



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 08:02 AM BST

PDB ID : 6B0N
Title : Crystal structure of the cleavage-independent prefusion HIV Env glycoprotein trimer of the clade A BG505 isolate (NFL construct) in complex with Fabs PGT122 and PGV19 at 3.39 Å
Authors : Sarkar, A.; Irimia, A.; Wilson, I.A.
Deposited on : 2017-09-14
Resolution : 3.40 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

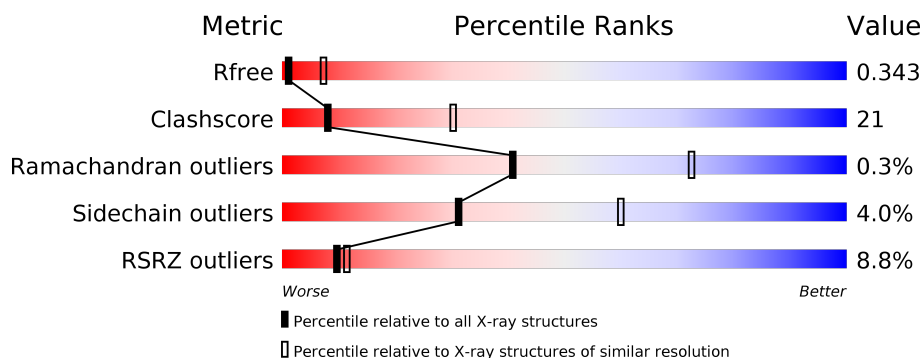
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	D	223	<div> <div>10%</div> <div> <div>52%</div> <div>22%</div> <div>•</div> <div>23%</div> </div> </div>
2	E	209	<div> <div>19%</div> <div> <div>73%</div> <div>13%</div> <div>13%</div> </div> </div>
3	G	638	<div> <div>5%</div> <div> <div>64%</div> <div>28%</div> <div>• •</div> </div> </div>
4	H	235	<div> <div>6%</div> <div> <div>74%</div> <div>22%</div> <div>• •</div> </div> </div>
5	L	213	<div> <div>8%</div> <div> <div>72%</div> <div>25%</div> <div>• •</div> </div> </div>
6	A	7	<div> <div>57%</div> <div>43%</div> </div>

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Mol	Chain	Length	Quality of chain
7	B	3	
7	C	3	
8	F	8	
9	I	5	
9	O	5	
10	J	2	
10	P	2	
10	R	2	
11	K	4	
12	M	8	
13	N	3	
14	Q	4	
15	S	8	

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
10	NAG	P	1	-	-	X	-
10	NAG	P	2	-	-	X	-
12	BMA	M	3	-	-	X	-
13	MAN	N	1	-	-	X	-
14	BMA	Q	1	-	-	X	-
16	NAG	G	1133	-	-	X	-
16	NAG	G	1235	-	-	-	X
16	NAG	G	1355	-	-	-	X
16	NAG	G	1840	-	-	-	X
17	MAN	G	1266	-	-	X	X
8	MAN	F	5	-	-	-	X
8	MAN	F	7	-	-	X	-
8	MAN	F	8	-	-	-	X
9	NAG	O	1	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 11789 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 PGV19 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	171	Total	C	N	O	S	0	0	0
			1341	851	237	244	9			

- Molecule 2 is a protein called PGV19 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	182	Total	C	N	O	S	0	0	0
			1375	866	233	272	4			

- Molecule 3 is a protein called Envelope glycoprotein gp140.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	610	Total	C	N	O	S	0	0	0
			4754	2992	832	898	32			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	507	GLY	-	linker	UNP Q2N0S6
G	508	GLY	-	linker	UNP Q2N0S6
G	509	GLY	-	linker	UNP Q2N0S6
G	509A	GLY	-	linker	UNP Q2N0S6
G	509B	GLY	-	linker	UNP Q2N0S6
G	509C	SER	-	linker	UNP Q2N0S6
G	509D	GLY	-	linker	UNP Q2N0S6
G	509E	GLY	-	linker	UNP Q2N0S6
G	509F	GLY	-	linker	UNP Q2N0S6
G	509G	GLY	-	linker	UNP Q2N0S6
G	511	SER	-	linker	UNP Q2N0S6
G	559	PRO	ILE	engineered mutation	UNP Q2N0S9

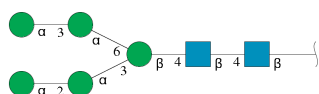
- Molecule 4 is a protein called PGT122 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	232	Total	C	N	O	S	0	0	0
			1767	1122	300	340	5			

- Molecule 5 is a protein called PGT122 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	210	Total	C	N	O	S	0	0	0
			1586	997	266	319	4			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-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.



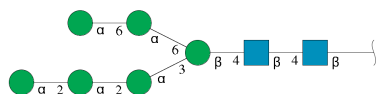
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	A	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 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.



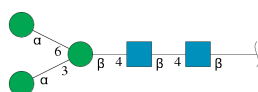
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-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.



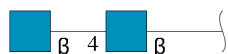
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	F	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-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.



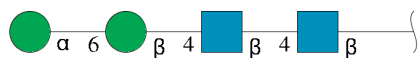
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
9	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



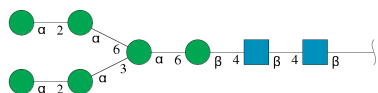
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 11 is an oligosaccharide called alpha-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
11	K	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-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.



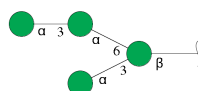
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
12	M	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



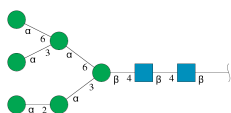
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	N	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose.



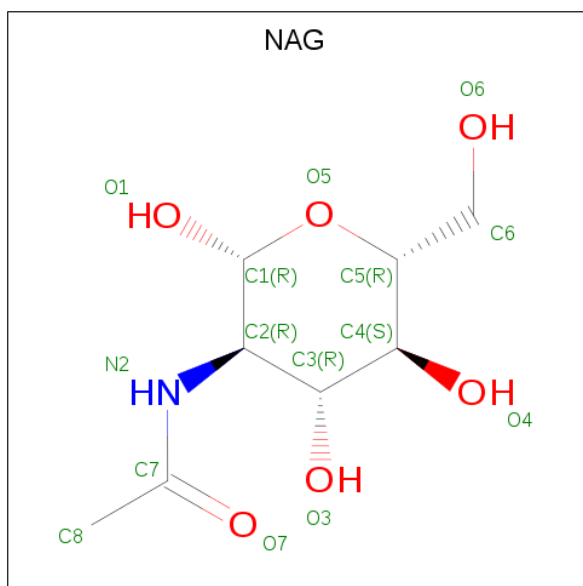
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
14	Q	4	Total	C	O	0	0	0
			44	24	20			

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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
15	S	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



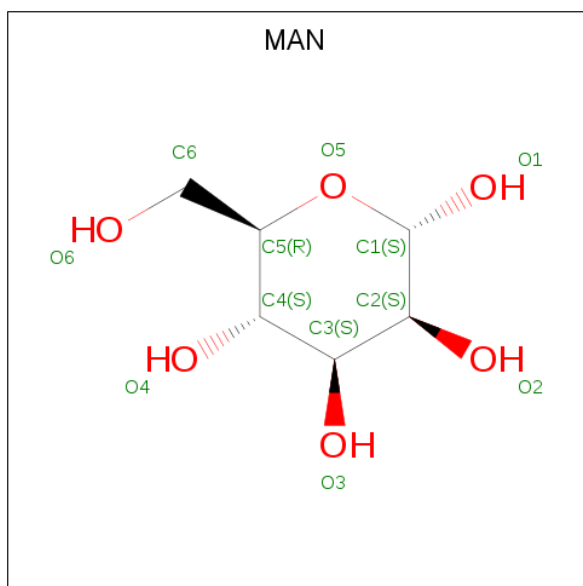
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		

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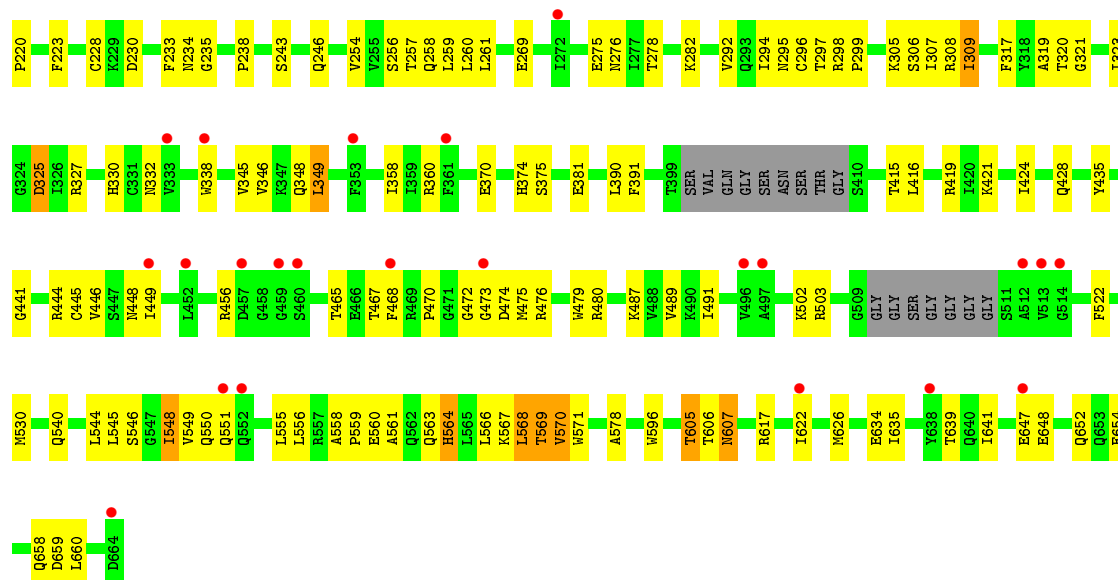
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		

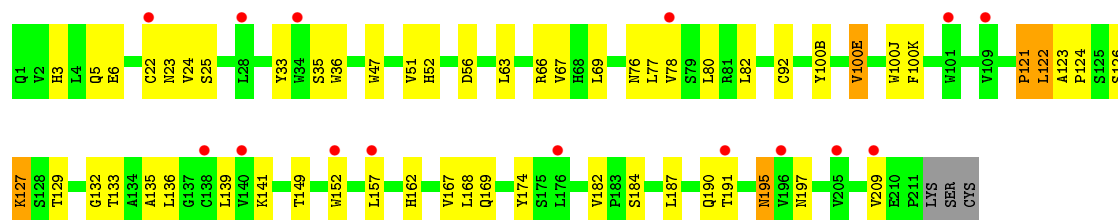
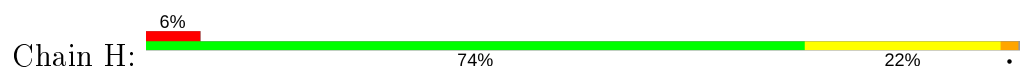
- Molecule 17 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



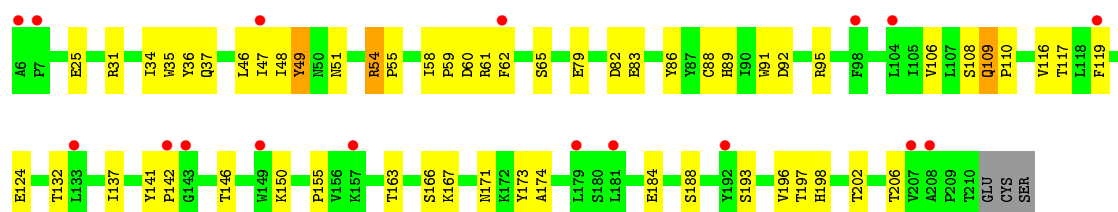
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	G	1	Total	C	O	0	0
			11	6	5		
17	G	1	Total	C	O	0	0
			11	6	5		



• Molecule 4: PGT122 Fab heavy chain



• Molecule 5: PGT122 light chain



• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-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



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  33% 67%

MAG1
MAG2
BGL3

- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  67% 33%

MAG1
MAG2
BGL3

- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-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

Chain F:  13% 75% 13%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-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

Chain I:  40% 60%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-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

Chain O:  20% 60% 20%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



- Molecule 11: alpha-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

Chain K:  75% 25%



- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-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

Chain M:  38% 63%



- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain N:  67% 33%



- Molecule 14: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose

Chain Q:  50% 25% 25%



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-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



HA1	HA2	HA3	HA4	HA5	HA6	HA7	HA8
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4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	161.25Å 161.25Å 245.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.85 – 3.40 48.85 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.85-3.40) 98.6 (48.85-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.12_2829: 000)	Depositor
R, R_{free}	0.335 , 0.346 0.335 , 0.343	Depositor DCC
R_{free} test set	2458 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	91.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	11789	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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, 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	D	0.33	0/1375	0.50	0/1861
2	E	0.28	0/1410	0.50	0/1914
3	G	0.40	0/4847	0.59	0/6582
4	H	0.32	0/1815	0.49	0/2479
5	L	0.33	0/1629	0.55	0/2232
All	All	0.36	0/11076	0.55	0/15068

There are no bond length outliers.

