



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:41 PM UTC

PDB ID : 4IIH / pdb_00004iih
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with thiocellobiose
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on : 2012-12-20
Resolution : 2.00 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

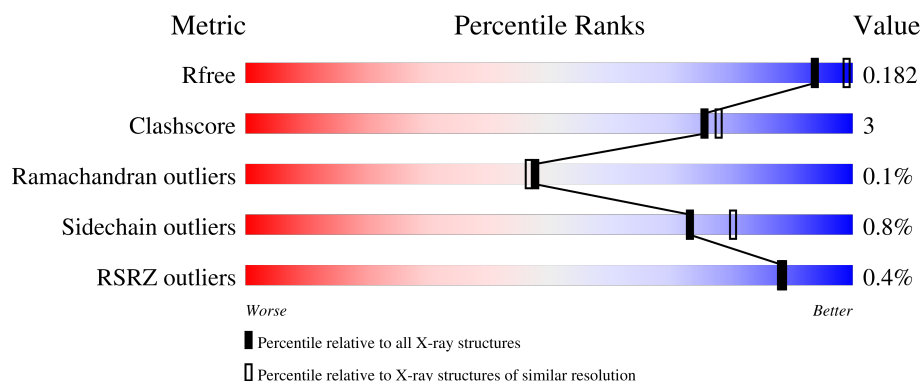
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



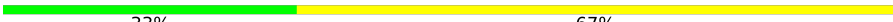
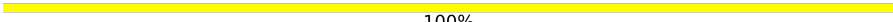
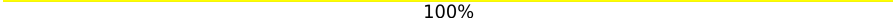
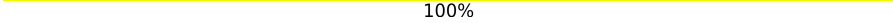
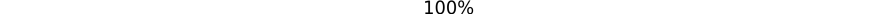
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	89% 10% ..
1	B	841	88% 10% ..
2	C	7	86% 14%
2	J	7	86% 14%
3	D	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	G	3	 100%
3	L	3	 33% 67%
3	N	3	 100%
4	E	2	 50% 50%
5	F	10	 10% 90%
5	M	10	 100%
6	H	7	 86% 14%
6	O	7	 71% 29%
7	I	7	 100%
8	K	6	 100%
9	P	8	 62% 38%
10	Q	2	 100%
10	R	2	 50% 50%

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	943	-	-	X	-

2 Entry composition [i](#)

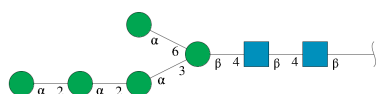
There are 13 unique types of molecules in this entry. The entry contains 15509 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

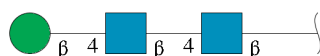
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6382	4028	1096	1240	18			
1	B	832	Total	C	N	O	S	0	0	0
			6375	4023	1095	1239	18			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
2	C	7	Total	C	N	O	0	0	0
			83	46	2	35			
2	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

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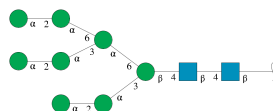
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



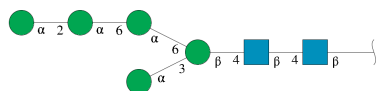
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



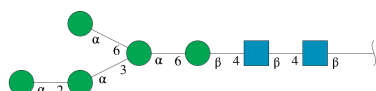
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	10	Total	C	N	O	0	0	0
			116	64	2	50			
5	M	10	Total	C	N	O	0	0	0
			116	64	2	50			

- 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.



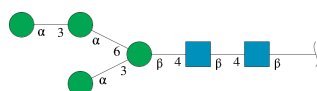
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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.



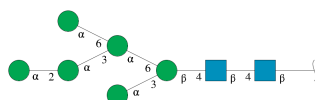
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
8	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 9 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.

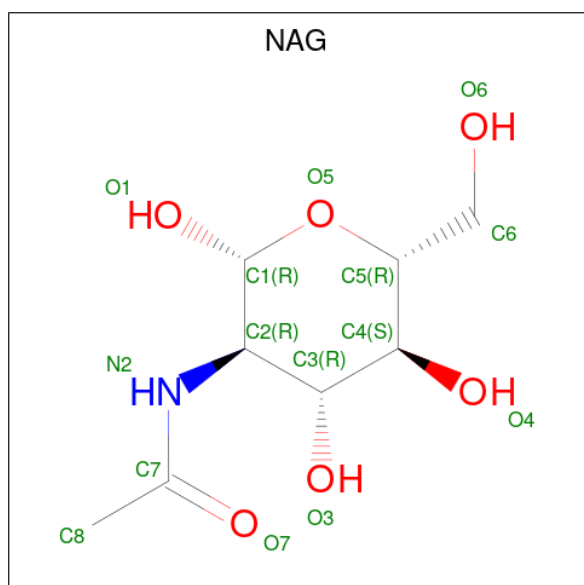


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 10 is an oligosaccharide called beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose.

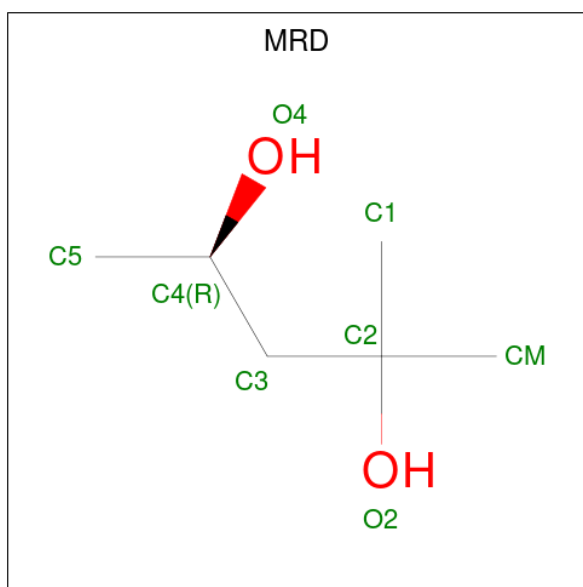
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	Q	2	Total	C	O	S	0	0	0
			23	12	10	1			
10	R	2	Total	C	O	S	0	0	0
			23	12	10	1			

- 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		
12	B	1	Total	C	O	0	0
			8	6	2		

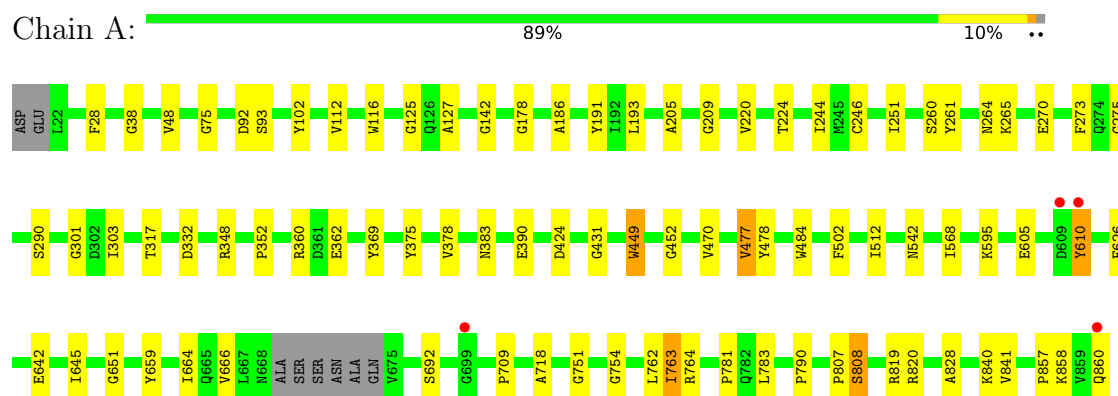
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	748	Total	O	0	0
			748	748		
13	B	859	Total	O	0	0
			859	859		

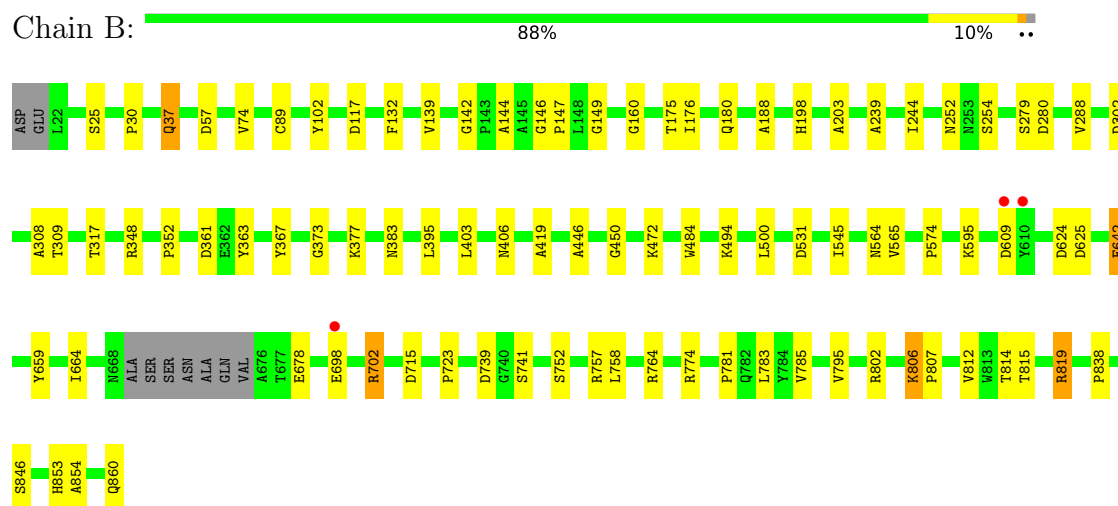
3 Residue-property plots

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.

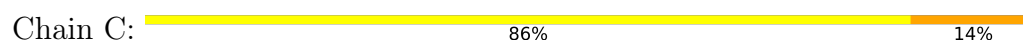
• Molecule 1: Beta-glucosidase 1



• Molecule 1: Beta-glucosidase 1

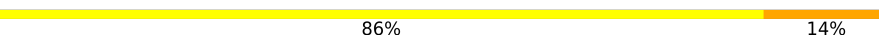


• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 2: 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%

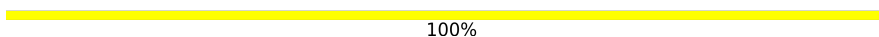


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67% 33%

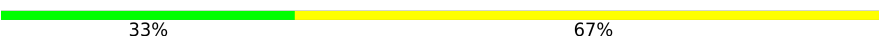


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

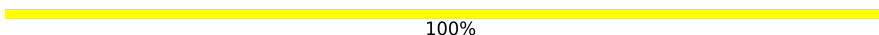


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  33% 67%



- 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%



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

Chain E:  50% 50%

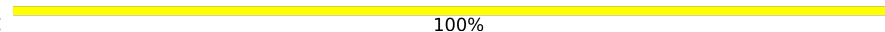


- Molecule 5: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain F:  10% 90%

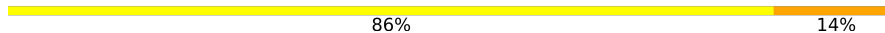
MAN1
MAN2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

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

Chain M:  100%

MAN1
MAN2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

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

Chain H:  86% 14%

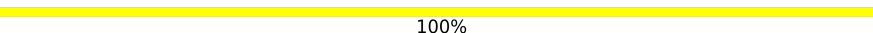
MAN1
MAN2
MAN3
MAN4
MAN5
MAN6
MAN7

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

Chain O:  71% 29%

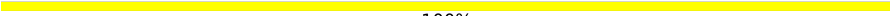
MAN1
MAN2
MAN3
MAN4
MAN5
MAN6
MAN7

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

Chain I:  100%

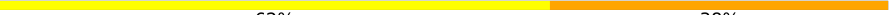
MAN1
MAN2
MAN3
MAN4
MAN5
MAN6
MAN7

- Molecule 8: α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain K:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 9: 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-glucopyranos e

Chain P:  62% 38%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 10: beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose

Chain Q:  100%

SGC1
BGC2

- Molecule 10: beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose

Chain R:  50% 50%

SGC1
BGC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.08Å 122.39Å 221.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.07 – 2.00 41.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.07-2.00) 99.6 (41.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.140 , 0.181 0.141 , 0.182	Depositor DCC
R_{free} test set	7569 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15509	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: SGC, BMA, MAN, MRD, NAG, BGC

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	1.57	36/6545 (0.6%)	1.26	9/8923 (0.1%)
1	B	1.62	42/6538 (0.6%)	1.29	17/8913 (0.2%)
All	All	1.60	78/13083 (0.6%)	1.28	26/17836 (0.1%)

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	PRO	CA-C	8.42	1.56	1.51
1	A	75	GLY	N-CA	7.53	1.53	1.45
1	A	275	GLY	N-CA	6.98	1.53	1.45
1	B	795	VAL	N-CA	6.97	1.54	1.46
1	B	280	ASP	CA-C	6.93	1.63	1.53
1	B	702	ARG	CD-NE	-6.77	1.36	1.46
1	A	205	ALA	CA-C	6.65	1.61	1.52
1	B	352	PRO	CA-C	6.52	1.55	1.51
1	B	812	VAL	C-O	-6.47	1.16	1.24
1	B	176	ILE	CA-CB	6.46	1.61	1.54
1	A	362	GLU	CA-C	6.45	1.61	1.52
1	B	37	GLN	N-CA	6.16	1.53	1.46
1	A	709	PRO	CA-C	6.16	1.59	1.52
1	B	564	ASN	C-O	6.14	1.32	1.23
1	A	332	ASP	CA-C	6.14	1.60	1.52
1	A	651	GLY	N-CA	6.13	1.51	1.45
1	A	127	ALA	N-CA	5.99	1.53	1.46
1	B	802	ARG	C-O	-5.98	1.17	1.24
1	A	718	ALA	C-O	-5.97	1.17	1.24
1	B	565	VAL	N-CA	5.95	1.53	1.46
1	B	609	ASP	C-O	5.91	1.31	1.23
1	A	178	GLY	N-CA	5.91	1.53	1.45
1	B	252	ASN	C-O	5.87	1.30	1.23
1	B	846	SER	N-CA	5.81	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	820	ARG	N-CA	5.81	1.53	1.46
1	B	807	PRO	C-O	5.78	1.30	1.23
1	A	317	THR	CA-C	5.74	1.60	1.52
1	A	477	VAL	C-O	5.73	1.30	1.23
1	A	224	THR	N-CA	5.70	1.53	1.46
1	A	478	TYR	C-O	5.68	1.30	1.23
1	B	419	ALA	CA-CB	5.66	1.60	1.53
1	A	112	VAL	N-CA	5.63	1.53	1.46
1	A	764	ARG	C-O	5.57	1.30	1.23
1	A	751	GLY	C-O	-5.57	1.19	1.24
1	B	715	ASP	CA-C	5.53	1.59	1.52
1	B	595	LYS	C-O	5.53	1.30	1.23
1	A	209	GLY	N-CA	5.50	1.53	1.45
1	A	48	VAL	N-CA	5.45	1.52	1.46
1	B	774	ARG	CZ-NH1	5.45	1.40	1.32
1	B	180	GLN	N-CA	5.45	1.53	1.46
1	B	317	THR	N-CA	5.45	1.52	1.46
1	A	369	TYR	N-CA	-5.44	1.41	1.46
1	B	89	CYS	CA-C	5.39	1.59	1.52
1	B	198	HIS	N-CA	5.38	1.53	1.46
1	B	175	THR	CA-C	5.37	1.59	1.52
1	A	290	SER	N-CA	5.37	1.52	1.46
1	A	270	GLU	CA-C	5.37	1.59	1.52
1	B	531	ASP	CA-C	5.35	1.59	1.52
1	A	261	TYR	CA-C	5.32	1.59	1.52
1	B	642	GLU	CD-OE1	5.32	1.35	1.25
1	B	117	ASP	C-O	5.29	1.29	1.23
1	B	361	ASP	CA-CB	5.26	1.62	1.53
1	B	254	SER	CA-C	5.23	1.58	1.52
1	A	378	VAL	N-CA	5.23	1.51	1.46
1	B	279	SER	N-CA	5.22	1.52	1.45
1	A	754	GLY	N-CA	5.21	1.49	1.45
1	A	828	ALA	N-CA	5.21	1.52	1.46
1	A	301	GLY	N-CA	5.21	1.51	1.45
1	A	645	ILE	CA-CB	5.20	1.60	1.54
1	A	568	ILE	C-O	5.20	1.29	1.24
1	B	758	LEU	CA-C	5.18	1.59	1.52
1	B	139	VAL	CA-CB	5.18	1.61	1.54
1	B	309	THR	CB-CG2	5.17	1.69	1.52
1	B	624	ASP	C-O	5.17	1.29	1.23
1	A	125	GLY	N-CA	5.17	1.52	1.45
1	B	472	LYS	C-O	-5.17	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	PHE	C-O	5.16	1.30	1.23
1	B	403	LEU	CA-C	5.16	1.59	1.52
1	A	92	ASP	CG-OD2	-5.15	1.15	1.25
1	B	132	PHE	CA-CB	5.12	1.61	1.53
1	B	308	ALA	CA-CB	5.12	1.61	1.53
1	B	757	ARG	CA-C	5.09	1.59	1.52
1	B	363	TYR	CA-C	-5.09	1.46	1.52
1	A	692	SER	C-O	-5.04	1.17	1.24
1	B	149	GLY	N-CA	5.04	1.52	1.45
1	A	186	ALA	N-CA	5.04	1.52	1.45
1	B	288	VAL	N-CA	5.03	1.52	1.46
1	B	785	VAL	N-CA	5.03	1.51	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	SER	CA-C-N	-7.82	112.32	120.38
1	B	25	SER	C-N-CA	-7.82	112.32	120.38
1	A	790	PRO	CA-C-N	-7.29	111.70	122.86
1	A	790	PRO	C-N-CA	-7.29	111.70	122.86
1	A	610	TYR	N-CA-C	6.99	120.52	110.10
1	B	741	SER	CA-C-N	6.85	126.89	119.90
1	B	741	SER	C-N-CA	6.85	126.89	119.90
1	B	806	LYS	CG-CD-CE	-6.24	96.96	111.30
1	A	431	GLY	N-CA-C	-6.09	105.00	112.68
1	A	808	SER	CA-CB-OG	-5.94	99.22	111.10
1	B	702	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	B	702	ARG	CB-CG-CD	-5.82	97.92	111.30
1	B	757	ARG	NE-CZ-NH1	-5.82	115.69	121.50
1	A	142	GLY	N-CA-C	-5.47	101.17	112.34
1	B	757	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	B	406	ASN	N-CA-C	-5.33	103.27	110.68
1	B	642	GLU	CG-CD-OE2	-5.23	106.38	118.40
1	B	142	GLY	N-CA-C	-5.22	101.69	112.34
1	B	348	ARG	N-CA-C	-5.21	106.88	113.18
1	B	239	ALA	N-CA-C	-5.14	106.96	113.18
1	A	645	ILE	N-CA-C	-5.09	105.75	110.53
1	B	450	GLY	N-CA-C	-5.08	106.43	111.56
1	A	449	TRP	N-CA-C	5.07	118.00	110.14
1	A	390	GLU	N-CA-C	-5.06	105.23	111.40
1	B	373	GLY	CA-C-N	-5.02	114.78	119.85
1	B	373	GLY	C-N-CA	-5.02	114.78	119.85

