



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 04:56 AM BST

PDB ID : 4TVP
Title : Crystal Structure of the HIV-1 BG505 SOSIP.664 Env Trimer Ectodomain, Comprising Atomic-Level Definition of Pre-Fusion gp120 and gp41, in Complex with Human Antibodies PGT122 and 35O22
Authors : Pancera, M.; Zhou, T.; Kwong, P.D.
Deposited on : 2014-06-27
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

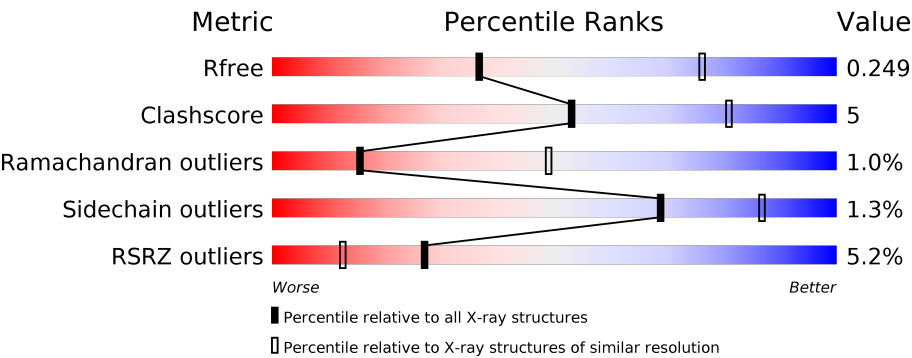
1 Overall quality at a glance i

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	G	481	<div><div>15%</div><div>78%15%6%</div></div>
2	B	153	<div><div>3%</div><div>66%14%18%</div></div>
3	L	213	<div><div></div><div>81%17%..</div></div>
4	H	235	<div><div>3%</div><div>81%16%. </div></div>
5	D	243	<div><div>15%</div><div>88%12%</div></div>
6	E	216	<div><div>12%</div><div>86%13%. </div></div>

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Mol	Chain	Length	Quality of chain
7	A	7	
8	C	4	
9	F	2	
9	J	2	
9	K	2	
9	M	2	
9	P	2	
9	Q	2	
9	R	2	
9	S	2	
10	I	6	
11	N	3	
12	O	5	
13	T	10	

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
15	SO4	G	606	-	-	-	X
8	MAN	C	4	-	-	-	X
9	NAG	K	2	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 12188 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	453	Total	C	N	O	S	0	0	0
			3565	2236	630	671	28			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S5
G	501	CYS	ALA	engineered mutation	UNP Q2N0S5
G	509	ARG	-	expression tag	UNP Q2N0S5
G	510	ARG	-	expression tag	UNP Q2N0S5
G	511	ARG	-	expression tag	UNP Q2N0S5
G	512	ARG	-	expression tag	UNP Q2N0S5
G	513	ARG	-	expression tag	UNP Q2N0S5

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S5
B	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 3 is a protein called PGT122 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 4 is a protein called PGT122 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

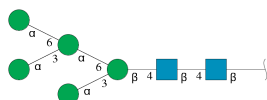
- Molecule 5 is a protein called 35O22 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			

- Molecule 6 is a protein called 35O22 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



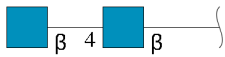
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



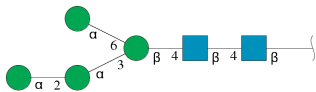
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 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
9	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



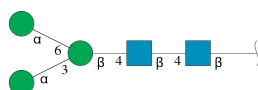
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 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.



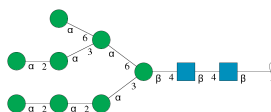
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 12 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
12	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



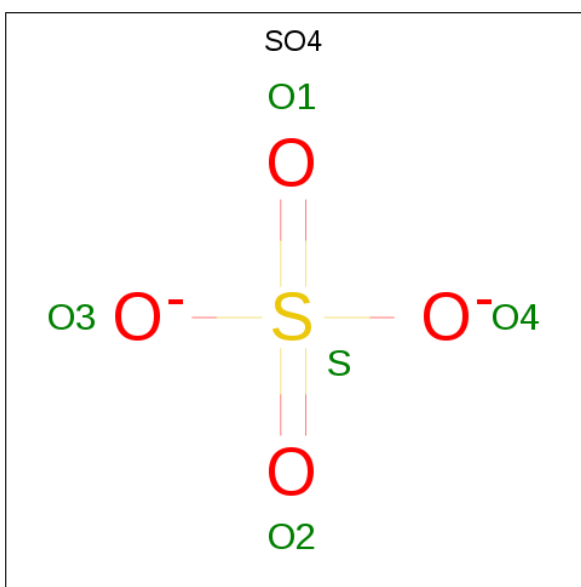
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	T	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 15 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	B	1	Total	O	S	0	0
			5	4	1		
15	B	1	Total	O	S	0	0
			5	4	1		
15	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	17	Total	O	0	0
			17	17		
16	B	2	Total	O	0	0
			2	2		

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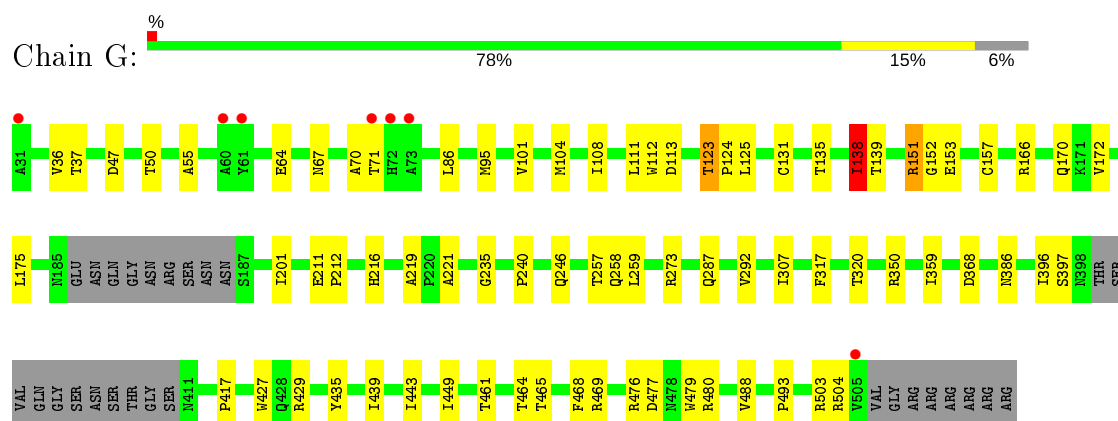
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	3	Total 3	O 3	0	0
16	H	2	Total 2	O 2	0	0
16	D	11	Total 11	O 11	0	0
16	E	2	Total 2	O 2	0	0

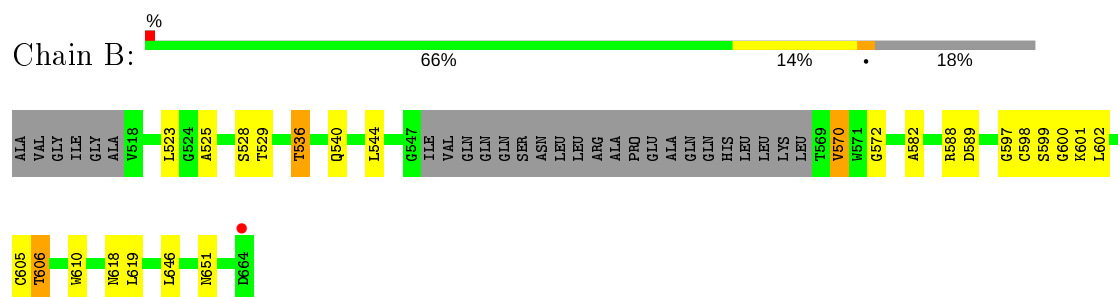
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

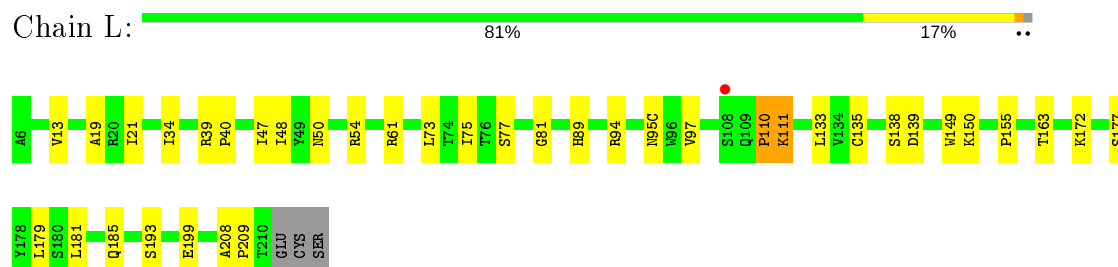
- Molecule 1: Envelope glycoprotein gp160



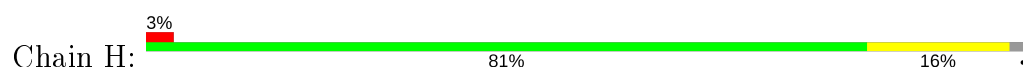
- Molecule 2: Envelope glycoprotein gp160

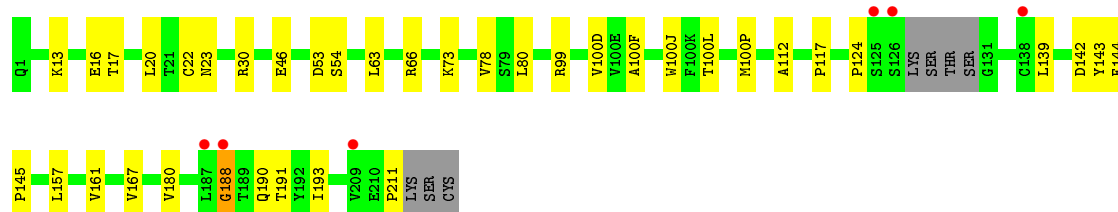


- Molecule 3: PGT122 Light chain

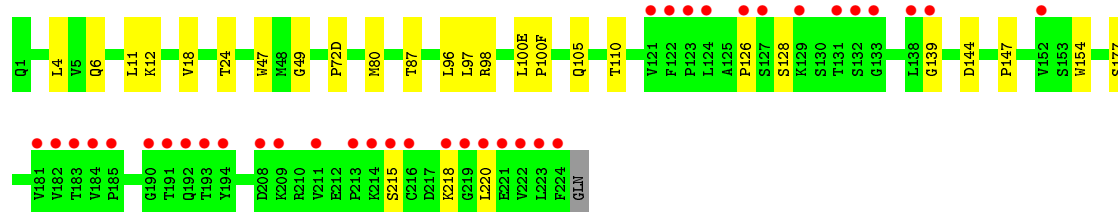
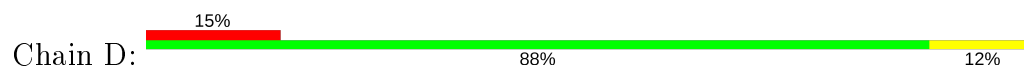


- Molecule 4: PGT122 Heavy chain

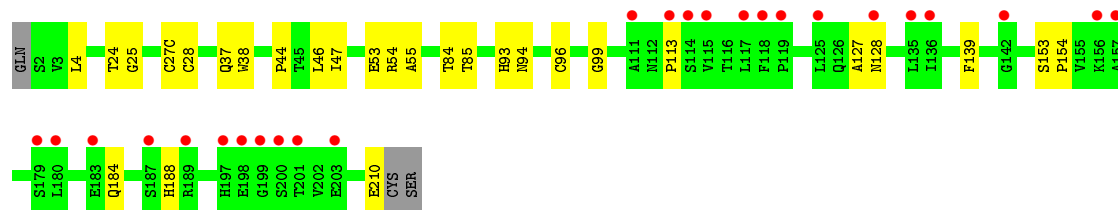
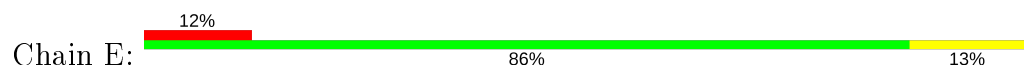




- Molecule 5: 35O22 Heavy chain



- Molecule 6: 35O22 Light chain



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%

GLU1
GLU2

- Molecule 10: alpha-D-mannopyranose-(1-2)-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:  50% 50%

GLU1
GLU2
GLU3
MAN4
MAN5
MAN6

- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

GLU1
GLU2
GLU3

- Molecule 12: 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:  60% 40%

GLU1
GLU2
GLU3
MAN4
MAN5

- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 T:  10% 70% 20%

GLU1
GLU2
GLU3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	128.89Å 128.89Å 313.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.74 – 3.10 40.74 – 3.10	Depositor EDS
% Data completeness (in resolution range)	55.0 (40.74-3.10) 55.1 (40.74-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.213 , 0.248 0.216 , 0.249	Depositor DCC
R_{free} test set	1451 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	76.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.086 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12188	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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: SO4, 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	G	0.21	0/3639	0.40	0/4941
2	B	0.20	0/1019	0.37	0/1382
3	L	0.20	0/1632	0.39	0/2236
4	H	0.20	0/1789	0.38	0/2443
5	D	0.20	0/1880	0.37	0/2560
6	E	0.20	0/1659	0.37	0/2269
All	All	0.20	0/11618	0.39	0/15831

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	G	3565	0	3495	43	0
2	B	1001	0	975	15	0
3	L	1589	0	1530	22	0
4	H	1742	0	1715	21	0
5	D	1832	0	1806	16	0
6	E	1615	0	1542	16	0
7	A	83	0	70	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	50	0	43	2	0
9	F	28	0	25	0	0
9	J	28	0	25	0	0
9	K	28	0	25	0	0
9	M	28	0	25	0	0
9	P	28	0	25	2	0
9	Q	28	0	25	0	0
9	R	28	0	25	0	0
9	S	28	0	25	0	0
10	I	72	0	61	0	0
11	N	39	0	34	0	0
12	O	61	0	52	0	0
13	T	116	0	97	2	0
14	B	42	0	39	2	0
14	G	56	0	52	1	0
14	H	14	0	13	0	0
15	B	10	0	0	1	0
15	G	35	0	0	2	0
15	L	5	0	0	0	0
16	B	2	0	0	0	0
16	D	11	0	0	0	0
16	E	2	0	0	0	0
16	G	17	0	0	0	0
16	H	2	0	0	0	0
16	L	3	0	0	0	0
All	All	12188	0	11724	128	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 5.