There are no bond angle outliers.

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	D	1341	0	1285	69	0
2	E	1375	0	1320	19	0
3	G	4754	0	4644	232	1
4	H	1767	0	1738	64	0
5	L	1586	0	1526	72	0
6	A	83	0	70	1	0
7	B	39	0	34	1	0
7	C	39	0	33	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	94	0	79	16	0
9	I	61	0	52	1	0
9	O	61	0	51	18	0
10	J	28	0	25	0	0
10	P	28	0	25	26	0
10	R	28	0	22	0	0
11	K	50	0	43	0	0
12	M	94	0	79	11	0
13	N	33	0	28	9	0
14	Q	44	0	34	6	0
15	S	94	0	79	1	0
16	G	168	0	156	12	0
17	G	22	0	20	16	0
All	All	11789	0	11343	493	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 21.

The worst 5 of 493 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)
3:G:133:ASN:HD21	16:G:1133:NAG:C1	1.06	1.63
3:G:64:GLU:HB2	3:G:66:HIS:CE1	1.37	1.55
5:L:35:TRP:CD1	5:L:48:ILE:HD11	1.45	1.52
3:G:64:GLU:CB	3:G:66:HIS:CE1	1.89	1.51
3:G:325:ASP:OD2	4:H:100(B):TYR:CD1	1.70	1.44

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)
3:G:103:GLN:NE2	3:G:560:GLU:OE2[3_685]	1.96	0.24

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	D	163/223 (73%)	157 (96%)	6 (4%)	0	100	100
2	E	176/209 (84%)	171 (97%)	5 (3%)	0	100	100
3	G	598/638 (94%)	572 (96%)	25 (4%)	1 (0%)	47	78
4	H	230/235 (98%)	222 (96%)	6 (3%)	2 (1%)	17	49
5	L	208/213 (98%)	201 (97%)	6 (3%)	1 (0%)	29	61
All	All	1375/1518 (91%)	1323 (96%)	48 (4%)	4 (0%)	41	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	100(E)	VAL
5	L	109	GLN
3	G	570	VAL
4	H	121	PRO

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	D	142/185 (77%)	136 (96%)	6 (4%)	30	59
2	E	153/176 (87%)	150 (98%)	3 (2%)	55	77
3	G	527/552 (96%)	500 (95%)	27 (5%)	24	54
4	H	201/205 (98%)	192 (96%)	9 (4%)	27	58
5	L	177/181 (98%)	174 (98%)	3 (2%)	60	80
All	All	1200/1299 (92%)	1152 (96%)	48 (4%)	31	60

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	218	CYS
3	G	548	ILE
4	H	195	ASN
3	G	307	ILE
3	G	325	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	216	HIS
5	L	109	GLN
3	G	246	GLN
1	D	64	GLN
3	G	348	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 ⓘ

64 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	$\# Z > 2$
6	NAG	A	1	3,6	14,14,15	0.53	0	17,19,21	0.85	0
6	NAG	A	2	6	14,14,15	0.52	0	17,19,21	0.80	0
6	BMA	A	3	6	11,11,12	0.36	0	15,15,17	0.76	0
6	MAN	A	4	6	11,11,12	0.49	0	15,15,17	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	A	5	6	11,11,12	0.47	0	15,15,17	0.82	0
6	MAN	A	6	6	11,11,12	0.42	0	15,15,17	0.91	1 (6%)
6	MAN	A	7	6	11,11,12	0.41	0	15,15,17	1.15	1 (6%)
7	NAG	B	1	3,7	14,14,15	0.62	0	17,19,21	0.73	0
7	NAG	B	2	7	14,14,15	0.88	0	17,19,21	1.82	2 (11%)
7	BMA	B	3	7	11,11,12	0.45	0	15,15,17	0.65	0
7	NAG	C	1	3,7	14,14,15	0.25	0	17,19,21	0.49	0
7	NAG	C	2	7	14,14,15	0.32	0	17,19,21	0.66	0
7	BMA	C	3	7	11,11,12	1.07	1 (9%)	15,15,17	1.22	2 (13%)
8	NAG	F	1	8,3	14,14,15	0.48	0	17,19,21	0.83	0
8	NAG	F	2	8	14,14,15	0.54	0	17,19,21	0.88	0
8	BMA	F	3	8	11,11,12	0.48	0	15,15,17	0.79	0
8	MAN	F	4	8	11,11,12	0.44	0	15,15,17	1.25	2 (13%)
8	MAN	F	5	8	11,11,12	0.47	0	15,15,17	1.97	4 (26%)
8	MAN	F	6	8	11,11,12	0.45	0	15,15,17	1.22	0
8	MAN	F	7	8	11,11,12	0.40	0	15,15,17	0.82	0
8	MAN	F	8	8	11,11,12	0.41	0	15,15,17	1.14	1 (6%)
9	NAG	I	1	9,3	14,14,15	0.83	0	17,19,21	1.76	3 (17%)
9	NAG	I	2	9	14,14,15	0.68	0	17,19,21	1.02	0
9	BMA	I	3	9	11,11,12	0.81	0	15,15,17	0.94	2 (13%)
9	MAN	I	4	9	11,11,12	0.46	0	15,15,17	0.66	0
9	MAN	I	5	9	11,11,12	0.63	0	15,15,17	0.80	0
10	NAG	J	1	10,3	14,14,15	0.49	0	17,19,21	0.76	0
10	NAG	J	2	10	14,14,15	0.58	0	17,19,21	0.85	0
11	NAG	K	1	11,3	14,14,15	0.57	0	17,19,21	0.93	1 (5%)
11	NAG	K	2	11	14,14,15	0.58	0	17,19,21	0.82	0
11	BMA	K	3	11	11,11,12	0.52	0	15,15,17	0.71	0
11	MAN	K	4	11	11,11,12	0.54	0	15,15,17	0.79	0
12	NAG	M	1	3,12	14,14,15	0.33	0	17,19,21	0.45	0
12	NAG	M	2	12	14,14,15	0.39	0	17,19,21	0.64	0
12	BMA	M	3	12	11,11,12	0.64	0	15,15,17	0.87	0
12	MAN	M	4	12	11,11,12	0.80	0	15,15,17	1.76	3 (20%)
12	MAN	M	5	12	11,11,12	0.38	0	15,15,17	1.12	1 (6%)
12	MAN	M	6	12	11,11,12	0.55	0	15,15,17	1.06	2 (13%)
12	MAN	M	7	12	11,11,12	0.45	0	15,15,17	0.82	0
12	MAN	M	8	12	11,11,12	0.44	0	15,15,17	0.73	0
13	MAN	N	1	13	11,11,12	0.40	0	15,15,17	0.74	0
13	MAN	N	2	13	11,11,12	0.41	0	15,15,17	0.81	0
13	MAN	N	3	13	11,11,12	0.42	0	15,15,17	0.76	0
9	NAG	O	1	9,3	14,14,15	0.64	0	17,19,21	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	O	2	9	14,14,15	0.61	0	17,19,21	2.66	5 (29%)
9	BMA	O	3	9	11,11,12	0.80	1 (9%)	15,15,17	1.73	4 (26%)
9	MAN	O	4	9	11,11,12	0.49	0	15,15,17	1.29	2 (13%)
9	MAN	O	5	9	11,11,12	0.63	0	15,15,17	1.04	0
10	NAG	P	1	10,3	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
10	NAG	P	2	10	14,14,15	0.80	0	17,19,21	0.85	0
14	BMA	Q	1	14	11,11,12	0.60	0	15,15,17	1.13	1 (6%)
14	MAN	Q	2	14	11,11,12	0.44	0	15,15,17	0.79	0
14	MAN	Q	3	14	11,11,12	0.46	0	15,15,17	0.81	0
14	MAN	Q	4	14	11,11,12	0.57	0	15,15,17	2.77	4 (26%)
10	NAG	R	1	10,3	14,14,15	0.64	0	17,19,21	0.89	0
10	NAG	R	2	10	14,14,15	0.71	0	17,19,21	0.84	0
15	NAG	S	1	3,15	14,14,15	0.55	0	17,19,21	0.85	0
15	NAG	S	2	15	14,14,15	0.61	0	17,19,21	0.90	1 (5%)
15	BMA	S	3	15	11,11,12	0.35	0	15,15,17	1.52	4 (26%)
15	MAN	S	4	15	11,11,12	0.44	0	15,15,17	0.69	0
15	MAN	S	5	15	11,11,12	0.44	0	15,15,17	0.69	0
15	MAN	S	6	15	11,11,12	0.43	0	15,15,17	1.10	1 (6%)
15	MAN	S	7	15	11,11,12	0.30	0	15,15,17	0.84	0
15	MAN	S	8	15	11,11,12	0.43	0	15,15,17	1.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	A	2	6	-	0/6/23/26	0/1/1/1
6	BMA	A	3	6	-	0/2/19/22	0/1/1/1
6	MAN	A	4	6	-	1/2/19/22	0/1/1/1
6	MAN	A	5	6	-	0/2/19/22	0/1/1/1
6	MAN	A	6	6	-	1/2/19/22	0/1/1/1
6	MAN	A	7	6	-	0/2/19/22	0/1/1/1
7	NAG	B	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	B	2	7	-	3/6/23/26	0/1/1/1
7	BMA	B	3	7	-	0/2/19/22	0/1/1/1
7	NAG	C	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	C	2	7	-	0/6/23/26	0/1/1/1
7	BMA	C	3	7	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	F	1	8,3	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	0/6/23/26	0/1/1/1
8	BMA	F	3	8	-	0/2/19/22	0/1/1/1
8	MAN	F	4	8	-	0/2/19/22	0/1/1/1
8	MAN	F	5	8	-	1/2/19/22	0/1/1/1
8	MAN	F	6	8	-	2/2/19/22	0/1/1/1
8	MAN	F	7	8	-	2/2/19/22	0/1/1/1
8	MAN	F	8	8	-	0/2/19/22	0/1/1/1
9	NAG	I	1	9,3	-	5/6/23/26	0/1/1/1
9	NAG	I	2	9	-	1/6/23/26	0/1/1/1
9	BMA	I	3	9	-	0/2/19/22	0/1/1/1
9	MAN	I	4	9	-	1/2/19/22	0/1/1/1
9	MAN	I	5	9	-	0/2/19/22	0/1/1/1
10	NAG	J	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	J	2	10	-	0/6/23/26	0/1/1/1
11	NAG	K	1	11,3	-	1/6/23/26	0/1/1/1
11	NAG	K	2	11	-	0/6/23/26	0/1/1/1
11	BMA	K	3	11	-	2/2/19/22	0/1/1/1
11	MAN	K	4	11	-	0/2/19/22	0/1/1/1
12	NAG	M	1	3,12	-	2/6/23/26	0/1/1/1
12	NAG	M	2	12	-	3/6/23/26	0/1/1/1
12	BMA	M	3	12	-	0/2/19/22	0/1/1/1
12	MAN	M	4	12	-	0/2/19/22	0/1/1/1
12	MAN	M	5	12	-	1/2/19/22	0/1/1/1
12	MAN	M	6	12	-	0/2/19/22	0/1/1/1
12	MAN	M	7	12	-	0/2/19/22	0/1/1/1
12	MAN	M	8	12	-	0/2/19/22	0/1/1/1
13	MAN	N	1	13	-	0/2/19/22	0/1/1/1
13	MAN	N	2	13	-	0/2/19/22	0/1/1/1
13	MAN	N	3	13	-	1/2/19/22	0/1/1/1
9	NAG	O	1	9,3	-	1/6/23/26	0/1/1/1
9	NAG	O	2	9	-	3/6/23/26	0/1/1/1
9	BMA	O	3	9	-	2/2/19/22	0/1/1/1
9	MAN	O	4	9	-	0/2/19/22	0/1/1/1
9	MAN	O	5	9	-	0/2/19/22	0/1/1/1
10	NAG	P	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	P	2	10	-	3/6/23/26	0/1/1/1
14	BMA	Q	1	14	-	0/2/19/22	0/1/1/1
14	MAN	Q	2	14	-	0/2/19/22	0/1/1/1
14	MAN	Q	3	14	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	MAN	Q	4	14	-	2/2/19/22	0/1/1/1
10	NAG	R	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	R	2	10	-	1/6/23/26	0/1/1/1
15	NAG	S	1	3,15	-	2/6/23/26	0/1/1/1
15	NAG	S	2	15	-	0/6/23/26	0/1/1/1
15	BMA	S	3	15	-	1/2/19/22	0/1/1/1
15	MAN	S	4	15	-	0/2/19/22	0/1/1/1
15	MAN	S	5	15	-	0/2/19/22	0/1/1/1
15	MAN	S	6	15	-	2/2/19/22	0/1/1/1
15	MAN	S	7	15	-	0/2/19/22	0/1/1/1
15	MAN	S	8	15	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	3	BMA	O5-C1	-2.17	1.40	1.43
7	C	3	BMA	C2-C3	2.17	1.55	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	O	2	NAG	O3-C3-C2	-6.71	95.57	109.47
14	Q	4	MAN	O3-C3-C4	-5.95	96.59	110.35
9	O	2	NAG	C1-O5-C5	5.78	120.03	112.19
14	Q	4	MAN	O4-C4-C5	-5.75	95.03	109.30
7	B	2	NAG	C2-N2-C7	5.74	131.07	122.90