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	6382	0	6092	32	0
1	B	6375	0	6082	34	0
2	C	83	0	70	1	0
2	J	83	0	70	1	0
3	D	39	0	33	2	0
3	G	39	0	34	0	0
3	L	39	0	34	0	0
3	N	39	0	34	0	0
4	E	28	0	25	3	0
5	F	116	0	96	0	0
5	M	116	0	97	0	0
6	H	83	0	70	1	0
6	O	83	0	69	3	0
7	I	83	0	70	0	0
8	K	72	0	61	0	0
9	P	94	0	79	4	0
10	Q	23	0	21	0	0
10	R	23	0	21	4	0
11	A	28	0	26	0	0
11	B	42	0	39	0	0
12	A	16	0	28	9	0
12	B	16	0	28	4	0
13	A	748	0	0	3	0
13	B	859	0	0	12	0
All	All	15509	0	13179	82	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 3.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:ARG:HH12	1:A:860:GLN:C	1.51	1.17
1:B:815:THR:HG22	13:B:1525:HOH:O	1.70	0.89
1:A:819:ARG:NH1	1:A:860:GLN:C	2.31	0.88
12:A:942:MRD:H5C2	13:A:1191:HOH:O	1.77	0.84
4:E:2:NAG:H83	4:E:2:NAG:H3	1.63	0.81
1:A:360:ARG:HH11	12:A:943:MRD:HMC3	1.45	0.80
12:A:943:MRD:HMC2	13:B:1105:HOH:O	1.85	0.74
12:A:943:MRD:H5C3	12:A:943:MRD:HMC1	1.70	0.72
1:B:764:ARG:HD3	1:B:814:THR:HG21	1.74	0.69
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.75	0.68
1:B:764:ARG:HD3	1:B:814:THR:CG2	2.25	0.67
1:B:484:TRP:CE2	6:O:3:BMA:H62	2.34	0.62
1:B:664:ILE:HD11	1:B:854:ALA:HB3	1.81	0.62
12:A:942:MRD:O2	12:A:942:MRD:H5C3	1.99	0.62
13:B:1464:HOH:O	9:P:3:BMA:H61	2.04	0.58
1:A:360:ARG:HH11	12:A:943:MRD:CM	2.15	0.57
1:A:193:LEU:HD13	1:A:220:VAL:HG21	1.88	0.55
4:E:2:NAG:H3	4:E:2:NAG:C8	2.36	0.55
12:A:943:MRD:HMC1	12:A:943:MRD:C5	2.37	0.55
1:B:819:ARG:HH22	1:B:860:GLN:C	2.16	0.54
1:B:494:LYS:HE2	13:B:1291:HOH:O	2.08	0.53
12:B:949:MRD:O2	12:B:949:MRD:C5	2.57	0.53
1:B:783:LEU:C	1:B:783:LEU:HD23	2.34	0.52
1:B:74:VAL:HG21	10:R:2:BGC:H6C1	1.91	0.52
1:B:74:VAL:CG2	10:R:2:BGC:H6C1	2.40	0.52
1:B:702:ARG:HD3	13:B:1175:HOH:O	2.10	0.52
1:B:819:ARG:NH2	1:B:860:GLN:C	2.68	0.52
1:A:605:GLU:HA	1:A:610:TYR:OH	2.11	0.51
1:A:666:VAL:CG2	1:A:857:PRO:HG3	2.40	0.51
1:B:659:TYR:HE1	1:B:781:PRO:HB3	1.76	0.51
1:A:260:SER:O	1:A:264:ASN:HB2	2.12	0.50
1:A:762:LEU:C	1:A:763:ILE:HG12	2.38	0.49
2:C:3:BMA:H61	2:C:7:MAN:H5	1.95	0.48
9:P:3:BMA:H62	9:P:4:MAN:H5	1.95	0.48
1:B:203:ALA:HB3	13:B:1726:HOH:O	2.13	0.48
1:A:191:TYR:O	1:A:246:CYS:HA	2.13	0.47
1:B:37:GLN:OE1	1:B:752:SER:HB2	2.15	0.47
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.97	0.47
12:B:948:MRD:H4	13:B:1363:HOH:O	2.15	0.47
1:A:424:ASP:HB3	1:A:502:PHE:HB3	1.96	0.47
12:A:942:MRD:O2	12:A:942:MRD:C5	2.63	0.46
1:B:57:ASP:OD1	1:B:57:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:VAL:HB	10:R:2:BGC:H6C1	1.96	0.46
1:A:542:ASN:ND2	13:A:1606:HOH:O	2.36	0.46
1:A:470:VAL:HG11	1:A:477:VAL:HB	1.98	0.46
1:A:303:ILE:HG21	4:E:2:NAG:H81	1.98	0.45
1:B:102:TYR:HB3	1:B:383:ASN:HA	1.98	0.45
1:A:484:TRP:CE2	6:H:3:BMA:H62	2.52	0.45
1:A:807:PRO:O	1:A:808:SER:HB2	2.16	0.45
9:P:3:BMA:H62	9:P:4:MAN:H3	1.99	0.45
1:B:377:LYS:HD3	13:B:1200:HOH:O	2.16	0.45
1:B:446:ALA:HA	1:B:574:PRO:HD2	1.98	0.45
1:B:723:PRO:HG2	13:B:1452:HOH:O	2.15	0.45
1:A:375:TYR:CG	9:P:7:MAN:H62	2.53	0.44
1:A:783:LEU:C	1:A:783:LEU:HD23	2.43	0.44
1:B:500:LEU:HD23	1:B:545:ILE:HB	2.00	0.44
12:B:948:MRD:H4	12:B:948:MRD:H1C2	1.38	0.44
1:B:494:LYS:CE	13:B:1291:HOH:O	2.64	0.44
1:A:360:ARG:HG2	12:A:943:MRD:HMC1	1.99	0.44
1:A:659:TYR:HE1	1:A:781:PRO:HB3	1.83	0.43
1:B:494:LYS:NZ	13:B:1291:HOH:O	2.51	0.43
1:A:93:SER:HB2	1:A:452:GLY:HA2	2.00	0.43
1:B:146:GLY:HA2	1:B:147:PRO:C	2.44	0.43
1:B:367:TYR:CZ	2:J:2:NAG:H83	2.54	0.42
1:A:840:LYS:HE2	1:A:840:LYS:HB3	1.91	0.42
1:A:449:TRP:CD1	1:A:512:ILE:HB	2.55	0.42
1:B:838:PRO:HD2	13:B:1672:HOH:O	2.20	0.42
1:B:395:LEU:O	1:B:395:LEU:HD23	2.20	0.42
1:B:625:ASP:HB3	12:B:949:MRD:HMC2	2.01	0.42
6:O:3:BMA:H61	6:O:4:MAN:H5	2.02	0.42
1:B:144:ALA:O	1:B:160:GLY:HA2	2.20	0.42
1:A:251:ILE:HG21	3:D:1:NAG:H82	2.01	0.41
1:A:220:VAL:HG22	1:A:626:PHE:CG	2.56	0.41
1:A:251:ILE:CG2	3:D:1:NAG:H82	2.50	0.41
1:A:28:PHE:CG	1:A:265:LYS:HB2	2.56	0.41
1:A:348:ARG:NH1	13:A:1479:HOH:O	2.52	0.41
1:B:30:PRO:HG3	1:B:739:ASP:O	2.21	0.41
1:A:116:TRP:CD1	1:A:595:LYS:HB2	2.57	0.40
1:A:193:LEU:HD13	1:A:220:VAL:CG2	2.50	0.40
1:B:74:VAL:CB	10:R:2:BGC:H6C1	2.50	0.40
1:A:102:TYR:HB3	1:A:383:ASN:HA	2.03	0.40
1:B:484:TRP:CZ2	6:O:3:BMA:H62	2.57	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	829/841 (99%)	803 (97%)	25 (3%)	1 (0%)	48	46
1	B	828/841 (98%)	804 (97%)	24 (3%)	0	100	100
All	All	1657/1682 (98%)	1607 (97%)	49 (3%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	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	A	671/677 (99%)	667 (99%)	4 (1%)	78	85
1	B	670/677 (99%)	663 (99%)	7 (1%)	68	75
All	All	1341/1354 (99%)	1330 (99%)	11 (1%)	73	80

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	ILE
1	A	642	GLU
1	A	763	ILE
1	A	858	LYS
1	B	302	ASP

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Mol	Chain	Res	Type
1	B	642	GLU
1	B	678	GLU
1	B	698	GLU
1	B	806	LYS
1	B	819	ARG
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	45	GLN
1	A	219	ASN
1	A	253	ASN
1	A	371	GLN
1	A	540	ASN
1	A	623	GLN
1	B	53	GLN
1	B	126	GLN
1	B	219	ASN
1	B	253	ASN
1	B	623	GLN
1	B	668	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

87 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	1.18	2 (14%)	17,19,21	1.45	2 (11%)
2	NAG	C	2	2	14,14,15	1.16	1 (7%)	17,19,21	1.41	3 (17%)
2	BMA	C	3	2	11,11,12	0.71	0	15,15,17	1.80	3 (20%)
2	MAN	C	4	2	11,11,12	0.97	1 (9%)	15,15,17	2.37	6 (40%)
2	MAN	C	5	2	11,11,12	0.87	0	15,15,17	1.99	5 (33%)
2	MAN	C	6	2	11,11,12	1.02	0	15,15,17	1.98	6 (40%)
2	MAN	C	7	2	11,11,12	0.85	0	15,15,17	0.98	0
3	NAG	D	1	1,3	14,14,15	1.06	1 (7%)	17,19,21	1.44	3 (17%)
3	NAG	D	2	3	14,14,15	1.46	2 (14%)	17,19,21	2.03	7 (41%)
3	BMA	D	3	3	11,11,12	1.26	0	15,15,17	2.54	7 (46%)
4	NAG	E	1	1,4	14,14,15	1.32	2 (14%)	17,19,21	1.80	3 (17%)
4	NAG	E	2	4	14,14,15	1.08	2 (14%)	17,19,21	1.83	7 (41%)
5	NAG	F	1	5,1	14,14,15	1.52	3 (21%)	17,19,21	1.30	3 (17%)
5	MAN	F	10	5	11,11,12	1.24	2 (18%)	15,15,17	2.23	5 (33%)
5	NAG	F	2	5	14,14,15	1.07	0	17,19,21	1.51	2 (11%)
5	BMA	F	3	5	11,11,12	0.67	0	15,15,17	1.25	3 (20%)
5	MAN	F	4	5	11,11,12	0.80	0	15,15,17	0.97	0
5	MAN	F	5	5	11,11,12	1.27	2 (18%)	15,15,17	1.16	2 (13%)
5	MAN	F	6	5	11,11,12	0.82	0	15,15,17	1.36	3 (20%)
5	MAN	F	7	5	11,11,12	1.43	3 (27%)	15,15,17	1.43	2 (13%)
5	MAN	F	8	5	11,11,12	0.88	0	15,15,17	0.94	1 (6%)
5	MAN	F	9	5	11,11,12	1.50	4 (36%)	15,15,17	1.95	6 (40%)
3	NAG	G	1	1,3	14,14,15	1.02	1 (7%)	17,19,21	2.07	5 (29%)
3	NAG	G	2	3	14,14,15	0.83	0	17,19,21	1.93	3 (17%)
3	BMA	G	3	3	11,11,12	1.26	2 (18%)	15,15,17	1.93	4 (26%)
6	NAG	H	1	6,1	14,14,15	1.18	1 (7%)	17,19,21	1.53	4 (23%)
6	NAG	H	2	6	14,14,15	0.82	0	17,19,21	1.44	3 (17%)
6	BMA	H	3	6	11,11,12	1.29	1 (9%)	15,15,17	1.59	3 (20%)
6	MAN	H	4	6	11,11,12	0.67	0	15,15,17	1.41	2 (13%)
6	MAN	H	5	6	11,11,12	0.82	0	15,15,17	2.13	4 (26%)
6	MAN	H	6	6	11,11,12	1.60	1 (9%)	15,15,17	1.59	3 (20%)
6	MAN	H	7	6	11,11,12	0.79	0	15,15,17	1.59	2 (13%)
7	NAG	I	1	1,7	14,14,15	1.06	1 (7%)	17,19,21	1.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	I	2	7	14,14,15	1.33	2 (14%)	17,19,21	1.46	3 (17%)
7	BMA	I	3	7	11,11,12	1.43	1 (9%)	15,15,17	1.67	3 (20%)
7	MAN	I	4	7	11,11,12	1.24	1 (9%)	15,15,17	1.11	0
7	MAN	I	5	7	11,11,12	1.23	0	15,15,17	2.29	6 (40%)
7	MAN	I	6	7	11,11,12	0.97	1 (9%)	15,15,17	1.82	4 (26%)
7	MAN	I	7	7	11,11,12	1.90	2 (18%)	15,15,17	1.12	1 (6%)
2	NAG	J	1	1,2	14,14,15	1.43	3 (21%)	17,19,21	2.17	5 (29%)
2	NAG	J	2	2	14,14,15	0.92	0	17,19,21	2.05	6 (35%)
2	BMA	J	3	2	11,11,12	1.75	2 (18%)	15,15,17	1.73	5 (33%)
2	MAN	J	4	2	11,11,12	0.68	0	15,15,17	1.60	4 (26%)
2	MAN	J	5	2	11,11,12	1.06	1 (9%)	15,15,17	1.03	0
2	MAN	J	6	2	11,11,12	0.88	0	15,15,17	1.29	1 (6%)
2	MAN	J	7	2	11,11,12	0.68	0	15,15,17	1.77	5 (33%)
8	NAG	K	1	1,8	14,14,15	0.92	0	17,19,21	1.71	3 (17%)
8	NAG	K	2	8	14,14,15	1.65	6 (42%)	17,19,21	1.88	6 (35%)
8	BMA	K	3	8	11,11,12	1.11	1 (9%)	15,15,17	1.79	4 (26%)
8	MAN	K	4	8	11,11,12	0.82	0	15,15,17	1.60	2 (13%)
8	MAN	K	5	8	11,11,12	0.83	0	15,15,17	1.97	4 (26%)
8	MAN	K	6	8	11,11,12	1.21	1 (9%)	15,15,17	1.32	2 (13%)
3	NAG	L	1	1,3	14,14,15	0.87	0	17,19,21	0.90	0
3	NAG	L	2	3	14,14,15	0.81	0	17,19,21	1.81	6 (35%)
3	BMA	L	3	3	11,11,12	0.91	0	15,15,17	1.84	5 (33%)
5	NAG	M	1	5,1	14,14,15	1.33	1 (7%)	17,19,21	1.63	3 (17%)
5	MAN	M	10	5	11,11,12	1.14	1 (9%)	15,15,17	2.22	4 (26%)
5	NAG	M	2	5	14,14,15	1.57	2 (14%)	17,19,21	1.54	3 (17%)
5	BMA	M	3	5	11,11,12	1.20	1 (9%)	15,15,17	1.34	2 (13%)
5	MAN	M	4	5	11,11,12	0.86	0	15,15,17	1.26	3 (20%)
5	MAN	M	5	5	11,11,12	0.97	0	15,15,17	1.93	4 (26%)
5	MAN	M	6	5	11,11,12	1.14	0	15,15,17	1.91	6 (40%)
5	MAN	M	7	5	11,11,12	0.83	0	15,15,17	1.91	3 (20%)
5	MAN	M	8	5	11,11,12	1.23	1 (9%)	15,15,17	1.40	1 (6%)
5	MAN	M	9	5	11,11,12	0.89	1 (9%)	15,15,17	2.18	6 (40%)
3	NAG	N	1	1,3	14,14,15	1.16	2 (14%)	17,19,21	1.49	5 (29%)
3	NAG	N	2	3	14,14,15	1.41	3 (21%)	17,19,21	2.80	7 (41%)
3	BMA	N	3	3	11,11,12	1.33	1 (9%)	15,15,17	2.71	8 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	O	1	6,1	14,14,15	1.07	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	O	2	6	14,14,15	1.18	1 (7%)	17,19,21	1.90	6 (35%)
6	BMA	O	3	6	11,11,12	1.29	2 (18%)	15,15,17	1.93	4 (26%)
6	MAN	O	4	6	11,11,12	0.87	0	15,15,17	1.62	4 (26%)
6	MAN	O	5	6	11,11,12	1.24	1 (9%)	15,15,17	1.66	4 (26%)
6	MAN	O	6	6	11,11,12	0.97	0	15,15,17	1.64	6 (40%)
6	MAN	O	7	6	11,11,12	1.19	2 (18%)	15,15,17	2.19	6 (40%)
9	NAG	P	1	1,9	14,14,15	0.96	1 (7%)	17,19,21	1.93	4 (23%)
9	NAG	P	2	9	14,14,15	0.81	0	17,19,21	1.11	1 (5%)
9	BMA	P	3	9	11,11,12	1.28	2 (18%)	15,15,17	3.37	6 (40%)
9	MAN	P	4	9	11,11,12	1.04	1 (9%)	15,15,17	1.87	4 (26%)
9	MAN	P	5	9	11,11,12	1.10	0	15,15,17	1.76	3 (20%)
9	MAN	P	6	9	11,11,12	0.85	0	15,15,17	3.41	7 (46%)
9	MAN	P	7	9	11,11,12	0.95	1 (9%)	15,15,17	2.67	7 (46%)
9	MAN	P	8	9	11,11,12	1.06	1 (9%)	15,15,17	2.11	6 (40%)
10	SGC	Q	1	10	11,12,12	2.75	2 (18%)	14,17,17	1.98	6 (42%)
10	BGC	Q	2	10	11,11,12	1.52	3 (27%)	15,15,17	1.51	3 (20%)
10	SGC	R	1	10	11,12,12	3.25	4 (36%)	14,17,17	2.12	3 (21%)
10	BGC	R	2	10	11,11,12	1.94	2 (18%)	15,15,17	2.80	6 (40%)

