



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:01 PM UTC

PDB ID : 4IID / pdb_00004iid
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with 1-deoxynojirimycin
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on : 2012-12-20
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

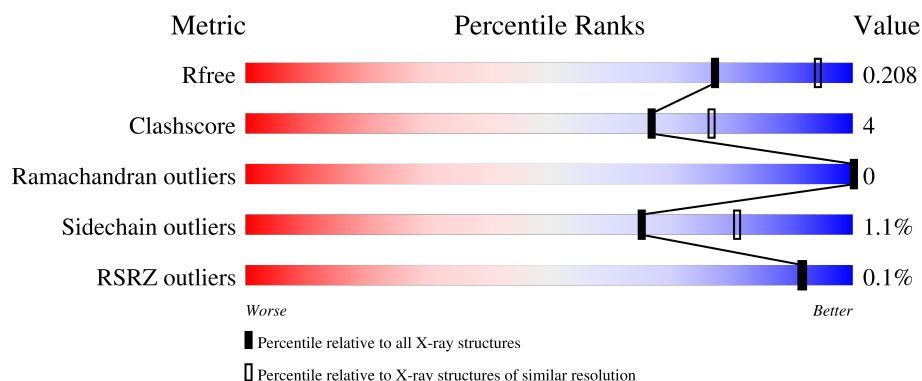
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

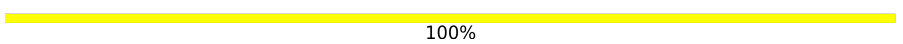
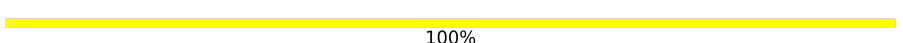
The reported resolution of this entry is 2.30 Å.

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



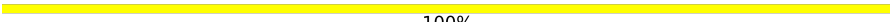
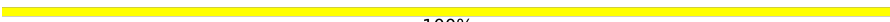
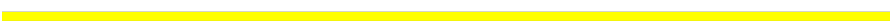
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	841	 90% 9% ..
1	B	841	 89% 10% .
2	C	4	 100%
3	D	3	 67% 33%
3	L	3	 100%

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Mol	Chain	Length	Quality of chain
3	N	3	 100%
4	E	2	 100%
4	G	2	 100%
5	F	10	 100%
5	M	10	 30% 70%
6	H	7	 29% 71%
6	O	7	 14% 57% 29%
7	I	7	 100%
8	J	7	 86% 14%
9	K	5	 100%
10	P	8	 100%

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
12	MRD	A	939	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 14782 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 Beta-glucosidase 1.

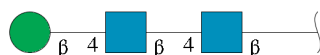
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	834	Total	C	N	O	S	0	0	0
			6387	4031	1097	1241	18			
1	B	832	Total	C	N	O	S	0	0	0
			6375	4023	1095	1239	18			

- Molecule 2 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
2	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 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.



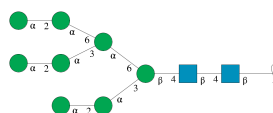
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



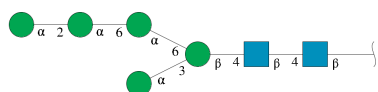
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



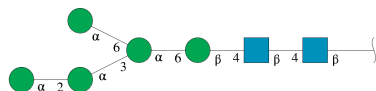
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	10	Total	C	N	O	0	0	0
			116	64	2	50			
5	M	10	Total	C	N	O	0	0	0
			116	64	2	50			

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



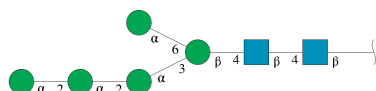
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is an oligosaccharide called 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.



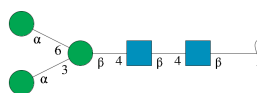
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



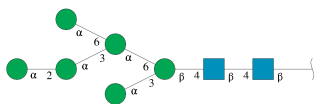
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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.



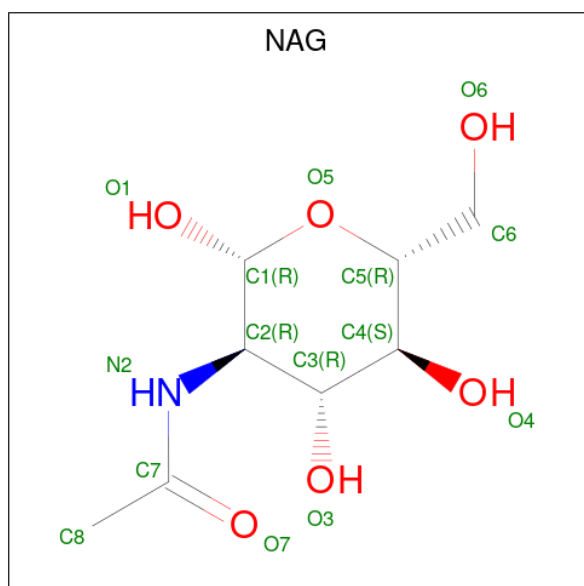
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



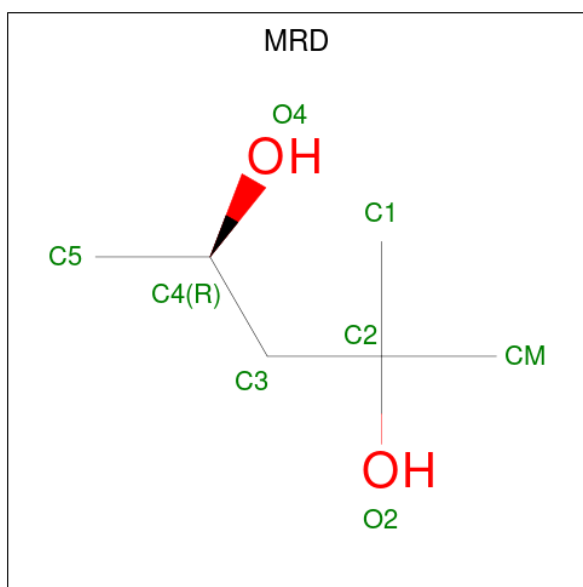
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



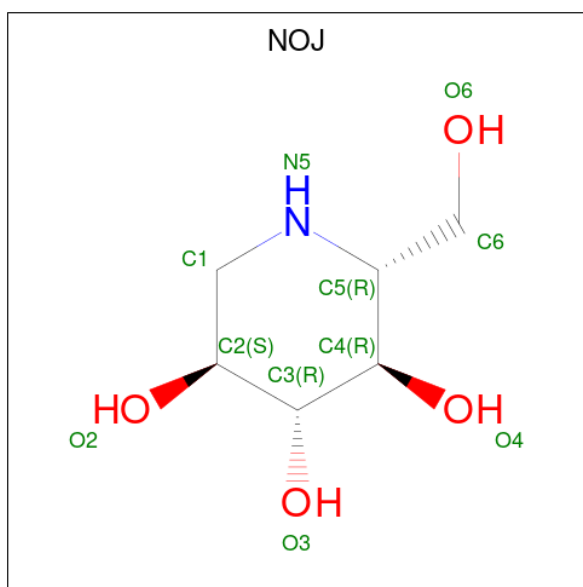
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			8	6	2		
12	A	1	Total	C	O	0	0
			8	6	2		
12	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 13 is 1-DEOXYNOJIRIMYCIN (CCD ID: NOJ) (formula: $C_6H_{13}NO_4$).



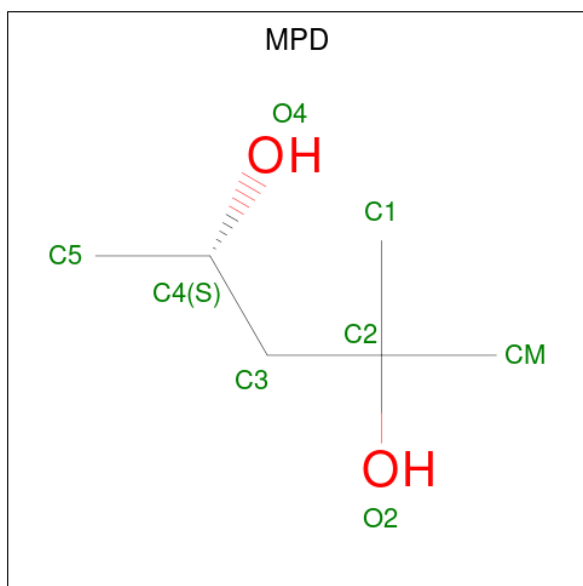
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			11	6	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 14 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	C	O	0	0
			8	6	2		

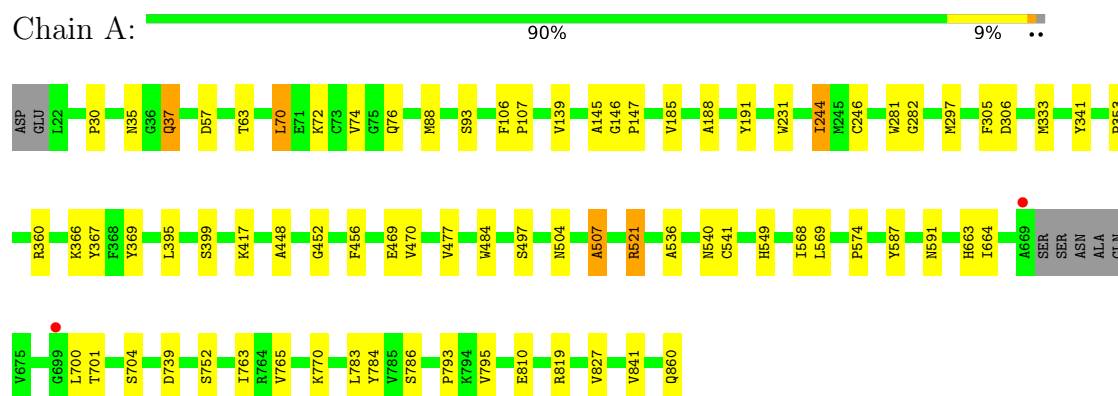
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	450	Total	O	0	0
			450	450		
15	B	504	Total	O	0	0
			504	504		

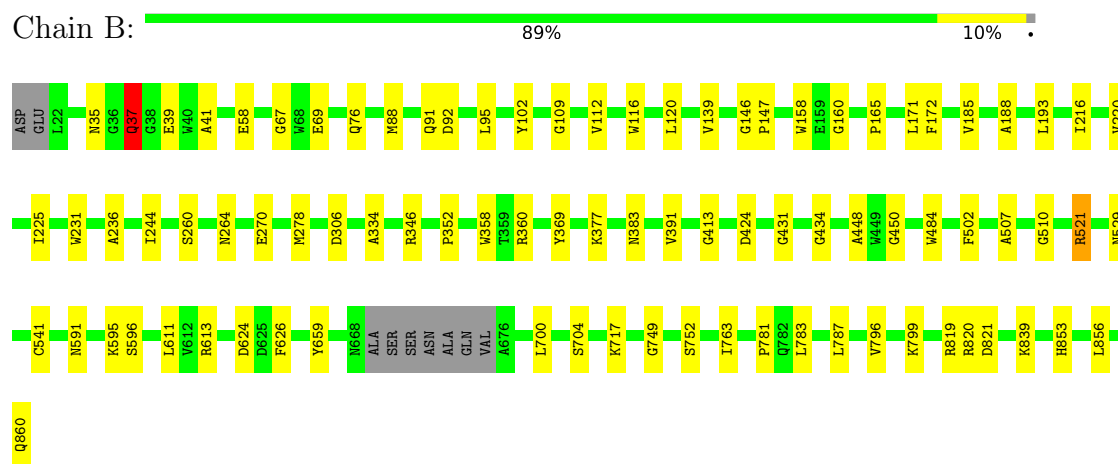
3 Residue-property plots

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

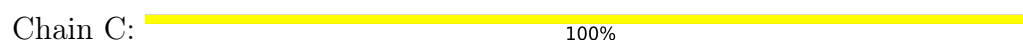
• Molecule 1: Beta-glucosidase 1



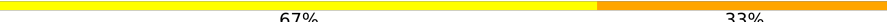
• Molecule 1: Beta-glucosidase 1



• Molecule 2: 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

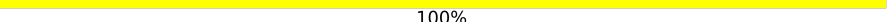


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67% 33%

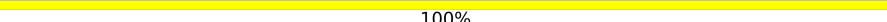
MAG1
MAG2
BMA3

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

Chain L:  100%

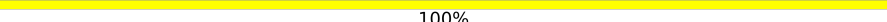
MAG1
MAG2
BMA3

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

Chain N:  100%

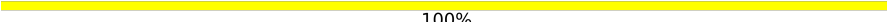
MAG1
MAG2
BMA3

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

Chain E:  100%

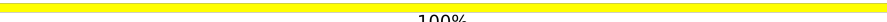
MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

- Molecule 5: 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)-[alpha-D-mannopyranose-(1-2)-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

Chain F:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

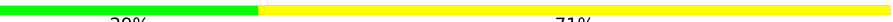
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(

1-2)-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

Chain M:  30% 70%

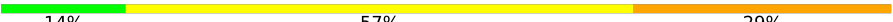


• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  29% 71%

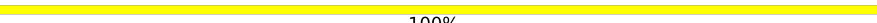


• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  14% 57% 29%

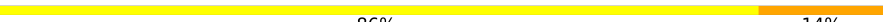


• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

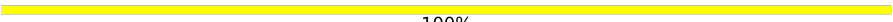


• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  86% 14%



• 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 K:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain P:

100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.45Å 121.60Å 221.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.07 – 2.30 39.07 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.07-2.30) 99.4 (39.07-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.155 , 0.207 0.157 , 0.208	Depositor DCC
R_{free} test set	4977 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14782	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: MPD, NOJ, MRD, NAG, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.19	8/6550 (0.1%)	1.15	17/8930 (0.2%)
1	B	1.26	16/6538 (0.2%)	1.15	20/8913 (0.2%)
All	All	1.22	24/13088 (0.2%)	1.15	37/17843 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	CYS	CA-CB	9.89	1.68	1.53
1	B	541	CYS	CA-CB	8.48	1.69	1.53
1	B	541	CYS	N-CA	7.54	1.55	1.46
1	B	596	SER	C-N	6.49	1.38	1.33
1	B	41	ALA	N-CA	6.35	1.53	1.46
1	A	231	TRP	CA-C	6.01	1.59	1.52
1	B	450	GLY	C-O	5.96	1.28	1.24
1	A	568	ILE	C-O	5.78	1.29	1.23
1	B	820	ARG	CZ-NH2	5.78	1.41	1.33
1	A	704	SER	CA-C	5.70	1.59	1.52
1	B	67	GLY	N-CA	5.67	1.50	1.45
1	B	521	ARG	CD-NE	-5.63	1.38	1.46
1	B	352	PRO	CA-C	5.54	1.57	1.52
1	B	704	SER	CA-C	5.38	1.59	1.52
1	B	369	TYR	CA-C	5.38	1.59	1.52
1	B	165	PRO	CA-C	5.29	1.60	1.52
1	B	278	MET	CA-C	-5.22	1.46	1.52
1	A	541	CYS	N-CA	5.22	1.52	1.46
1	B	334	ALA	CA-C	5.17	1.59	1.52
1	A	793	PRO	C-O	5.08	1.29	1.23
1	B	749	GLY	N-CA	5.06	1.52	1.44
1	B	796	VAL	C-O	5.04	1.29	1.24
1	A	507	ALA	C-O	5.02	1.28	1.23
1	A	369	TYR	CA-C	5.01	1.58	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	CYS	N-CA-CB	8.42	124.82	110.68
1	B	434	GLY	N-CA-C	7.86	123.13	114.40
1	A	541	CYS	N-CA-CB	7.71	122.67	110.57
1	B	521	ARG	NE-CZ-NH2	-7.70	112.27	119.20
1	A	521	ARG	NE-CZ-NH2	-7.56	112.39	119.20
1	A	536	ALA	N-CA-C	-7.56	103.11	111.36
1	B	541	CYS	N-CA-C	-6.56	98.20	108.90
1	B	231	TRP	CA-C-N	-6.33	112.48	119.19
1	B	231	TRP	C-N-CA	-6.33	112.48	119.19
1	A	456	PHE	CA-C-N	-6.25	113.24	119.56
1	A	456	PHE	C-N-CA	-6.25	113.24	119.56
1	B	510	GLY	N-CA-C	6.13	121.83	113.99
1	A	70	LEU	CA-CB-CG	-6.09	94.98	116.30
1	B	591	ASN	CA-C-N	-6.06	113.52	119.76
1	B	591	ASN	C-N-CA	-6.06	113.52	119.76
1	A	282	GLY	N-CA-C	-5.94	106.90	115.27
1	B	37	GLN	CA-CB-CG	5.93	125.96	114.10
1	A	399	SER	N-CA-C	-5.71	104.89	112.94
1	A	541	CYS	N-CA-C	-5.69	99.90	109.07
1	A	591	ASN	CA-C-N	-5.59	114.00	119.76
1	A	591	ASN	C-N-CA	-5.59	114.00	119.76
1	B	360	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	B	704	SER	N-CA-CB	-5.50	101.52	109.83
1	A	521	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	A	786	SER	N-CA-C	-5.47	99.49	108.41
1	A	540	ASN	N-CA-C	5.42	121.44	114.56
1	B	431	GLY	N-CA-C	-5.32	106.05	112.48
1	B	171	LEU	CA-C-N	5.26	127.28	120.44
1	B	171	LEU	C-N-CA	5.26	127.28	120.44
1	B	521	ARG	NE-CZ-NH1	5.19	126.69	121.50
1	B	820	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	B	112	VAL	N-CA-C	-5.13	105.39	110.62
1	A	145	ALA	N-CA-C	-5.12	105.05	113.50
1	B	413	GLY	N-CA-C	-5.08	108.31	115.32
1	B	270	GLU	N-CA-C	5.07	116.66	111.03
1	A	106	PHE	CA-C-N	-5.02	115.06	120.03
1	A	106	PHE	C-N-CA	-5.02	115.06	120.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6387	0	6096	53	0
1	B	6375	0	6082	35	0
2	C	50	0	43	0	0
3	D	39	0	34	1	0
3	L	39	0	34	0	0
3	N	39	0	34	0	0
4	E	28	0	25	0	0
4	G	28	0	25	0	0
5	F	116	0	97	0	0
5	M	116	0	97	0	0
6	H	83	0	70	3	0
6	O	83	0	70	2	0
7	I	83	0	70	0	0
8	J	83	0	70	1	0
9	K	61	0	52	0	0
10	P	94	0	79	0	0
11	A	28	0	26	0	0
11	B	42	0	39	0	0
12	A	16	0	28	11	0
12	B	8	0	14	2	0
13	A	11	0	13	0	0
13	B	11	0	13	0	0
14	B	8	0	14	4	0
15	A	450	0	0	0	0
15	B	504	0	0	5	0
All	All	14782	0	13125	100	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 4.

