



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 01:25 AM BST

PDB ID : 3CIG
Title : Crystal structure of mouse TLR3 ectodomain
Authors : Liu, L.; Botos, I.; Wang, Y.; Leonard, J.N.; Shiloach, J.; Segal, D.M.; Davies, D.R.
Deposited on : 2008-03-11
Resolution : 2.66 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

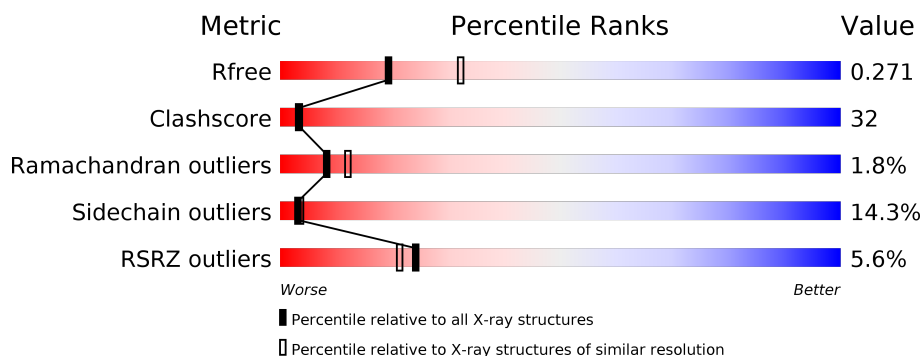
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	697	<div> <div>5%</div> <div>48%</div> <div>39%</div> <div>8%</div> <div>5%</div> </div>
2	B	2	<div>100%</div>
2	E	2	<div>100%</div>
3	C	3	<div>33%</div> <div>67%</div>
4	D	2	<div>50%</div> <div>50%</div>
4	H	2	<div>100%</div>

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Mol	Chain	Length	Quality of chain
5	F	5	 20%80%
6	G	4	 25%75%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1	-	-	X	-
2	NDG	E	2	-	-	-	X
4	NAG	H	1	X	-	-	-
5	NAG	F	1	X	-	-	-
5	BMA	F	4	-	-	-	X
6	NAG	G	1	X	-	-	-
6	FUL	G	4	-	-	-	X
7	NAG	A	6621	X	-	-	X
8	FUC	A	2916	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5736 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.

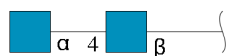
- Molecule 1 is a protein called Toll-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5330	3404	908	1004	14			

There are 20 discrepancies between the modelled and reference sequences:

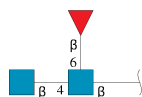
Chain	Residue	Modelled	Actual	Comment	Reference
A	704	ASN	-	expression tag	UNP Q99MB1
A	705	LEU	-	expression tag	UNP Q99MB1
A	706	TYR	-	expression tag	UNP Q99MB1
A	707	PHE	-	expression tag	UNP Q99MB1
A	708	GLN	-	expression tag	UNP Q99MB1
A	709	GLY	-	expression tag	UNP Q99MB1
A	710	HIS	-	expression tag	UNP Q99MB1
A	711	HIS	-	expression tag	UNP Q99MB1
A	712	HIS	-	expression tag	UNP Q99MB1
A	713	HIS	-	expression tag	UNP Q99MB1
A	714	HIS	-	expression tag	UNP Q99MB1
A	715	HIS	-	expression tag	UNP Q99MB1
A	716	TRP	-	expression tag	UNP Q99MB1
A	717	SER	-	expression tag	UNP Q99MB1
A	718	HIS	-	expression tag	UNP Q99MB1
A	719	PRO	-	expression tag	UNP Q99MB1
A	720	GLN	-	expression tag	UNP Q99MB1
A	721	PHE	-	expression tag	UNP Q99MB1
A	722	GLU	-	expression tag	UNP Q99MB1
A	723	LYS	-	expression tag	UNP Q99MB1

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



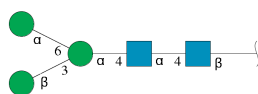
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



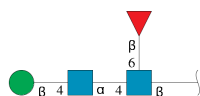
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



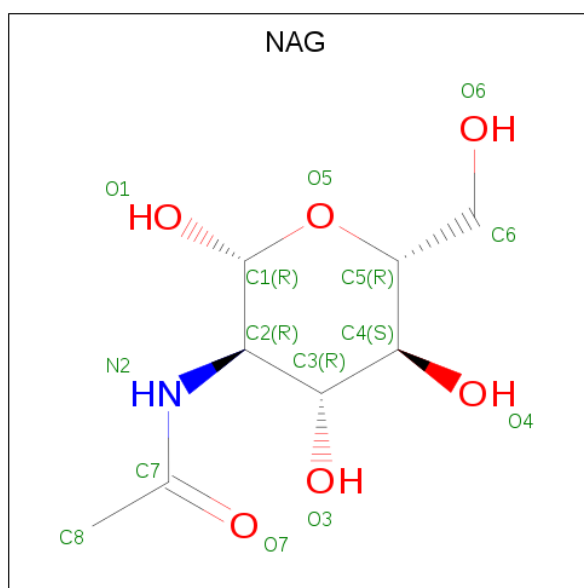
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



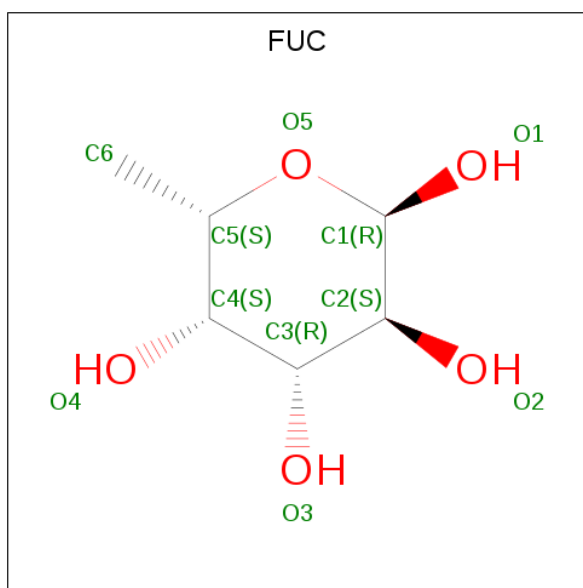
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		

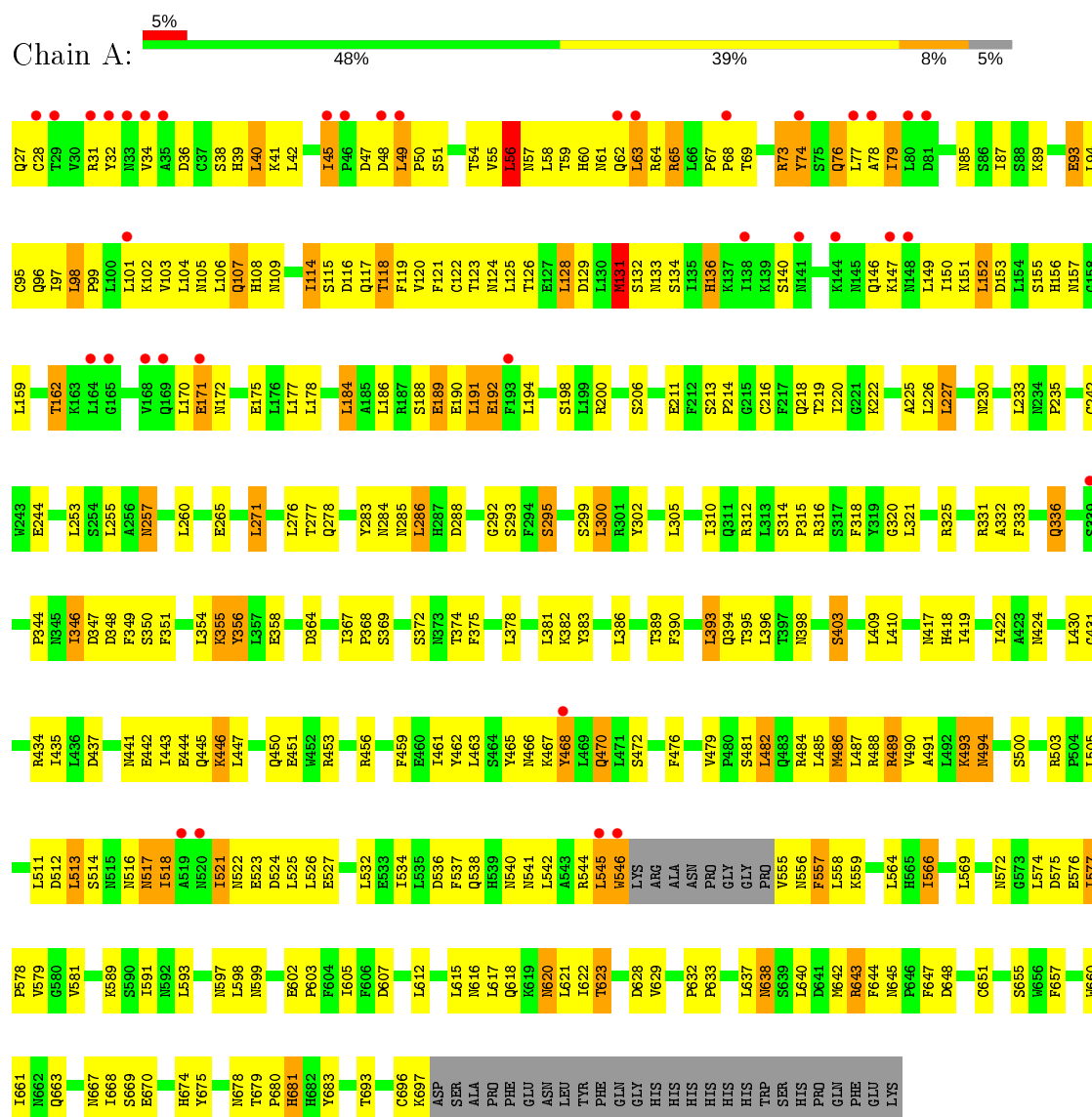
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	79	Total	O	0	0
			79	79		