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	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	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	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	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

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

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

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	R	1	SGC	C5-C4	8.99	1.60	1.53
10	Q	1	SGC	C5-C4	7.64	1.59	1.53
10	R	2	BGC	O5-C1	4.91	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	7	MAN	O5-C1	-4.87	1.35	1.43
10	R	1	SGC	C6-C5	4.39	1.66	1.51
2	J	3	BMA	C2-C3	4.29	1.59	1.52
5	M	2	NAG	C1-C2	3.90	1.57	1.52
5	M	1	NAG	C1-C2	3.79	1.57	1.52
7	I	7	MAN	C2-C3	3.74	1.58	1.52
7	I	3	BMA	O5-C1	-3.71	1.37	1.43
5	F	1	NAG	C2-N2	3.40	1.51	1.46
2	C	2	NAG	C1-C2	3.35	1.56	1.52
10	Q	1	SGC	C3-C4	-3.23	1.50	1.53
6	H	1	NAG	O5-C5	-3.21	1.37	1.43
6	H	6	MAN	C4-C5	3.14	1.59	1.53
10	Q	2	BGC	O5-C5	3.09	1.49	1.43
8	K	6	MAN	C2-C3	3.04	1.57	1.52
6	H	3	BMA	C2-C3	3.00	1.57	1.52
7	I	2	NAG	O5-C1	-2.95	1.38	1.43
6	O	7	MAN	C2-C3	2.91	1.56	1.52
5	M	2	NAG	C4-C3	2.90	1.59	1.52
3	N	2	NAG	O7-C7	2.88	1.29	1.23
5	M	8	MAN	O5-C5	2.80	1.48	1.43
2	J	1	NAG	C1-C2	2.79	1.56	1.52
8	K	2	NAG	C8-C7	2.73	1.56	1.50
3	N	3	BMA	C2-C3	2.72	1.56	1.52
10	R	2	BGC	C6-C5	2.68	1.60	1.51
3	D	2	NAG	C3-C2	2.68	1.58	1.52
2	J	3	BMA	C4-C5	2.67	1.58	1.53
5	F	10	MAN	O5-C1	-2.67	1.39	1.43
10	R	1	SGC	O5-C1	2.65	1.49	1.42
2	J	1	NAG	C4-C5	2.63	1.58	1.53
5	F	5	MAN	O3-C3	-2.62	1.36	1.43
3	D	2	NAG	O5-C1	-2.61	1.39	1.43
4	E	1	NAG	O5-C5	-2.58	1.38	1.43
9	P	7	MAN	C2-C3	2.58	1.56	1.52
5	F	9	MAN	O5-C1	2.57	1.48	1.43
7	I	2	NAG	C2-N2	-2.56	1.42	1.46
4	E	2	NAG	C8-C7	-2.55	1.45	1.50
5	M	10	MAN	O5-C1	-2.53	1.39	1.43
5	F	7	MAN	C4-C3	2.52	1.58	1.52
6	O	2	NAG	C2-N2	-2.52	1.42	1.46
5	F	7	MAN	C1-C2	2.52	1.58	1.52
3	N	2	NAG	C4-C5	2.51	1.58	1.53
6	O	3	BMA	C1-C2	2.51	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C8-C7	2.50	1.55	1.50
8	K	2	NAG	O5-C1	-2.49	1.39	1.43
10	Q	2	BGC	O5-C1	2.49	1.47	1.43
6	O	5	MAN	C1-C2	2.48	1.58	1.52
5	M	3	BMA	O5-C5	-2.48	1.38	1.43
6	O	3	BMA	O4-C4	-2.48	1.36	1.43
6	O	1	NAG	C4-C5	2.44	1.58	1.53
3	N	2	NAG	C1-C2	2.42	1.55	1.52
7	I	6	MAN	C2-C3	2.40	1.56	1.52
5	F	9	MAN	C2-C3	-2.39	1.48	1.52
8	K	2	NAG	C3-C2	2.36	1.57	1.52
5	F	1	NAG	C4-C3	2.36	1.58	1.52
4	E	1	NAG	C1-C2	-2.34	1.49	1.52
10	Q	2	BGC	C6-C5	2.33	1.59	1.51
2	J	1	NAG	O5-C1	-2.30	1.39	1.43
9	P	1	NAG	O3-C3	-2.29	1.37	1.43
3	G	3	BMA	C2-C3	2.29	1.56	1.52
8	K	2	NAG	O7-C7	2.28	1.28	1.23
9	P	3	BMA	O5-C1	-2.28	1.39	1.43
2	J	5	MAN	C1-C2	2.28	1.57	1.52
5	F	10	MAN	O5-C5	-2.25	1.39	1.43
2	C	1	NAG	C1-C2	2.25	1.55	1.52
9	P	3	BMA	O4-C4	-2.23	1.37	1.43
5	F	9	MAN	O3-C3	-2.23	1.37	1.43
9	P	8	MAN	C2-C3	2.23	1.55	1.52
3	G	3	BMA	C1-C2	2.22	1.57	1.52
10	R	1	SGC	O5-C5	2.21	1.49	1.44
3	N	1	NAG	C8-C7	2.20	1.55	1.50
8	K	2	NAG	C1-C2	2.18	1.55	1.52
7	I	4	MAN	O5-C5	2.17	1.47	1.43
3	G	1	NAG	O4-C4	-2.17	1.37	1.43
5	M	9	MAN	O3-C3	-2.16	1.37	1.43
4	E	2	NAG	O7-C7	2.13	1.28	1.23
7	I	1	NAG	C7-N2	-2.13	1.27	1.34
3	N	1	NAG	C1-C2	2.12	1.55	1.52
5	F	5	MAN	O4-C4	-2.10	1.37	1.43
3	D	1	NAG	C1-C2	2.10	1.55	1.52
5	F	9	MAN	O4-C4	-2.08	1.37	1.43
9	P	4	MAN	O3-C3	-2.07	1.37	1.43
2	C	4	MAN	C1-C2	2.06	1.57	1.52
5	F	7	MAN	O5-C1	-2.05	1.40	1.43
8	K	3	BMA	C2-C3	2.03	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	NAG	C8-C7	2.03	1.54	1.50
8	K	2	NAG	C4-C5	2.02	1.57	1.53
6	O	7	MAN	C1-C2	2.01	1.57	1.52