All (100) 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)
14:B:947:MPD:HM1	14:B:947:MPD:C5	1.66	1.16
14:B:947:MPD:H53	14:B:947:MPD:CM	1.79	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:HG21	1:A:333:MET:CE	1.83	1.08
1:A:63:THR:HG21	1:A:333:MET:HE2	1.35	1.05
1:A:63:THR:CG2	1:A:333:MET:CE	2.39	1.01
12:A:939:MRD:HMC2	15:B:1083:HOH:O	1.61	0.99
14:B:947:MPD:C5	14:B:947:MPD:CM	2.42	0.95
1:A:63:THR:CG2	1:A:333:MET:HE2	2.03	0.89
14:B:947:MPD:HM1	14:B:947:MPD:H53	0.90	0.88
1:A:360:ARG:HH21	12:A:939:MRD:HMC3	1.49	0.78
6:O:3:BMA:H62	6:O:4:MAN:H5	1.68	0.75
1:B:260:SER:O	1:B:264:ASN:HB2	1.89	0.72
1:A:63:THR:HG21	1:A:333:MET:HE1	1.72	0.69
1:A:819:ARG:HH12	1:A:860:GLN:C	1.99	0.69
12:A:938:MRD:O2	12:A:938:MRD:H5C3	1.94	0.66
1:B:717:LYS:HE3	15:B:1158:HOH:O	1.95	0.66
1:A:360:ARG:HH21	12:A:939:MRD:CM	2.08	0.66
1:A:35:ASN:OD1	1:A:37:GLN:HB3	1.96	0.65
1:A:360:ARG:HG2	12:A:939:MRD:HMC1	1.78	0.65
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.78	0.64
1:B:146:GLY:HA2	1:B:147:PRO:C	2.23	0.64
1:A:360:ARG:CG	12:A:939:MRD:HMC1	2.32	0.60
1:A:484:TRP:CZ2	6:H:3:BMA:H62	2.37	0.60
1:A:63:THR:CG2	1:A:333:MET:HE1	2.29	0.60
1:A:507:ALA:HB2	1:A:521:ARG:HG3	1.83	0.59
1:B:763:ILE:HD13	1:B:856:LEU:HD22	1.85	0.59
1:B:611:LEU:HD12	1:B:613:ARG:NH2	2.18	0.58
6:O:3:BMA:H62	6:O:4:MAN:C5	2.34	0.58
1:A:827:VAL:HG11	3:D:2:NAG:O3	2.04	0.58
1:A:819:ARG:NH1	1:A:860:GLN:O	2.28	0.57
1:A:188:ALA:HB3	1:A:244:ILE:HD13	1.87	0.56
1:A:819:ARG:NH1	1:A:860:GLN:C	2.63	0.56
1:B:819:ARG:HH22	1:B:860:GLN:C	2.12	0.56
1:A:63:THR:HG22	1:A:333:MET:CE	2.33	0.56
1:B:424:ASP:HB3	1:B:502:PHE:HB3	1.88	0.56
1:A:784:TYR:HB3	1:A:795:VAL:HB	1.88	0.55
12:B:948:MRD:O2	12:B:948:MRD:C5	2.55	0.54
1:B:783:LEU:C	1:B:783:LEU:HD23	2.33	0.54
1:B:193:LEU:HD11	1:B:225:ILE:HD12	1.90	0.54
1:A:191:TYR:O	1:A:246:CYS:HA	2.10	0.51
1:B:507:ALA:HB2	1:B:521:ARG:HG3	1.93	0.51
1:B:787:LEU:HA	1:B:839:LYS:HG2	1.93	0.51
1:A:448:ALA:HB1	1:A:507:ALA:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLN:HA	1:B:88:MET:O	2.12	0.50
1:A:88:MET:HE2	1:A:341:TYR:CD1	2.47	0.50
1:A:360:ARG:HD2	12:A:939:MRD:CM	2.42	0.50
1:A:107:PRO:HG3	1:A:574:PRO:O	2.11	0.50
1:A:484:TRP:CE2	6:H:3:BMA:H62	2.47	0.49
1:B:799:LYS:NZ	1:B:821:ASP:OD2	2.43	0.49
1:B:109:GLY:HA3	1:B:160:GLY:O	2.12	0.49
1:A:664:ILE:HD12	1:A:765:VAL:HG22	1.95	0.48
1:A:484:TRP:CE2	6:H:3:BMA:C6	2.97	0.48
1:A:93:SER:HB2	1:A:452:GLY:HA2	1.96	0.48
1:A:360:ARG:CG	12:A:939:MRD:CM	2.91	0.48
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.94	0.48
1:B:611:LEU:HD12	1:B:613:ARG:CZ	2.43	0.47
1:A:37:GLN:OE1	1:A:752:SER:HB2	2.14	0.47
1:A:770:LYS:HG3	1:A:810:GLU:HG2	1.97	0.47
1:A:470:VAL:HG11	1:A:477:VAL:HB	1.97	0.47
12:A:938:MRD:O2	12:A:938:MRD:C5	2.63	0.46
1:A:63:THR:O	1:A:297:MET:HA	2.16	0.46
1:A:360:ARG:HD2	12:A:939:MRD:HMC3	1.97	0.46
1:B:158:TRP:CE2	1:B:448:ALA:HB3	2.51	0.45
1:B:139:VAL:HG22	1:B:185:VAL:HB	1.99	0.45
1:B:35:ASN:OD1	1:B:37:GLN:HB3	2.17	0.45
1:B:484:TRP:CZ2	1:B:529:ASN:HB2	2.52	0.45
1:B:172:PHE:CE2	1:B:236:ALA:HB2	2.52	0.45
1:B:613:ARG:NH1	15:B:1147:HOH:O	2.31	0.45
1:A:504:ASN:HA	1:A:549:HIS:O	2.17	0.44
1:A:30:PRO:HG3	1:A:739:ASP:O	2.18	0.44
1:A:146:GLY:HA2	1:A:147:PRO:C	2.43	0.44
1:A:469:GLU:HG2	1:A:587:TYR:CE2	2.52	0.44
1:A:63:THR:CB	1:A:333:MET:HE1	2.48	0.44
1:B:220:VAL:HG22	1:B:626:PHE:CG	2.52	0.43
1:A:663:HIS:O	1:A:664:ILE:HD13	2.18	0.43
1:A:63:THR:HB	1:A:333:MET:HE1	1.99	0.43
1:A:139:VAL:HG22	1:A:185:VAL:HB	2.00	0.43
1:B:116:TRP:NE1	1:B:595:LYS:HB2	2.34	0.43
1:A:569:LEU:HD12	1:A:569:LEU:N	2.34	0.42
1:B:95:LEU:C	1:B:95:LEU:HD12	2.44	0.42
1:A:366:LYS:HE2	1:A:367:TYR:OH	2.19	0.42
1:B:346:ARG:HA	1:B:346:ARG:HD2	1.84	0.42
1:B:39:GLU:HG2	15:B:1350:HOH:O	2.19	0.42
1:B:102:TYR:HB3	1:B:383:ASN:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:PHE:O	1:A:306:ASP:HB2	2.20	0.42
1:A:783:LEU:C	1:A:783:LEU:HD23	2.45	0.41
12:A:939:MRD:HMC1	12:A:939:MRD:H5C3	2.03	0.41
1:A:72:LYS:HG3	1:A:353:PRO:HG2	2.02	0.41
1:A:281:TRP:N	1:A:281:TRP:HE3	2.18	0.41
12:B:948:MRD:O2	12:B:948:MRD:H5C3	2.21	0.41
1:A:76:GLN:HA	1:A:88:MET:O	2.20	0.41
1:B:37:GLN:OE1	1:B:752:SER:HB2	2.21	0.41
1:A:417:LYS:HB2	1:A:417:LYS:HE2	1.83	0.41
1:B:69:GLU:HG2	1:B:358:TRP:CE3	2.56	0.41
1:B:58:GLU:HG3	8:J:1:NAG:H81	2.02	0.40
1:B:91:GLN:HG3	1:B:92:ASP:O	2.21	0.40
1:B:306:ASP:HA	15:B:1075:HOH:O	2.20	0.40
1:A:57:ASP:OD1	1:A:57:ASP:N	2.54	0.40
1:B:659:TYR:HE1	1:B:781:PRO:HB3	1.87	0.40
1:B:216:ILE:HD11	1:B:624:ASP:HB2	2.03	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	A	830/841 (99%)	795 (96%)	35 (4%)	0	100	100
1	B	828/841 (98%)	799 (96%)	29 (4%)	0	100	100
All	All	1658/1682 (99%)	1594 (96%)	64 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	671/677 (99%)	662 (99%)	9 (1%)	61	77
1	B	670/677 (99%)	664 (99%)	6 (1%)	70	84
All	All	1341/1354 (99%)	1326 (99%)	15 (1%)	65	81

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	70	LEU
1	A	74	VAL
1	A	244	ILE
1	A	395	LEU
1	A	497	SER
1	A	700	LEU
1	A	701	THR
1	A	763	ILE
1	B	37	GLN
1	B	120	LEU
1	B	377	LYS
1	B	391	VAL
1	B	700	LEU
1	B	853	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	253	ASN
1	A	371	GLN
1	A	539	ASN
1	A	619	ASN
1	A	623	GLN
1	A	658	ASN

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Mol	Chain	Res	Type
1	A	663	HIS
1	B	126	GLN
1	B	371	GLN
1	B	539	ASN
1	B	540	ASN

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 ⓘ

78 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	1.02	1 (7%)	17,19,21	1.54	3 (17%)
2	NAG	C	2	2	14,14,15	0.95	1 (7%)	17,19,21	1.74	5 (29%)
2	BMA	C	3	2	11,11,12	1.26	1 (9%)	15,15,17	1.71	3 (20%)
2	MAN	C	4	2	11,11,12	1.02	0	15,15,17	2.09	3 (20%)
3	NAG	D	1	1,3	14,14,15	1.06	2 (14%)	17,19,21	1.49	3 (17%)
3	NAG	D	2	3	14,14,15	0.83	0	17,19,21	1.46	3 (17%)
3	BMA	D	3	3	11,11,12	1.08	0	15,15,17	2.67	7 (46%)
4	NAG	E	1	1,4	14,14,15	0.60	0	17,19,21	1.32	2 (11%)
4	NAG	E	2	4	14,14,15	0.60	0	17,19,21	1.60	3 (17%)
5	NAG	F	1	1,5	14,14,15	1.24	2 (14%)	17,19,21	0.72	0
5	MAN	F	10	5	11,11,12	1.12	2 (18%)	15,15,17	1.93	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	2	5	14,14,15	0.78	0	17,19,21	1.29	2 (11%)
5	BMA	F	3	5	11,11,12	0.90	0	15,15,17	1.70	4 (26%)
5	MAN	F	4	5	11,11,12	0.63	0	15,15,17	1.68	2 (13%)
5	MAN	F	5	5	11,11,12	0.94	0	15,15,17	1.89	4 (26%)
5	MAN	F	6	5	11,11,12	0.92	1 (9%)	15,15,17	1.42	3 (20%)
5	MAN	F	7	5	11,11,12	0.64	0	15,15,17	1.43	2 (13%)
5	MAN	F	8	5	11,11,12	0.61	0	15,15,17	1.50	4 (26%)
5	MAN	F	9	5	11,11,12	0.75	0	15,15,17	1.11	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.80	0	17,19,21	1.55	3 (17%)
4	NAG	G	2	4	14,14,15	0.88	1 (7%)	17,19,21	1.45	3 (17%)
6	NAG	H	1	1,6	14,14,15	0.69	0	17,19,21	0.83	0
6	NAG	H	2	6	14,14,15	0.93	1 (7%)	17,19,21	2.04	5 (29%)
6	BMA	H	3	6	11,11,12	0.83	0	15,15,17	1.07	0
6	MAN	H	4	6	11,11,12	0.79	0	15,15,17	0.99	0
6	MAN	H	5	6	11,11,12	0.84	0	15,15,17	1.76	5 (33%)
6	MAN	H	6	6	11,11,12	0.63	0	15,15,17	1.54	3 (20%)
6	MAN	H	7	6	11,11,12	0.69	0	15,15,17	1.46	2 (13%)
7	NAG	I	1	1,7	14,14,15	1.02	1 (7%)	17,19,21	1.94	4 (23%)
7	NAG	I	2	7	14,14,15	0.79	1 (7%)	17,19,21	1.33	2 (11%)
7	BMA	I	3	7	11,11,12	1.11	0	15,15,17	1.82	3 (20%)
7	MAN	I	4	7	11,11,12	0.92	0	15,15,17	1.35	2 (13%)
7	MAN	I	5	7	11,11,12	0.91	0	15,15,17	1.52	3 (20%)
7	MAN	I	6	7	11,11,12	0.57	0	15,15,17	1.98	5 (33%)
7	MAN	I	7	7	11,11,12	1.13	2 (18%)	15,15,17	3.45	7 (46%)
8	NAG	J	1	8,1	14,14,15	1.22	1 (7%)	17,19,21	1.54	4 (23%)
8	NAG	J	2	8	14,14,15	0.68	0	17,19,21	1.76	4 (23%)
8	BMA	J	3	8	11,11,12	0.94	0	15,15,17	1.67	2 (13%)
8	MAN	J	4	8	11,11,12	0.54	0	15,15,17	1.57	2 (13%)
8	MAN	J	5	8	11,11,12	0.89	0	15,15,17	1.27	1 (6%)
8	MAN	J	6	8	11,11,12	0.83	0	15,15,17	1.45	3 (20%)
8	MAN	J	7	8	11,11,12	1.01	0	15,15,17	2.30	8 (53%)
9	NAG	K	1	1,9	14,14,15	1.11	0	17,19,21	1.58	4 (23%)
9	NAG	K	2	9	14,14,15	0.84	0	17,19,21	1.56	4 (23%)
9	BMA	K	3	9	11,11,12	0.56	0	15,15,17	1.66	1 (6%)
9	MAN	K	4	9	11,11,12	1.07	1 (9%)	15,15,17	1.43	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	K	5	9	11,11,12	0.93	0	15,15,17	1.64	3 (20%)
3	NAG	L	1	1,3	14,14,15	0.81	0	17,19,21	1.76	4 (23%)
3	NAG	L	2	3	14,14,15	0.73	0	17,19,21	1.69	4 (23%)
3	BMA	L	3	3	11,11,12	0.82	0	15,15,17	1.64	3 (20%)
5	NAG	M	1	1,5	14,14,15	1.19	2 (14%)	17,19,21	1.84	6 (35%)
5	MAN	M	10	5	11,11,12	1.24	2 (18%)	15,15,17	1.92	6 (40%)
5	NAG	M	2	5	14,14,15	1.05	1 (7%)	17,19,21	1.54	3 (17%)
5	BMA	M	3	5	11,11,12	0.77	0	15,15,17	1.05	0
5	MAN	M	4	5	11,11,12	0.80	0	15,15,17	2.15	5 (33%)
5	MAN	M	5	5	11,11,12	0.58	0	15,15,17	2.35	5 (33%)
5	MAN	M	6	5	11,11,12	0.67	0	15,15,17	1.05	0
5	MAN	M	7	5	11,11,12	0.97	0	15,15,17	1.34	2 (13%)
5	MAN	M	8	5	11,11,12	1.41	2 (18%)	15,15,17	1.90	3 (20%)
5	MAN	M	9	5	11,11,12	0.85	0	15,15,17	0.73	0
3	NAG	N	1	1,3	14,14,15	0.76	0	17,19,21	1.36	1 (5%)
3	NAG	N	2	3	14,14,15	0.97	0	17,19,21	1.48	3 (17%)
3	BMA	N	3	3	11,11,12	0.89	0	15,15,17	2.14	4 (26%)
6	NAG	O	1	1,6	14,14,15	0.85	0	17,19,21	1.73	6 (35%)
6	NAG	O	2	6	14,14,15	1.16	1 (7%)	17,19,21	2.12	7 (41%)
6	BMA	O	3	6	11,11,12	0.59	0	15,15,17	2.95	4 (26%)
6	MAN	O	4	6	11,11,12	1.34	1 (9%)	15,15,17	2.01	4 (26%)
6	MAN	O	5	6	11,11,12	0.60	0	15,15,17	1.04	0
6	MAN	O	6	6	11,11,12	0.91	0	15,15,17	1.27	2 (13%)
6	MAN	O	7	6	11,11,12	1.02	1 (9%)	15,15,17	1.70	4 (26%)
10	NAG	P	1	1,10	14,14,15	0.71	0	17,19,21	1.96	3 (17%)
10	NAG	P	2	10	14,14,15	0.89	1 (7%)	17,19,21	1.44	1 (5%)
10	BMA	P	3	10	11,11,12	1.05	0	15,15,17	1.35	3 (20%)
10	MAN	P	4	10	11,11,12	0.70	0	15,15,17	1.22	1 (6%)
10	MAN	P	5	10	11,11,12	0.72	0	15,15,17	2.14	4 (26%)
10	MAN	P	6	10	11,11,12	0.71	0	15,15,17	1.74	5 (33%)
10	MAN	P	7	10	11,11,12	1.00	1 (9%)	15,15,17	1.59	4 (26%)
10	MAN	P	8	10	11,11,12	0.97	1 (9%)	15,15,17	1.63	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	F	10	5	-	2/2/19/22	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	1/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
5	MAN	F	7	5	-	0/2/19/22	0/1/1/1
5	MAN	F	8	5	-	0/2/19/22	0/1/1/1
5	MAN	F	9	5	-	0/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
6	NAG	H	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
6	MAN	H	5	6	-	0/2/19/22	0/1/1/1
6	MAN	H	6	6	-	0/2/19/22	0/1/1/1
6	MAN	H	7	6	-	2/2/19/22	0/1/1/1
7	NAG	I	1	1,7	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
7	MAN	I	4	7	-	2/2/19/22	0/1/1/1
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
7	MAN	I	6	7	-	2/2/19/22	0/1/1/1
7	MAN	I	7	7	-	2/2/19/22	0/1/1/1
8	NAG	J	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	2/6/23/26	0/1/1/1
8	BMA	J	3	8	-	0/2/19/22	0/1/1/1
8	MAN	J	4	8	-	0/2/19/22	0/1/1/1
8	MAN	J	5	8	-	1/2/19/22	0/1/1/1

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

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	4	MAN	O5-C1	-3.32	1.38	1.43
5	M	8	MAN	C2-C3	3.07	1.57	1.52
7	I	1	NAG	C2-N2	-3.05	1.41	1.46
5	F	1	NAG	O5-C1	-2.98	1.38	1.43
9	K	4	MAN	C2-C3	2.78	1.56	1.52
6	O	7	MAN	C2-C3	2.76	1.56	1.52
5	M	10	MAN	C2-C3	2.62	1.56	1.52
5	M	8	MAN	O5-C1	-2.61	1.39	1.43
10	P	7	MAN	C2-C3	2.59	1.56	1.52
5	M	10	MAN	O5-C1	-2.54	1.39	1.43
7	I	7	MAN	C2-C3	2.53	1.56	1.52
2	C	1	NAG	C1-C2	2.48	1.55	1.52
5	M	1	NAG	C2-N2	-2.45	1.42	1.46
10	P	8	MAN	C2-C3	2.37	1.56	1.52
6	O	2	NAG	O5-C1	-2.34	1.39	1.43
5	F	6	MAN	C2-C3	2.26	1.55	1.52
5	M	1	NAG	C1-C2	2.23	1.55	1.52
8	J	1	NAG	C1-C2	2.21	1.55	1.52
2	C	2	NAG	O5-C1	-2.18	1.40	1.43
10	P	2	NAG	O5-C1	-2.16	1.40	1.43
4	G	2	NAG	O5-C1	-2.14	1.40	1.43
5	F	10	MAN	C2-C3	2.12	1.55	1.52
3	D	1	NAG	C1-C2	2.11	1.55	1.52
3	D	1	NAG	O5-C1	-2.09	1.40	1.43
2	C	3	BMA	C2-C3	2.08	1.55	1.52
5	F	1	NAG	C2-N2	2.06	1.49	1.46
7	I	7	MAN	O5-C1	2.04	1.47	1.43
5	F	10	MAN	O3-C3	-2.03	1.37	1.43
6	H	2	NAG	C2-N2	-2.02	1.42	1.46
5	M	2	NAG	C2-N2	-2.01	1.42	1.46
7	I	2	NAG	O3-C3	-2.00	1.38	1.43