3 Residue-property plots

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 3



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

Chain B: 

100%

MAG1
NDG2

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

Chain E:  100%

MAG1
NDG2

- Molecule 3: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[β -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain C:  33% 67%

MAG1
MAG2
FUL3

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

Chain D:  50% 50%

MAG1
MAG2

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

Chain H:  100%

MAG1
MAG2

- Molecule 5: β -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- α -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain F:  20% 80%

MAG1
NDG2
MAN3
ENM4
MAN5

- Molecule 6: β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- α -D-glucopyranose-(1-4)-[β -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain G:  25% 75%

MAG1
NDG2
ENM3
FUL4

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.68Å 158.02Å 185.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.66 49.48 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-2.66) 95.2 (49.48-2.66)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.272 0.246 , 0.271	Depositor DCC
R_{free} test set	1693 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	51.3	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5736	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: BMA, NAG, NDG, FUC, FUL, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	0/5440	0.83	4/7386 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	286	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	A	227	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	A	489	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	393	LEU	CB-CG-CD2	-5.22	102.13	111.00

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	5330	0	5334	347	0
2	B	28	0	24	7	0
2	E	28	0	24	0	0
3	C	38	0	34	0	0
4	D	28	0	25	1	0
4	H	28	0	25	3	0
5	F	61	0	51	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	49	0	42	5	0
7	A	56	0	52	4	0
8	A	11	0	12	1	0
9	A	79	0	0	5	1
All	All	5736	0	5623	365	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 32.

The worst 5 of 365 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:556:ASN:HB2	9:A:6725:HOH:O	1.51	1.11
1:A:393:LEU:HD21	1:A:396:LEU:HD23	1.34	1.08
1:A:107:GLN:NE2	1:A:107:GLN:H	1.52	1.06
1:A:107:GLN:N	1:A:107:GLN:HE21	1.60	0.97
1:A:77:LEU:HB2	1:A:98:LEU:HD21	1.43	0.97

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)
9:A:6718:HOH:O	9:A:6718:HOH:O[2_655]	1.90	0.30

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	659/697 (94%)	546 (83%)	101 (15%)	12 (2%)	8 12

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	517	ASN
1	A	131	MET
1	A	372	SER
1	A	398	ASN
1	A	56	LEU

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	622/651 (96%)	533 (86%)	89 (14%)	3 3

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	SER
1	A	403	SER
1	A	643	ARG
1	A	300	LEU
1	A	355	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	445	GLN
1	A	638	ASN
1	A	309	ASN
1	A	450	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 ⓘ

20 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	B	1	1,2	14,14,15	0.45	0	17,19,21	1.47	2 (11%)
2	NDG	B	2	2	14,14,15	0.54	0	17,19,21	1.69	4 (23%)
3	NAG	C	1	1,3	14,14,15	0.52	0	17,19,21	1.27	1 (5%)
3	NAG	C	2	3	14,14,15	0.55	0	17,19,21	1.72	4 (23%)
3	FUL	C	3	3	10,10,11	0.61	0	14,14,16	0.70	0
4	NAG	D	1	1,4	14,14,15	0.65	0	17,19,21	1.45	1 (5%)
4	NAG	D	2	4	14,14,15	0.53	0	17,19,21	1.00	0
2	NAG	E	1	1,2	14,14,15	0.49	0	17,19,21	1.18	1 (5%)
2	NDG	E	2	2	14,14,15	0.50	0	17,19,21	1.28	4 (23%)
5	NAG	F	1	1,5	14,14,15	0.70	0	17,19,21	1.48	3 (17%)
5	NDG	F	2	5	14,14,15	0.55	0	17,19,21	1.03	1 (5%)
5	MAN	F	3	5	11,11,12	0.58	0	15,15,17	1.95	5 (33%)
5	BMA	F	4	5	11,11,12	0.58	0	15,15,17	1.03	1 (6%)
5	MAN	F	5	5	11,11,12	0.56	0	15,15,17	1.22	1 (6%)
6	NAG	G	1	1,6	14,14,15	0.48	0	17,19,21	1.18	1 (5%)
6	NDG	G	2	6	14,14,15	0.54	0	17,19,21	0.81	1 (5%)
6	BMA	G	3	6	11,11,12	0.63	0	15,15,17	1.23	2 (13%)
6	FUL	G	4	6	10,10,11	0.65	0	14,14,16	1.25	2 (14%)
4	NAG	H	1	1,4	14,14,15	0.53	0	17,19,21	1.74	4 (23%)
4	NAG	H	2	4	14,14,15	0.46	0	17,19,21	1.55	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
2	NAG	B	1	1,2	-	4/6/23/26	0/1/1/1
2	NDG	B	2	2	-	4/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
3	FUL	C	3	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	4/6/23/26	0/1/1/1
2	NDG	E	2	2	-	5/6/23/26	0/1/1/1
5	NAG	F	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NDG	F	2	5	-	4/6/23/26	0/1/1/1
5	MAN	F	3	5	-	2/2/19/22	0/1/1/1
5	BMA	F	4	5	-	1/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
6	NAG	G	1	1,6	1/1/5/7	2/6/23/26	0/1/1/1
6	NDG	G	2	6	-	4/6/23/26	0/1/1/1
6	BMA	G	3	6	-	2/2/19/22	0/1/1/1
6	FUL	G	4	6	-	-	0/1/1/1
4	NAG	H	1	1,4	1/1/5/7	5/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3	MAN	C1-O5-C5	4.68	118.54	112.19
3	C	1	NAG	C1-O5-C5	4.63	118.46	112.19
4	D	1	NAG	C3-C4-C5	-4.49	102.23	110.24
2	B	2	NDG	C2-N2-C7	4.23	128.92	122.90
4	H	1	NAG	C1-O5-C5	4.20	117.88	112.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	G	1	NAG	C1
4	H	1	NAG	C1
5	F	1	NAG	C1

5 of 53 torsion outliers are listed below:

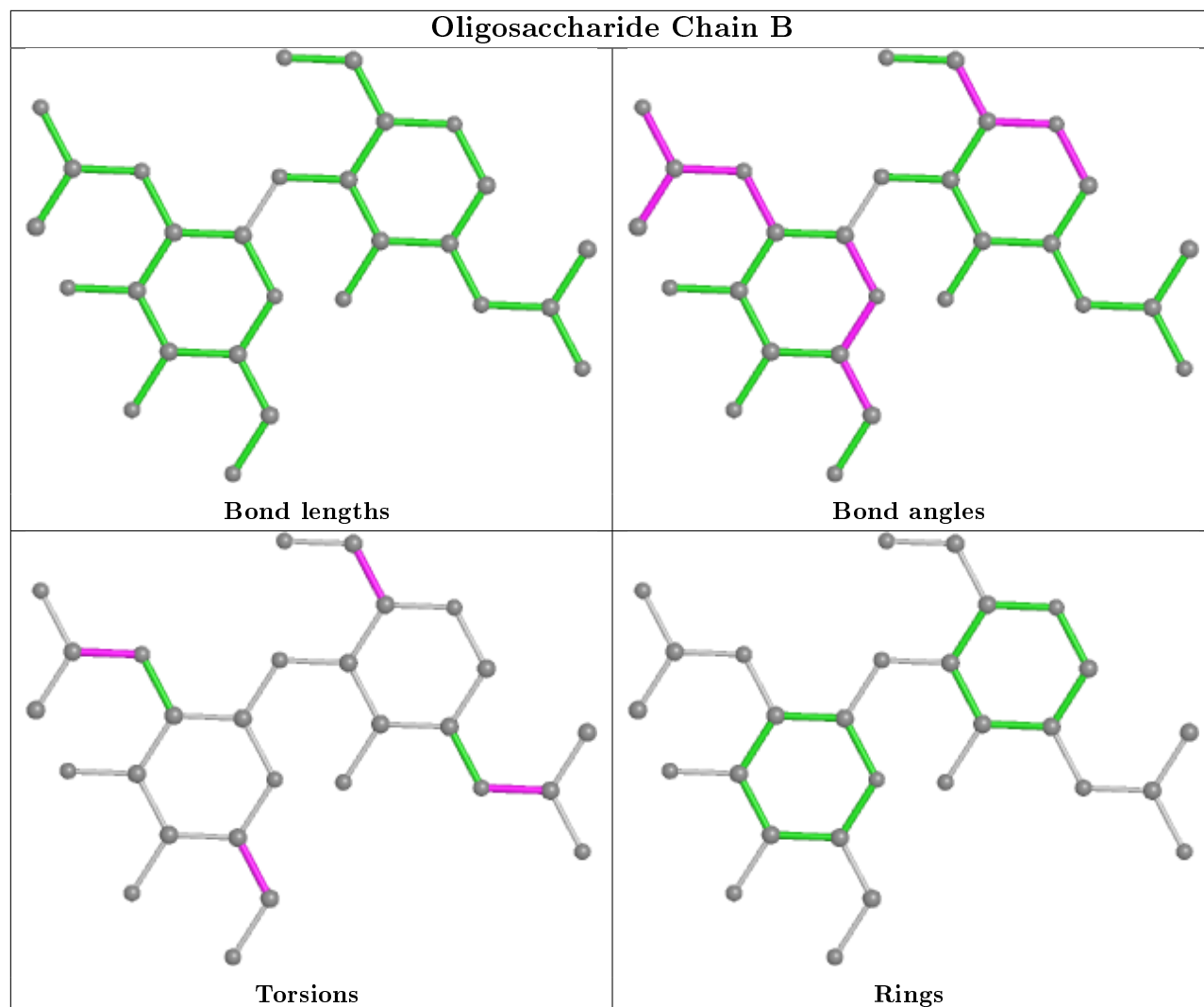
Mol	Chain	Res	Type	Atoms
6	G	2	NDG	C8-C7-N2-C2
6	G	2	NDG	O7-C7-N2-C2
2	E	2	NDG	C8-C7-N2-C2
2	E	2	NDG	O7-C7-N2-C2
2	B	2	NDG	C8-C7-N2-C2

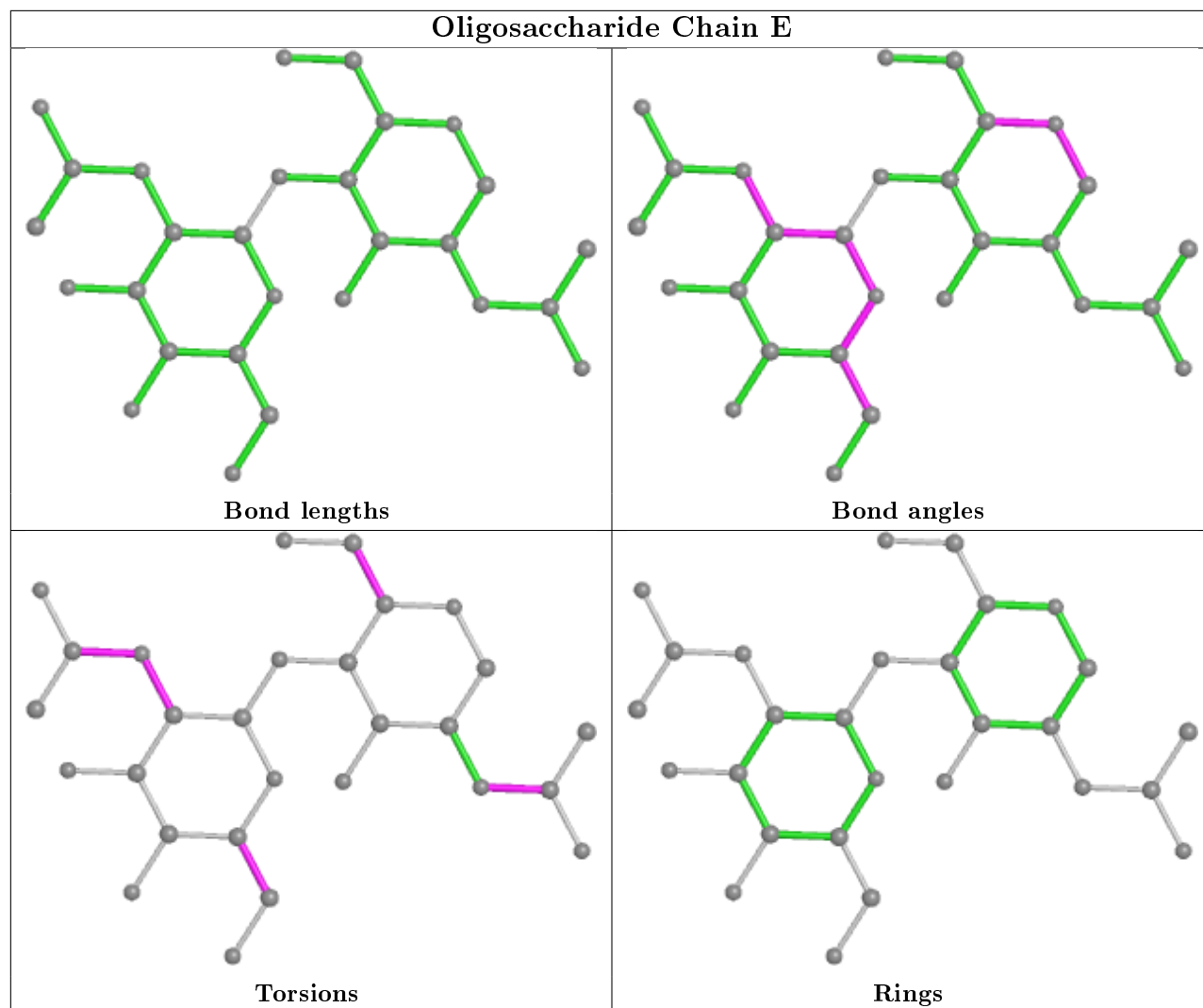
There are no ring outliers.