All (331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	6	MAN	C1-O5-C5	10.51	126.27	112.19
9	P	3	BMA	C1-O5-C5	8.47	123.54	112.19
3	N	2	NAG	C1-O5-C5	-8.16	101.25	112.19
9	P	3	BMA	C6-C5-C4	-7.40	94.84	113.02
10	R	2	BGC	C1-O5-C5	7.10	121.71	112.19
9	P	7	MAN	C1-O5-C5	5.76	119.91	112.19
3	D	3	BMA	C3-C4-C5	5.45	120.11	110.23
5	M	7	MAN	C1-O5-C5	5.39	119.42	112.19
3	N	3	BMA	C1-O5-C5	5.38	119.40	112.19
5	F	10	MAN	C1-O5-C5	5.37	119.39	112.19
6	H	5	MAN	C1-O5-C5	5.19	119.14	112.19
3	D	3	BMA	C1-C2-C3	5.03	116.97	109.64
6	O	3	BMA	O3-C3-C2	5.01	120.27	110.05
10	R	1	SGC	C6-C5-C4	5.00	123.21	112.76
2	C	4	MAN	O2-C2-C3	-4.94	99.91	110.15
9	P	1	NAG	C1-O5-C5	4.86	118.70	112.19
10	R	1	SGC	O1-C1-C2	-4.78	95.10	108.98
8	K	5	MAN	C1-O5-C5	4.76	118.57	112.19
10	R	2	BGC	C1-C2-C3	-4.70	102.80	109.64
5	M	10	MAN	C1-O5-C5	4.61	118.36	112.19
2	J	2	NAG	O6-C6-C5	-4.60	95.67	111.33
3	G	1	NAG	C1-O5-C5	4.58	118.33	112.19
9	P	6	MAN	O2-C2-C3	4.54	119.56	110.15
7	I	6	MAN	C1-O5-C5	4.48	118.20	112.19
3	G	1	NAG	C1-C2-N2	-4.48	103.37	110.43
7	I	5	MAN	O2-C2-C3	-4.47	100.90	110.15
3	L	3	BMA	O4-C4-C3	-4.45	99.88	110.38
3	N	3	BMA	C3-C4-C5	4.43	118.27	110.23
2	J	1	NAG	C4-C3-C2	-4.39	104.58	111.02
8	K	4	MAN	O5-C5-C6	4.36	116.16	107.66
2	J	1	NAG	O5-C1-C2	-4.32	104.61	111.29
4	E	1	NAG	O4-C4-C5	-4.29	98.77	109.32
9	P	8	MAN	C2-C3-C4	4.28	118.39	110.86
2	C	3	BMA	O3-C3-C2	-4.24	101.39	110.05
3	N	2	NAG	C2-N2-C7	-4.24	117.22	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	5	MAN	O6-C6-C5	-4.22	96.95	111.33
2	C	5	MAN	O2-C2-C3	-4.19	101.47	110.15
3	L	2	NAG	C3-C4-C5	-4.19	102.63	110.23
9	P	4	MAN	O2-C2-C1	-4.18	99.65	109.22
6	H	3	BMA	O3-C3-C2	4.15	118.52	110.05
3	G	2	NAG	C1-C2-N2	-4.11	103.95	110.43
6	O	7	MAN	O5-C5-C6	4.08	115.61	107.66
5	M	1	NAG	C1-C2-N2	-4.08	104.01	110.43
3	G	2	NAG	C2-N2-C7	-4.02	117.52	122.90
3	D	2	NAG	O5-C1-C2	-4.02	105.08	111.29
6	O	2	NAG	O5-C1-C2	-3.97	105.15	111.29
2	C	4	MAN	O6-C6-C5	-3.97	97.83	111.33
9	P	3	BMA	C3-C4-C5	3.97	117.42	110.23
2	C	3	BMA	C3-C4-C5	3.95	117.39	110.23
5	M	9	MAN	C1-C2-C3	3.92	115.35	109.64
9	P	8	MAN	C3-C4-C5	3.92	117.34	110.23
9	P	7	MAN	C6-C5-C4	-3.92	103.40	113.02
8	K	1	NAG	O5-C5-C4	-3.91	101.31	110.83
3	G	2	NAG	C4-C3-C2	3.91	116.75	111.02
5	M	9	MAN	C1-O5-C5	3.90	117.42	112.19
2	C	4	MAN	O5-C5-C6	3.86	115.17	107.66
8	K	5	MAN	C1-C2-C3	-3.85	104.04	109.64
7	I	5	MAN	C6-C5-C4	3.83	122.42	113.02
2	C	6	MAN	O6-C6-C5	-3.82	98.34	111.33
9	P	5	MAN	C6-C5-C4	3.80	122.36	113.02
5	M	10	MAN	O6-C6-C5	-3.80	98.39	111.33
5	F	9	MAN	C1-O5-C5	3.80	117.28	112.19
5	M	10	MAN	C6-C5-C4	-3.79	103.72	113.02
9	P	7	MAN	O2-C2-C3	3.78	117.97	110.15
2	C	5	MAN	C2-C3-C4	-3.75	104.27	110.86
3	D	2	NAG	C6-C5-C4	3.74	122.20	113.02
2	J	7	MAN	O4-C4-C3	-3.71	101.64	110.38
3	G	3	BMA	O3-C3-C4	3.70	119.09	110.38
6	O	7	MAN	C2-C3-C4	3.67	117.32	110.86
8	K	3	BMA	C1-O5-C5	3.65	117.07	112.19
2	J	2	NAG	O7-C7-C8	-3.62	115.61	122.05
7	I	3	BMA	C1-C2-C3	3.62	114.91	109.64
5	M	10	MAN	O5-C5-C6	-3.60	100.66	107.66
5	M	5	MAN	C1-O5-C5	3.58	116.98	112.19
7	I	1	NAG	C1-C2-N2	-3.55	104.85	110.43
9	P	3	BMA	O6-C6-C5	-3.53	99.30	111.33
3	D	2	NAG	C3-C4-C5	-3.53	103.84	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	6	MAN	C1-O5-C5	3.51	116.89	112.19
3	G	1	NAG	O5-C1-C2	-3.51	105.87	111.29
5	M	9	MAN	O3-C3-C2	-3.48	102.96	110.05
2	C	1	NAG	O5-C5-C4	-3.48	102.37	110.83
5	F	2	NAG	O4-C4-C3	-3.47	102.20	110.38
6	H	7	MAN	C2-C3-C4	3.44	116.90	110.86
3	N	2	NAG	O7-C7-C8	-3.41	115.97	122.05
5	M	8	MAN	C1-O5-C5	3.41	116.76	112.19
6	H	1	NAG	C1-O5-C5	3.41	116.75	112.19
3	G	3	BMA	O5-C5-C6	3.40	114.28	107.66
3	N	3	BMA	O5-C1-C2	-3.38	102.74	110.79
10	R	2	BGC	C3-C4-C5	3.36	116.33	110.23
2	J	7	MAN	O3-C3-C2	3.36	116.91	110.05
6	H	5	MAN	C6-C5-C4	-3.34	104.82	113.02
6	H	5	MAN	O3-C3-C4	-3.34	102.50	110.38
10	R	2	BGC	O5-C5-C4	-3.34	102.70	110.83
5	M	2	NAG	C1-O5-C5	-3.32	107.73	112.19
6	O	5	MAN	C6-C5-C4	-3.32	104.86	113.02
5	F	10	MAN	O5-C5-C6	-3.31	101.22	107.66
9	P	5	MAN	O2-C2-C3	-3.30	103.31	110.15
9	P	7	MAN	O5-C5-C6	3.29	114.07	107.66
3	N	3	BMA	O3-C3-C2	3.29	116.77	110.05
7	I	5	MAN	C3-C4-C5	-3.29	104.27	110.23
3	D	3	BMA	O2-C2-C3	-3.28	103.36	110.15
7	I	2	NAG	O5-C5-C4	-3.28	102.85	110.83
3	D	1	NAG	O5-C5-C4	-3.27	102.88	110.83
5	M	9	MAN	O2-C2-C3	-3.23	103.45	110.15
3	N	2	NAG	C6-C5-C4	3.19	120.85	113.02
8	K	2	NAG	C4-C3-C2	-3.17	106.37	111.02
4	E	1	NAG	C1-O5-C5	3.13	116.38	112.19
4	E	2	NAG	C3-C4-C5	-3.12	104.57	110.23
9	P	8	MAN	O2-C2-C3	3.12	116.61	110.15
9	P	7	MAN	C2-C3-C4	3.12	116.35	110.86
10	Q	1	SGC	C6-C5-C4	3.11	119.27	112.76
5	M	6	MAN	O2-C2-C1	-3.10	102.12	109.22
10	Q	2	BGC	C1-O5-C5	3.10	116.34	112.19
6	O	7	MAN	C1-C2-C3	3.10	114.16	109.64
9	P	7	MAN	C1-C2-C3	3.09	114.14	109.64
6	H	6	MAN	C3-C4-C5	3.06	115.79	110.23
6	H	3	BMA	O2-C2-C1	-3.06	102.23	109.22
2	C	5	MAN	O6-C6-C5	-3.05	100.94	111.33
4	E	2	NAG	O4-C4-C3	-3.05	103.18	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	3	BMA	O2-C2-C1	-3.04	102.27	109.22
6	H	2	NAG	C2-N2-C7	-3.04	118.83	122.90
2	J	1	NAG	O4-C4-C3	-3.04	103.22	110.38
10	Q	1	SGC	C5-C4-S4	3.03	117.53	110.16
7	I	5	MAN	O3-C3-C2	-3.03	103.86	110.05
5	F	7	MAN	C1-O5-C5	3.03	116.24	112.19
3	N	3	BMA	O5-C5-C6	3.02	113.54	107.66
8	K	1	NAG	C4-C3-C2	-3.01	106.61	111.02
8	K	2	NAG	C6-C5-C4	3.00	120.40	113.02
7	I	2	NAG	O5-C1-C2	-3.00	106.65	111.29
5	M	6	MAN	C1-O5-C5	2.99	116.19	112.19
10	R	2	BGC	O5-C1-C2	2.99	117.91	110.79
2	C	2	NAG	O6-C6-C5	-2.99	101.17	111.33
9	P	6	MAN	C1-C2-C3	-2.97	105.31	109.64
5	M	6	MAN	O5-C5-C6	2.97	113.45	107.66
6	O	2	NAG	C6-C5-C4	2.96	120.30	113.02
5	F	10	MAN	O2-C2-C3	2.96	116.29	110.15
9	P	5	MAN	O4-C4-C3	-2.96	103.40	110.38
6	H	6	MAN	C1-O5-C5	2.95	116.14	112.19
6	H	1	NAG	C1-C2-N2	-2.94	105.80	110.43
7	I	3	BMA	O4-C4-C5	-2.93	102.11	109.32
5	F	9	MAN	O4-C4-C3	-2.93	103.48	110.38
5	M	9	MAN	C3-C4-C5	-2.92	104.93	110.23
6	O	4	MAN	C1-O5-C5	2.92	116.10	112.19
2	C	6	MAN	O5-C5-C6	2.92	113.35	107.66
9	P	8	MAN	O3-C3-C4	-2.92	103.50	110.38
2	J	4	MAN	O3-C3-C2	-2.92	104.10	110.05
8	K	3	BMA	O3-C3-C4	-2.91	103.52	110.38
5	F	3	BMA	C1-O5-C5	2.90	116.07	112.19
8	K	2	NAG	O4-C4-C5	-2.88	102.22	109.32
6	O	5	MAN	C2-C3-C4	-2.86	105.83	110.86
5	M	2	NAG	C1-C2-N2	-2.86	105.92	110.43
5	M	3	BMA	C2-C3-C4	-2.86	105.83	110.86
2	J	3	BMA	C1-C2-C3	-2.86	105.48	109.64
3	N	2	NAG	O7-C7-N2	2.86	127.04	121.98
6	H	4	MAN	O2-C2-C1	-2.86	102.67	109.22
3	D	3	BMA	O4-C4-C5	-2.84	102.33	109.32
2	J	2	NAG	C2-N2-C7	-2.83	119.11	122.90
9	P	4	MAN	O3-C3-C4	-2.82	103.73	110.38
3	G	3	BMA	O2-C2-C1	2.81	115.66	109.22
7	I	6	MAN	C6-C5-C4	-2.79	106.16	113.02
3	L	2	NAG	O6-C6-C5	-2.79	101.84	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	9	MAN	C3-C4-C5	-2.79	105.18	110.23
5	F	10	MAN	C1-C2-C3	2.78	113.69	109.64
3	N	3	BMA	C6-C5-C4	-2.78	106.20	113.02
6	O	7	MAN	O4-C4-C5	-2.77	102.51	109.32
2	C	6	MAN	O3-C3-C4	2.76	116.89	110.38
6	O	3	BMA	O4-C4-C5	-2.75	102.55	109.32
8	K	5	MAN	O6-C6-C5	-2.75	101.97	111.33
2	J	4	MAN	C2-C3-C4	-2.75	106.03	110.86
6	O	7	MAN	O6-C6-C5	-2.74	102.01	111.33
5	M	7	MAN	O2-C2-C1	-2.73	102.97	109.22
5	M	6	MAN	O5-C5-C4	-2.71	104.23	110.83
2	C	2	NAG	C6-C5-C4	2.71	119.68	113.02
6	H	2	NAG	O4-C4-C3	-2.71	103.99	110.38
6	O	7	MAN	C1-O5-C5	-2.71	108.56	112.19
5	M	4	MAN	C1-O5-C5	2.70	115.81	112.19
9	P	1	NAG	O4-C4-C5	-2.68	102.73	109.32
2	J	3	BMA	C2-C3-C4	-2.67	106.16	110.86
2	J	6	MAN	O3-C3-C2	2.67	115.50	110.05
3	D	2	NAG	C4-C3-C2	-2.66	107.12	111.02
10	Q	2	BGC	O5-C5-C6	2.66	112.84	107.66
8	K	1	NAG	C1-C2-N2	2.65	114.60	110.43
4	E	2	NAG	C1-C2-N2	2.64	114.59	110.43
8	K	2	NAG	O5-C5-C4	-2.64	104.40	110.83
3	N	2	NAG	O5-C5-C6	2.64	112.79	107.66
2	J	7	MAN	C6-C5-C4	2.62	119.45	113.02
5	M	5	MAN	C6-C5-C4	-2.61	106.61	113.02
3	D	1	NAG	C1-C2-N2	2.61	114.55	110.43
2	C	3	BMA	C2-C3-C4	-2.61	106.27	110.86
10	Q	1	SGC	O1-C1-C2	-2.60	101.43	108.98
10	R	1	SGC	O5-C5-C6	2.60	112.88	106.44
3	D	3	BMA	O6-C6-C5	2.60	120.18	111.33
2	C	2	NAG	O5-C5-C4	-2.59	104.53	110.83
4	E	1	NAG	C2-N2-C7	2.58	126.36	122.90
3	G	1	NAG	O4-C4-C3	-2.58	104.30	110.38
5	M	6	MAN	C1-C2-C3	-2.58	105.89	109.64
4	E	2	NAG	O6-C6-C5	-2.57	102.57	111.33
5	F	6	MAN	O5-C5-C6	2.57	112.67	107.66
3	L	3	BMA	C1-O5-C5	-2.57	108.75	112.19
10	Q	1	SGC	O2-C2-C1	2.56	115.14	109.25
2	C	5	MAN	O2-C2-C1	2.55	115.06	109.22
2	J	3	BMA	O5-C5-C4	-2.55	104.62	110.83
3	L	2	NAG	O5-C5-C6	2.53	112.59	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	NAG	O7-C7-N2	2.53	126.45	121.98
8	K	3	BMA	C3-C4-C5	-2.53	105.65	110.23
8	K	6	MAN	O4-C4-C5	2.52	115.54	109.32
9	P	6	MAN	O5-C1-C2	2.52	116.80	110.79
6	O	2	NAG	O4-C4-C3	-2.51	104.46	110.38
8	K	2	NAG	O6-C6-C5	-2.51	102.79	111.33
9	P	3	BMA	O4-C4-C5	-2.50	103.17	109.32
2	J	7	MAN	C3-C4-C5	-2.50	105.70	110.23
2	J	1	NAG	O5-C5-C4	-2.50	104.75	110.83
6	O	4	MAN	O5-C5-C6	2.50	112.52	107.66
2	J	2	NAG	O4-C4-C5	-2.49	103.18	109.32
5	F	7	MAN	C1-C2-C3	-2.49	106.02	109.64
6	H	6	MAN	C2-C3-C4	-2.48	106.50	110.86
10	R	2	BGC	O2-C2-C1	2.47	114.89	109.22
5	F	3	BMA	O6-C6-C5	-2.47	102.92	111.33
6	O	2	NAG	O5-C5-C4	-2.47	104.82	110.83
8	K	3	BMA	O3-C3-C2	2.47	115.09	110.05
10	Q	2	BGC	O5-C1-C2	2.46	116.67	110.79
6	H	1	NAG	O5-C1-C2	2.46	115.10	111.29
3	N	1	NAG	C4-C3-C2	-2.45	107.42	111.02
2	C	6	MAN	O2-C2-C3	-2.45	105.08	110.15
2	J	4	MAN	O6-C6-C5	-2.44	103.03	111.33
5	M	5	MAN	O4-C4-C5	-2.43	103.35	109.32
7	I	6	MAN	O3-C3-C2	2.42	115.00	110.05
5	M	3	BMA	O5-C5-C4	-2.42	104.94	110.83
3	L	2	NAG	O5-C1-C2	-2.42	107.55	111.29
3	N	2	NAG	C3-C4-C5	-2.42	105.85	110.23
5	F	9	MAN	O4-C4-C5	-2.41	103.39	109.32
8	K	6	MAN	C1-O5-C5	2.41	115.41	112.19
3	N	3	BMA	O4-C4-C3	-2.40	104.71	110.38
3	D	2	NAG	O6-C6-C5	-2.40	103.16	111.33
8	K	2	NAG	C1-O5-C5	-2.40	108.97	112.19
3	L	3	BMA	O5-C5-C6	2.39	112.32	107.66
2	J	4	MAN	O5-C5-C6	2.39	112.31	107.66
9	P	4	MAN	O4-C4-C3	-2.38	104.75	110.38
2	C	4	MAN	C2-C3-C4	-2.38	106.67	110.86
5	F	2	NAG	C1-O5-C5	-2.38	109.00	112.19
7	I	7	MAN	O2-C2-C1	-2.38	103.78	109.22
2	J	2	NAG	C1-O5-C5	2.37	115.37	112.19
5	M	6	MAN	O3-C3-C2	-2.36	105.24	110.05
6	O	4	MAN	O3-C3-C4	2.36	115.93	110.38
7	I	5	MAN	O5-C5-C4	-2.36	105.09	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	3	BMA	C1-O5-C5	2.35	115.34	112.19
5	F	1	NAG	O5-C1-C2	2.35	114.92	111.29
6	O	6	MAN	O4-C4-C3	-2.34	104.87	110.38
5	F	5	MAN	O6-C6-C5	-2.33	103.39	111.33
6	O	6	MAN	O2-C2-C1	2.33	114.56	109.22
3	D	1	NAG	C4-C3-C2	-2.33	107.61	111.02
5	F	10	MAN	O5-C1-C2	2.33	116.34	110.79
4	E	2	NAG	C2-N2-C7	2.32	126.02	122.90
3	D	2	NAG	O3-C3-C2	-2.32	104.59	109.40
2	C	6	MAN	C2-C3-C4	-2.32	106.78	110.86
3	N	1	NAG	O7-C7-C8	2.31	126.17	122.05
5	F	1	NAG	C2-N2-C7	-2.31	119.80	122.90
3	N	1	NAG	O4-C4-C3	-2.31	104.94	110.38
6	O	2	NAG	O6-C6-C5	-2.30	103.50	111.33
5	F	9	MAN	O5-C5-C4	-2.30	105.24	110.83
6	O	2	NAG	O7-C7-C8	2.30	126.14	122.05
9	P	6	MAN	O2-C2-C1	-2.29	103.97	109.22
6	H	7	MAN	O5-C5-C6	2.29	112.13	107.66
8	K	4	MAN	O3-C3-C4	-2.29	104.99	110.38
5	F	5	MAN	C1-O5-C5	2.28	115.25	112.19
2	C	1	NAG	C6-C5-C4	-2.28	107.42	113.02
5	F	6	MAN	O2-C2-C1	-2.28	104.00	109.22
2	C	4	MAN	C1-C2-C3	2.28	112.96	109.64
3	N	1	NAG	O7-C7-N2	-2.28	117.95	121.98
3	N	1	NAG	O3-C3-C2	-2.27	104.68	109.40
6	O	5	MAN	O6-C6-C5	-2.27	103.60	111.33
3	G	3	BMA	C1-O5-C5	2.27	115.22	112.19
10	Q	1	SGC	O5-C5-C6	-2.25	100.86	106.44
2	J	7	MAN	O5-C5-C6	2.25	112.04	107.66
9	P	6	MAN	O5-C5-C6	2.25	112.04	107.66
4	E	2	NAG	O7-C7-C8	-2.24	118.06	122.05
5	M	7	MAN	O6-C6-C5	-2.24	103.72	111.33
6	O	4	MAN	O4-C4-C5	-2.23	103.83	109.32
3	D	2	NAG	C1-O5-C5	-2.23	109.20	112.19
6	O	5	MAN	C1-C2-C3	-2.23	106.40	109.64
7	I	6	MAN	O6-C6-C5	-2.22	103.77	111.33
9	P	6	MAN	O4-C4-C5	-2.22	103.85	109.32
7	I	1	NAG	O5-C5-C6	2.22	111.98	107.66
6	O	6	MAN	O6-C6-C5	-2.21	103.79	111.33
6	H	1	NAG	O3-C3-C2	-2.21	104.81	109.40
9	P	2	NAG	O6-C6-C5	-2.21	103.80	111.33
5	M	1	NAG	C2-N2-C7	-2.21	119.94	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	O5-C5-C6	2.20	111.94	107.66
7	I	5	MAN	O6-C6-C5	-2.19	103.87	111.33
9	P	1	NAG	C3-C4-C5	-2.19	106.26	110.23
3	D	3	BMA	C6-C5-C4	-2.19	107.65	113.02
5	M	2	NAG	O4-C4-C3	-2.17	105.26	110.38
7	I	2	NAG	O6-C6-C5	-2.17	103.95	111.33
2	C	6	MAN	O4-C4-C3	2.16	115.47	110.38
3	L	3	BMA	C6-C5-C4	2.16	118.31	113.02
2	J	3	BMA	O3-C3-C4	-2.15	105.30	110.38
6	H	3	BMA	C6-C5-C4	-2.15	107.73	113.02
3	L	2	NAG	O7-C7-C8	-2.15	118.22	122.05
2	J	2	NAG	C8-C7-N2	2.15	119.69	116.12
8	K	5	MAN	O5-C5-C6	-2.15	103.48	107.66
9	P	8	MAN	O2-C2-C1	2.15	114.14	109.22
5	F	6	MAN	O5-C5-C4	-2.14	105.63	110.83
9	P	7	MAN	O3-C3-C4	-2.14	105.34	110.38
6	H	4	MAN	O4-C4-C5	-2.14	104.06	109.32
6	O	6	MAN	C2-C3-C4	-2.13	107.11	110.86
6	H	2	NAG	O6-C6-C5	-2.13	104.08	111.33
6	O	6	MAN	C1-C2-C3	-2.11	106.57	109.64
5	M	9	MAN	C6-C5-C4	-2.11	107.84	113.02
5	F	8	MAN	C1-O5-C5	2.11	115.01	112.19
10	Q	1	SGC	O3-C3-C2	-2.09	105.44	110.38
5	F	1	NAG	C4-C3-C2	2.09	114.08	111.02
2	C	4	MAN	C6-C5-C4	-2.09	107.89	113.02
3	L	2	NAG	C8-C7-N2	2.09	119.58	116.12
3	N	3	BMA	O5-C5-C4	2.09	115.90	110.83
9	P	3	BMA	O5-C5-C4	2.08	115.89	110.83
3	G	1	NAG	C4-C3-C2	-2.08	107.97	111.02
2	C	5	MAN	O5-C5-C4	2.07	115.87	110.83
5	M	1	NAG	O5-C1-C2	-2.07	108.10	111.29
5	F	9	MAN	C6-C5-C4	-2.06	107.96	113.02
3	L	3	BMA	O3-C3-C2	2.06	114.26	110.05
3	D	3	BMA	O3-C3-C2	-2.06	105.86	110.05
6	O	3	BMA	O2-C2-C3	2.05	114.40	110.15
5	M	4	MAN	O5-C5-C4	-2.03	105.88	110.83
2	J	3	BMA	C6-C5-C4	-2.03	108.04	113.02
5	M	4	MAN	C1-C2-C3	-2.02	106.70	109.64
9	P	4	MAN	C1-O5-C5	2.02	114.90	112.19
9	P	1	NAG	O3-C3-C2	-2.02	105.20	109.40
6	H	5	MAN	O4-C4-C3	2.01	115.12	110.38
5	F	3	BMA	O3-C3-C2	-2.01	105.95	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	1	NAG	C1-C2-N2	-2.01	107.27	110.43
9	P	8	MAN	O4-C4-C3	-2.00	105.65	110.38