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

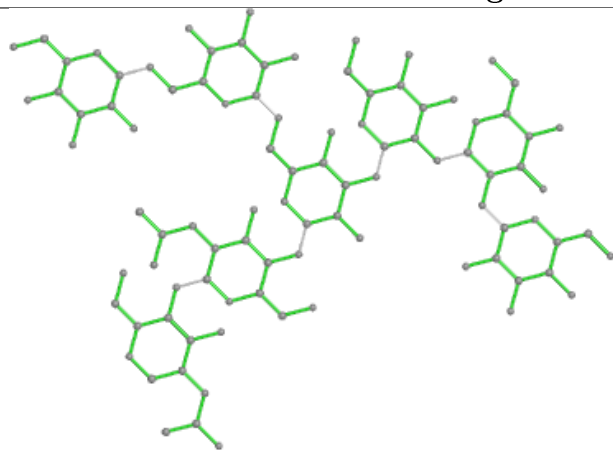
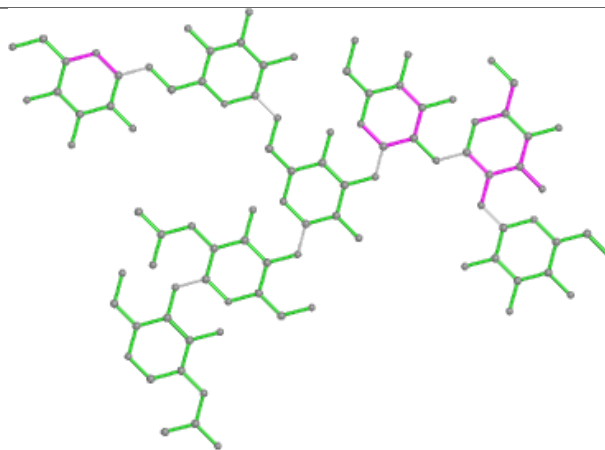
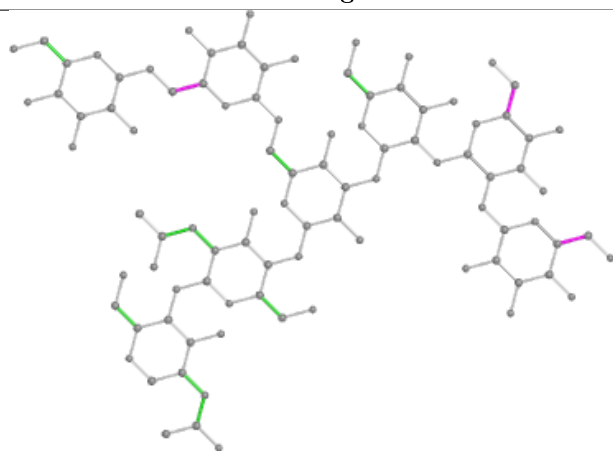
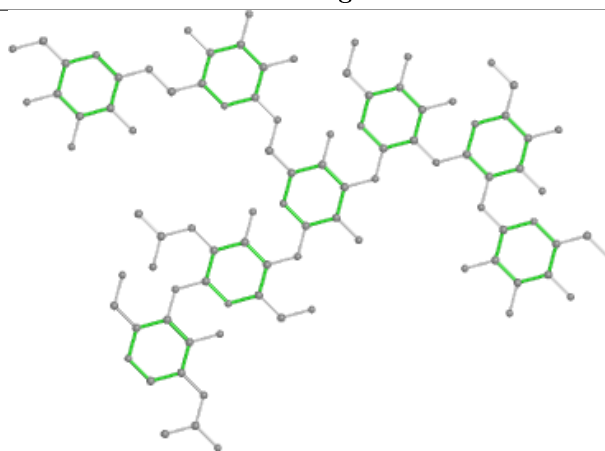
Mol	Chain	Res	Type	Atoms
9	O	2	NAG	C1-C2-N2-C7
9	O	2	NAG	C8-C7-N2-C2
9	O	2	NAG	O7-C7-N2-C2
14	Q	4	MAN	O5-C5-C6-O6
12	M	2	NAG	O5-C5-C6-O6

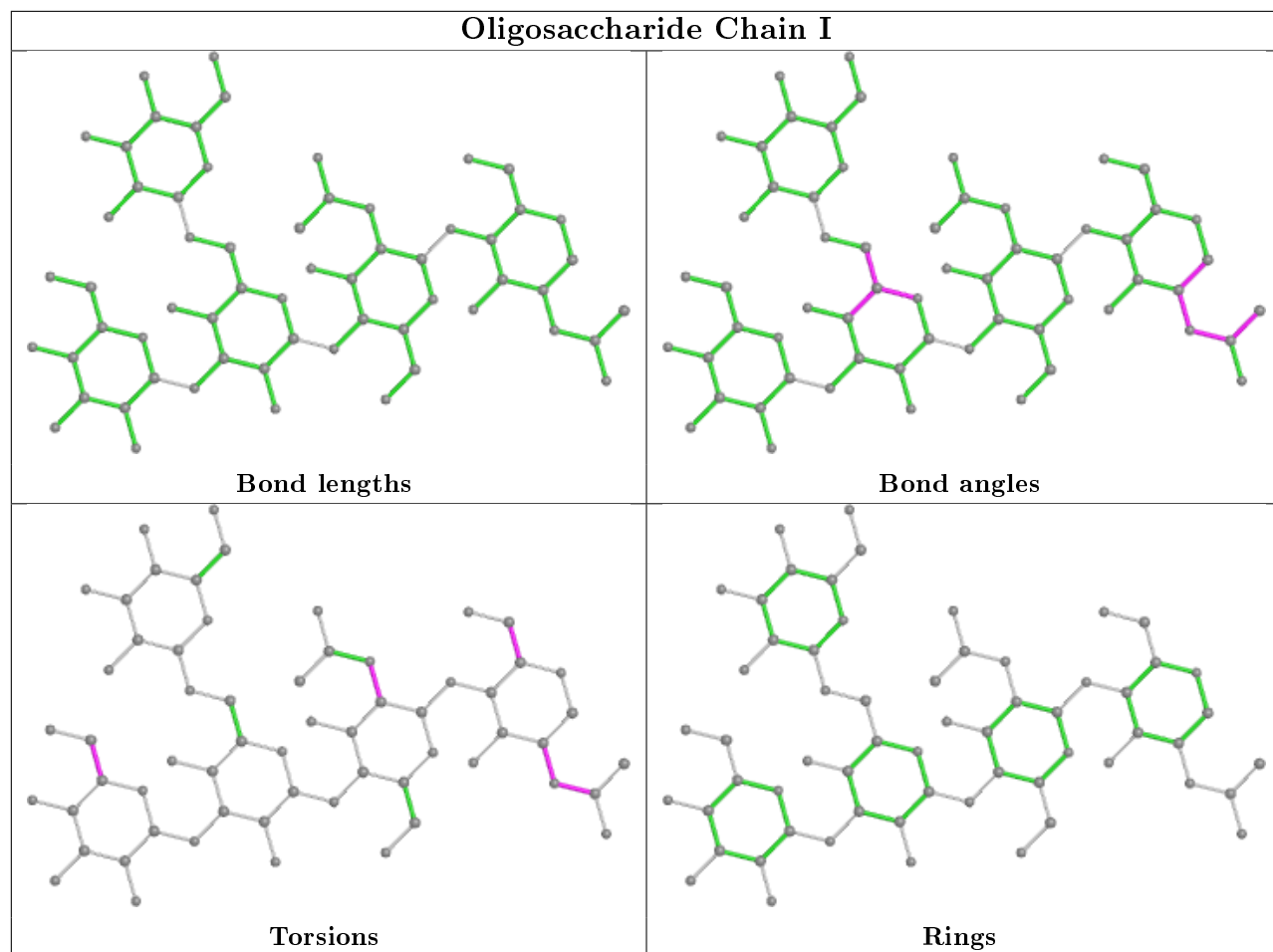
There are no ring outliers.

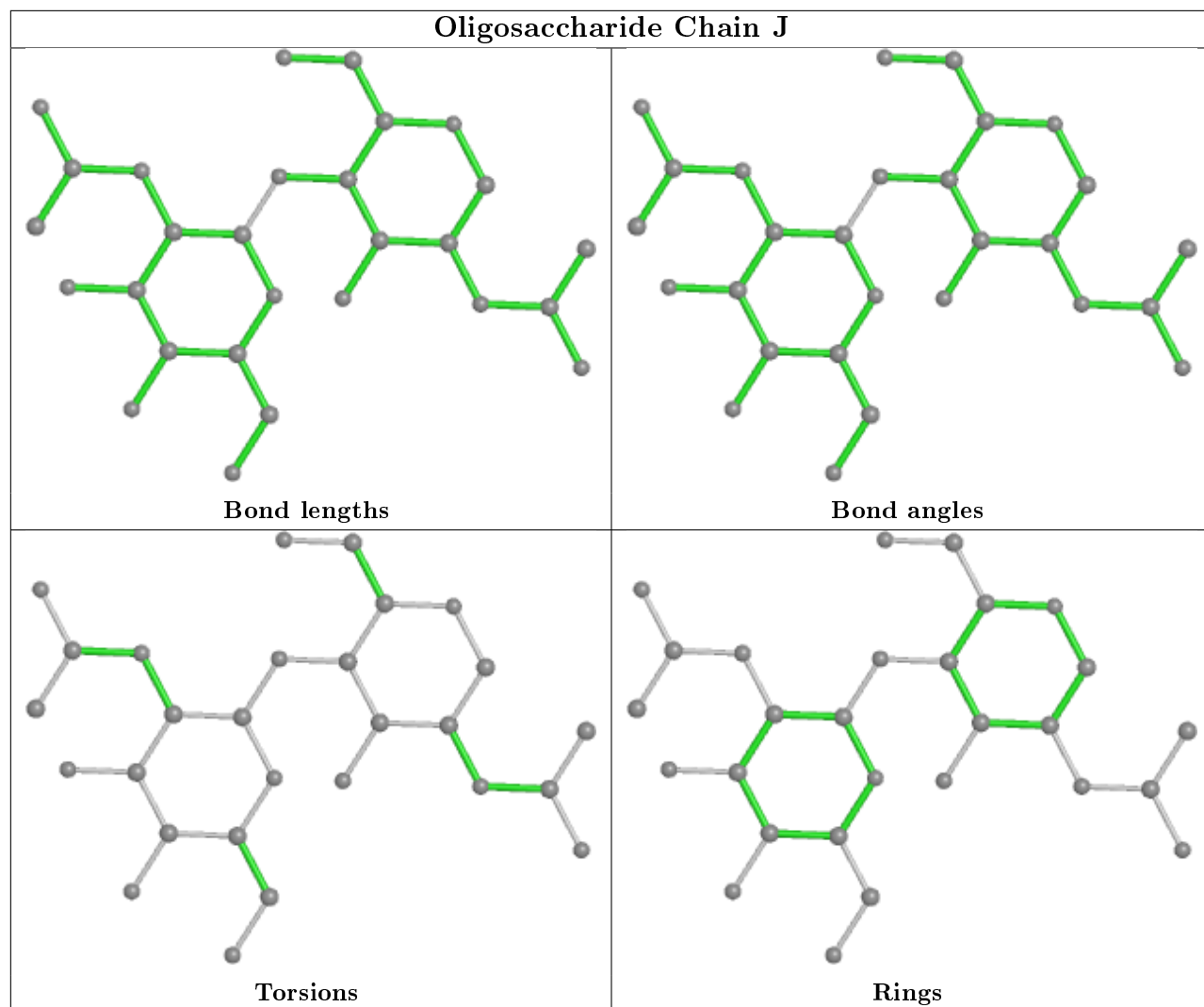
18 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	2	NAG	1	0
8	F	2	NAG	1	0
7	C	3	BMA	2	0
8	F	3	BMA	1	0
13	N	1	MAN	9	0
9	O	1	NAG	18	0
8	F	7	MAN	14	0
14	Q	1	BMA	6	0
10	P	1	NAG	20	0
6	A	1	NAG	1	0
9	O	2	NAG	1	0
7	B	1	NAG	1	0
12	M	1	NAG	2	0
8	F	4	MAN	1	0
15	S	1	NAG	1	0
12	M	3	BMA	9	0
10	P	2	NAG	9	0
8	F	1	NAG	1	0