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	3	BMA	C6-C5-C4	-9.22	90.39	113.02
7	I	7	MAN	C1-O5-C5	8.15	123.11	112.19
10	P	5	MAN	C1-O5-C5	6.25	120.56	112.19
10	P	1	NAG	C1-O5-C5	6.00	120.23	112.19
7	I	7	MAN	C1-C2-C3	-5.80	101.20	109.64
3	D	3	BMA	C1-O5-C5	5.67	119.78	112.19
9	K	3	BMA	C1-O5-C5	5.53	119.59	112.19
5	M	4	MAN	C1-O5-C5	5.47	119.52	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	5	MAN	O6-C6-C5	-5.41	92.91	111.33
6	H	2	NAG	O5-C1-C2	-5.30	103.09	111.29
2	C	4	MAN	C1-O5-C5	5.27	119.25	112.19
5	M	8	MAN	C1-O5-C5	5.23	119.19	112.19
8	J	2	NAG	C1-O5-C5	5.04	118.94	112.19
7	I	1	NAG	C1-O5-C5	5.00	118.89	112.19
3	N	3	BMA	C1-O5-C5	4.95	118.82	112.19
7	I	7	MAN	O2-C2-C3	4.90	120.31	110.15
7	I	6	MAN	C1-O5-C5	4.83	118.66	112.19
5	M	5	MAN	C1-O5-C5	4.81	118.63	112.19
6	O	4	MAN	C1-O5-C5	4.61	118.36	112.19
5	F	10	MAN	O2-C2-C3	4.58	119.63	110.15
3	N	1	NAG	C1-O5-C5	4.54	118.28	112.19
6	O	3	BMA	C1-O5-C5	4.50	118.21	112.19
10	P	2	NAG	C1-O5-C5	4.43	118.13	112.19
6	O	2	NAG	O7-C7-N2	-4.42	114.17	121.98
5	M	2	NAG	C1-C2-N2	-4.33	103.62	110.43
4	G	1	NAG	C1-O5-C5	4.29	117.93	112.19
3	L	1	NAG	O4-C4-C5	-4.24	98.88	109.32
7	I	7	MAN	O5-C5-C6	4.17	115.78	107.66
4	E	2	NAG	O5-C5-C6	4.16	115.76	107.66
3	L	2	NAG	C2-N2-C7	4.15	128.47	122.90
2	C	3	BMA	C1-C2-C3	4.06	115.56	109.64
8	J	7	MAN	O6-C6-C5	4.01	124.98	111.33
6	H	6	MAN	C1-O5-C5	3.97	117.51	112.19
3	D	1	NAG	C1-C2-N2	3.97	116.69	110.43
6	H	2	NAG	C2-N2-C7	-3.96	117.59	122.90
5	F	3	BMA	O2-C2-C3	-3.95	101.97	110.15
7	I	3	BMA	C1-O5-C5	3.93	117.46	112.19
8	J	3	BMA	C1-O5-C5	3.92	117.44	112.19
6	O	4	MAN	C1-C2-C3	3.92	115.35	109.64
5	F	5	MAN	C1-O5-C5	3.87	117.37	112.19
9	K	5	MAN	O3-C3-C4	3.86	119.48	110.38
3	D	3	BMA	O3-C3-C2	-3.85	102.19	110.05
2	C	4	MAN	O5-C5-C6	3.84	115.14	107.66
7	I	3	BMA	O3-C3-C4	3.79	119.32	110.38
7	I	7	MAN	C3-C4-C5	-3.76	103.42	110.23
3	L	3	BMA	C1-O5-C5	3.70	117.15	112.19
3	D	3	BMA	C3-C4-C5	3.70	116.94	110.23
5	F	4	MAN	O6-C6-C5	-3.67	98.82	111.33
5	F	5	MAN	O6-C6-C5	-3.67	98.83	111.33
5	M	1	NAG	O4-C4-C5	-3.64	100.36	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	4	MAN	O2-C2-C3	-3.63	102.64	110.15
6	O	7	MAN	O2-C2-C1	-3.53	101.14	109.22
5	F	6	MAN	C1-O5-C5	3.48	116.85	112.19
5	F	3	BMA	C1-O5-C5	3.46	116.83	112.19
2	C	2	NAG	C2-N2-C7	3.46	127.54	122.90
3	N	3	BMA	C3-C4-C5	3.45	116.49	110.23
3	N	3	BMA	C1-C2-C3	3.45	114.66	109.64
8	J	5	MAN	O6-C6-C5	-3.44	99.60	111.33
5	F	4	MAN	O3-C3-C4	-3.44	102.27	110.38
4	E	1	NAG	C2-N2-C7	3.43	127.49	122.90
3	D	3	BMA	C1-C2-C3	3.41	114.61	109.64
10	P	8	MAN	C2-C3-C4	3.40	116.84	110.86
2	C	1	NAG	C2-N2-C7	-3.40	118.34	122.90
3	D	3	BMA	O6-C6-C5	3.39	122.87	111.33
3	L	2	NAG	C3-C4-C5	-3.37	104.12	110.23
5	M	7	MAN	O2-C2-C3	-3.37	103.17	110.15
6	O	3	BMA	C3-C4-C5	3.37	116.34	110.23
6	O	6	MAN	C1-O5-C5	3.35	116.68	112.19
6	H	7	MAN	O5-C1-C2	-3.34	102.83	110.79
10	P	6	MAN	O5-C5-C6	3.33	114.15	107.66
6	H	5	MAN	C3-C4-C5	-3.31	104.22	110.23
9	K	1	NAG	C4-C3-C2	-3.31	106.16	111.02
6	H	2	NAG	O6-C6-C5	-3.22	100.38	111.33
4	G	2	NAG	C4-C3-C2	3.22	115.73	111.02
8	J	7	MAN	O5-C5-C6	3.21	113.92	107.66
5	M	10	MAN	O2-C2-C3	3.21	116.80	110.15
6	O	2	NAG	C8-C7-N2	3.20	121.42	116.12
7	I	1	NAG	C1-C2-N2	-3.19	105.41	110.43
5	M	10	MAN	O3-C3-C2	3.18	116.55	110.05
6	H	5	MAN	O2-C2-C3	-3.15	103.62	110.15
3	D	2	NAG	C2-N2-C7	-3.14	118.69	122.90
6	O	1	NAG	O5-C1-C2	-3.11	106.47	111.29
2	C	4	MAN	O6-C6-C5	3.11	121.91	111.33
2	C	2	NAG	O7-C7-C8	-3.09	116.55	122.05
2	C	3	BMA	O3-C3-C4	3.09	117.66	110.38
8	J	7	MAN	O4-C4-C3	-3.07	103.14	110.38
7	I	7	MAN	O3-C3-C2	3.07	116.32	110.05
5	F	2	NAG	C1-O5-C5	3.05	116.27	112.19
6	O	2	NAG	O5-C1-C2	-3.05	106.58	111.29
8	J	4	MAN	O5-C5-C6	3.04	113.58	107.66
7	I	6	MAN	O3-C3-C4	3.04	117.54	110.38
8	J	2	NAG	O6-C6-C5	-3.01	101.07	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	6	MAN	C1-O5-C5	3.01	116.21	112.19
9	K	2	NAG	C1-C2-N2	3.00	115.16	110.43
3	N	2	NAG	C2-N2-C7	2.98	126.89	122.90
3	L	3	BMA	O4-C4-C5	2.96	116.60	109.32
7	I	6	MAN	O5-C5-C6	-2.95	101.91	107.66
8	J	7	MAN	C1-O5-C5	2.91	116.08	112.19
8	J	1	NAG	C2-N2-C7	-2.91	119.00	122.90
3	D	3	BMA	O5-C5-C6	2.89	113.29	107.66
9	K	5	MAN	C6-C5-C4	2.88	120.08	113.02
8	J	7	MAN	O3-C3-C4	2.87	117.15	110.38
5	F	10	MAN	C2-C3-C4	2.87	115.91	110.86
8	J	7	MAN	C6-C5-C4	2.87	120.06	113.02
5	F	2	NAG	O4-C4-C3	-2.86	103.63	110.38
2	C	1	NAG	C1-O5-C5	2.86	116.02	112.19
7	I	4	MAN	O5-C5-C6	2.86	113.23	107.66
8	J	1	NAG	C1-O5-C5	2.85	116.01	112.19
10	P	5	MAN	O2-C2-C3	-2.83	104.29	110.15
5	F	7	MAN	O2-C2-C3	-2.83	104.30	110.15
10	P	6	MAN	O3-C3-C4	2.83	117.04	110.38
10	P	7	MAN	C1-C2-C3	-2.83	105.53	109.64
7	I	6	MAN	O2-C2-C1	2.82	115.69	109.22
7	I	4	MAN	C1-O5-C5	2.82	115.96	112.19
6	O	1	NAG	C1-C2-N2	-2.82	105.99	110.43
9	K	1	NAG	C1-O5-C5	2.82	115.96	112.19
5	F	8	MAN	C1-O5-C5	2.81	115.95	112.19
9	K	4	MAN	O5-C5-C6	2.80	113.12	107.66
3	N	3	BMA	O5-C5-C6	2.79	113.09	107.66
5	M	2	NAG	O5-C5-C6	-2.79	102.24	107.66
5	M	1	NAG	C8-C7-N2	2.78	120.73	116.12
10	P	3	BMA	O5-C5-C6	-2.78	102.26	107.66
4	E	2	NAG	C3-C4-C5	-2.77	105.21	110.23
2	C	1	NAG	O5-C1-C2	2.76	115.55	111.29
7	I	5	MAN	C6-C5-C4	2.75	119.78	113.02
5	F	8	MAN	O3-C3-C2	-2.75	104.44	110.05
3	N	2	NAG	O7-C7-N2	2.73	126.81	121.98
5	M	10	MAN	C6-C5-C4	-2.73	106.32	113.02
5	M	8	MAN	O4-C4-C3	2.71	116.77	110.38
10	P	8	MAN	C1-C2-C3	2.71	113.59	109.64
5	M	1	NAG	C3-C4-C5	-2.71	105.32	110.23
4	E	1	NAG	O5-C5-C6	2.71	112.94	107.66
3	L	1	NAG	C1-O5-C5	2.71	115.81	112.19
9	K	2	NAG	C1-O5-C5	-2.70	108.56	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6	MAN	O5-C5-C6	2.69	112.90	107.66
3	D	3	BMA	O3-C3-C4	2.69	116.71	110.38
5	M	4	MAN	O6-C6-C5	-2.68	102.21	111.33
5	M	4	MAN	O2-C2-C3	2.67	115.67	110.15
10	P	8	MAN	C3-C4-C5	2.66	115.05	110.23
8	J	7	MAN	C1-C2-C3	2.65	113.50	109.64
7	I	2	NAG	C1-O5-C5	2.62	115.69	112.19
5	M	5	MAN	C6-C5-C4	-2.61	106.62	113.02
5	M	5	MAN	O2-C2-C1	2.60	115.18	109.22
6	H	6	MAN	C3-C4-C5	2.59	114.93	110.23
5	F	10	MAN	C1-O5-C5	2.59	115.66	112.19
6	O	4	MAN	O3-C3-C4	2.59	116.47	110.38
10	P	4	MAN	O3-C3-C2	-2.58	104.80	110.05
10	P	1	NAG	O6-C6-C5	-2.57	102.58	111.33
3	N	2	NAG	O5-C5-C6	-2.57	102.66	107.66
9	K	4	MAN	O2-C2-C3	2.57	115.47	110.15
5	M	10	MAN	O2-C2-C1	2.56	115.08	109.22
3	D	2	NAG	C1-O5-C5	-2.54	108.78	112.19
5	F	3	BMA	C1-C2-C3	2.53	113.33	109.64
7	I	5	MAN	O2-C2-C3	-2.52	104.92	110.15
6	O	7	MAN	O3-C3-C2	2.51	115.18	110.05
5	M	1	NAG	O5-C1-C2	-2.49	107.44	111.29
5	M	4	MAN	O3-C3-C4	-2.48	104.53	110.38
5	F	5	MAN	C6-C5-C4	-2.48	106.93	113.02
5	F	10	MAN	O2-C2-C1	2.47	114.88	109.22
4	G	1	NAG	O3-C3-C2	-2.46	104.28	109.40
5	M	10	MAN	O6-C6-C5	-2.46	102.96	111.33
6	O	7	MAN	O2-C2-C3	2.46	115.24	110.15
7	I	2	NAG	C2-N2-C7	-2.45	119.61	122.90
8	J	6	MAN	O5-C5-C6	2.45	112.43	107.66
3	L	2	NAG	C1-O5-C5	2.45	115.46	112.19
10	P	3	BMA	O5-C5-C4	-2.43	104.90	110.83
4	G	2	NAG	C1-C2-N2	-2.43	106.60	110.43
6	H	5	MAN	C6-C5-C4	2.43	118.99	113.02
6	O	1	NAG	C2-N2-C7	-2.42	119.66	122.90
10	P	7	MAN	O2-C2-C3	2.42	115.16	110.15
5	F	6	MAN	O3-C3-C2	2.42	114.99	110.05
5	M	1	NAG	C4-C3-C2	2.42	114.56	111.02
4	G	2	NAG	C2-N2-C7	-2.40	119.68	122.90
2	C	2	NAG	O5-C5-C4	-2.39	105.00	110.83
7	I	6	MAN	O6-C6-C5	-2.39	103.19	111.33
10	P	6	MAN	C3-C4-C5	-2.38	105.92	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	3	BMA	O3-C3-C2	-2.38	105.20	110.05
5	F	10	MAN	O4-C4-C3	-2.37	104.78	110.38
7	I	5	MAN	O4-C4-C3	-2.37	104.78	110.38
8	J	6	MAN	C3-C4-C5	-2.37	105.93	110.23
6	O	4	MAN	O5-C1-C2	2.37	116.43	110.79
7	I	3	BMA	O2-C2-C3	2.36	115.05	110.15
7	I	1	NAG	O5-C1-C2	-2.36	107.64	111.29
6	H	7	MAN	C1-C2-C3	-2.34	106.24	109.64
6	O	2	NAG	C1-C2-N2	-2.34	106.75	110.43
8	J	2	NAG	O4-C4-C5	-2.34	103.57	109.32
8	J	6	MAN	O3-C3-C4	-2.33	104.88	110.38
6	O	7	MAN	O5-C1-C2	-2.33	105.23	110.79
9	K	4	MAN	C2-C3-C4	2.31	114.92	110.86
3	L	2	NAG	O6-C6-C5	-2.30	103.51	111.33
10	P	7	MAN	C3-C4-C5	2.29	114.39	110.23
3	D	1	NAG	O5-C5-C4	-2.29	105.25	110.83
9	K	5	MAN	O5-C5-C6	2.29	112.12	107.66
5	M	5	MAN	O2-C2-C3	-2.29	105.41	110.15
10	P	5	MAN	O6-C6-C5	-2.28	103.57	111.33
9	K	2	NAG	O6-C6-C5	-2.28	103.57	111.33
6	O	1	NAG	O4-C4-C3	-2.28	105.01	110.38
2	C	3	BMA	O3-C3-C2	2.27	114.69	110.05
8	J	1	NAG	O7-C7-C8	-2.26	118.03	122.05
10	P	6	MAN	O2-C2-C3	2.26	114.83	110.15
5	F	8	MAN	O3-C3-C4	-2.25	105.08	110.38
6	O	6	MAN	O4-C4-C3	-2.24	105.08	110.38
6	O	2	NAG	O4-C4-C5	2.23	114.81	109.32
6	H	6	MAN	C6-C5-C4	-2.23	107.55	113.02
10	P	5	MAN	O5-C5-C4	2.21	116.22	110.83
9	K	1	NAG	O7-C7-N2	2.20	125.86	121.98
5	F	9	MAN	O4-C4-C3	-2.19	105.21	110.38
10	P	3	BMA	O6-C6-C5	-2.19	103.87	111.33
5	M	1	NAG	C1-C2-N2	-2.19	106.98	110.43
4	E	2	NAG	O7-C7-C8	-2.19	118.16	122.05
6	H	2	NAG	C3-C4-C5	-2.18	106.27	110.23
8	J	2	NAG	O7-C7-C8	-2.18	118.17	122.05
9	K	2	NAG	O5-C5-C4	-2.17	105.54	110.83
5	M	10	MAN	C1-O5-C5	2.17	115.10	112.19
7	I	1	NAG	O6-C6-C5	-2.17	103.94	111.33
10	P	1	NAG	O4-C4-C5	-2.16	104.01	109.32
2	C	2	NAG	C4-C3-C2	2.15	114.17	111.02
6	O	3	BMA	O3-C3-C4	-2.15	105.32	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	O5-C5-C6	2.14	111.83	107.66
2	C	2	NAG	O6-C6-C5	-2.14	104.05	111.33
6	O	2	NAG	O5-C5-C4	-2.13	105.63	110.83
5	F	8	MAN	O4-C4-C5	2.13	114.58	109.32
5	M	8	MAN	C1-C2-C3	2.13	112.75	109.64
7	I	7	MAN	O4-C4-C3	2.12	115.38	110.38
5	F	9	MAN	O2-C2-C3	-2.12	105.77	110.15
6	H	2	NAG	O4-C4-C3	-2.11	105.40	110.38
4	G	1	NAG	C1-C2-N2	-2.11	107.11	110.43
3	L	1	NAG	C2-N2-C7	2.10	125.71	122.90
6	H	5	MAN	C2-C3-C4	-2.10	107.17	110.86
6	O	1	NAG	O3-C3-C2	-2.09	105.06	109.40
6	O	1	NAG	C4-C3-C2	2.08	114.07	111.02
9	K	1	NAG	O4-C4-C3	-2.08	105.47	110.38
8	J	1	NAG	C4-C3-C2	2.08	114.06	111.02
6	O	2	NAG	C6-C5-C4	2.08	118.12	113.02
5	F	5	MAN	O5-C5-C4	2.07	115.87	110.83
8	J	3	BMA	O2-C2-C1	-2.06	104.50	109.22
8	J	7	MAN	C3-C4-C5	2.06	113.96	110.23
3	D	1	NAG	C2-N2-C7	-2.05	120.15	122.90
3	L	1	NAG	O5-C1-C2	-2.05	108.12	111.29
6	H	5	MAN	O5-C5-C6	2.04	111.64	107.66
5	M	7	MAN	O6-C6-C5	-2.02	104.45	111.33
9	K	4	MAN	O3-C3-C2	2.02	114.17	110.05
5	M	2	NAG	O6-C6-C5	-2.02	104.47	111.33
3	L	3	BMA	C1-C2-C3	2.01	112.57	109.64
5	M	4	MAN	C3-C4-C5	-2.01	106.59	110.23
5	F	7	MAN	O3-C3-C4	-2.01	105.64	110.38
10	P	7	MAN	O3-C3-C2	2.00	114.14	110.05