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	MAN	C4-C5-C6-O6
2	J	5	MAN	O5-C5-C6-O6
7	I	6	MAN	O5-C5-C6-O6
7	I	4	MAN	O5-C5-C6-O6
9	P	7	MAN	O5-C5-C6-O6
9	P	6	MAN	C4-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
9	P	3	BMA	C4-C5-C6-O6
9	P	7	MAN	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
5	F	10	MAN	C4-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
5	F	10	MAN	O5-C5-C6-O6
6	O	7	MAN	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
9	P	3	BMA	O5-C5-C6-O6
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
7	I	6	MAN	C4-C5-C6-O6
2	J	5	MAN	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
9	P	6	MAN	O5-C5-C6-O6
10	R	2	BGC	C4-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
7	I	4	MAN	C4-C5-C6-O6
5	M	10	MAN	C4-C5-C6-O6
8	K	5	MAN	O5-C5-C6-O6
10	Q	1	SGC	O5-C5-C6-O6
5	M	10	MAN	O5-C5-C6-O6
9	P	8	MAN	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
6	O	7	MAN	C4-C5-C6-O6
10	R	1	SGC	O5-C5-C6-O6
9	P	5	MAN	O5-C5-C6-O6

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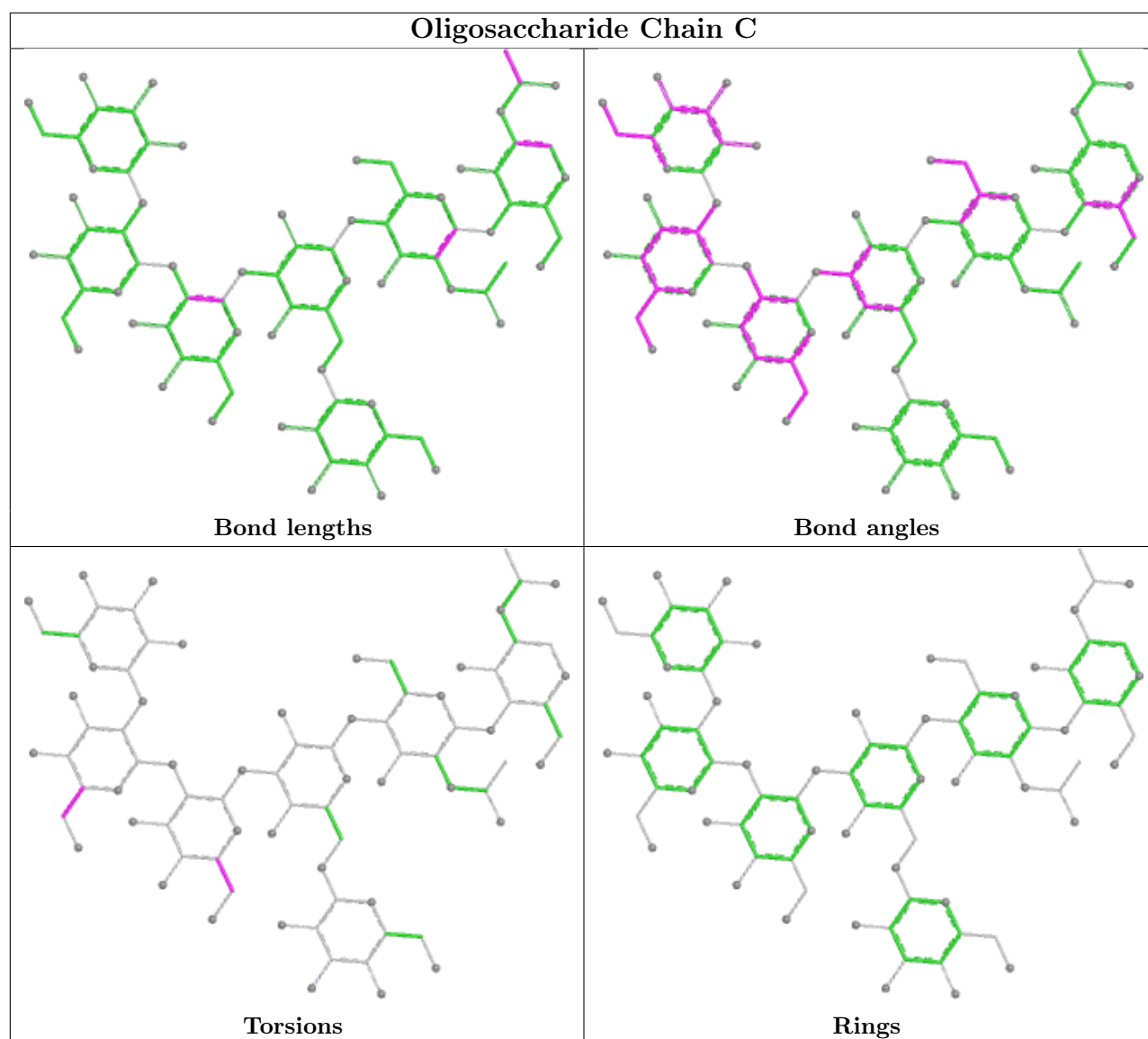
Mol	Chain	Res	Type	Atoms
6	H	7	MAN	O5-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
2	J	6	MAN	O5-C5-C6-O6
3	L	2	NAG	C1-C2-N2-C7
6	H	6	MAN	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	J	4	MAN	O5-C5-C6-O6

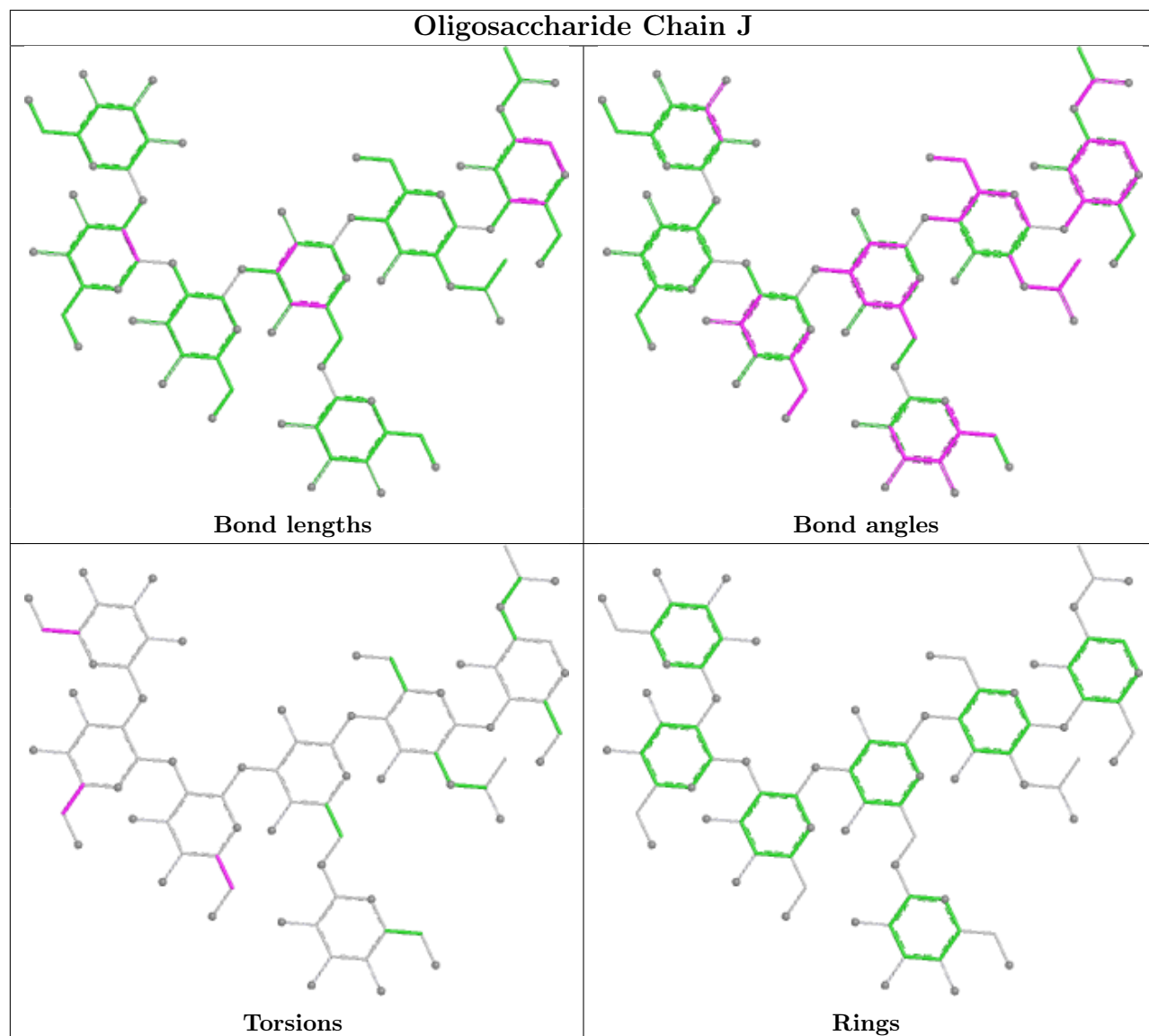
There are no ring outliers.

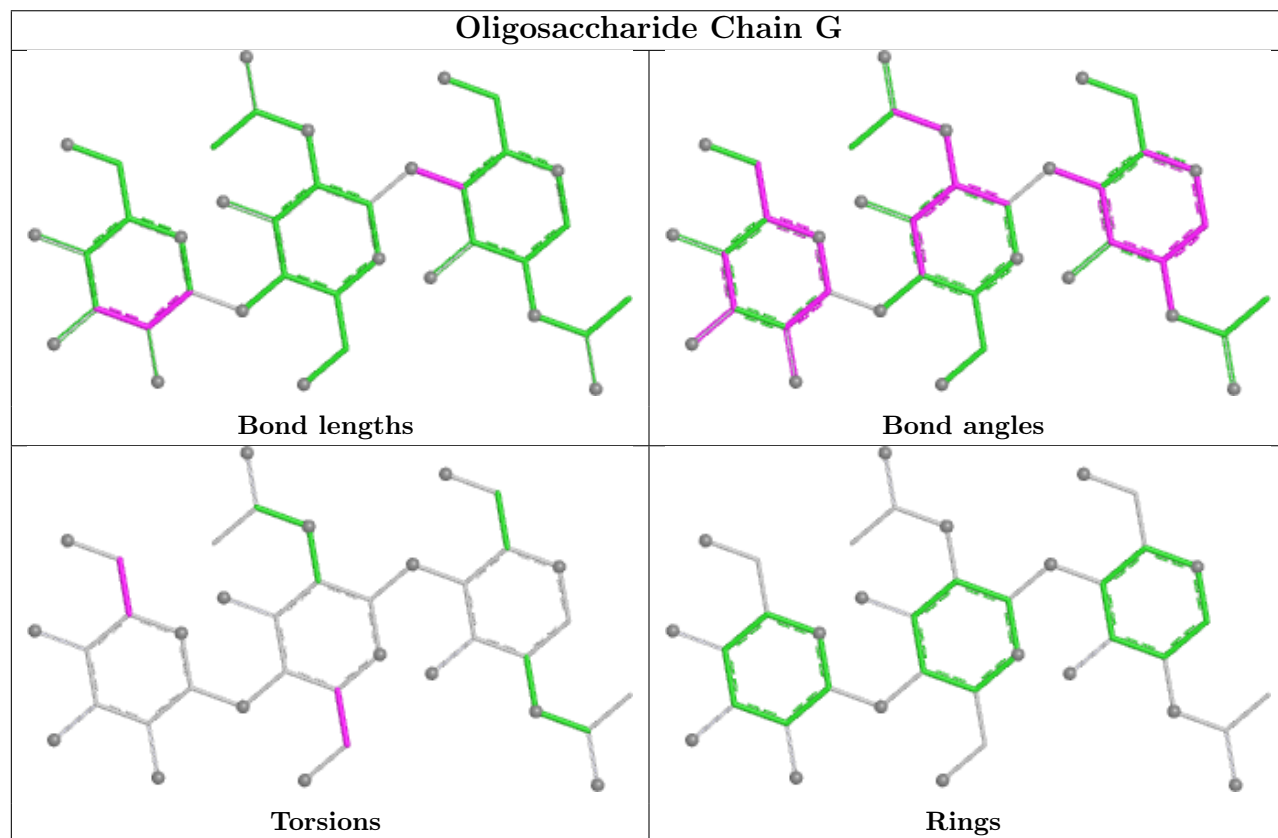
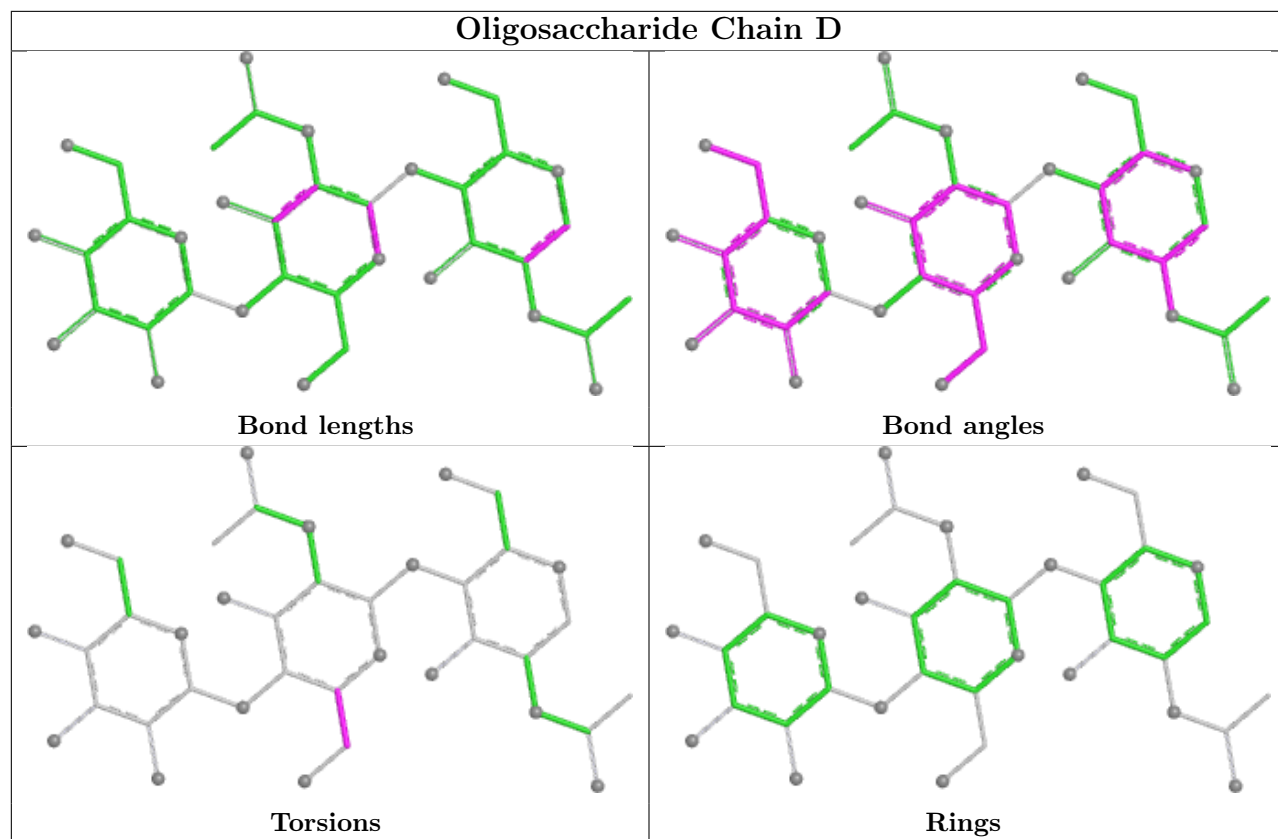
12 monomers are involved in 19 short contacts:

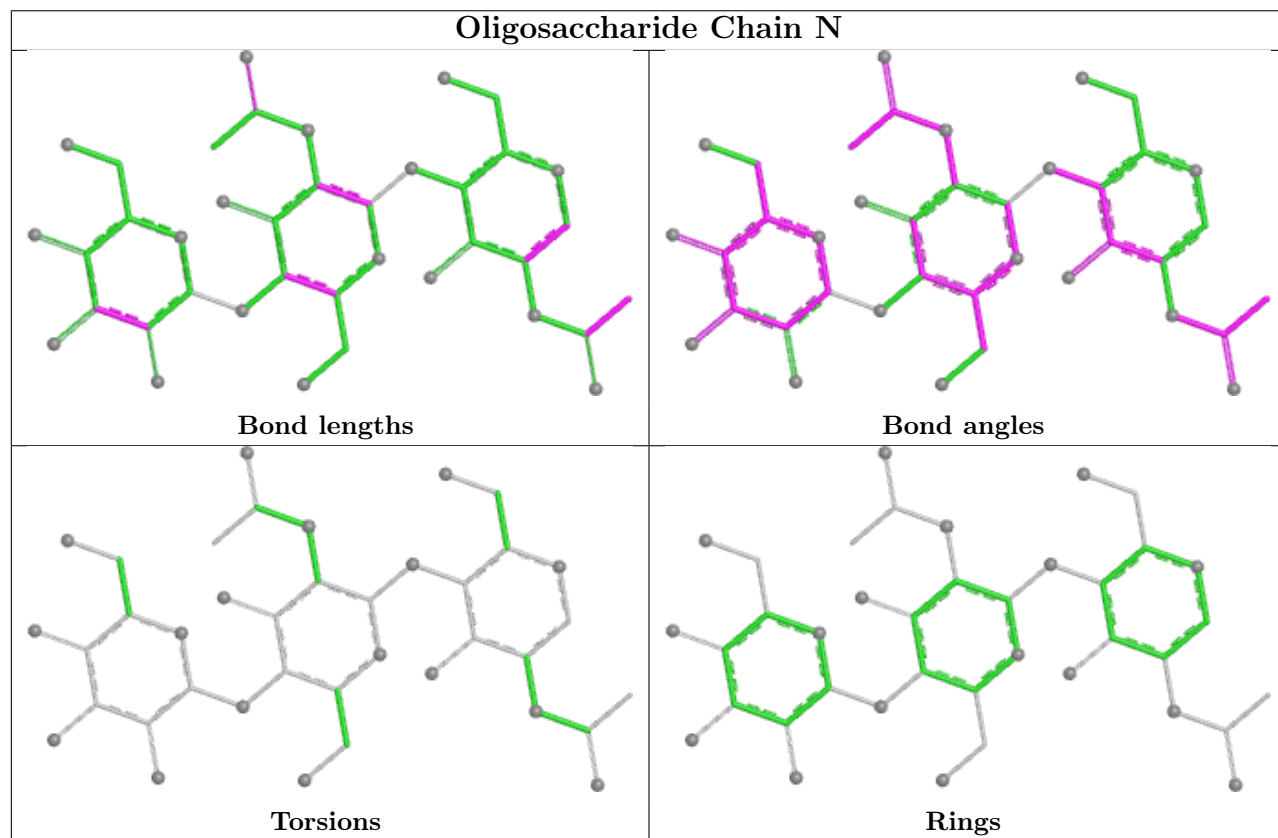
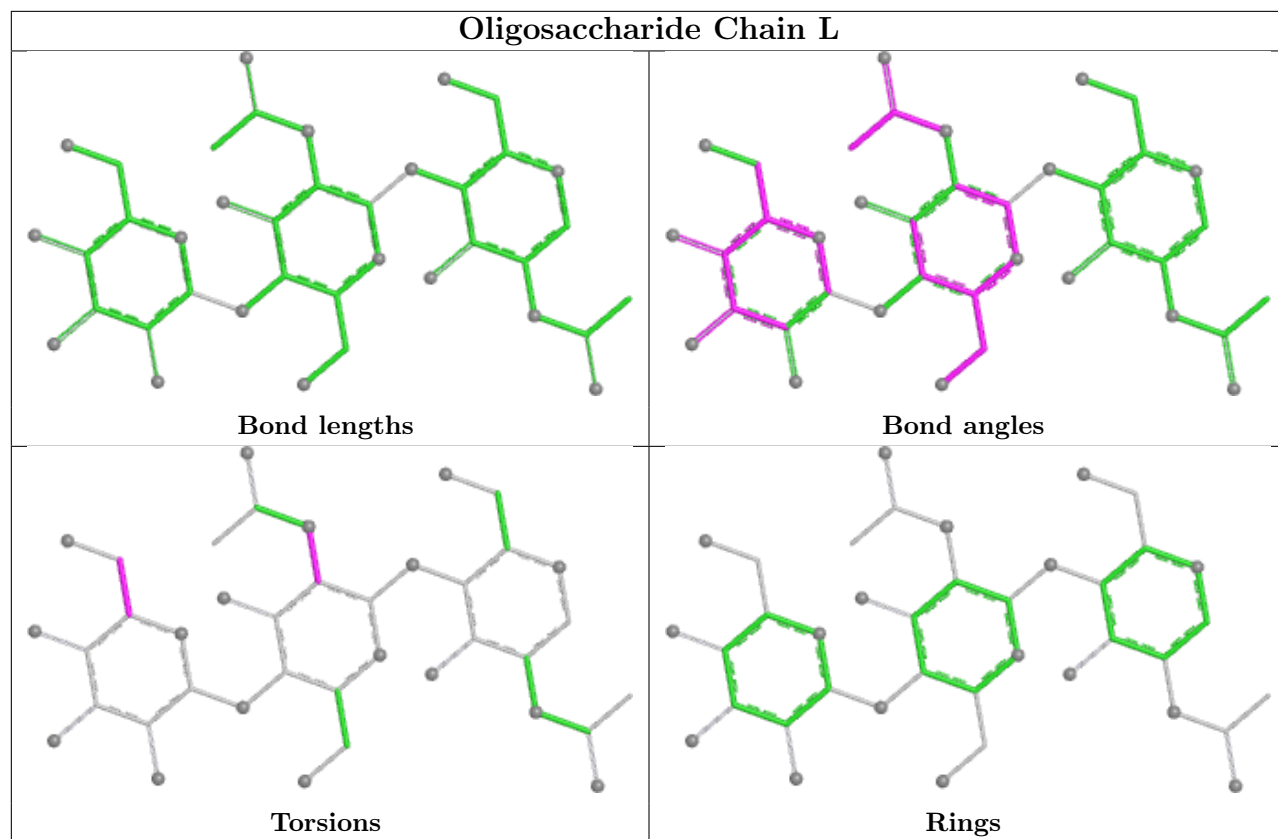
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	BMA	1	0
2	C	7	MAN	1	0
6	O	3	BMA	3	0
9	P	4	MAN	2	0
9	P	7	MAN	1	0
10	R	2	BGC	4	0
6	O	4	MAN	1	0
6	H	3	BMA	1	0
9	P	3	BMA	3	0
2	J	2	NAG	1	0
3	D	1	NAG	2	0
4	E	2	NAG	3	0

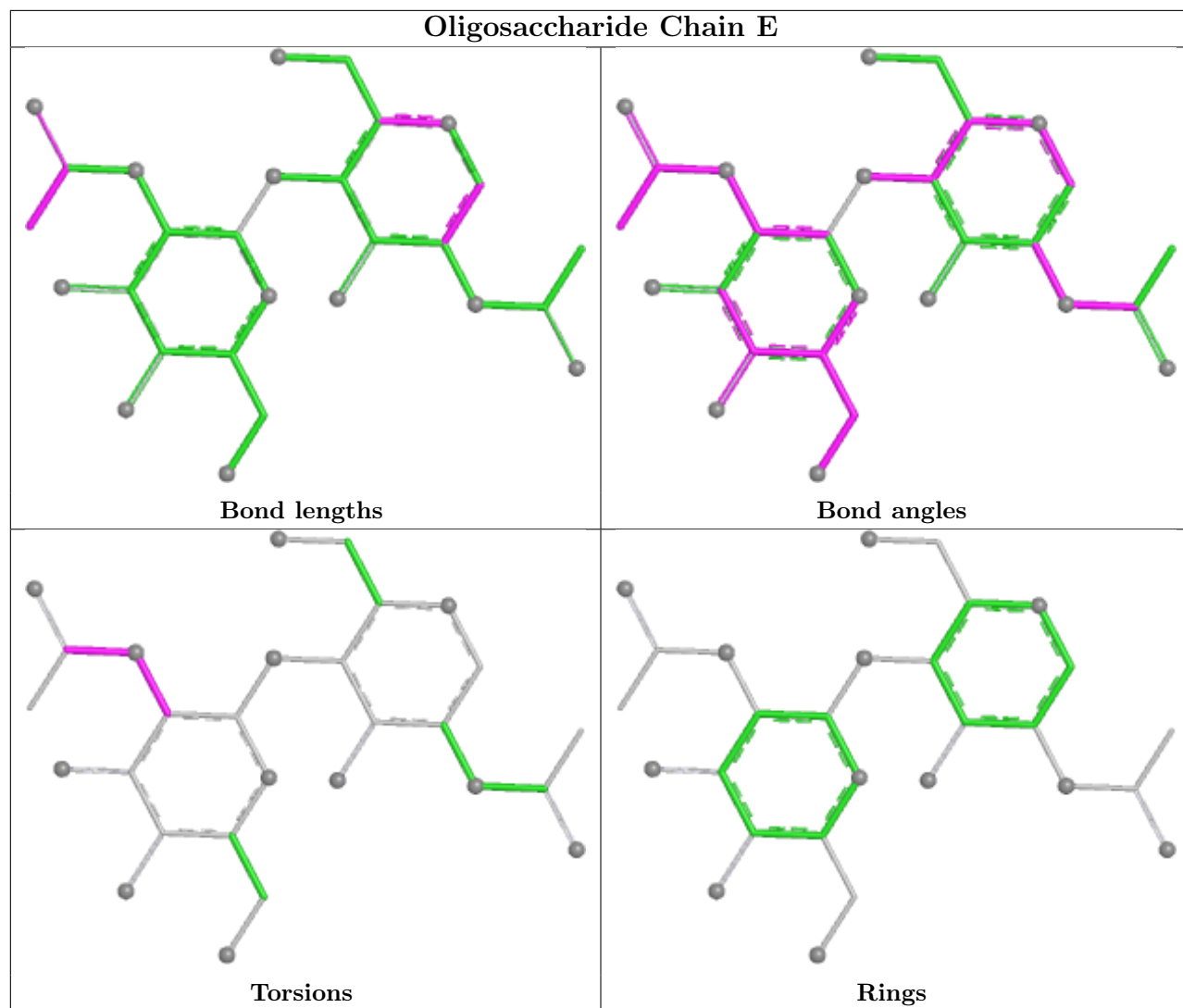
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