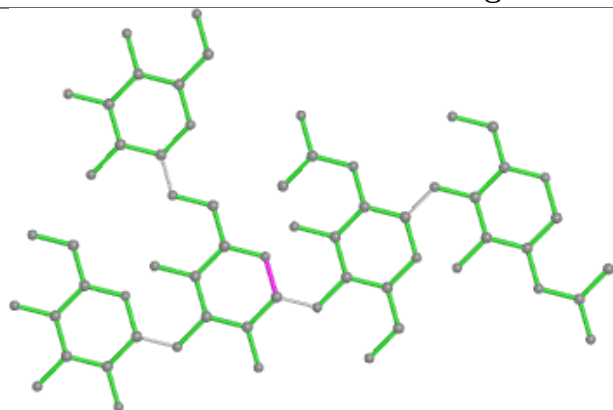
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

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

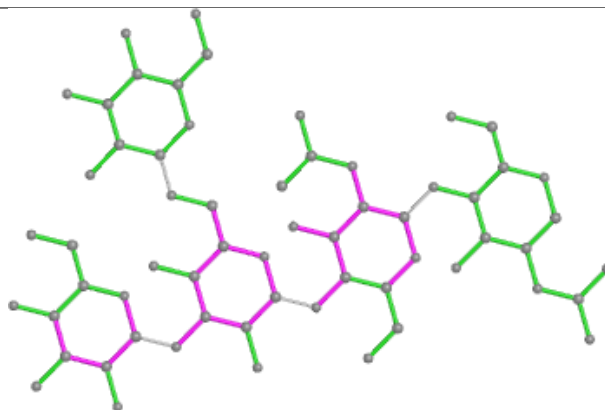




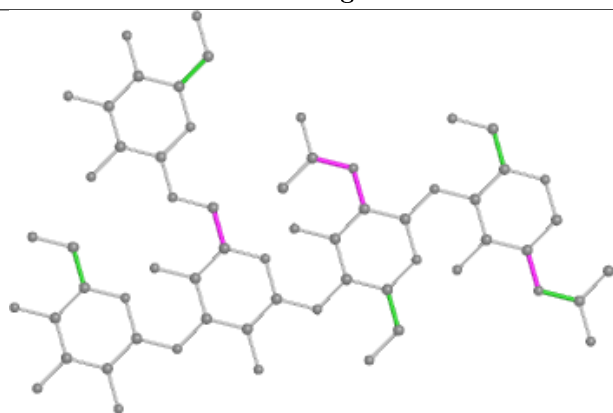
Oligosaccharide Chain O



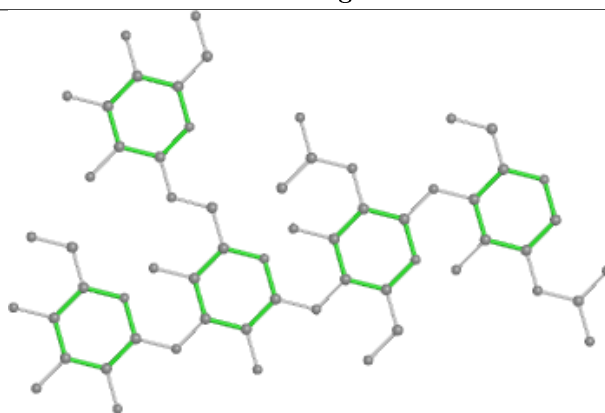
Bond lengths



Bond angles

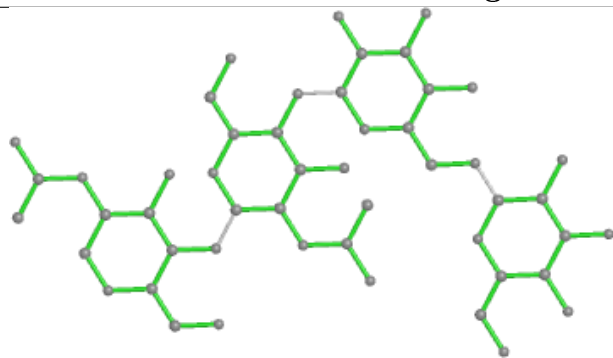