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	4	MAN	O5-C5-C6-O6
7	I	6	MAN	O5-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
7	I	7	MAN	O5-C5-C6-O6
7	I	4	MAN	C4-C5-C6-O6
5	F	10	MAN	O5-C5-C6-O6
9	K	4	MAN	O5-C5-C6-O6
10	P	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	J	6	MAN	O5-C5-C6-O6
7	I	6	MAN	C4-C5-C6-O6
9	K	4	MAN	C4-C5-C6-O6
5	F	10	MAN	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
6	H	7	MAN	O5-C5-C6-O6
7	I	7	MAN	C4-C5-C6-O6
10	P	6	MAN	C4-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
10	P	8	MAN	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
8	J	6	MAN	C4-C5-C6-O6
8	J	5	MAN	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
6	H	7	MAN	C4-C5-C6-O6
10	P	1	NAG	C4-C5-C6-O6
8	J	2	NAG	C4-C5-C6-O6
6	O	5	MAN	O5-C5-C6-O6
10	P	4	MAN	C4-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
3	N	3	BMA	O5-C5-C6-O6
9	K	5	MAN	O5-C5-C6-O6
10	P	8	MAN	C4-C5-C6-O6
3	D	3	BMA	C4-C5-C6-O6
8	J	2	NAG	O5-C5-C6-O6
6	O	6	MAN	O5-C5-C6-O6
3	L	2	NAG	C1-C2-N2-C7
6	O	7	MAN	C4-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
5	F	5	MAN	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 7 short contacts:

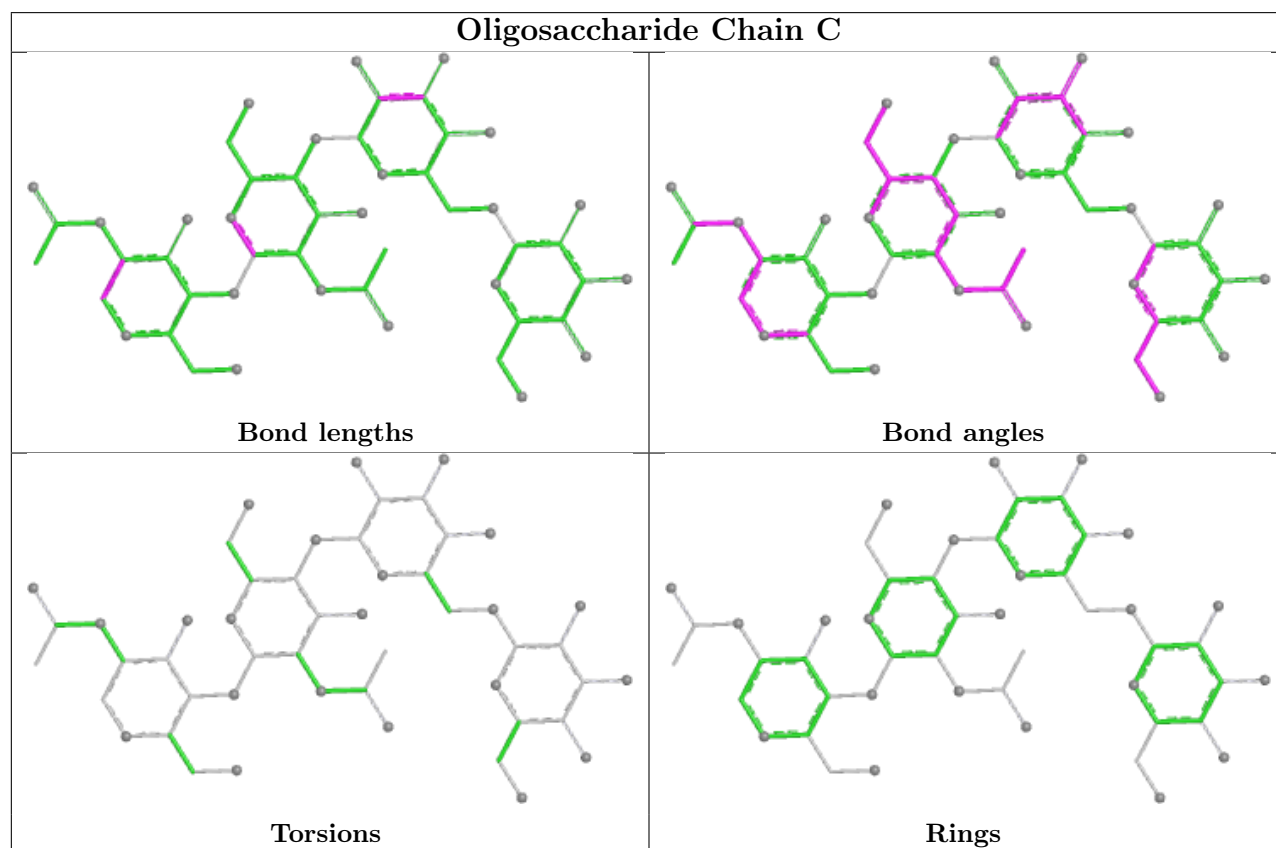
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	3	BMA	3	0
6	O	4	MAN	2	0

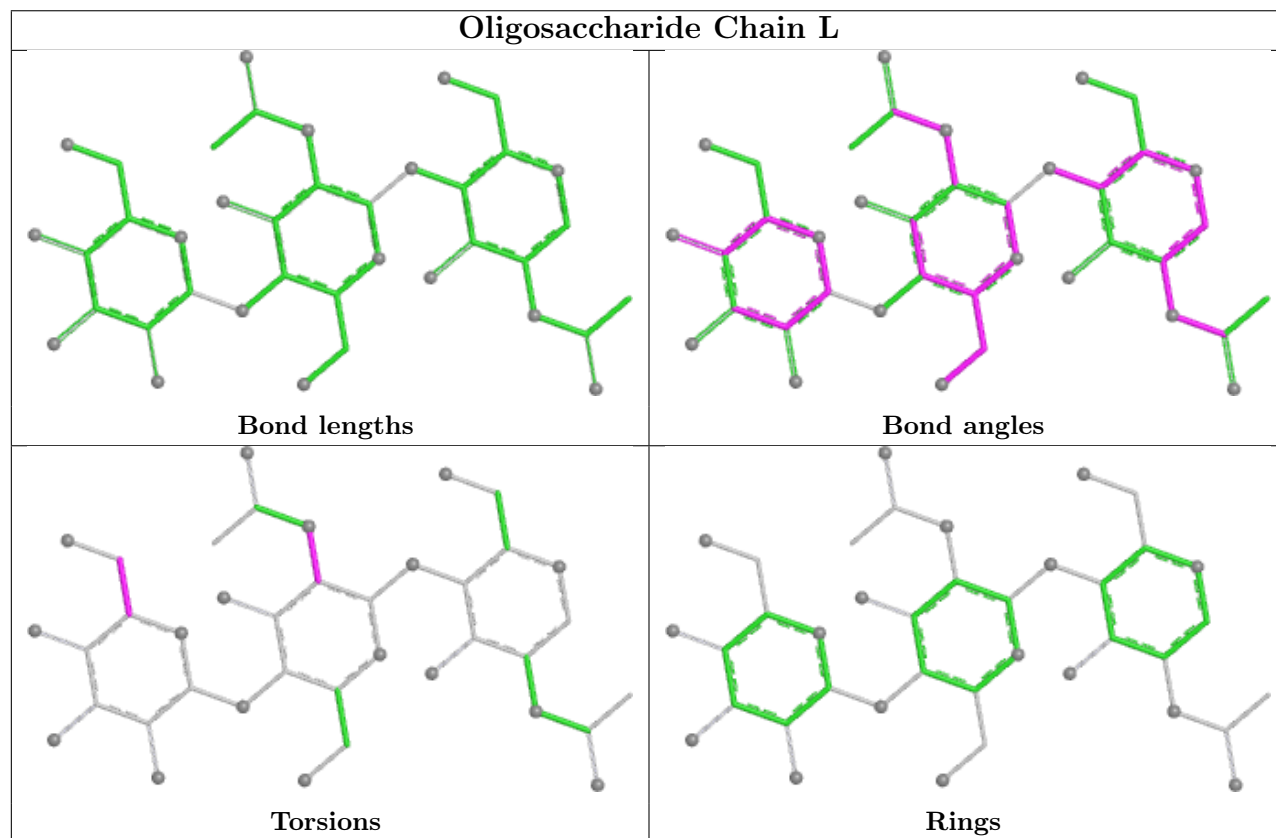
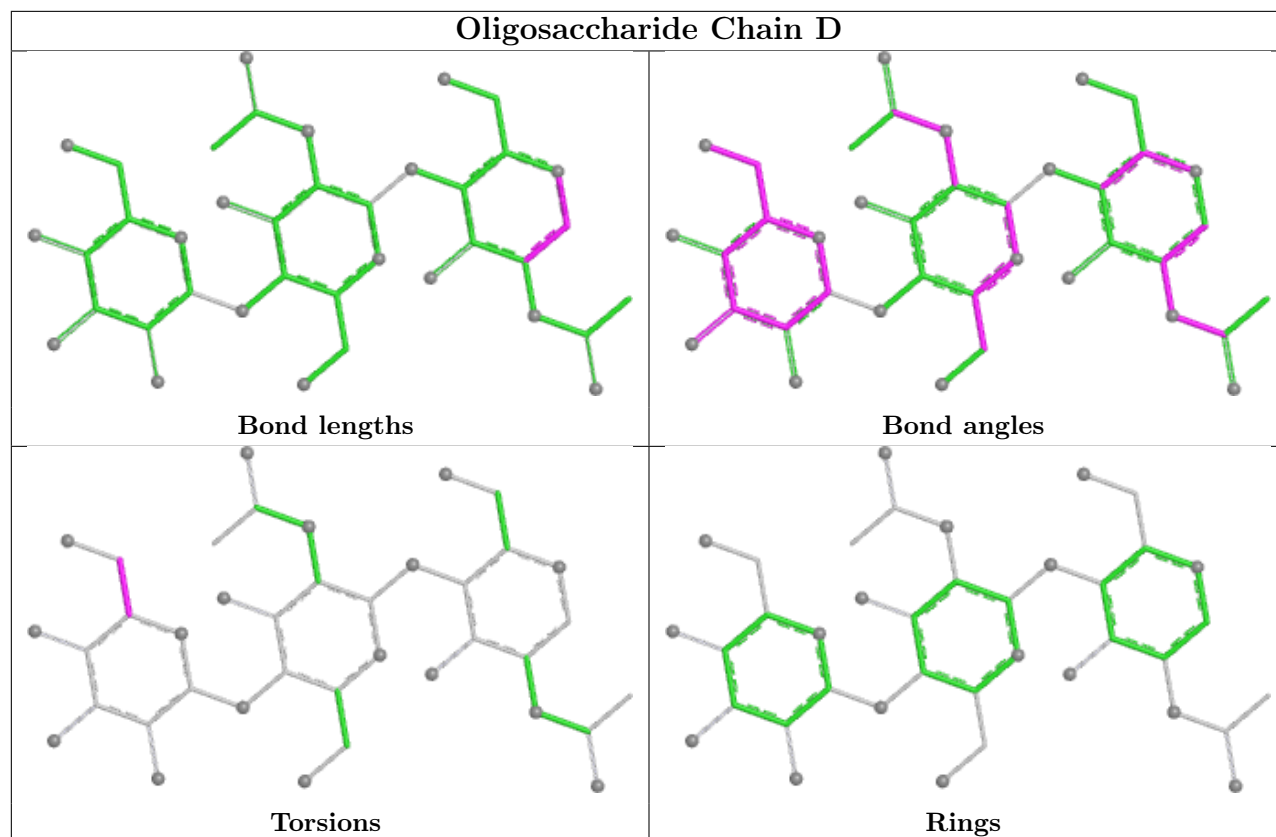
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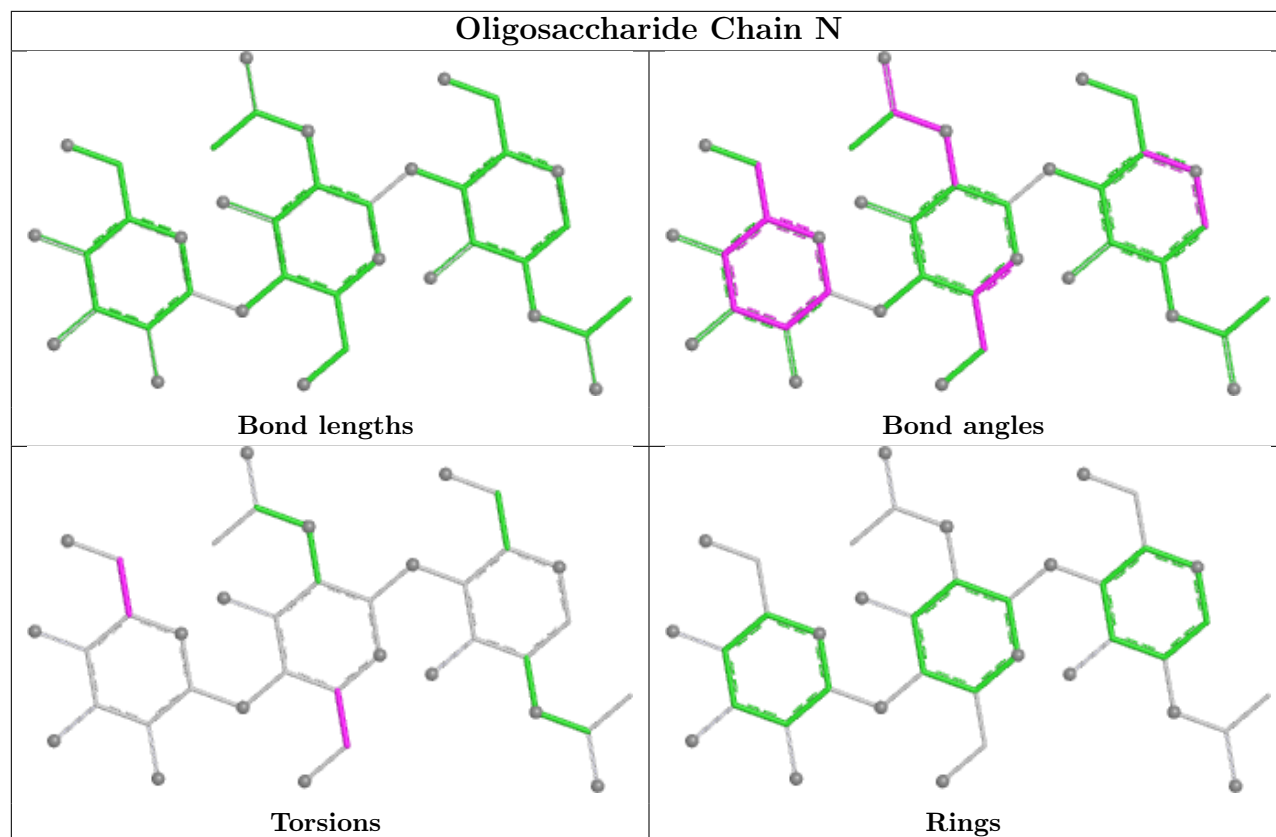
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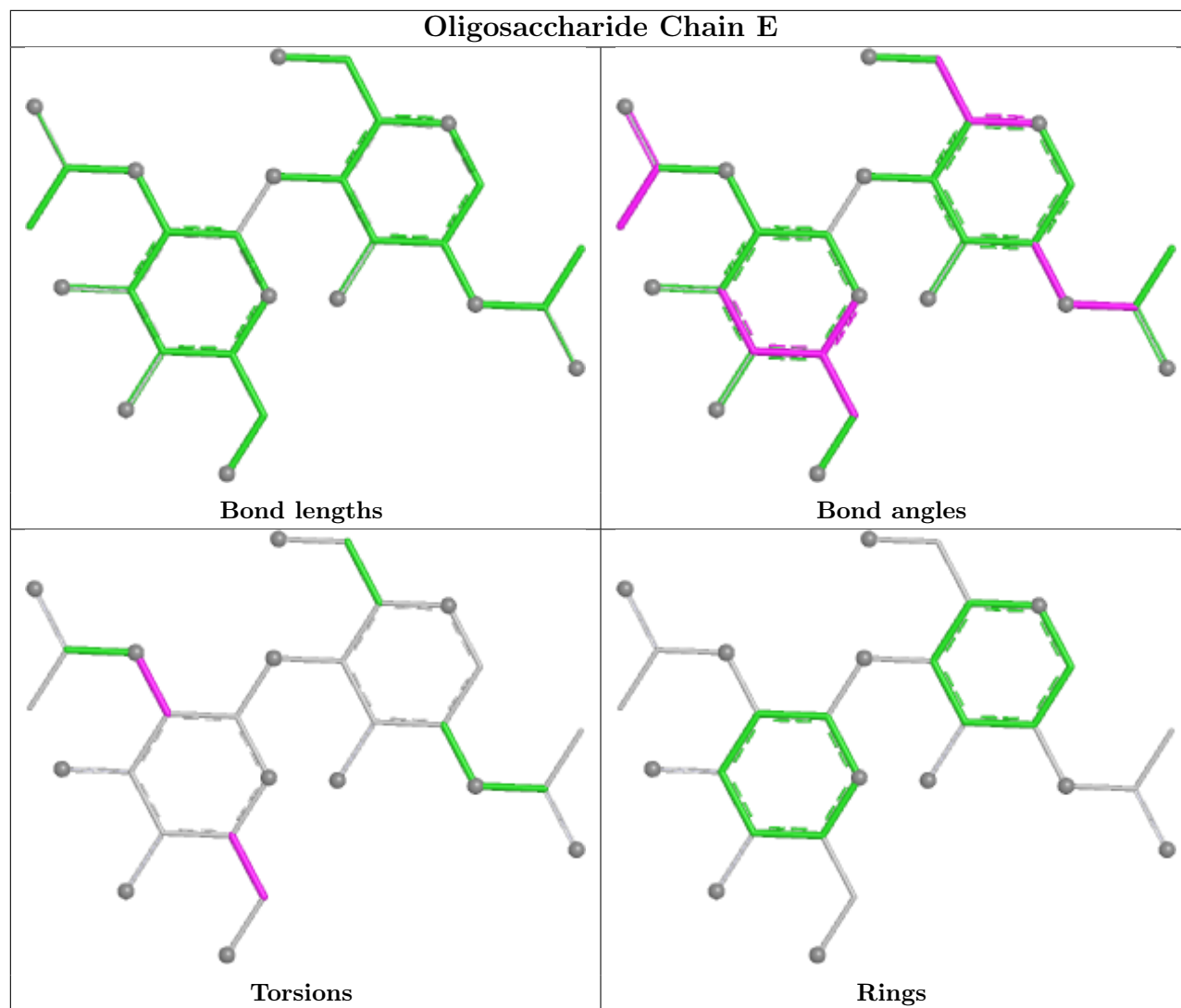
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	3	BMA	2	0
3	D	2	NAG	1	0
8	J	1	NAG	1	0