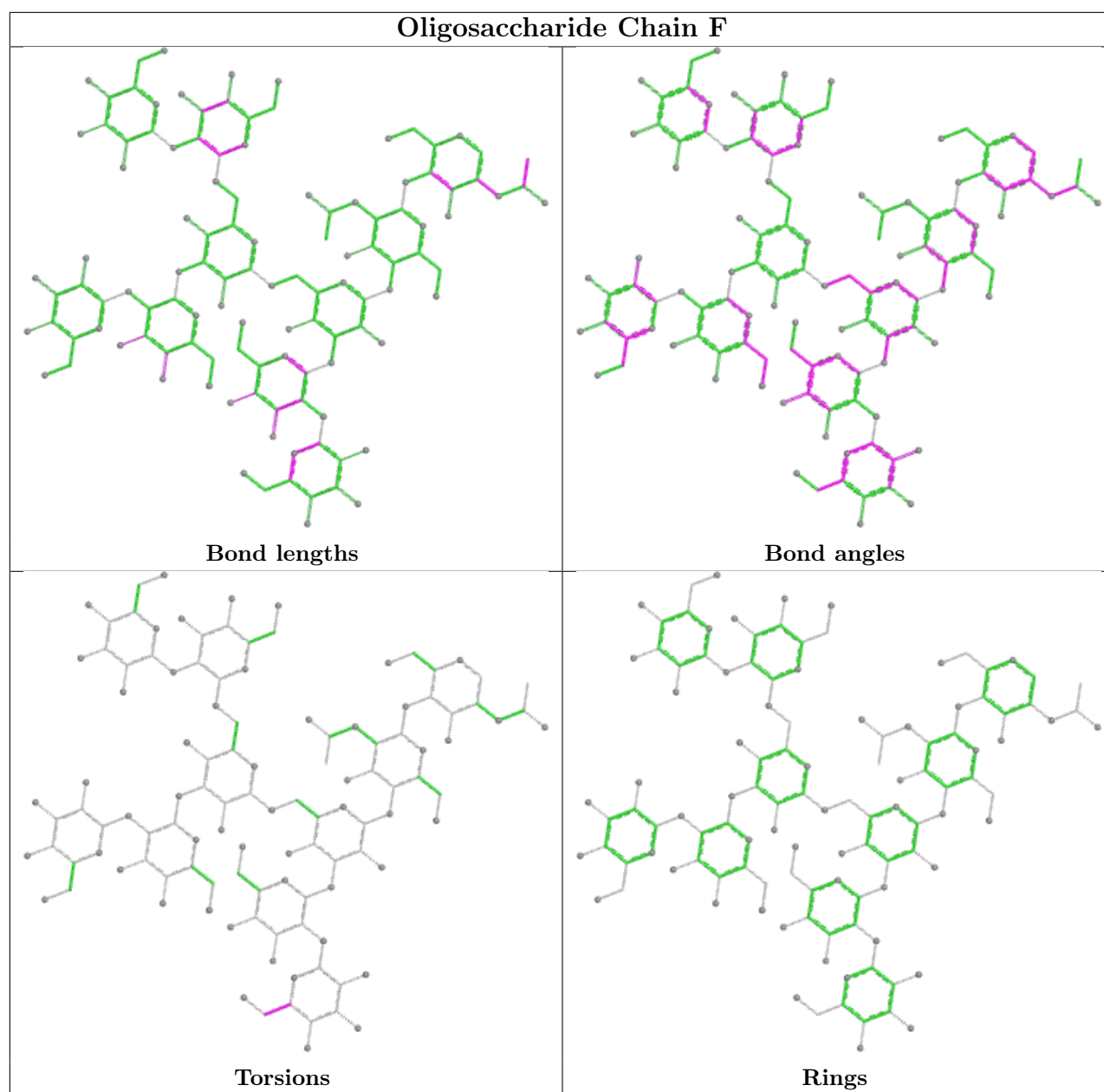




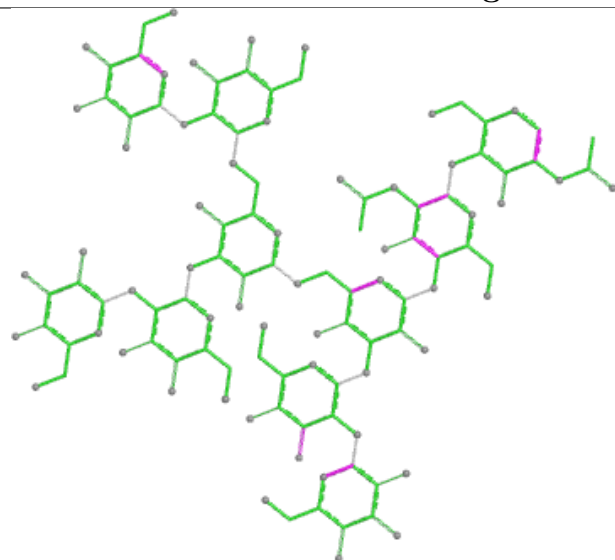




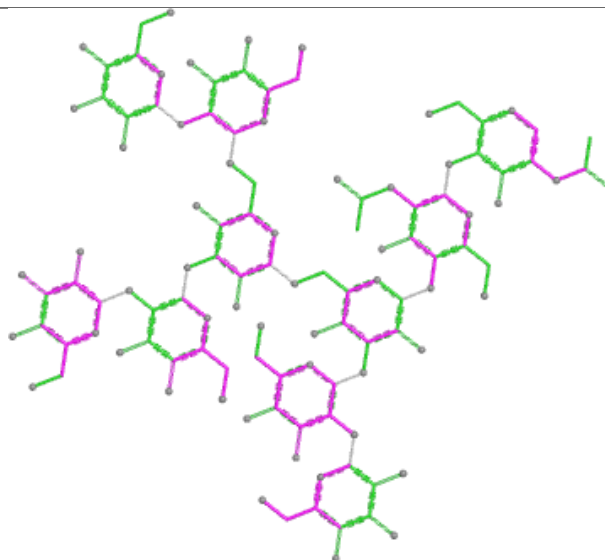




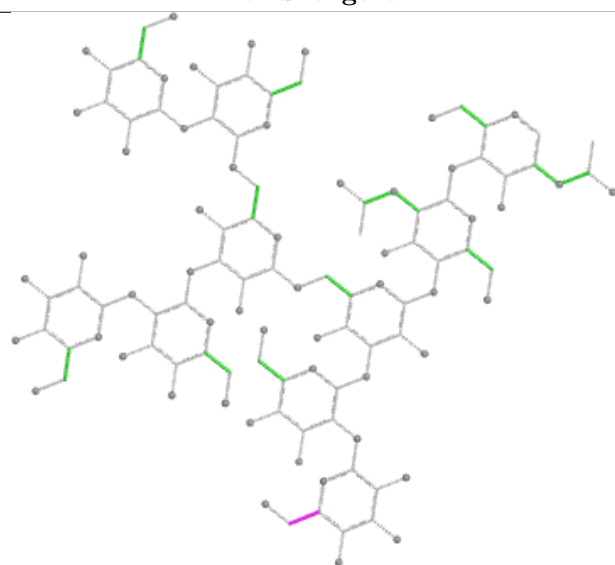
Oligosaccharide Chain M



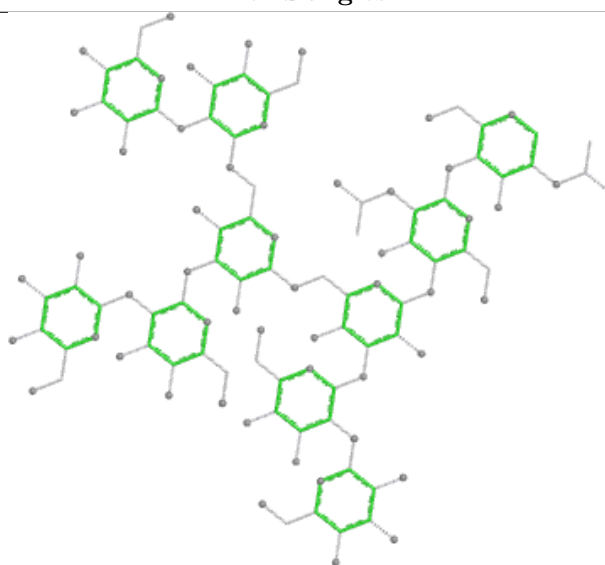
Bond lengths



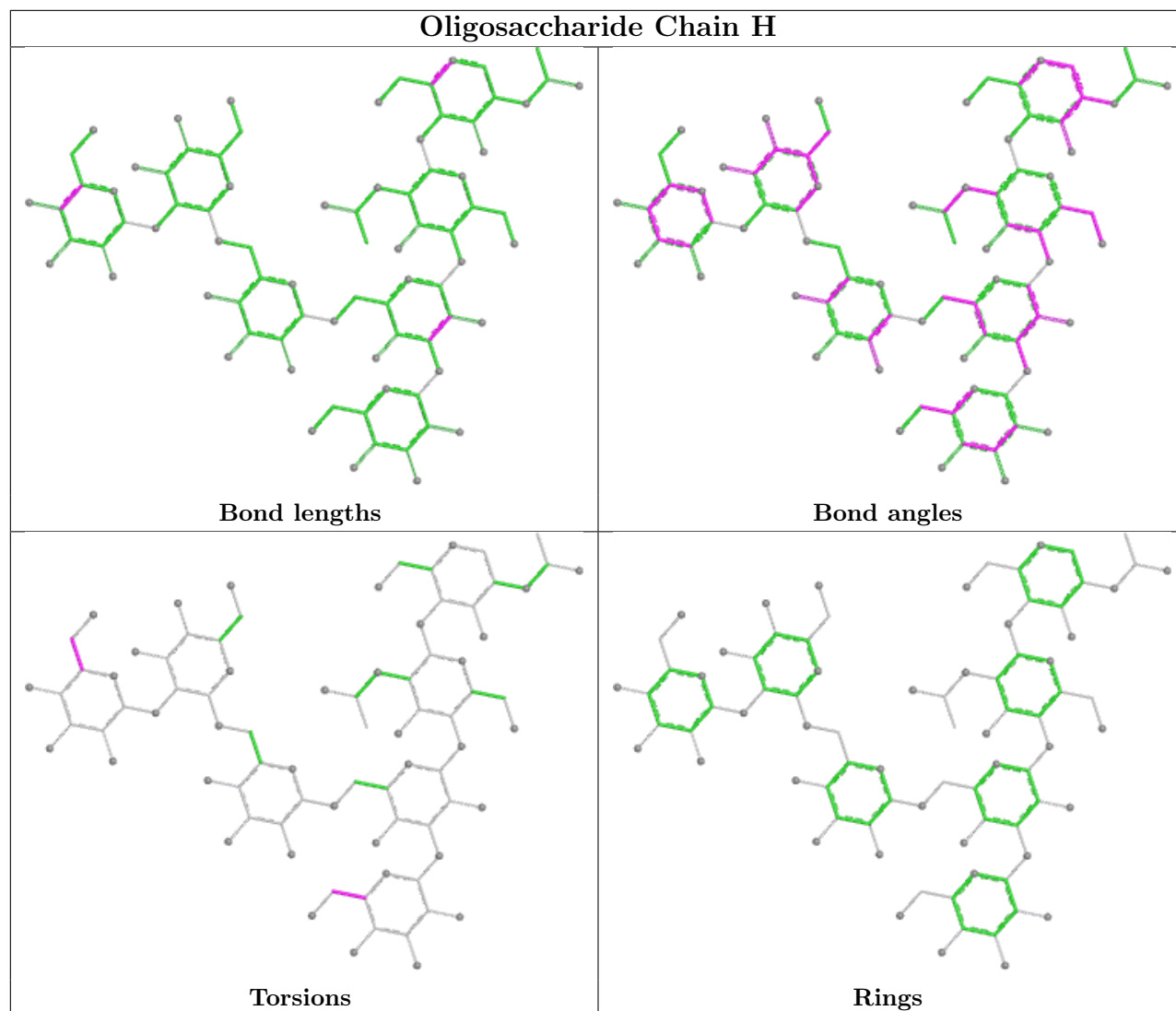
Bond angles

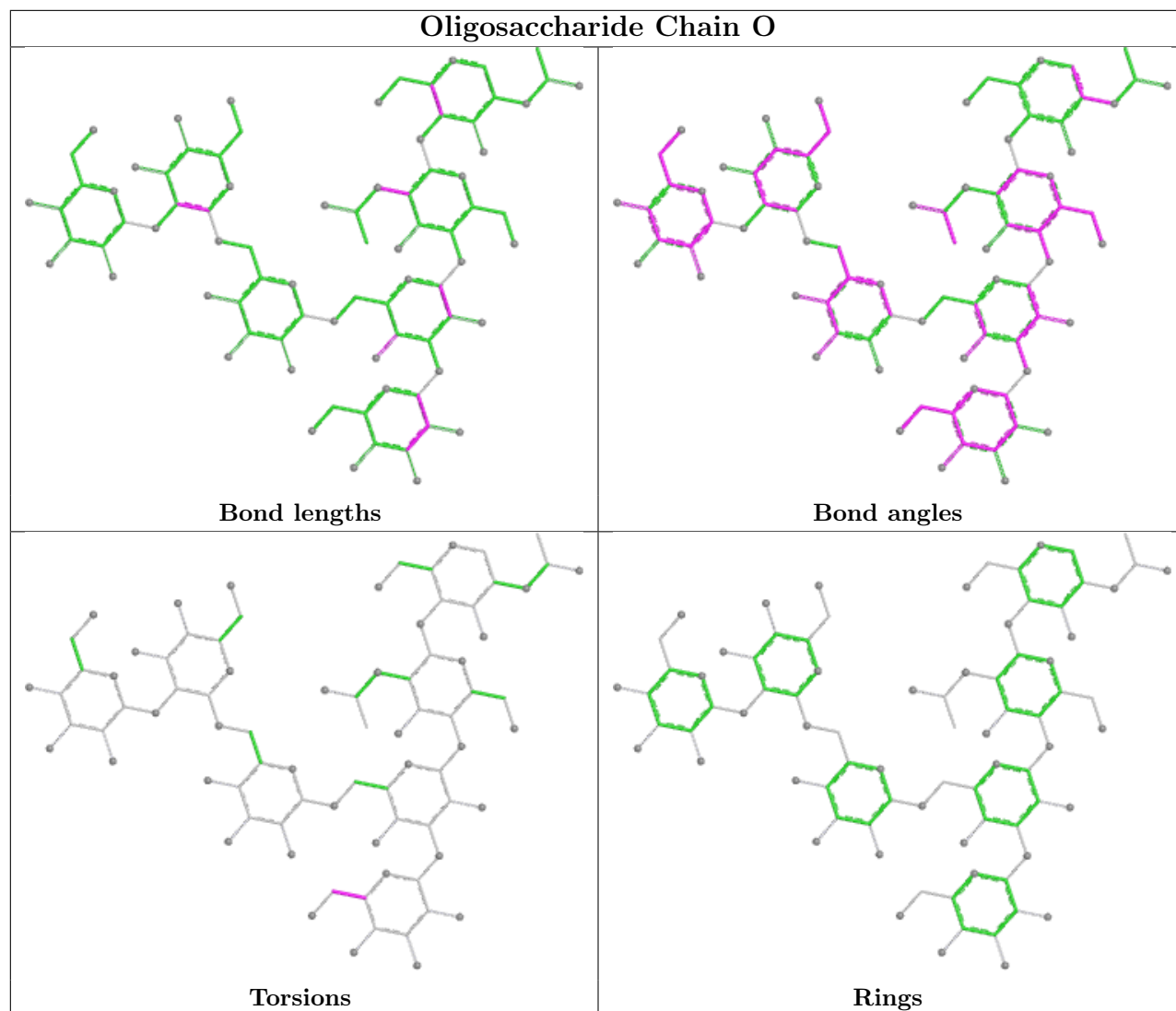


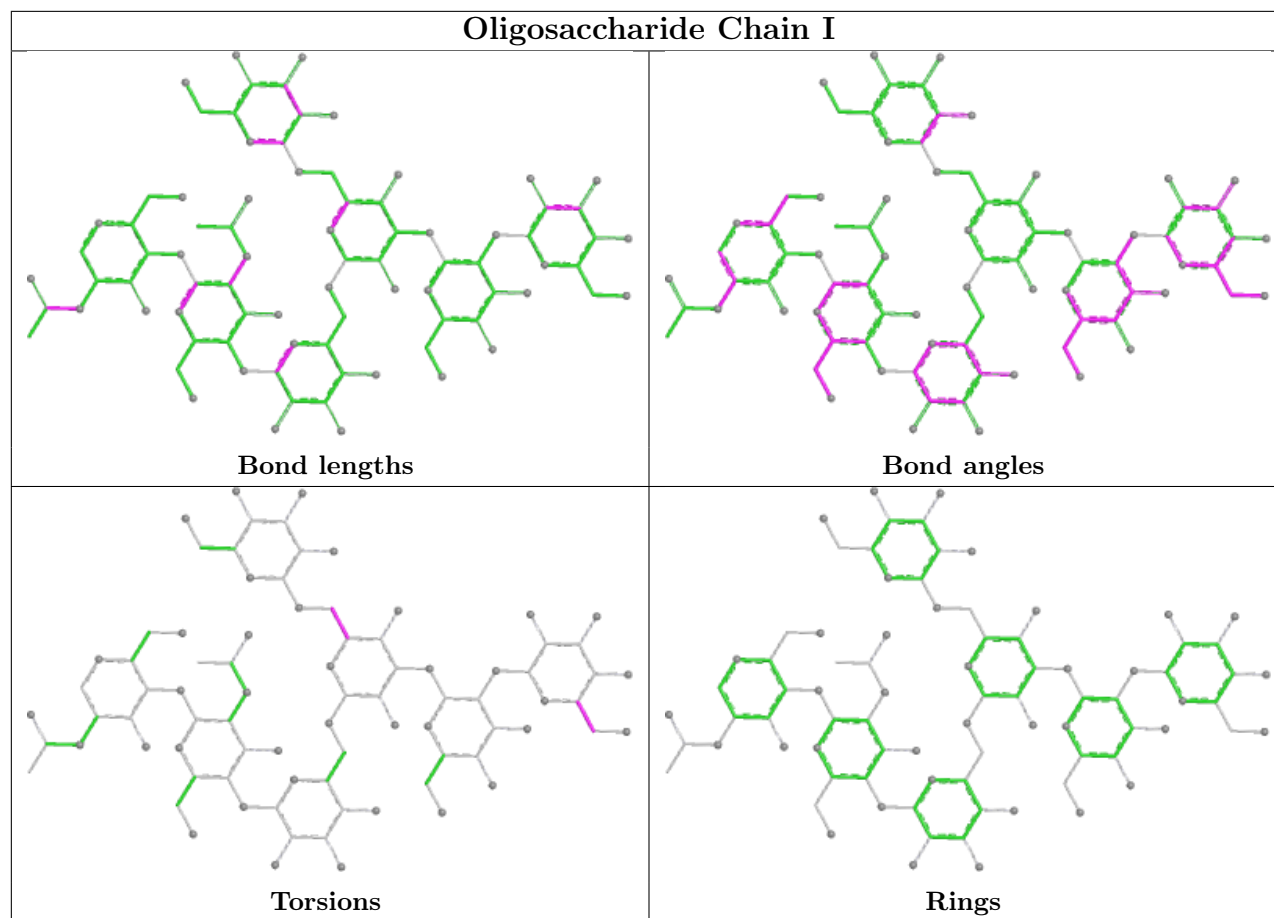
Torsions

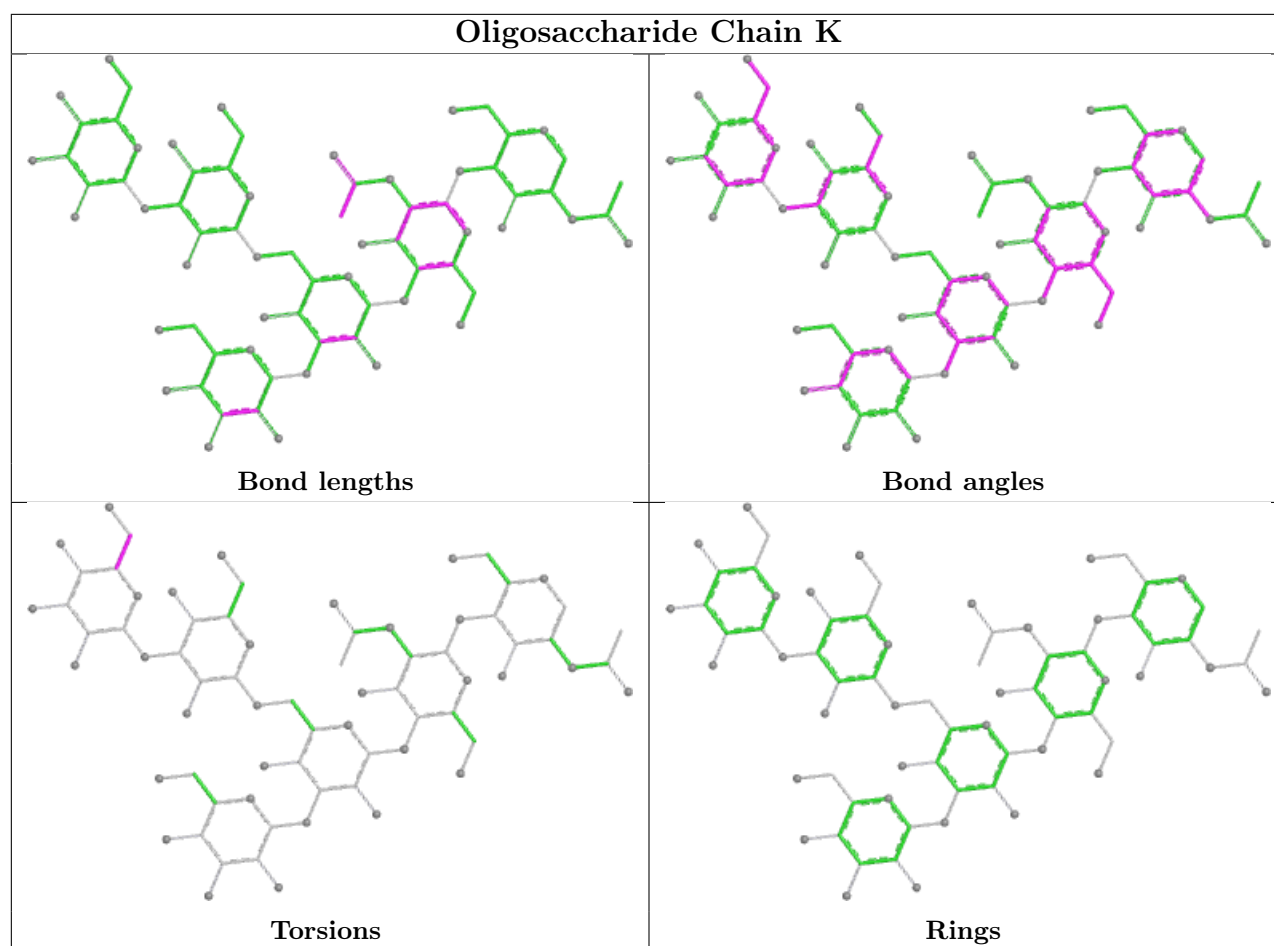


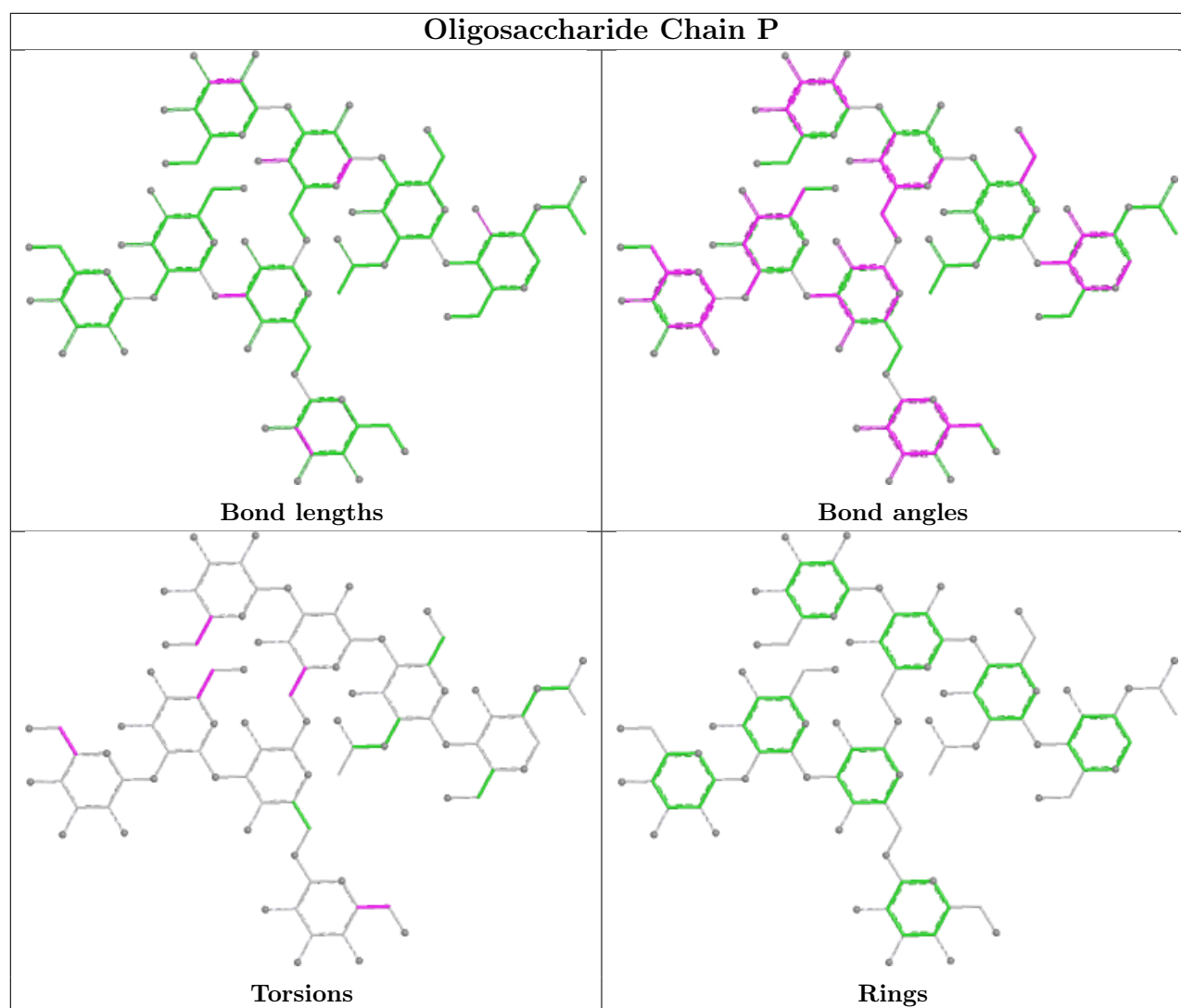
Rings

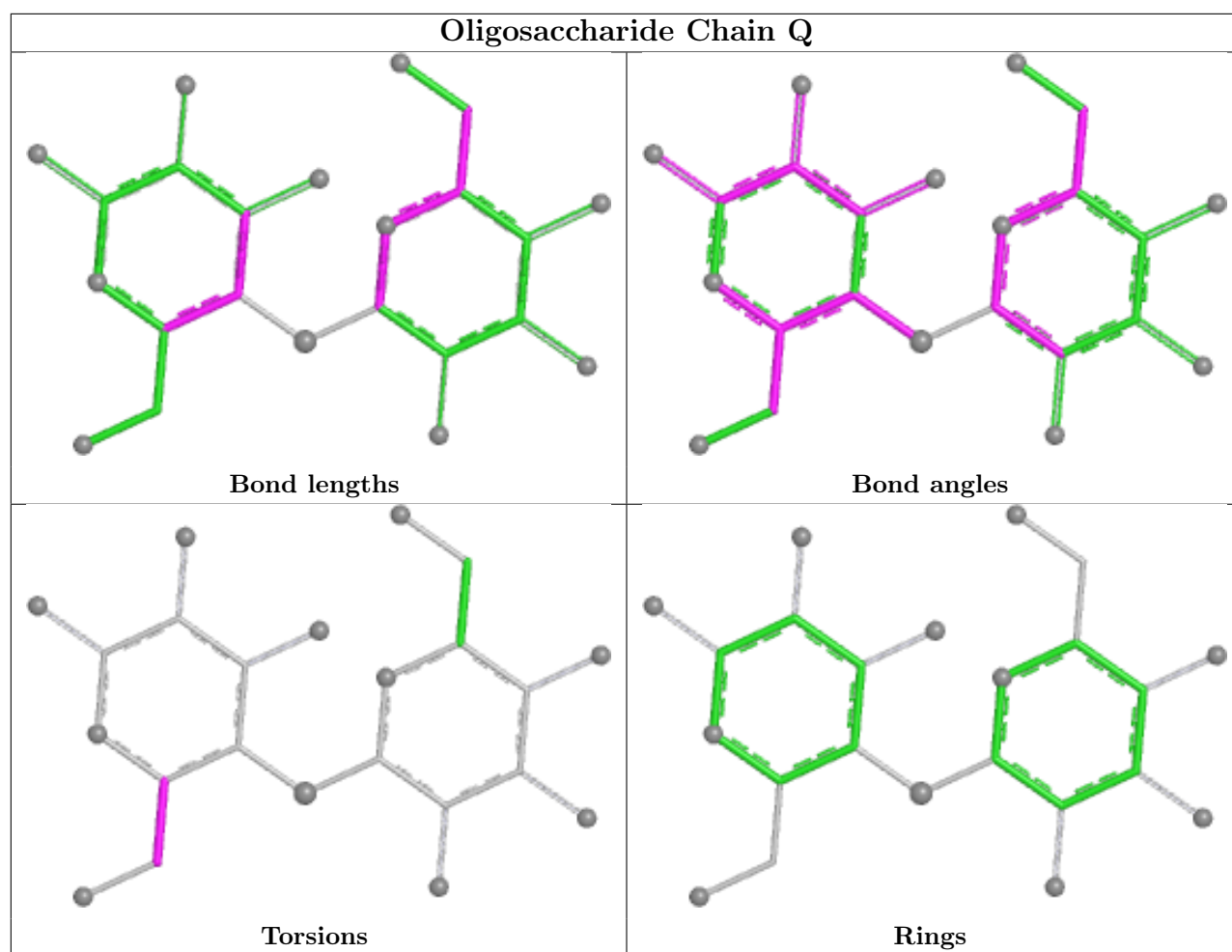


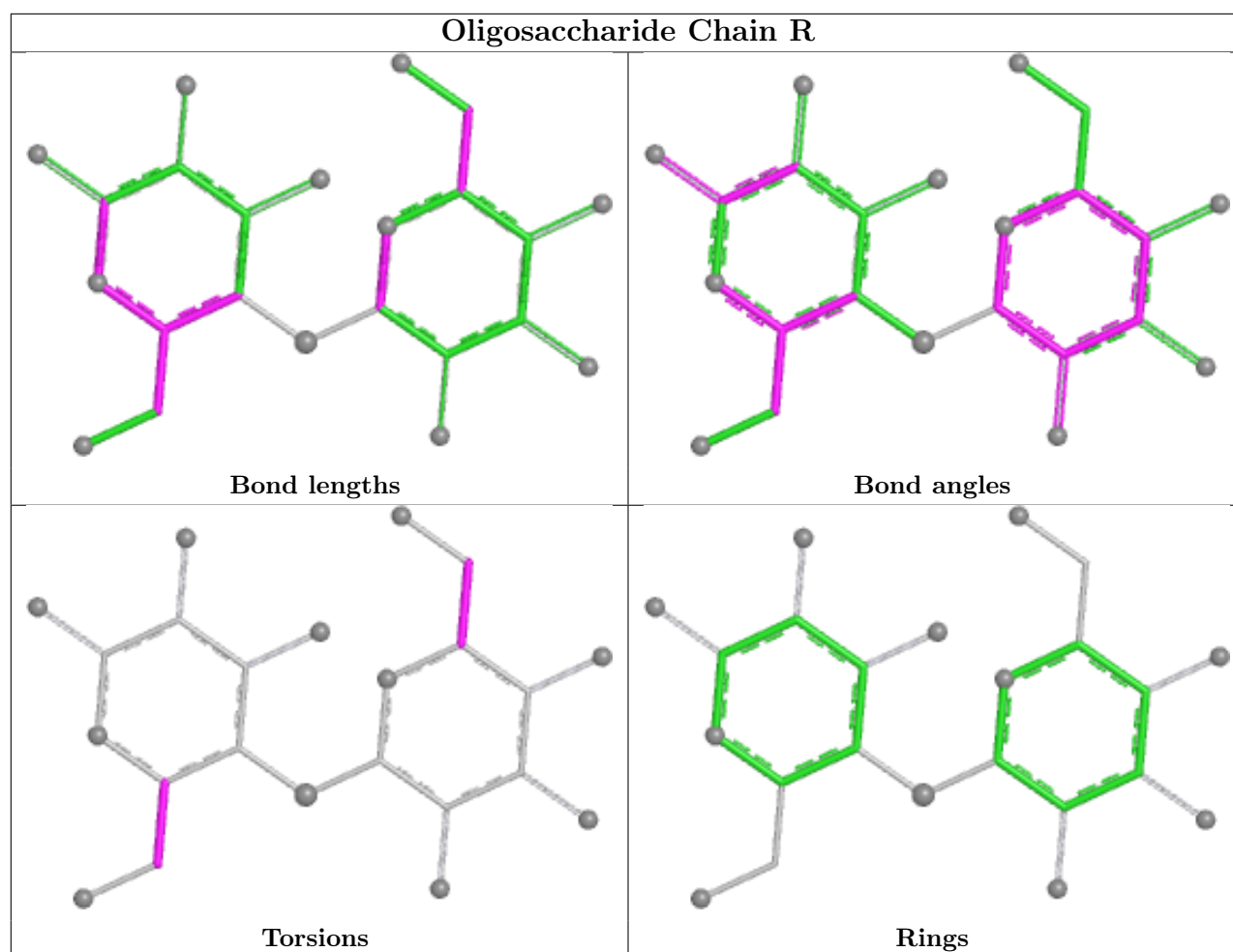












5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
11	NAG	A	908	1	14,14,15	1.14	1 (7%)	17,19,21	1.56	3 (17%)
11	NAG	A	941	1	14,14,15	0.87	0	17,19,21	2.23	8 (47%)
12	MRD	A	942	-	7,7,7	1.50	2 (28%)	9,10,10	1.17	0
11	NAG	B	908	1	14,14,15	1.10	2 (14%)	17,19,21	3.56	9 (52%)
12	MRD	B	948	-	7,7,7	0.77	0	9,10,10	1.34	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MRD	B	949	-	7,7,7	1.13	1 (14%)	9,10,10	0.94	0
11	NAG	B	947	1	14,14,15	0.86	0	17,19,21	1.24	0
12	MRD	A	943	-	7,7,7	0.92	0	9,10,10	1.27	2 (22%)
11	NAG	B	946	1	14,14,15	1.17	2 (14%)	17,19,21	1.95	5 (29%)

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
11	NAG	A	908	1	-	0/6/23/26	0/1/1/1
11	NAG	A	941	1	-	0/6/23/26	0/1/1/1
12	MRD	A	942	-	-	1/5/5/5	-
11	NAG	B	908	1	-	2/6/23/26	0/1/1/1
12	MRD	B	948	-	-	2/5/5/5	-
12	MRD	B	949	-	-	4/5/5/5	-
11	NAG	B	947	1	-	0/6/23/26	0/1/1/1
12	MRD	A	943	-	-	3/5/5/5	-
11	NAG	B	946	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	908	NAG	O5-C1	-2.93	1.38	1.43
11	B	908	NAG	O5-C1	-2.75	1.39	1.43
12	B	949	MRD	O2-C2	-2.59	1.38	1.44
12	A	942	MRD	C1-C2	2.50	1.59	1.52
11	B	946	NAG	O5-C5	-2.49	1.38	1.43
12	A	942	MRD	C3-C2	2.19	1.60	1.54
11	B	908	NAG	O3-C3	-2.15	1.37	1.43