All (128) 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:G:70:ALA:HB2	1:G:111:LEU:HD11	1.69	0.75
1:G:55:ALA:HB3	1:G:216:HIS:HB2	1.71	0.71
6:E:37:GLN:HB2	6:E:47:ILE:HD11	1.74	0.68
1:G:350:ARG:NH2	1:G:396:ILE:O	2.27	0.66
5:D:6:GLN:H	5:D:105:GLN:HE22	1.43	0.66
2:B:536:THR:O	2:B:540:GLN:NE2	2.29	0.66
3:L:110:PRO:HG2	3:L:111:LYS:HD2	1.79	0.64
5:D:12:LYS:HG3	5:D:18:VAL:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:ALA:O	1:G:246:GLN:NE2	2.31	0.63
3:L:163:THR:HG22	4:H:167:VAL:HB	1.81	0.62
3:L:47:ILE:HG22	3:L:48:ILE:HG13	1.80	0.62
1:G:37:THR:HG22	2:B:605:CYS:HA	1.81	0.62
4:H:99:ARG:HG2	4:H:100(L):THR:HG22	1.83	0.60
3:L:181:LEU:HD22	3:L:185:GLN:HG2	1.83	0.60
1:G:201:ILE:HD11	1:G:435:TYR:HB2	1.82	0.60
3:L:139:ASP:H	3:L:172:LYS:HG3	1.67	0.59
3:L:39:ARG:NH1	3:L:81:GLY:O	2.35	0.59
1:G:166:ARG:NH2	15:G:606:SO4:O2	2.34	0.59
1:G:464:THR:OG1	1:G:465:THR:N	2.34	0.58
4:H:100(D):VAL:HA	13:T:2:NAG:H2	1.86	0.58
1:G:113:ASP:OD1	1:G:429:ARG:NH1	2.37	0.58
2:B:588:ARG:NH2	15:B:701:SO4:O3	2.37	0.57
1:G:292:VAL:HB	1:G:449:ILE:HB	1.85	0.57
9:P:2:NAG:H83	9:P:2:NAG:H3	1.87	0.57
5:D:100(E):LEU:HD12	5:D:100(F):PRO:HD2	1.87	0.57
7:A:2:NAG:H3	7:A:2:NAG:H83	1.87	0.56
3:L:39:ARG:HG3	3:L:40:PRO:HD2	1.87	0.56
14:G:1276:NAG:H3	14:G:1276:NAG:H83	1.88	0.55
5:D:128:SER:HB2	5:D:220:LEU:HB2	1.89	0.55
1:G:469:ARG:NH2	15:G:602:SO4:O4	2.40	0.55
5:D:4:LEU:HG	5:D:24:THR:HG22	1.90	0.54
1:G:36:VAL:HG12	2:B:610:TRP:HE3	1.74	0.53
6:E:127:ALA:N	6:E:128:ASN:HA	2.22	0.53
5:D:126:PRO:HB2	5:D:215:SER:HB2	1.91	0.53
1:G:257:THR:O	1:G:259:LEU:N	2.40	0.52
4:H:30:ARG:HD3	4:H:73:LYS:HD2	1.91	0.52
5:D:218:LYS:NZ	6:E:210:GLU:OE1	2.42	0.52
6:E:84:THR:OG1	6:E:85:THR:N	2.41	0.52
5:D:87:THR:HG23	5:D:110:THR:HA	1.92	0.52
3:L:97:VAL:HG22	4:H:46:GLU:HG3	1.93	0.51
1:G:175:LEU:HB3	1:G:320:THR:HB	1.92	0.51
4:H:188:GLY:HA3	4:H:190:GLN:N	2.26	0.51
2:B:529:THR:HG23	5:D:98:ARG:HD2	1.93	0.50
1:G:359:ILE:HD12	1:G:468:PHE:HE2	1.76	0.50
5:D:11:LEU:HD13	5:D:147:PRO:HG3	1.94	0.50
2:B:618:ASN:OD1	2:B:619:LEU:N	2.43	0.50
9:P:1:NAG:H62	9:P:2:NAG:H82	1.94	0.49
6:E:113:PRO:HB3	6:E:139:PHE:HB3	1.93	0.49
4:H:63:LEU:HD22	4:H:66:ARG:HH21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:PRO:HG3	5:D:72(D):PRO:HG2	1.93	0.49
1:G:477:ASP:OD1	1:G:480:ARG:NH1	2.46	0.49
14:B:1618:NAG:H83	6:E:54:ARG:HH21	1.78	0.49
1:G:439:ILE:HB	1:G:443:ILE:HD11	1.95	0.49
3:L:150:LYS:HB2	3:L:193:SER:HB2	1.95	0.49
6:E:24:THR:OG1	6:E:25:GLY:N	2.45	0.49
3:L:133:LEU:HD12	3:L:179:LEU:HD23	1.95	0.49
2:B:588:ARG:NH1	2:B:589:ASP:OD1	2.46	0.48
4:H:117:PRO:HB3	4:H:143:TYR:HB3	1.94	0.48
3:L:61:ARG:HD2	3:L:77:SER:HB2	1.95	0.48
3:L:149:TRP:HE1	3:L:177:SER:HG	1.62	0.48
2:B:598:CYS:O	2:B:600:GLY:N	2.45	0.47
4:H:191:THR:HG22	4:H:193:ILE:HG13	1.96	0.47
1:G:476:ARG:HA	1:G:479:TRP:CD1	2.49	0.47
1:G:221:ALA:HB3	2:B:582:ALA:HB1	1.96	0.47
1:G:170:GLN:HG2	1:G:172:VAL:HG13	1.96	0.47
1:G:95:MET:SD	1:G:273:ARG:HD3	2.55	0.47
4:H:100(D):VAL:O	4:H:100(F):ALA:N	2.43	0.47
4:H:53:ASP:OD1	4:H:54:SER:N	2.42	0.46
5:D:47:TRP:CZ2	5:D:49:GLY:HA2	2.51	0.46
1:G:386:ASN:HB3	1:G:417:PRO:HD2	1.97	0.46
5:D:144:ASP:H	5:D:177:SER:HG	1.62	0.46
1:G:123:THR:HG23	1:G:124:PRO:HD3	1.97	0.46
1:G:138:ILE:CB	1:G:139:THR:HA	2.46	0.46
2:B:525:ALA:HB1	2:B:528:SER:HB2	1.97	0.45
5:D:96:LEU:HG	5:D:97:LEU:HG	1.98	0.45
1:G:138:ILE:HB	1:G:139:THR:HA	1.98	0.45
3:L:138:SER:HB2	3:L:172:LYS:HE2	1.99	0.45
1:G:101:VAL:HG13	1:G:479:TRP:HB2	1.99	0.45
1:G:101:VAL:HG21	1:G:480:ARG:HG2	1.98	0.45
4:H:20:LEU:HD12	4:H:80:LEU:HD22	1.98	0.45
3:L:150:LYS:HD3	3:L:155:PRO:HA	1.99	0.45
6:E:153:SER:HA	6:E:154:PRO:HD2	1.76	0.44
4:H:144:PHE:HA	4:H:145:PRO:HA	1.78	0.44
2:B:606:THR:HG21	2:B:646:LEU:HD22	1.98	0.44
4:H:100(L):THR:HG21	8:C:4:MAN:H62	1.99	0.44
1:G:135:THR:O	3:L:94:ARG:NE	2.42	0.44
3:L:21:ILE:HB	3:L:73:LEU:HB3	1.98	0.44
6:E:4:LEU:HB3	6:E:99:GLY:HA2	1.99	0.43
4:H:161:VAL:HG22	4:H:180:VAL:HG22	2.00	0.43
4:H:16:GLU:HG2	4:H:17:THR:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:38:TRP:CG	6:E:44:PRO:HB3	2.53	0.43
4:H:22:CYS:HB3	4:H:78:VAL:HB	2.01	0.43
3:L:19:ALA:HB3	3:L:75:ILE:HB	1.99	0.43
2:B:570:VAL:C	2:B:572:GLY:H	2.22	0.43
6:E:184:GLN:O	6:E:188:HIS:ND1	2.47	0.43
4:H:157:LEU:HD21	4:H:180:VAL:HG11	2.00	0.43
5:D:126:PRO:O	5:D:215:SER:OG	2.31	0.42
6:E:27(C):CYS:HA	6:E:28:CYS:HA	1.58	0.42
1:G:493:PRO:HG3	2:B:544:LEU:HD21	2.00	0.42
4:H:13:LYS:NZ	4:H:112:ALA:O	2.52	0.42
6:E:94:ASN:HD21	7:A:6:MAN:H2	1.85	0.42
3:L:13:VAL:HG21	3:L:19:ALA:HA	2.01	0.42
7:A:3:BMA:H61	7:A:4:MAN:H2	1.29	0.42
6:E:93:HIS:CG	7:A:7:MAN:H2	2.55	0.42
1:G:396:ILE:HG22	1:G:397:SER:H	1.84	0.42
1:G:86:LEU:HD22	2:B:523:LEU:O	2.20	0.41
3:L:135:CYS:HB3	3:L:177:SER:HB3	2.01	0.41
1:G:503:ARG:HB3	1:G:504:ARG:H	1.76	0.41
3:L:208:ALA:HA	3:L:209:PRO:HD3	1.88	0.41
13:T:8:MAN:H2	13:T:9:MAN:H2	1.86	0.41
1:G:131:CYS:HA	1:G:157:CYS:HA	2.02	0.41
1:G:211:GLU:HA	1:G:212:PRO:HD3	1.90	0.41
1:G:273:ARG:NH1	1:G:287:GLN:OE1	2.52	0.41
1:G:138:ILE:HB	8:C:1:NAG:H61	2.03	0.41
3:L:34:ILE:HD13	3:L:50:ASN:H	1.86	0.41
6:E:46:LEU:HG	6:E:55:ALA:HB2	2.03	0.41
1:G:151:ARG:O	1:G:153:GLU:N	2.54	0.41
1:G:307:ILE:HD11	1:G:317:PHE:HD2	1.86	0.41
4:H:124:PRO:HD2	4:H:211:PRO:HA	2.02	0.41
1:G:50:THR:HG22	1:G:488:VAL:HG11	2.03	0.41
3:L:89:HIS:NE2	3:L:95(C):ASN:O	2.38	0.41
5:D:139:GLY:HA2	5:D:154:TRP:CZ2	2.56	0.40
14:B:1618:NAG:H4	6:E:53:GLU:HG2	2.04	0.40
1:G:112:TRP:CG	1:G:427:TRP:HZ3	2.39	0.40
4:H:100(P):MET:SD	4:H:100(P):MET:N	2.94	0.40
2:B:597:GLY:HA2	2:B:651:ASN:HD21	1.87	0.40
1:G:95:MET:SD	1:G:235:GLY:HA3	2.61	0.40
1:G:104:MET:O	1:G:108:ILE:HG12	2.21	0.40

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	G	447/481 (93%)	405 (91%)	35 (8%)	7 (2%)	9	37
2	B	122/153 (80%)	108 (88%)	11 (9%)	3 (2%)	5	27
3	L	208/213 (98%)	196 (94%)	10 (5%)	2 (1%)	15	49
4	H	224/235 (95%)	211 (94%)	11 (5%)	2 (1%)	17	52
5	D	240/243 (99%)	228 (95%)	12 (5%)	0	100	100
6	E	211/216 (98%)	197 (93%)	14 (7%)	0	100	100
All	All	1452/1541 (94%)	1345 (93%)	93 (6%)	14 (1%)	15	49

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	138	ILE
3	L	110	PRO
1	G	71	THR
1	G	152	GLY
2	B	602	LEU
1	G	151	ARG
1	G	258	GLN
3	L	199	GLU
4	H	142	ASP
1	G	64	GLU
1	G	67	ASN
2	B	599	SER
2	B	601	LYS
4	H	188	GLY

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	G	404/428 (94%)	398 (98%)	6 (2%)	65	85
2	B	108/129 (84%)	105 (97%)	3 (3%)	43	73
3	L	178/181 (98%)	176 (99%)	2 (1%)	73	89
4	H	198/205 (97%)	195 (98%)	3 (2%)	65	85
5	D	205/206 (100%)	204 (100%)	1 (0%)	88	94
6	E	186/189 (98%)	185 (100%)	1 (0%)	88	94
All	All	1279/1338 (96%)	1263 (99%)	16 (1%)	69	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	47	ASP
1	G	123	THR
1	G	125	LEU
1	G	138	ILE
1	G	368	ASP
1	G	461	THR
2	B	536	THR
2	B	570	VAL
2	B	606	THR
3	L	54	ARG
3	L	111	LYS
4	H	23	ASN
4	H	100(J)	TRP
4	H	139	LEU
5	D	80	MET
6	E	96	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