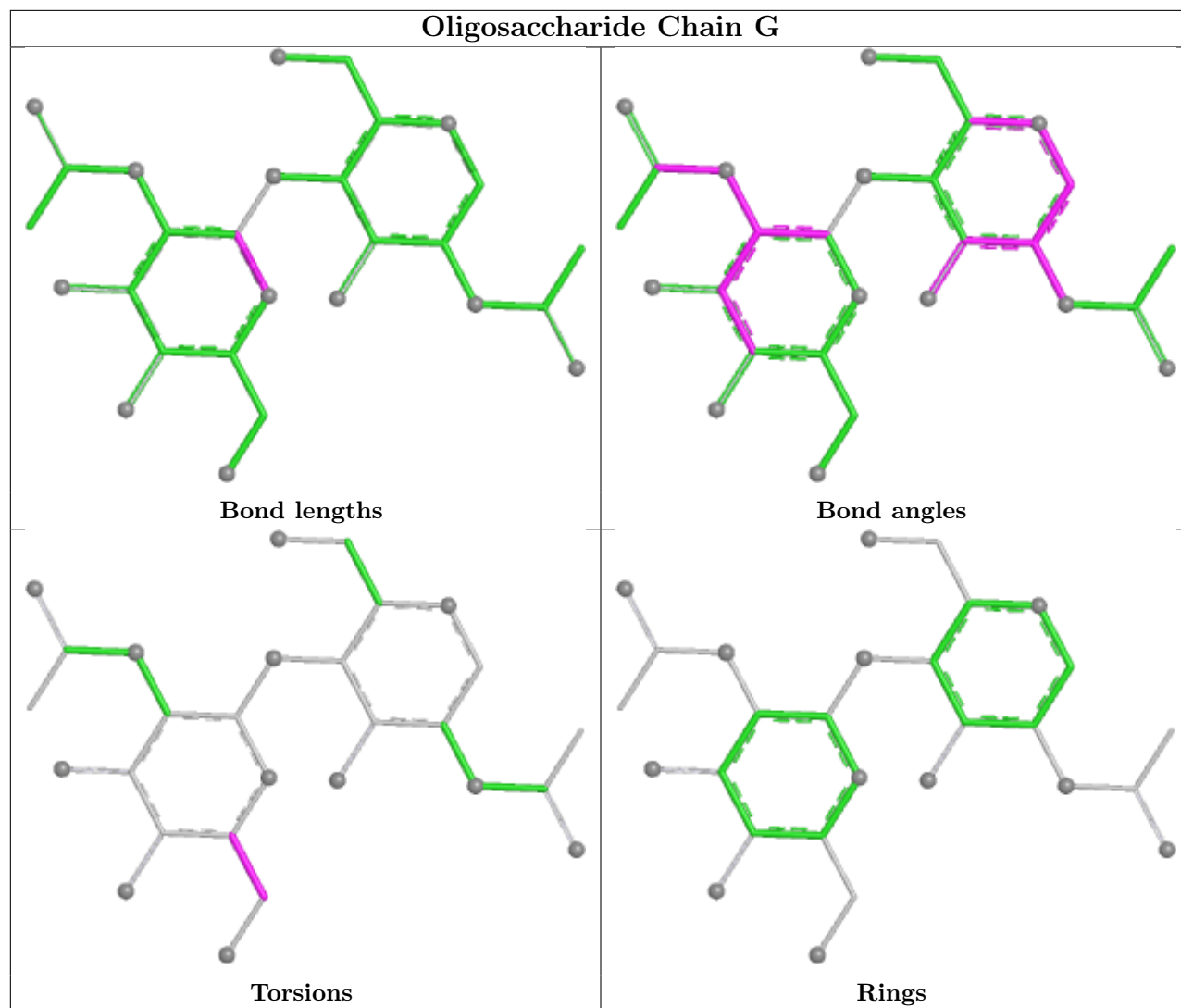
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

