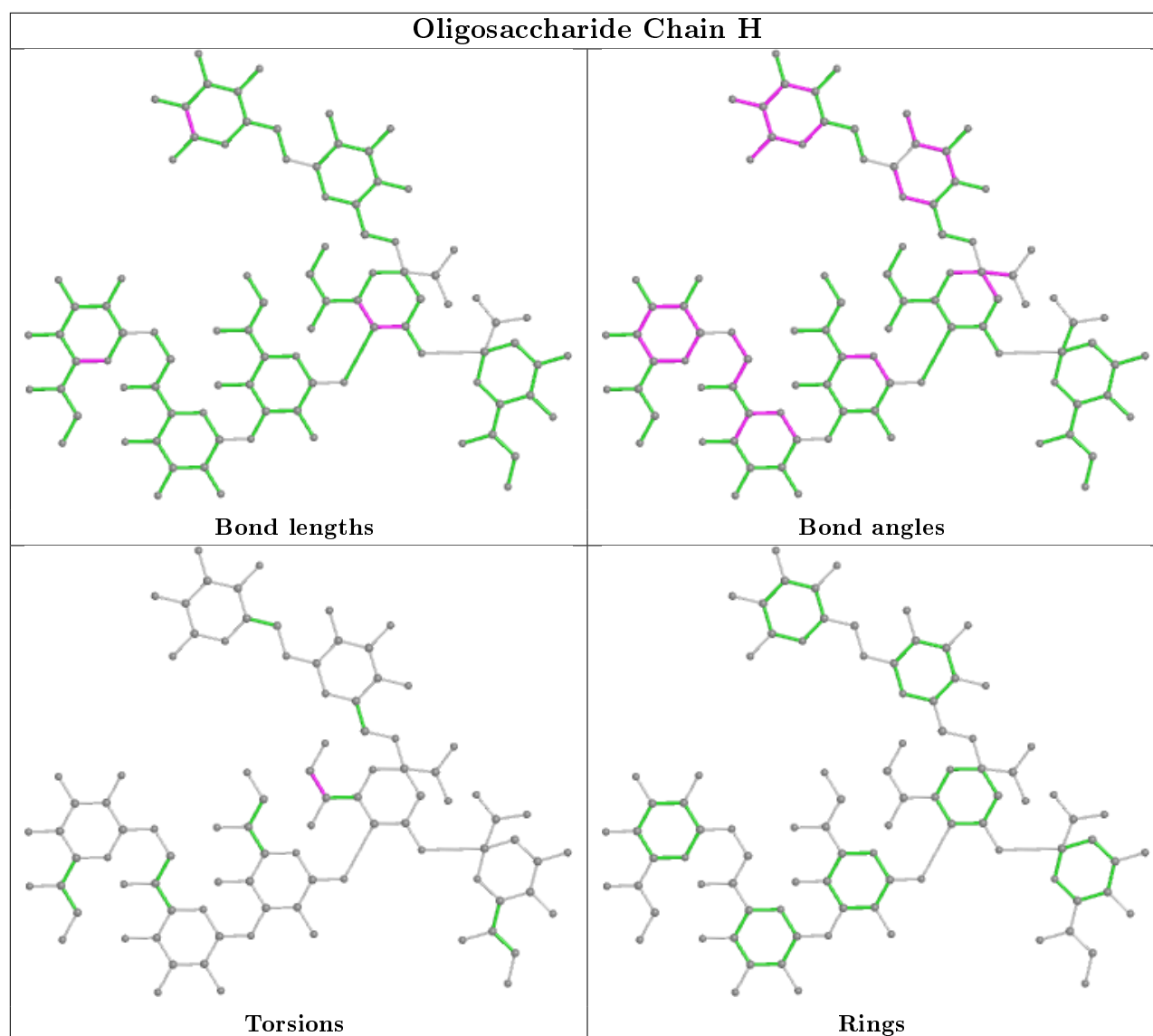
Oligosaccharide Chain E**Bond lengths****Bond angles****Torsions****Rings**