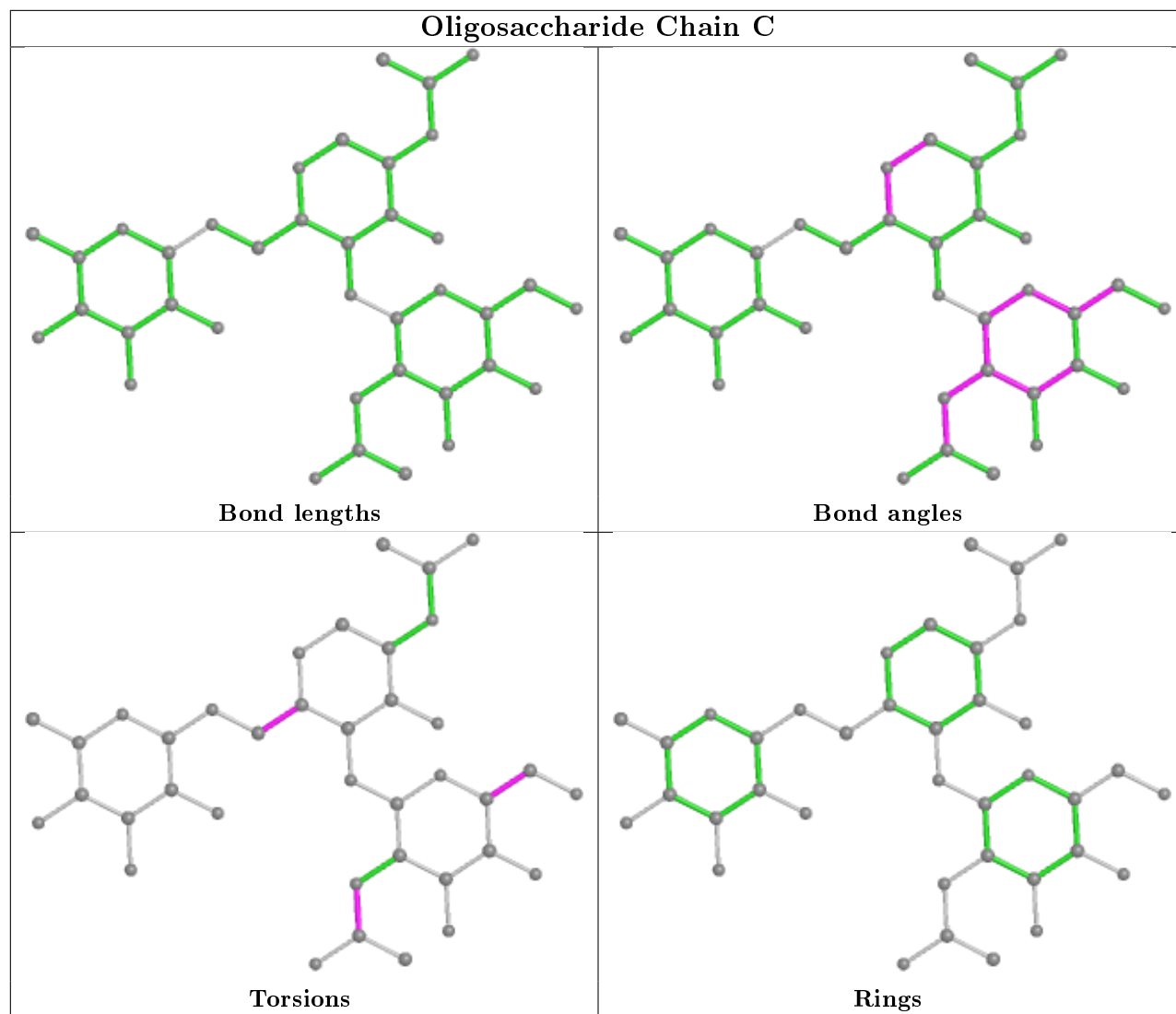
12 monomers are involved in 21 short contacts:

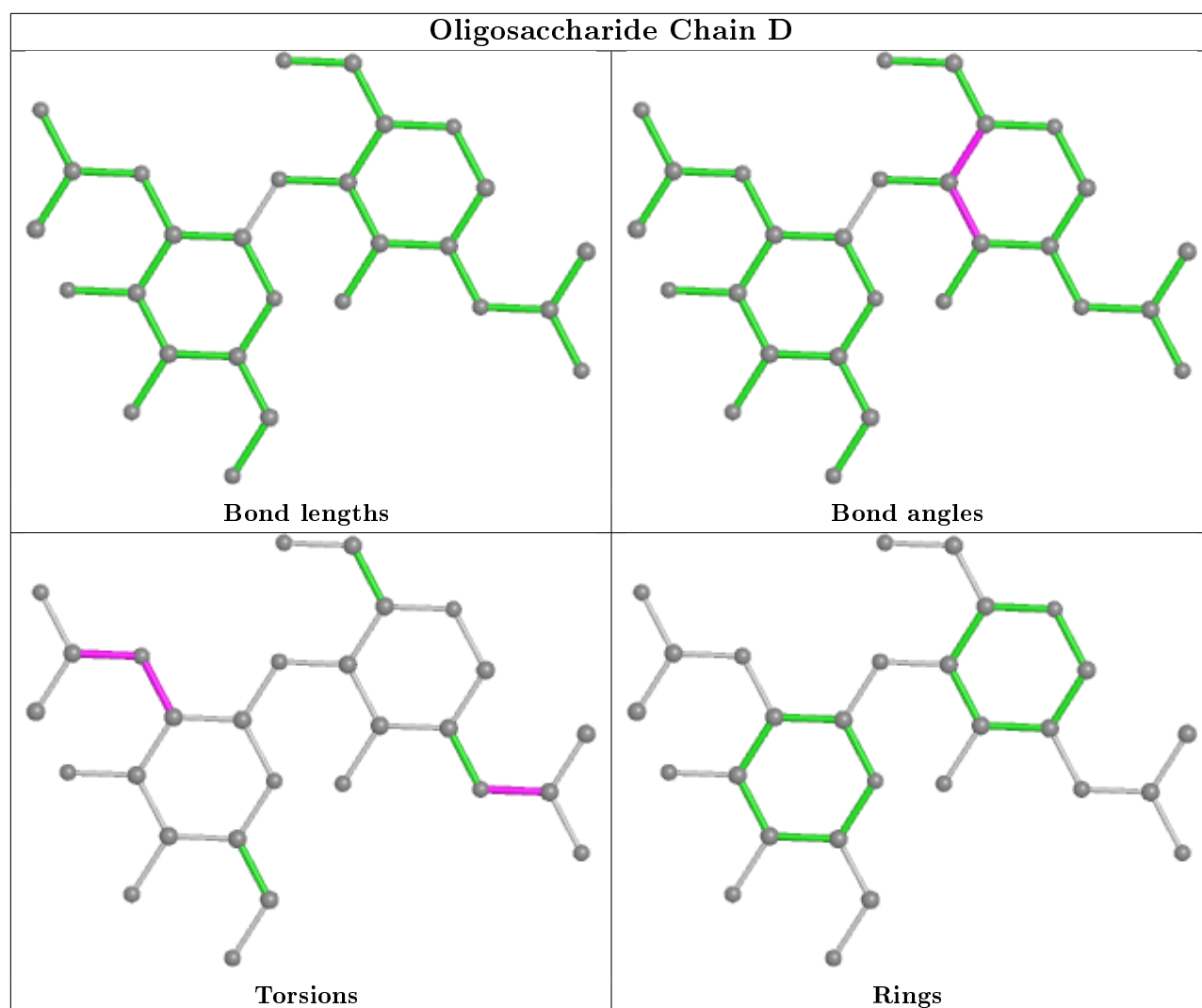
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	3	MAN	5	0
6	G	2	NDG	2	0
2	B	2	NDG	3	0
4	H	1	NAG	3	0
4	H	2	NAG	2	0
6	G	3	BMA	2	0
5	F	2	NDG	3	0
5	F	4	BMA	1	0
2	B	1	NAG	7	0
5	F	5	MAN	1	0
4	D	1	NAG	1	0
6	G	1	NAG	3	0