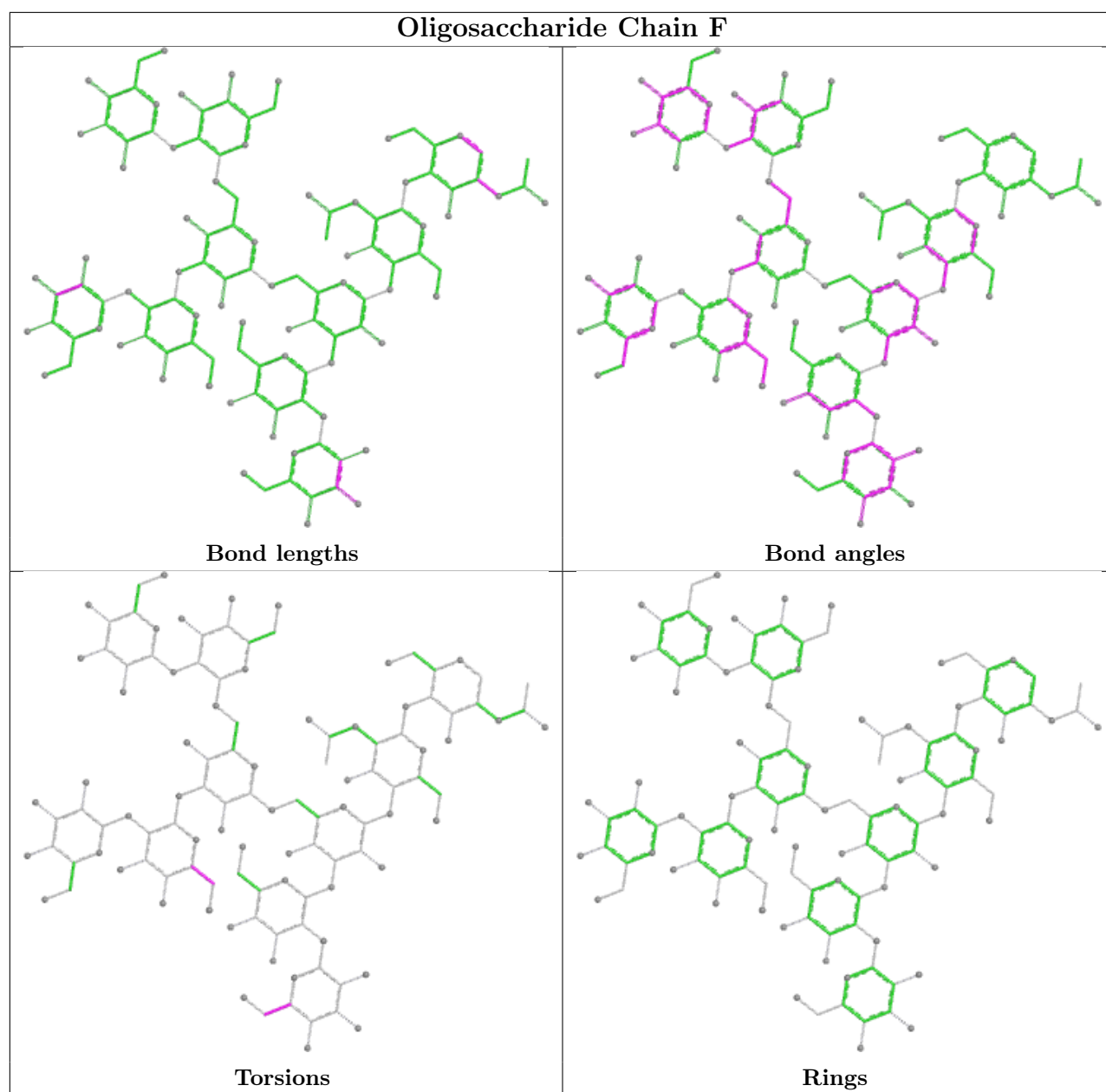


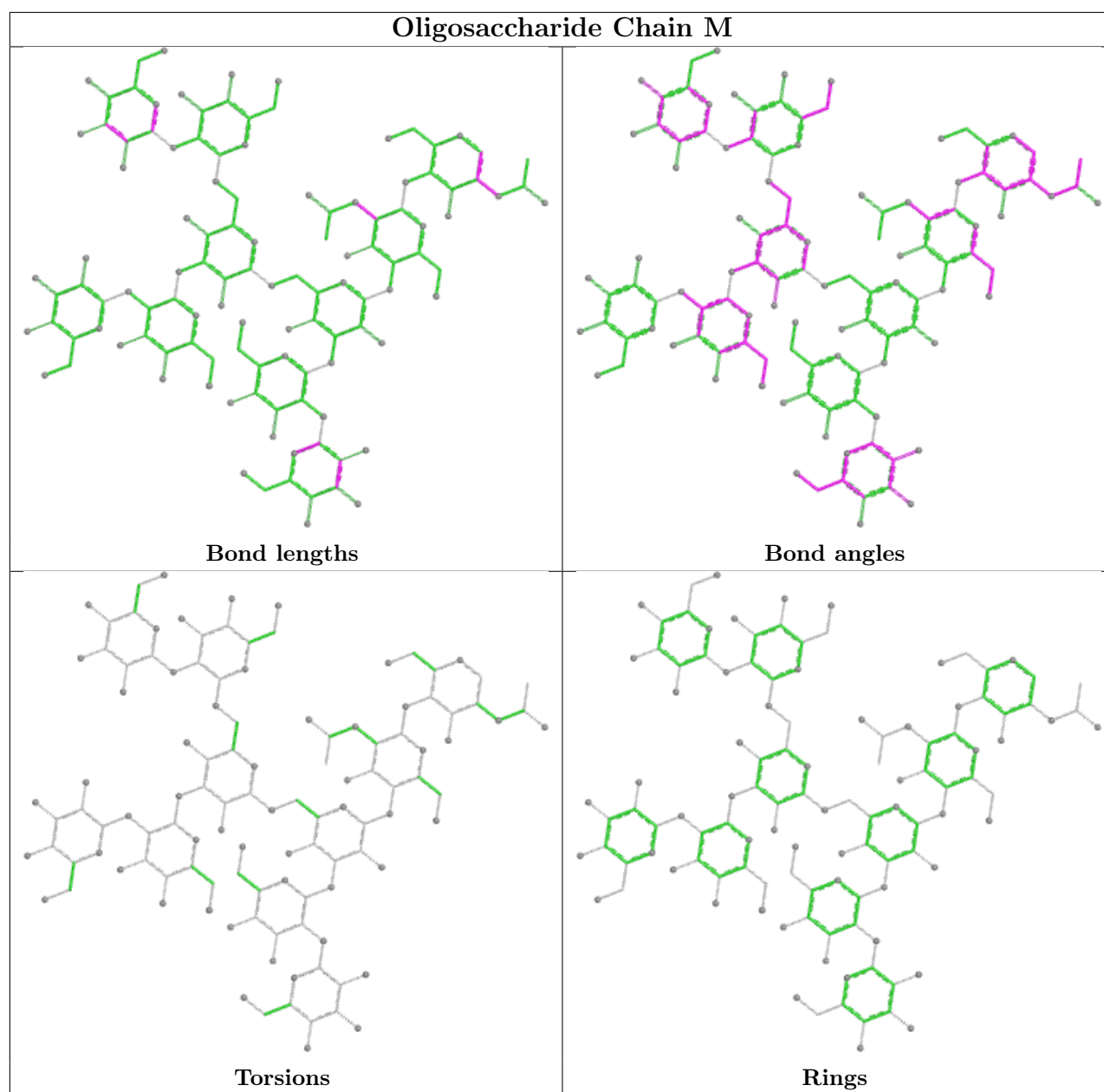


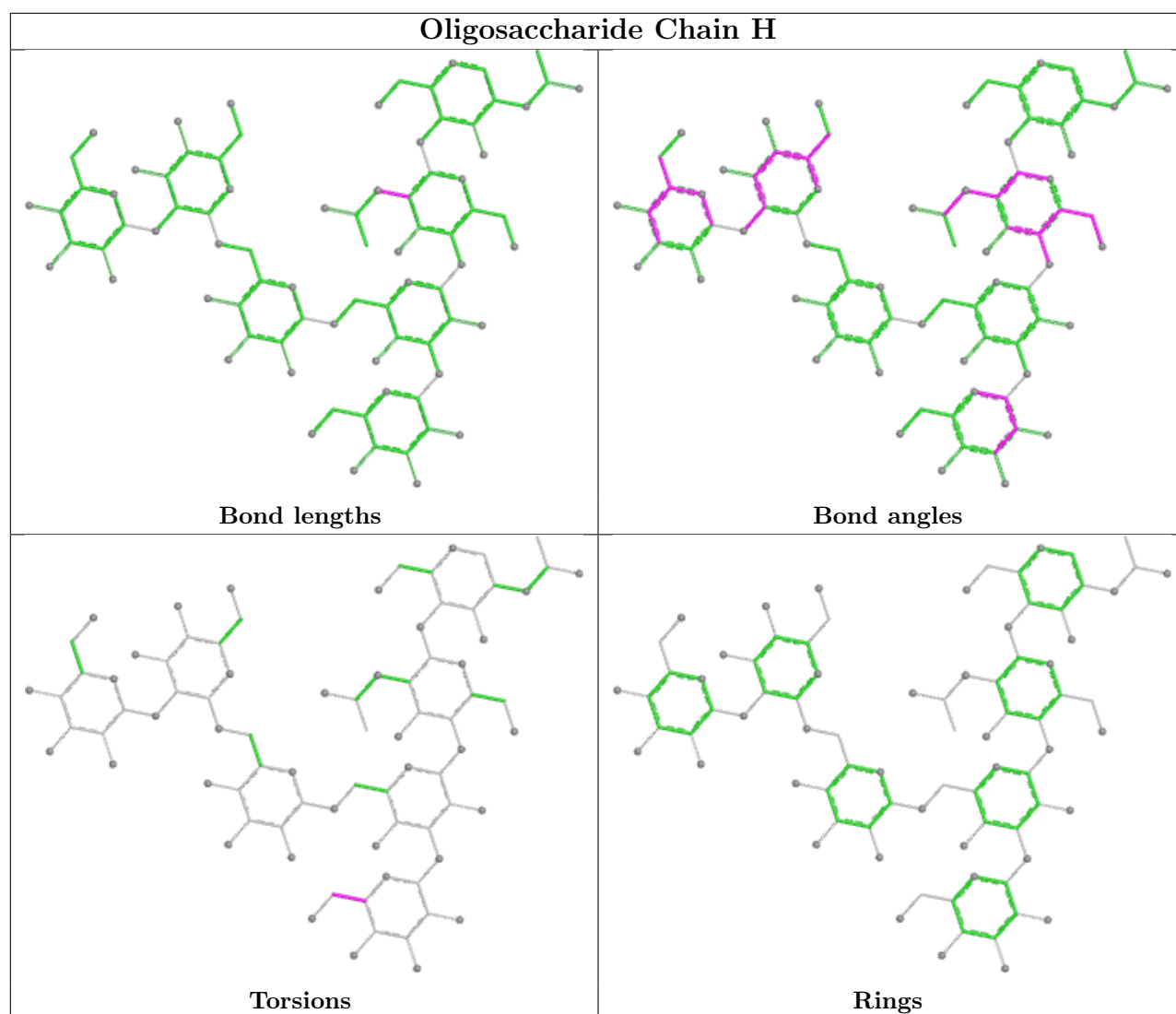


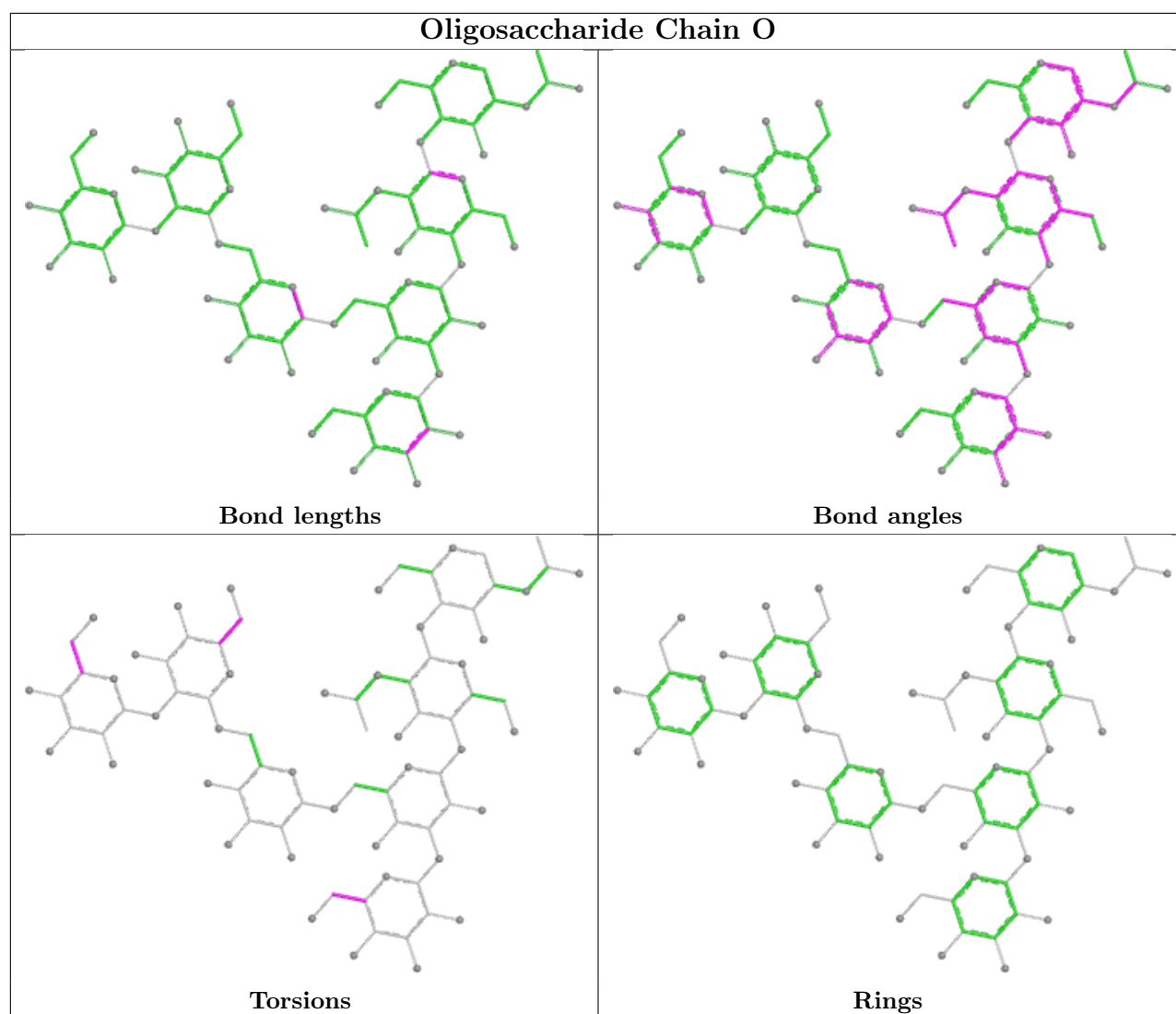


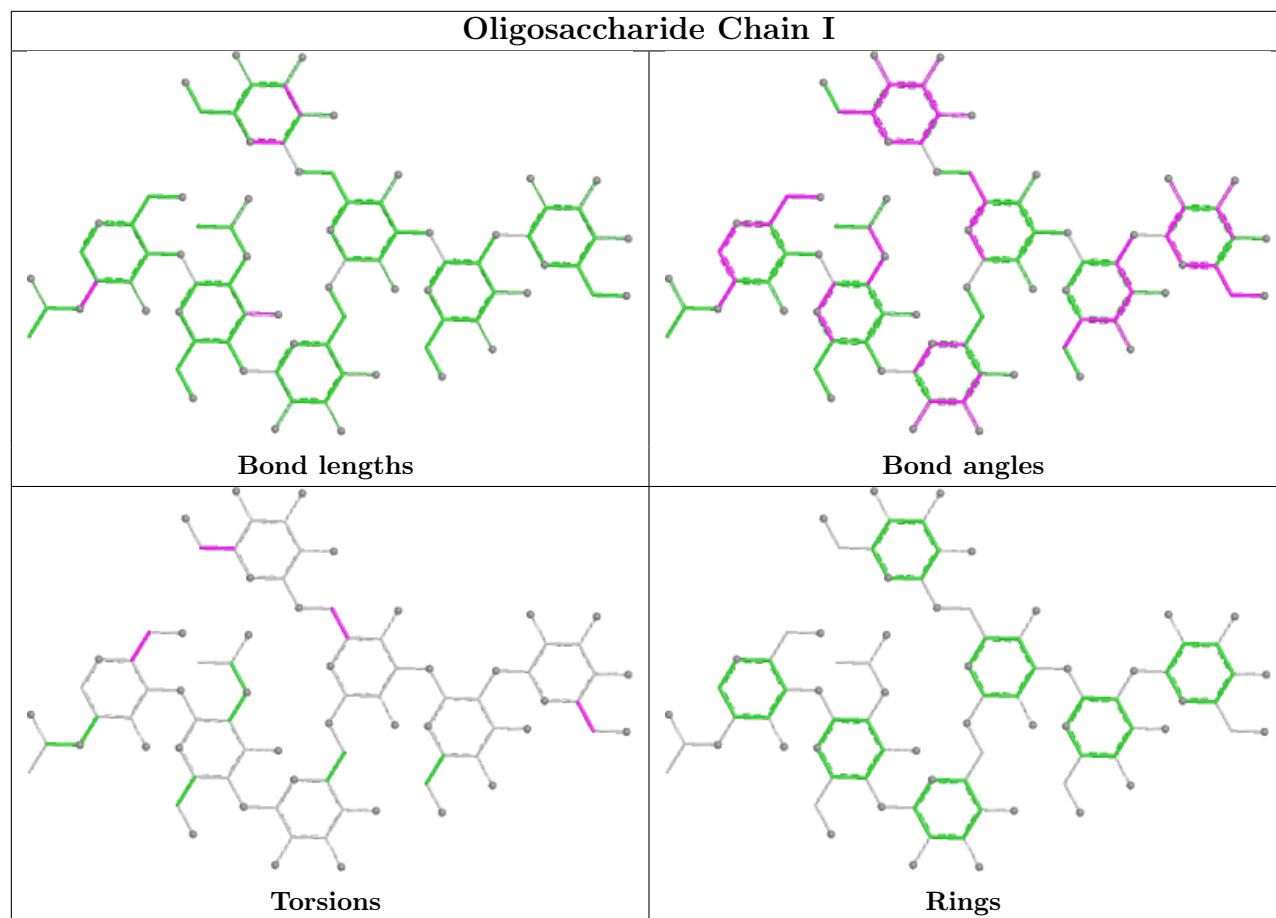


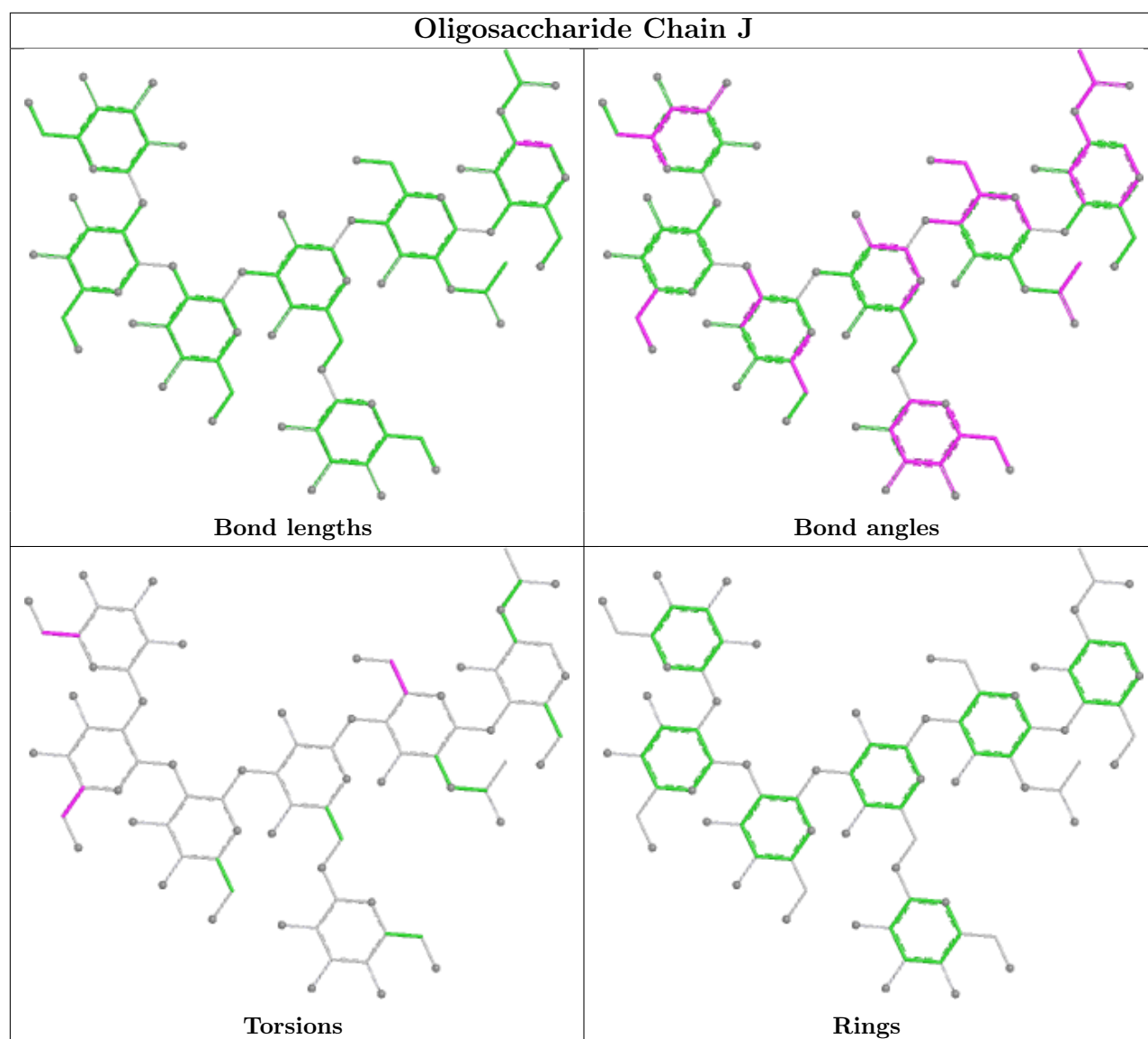


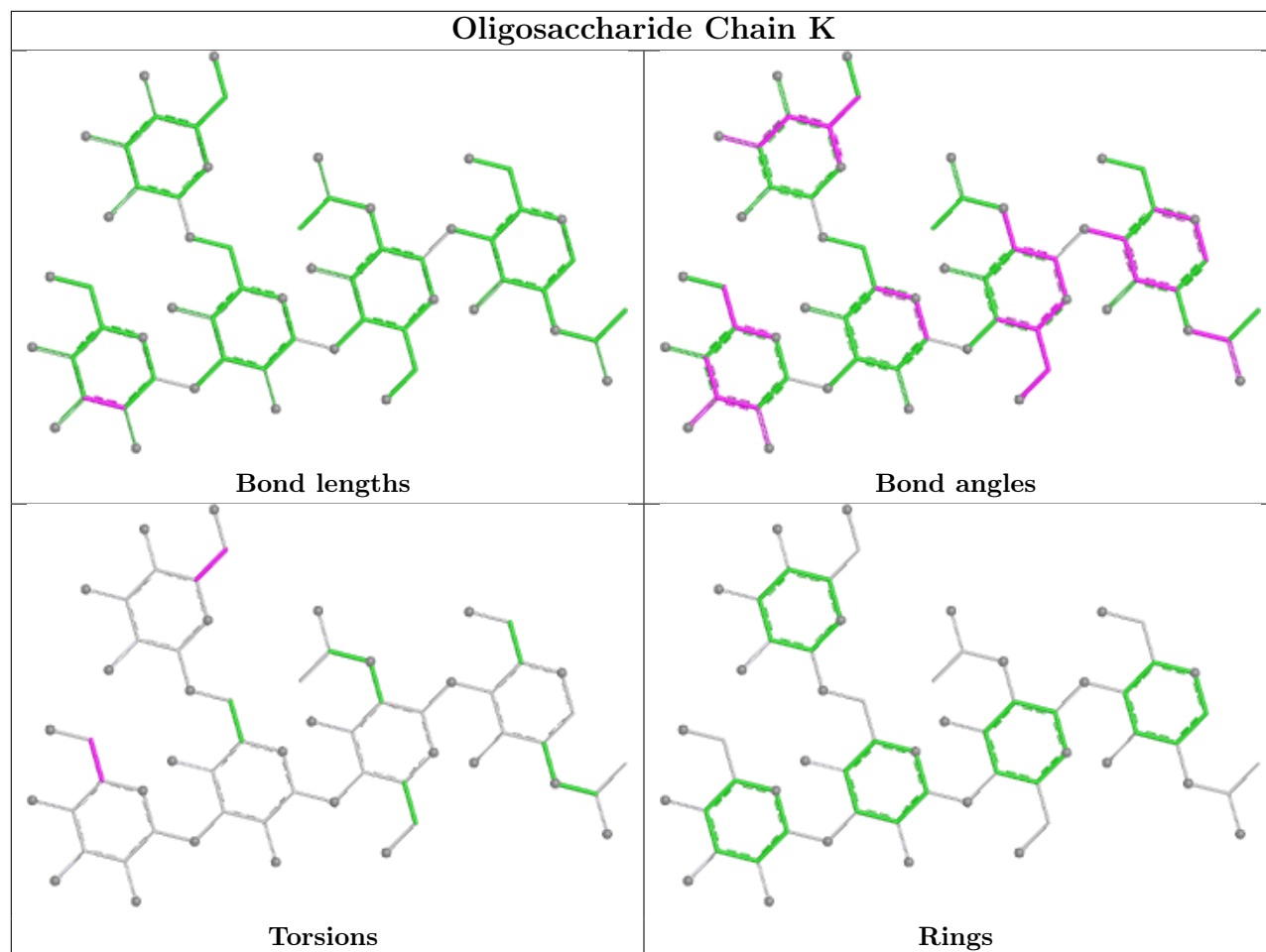


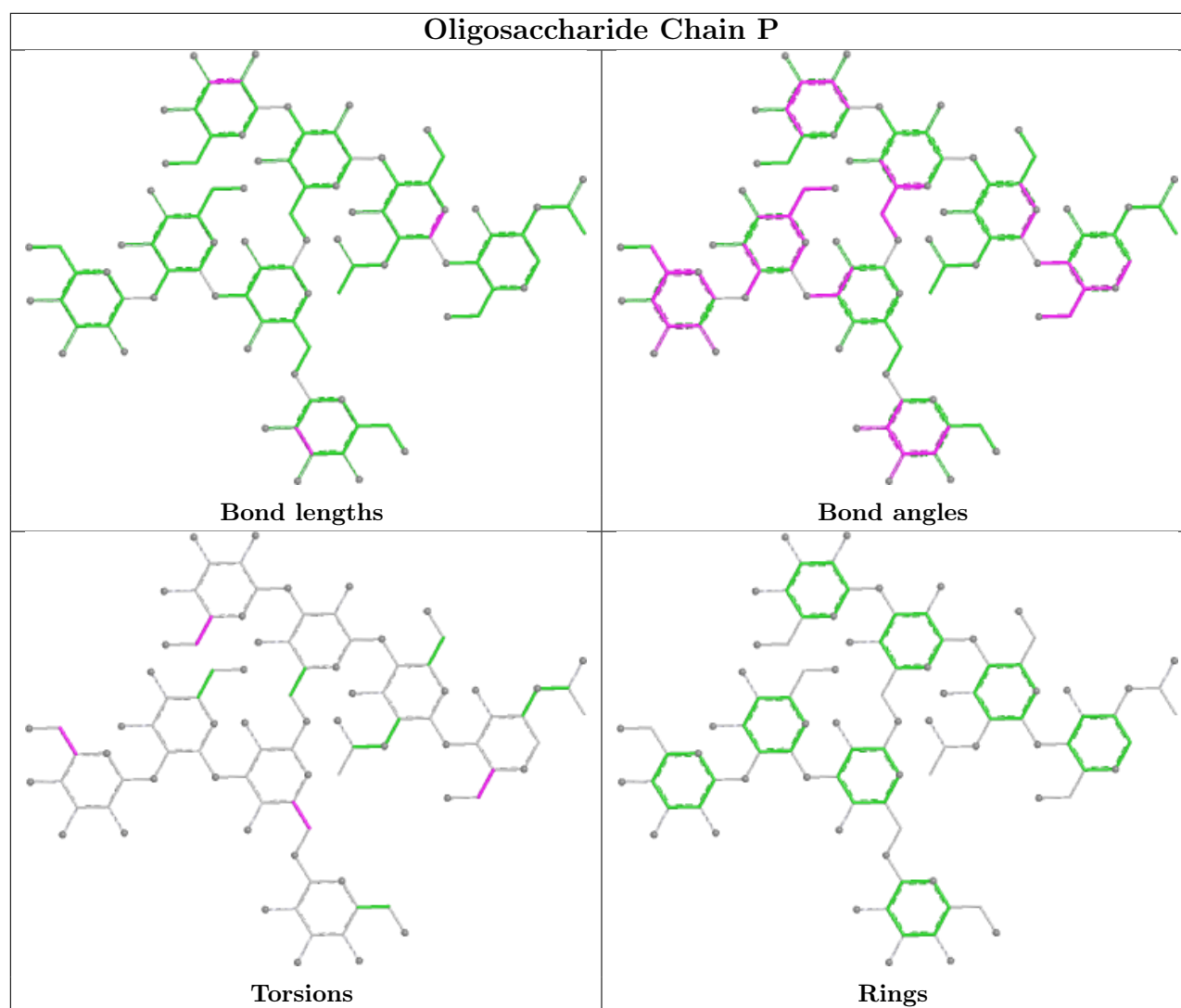












5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
12	MRD	A	938	-	7,7,7	0.55	0	9,10,10	0.60	0
12	MRD	B	948	-	7,7,7	0.92	0	9,10,10	0.43	0
11	NAG	A	937	1	14,14,15	0.57	0	17,19,21	1.79	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	MPD	B	947	-	7,7,7	0.53	0	9,10,10	1.58	1 (11%)
11	NAG	B	946	1	14,14,15	0.70	0	17,19,21	1.10	0
11	NAG	B	945	1	14,14,15	0.59	0	17,19,21	1.42	2 (11%)
11	NAG	A	905	1	14,14,15	0.94	0	17,19,21	1.62	3 (17%)
13	NOJ	B	949	-	11,11,11	1.47	2 (18%)	13,15,15	1.81	4 (30%)
13	NOJ	A	940	-	11,11,11	0.48	0	13,15,15	1.19	2 (15%)
12	MRD	A	939	-	7,7,7	0.75	0	9,10,10	0.76	0
11	NAG	B	908	1	14,14,15	0.79	0	17,19,21	1.25	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MRD	A	938	-	-	1/5/5/5	-
12	MRD	B	948	-	-	2/5/5/5	-
11	NAG	A	937	1	-	2/6/23/26	0/1/1/1
14	MPD	B	947	-	-	0/5/5/5	-
11	NAG	B	946	1	-	2/6/23/26	0/1/1/1
11	NAG	B	945	1	-	1/6/23/26	0/1/1/1
11	NAG	A	905	1	-	0/6/23/26	0/1/1/1
13	NOJ	B	949	-	-	0/2/19/19	0/1/1/1
13	NOJ	A	940	-	-	0/2/19/19	0/1/1/1
12	MRD	A	939	-	-	4/5/5/5	-
11	NAG	B	908	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	949	NOJ	C1-C2	3.20	1.55	1.52
13	B	949	NOJ	C2-C3	2.40	1.56	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	905	NAG	C1-C2-N2	4.11	116.91	110.43
11	B	945	NAG	O5-C1-C2	-3.66	105.64	111.29
11	A	937	NAG	O5-C5-C6	3.64	114.75	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	937	NAG	C3-C4-C5	-3.51	103.87	110.23
13	B	949	NOJ	C1-N5-C5	3.40	117.18	109.71
13	B	949	NOJ	O2-C2-C1	-3.12	103.61	109.65
11	A	937	NAG	C4-C3-C2	-3.08	106.50	111.02
11	B	945	NAG	C4-C3-C2	3.08	115.53	111.02
11	A	905	NAG	O7-C7-C8	-2.96	116.79	122.05
14	B	947	MPD	O2-C2-C1	-2.82	99.21	107.99
11	A	905	NAG	C1-O5-C5	2.61	115.69	112.19
11	B	908	NAG	C2-N2-C7	2.41	126.14	122.90
13	B	949	NOJ	O4-C4-C5	2.34	114.27	109.40
13	A	940	NOJ	C1-N5-C5	2.10	114.32	109.71
13	B	949	NOJ	O2-C2-C3	-2.02	105.96	110.15
13	A	940	NOJ	C1-C2-C3	2.02	112.72	110.25

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	939	MRD	C2-C3-C4-O4
12	A	939	MRD	C2-C3-C4-C5
12	B	948	MRD	C2-C3-C4-O4
12	B	948	MRD	C2-C3-C4-C5
11	B	946	NAG	O5-C5-C6-O6
11	A	937	NAG	O5-C5-C6-O6
11	B	946	NAG	C4-C5-C6-O6
11	A	937	NAG	C4-C5-C6-O6
11	B	908	NAG	O5-C5-C6-O6
11	B	908	NAG	C4-C5-C6-O6
11	B	908	NAG	C1-C2-N2-C7
12	A	939	MRD	C1-C2-C3-C4
12	A	939	MRD	CM-C2-C3-C4
11	B	908	NAG	C3-C2-N2-C7
12	A	938	MRD	C2-C3-C4-C5
11	B	945	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	938	MRD	2	0
12	B	948	MRD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	947	MPD	4	0
12	A	939	MRD	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	834/841 (99%)	-0.70	2 (0%) 91 91	11, 21, 36, 74	0
1	B	832/841 (98%)	-0.81	0 100 100	11, 18, 32, 56	0
All	All	1666/1682 (99%)	-0.75	2 (0%) 92 91	11, 20, 34, 74	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	669	ALA	5.1
1	A	699	GLY	2.6