Torsions

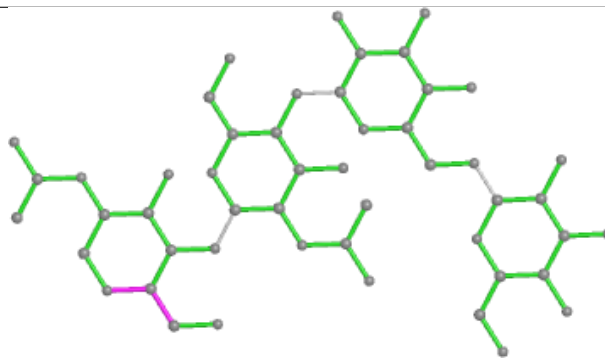


Rings

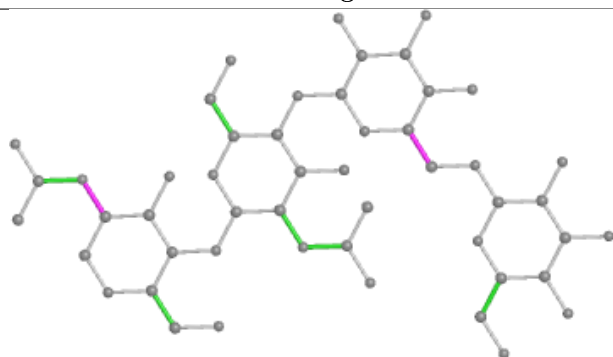
Oligosaccharide Chain K



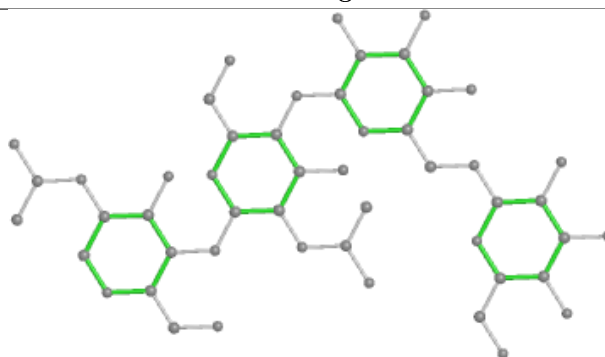
Bond lengths



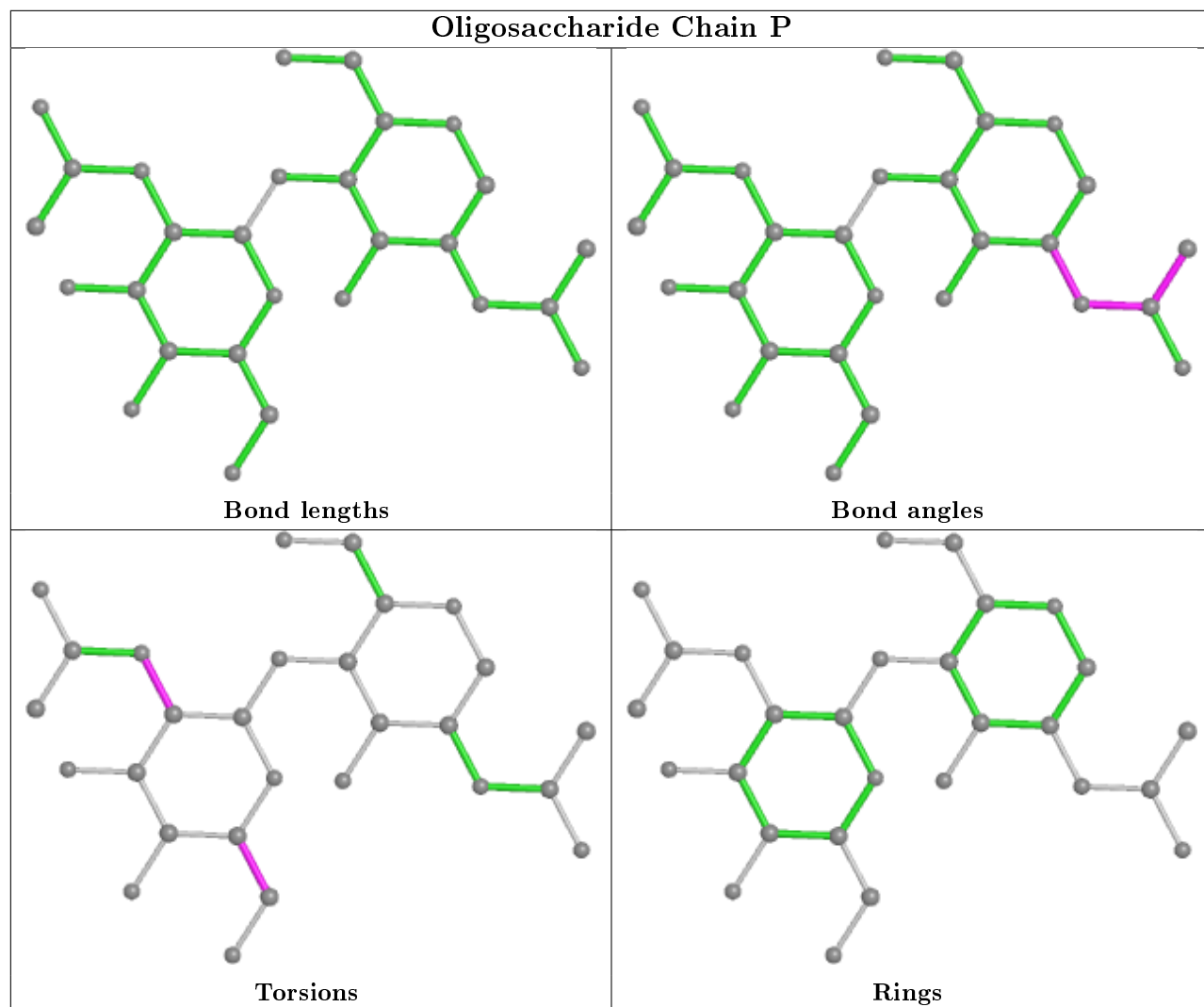
Bond angles

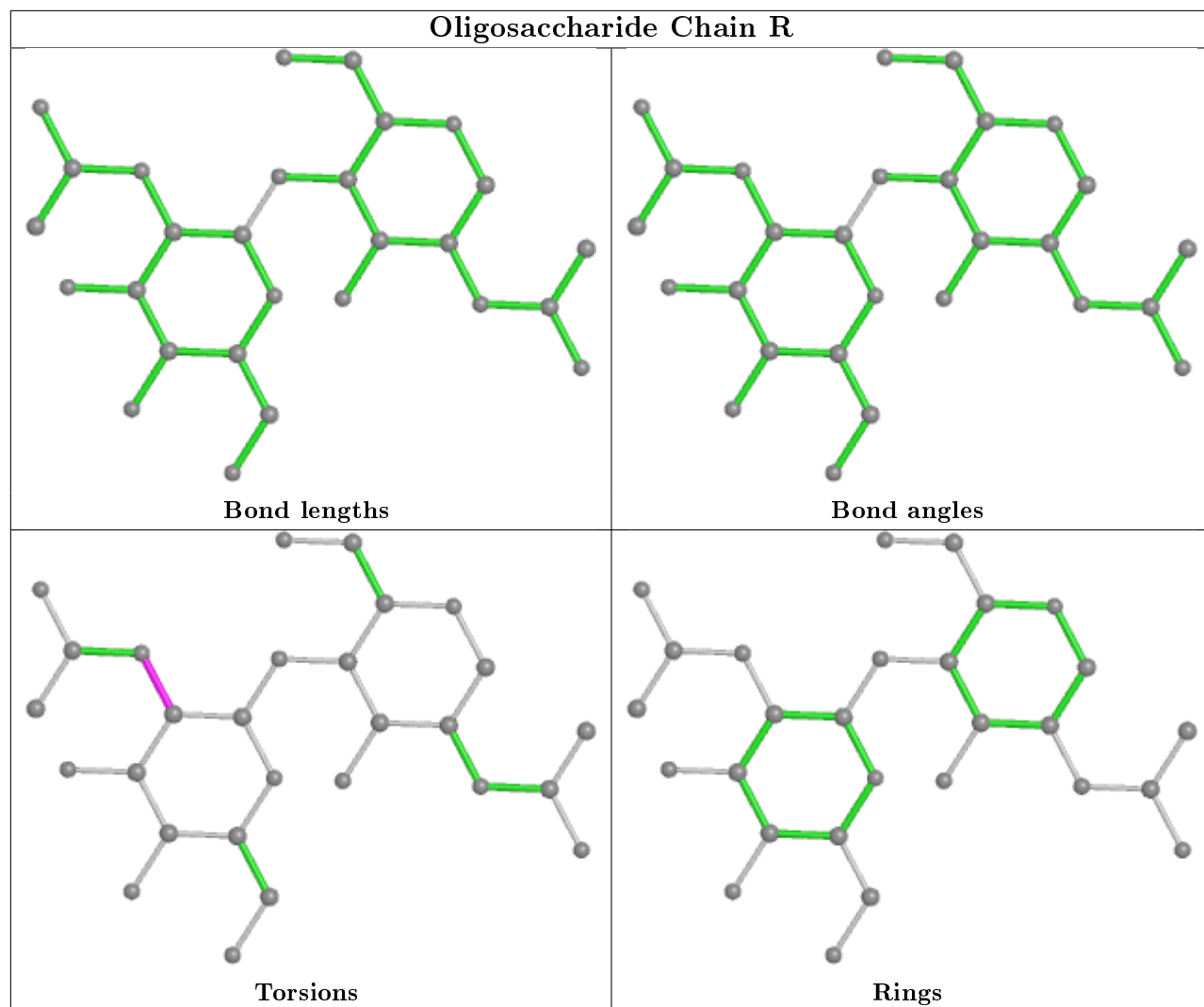


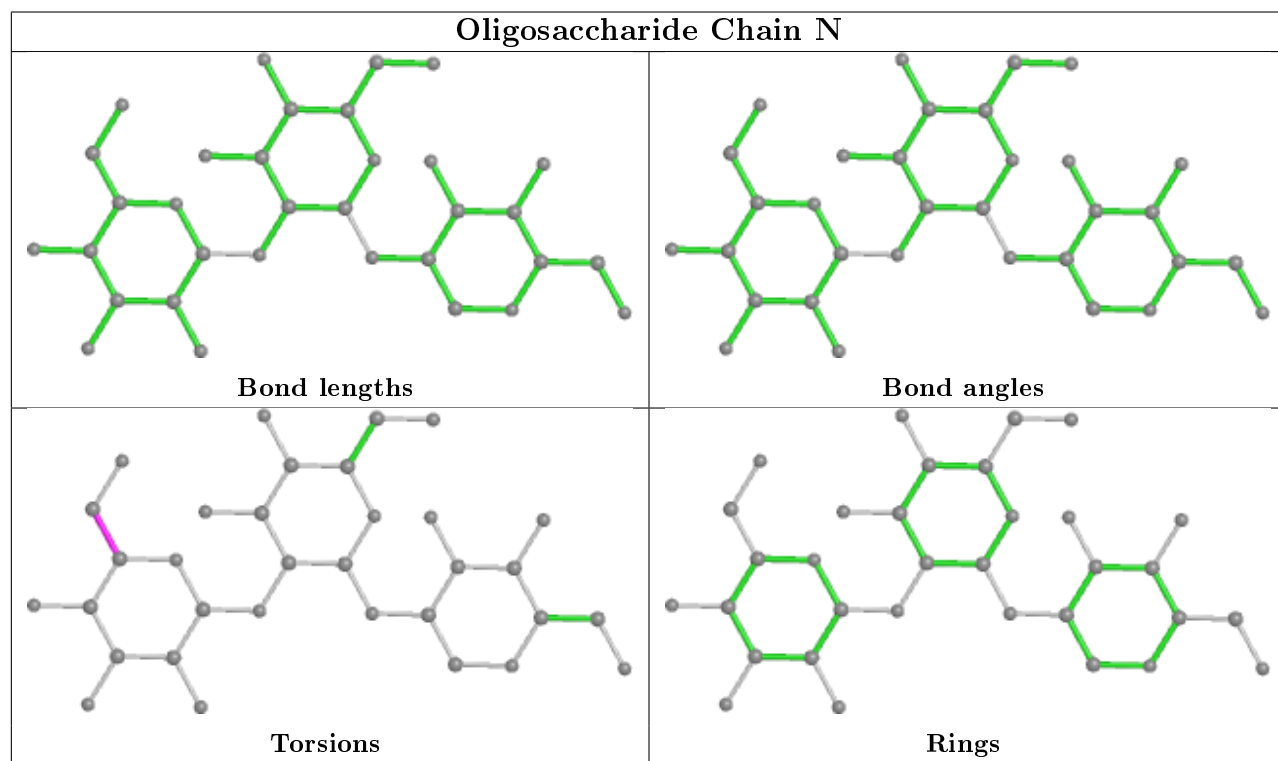
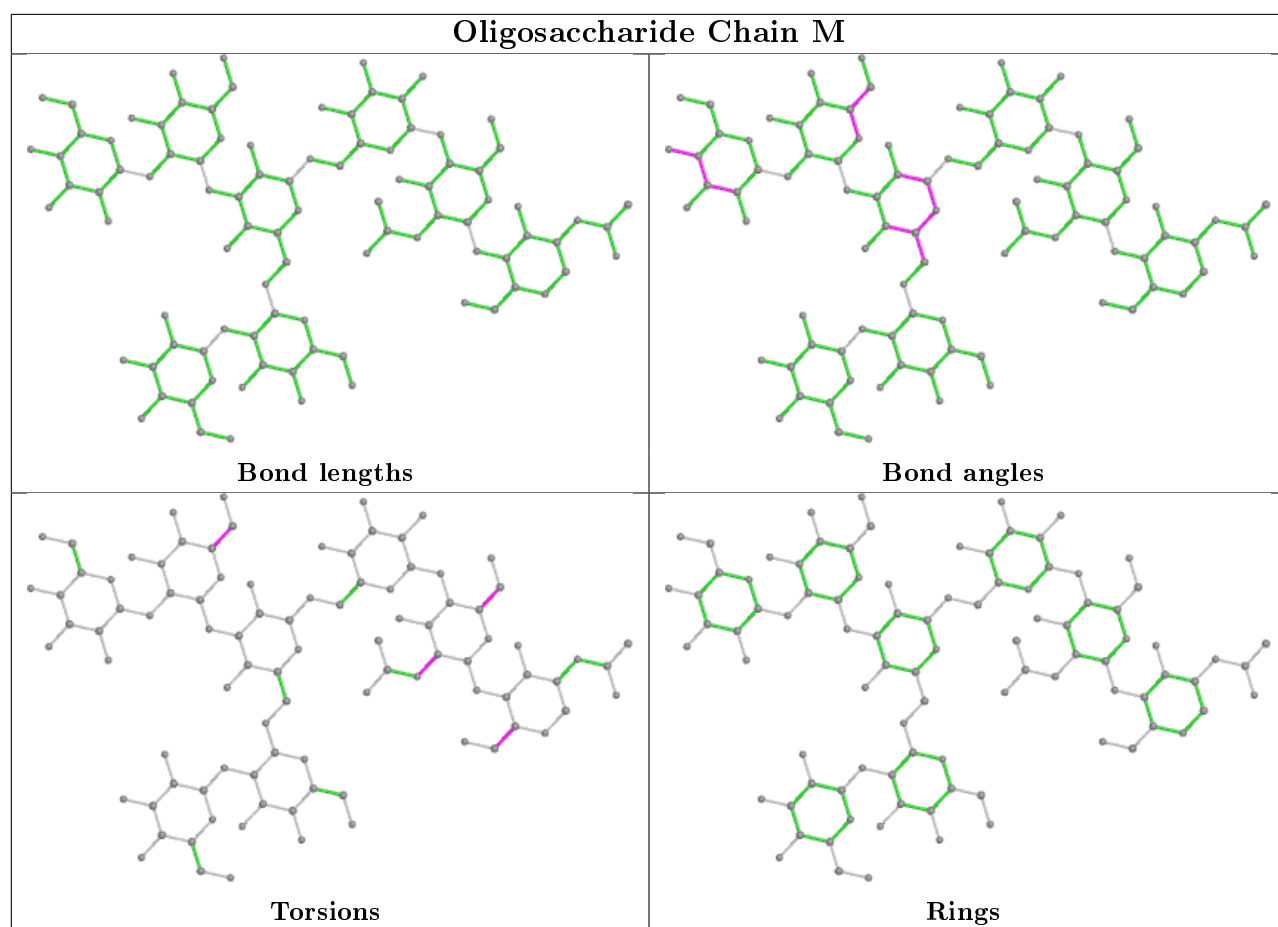
Torsions