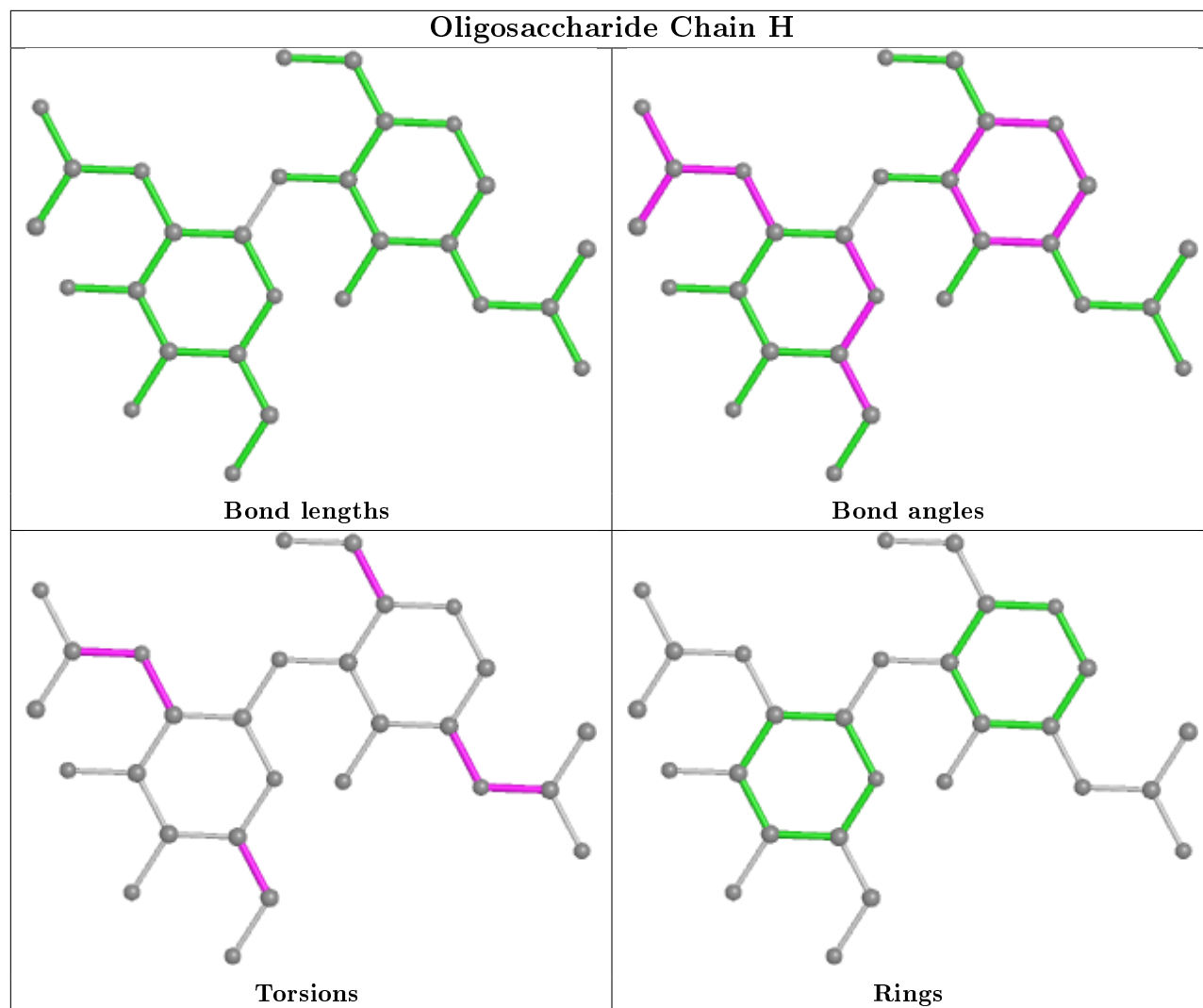
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