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
9	MAN	K	4	11/12	0.64	0.19	71,78,86,88	0
6	MAN	O	7	11/12	0.65	0.17	71,76,79,85	0
9	MAN	K	5	11/12	0.72	0.15	56,66,70,73	0
10	MAN	P	8	11/12	0.72	0.15	62,72,77,79	0
6	MAN	H	7	11/12	0.73	0.16	66,68,75,77	0
10	MAN	P	7	11/12	0.76	0.16	45,61,66,70	0
3	BMA	L	3	11/12	0.76	0.16	57,75,80,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	C	4	11/12	0.79	0.12	42,50,53,58	0
3	BMA	N	3	11/12	0.79	0.14	56,65,69,69	0
7	MAN	I	7	11/12	0.81	0.14	51,57,67,69	0
4	NAG	G	2	14/15	0.82	0.15	49,56,64,65	0
10	MAN	P	6	11/12	0.83	0.14	51,58,63,67	0
7	MAN	I	6	11/12	0.84	0.14	50,56,59,62	0
7	BMA	I	3	11/12	0.86	0.11	38,43,49,53	0
3	BMA	D	3	11/12	0.86	0.10	38,43,52,56	0
8	MAN	J	7	11/12	0.87	0.10	34,38,42,44	0
10	BMA	P	3	11/12	0.89	0.10	37,44,55,66	0
2	BMA	C	3	11/12	0.89	0.08	32,39,46,47	0
8	MAN	J	5	11/12	0.90	0.10	33,37,46,61	0
5	MAN	M	10	11/12	0.90	0.10	32,38,45,48	0
9	BMA	K	3	11/12	0.90	0.09	47,53,62,78	0
6	MAN	O	4	11/12	0.91	0.09	30,35,41,41	0
5	MAN	F	10	11/12	0.91	0.11	35,45,55,58	0
6	BMA	H	3	11/12	0.92	0.09	32,35,43,53	0
6	BMA	O	3	11/12	0.92	0.08	34,39,47,54	0
6	MAN	H	4	11/12	0.92	0.08	30,36,41,46	0
10	NAG	P	2	14/15	0.92	0.09	25,35,42,44	0
3	NAG	L	2	14/15	0.93	0.09	20,32,45,51	0
10	MAN	P	4	11/12	0.93	0.09	27,35,47,52	0
4	NAG	E	2	14/15	0.93	0.07	32,37,42,47	0
3	NAG	N	2	14/15	0.93	0.08	39,42,50,57	0
7	MAN	I	4	11/12	0.93	0.09	27,34,41,52	0
6	NAG	O	2	14/15	0.94	0.09	23,28,38,38	0
7	MAN	I	5	11/12	0.94	0.09	28,35,45,49	0
6	NAG	H	1	14/15	0.94	0.07	18,26,39,42	0
5	MAN	F	5	11/12	0.94	0.07	24,28,35,39	0
8	BMA	J	3	11/12	0.94	0.07	26,28,32,32	0
5	MAN	M	6	11/12	0.94	0.08	29,37,42,43	0
8	MAN	J	6	11/12	0.94	0.07	28,31,36,40	0
5	MAN	F	6	11/12	0.94	0.07	33,38,43,43	0
9	NAG	K	2	14/15	0.94	0.07	27,29,35,42	0
2	NAG	C	2	14/15	0.95	0.07	27,31,36,39	0
5	NAG	F	1	14/15	0.95	0.07	24,28,31,31	0
6	NAG	O	1	14/15	0.95	0.08	16,24,41,41	0
3	NAG	D	2	14/15	0.95	0.06	24,31,38,39	0
4	NAG	G	1	14/15	0.95	0.07	29,36,44,47	0
6	NAG	H	2	14/15	0.95	0.06	18,26,37,39	0
8	MAN	J	4	11/12	0.95	0.07	28,34,39,41	0
10	MAN	P	5	11/12	0.95	0.07	26,33,38,48	0

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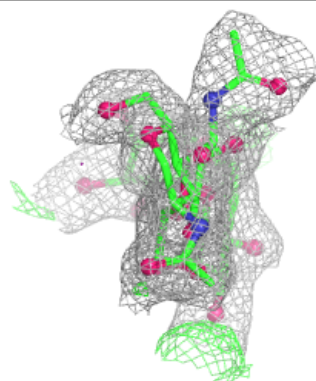
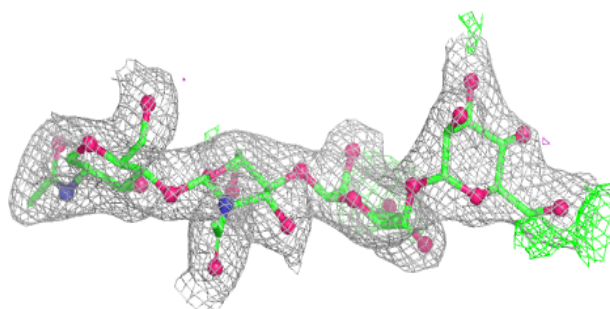
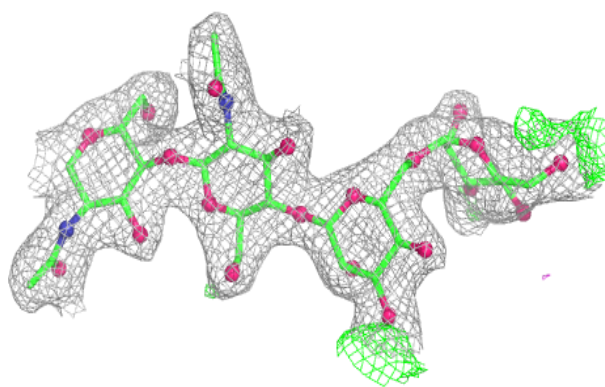
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	O	6	11/12	0.95	0.07	26,31,37,39	0
5	MAN	F	9	11/12	0.95	0.06	30,34,38,41	0
7	NAG	I	2	14/15	0.95	0.07	26,32,42,45	0
7	NAG	I	1	14/15	0.96	0.06	21,24,26,31	0
6	MAN	H	6	11/12	0.96	0.06	29,31,40,49	0
8	NAG	J	2	14/15	0.96	0.06	16,21,25,31	0
4	NAG	E	1	14/15	0.96	0.06	18,24,27,29	0
5	MAN	F	8	11/12	0.96	0.06	21,22,26,27	0
5	MAN	M	5	11/12	0.96	0.06	21,23,30,32	0
10	NAG	P	1	14/15	0.96	0.06	19,23,26,27	0
9	NAG	K	1	14/15	0.97	0.06	21,24,27,28	0
5	BMA	M	3	11/12	0.97	0.05	20,22,25,26	0
3	NAG	D	1	14/15	0.97	0.05	19,25,30,34	0
3	NAG	N	1	14/15	0.97	0.06	26,33,46,54	0
5	MAN	M	8	11/12	0.97	0.05	18,20,20,25	0
2	NAG	C	1	14/15	0.97	0.06	19,25,26,27	0
8	NAG	J	1	14/15	0.97	0.05	14,17,20,21	0
5	NAG	F	2	14/15	0.97	0.06	26,27,31,31	0
6	MAN	O	5	11/12	0.97	0.05	27,30,34,40	0
5	BMA	F	3	11/12	0.97	0.05	24,26,29,31	0
5	NAG	M	1	14/15	0.97	0.06	17,20,23,25	0
5	NAG	M	2	14/15	0.97	0.06	18,20,27,30	0
6	MAN	H	5	11/12	0.97	0.05	25,27,28,32	0
5	MAN	M	4	11/12	0.98	0.04	17,19,20,21	0
3	NAG	L	1	14/15	0.98	0.04	15,19,22,23	0
5	MAN	F	4	11/12	0.98	0.04	17,20,23,23	0
5	MAN	M	7	11/12	0.98	0.04	15,17,20,24	0
5	MAN	F	7	11/12	0.98	0.04	23,25,27,27	0
5	MAN	M	9	11/12	0.98	0.05	19,22,24,31	0

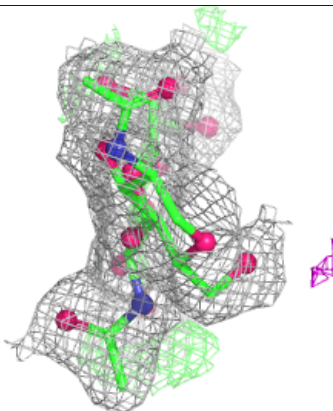
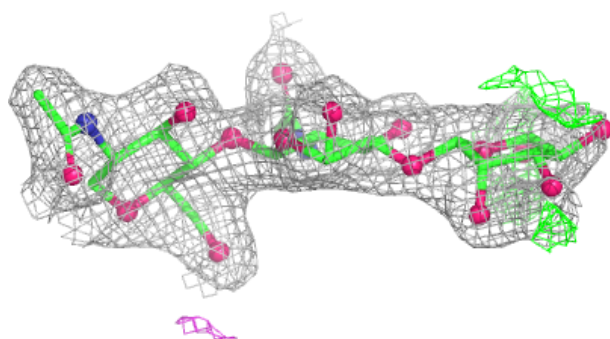
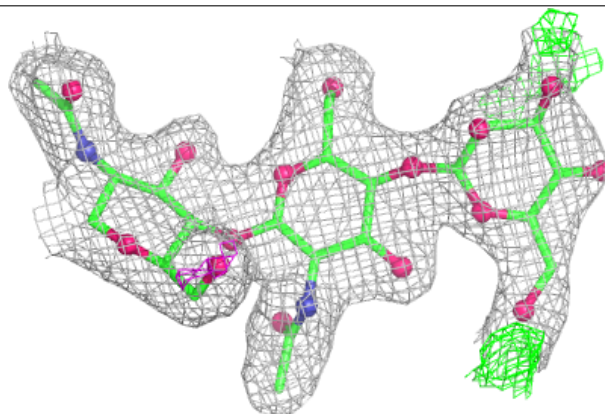
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

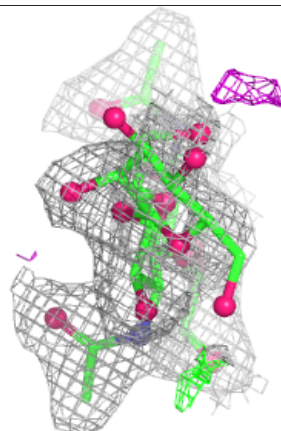
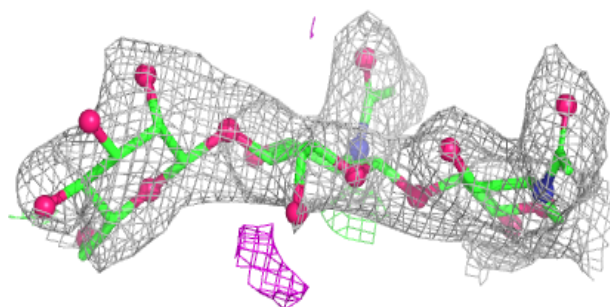
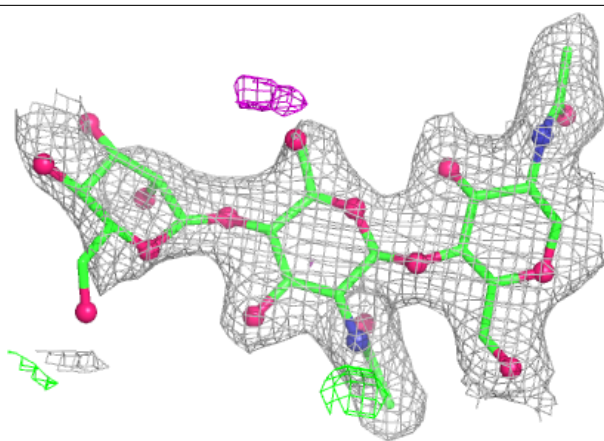
**Electron density around Chain D:**

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

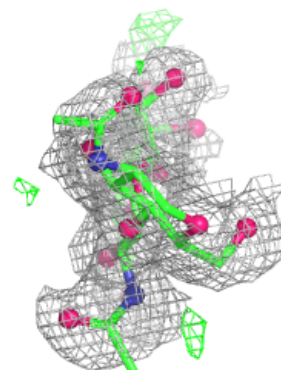
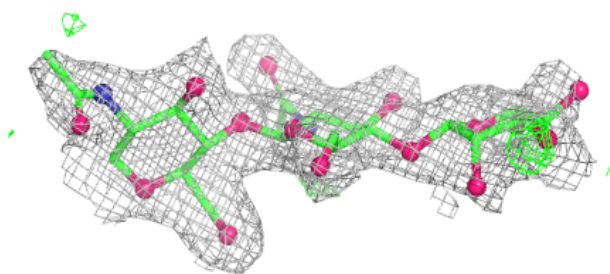
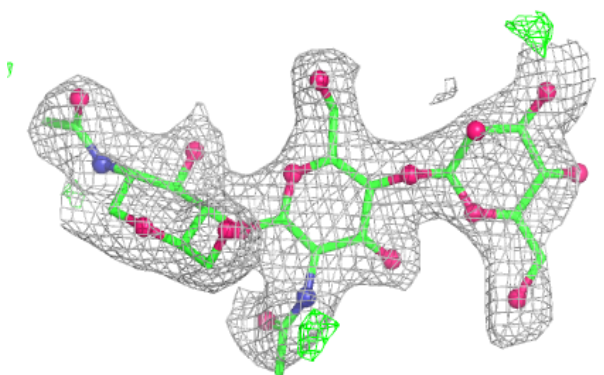


Electron density around Chain L:

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

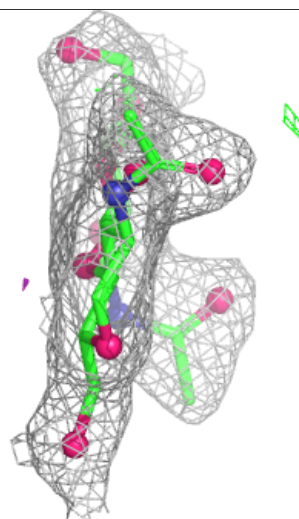
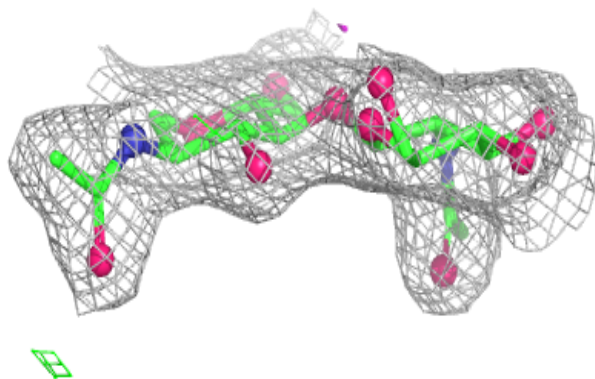
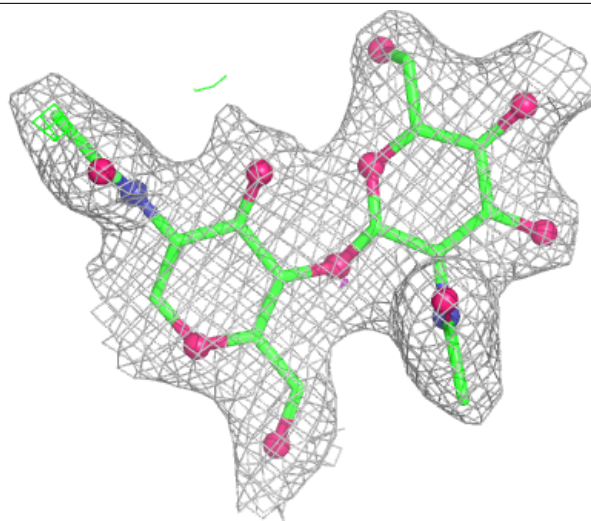
**Electron density around Chain N:**

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



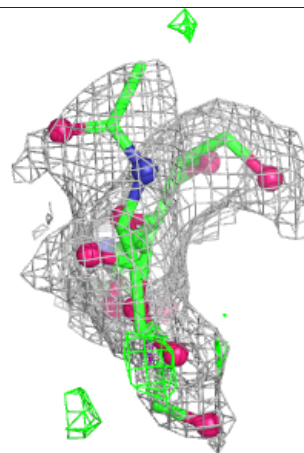
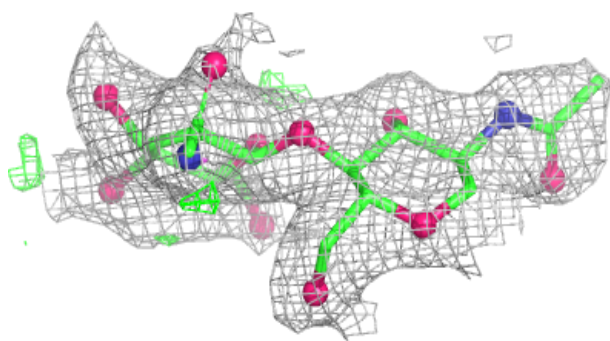
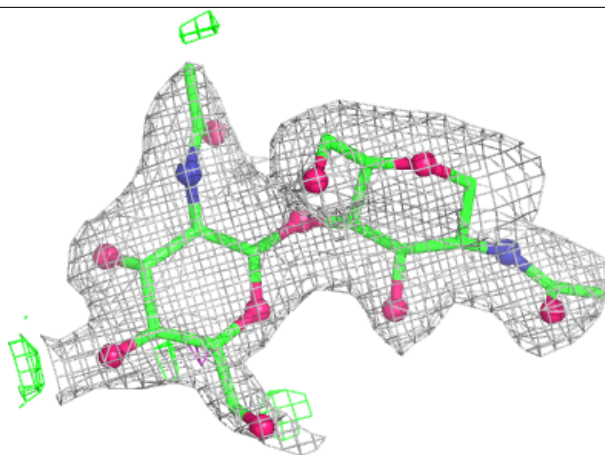
Electron density around Chain E:

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



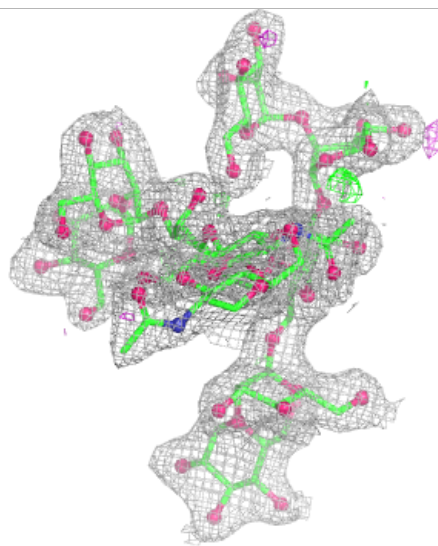
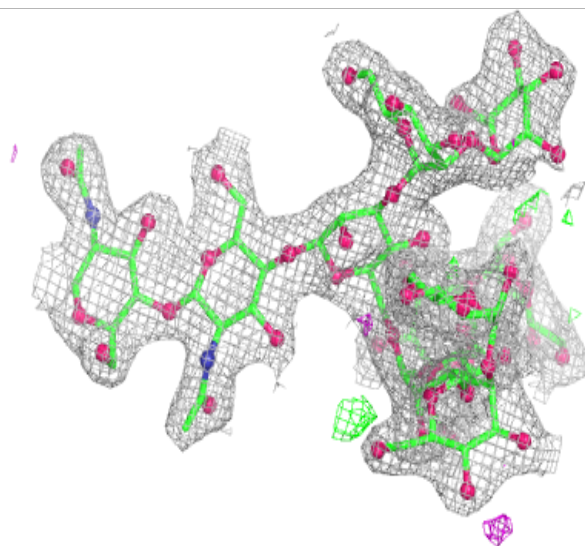
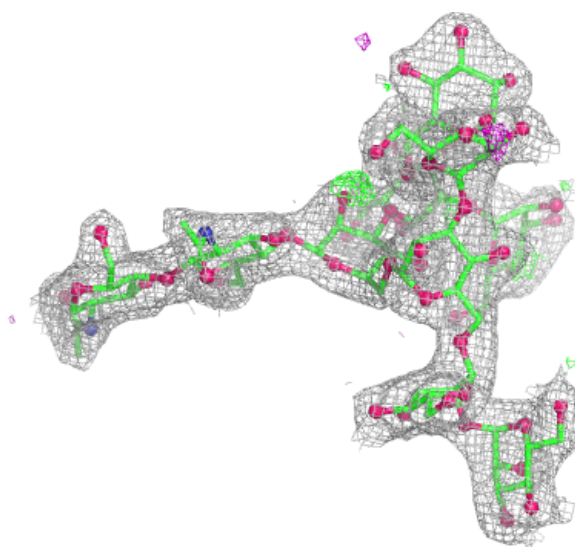
Electron density around Chain G:

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



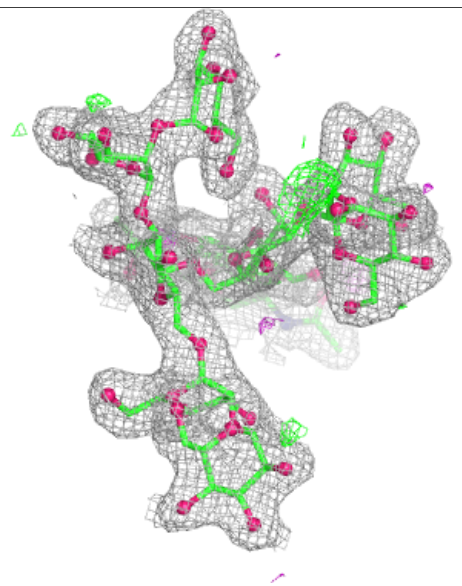
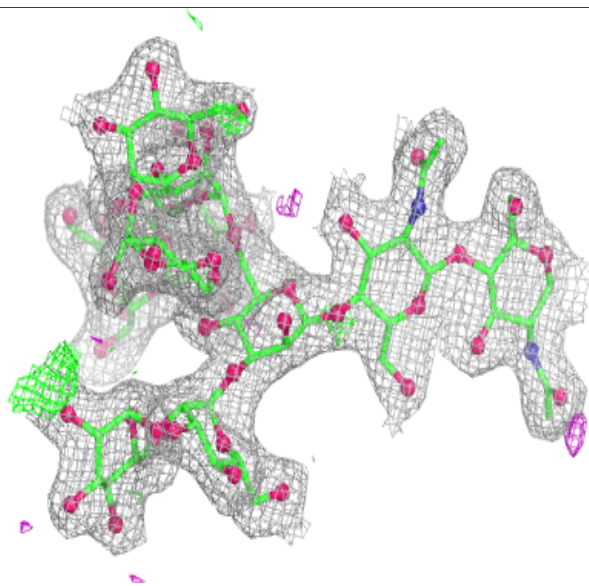
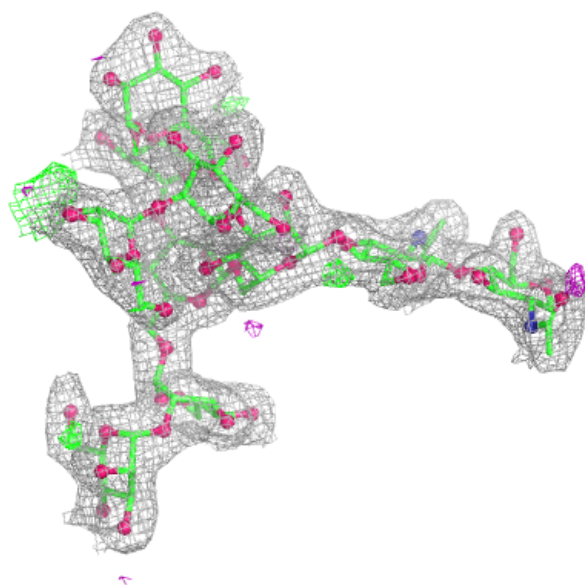
Electron density around Chain F:

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



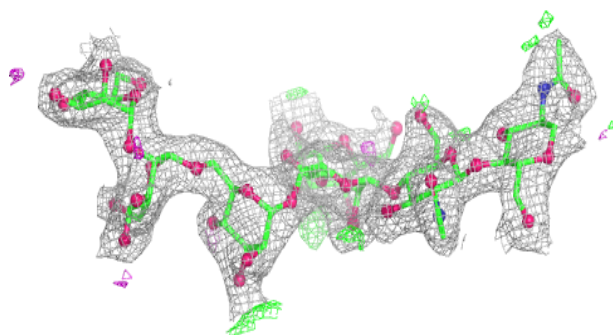
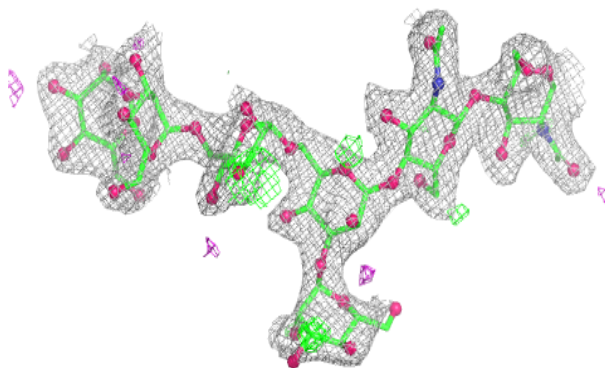
Electron density around Chain M:

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

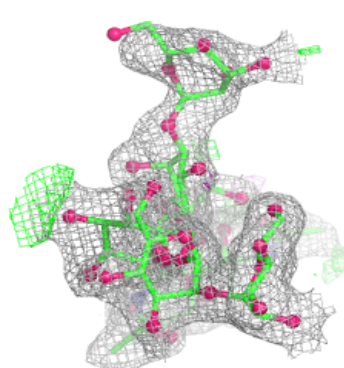
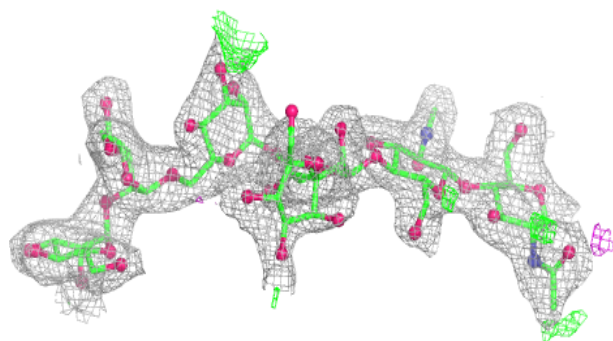
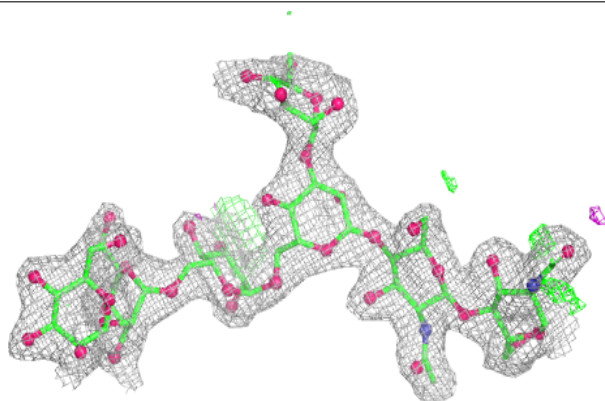


Electron density around Chain H:

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

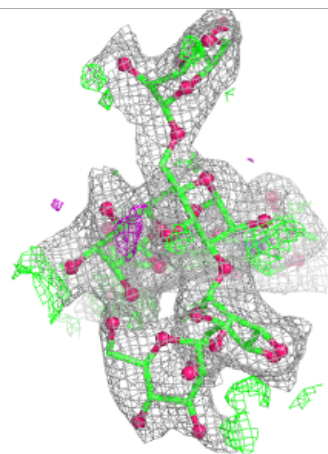
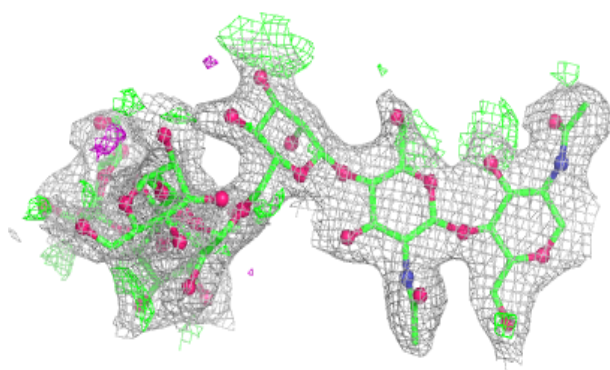
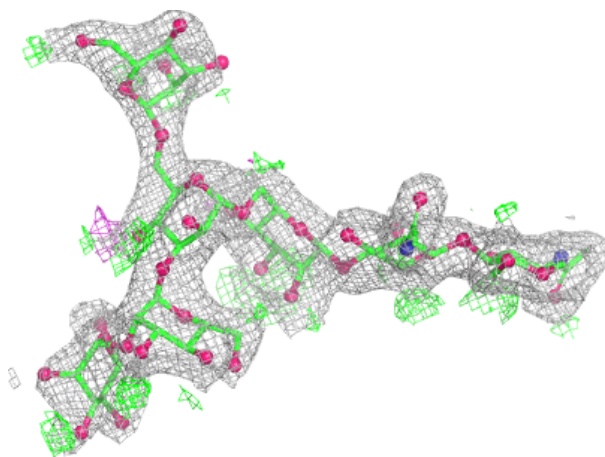
**Electron density around Chain O:**

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



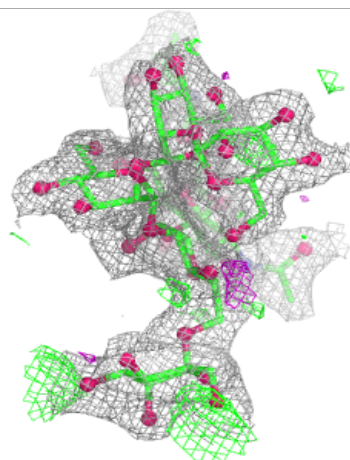
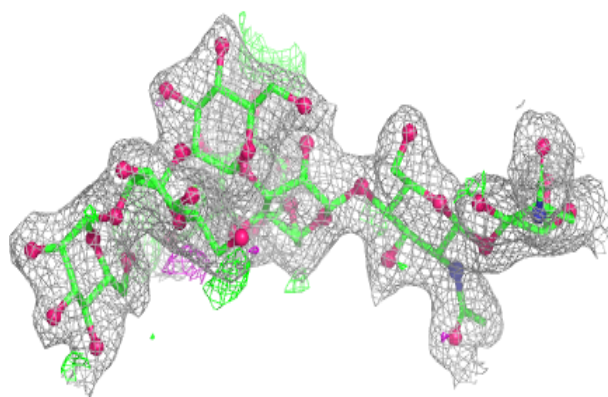
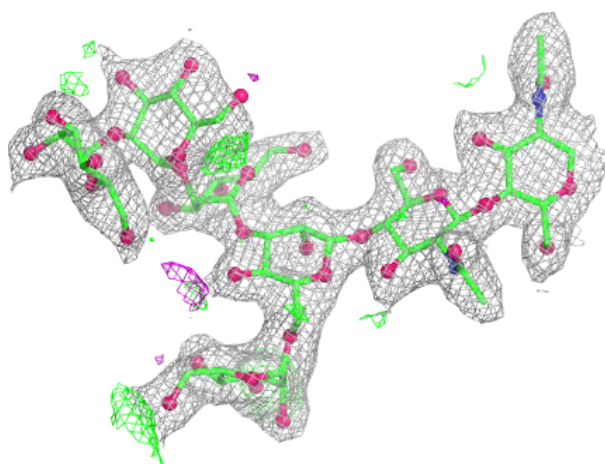
Electron density around Chain I:

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



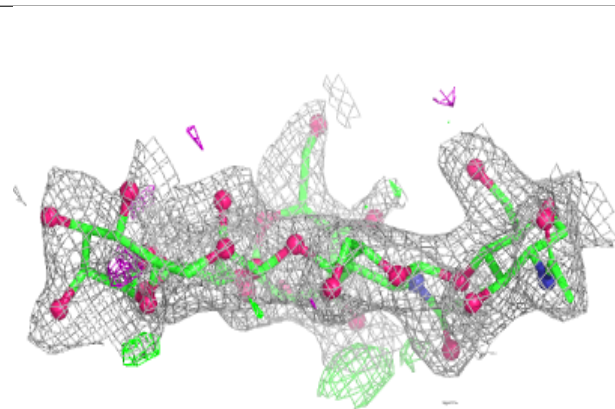
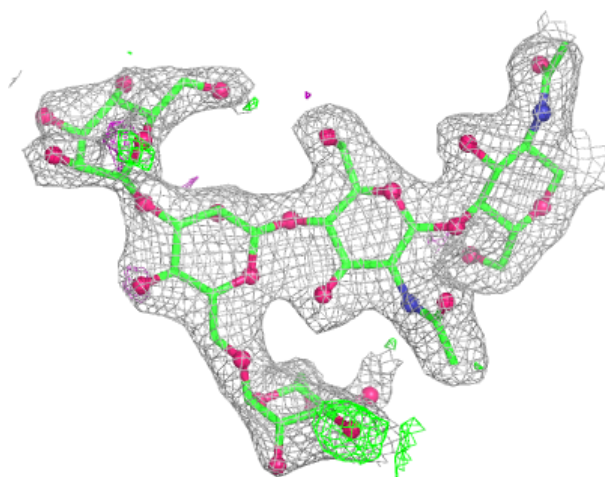
Electron density around Chain J:

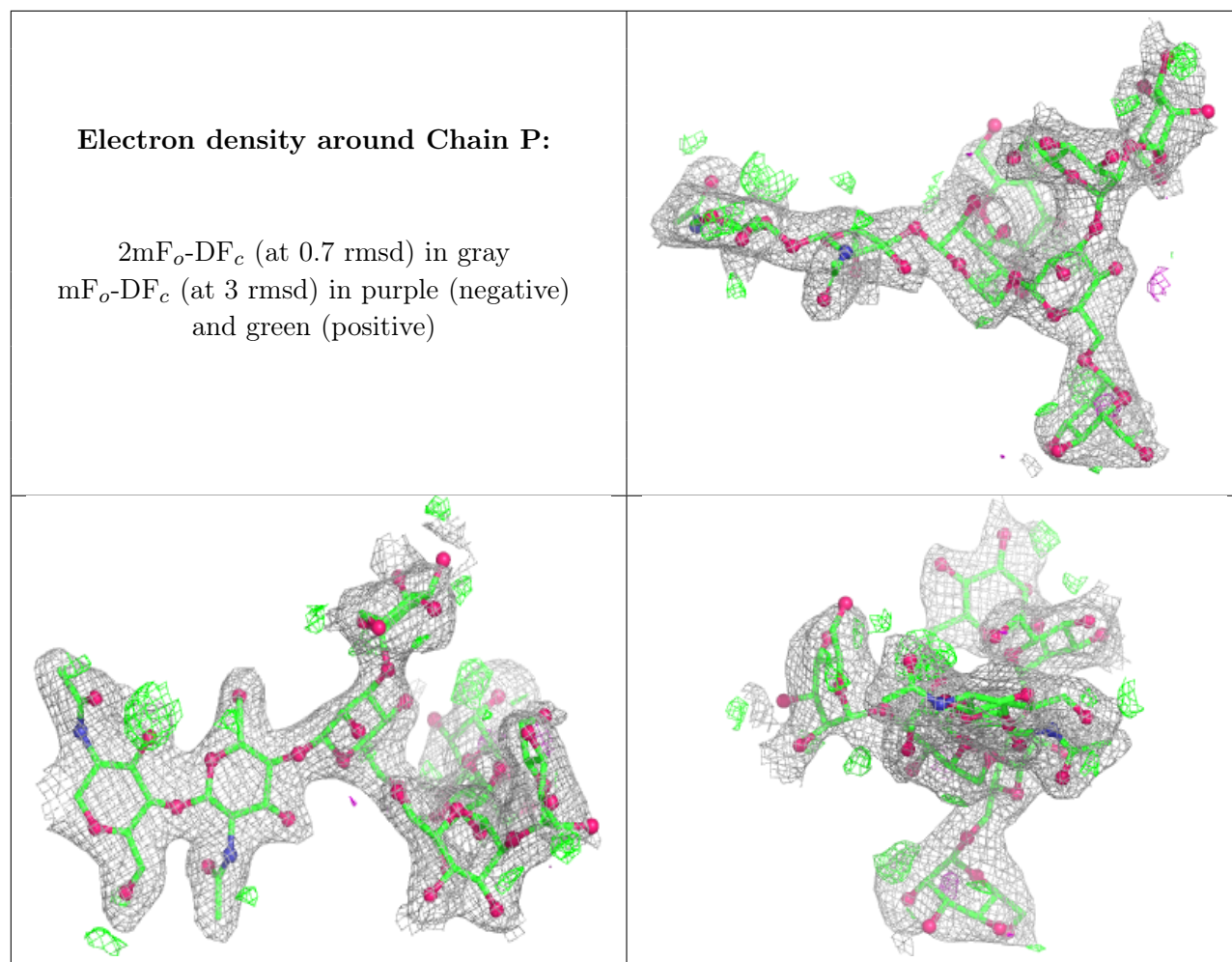
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	A	905	14/15	0.78	0.15	49,63,72,73	0
11	NAG	B	908	14/15	0.81	0.15	44,58,67,69	0
12	MRD	A	939	8/8	0.88	0.12	24,28,37,37	0
11	NAG	B	945	14/15	0.89	0.12	45,60,67,70	0
14	MPD	B	947	8/8	0.90	0.13	26,32,40,44	0
12	MRD	B	948	8/8	0.93	0.11	38,45,48,52	0
12	MRD	A	938	8/8	0.94	0.10	36,38,40,41	0
11	NAG	A	937	14/15	0.94	0.09	39,45,50,52	0
11	NAG	B	946	14/15	0.95	0.06	29,35,40,43	0
13	NOJ	B	949	11/11	0.98	0.04	14,15,17,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	NOJ	A	940	11/11	0.98	0.05	17,21,22,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.