51 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	$\# Z > 2$
7	NAG	A	1	1,7	14,14,15	0.33	0	17,19,21	0.41	0
7	NAG	A	2	7	14,14,15	0.42	0	17,19,21	1.28	1 (5%)
7	BMA	A	3	7	11,11,12	0.68	0	15,15,17	0.78	0
7	MAN	A	4	7	11,11,12	0.85	1 (9%)	15,15,17	1.32	4 (26%)
7	MAN	A	5	7	11,11,12	0.71	0	15,15,17	1.02	2 (13%)
7	MAN	A	6	7	11,11,12	0.63	0	15,15,17	1.10	2 (13%)
7	MAN	A	7	7	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
8	NAG	C	1	1,8	14,14,15	0.44	0	17,19,21	0.47	0
8	NAG	C	2	8	14,14,15	0.41	0	17,19,21	0.37	0
8	BMA	C	3	8	11,11,12	0.54	0	15,15,17	0.81	0
8	MAN	C	4	8	11,11,12	0.70	0	15,15,17	1.06	2 (13%)
9	NAG	F	1	1,9	14,14,15	0.18	0	17,19,21	0.41	0
9	NAG	F	2	9	14,14,15	0.22	0	17,19,21	0.38	0
10	NAG	I	1	1,10	14,14,15	0.25	0	17,19,21	0.48	0
10	NAG	I	2	10	14,14,15	0.34	0	17,19,21	0.42	0
10	BMA	I	3	10	11,11,12	0.67	0	15,15,17	0.71	0
10	MAN	I	4	10	11,11,12	0.70	0	15,15,17	1.05	2 (13%)
10	MAN	I	5	10	11,11,12	0.79	0	15,15,17	1.21	2 (13%)
10	MAN	I	6	10	11,11,12	0.65	0	15,15,17	1.12	2 (13%)
9	NAG	J	1	1,9	14,14,15	0.23	0	17,19,21	0.37	0
9	NAG	J	2	9	14,14,15	0.21	0	17,19,21	0.43	0
9	NAG	K	1	1,9	14,14,15	0.23	0	17,19,21	0.61	0
9	NAG	K	2	9	14,14,15	0.23	0	17,19,21	0.40	0
9	NAG	M	1	1,9	14,14,15	0.25	0	17,19,21	0.44	0
9	NAG	M	2	9	14,14,15	0.30	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	N	1	1,11	14,14,15	0.20	0	17,19,21	0.50	0
11	NAG	N	2	11	14,14,15	0.26	0	17,19,21	0.35	0
11	BMA	N	3	11	11,11,12	0.57	0	15,15,17	0.86	0
12	NAG	O	1	1,12	14,14,15	0.26	0	17,19,21	0.36	0
12	NAG	O	2	12	14,14,15	0.23	0	17,19,21	0.37	0
12	BMA	O	3	12	11,11,12	0.61	0	15,15,17	0.78	0
12	MAN	O	4	12	11,11,12	0.72	0	15,15,17	1.07	2 (13%)
12	MAN	O	5	12	11,11,12	0.71	0	15,15,17	1.12	2 (13%)
9	NAG	P	1	1,9	14,14,15	0.28	0	17,19,21	0.45	0
9	NAG	P	2	9	14,14,15	0.44	0	17,19,21	1.25	1 (5%)
9	NAG	Q	1	1,9	14,14,15	0.21	0	17,19,21	0.41	0
9	NAG	Q	2	9	14,14,15	0.22	0	17,19,21	0.41	0
9	NAG	R	1	1,9	14,14,15	0.26	0	17,19,21	0.47	0
9	NAG	R	2	9	14,14,15	0.19	0	17,19,21	0.40	0
9	NAG	S	1	1,9	14,14,15	0.20	0	17,19,21	0.38	0
9	NAG	S	2	9	14,14,15	0.23	0	17,19,21	0.42	0
13	NAG	T	1	1,13	14,14,15	0.26	0	17,19,21	0.38	0
13	MAN	T	10	13	11,11,12	0.73	0	15,15,17	1.03	2 (13%)
13	NAG	T	2	13	14,14,15	0.31	0	17,19,21	0.52	0
13	BMA	T	3	13	11,11,12	0.78	0	15,15,17	1.29	3 (20%)
13	MAN	T	4	13	11,11,12	0.64	0	15,15,17	1.13	1 (6%)
13	MAN	T	5	13	11,11,12	0.60	0	15,15,17	1.05	1 (6%)
13	MAN	T	6	13	11,11,12	0.61	0	15,15,17	1.41	3 (20%)
13	MAN	T	7	13	11,11,12	0.81	0	15,15,17	1.01	2 (13%)
13	MAN	T	8	13	11,11,12	0.71	0	15,15,17	1.03	2 (13%)
13	MAN	T	9	13	11,11,12	0.82	0	15,15,17	1.19	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
7	NAG	A	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	3/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	0/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	T	2	13	-	3/6/23/26	0/1/1/1
13	BMA	T	3	13	-	0/2/19/22	0/1/1/1
13	MAN	T	4	13	-	0/2/19/22	0/1/1/1
13	MAN	T	5	13	-	0/2/19/22	0/1/1/1
13	MAN	T	6	13	-	1/2/19/22	0/1/1/1
13	MAN	T	7	13	-	2/2/19/22	0/1/1/1
13	MAN	T	8	13	-	0/2/19/22	0/1/1/1
13	MAN	T	9	13	-	0/2/19/22	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	4	MAN	C1-C2	2.33	1.57	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2	NAG	C2-N2-C7	4.35	129.10	122.90
9	P	2	NAG	C2-N2-C7	4.29	129.01	122.90
13	T	6	MAN	C1-O5-C5	3.87	117.44	112.19
10	I	5	MAN	C1-O5-C5	3.32	116.69	112.19
13	T	9	MAN	C1-O5-C5	3.27	116.62	112.19
7	A	4	MAN	C1-O5-C5	2.87	116.08	112.19
13	T	4	MAN	C1-O5-C5	2.84	116.03	112.19
7	A	7	MAN	C1-O5-C5	2.77	115.95	112.19
10	I	4	MAN	O2-C2-C3	-2.71	104.71	110.14
13	T	3	BMA	C1-O5-C5	2.68	115.83	112.19
13	T	5	MAN	C1-O5-C5	2.63	115.76	112.19
7	A	6	MAN	C1-O5-C5	2.52	115.60	112.19
10	I	6	MAN	C1-O5-C5	2.50	115.58	112.19
10	I	4	MAN	C1-O5-C5	2.40	115.44	112.19
12	O	5	MAN	C1-O5-C5	2.38	115.42	112.19
13	T	8	MAN	C1-O5-C5	2.36	115.39	112.19
13	T	6	MAN	O5-C1-C2	2.34	114.38	110.77
7	A	7	MAN	O2-C2-C3	-2.31	105.50	110.14
10	I	6	MAN	O2-C2-C3	-2.29	105.55	110.14
7	A	6	MAN	O2-C2-C3	-2.29	105.55	110.14
13	T	3	BMA	C1-C2-C3	2.27	112.46	109.67
12	O	5	MAN	O2-C2-C3	-2.27	105.59	110.14
8	C	4	MAN	O2-C2-C3	-2.26	105.60	110.14
12	O	4	MAN	O2-C2-C3	-2.25	105.62	110.14
8	C	4	MAN	C1-O5-C5	2.24	115.22	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	5	MAN	O2-C2-C3	-2.23	105.68	110.14
13	T	6	MAN	O2-C2-C3	-2.22	105.69	110.14
10	I	5	MAN	O2-C2-C3	-2.22	105.70	110.14
12	O	4	MAN	C1-O5-C5	2.21	115.19	112.19
7	A	4	MAN	O2-C2-C3	-2.20	105.73	110.14
13	T	10	MAN	O2-C2-C3	-2.19	105.75	110.14
13	T	9	MAN	O2-C2-C3	-2.18	105.77	110.14
13	T	10	MAN	C1-O5-C5	2.15	115.11	112.19
13	T	7	MAN	O2-C2-C3	-2.14	105.86	110.14
7	A	5	MAN	C1-O5-C5	2.13	115.08	112.19
13	T	3	BMA	O5-C1-C2	2.10	114.01	110.77
13	T	8	MAN	O2-C2-C3	-2.08	105.96	110.14
7	A	4	MAN	O5-C1-C2	2.08	113.98	110.77
13	T	7	MAN	C1-O5-C5	2.04	114.95	112.19
7	A	4	MAN	C1-C2-C3	2.02	112.14	109.67

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	O	3	BMA	C4-C5-C6-O6
9	R	1	NAG	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
12	O	2	NAG	O5-C5-C6-O6
13	T	2	NAG	O5-C5-C6-O6
12	O	2	NAG	C4-C5-C6-O6
11	N	3	BMA	O5-C5-C6-O6
9	J	2	NAG	O5-C5-C6-O6
12	O	3	BMA	O5-C5-C6-O6
9	R	1	NAG	C4-C5-C6-O6
10	I	4	MAN	O5-C5-C6-O6
9	J	2	NAG	C4-C5-C6-O6
9	P	1	NAG	C4-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
9	Q	2	NAG	O5-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
9	P	1	NAG	O5-C5-C6-O6
11	N	1	NAG	C4-C5-C6-O6
9	K	1	NAG	O5-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6
10	I	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	T	2	NAG	C4-C5-C6-O6
9	P	2	NAG	C8-C7-N2-C2
9	P	2	NAG	O7-C7-N2-C2
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
9	P	1	NAG	C8-C7-N2-C2
9	P	1	NAG	O7-C7-N2-C2
9	Q	1	NAG	C8-C7-N2-C2
9	Q	1	NAG	O7-C7-N2-C2
11	N	1	NAG	C8-C7-N2-C2
11	N	1	NAG	O7-C7-N2-C2
9	S	2	NAG	O5-C5-C6-O6
9	M	2	NAG	O5-C5-C6-O6
9	K	1	NAG	C4-C5-C6-O6
11	N	1	NAG	O5-C5-C6-O6
12	O	1	NAG	C4-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
13	T	7	MAN	O5-C5-C6-O6
9	S	2	NAG	C4-C5-C6-O6
11	N	3	BMA	C4-C5-C6-O6
9	M	2	NAG	C4-C5-C6-O6
12	O	1	NAG	O5-C5-C6-O6
13	T	7	MAN	C4-C5-C6-O6
13	T	6	MAN	O5-C5-C6-O6
13	T	1	NAG	C4-C5-C6-O6
13	T	1	NAG	O5-C5-C6-O6
9	R	2	NAG	C4-C5-C6-O6
9	Q	2	NAG	C4-C5-C6-O6
10	I	2	NAG	C4-C5-C6-O6
12	O	4	MAN	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
9	P	2	NAG	O5-C5-C6-O6
8	C	4	MAN	O5-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6
10	I	2	NAG	O5-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
9	S	1	NAG	O5-C5-C6-O6
9	K	1	NAG	C3-C2-N2-C7
13	T	2	NAG	C3-C2-N2-C7
9	P	2	NAG	C3-C2-N2-C7
7	A	2	NAG	C3-C2-N2-C7

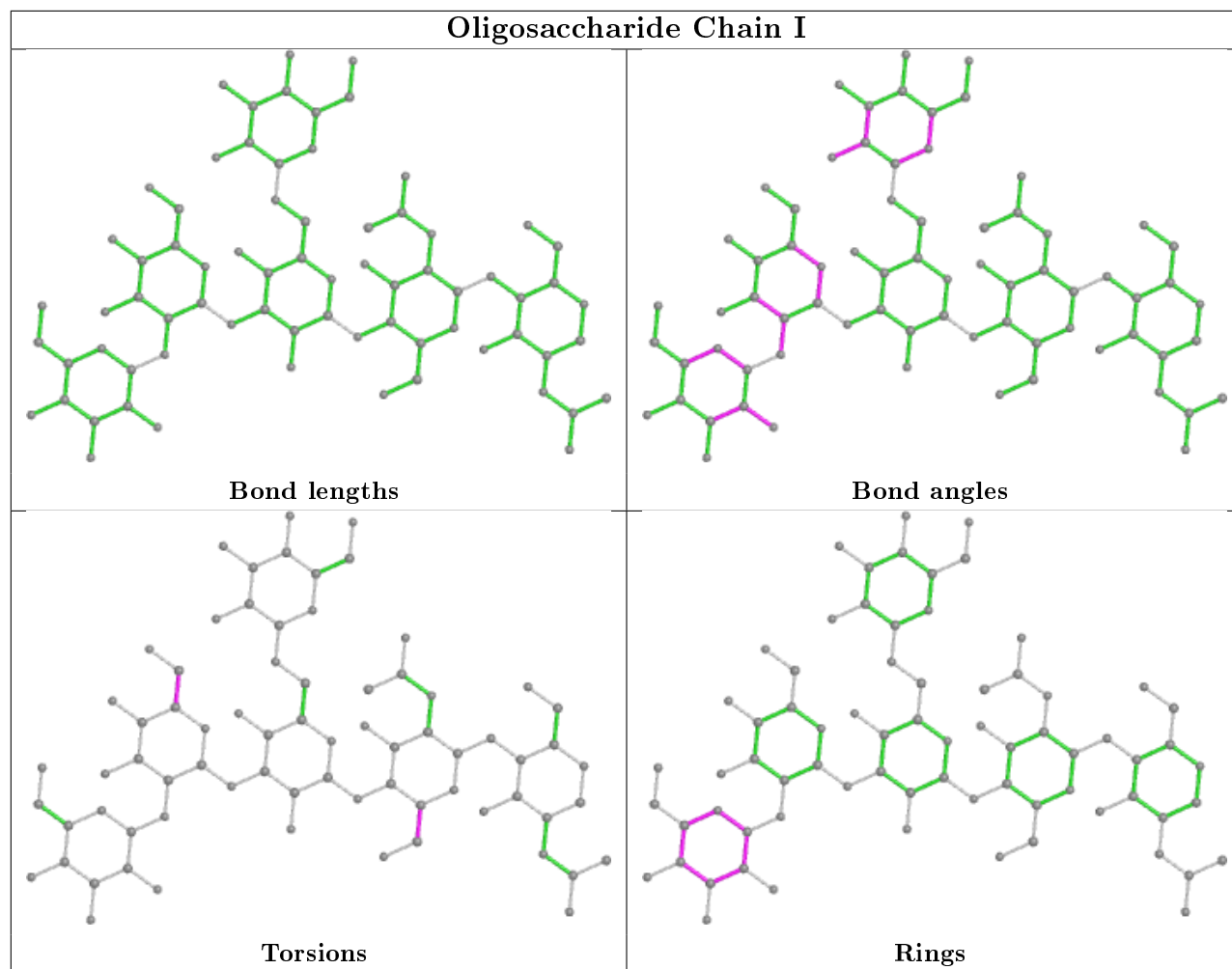
All (2) ring outliers are listed below:

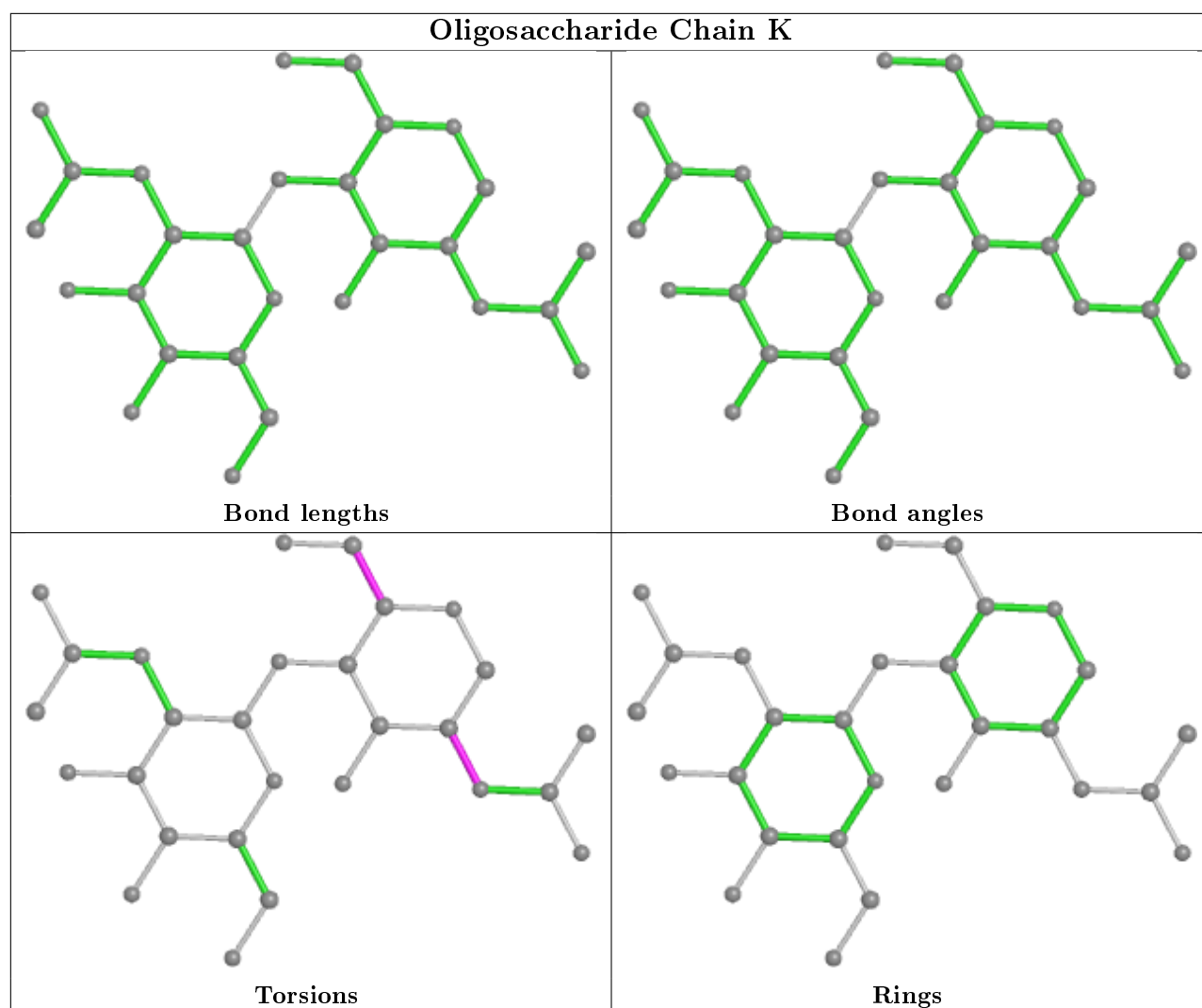
Mol	Chain	Res	Type	Atoms
13	T	9	MAN	C1-C2-C3-C4-C5-O5
10	I	5	MAN	C1-C2-C3-C4-C5-O5

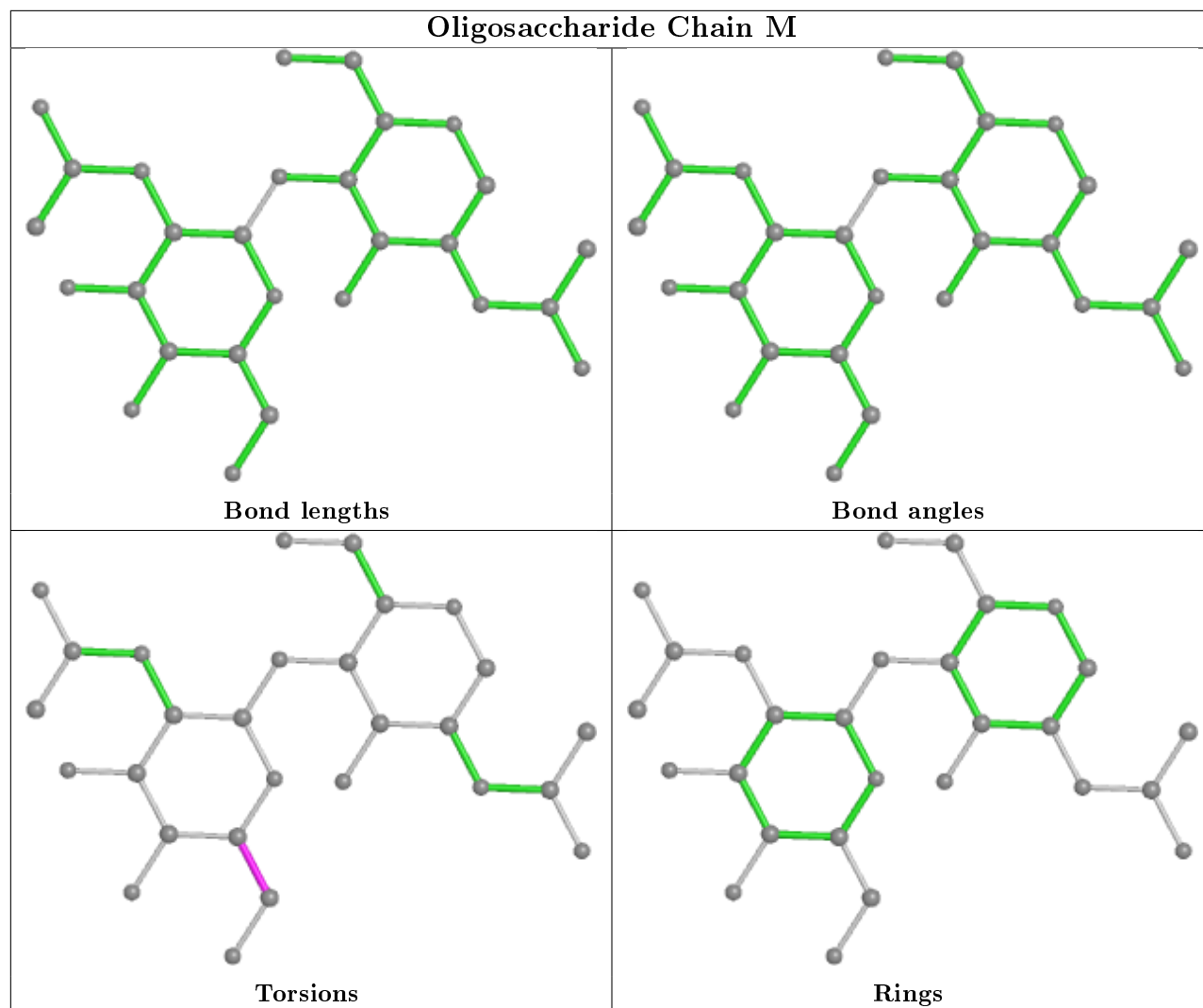
12 monomers are involved in 10 short contacts:

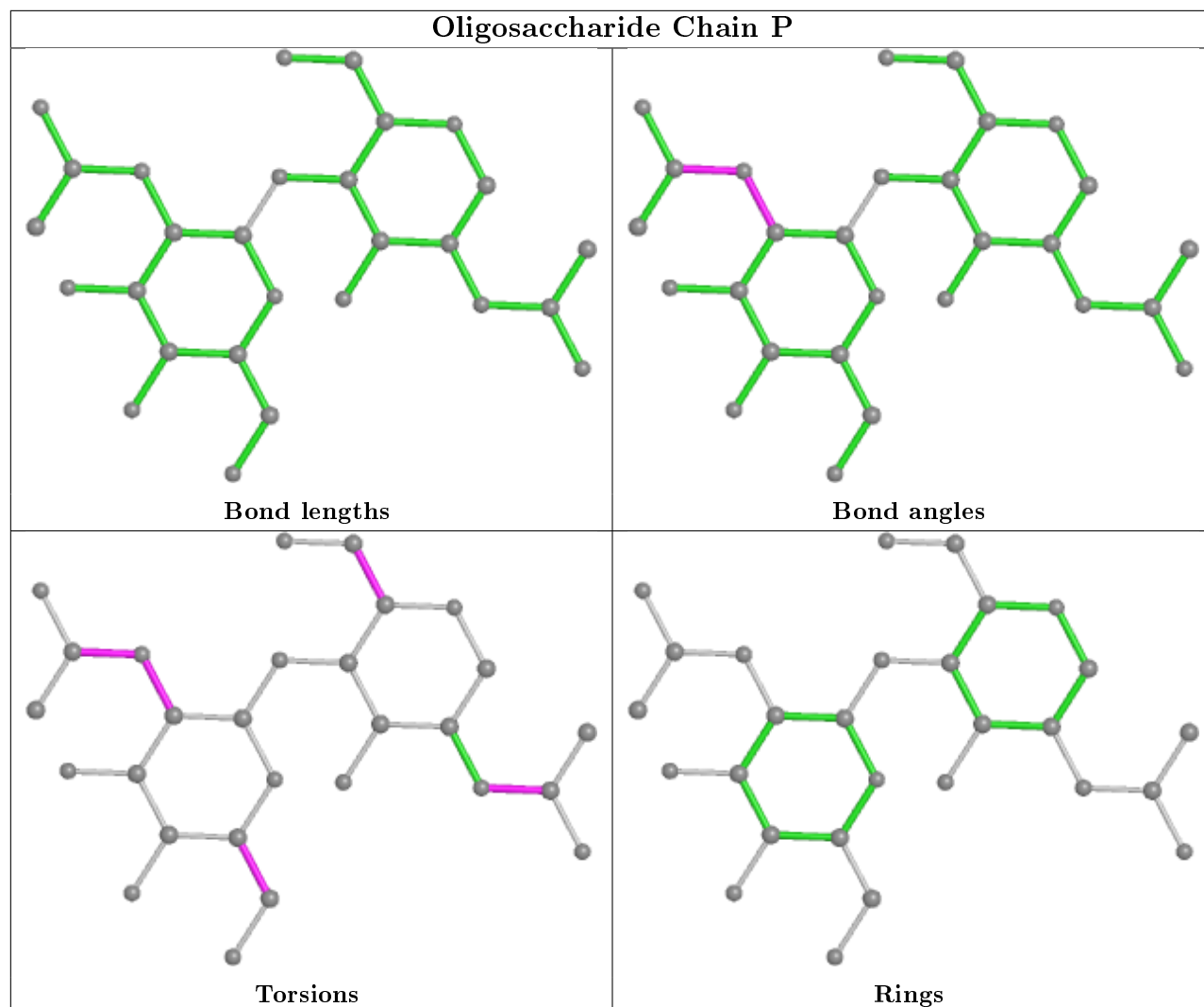
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1	NAG	1	0
7	A	3	BMA	1	0
13	T	8	MAN	1	0
9	P	2	NAG	2	0
13	T	9	MAN	1	0
7	A	6	MAN	1	0
7	A	2	NAG	1	0
7	A	7	MAN	1	0
13	T	2	NAG	1	0
9	P	1	NAG	1	0
7	A	4	MAN	1	0
8	C	4	MAN	1	0

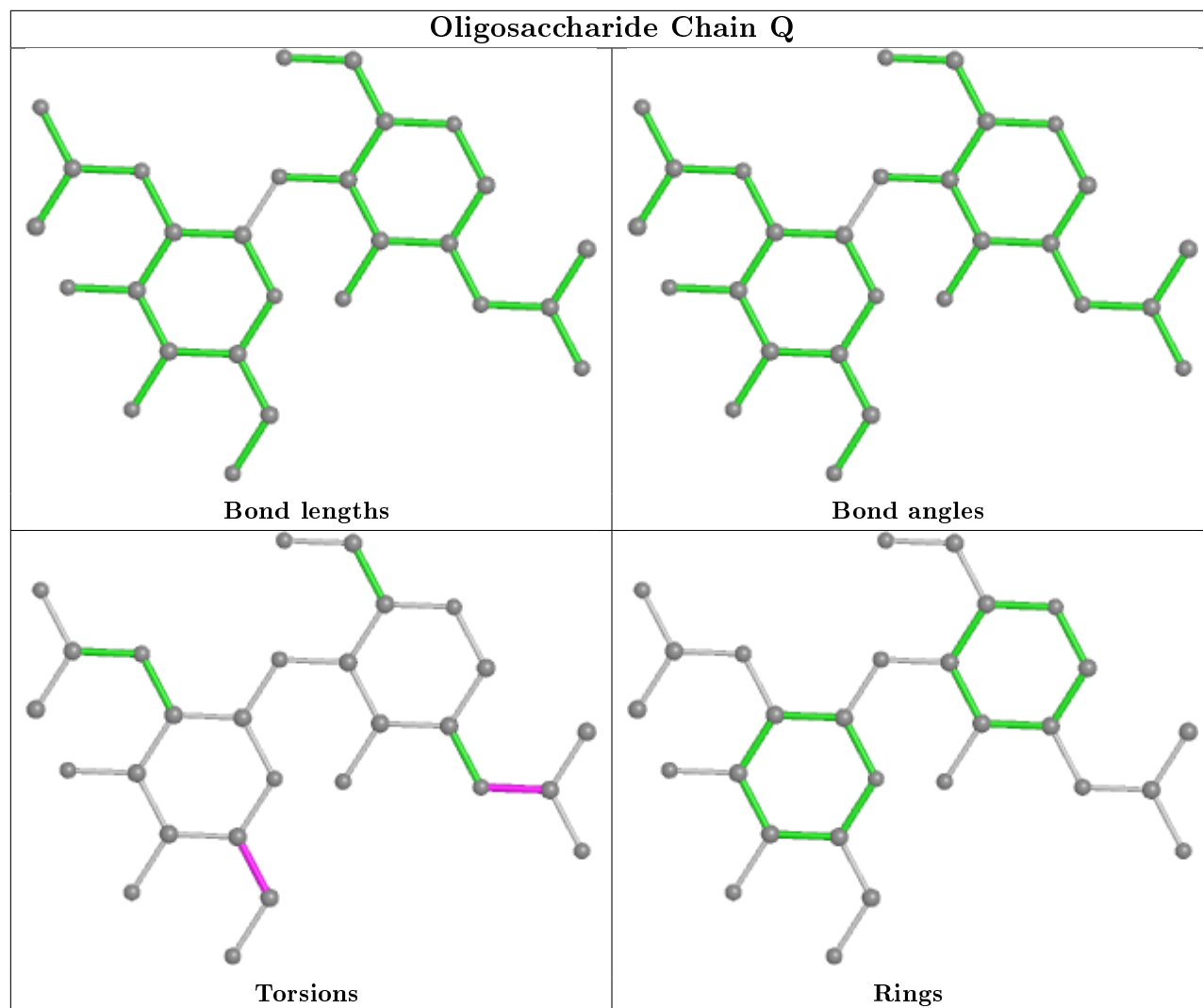
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