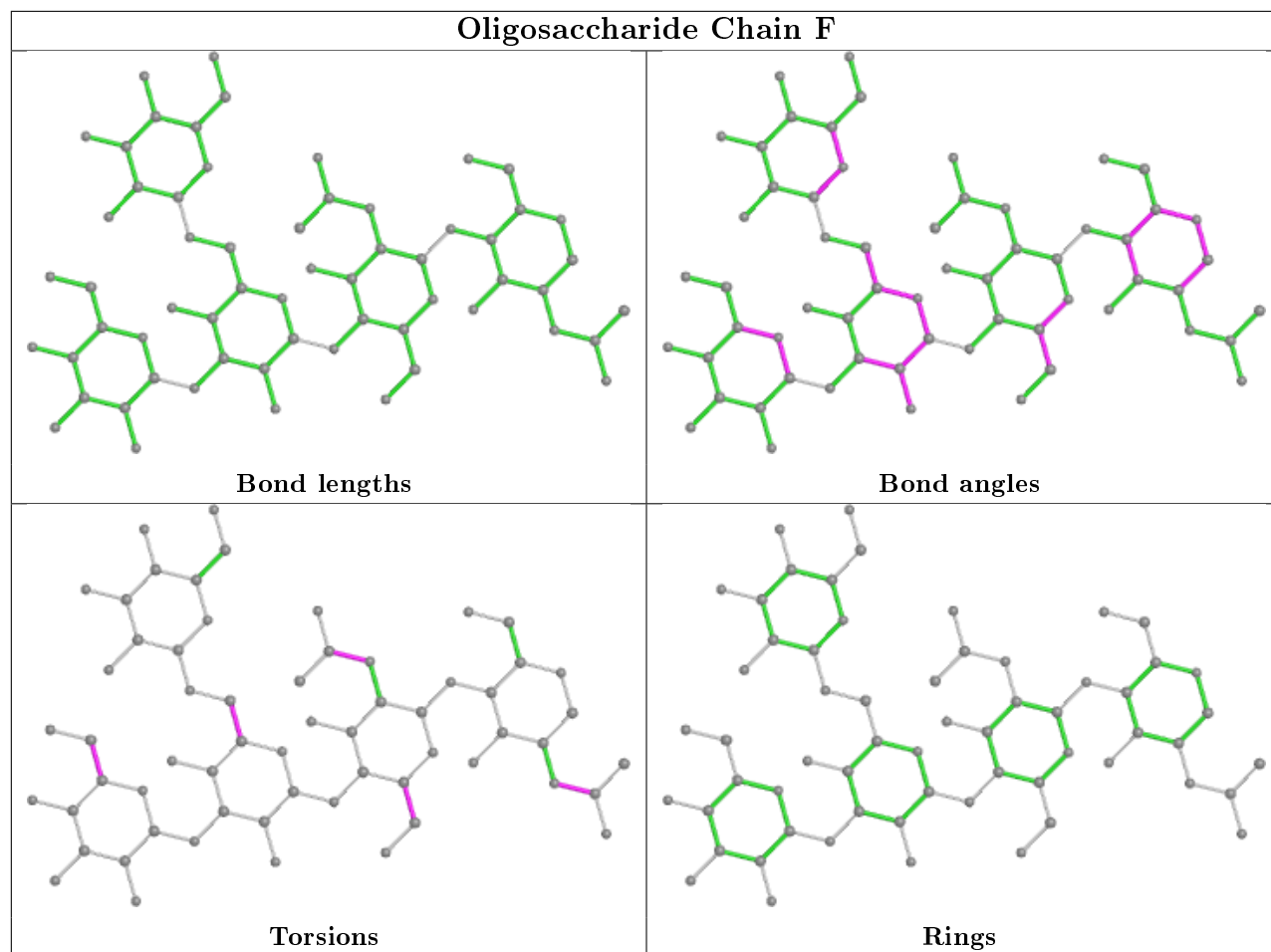


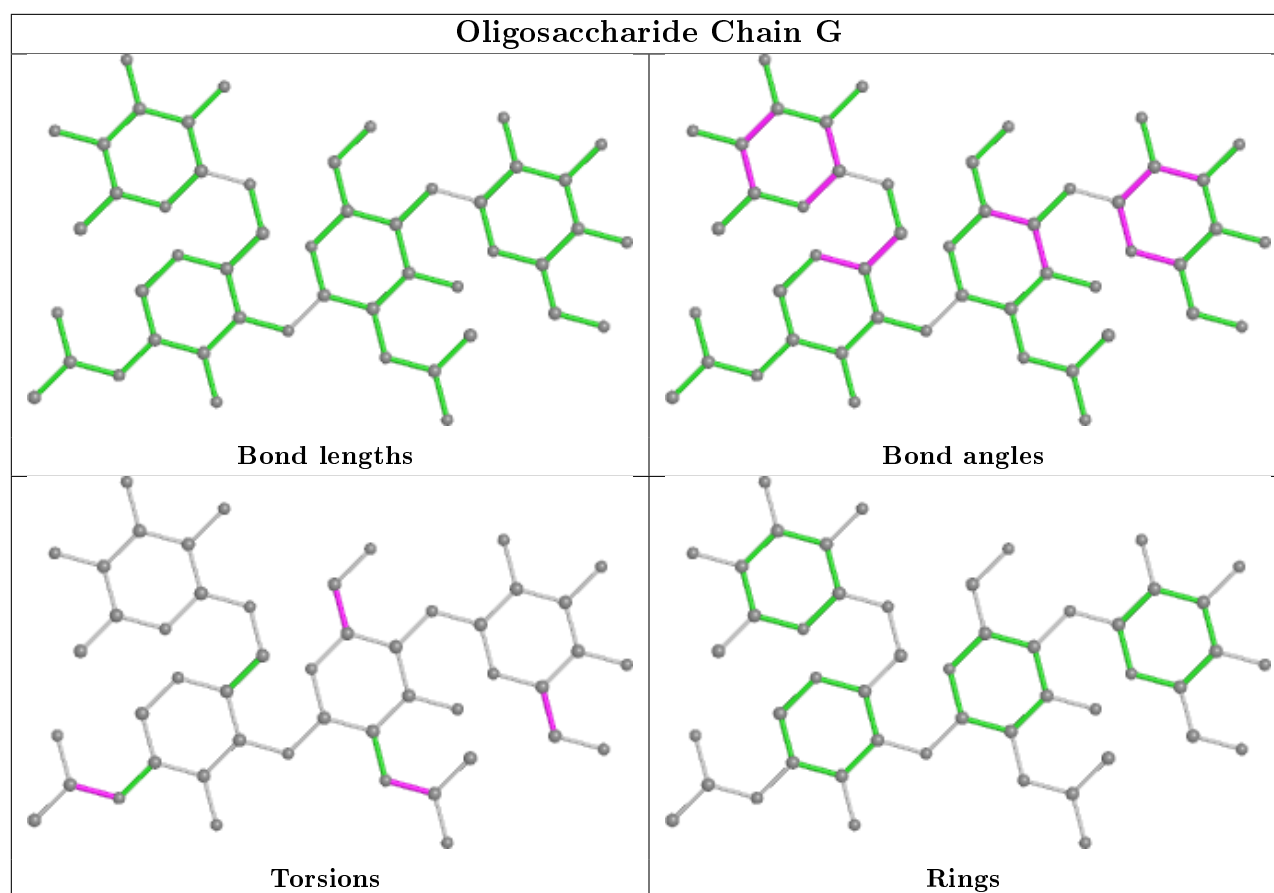












5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
7	NAG	A	724	1	14,14,15	0.51	0	17,19,21	0.97	1 (5%)
7	NAG	A	6621	1	14,14,15	0.51	0	17,19,21	0.88	1 (5%)
7	NAG	A	1961	1	14,14,15	0.48	0	17,19,21	1.33	2 (11%)
8	FUC	A	2916	-	11,11,11	0.60	0	15,16,16	1.20	2 (13%)
7	NAG	A	6671	1	14,14,15	0.49	0	17,19,21	1.33	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
7	NAG	A	724	1	-	3/6/23/26	0/1/1/1
7	NAG	A	6621	1	1/1/5/7	5/6/23/26	0/1/1/1
7	NAG	A	1961	1	-	6/6/23/26	0/1/1/1
8	FUC	A	2916	-	-	-	0/1/1/1
7	NAG	A	6671	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	6671	NAG	C1-O5-C5	4.01	117.62	112.19
7	A	1961	NAG	C1-O5-C5	3.90	117.48	112.19
7	A	724	NAG	C1-O5-C5	2.98	116.23	112.19
8	A	2916	FUC	O5-C5-C4	2.65	114.28	109.52
7	A	6621	NAG	O5-C5-C6	2.31	110.83	107.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	6621	NAG	C1

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	724	NAG	C8-C7-N2-C2
7	A	724	NAG	O7-C7-N2-C2
7	A	6621	NAG	C3-C2-N2-C7
7	A	6621	NAG	C8-C7-N2-C2
7	A	6621	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	724	NAG	1	0
7	A	6621	NAG	1	0
8	A	2916	FUC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	6671	NAG	2	0

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	663/697 (95%)	0.41	37 (5%) 24 21	38, 59, 95, 115	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	PRO	5.5
1	A	33	ASN	5.2
1	A	164	LEU	5.0
1	A	78	ALA	5.0
1	A	49	LEU	4.4

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.

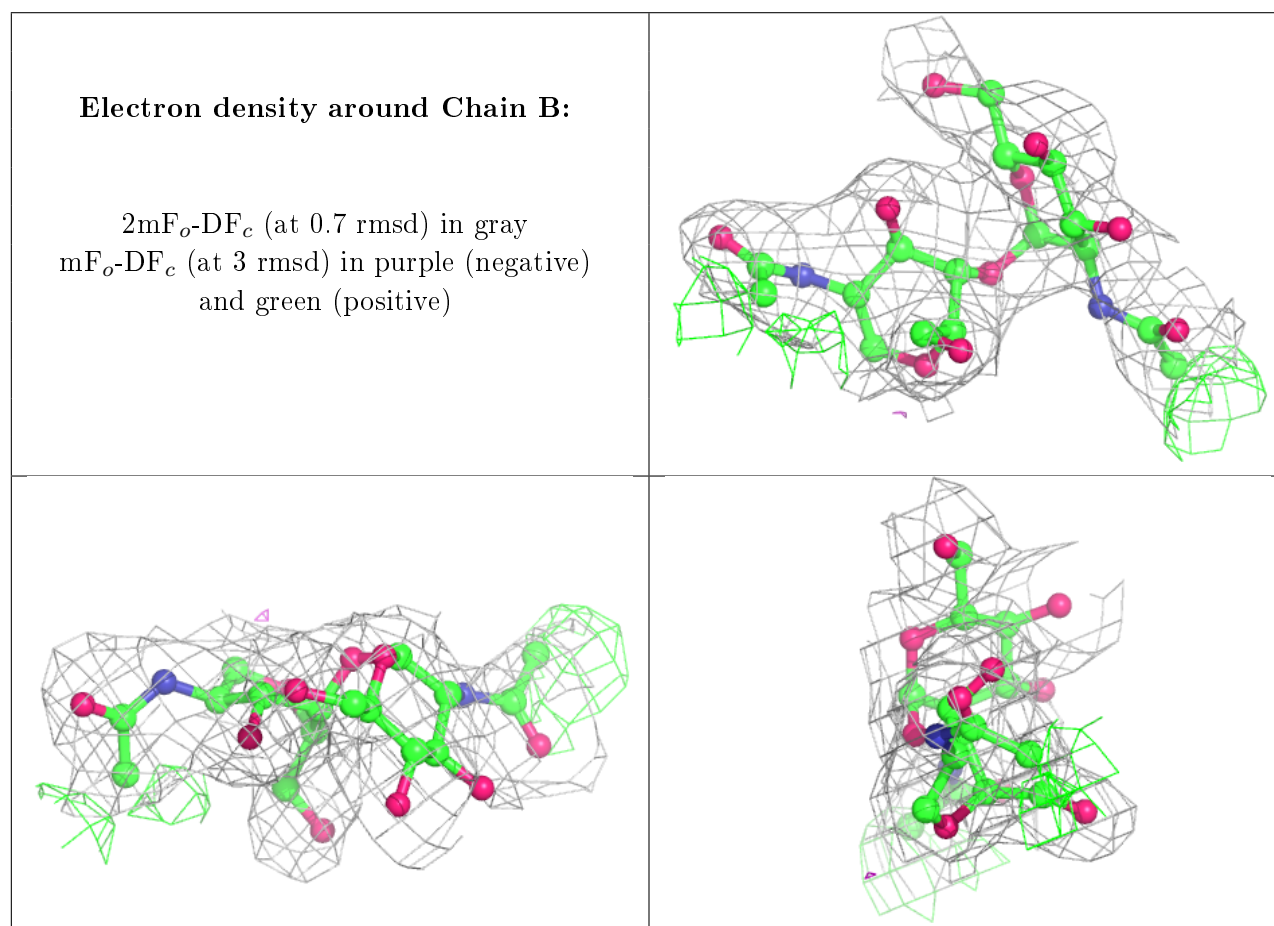
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	F	4	11/12	0.42	0.50	113,120,121,123	0
5	MAN	F	5	11/12	0.47	0.36	112,126,127,127	0
2	NDG	B	2	14/15	0.49	0.28	96,104,109,109	0
2	NDG	E	2	14/15	0.58	0.50	106,109,111,114	0
5	MAN	F	3	11/12	0.62	0.38	108,115,120,124	0
6	FUL	G	4	10/11	0.70	0.63	97,99,102,102	0
6	NDG	G	2	14/15	0.71	0.30	90,91,93,95	0