5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	DAO	B	1007	6	12,12,13	0.28	0	11,11,13	1.69	3 (27%)
9	PO4	A	1011	-	0,3,4	0.00	-	0,3,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DAO	A	1007	6	12,12,13	0.32	0	11,11,13	1.69	3 (27%)
10	NAG	B	841	1	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
6	FTT	A	1005	7	15,15,16	0.56	0	15,15,17	1.85	4 (26%)
9	PO4	A	1010	-	0,3,4	0.00	-	0,3,6	0.00	-
10	NAG	A	741	1	14,14,15	0.91	1 (7%)	17,19,21	0.64	0
9	PO4	B	1017	5	0,3,4	0.00	-	0,3,6	0.00	-
9	PO4	B	1018	5	0,3,4	0.00	-	0,3,6	0.00	-
10	NAG	B	821	1	14,14,15	0.80	0	17,19,21	0.72	0
10	NAG	D	851	2	14,14,15	0.72	0	17,19,21	0.84	0
10	NAG	A	721	1	14,14,15	0.78	0	17,19,21	0.92	1 (5%)
9	PO4	A	1018	3	0,3,4	0.00	-	0,3,6	0.00	-
6	FTT	B	1005	7	15,15,16	0.48	0	15,15,17	1.86	3 (20%)
6	FTT	B	1004	-	15,15,16	0.38	0	15,15,17	3.17	4 (26%)
9	PO4	B	1011	-	0,3,4	0.00	-	0,3,6	0.00	-
6	FTT	B	1006	8	15,15,16	0.53	0	15,15,17	1.69	2 (13%)
9	PO4	B	1010	-	0,3,4	0.00	-	0,3,6	0.00	-
10	NAG	C	751	2	14,14,15	0.79	1 (7%)	17,19,21	0.85	1 (5%)
8	MYR	A	1008	6	14,14,15	0.25	0	13,13,15	1.19	2 (15%)
10	NAG	B	811	1	14,14,15	0.85	1 (7%)	17,19,21	0.68	1 (5%)
10	NAG	A	711	1	14,14,15	0.99	1 (7%)	17,19,21	0.68	0
6	FTT	A	1004	-	15,15,16	0.43	0	15,15,17	3.16	4 (26%)
6	FTT	A	1003	-	15,15,16	0.61	0	15,15,17	1.16	1 (6%)
6	FTT	B	1003	-	15,15,16	0.75	1 (6%)	15,15,17	1.13	1 (6%)
8	MYR	B	1008	6	14,14,15	0.23	0	13,13,15	1.21	2 (15%)
9	PO4	A	1017	3	0,3,4	0.00	-	0,3,6	0.00	-
6	FTT	A	1006	8	15,15,16	0.53	0	15,15,17	1.69	2 (13%)

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
10	NAG	A	711	1	-	2/6/23/26	0/1/1/1
10	NAG	A	741	1	-	3/6/23/26	0/1/1/1
10	NAG	B	811	1	-	4/6/23/26	0/1/1/1
6	FTT	B	1004	-	-	5/14/14/15	-
7	DAO	B	1007	6	-	3/9/10/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MYR	A	1008	6	-	4/11/12/13	-
6	FTT	A	1004	-	-	5/14/14/15	-
6	FTT	A	1003	-	-	6/14/14/15	-
7	DAO	A	1007	6	-	3/9/10/11	-
10	NAG	B	821	1	-	6/6/23/26	0/1/1/1
10	NAG	D	851	2	-	2/6/23/26	0/1/1/1
8	MYR	B	1008	6	-	4/11/12/13	-
6	FTT	B	1003	-	-	6/14/14/15	-
10	NAG	C	751	2	-	4/6/23/26	0/1/1/1
10	NAG	B	841	1	-	3/6/23/26	0/1/1/1
6	FTT	B	1005	7	-	7/14/14/15	-
6	FTT	A	1006	8	-	3/14/14/15	-
6	FTT	B	1006	8	-	3/14/14/15	-
10	NAG	A	721	1	-	4/6/23/26	0/1/1/1
6	FTT	A	1005	7	-	7/14/14/15	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1003	FTT	C2-C1	2.33	1.55	1.49
10	A	741	NAG	C1-C2	2.28	1.55	1.52
10	B	811	NAG	C1-C2	2.27	1.55	1.52
10	A	711	NAG	C1-C2	2.25	1.55	1.52
10	C	751	NAG	C1-C2	2.12	1.55	1.52