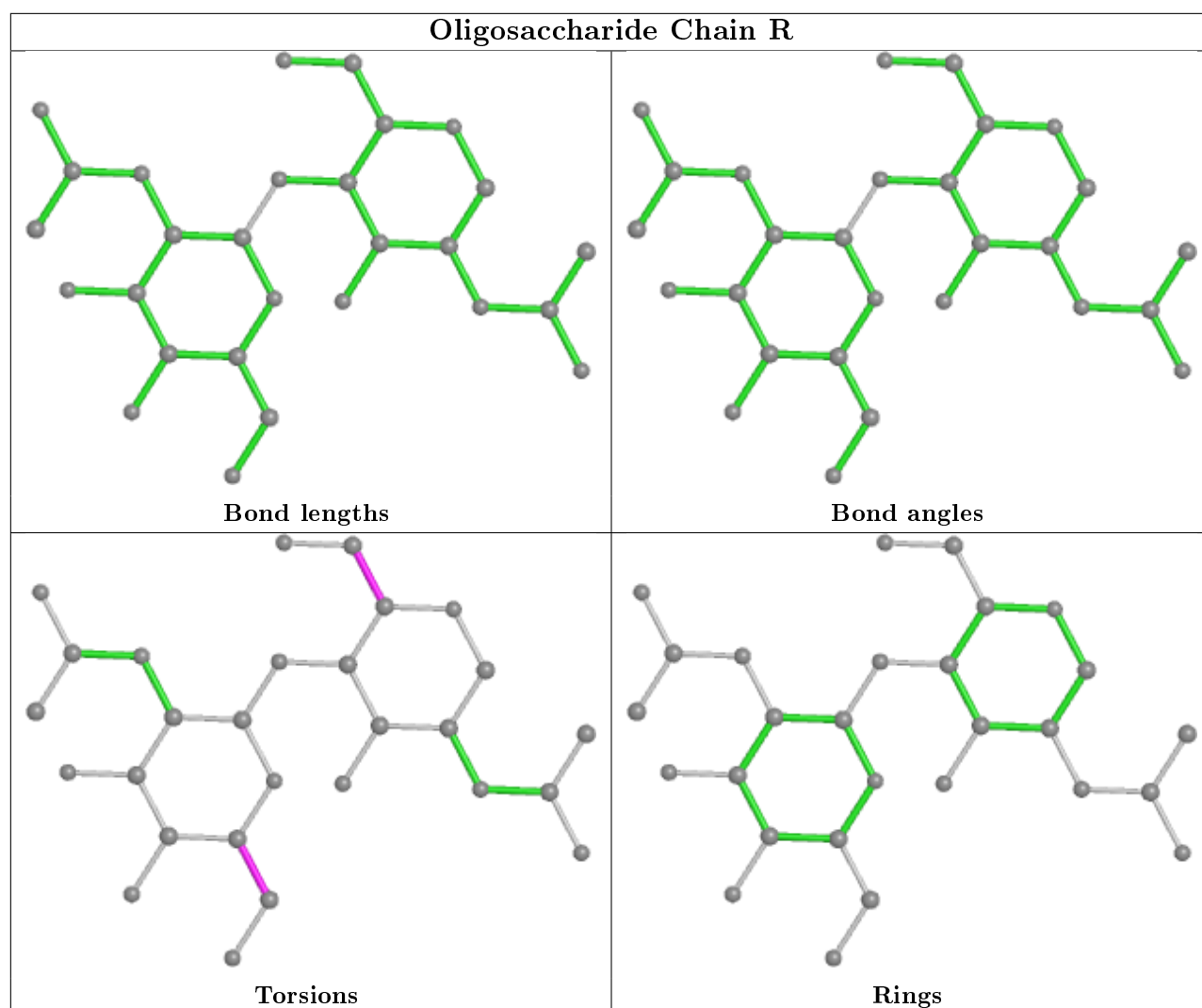


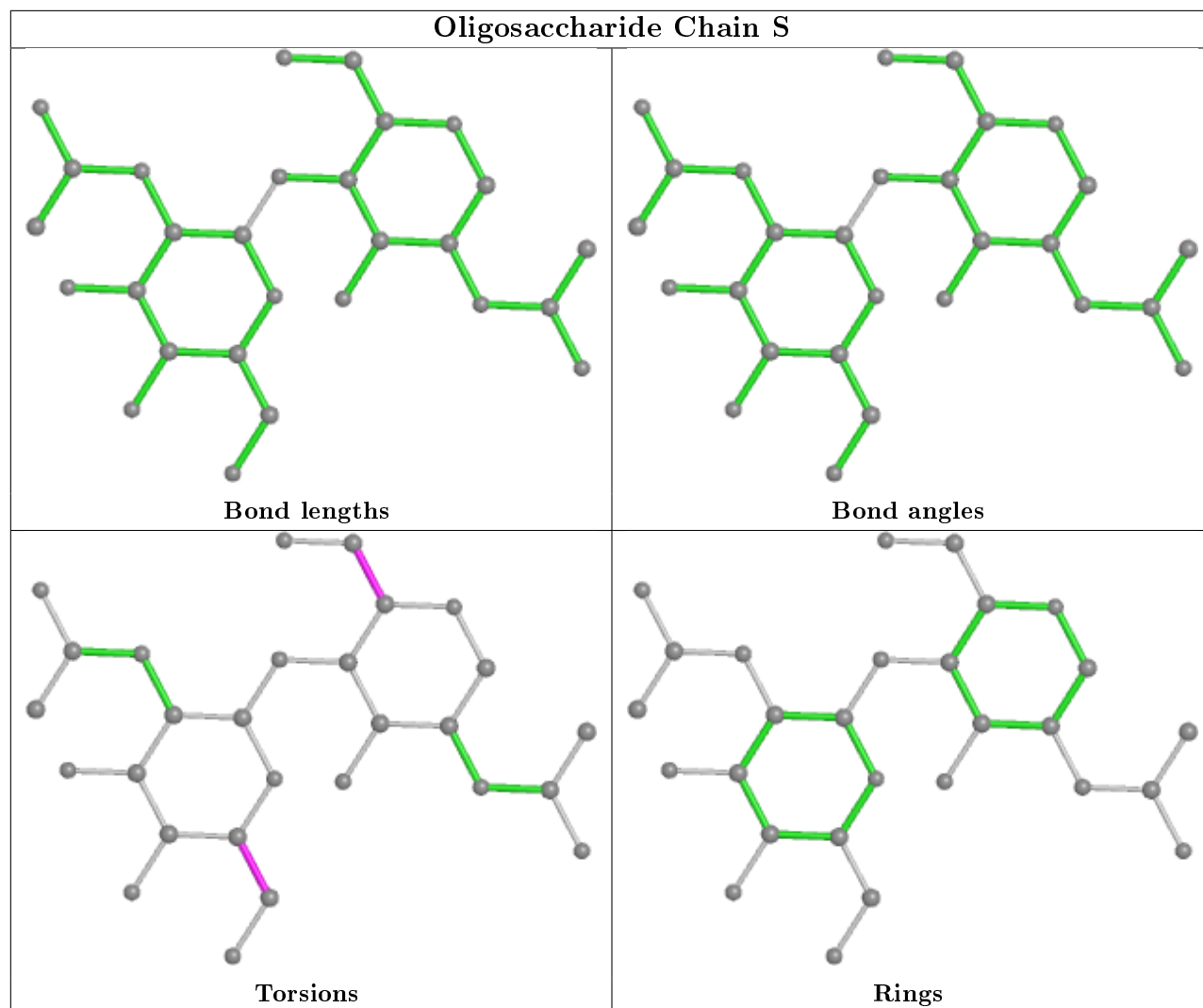


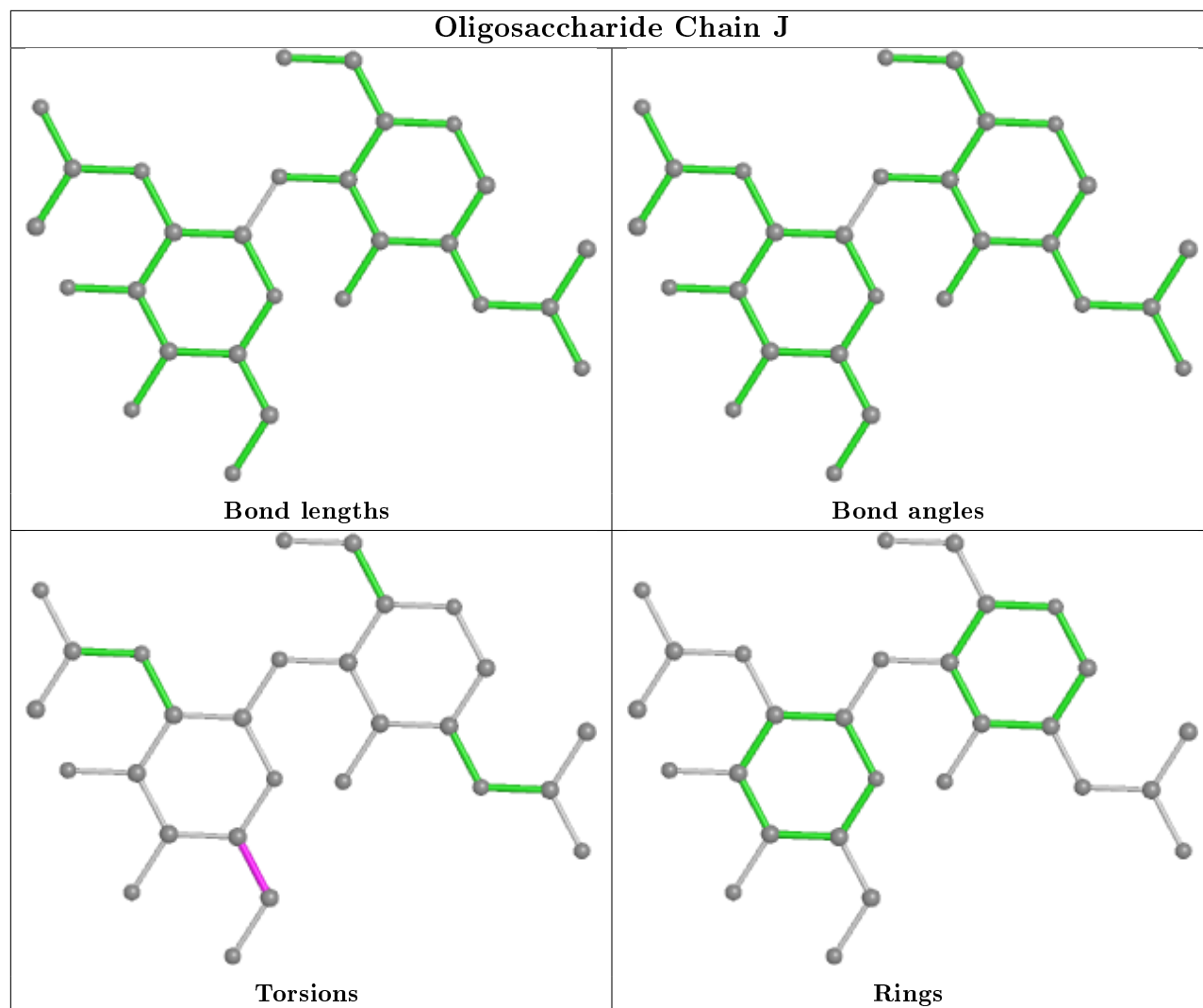


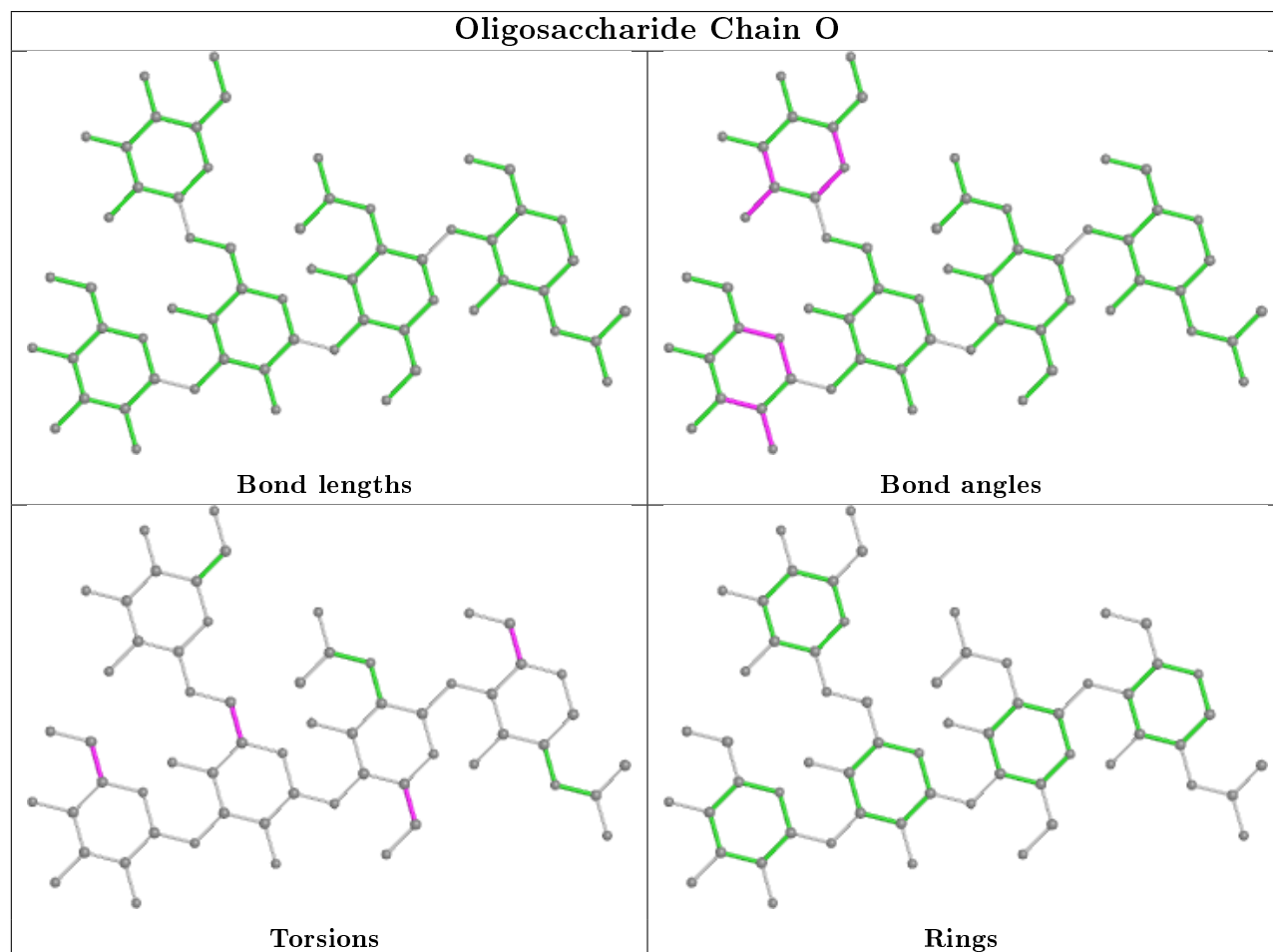
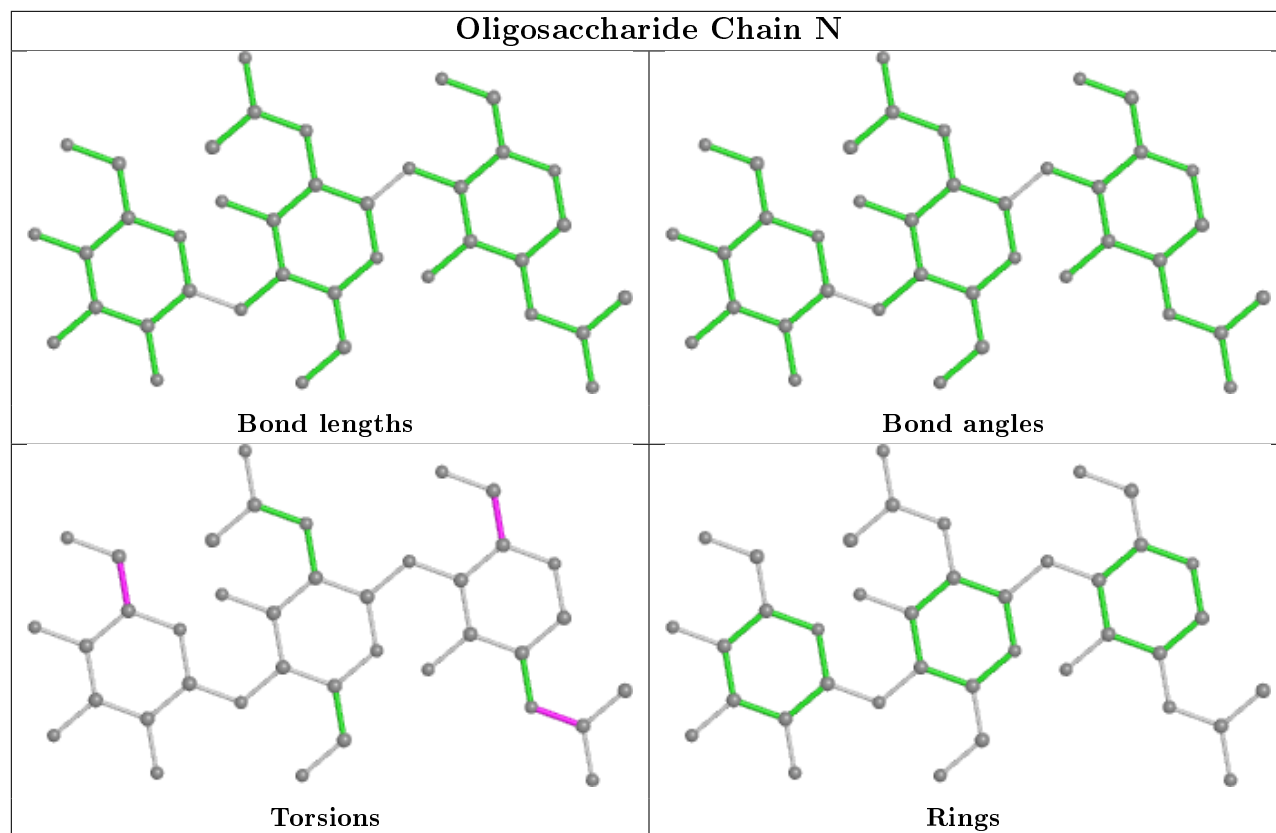


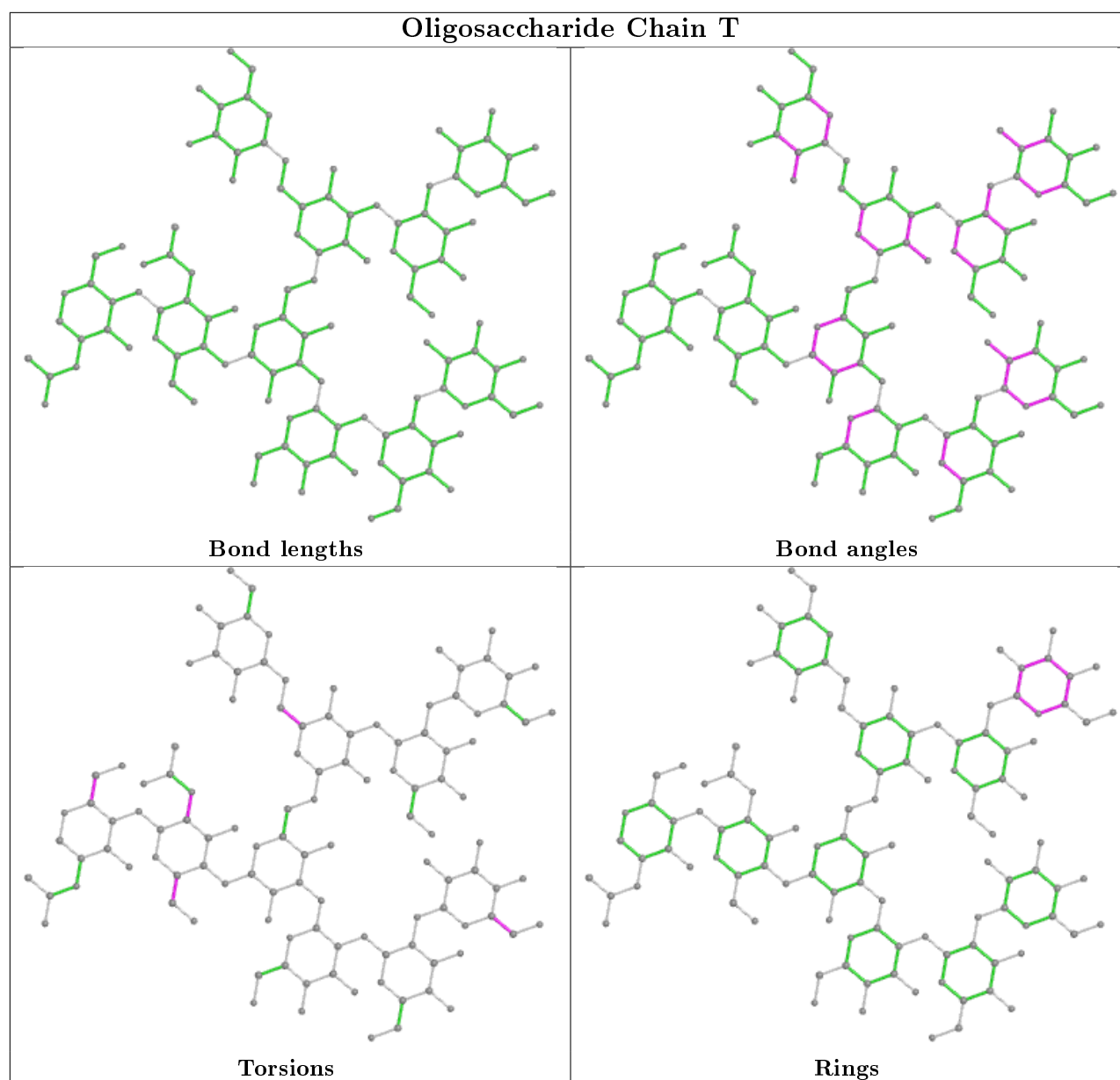












5.6 Ligand geometry [i](#)

18 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
14	NAG	G	1839	1	14,14,15	0.25	0	17,19,21	0.40	0
14	NAG	H	523	4	14,14,15	0.24	0	17,19,21	0.39	0
15	SO4	L	301	-	4,4,4	0.13	0	6,6,6	0.06	0
15	SO4	G	604	-	4,4,4	0.14	0	6,6,6	0.05	0
15	SO4	G	603	-	4,4,4	0.13	0	6,6,6	0.04	0
15	SO4	B	702	-	4,4,4	0.14	0	6,6,6	0.05	0
14	NAG	G	1276	1	14,14,15	0.43	0	17,19,21	1.26	2 (11%)
15	SO4	G	601	-	4,4,4	0.14	0	6,6,6	0.05	0
14	NAG	G	1355	1	14,14,15	0.23	0	17,19,21	0.37	0
14	NAG	B	1618	2	14,14,15	0.21	0	17,19,21	0.35	0
15	SO4	G	605	-	4,4,4	0.14	0	6,6,6	0.05	0
14	NAG	B	1637	2	14,14,15	0.25	0	17,19,21	0.41	0
15	SO4	G	602	-	4,4,4	0.14	0	6,6,6	0.05	0
15	SO4	G	607	-	4,4,4	0.14	0	6,6,6	0.05	0
15	SO4	G	606	-	4,4,4	0.17	0	6,6,6	0.20	0
14	NAG	G	1133	1	14,14,15	0.24	0	17,19,21	0.39	0
15	SO4	B	701	-	4,4,4	0.14	0	6,6,6	0.05	0
14	NAG	B	1611	2	14,14,15	0.23	0	17,19,21	0.41	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
14	NAG	G	1839	1	-	1/6/23/26	0/1/1/1
14	NAG	H	523	4	-	2/6/23/26	0/1/1/1
14	NAG	G	1276	1	-	5/6/23/26	0/1/1/1
14	NAG	G	1355	1	-	2/6/23/26	0/1/1/1
14	NAG	B	1618	2	-	2/6/23/26	0/1/1/1
14	NAG	B	1637	2	-	2/6/23/26	0/1/1/1
14	NAG	G	1133	1	-	1/6/23/26	0/1/1/1
14	NAG	B	1611	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1276	NAG	C2-N2-C7	4.34	129.09	122.90
14	G	1276	NAG	C1-C2-N2	2.01	113.91	110.49

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	1276	NAG	O5-C5-C6-O6
14	G	1276	NAG	C4-C5-C6-O6
14	B	1618	NAG	O5-C5-C6-O6
14	B	1618	NAG	C4-C5-C6-O6
14	G	1276	NAG	C8-C7-N2-C2
14	G	1276	NAG	O7-C7-N2-C2
14	G	1355	NAG	C8-C7-N2-C2
14	G	1355	NAG	O7-C7-N2-C2
14	B	1637	NAG	O5-C5-C6-O6
14	H	523	NAG	O5-C5-C6-O6
14	B	1637	NAG	C4-C5-C6-O6
14	B	1611	NAG	C4-C5-C6-O6
14	G	1133	NAG	O5-C5-C6-O6
14	B	1611	NAG	O5-C5-C6-O6
14	H	523	NAG	C4-C5-C6-O6
14	G	1839	NAG	O5-C5-C6-O6
14	G	1276	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	1276	NAG	1	0
14	B	1618	NAG	2	0
15	G	602	SO4	1	0
15	G	606	SO4	1	0
15	B	701	SO4	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	G	453/481 (94%)	-0.36	7 (1%) 73 54	33, 72, 145, 193	0