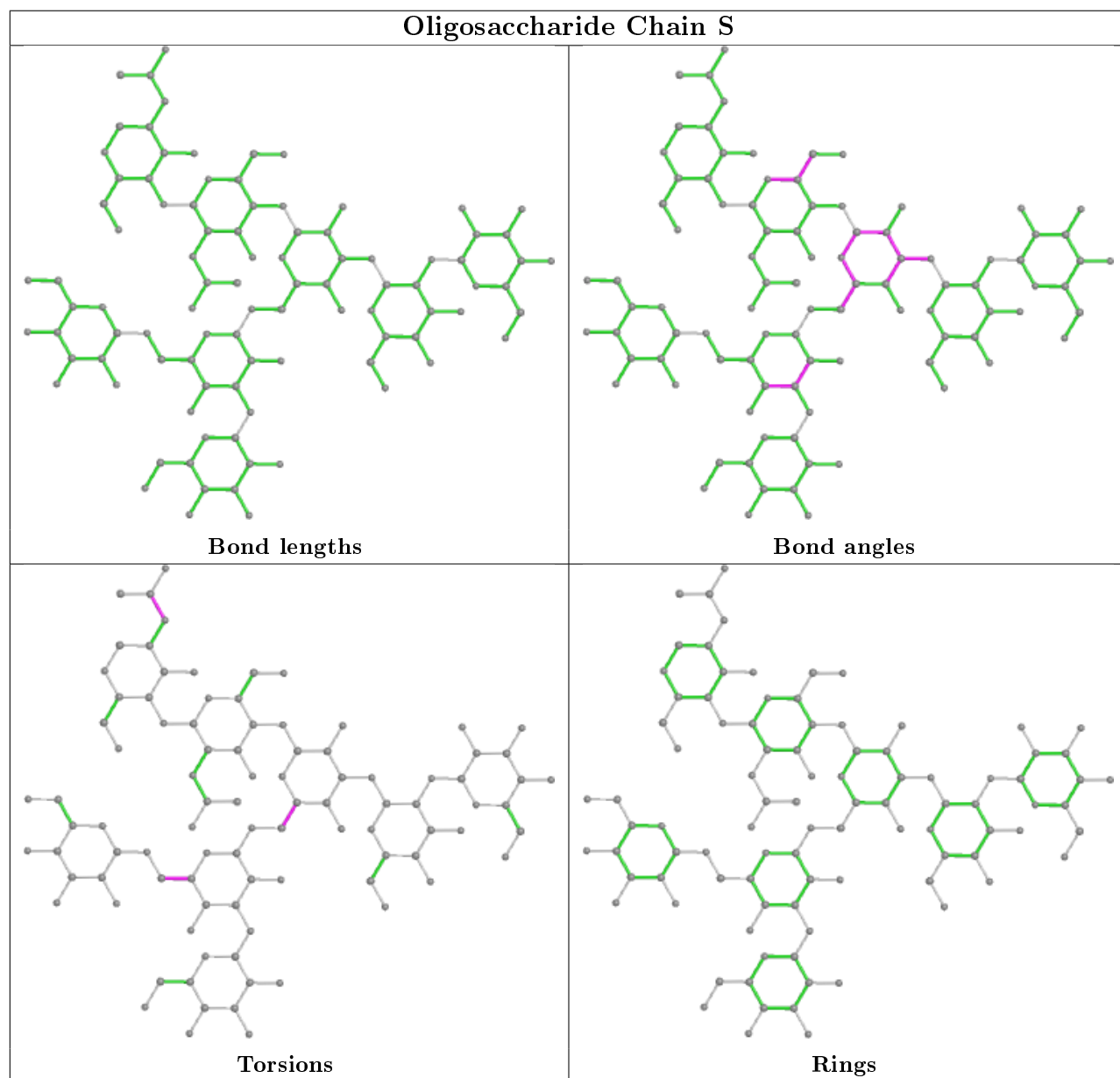
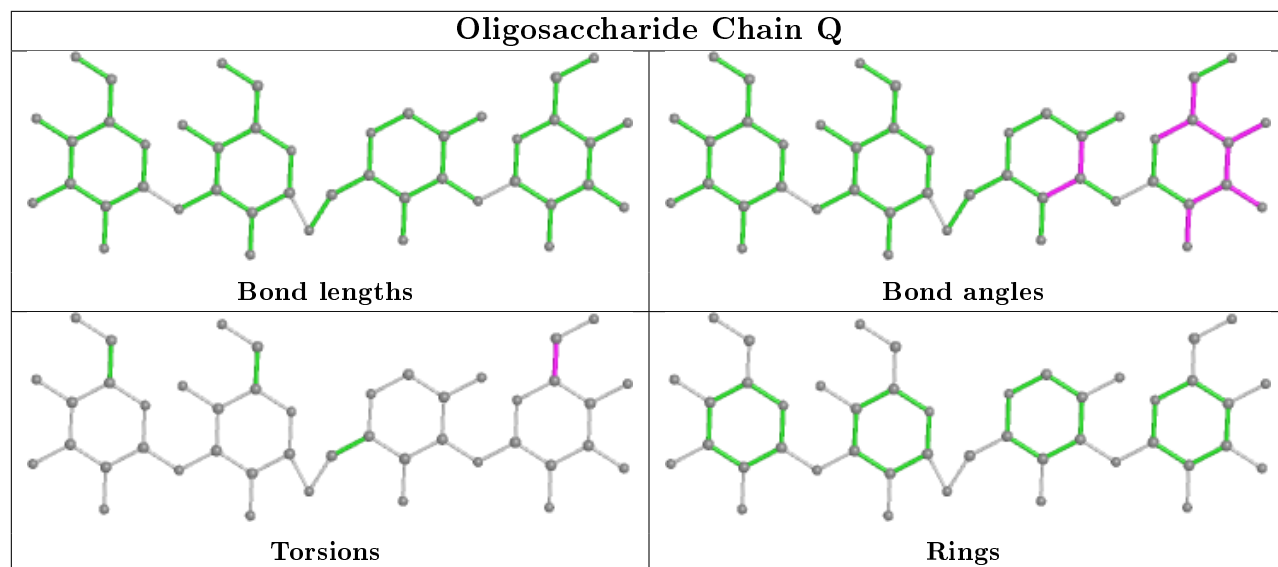


Rings









5.6 Ligand geometry

14 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	$\# Z > 2$
16	NAG	G	1840	3	14,14,15	0.97	0	17,19,21	1.69	2 (11%)
16	NAG	G	1235	-	14,14,15	0.56	0	17,19,21	0.84	0
16	NAG	G	1133	-	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
17	MAN	G	1266	-	11,11,12	0.36	0	15,15,17	0.78	0
16	NAG	G	1137	3	14,14,15	0.60	0	17,19,21	0.81	0
16	NAG	G	1839	3	14,14,15	0.59	0	17,19,21	0.81	0
16	NAG	G	1234	-	14,14,15	0.42	0	17,19,21	1.18	2 (11%)
17	MAN	G	1201	-	11,11,12	0.58	0	15,15,17	3.36	4 (26%)
16	NAG	G	1611	3	14,14,15	0.60	0	17,19,21	1.03	0
16	NAG	G	1355	3	14,14,15	0.42	0	17,19,21	0.81	0
16	NAG	G	1088	3	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
16	NAG	G	1625	3	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
16	NAG	G	1637	3	14,14,15	0.54	0	17,19,21	0.90	0
16	NAG	G	1618	3	14,14,15	0.62	0	17,19,21	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	NAG	G	1840	3	-	3/6/23/26	0/1/1/1
16	NAG	G	1235	-	-	0/6/23/26	0/1/1/1
16	NAG	G	1133	-	-	0/6/23/26	0/1/1/1
17	MAN	G	1266	-	-	1/2/19/22	0/1/1/1
16	NAG	G	1137	3	-	1/6/23/26	0/1/1/1
16	NAG	G	1839	3	-	0/6/23/26	0/1/1/1
16	NAG	G	1234	-	-	0/6/23/26	0/1/1/1
17	MAN	G	1201	-	-	0/2/19/22	0/1/1/1
16	NAG	G	1611	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	NAG	G	1355	3	-	0/6/23/26	0/1/1/1
16	NAG	G	1088	3	-	0/6/23/26	0/1/1/1
16	NAG	G	1625	3	-	0/6/23/26	0/1/1/1
16	NAG	G	1637	3	-	0/6/23/26	0/1/1/1
16	NAG	G	1618	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	1201	MAN	O2-C2-C3	8.18	126.53	110.14
17	G	1201	MAN	O3-C3-C4	-5.93	96.63	110.35
17	G	1201	MAN	O4-C4-C5	-5.75	95.01	109.30
16	G	1840	NAG	C2-N2-C7	5.40	130.60	122.90
17	G	1201	MAN	O5-C5-C6	-5.06	99.27	107.20

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	G	1840	NAG	C8-C7-N2-C2
16	G	1840	NAG	O7-C7-N2-C2
17	G	1266	MAN	O5-C5-C6-O6
16	G	1137	NAG	O5-C5-C6-O6
16	G	1611	NAG	C3-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	1235	NAG	2	0
16	G	1133	NAG	8	0
17	G	1266	MAN	14	0
16	G	1137	NAG	1	0
16	G	1234	NAG	2	0
17	G	1201	MAN	2	0
16	G	1088	NAG	1	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	D	171/223 (76%)	0.55	22 (12%) 3 4	81, 125, 206, 214	0
2	E	182/209 (87%)	1.01	40 (21%) 0 1	130, 168, 244, 255	0
3	G	610/638 (95%)	0.39	29 (4%) 30 31	58, 91, 145, 196	2 (0%)
4	H	232/235 (98%)	0.24	15 (6%) 18 20	96, 123, 149, 161	0
5	L	210/213 (98%)	0.31	17 (8%) 12 13	90, 119, 177, 199	0
All	All	1405/1518 (92%)	0.45	123 (8%) 10 11	58, 115, 211, 255	2 (0%)

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	179	SER	11.7
2	E	133	VAL	8.0
3	G	150	MET	7.1
5	L	6	ALA	6.5
2	E	120	PRO	6.4

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
7	BMA	C	3	11/12	0.34	0.26	171,177,190,195	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MAN	F	5	11/12	0.54	0.47	126,128,129,129	11
8	MAN	F	7	11/12	0.55	0.29	151,153,155,156	11
9	BMA	I	3	11/12	0.65	0.19	157,158,162,162	0
11	BMA	K	3	11/12	0.67	0.23	148,150,153,154	0
9	MAN	I	4	11/12	0.68	0.32	153,155,157,157	11
15	MAN	S	4	11/12	0.70	0.36	157,158,159,160	11
8	BMA	F	3	11/12	0.70	0.36	143,144,147,149	11
15	MAN	S	5	11/12	0.70	0.27	161,162,163,163	11
15	MAN	S	6	11/12	0.72	0.13	159,160,162,163	0
11	MAN	K	4	11/12	0.72	0.25	145,147,150,150	0
12	BMA	M	3	11/12	0.73	0.16	84,102,116,128	0
8	MAN	F	8	11/12	0.74	0.42	53,53,53,53	0
9	NAG	O	1	14/15	0.76	0.26	142,144,145,146	0
9	NAG	I	2	14/15	0.77	0.36	156,159,161,163	14
14	MAN	Q	3	11/12	0.77	0.21	144,152,155,158	0
10	NAG	P	2	14/15	0.77	0.24	141,142,143,143	0
15	NAG	S	2	14/15	0.79	0.18	154,155,157,157	0
9	MAN	I	5	11/12	0.79	0.34	161,163,165,166	0
7	NAG	C	2	14/15	0.81	0.31	136,151,158,165	0
15	BMA	S	3	11/12	0.81	0.11	157,159,160,160	0
12	MAN	M	8	11/12	0.81	0.27	155,160,166,168	11
7	BMA	B	3	11/12	0.81	0.28	138,140,141,141	0
14	BMA	Q	1	11/12	0.82	0.19	39,39,39,39	0
14	MAN	Q	4	11/12	0.82	0.25	39,39,39,39	0
10	NAG	R	2	14/15	0.82	0.17	157,159,161,162	0
7	NAG	B	2	14/15	0.82	0.25	136,136,138,139	0
10	NAG	R	1	14/15	0.82	0.21	142,150,157,158	0
7	NAG	C	1	14/15	0.83	0.28	123,140,152,157	0
6	MAN	A	5	11/12	0.83	0.24	133,134,135,137	11
15	MAN	S	8	11/12	0.84	0.29	39,39,39,39	0
12	MAN	M	6	11/12	0.84	0.21	39,39,39,39	11
13	MAN	N	3	11/12	0.84	0.30	142,143,147,150	0
8	MAN	F	6	11/12	0.84	0.29	39,39,39,39	0
9	NAG	I	1	14/15	0.84	0.23	154,157,161,162	0
7	NAG	B	1	14/15	0.85	0.19	133,134,135,135	0
10	NAG	P	1	14/15	0.85	0.18	53,53,53,53	0
6	MAN	A	6	11/12	0.85	0.13	136,136,139,139	0
12	NAG	M	2	14/15	0.86	0.22	61,89,109,117	0
14	MAN	Q	2	11/12	0.86	0.22	152,155,159,159	11
9	BMA	O	3	11/12	0.87	0.10	53,53,53,53	0
12	MAN	M	5	11/12	0.87	0.24	150,152,158,158	11
15	NAG	S	1	14/15	0.88	0.19	149,150,153,153	0

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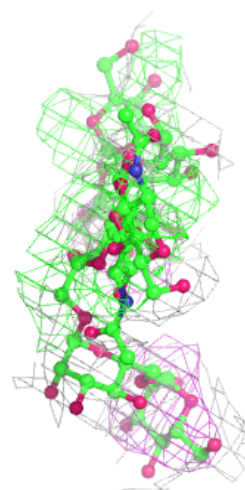
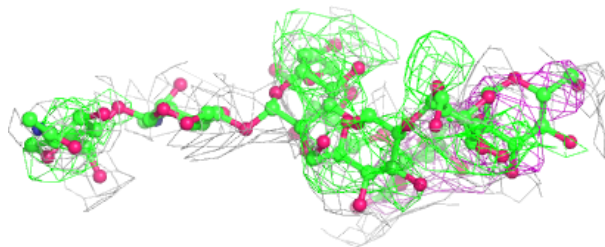
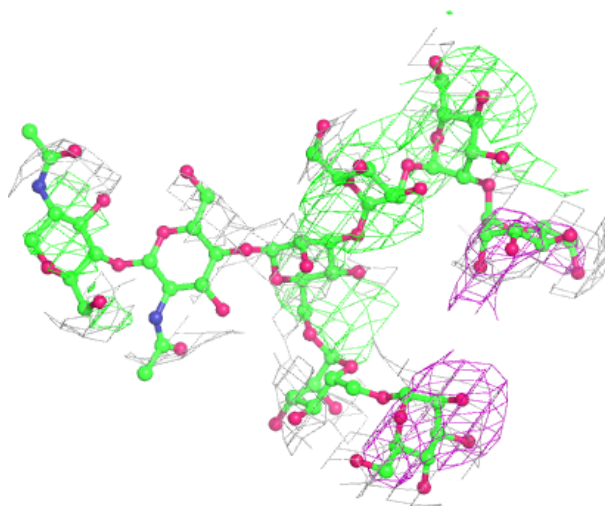
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	MAN	M	4	11/12	0.88	0.13	147,149,152,154	0
9	NAG	O	2	14/15	0.88	0.15	39,39,39,39	0
13	MAN	N	1	11/12	0.89	0.26	134,136,138,138	0
11	NAG	K	2	14/15	0.89	0.14	140,143,146,146	0
12	NAG	M	1	14/15	0.89	0.16	87,106,110,121	0
15	MAN	S	7	11/12	0.89	0.13	157,158,159,159	0
9	MAN	O	5	11/12	0.90	0.23	39,39,39,39	0
8	MAN	F	4	11/12	0.90	0.32	136,140,142,142	11
6	MAN	A	7	11/12	0.90	0.29	53,53,53,53	0
6	NAG	A	2	14/15	0.91	0.19	130,131,132,132	0
6	NAG	A	1	14/15	0.91	0.28	128,129,130,130	0
10	NAG	J	2	14/15	0.91	0.12	146,148,151,152	0
10	NAG	J	1	14/15	0.92	0.17	138,142,145,146	0
13	MAN	N	2	11/12	0.92	0.21	139,140,143,145	0
11	NAG	K	1	14/15	0.93	0.19	136,137,140,140	0
12	MAN	M	7	11/12	0.93	0.14	155,159,162,164	0
6	BMA	A	3	11/12	0.93	0.07	132,134,135,135	0
6	MAN	A	4	11/12	0.93	0.16	133,134,135,135	0
8	NAG	F	2	14/15	0.93	0.19	138,144,151,153	0
9	MAN	O	4	11/12	0.93	0.18	141,146,148,149	0
8	NAG	F	1	14/15	0.95	0.27	136,142,148,149	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.