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1004	FTT	C5-C4-C3	9.83	143.14	114.85
6	A	1004	FTT	C5-C4-C3	9.78	143.00	114.85
6	B	1005	FTT	C3-C2-C1	5.02	121.57	112.75
6	A	1005	FTT	C3-C2-C1	4.88	121.32	112.75
6	A	1004	FTT	C3-C2-C1	4.63	120.89	112.75

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	841	NAG	C8-C7-N2-C2
10	B	841	NAG	O7-C7-N2-C2
6	A	1005	FTT	C1-C2-C3-C4
6	A	1005	FTT	C1-C2-C3-O3
6	A	1005	FTT	O3-C3-C4-C5

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1007	DAO	1	0
7	A	1007	DAO	1	0
6	A	1005	FTT	1	0
10	A	741	NAG	1	0
6	B	1005	FTT	1	0
6	B	1004	FTT	2	0
6	B	1006	FTT	2	0
10	C	751	NAG	1	0
6	A	1004	FTT	3	0
6	A	1006	FTT	2	0

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 [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	601/605 (99%)	-0.01	12 (1%) 65 44	39, 74, 157, 178	0
1	B	601/605 (99%)	0.04	26 (4%) 35 17	40, 74, 158, 178	0
2	C	140/142 (98%)	-0.27	0 100 100	52, 70, 93, 110	0
2	D	140/142 (98%)	-0.23	1 (0%) 87 75	52, 71, 93, 110	0
All	All	1482/1494 (99%)	-0.03	39 (2%) 56 33	39, 73, 152, 178	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	614	ASP	4.7
1	A	563	GLU	4.5
1	A	562	GLN	4.4
1	A	582	ALA	4.3
1	B	569	SER	3.7

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GMH	H	5	13/14	0.72	0.32	128,130,131,131	0
3	GMH	E	5	13/14	0.77	0.24	128,130,131,131	0