2	B	126/153 (82%)	-0.28	1 (0%) 86 72	38, 77, 145, 176	0
3	L	210/213 (98%)	-0.47	1 (0%) 91 81	60, 96, 142, 172	0
4	H	228/235 (97%)	-0.22	6 (2%) 56 33	65, 111, 160, 199	0
5	D	242/243 (99%)	0.41	37 (15%) 2 1	51, 123, 284, 386	0
6	E	213/216 (98%)	0.36	25 (11%) 4 2	82, 146, 238, 257	0
All	All	1472/1541 (95%)	-0.12	77 (5%) 27 12	33, 97, 220, 386	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	218	LYS	7.1
5	D	214	LYS	7.0
6	E	157	ALA	7.0
5	D	185	PRO	6.6
6	E	197	HIS	6.4
5	D	215	SER	5.9
5	D	222	VAL	5.8
5	D	127	SER	5.5
5	D	213	PRO	5.5
5	D	216	CYS	5.2
6	E	180	LEU	5.0
5	D	221	GLU	5.0
5	D	192	GLN	4.7
6	E	199	GLY	4.6
1	G	31	ALA	4.4
5	D	184	VAL	4.4
6	E	117	LEU	4.4
1	G	61	TYR	4.3
5	D	132	SER	4.3

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Mol	Chain	Res	Type	RSRZ
5	D	138	LEU	4.3
5	D	224	PHE	4.2
6	E	156	LYS	4.0
5	D	191	THR	3.9
6	E	198	GLU	3.9
5	D	190	GLY	3.8
6	E	118	PHE	3.7
1	G	60	ALA	3.6
5	D	139	GLY	3.6
5	D	211	VAL	3.5
5	D	126	PRO	3.5
3	L	108	SER	3.5
4	H	209	VAL	3.4
6	E	203	GLU	3.3
5	D	121	VAL	3.3
5	D	193	THR	3.2
5	D	183	THR	3.2
5	D	123	PRO	3.1
1	G	73	ALA	3.1
6	E	142	GLY	3.0
5	D	122	PHE	3.0
5	D	220	LEU	2.9
2	B	664	ASP	2.9
4	H	126	SER	2.8
6	E	119	PRO	2.8
1	G	72	HIS	2.7
5	D	223	LEU	2.7
6	E	111	ALA	2.7
6	E	200	SER	2.7
6	E	115	VAL	2.7
6	E	136	ILE	2.7
5	D	182	VAL	2.6
5	D	181	VAL	2.6
5	D	208	ASP	2.6
6	E	114	SER	2.5
5	D	219	GLY	2.5
1	G	505	VAL	2.5
4	H	138	CYS	2.5
5	D	194	TYR	2.4
6	E	201	THR	2.4
5	D	152	VAL	2.4
6	E	128	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
6	E	179	SER	2.3
6	E	125	LEU	2.3
5	D	131	THR	2.2
6	E	183	GLU	2.2
4	H	187	LEU	2.2
4	H	125	SER	2.2
5	D	133	GLY	2.1
4	H	188	GLY	2.1
6	E	113	PRO	2.1
6	E	187	SER	2.1
5	D	129	LYS	2.1
6	E	189	ARG	2.0
1	G	71	THR	2.0
5	D	124	LEU	2.0
5	D	209	LYS	2.0
6	E	135	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
9	NAG	K	2	14/15	0.73	0.41	131,149,156,158	0
8	MAN	C	4	11/12	0.74	0.59	139,156,166,167	0
10	MAN	I	6	11/12	0.74	0.38	122,141,149,150	0
11	BMA	N	3	11/12	0.77	0.27	161,197,227,281	0
12	MAN	O	5	11/12	0.79	0.32	153,155,158,160	0
13	MAN	T	9	11/12	0.79	0.25	142,149,153,154	0
10	BMA	I	3	11/12	0.80	0.14	123,129,144,150	0
9	NAG	Q	2	14/15	0.81	0.33	143,152,162,166	0
9	NAG	M	2	14/15	0.82	0.34	121,142,144,145	0
9	NAG	S	2	14/15	0.83	0.39	117,131,141,146	0
9	NAG	J	2	14/15	0.83	0.35	142,148,156,161	0
12	BMA	O	3	11/12	0.84	0.21	126,135,145,155	0