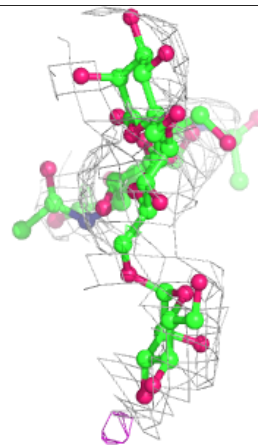
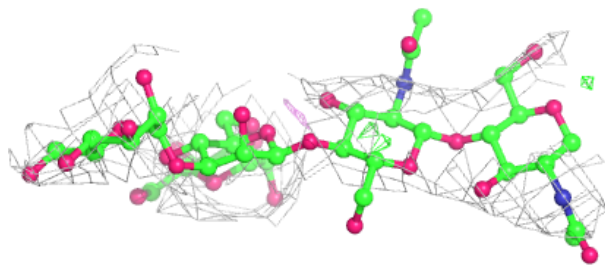
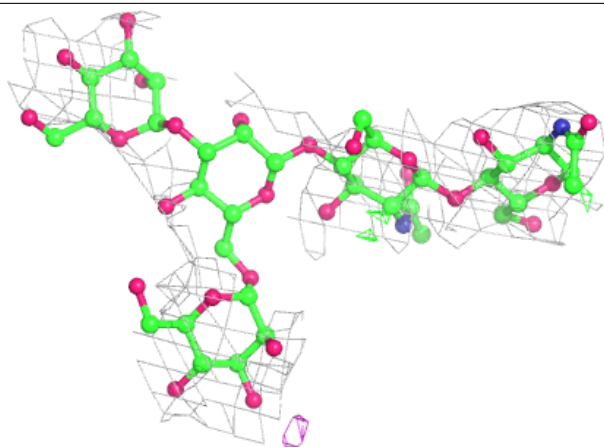
Electron density around Chain F:

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



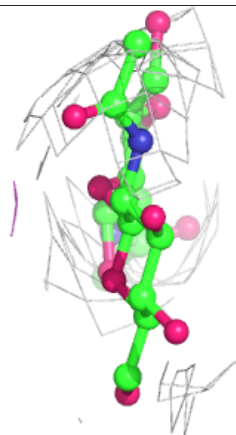
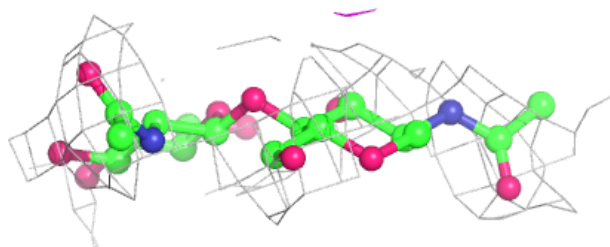
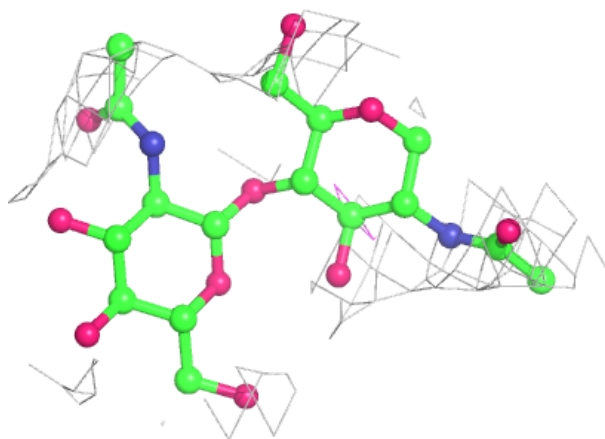
Electron density around Chain I:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



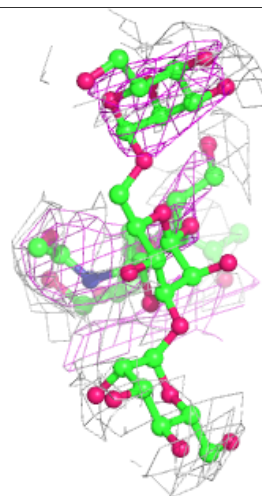
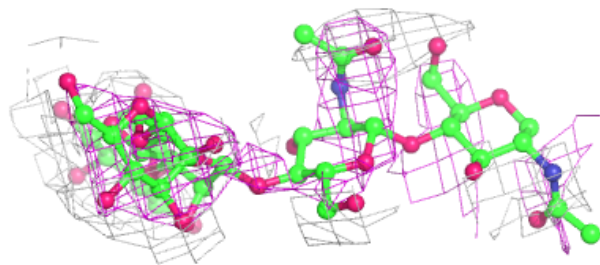
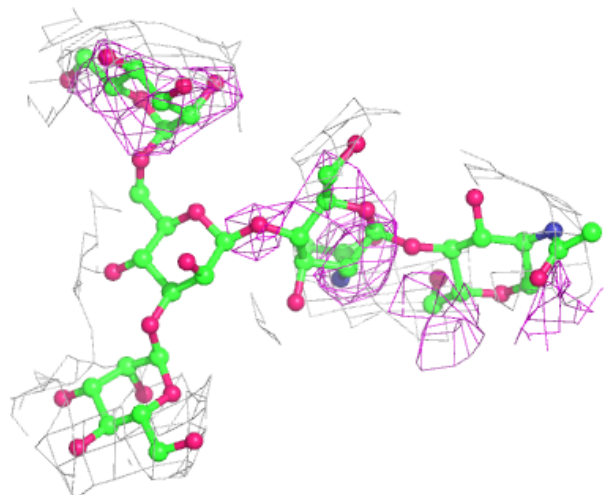
Electron density around Chain J:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



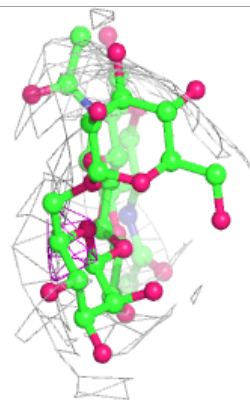
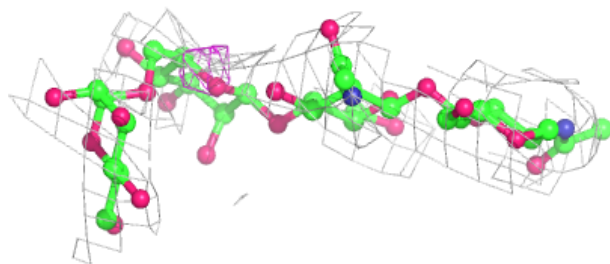
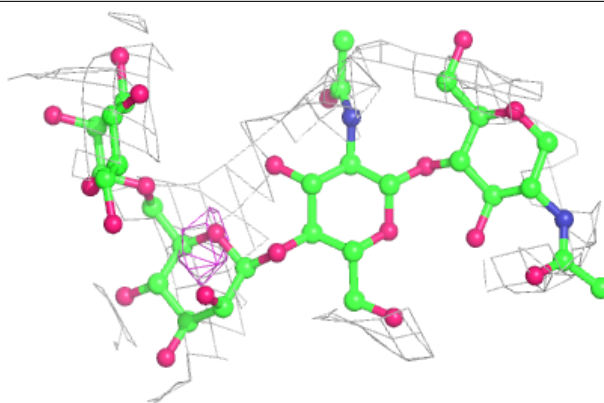
Electron density around Chain O:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



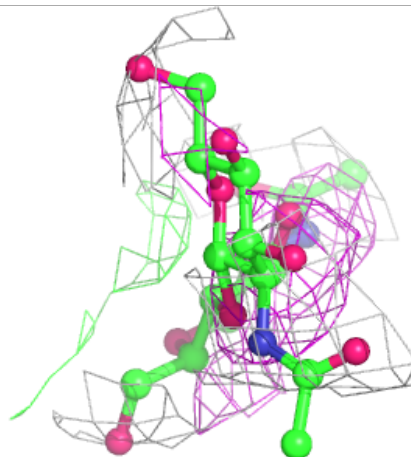
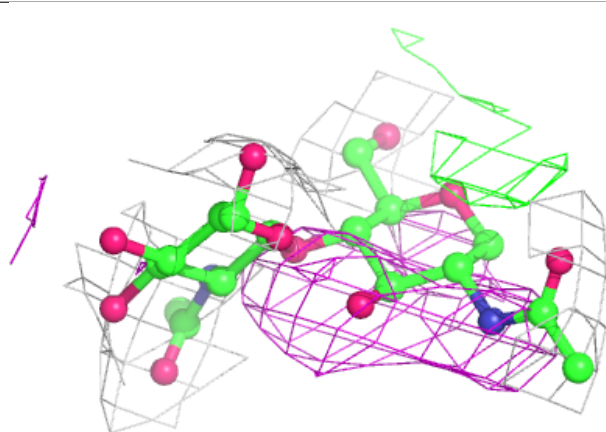
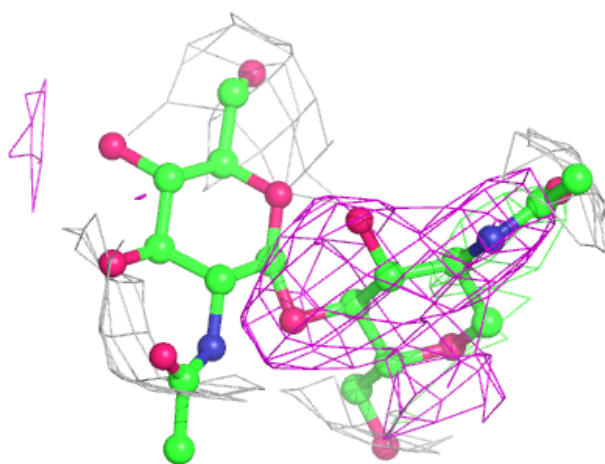
Electron density around Chain K:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



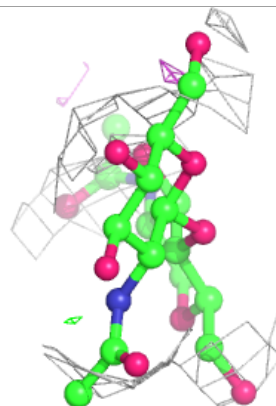
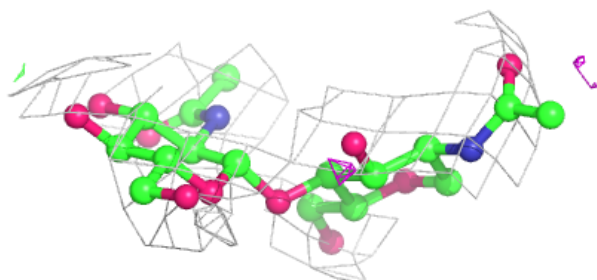
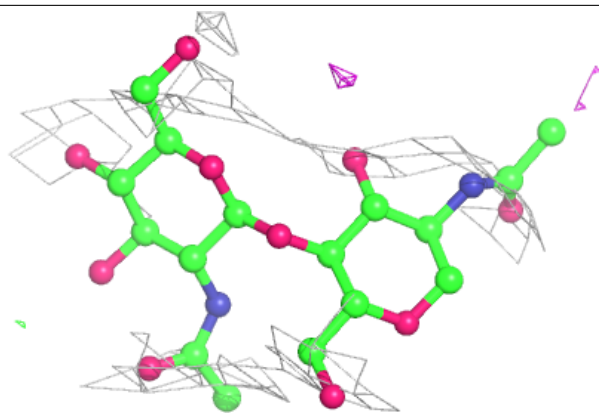
Electron density around Chain P:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