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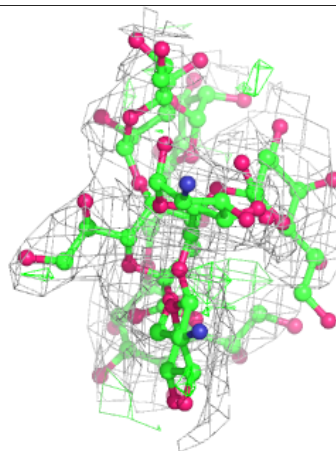
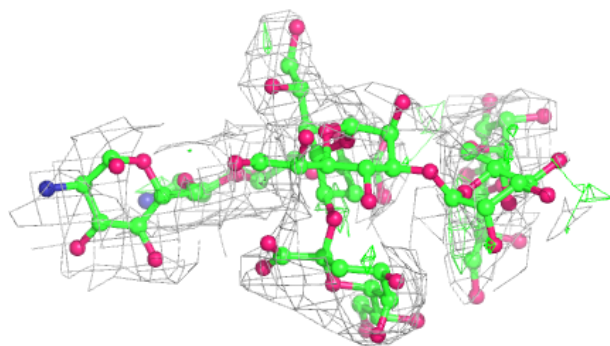
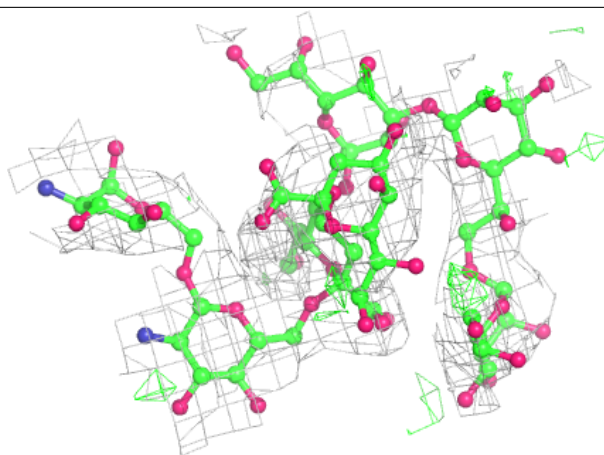
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	G	2	14/15	0.77	0.27	116,118,118,119	0
4	NAG	J	2	14/15	0.78	0.35	109,111,111,112	0
3	GMH	E	6	13/14	0.79	0.30	132,133,134,134	0
4	NAG	F	2	14/15	0.80	0.19	83,85,87,87	0
5	GMH	H	6	13/14	0.82	0.29	132,133,134,134	0
4	NAG	J	1	14/15	0.84	0.29	102,107,111,113	0
3	KDO	E	7	15/16	0.85	0.26	109,110,112,113	0
4	NAG	I	2	14/15	0.86	0.20	91,95,99,99	0
5	KDO	H	7	15/16	0.86	0.27	109,110,112,112	0
4	NAG	G	1	14/15	0.86	0.42	108,110,113,115	0
3	GMH	E	4	13/14	0.89	0.25	116,123,127,127	0
5	GMH	H	4	13/14	0.90	0.24	116,123,126,127	0
5	KDO	H	3	15/16	0.91	0.22	94,97,105,107	0
3	KDO	E	3	15/16	0.92	0.22	93,96,104,107	0
4	NAG	F	1	14/15	0.94	0.22	75,77,82,84	0
3	PA1	E	1	12/12	0.94	0.18	69,78,82,84	0
5	GCS	H	2	11/12	0.95	0.20	67,70,79,88	0
4	NAG	I	1	14/15	0.95	0.19	78,80,84,86	0
3	PA1	E	2	11/12	0.96	0.22	67,69,78,87	0
5	PA1	H	1	12/12	0.98	0.20	71,77,81,83	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

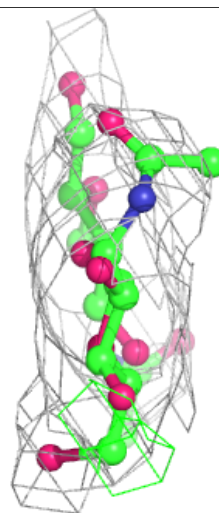
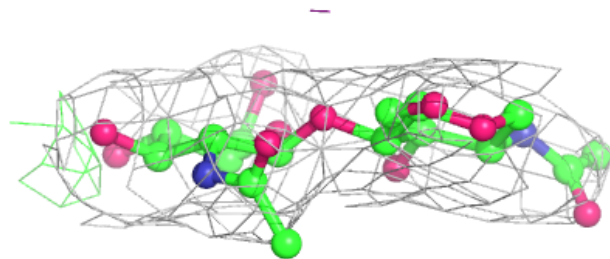
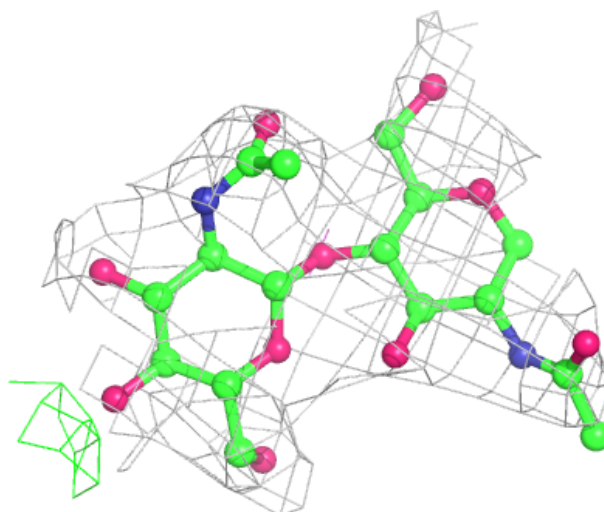
Electron density around Chain E:

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



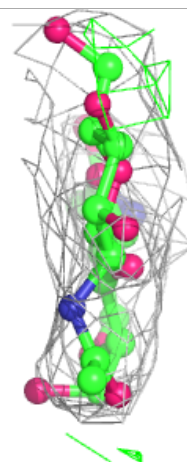
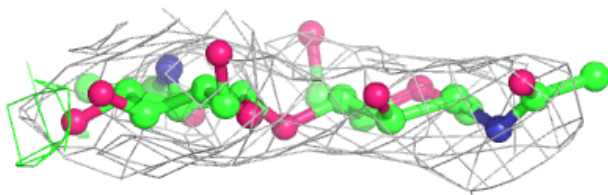
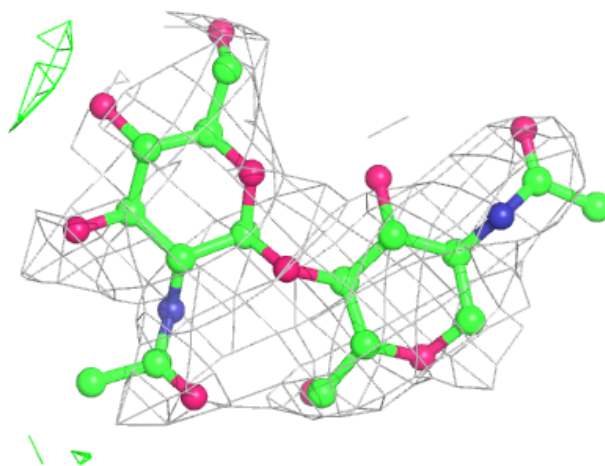
Electron density around Chain F:

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



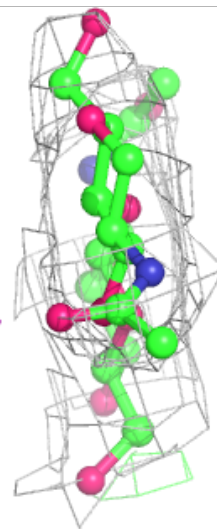
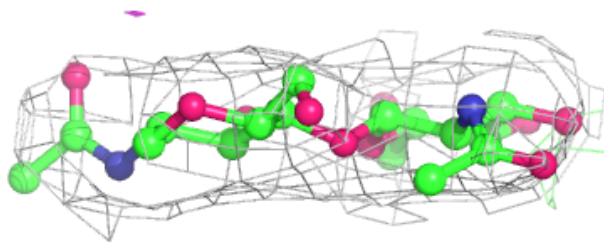
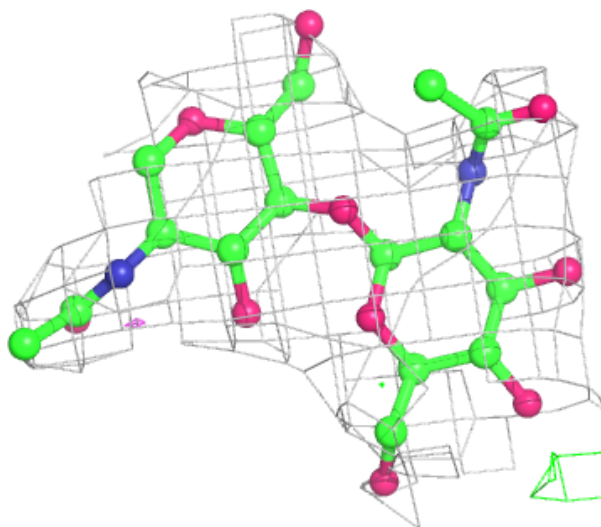
Electron density around Chain G:

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



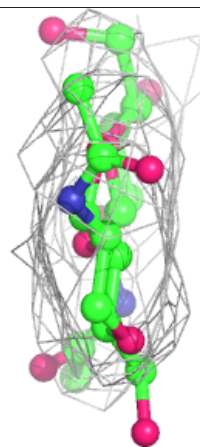
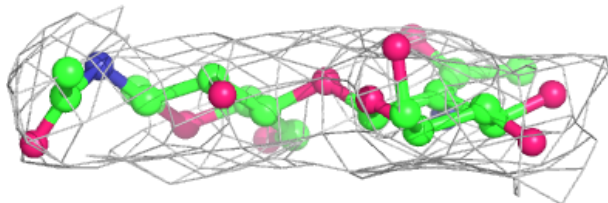
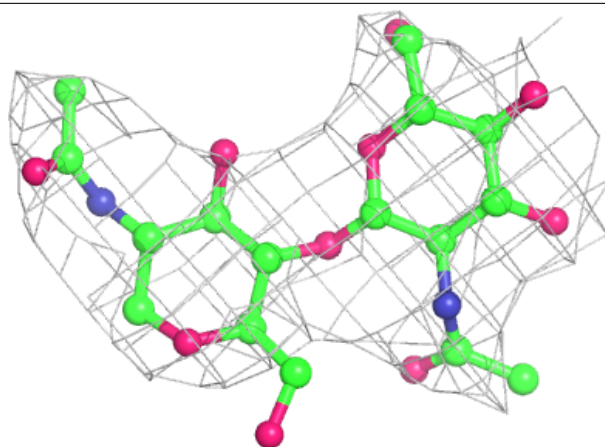
Electron density around Chain I:

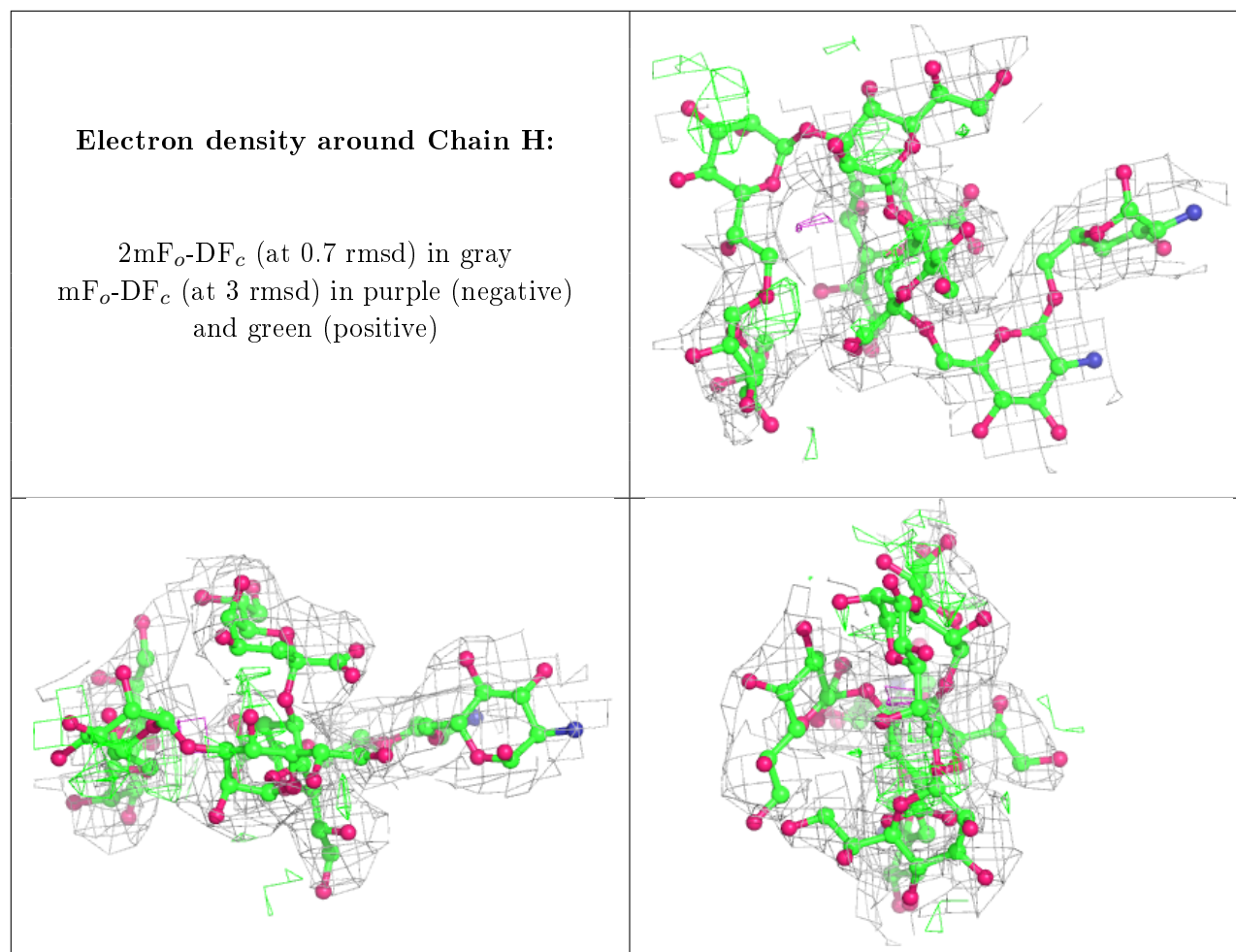
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