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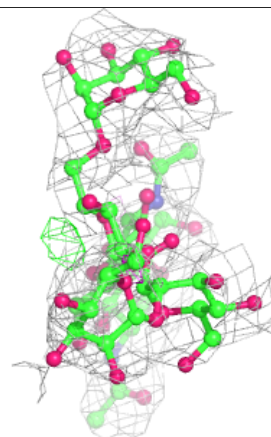
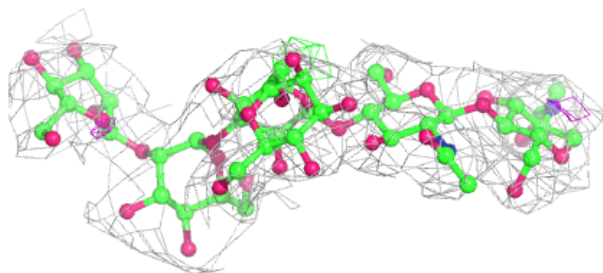
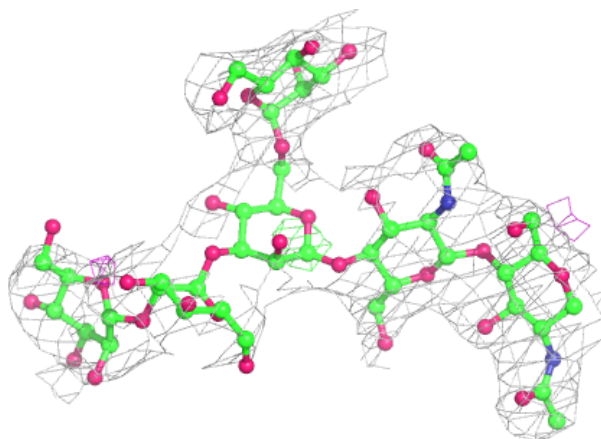
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	BMA	C	3	11/12	0.84	0.30	123,133,142,149	0
9	NAG	K	1	14/15	0.85	0.22	74,111,130,137	0
13	MAN	T	6	11/12	0.85	0.24	115,120,125,126	0
10	MAN	I	5	11/12	0.86	0.29	131,135,139,140	0
9	NAG	F	2	14/15	0.86	0.49	135,137,140,141	0
7	MAN	A	4	11/12	0.86	0.16	107,114,122,123	0
9	NAG	R	2	14/15	0.87	0.40	117,131,142,150	0
9	NAG	P	2	14/15	0.88	0.24	93,107,118,125	0
7	MAN	A	5	11/12	0.88	0.19	116,133,144,153	0
13	MAN	T	7	11/12	0.88	0.11	100,117,123,132	0
12	MAN	O	4	11/12	0.88	0.18	110,122,126,127	0
11	NAG	N	2	14/15	0.89	0.28	102,124,150,177	0
9	NAG	M	1	14/15	0.90	0.37	110,120,137,140	0
8	NAG	C	2	14/15	0.90	0.21	109,118,126,127	0
13	MAN	T	10	11/12	0.90	0.16	94,109,115,117	0
12	NAG	O	2	14/15	0.90	0.20	91,105,116,127	0
13	NAG	T	2	14/15	0.91	0.16	71,88,108,114	0
9	NAG	F	1	14/15	0.91	0.17	85,99,116,124	0
13	MAN	T	8	11/12	0.91	0.24	135,138,146,152	0
10	MAN	I	4	11/12	0.91	0.14	117,128,138,144	0
11	NAG	N	1	14/15	0.91	0.16	73,91,103,106	0
9	NAG	Q	1	14/15	0.91	0.17	75,106,125,140	0
7	MAN	A	6	11/12	0.92	0.22	97,104,117,118	0
9	NAG	J	1	14/15	0.92	0.17	81,90,114,132	0
13	MAN	T	5	11/12	0.93	0.18	76,80,93,100	0
7	BMA	A	3	11/12	0.94	0.14	66,77,101,104	0
9	NAG	P	1	14/15	0.94	0.16	66,90,98,111	0
8	NAG	C	1	14/15	0.95	0.15	72,98,116,118	0
7	MAN	A	7	11/12	0.95	0.15	68,74,91,105	0
13	BMA	T	3	11/12	0.95	0.13	65,82,97,99	0
10	NAG	I	2	14/15	0.96	0.12	77,92,102,112	0
9	NAG	S	1	14/15	0.96	0.13	62,77,90,104	0
9	NAG	R	1	14/15	0.96	0.11	59,75,100,110	0
12	NAG	O	1	14/15	0.96	0.12	27,73,91,94	0
7	NAG	A	2	14/15	0.97	0.13	44,56,72,76	0
13	MAN	T	4	11/12	0.97	0.14	49,55,72,92	0
13	NAG	T	1	14/15	0.97	0.12	51,62,79,84	0
10	NAG	I	1	14/15	0.98	0.14	34,54,70,80	0
7	NAG	A	1	14/15	0.98	0.15	35,43,56,57	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.

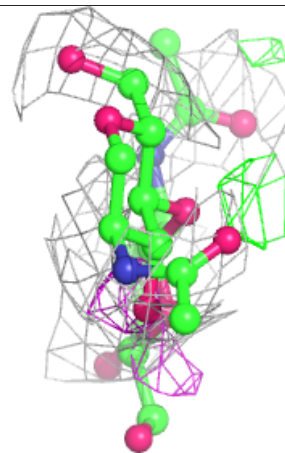
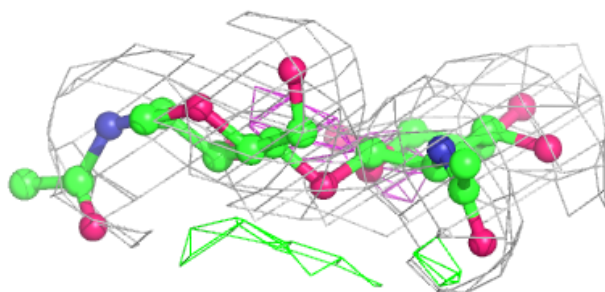
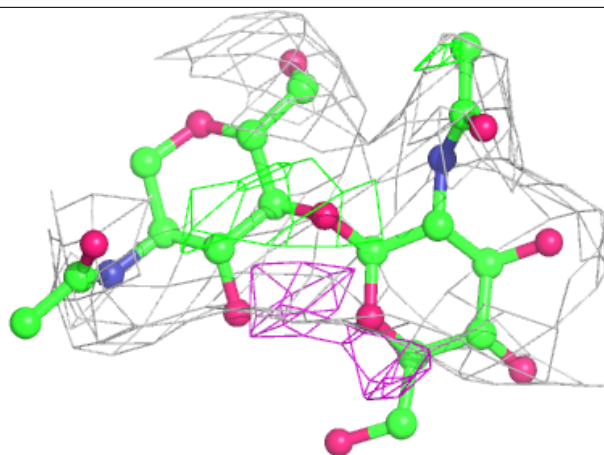
Electron density around Chain I:

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



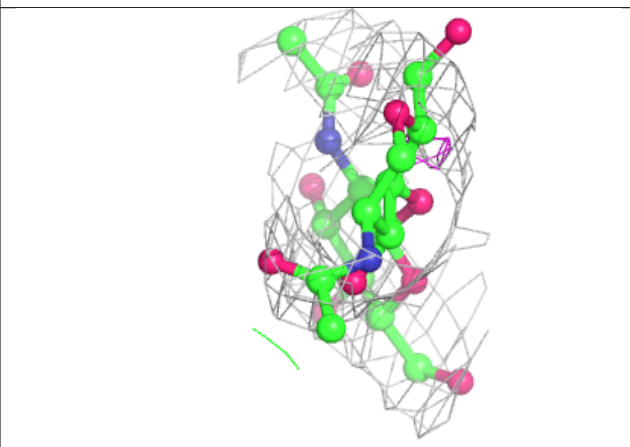
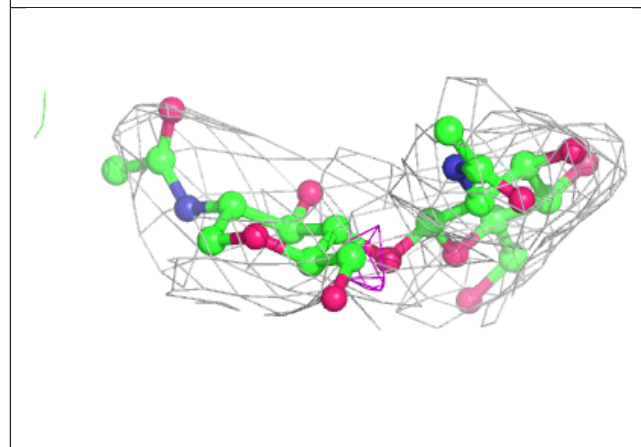
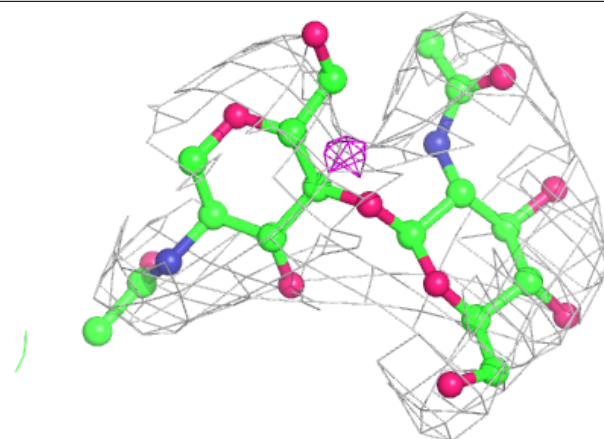
Electron density around Chain K:

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



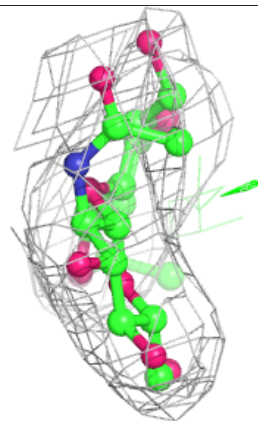
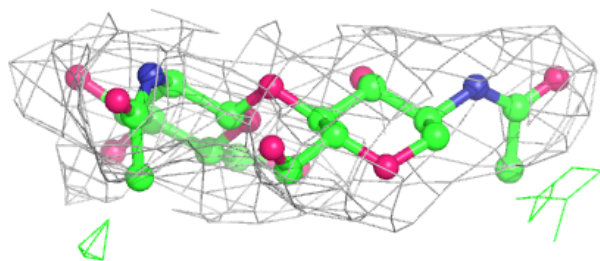
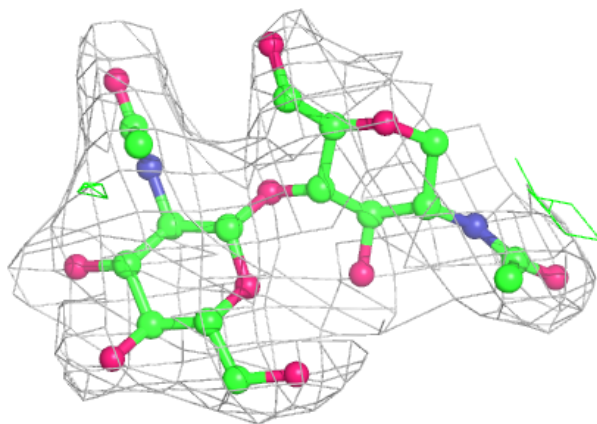
Electron density around Chain M:

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



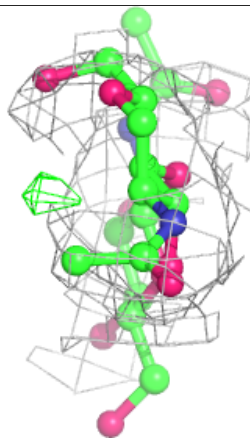
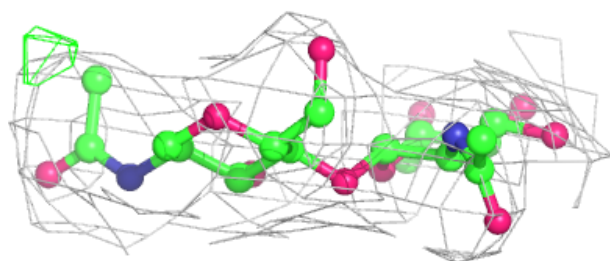
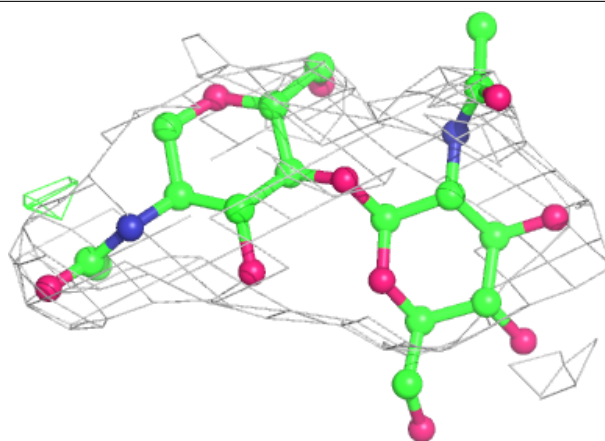
Electron density around Chain P:

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



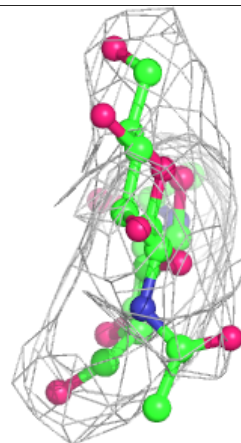
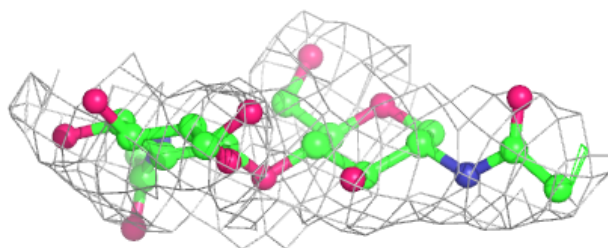
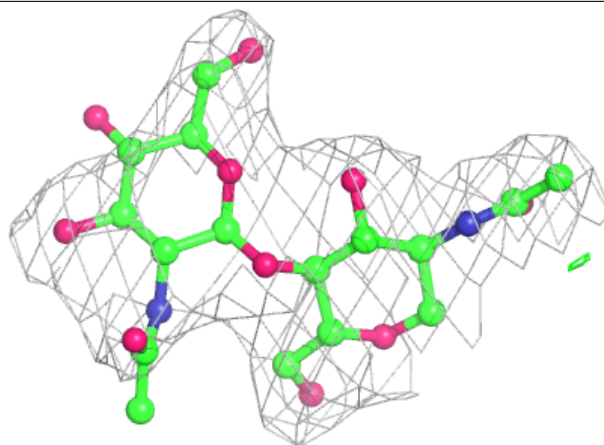
Electron density around Chain Q:

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



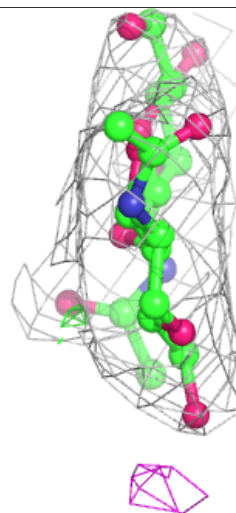
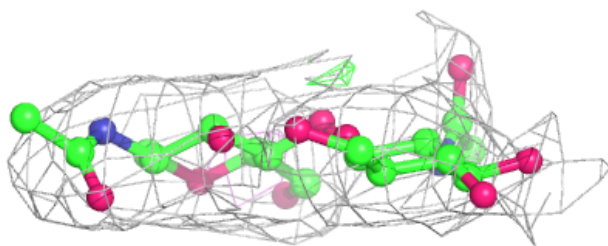
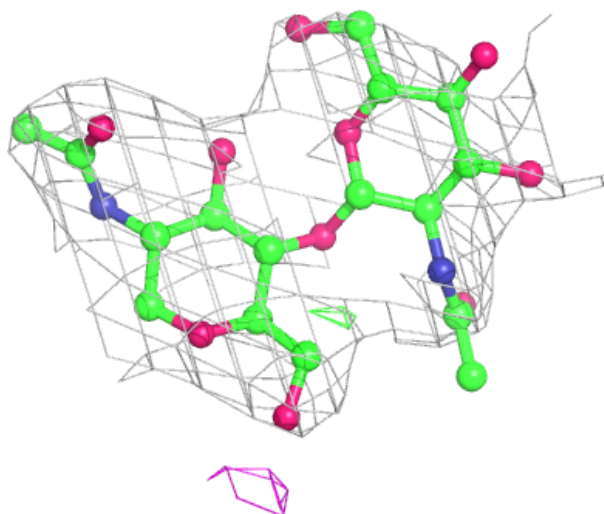
Electron density around Chain R:

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



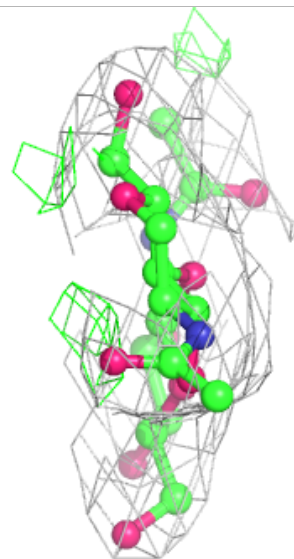
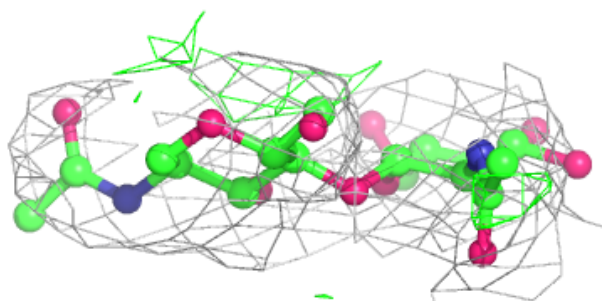
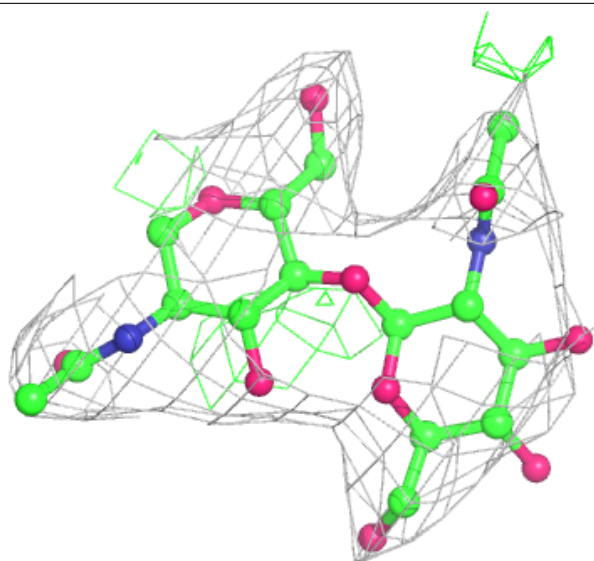
Electron density around Chain S:

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



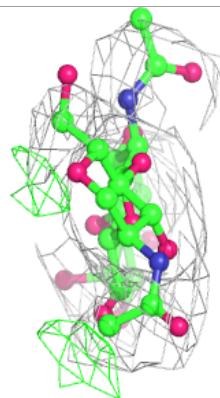
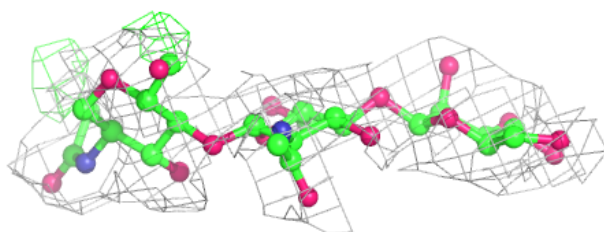
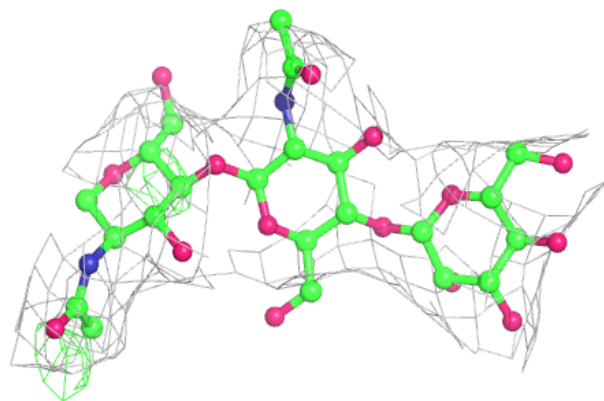
Electron density around Chain J:

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

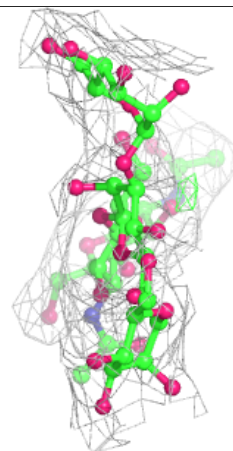
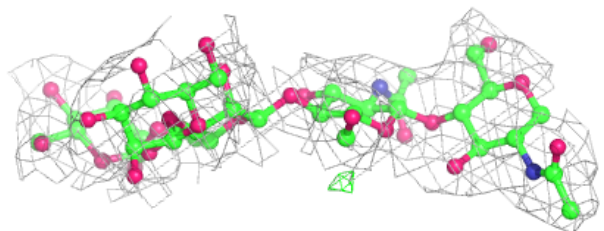
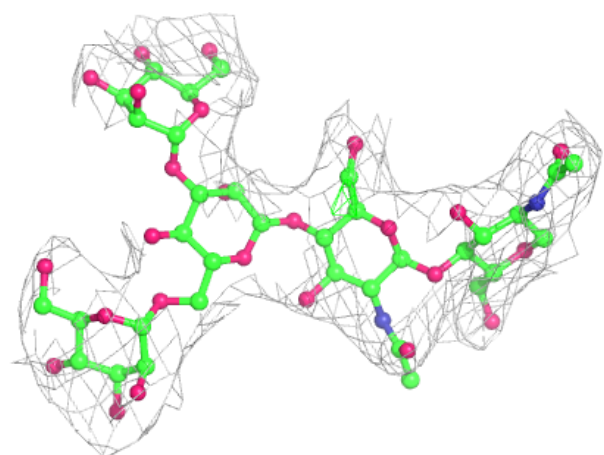


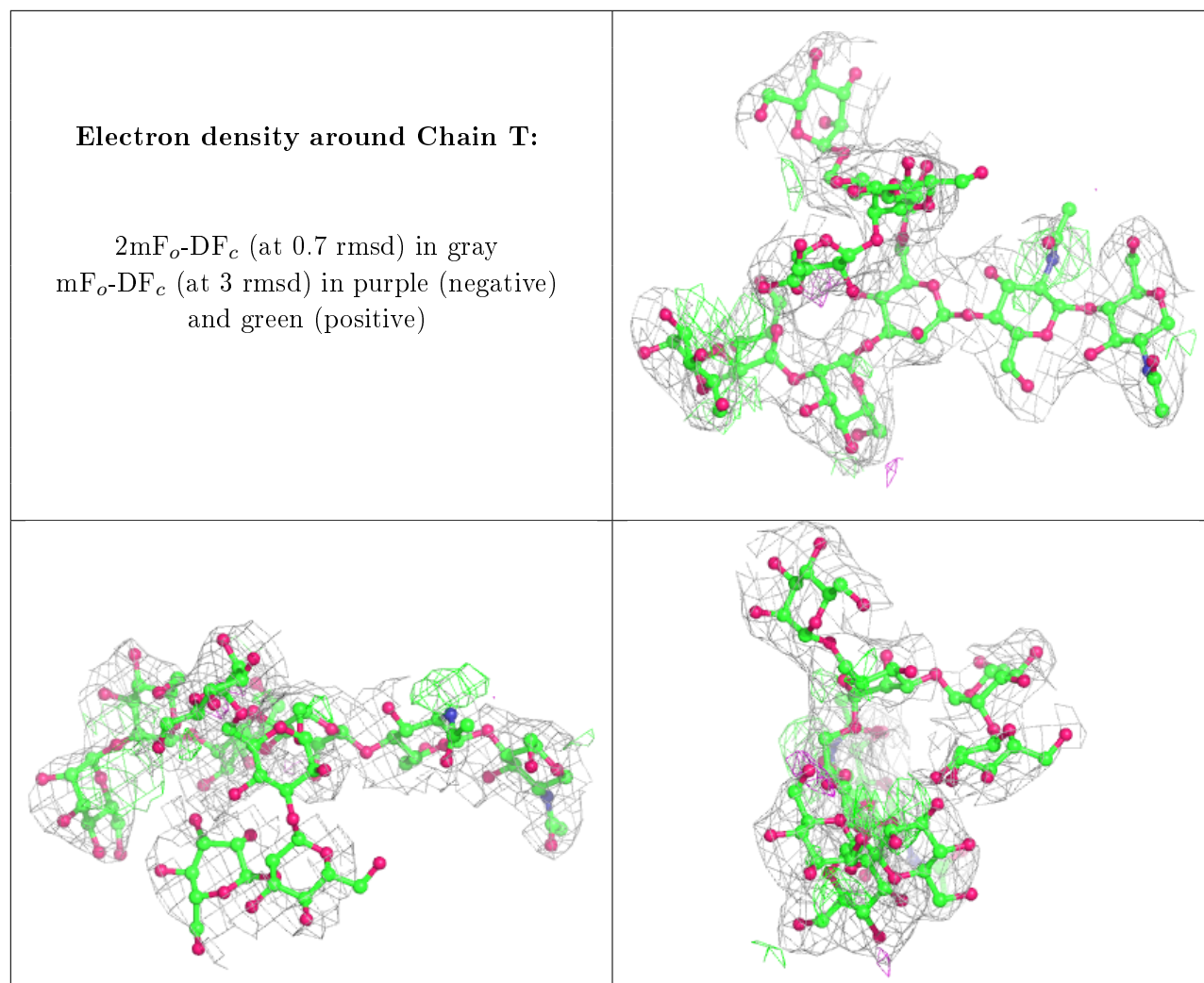
Electron density around Chain N:

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

**Electron density around Chain O:**

$2mF_o - DF_c$ (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(\AA^2)	Q<0.9
15	SO4	G	606	5/5	0.45	0.41	229,229,230,246	5
14	NAG	B	1611	14/15	0.80	0.23	110,127,140,144	0
14	NAG	B	1618	14/15	0.82	0.38	95,108,114,122	0
14	NAG	G	1355	14/15	0.84	0.29	121,137,144,146	0
15	SO4	G	607	5/5	0.84	0.24	155,157,158,160	0
14	NAG	G	1839	14/15	0.87	0.30	107,125,132,137	0
14	NAG	G	1276	14/15	0.90	0.33	113,122,128,128	0
14	NAG	H	523	14/15	0.90	0.24	113,124,132,136	0
15	SO4	B	702	5/5	0.90	0.17	154,155,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	NAG	B	1637	14/15	0.91	0.26	99,117,130,131	0
15	SO4	G	603	5/5	0.91	0.19	147,147,152,153	0
15	SO4	G	604	5/5	0.92	0.13	135,139,141,142	0
14	NAG	G	1133	14/15	0.93	0.28	104,119,131,133	0
15	SO4	G	605	5/5	0.94	0.14	147,147,151,157	0
15	SO4	G	601	5/5	0.95	0.15	123,126,128,132	0
15	SO4	G	602	5/5	0.96	0.18	107,114,116,121	0
15	SO4	B	701	5/5	0.97	0.15	81,82,86,101	0
15	SO4	L	301	5/5	0.98	0.11	90,90,92,93	5

6.5 Other polymers [i](#)

There are no such residues in this entry.