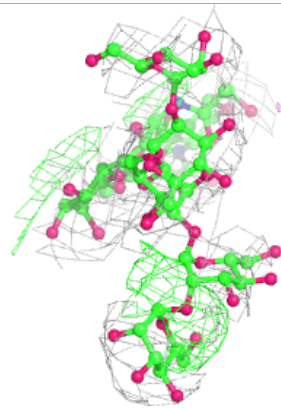
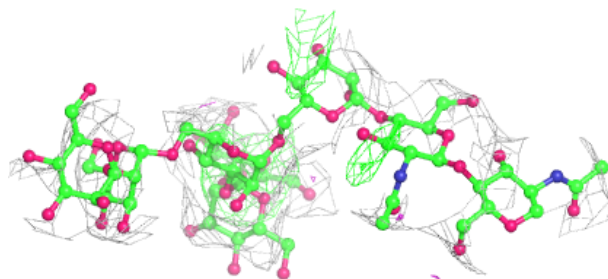
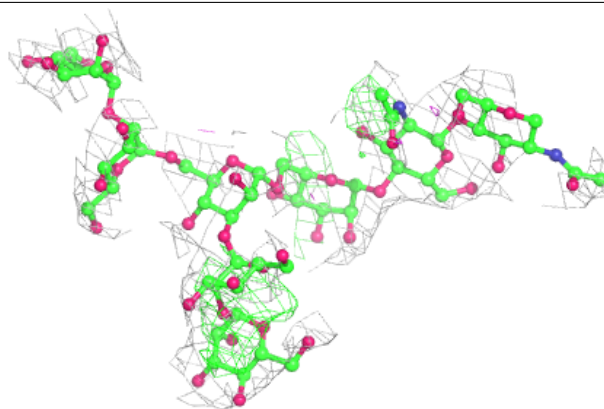


Electron density around Chain R:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

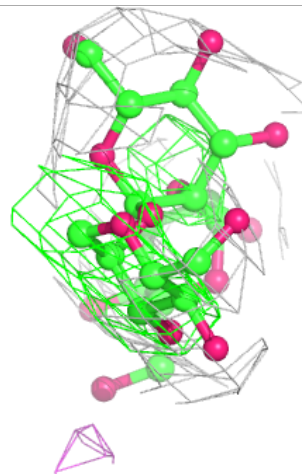
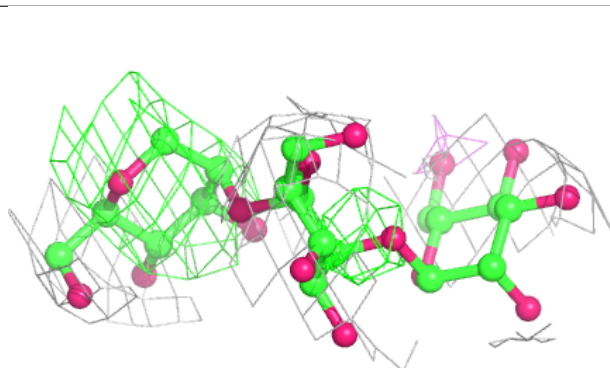
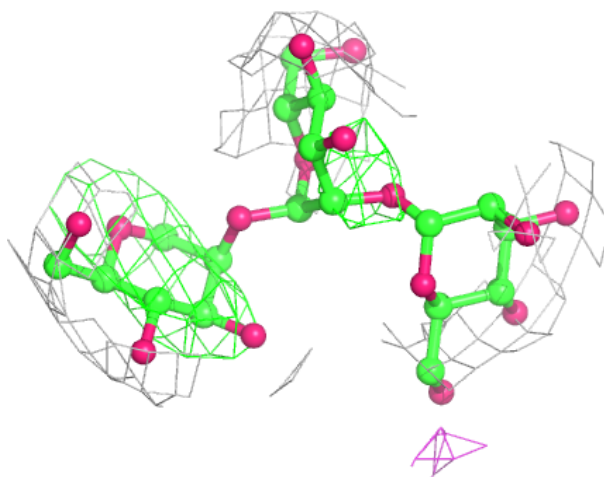
**Electron density around Chain M:**

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



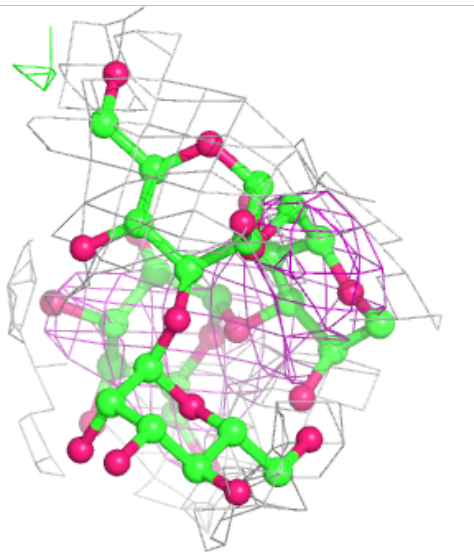
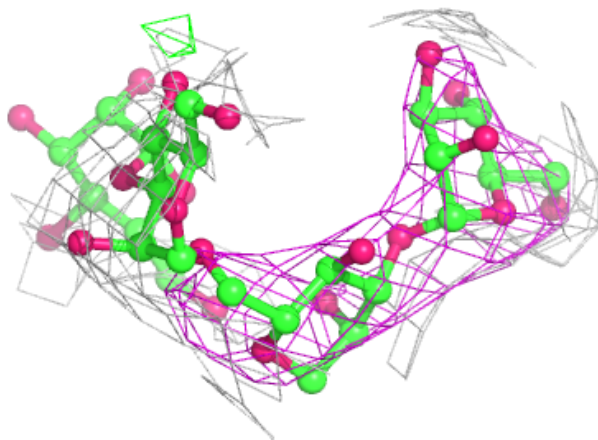
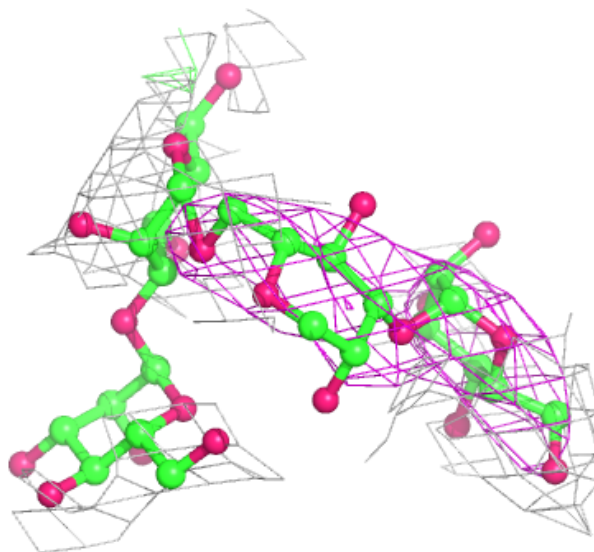
Electron density around Chain N:

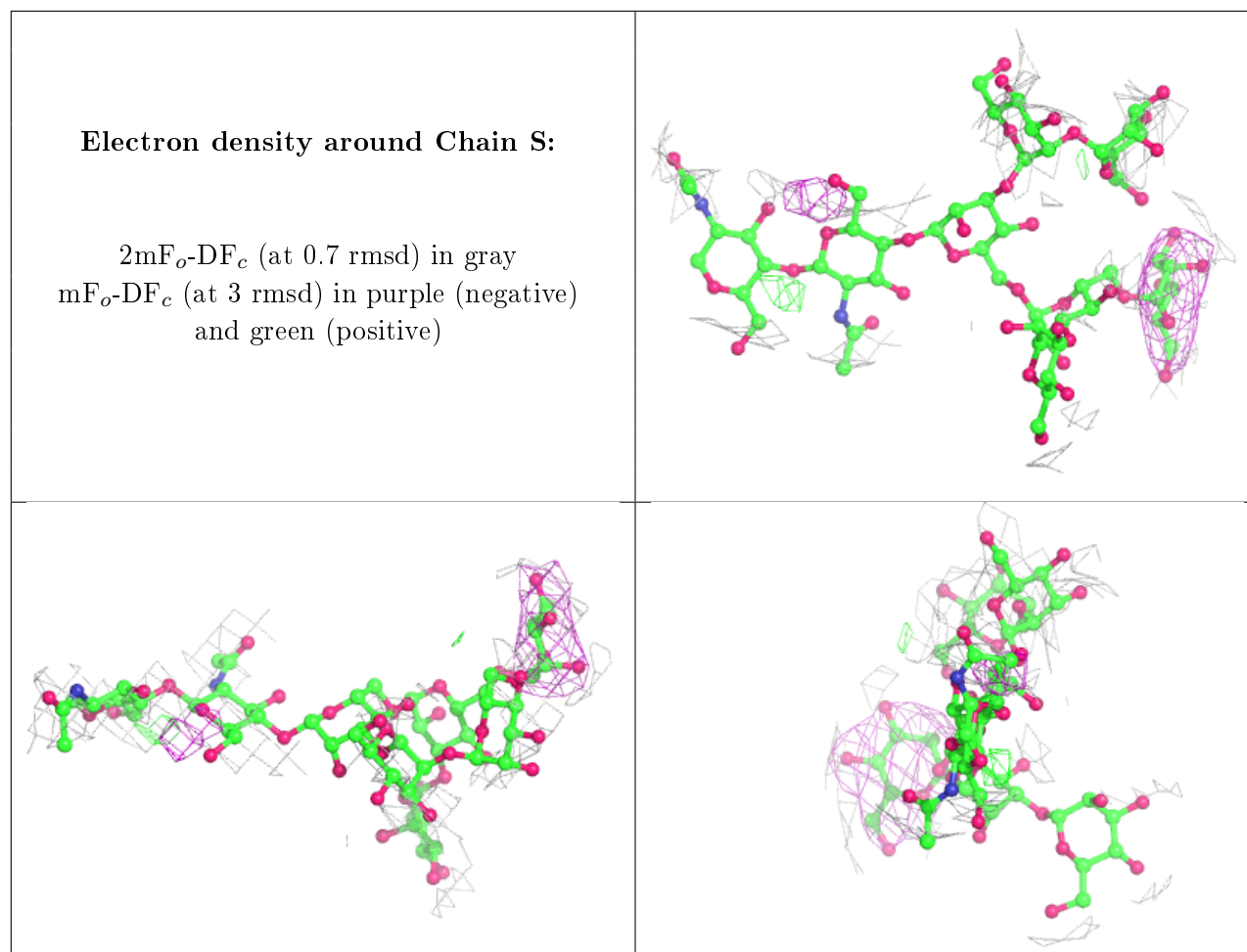
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Q:

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	MAN	G	1266	11/12	0.61	0.46	126,128,129,129	11
16	NAG	G	1088	14/15	0.67	0.29	53,53,53,53	0
16	NAG	G	1840	14/15	0.68	0.63	130,132,133,133	0
16	NAG	G	1355	14/15	0.70	0.44	63,63,63,63	14
16	NAG	G	1235	14/15	0.72	0.45	152,153,156,158	14
16	NAG	G	1839	14/15	0.72	0.30	159,165,169,170	0
16	NAG	G	1137	14/15	0.75	0.31	132,135,138,139	0
17	MAN	G	1201	11/12	0.76	0.37	39,39,39,39	0
16	NAG	G	1133	14/15	0.78	0.25	53,53,53,53	0
16	NAG	G	1625	14/15	0.78	0.36	53,53,53,53	0
16	NAG	G	1611	14/15	0.86	0.27	157,160,162,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	NAG	G	1234	14/15	0.86	0.23	53,53,53,53	0
16	NAG	G	1618	14/15	0.87	0.18	170,176,181,184	0
16	NAG	G	1637	14/15	0.91	0.21	155,156,158,159	0

6.5 Other polymers [i](#)

There are no such residues in this entry.