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





6.4 Ligands [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
11	MG	B	2001	1/1	0.35	0.59	83,83,83,83	0
10	NAG	A	711	14/15	0.73	0.18	111,113,114,115	0
10	NAG	B	811	14/15	0.74	0.22	108,109,111,111	0
6	FTT	B	1003	16/17	0.76	0.56	85,93,111,111	0
10	NAG	A	741	14/15	0.78	0.21	99,102,103,104	0
10	NAG	A	721	14/15	0.78	0.29	98,101,103,103	0
6	FTT	A	1003	16/17	0.81	0.53	86,95,110,110	0
10	NAG	C	751	14/15	0.81	0.27	91,95,96,96	0
10	NAG	B	821	14/15	0.82	0.22	92,95,98,100	0
11	MG	A	2001	1/1	0.82	0.67	72,72,72,72	0
10	NAG	D	851	14/15	0.83	0.22	84,90,93,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	DAO	B	1007	13/14	0.84	0.54	70,71,76,77	0
6	FTT	A	1004	16/17	0.86	0.55	77,78,83,84	0
9	PO4	A	1017	4/5	0.86	0.39	129,130,131,131	0
6	FTT	B	1004	16/17	0.87	0.51	75,77,84,85	0
9	PO4	A	1018	4/5	0.88	0.34	126,126,126,127	0
8	MYR	B	1008	15/16	0.89	0.41	65,73,78,78	0
6	FTT	A	1005	16/17	0.89	0.43	68,70,81,83	0
10	NAG	B	841	14/15	0.90	0.13	87,89,91,91	0
9	PO4	B	1018	4/5	0.90	0.41	125,125,126,126	0
7	DAO	A	1007	13/14	0.90	0.47	70,72,75,76	0
9	PO4	B	1017	4/5	0.93	0.33	129,129,130,130	0
6	FTT	B	1005	16/17	0.93	0.36	68,70,81,83	0
8	MYR	A	1008	15/16	0.93	0.60	66,74,79,79	0
6	FTT	A	1006	16/17	0.93	0.36	55,59,69,72	0
6	FTT	B	1006	16/17	0.94	0.30	56,61,68,72	0
9	PO4	A	1011	4/5	0.96	0.20	81,82,82,84	0
9	PO4	B	1010	4/5	0.96	0.22	69,69,69,73	0
9	PO4	B	1011	4/5	0.97	0.24	81,82,83,83	0
9	PO4	A	1010	4/5	0.99	0.24	66,66,67,68	0

6.5 Other polymers

There are no such residues in this entry.