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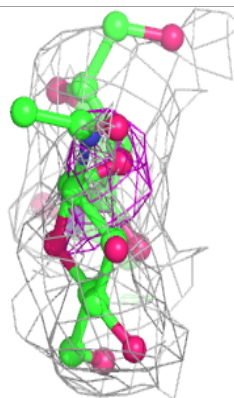
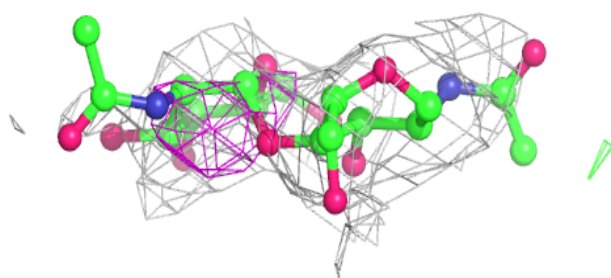
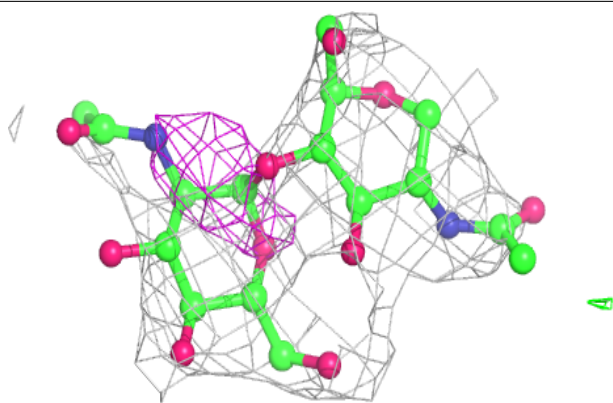
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	BMA	G	3	11/12	0.75	0.18	79,83,88,90	0
4	NAG	D	2	14/15	0.82	0.17	85,91,94,95	0
2	NAG	E	1	14/15	0.83	0.31	90,99,104,105	0
2	NAG	B	1	14/15	0.87	0.13	74,82,88,96	0
3	NAG	C	1	14/15	0.88	0.16	60,64,73,83	0
3	FUL	C	3	10/11	0.88	0.22	86,91,93,95	0
4	NAG	H	2	14/15	0.88	0.17	82,87,91,92	0
5	NDG	F	2	14/15	0.89	0.28	73,84,93,105	0
3	NAG	C	2	14/15	0.90	0.16	51,62,65,66	0
6	NAG	G	1	14/15	0.90	0.16	72,76,87,91	0
4	NAG	D	1	14/15	0.92	0.14	70,75,81,83	0
4	NAG	H	1	14/15	0.94	0.15	55,67,74,80	0
5	NAG	F	1	14/15	0.95	0.14	34,54,64,78	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.



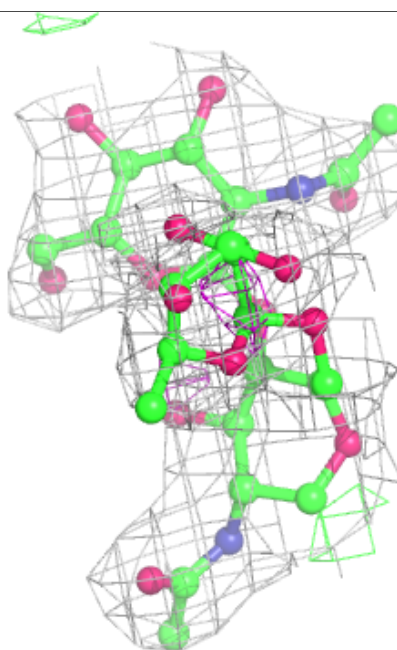
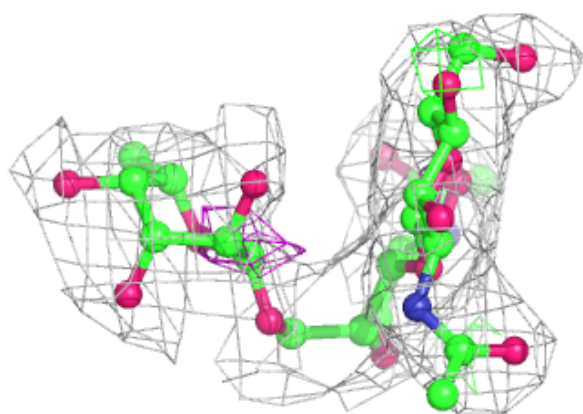
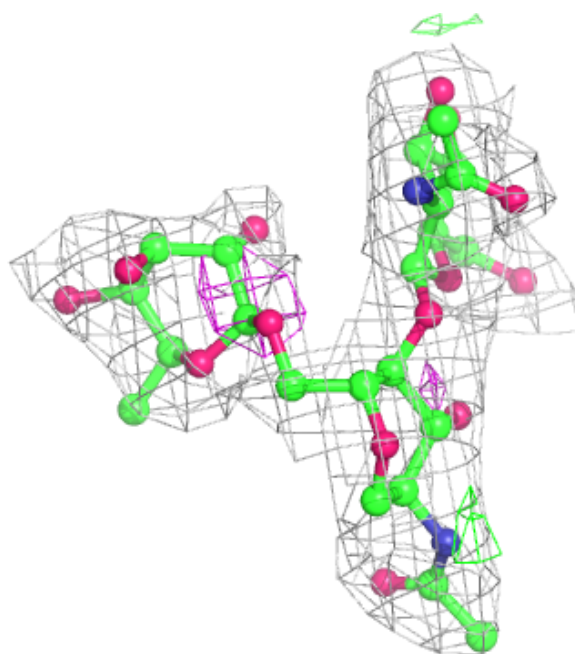
Electron density around Chain E:

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



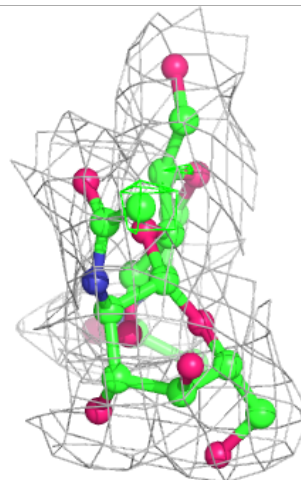
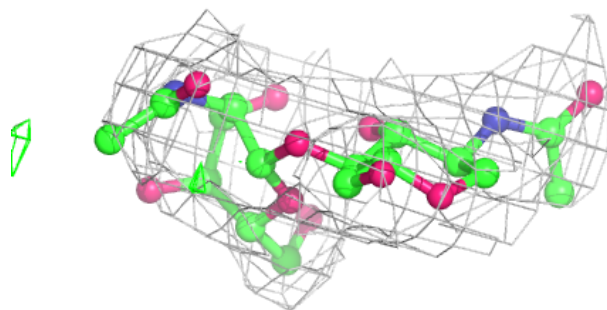
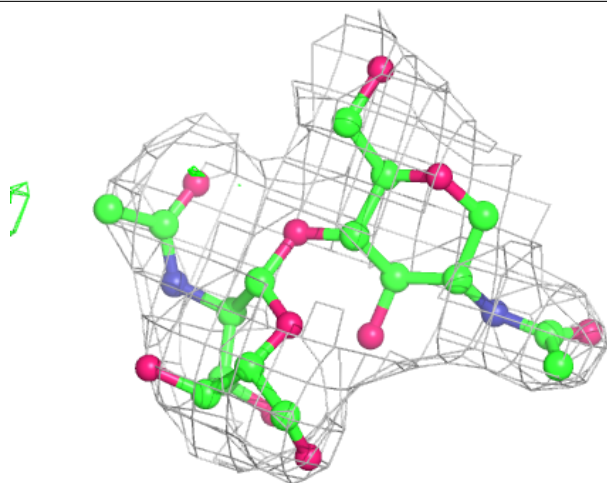
Electron density around Chain C:

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



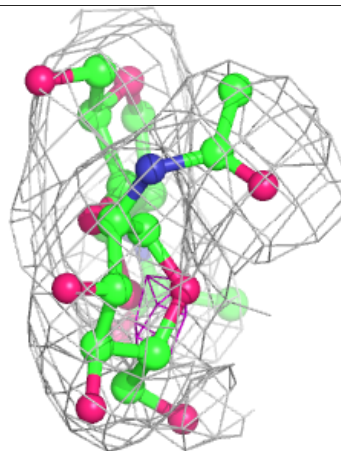
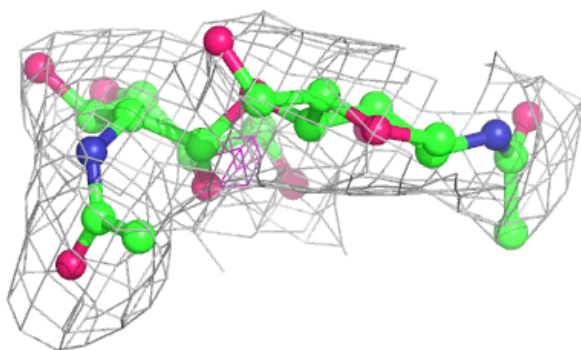
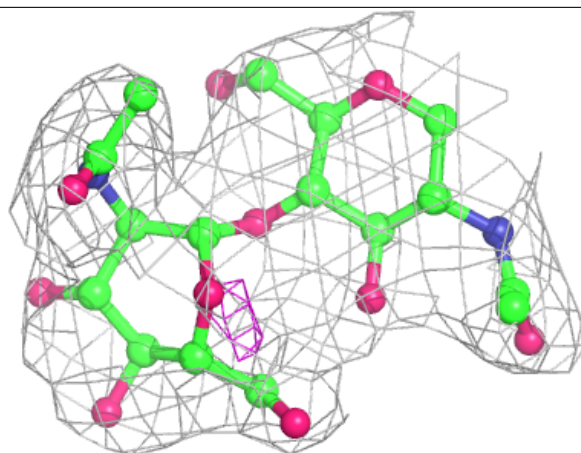
Electron density around Chain D:

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



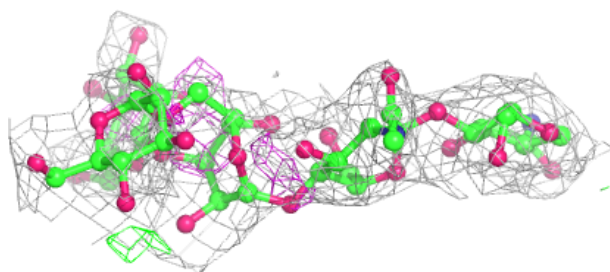
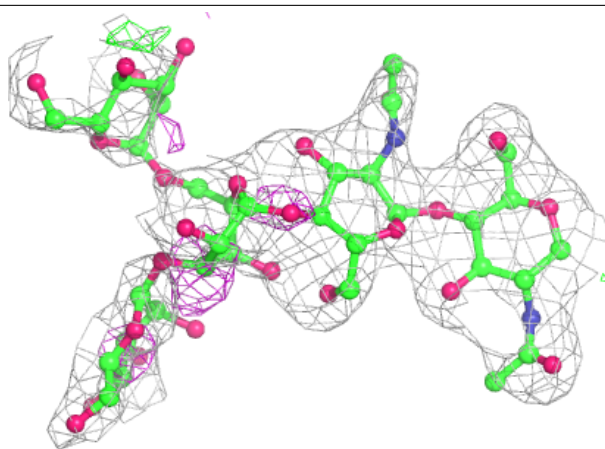
Electron density around Chain H:

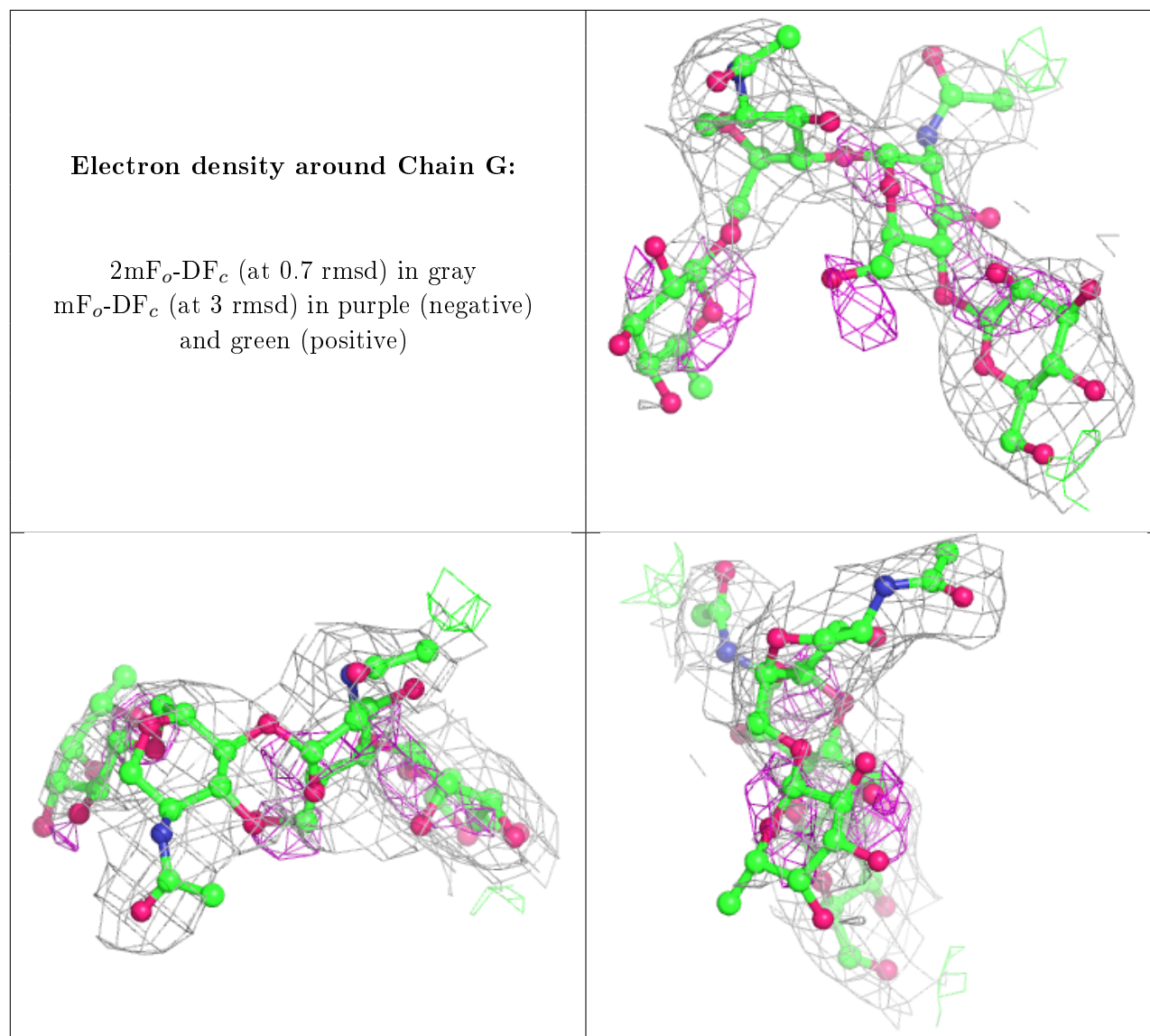
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain F:

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





6.4 Ligands [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
7	NAG	A	6621	14/15	0.57	0.41	67,79,81,82	0
8	FUC	A	2916	11/11	0.57	0.41	105,113,116,116	0
7	NAG	A	1961	14/15	0.64	0.39	74,83,87,88	0
7	NAG	A	6671	14/15	0.71	0.32	79,81,84,85	0
7	NAG	A	724	14/15	0.79	0.30	86,89,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.