11	B	946	NAG	O5-C1	-2.08	1.40	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	908	NAG	C4-C3-C2	-7.33	100.27	111.02
11	B	908	NAG	O5-C1-C2	-6.70	100.92	111.29
11	B	908	NAG	C2-N2-C7	6.19	131.20	122.90
11	B	908	NAG	C6-C5-C4	-4.01	103.17	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	908	NAG	O5-C1-C2	-3.89	105.28	111.29
11	B	946	NAG	O5-C5-C4	-3.85	101.46	110.83
11	B	908	NAG	C8-C7-N2	-3.82	109.79	116.12
11	B	908	NAG	C1-C2-N2	3.67	116.22	110.43
11	A	941	NAG	O7-C7-C8	-3.67	115.52	122.05
11	B	946	NAG	O3-C3-C4	-3.57	101.96	110.38
11	A	941	NAG	C8-C7-N2	3.43	121.81	116.12
11	A	908	NAG	C1-C2-N2	3.39	115.78	110.43
11	A	941	NAG	C2-N2-C7	-3.32	118.45	122.90
11	A	941	NAG	O6-C6-C5	-3.28	100.16	111.33
11	B	908	NAG	C1-O5-C5	3.24	116.52	112.19
11	B	946	NAG	O5-C1-C2	-2.91	106.78	111.29
11	A	941	NAG	O5-C5-C4	-2.88	103.83	110.83
11	A	941	NAG	C3-C4-C5	-2.78	105.20	110.23
11	B	908	NAG	O4-C4-C5	-2.77	102.51	109.32
12	B	948	MRD	O4-C4-C3	-2.60	101.00	111.35
11	A	941	NAG	C4-C3-C2	-2.58	107.23	111.02
11	A	941	NAG	O5-C1-C2	2.40	115.01	111.29
11	A	908	NAG	O4-C4-C5	-2.35	103.53	109.32
11	B	946	NAG	O4-C4-C3	-2.33	104.88	110.38
11	B	908	NAG	O5-C5-C6	2.25	112.04	107.66
12	A	943	MRD	O2-C2-C3	-2.16	101.18	109.27
12	A	943	MRD	O4-C4-C3	-2.15	102.80	111.35
11	B	946	NAG	C1-C2-N2	2.04	113.65	110.43
12	B	948	MRD	O2-C2-C1	2.03	114.30	107.99

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	948	MRD	C2-C3-C4-O4
12	B	948	MRD	C2-C3-C4-C5
12	B	949	MRD	C2-C3-C4-O4
12	B	949	MRD	C2-C3-C4-C5
11	B	946	NAG	O5-C5-C6-O6
11	B	946	NAG	C4-C5-C6-O6
12	A	943	MRD	C1-C2-C3-C4
12	A	942	MRD	C2-C3-C4-C5
12	A	943	MRD	C2-C3-C4-C5
11	B	908	NAG	C1-C2-N2-C7
11	B	908	NAG	C3-C2-N2-C7
12	B	949	MRD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
12	A	943	MRD	CM-C2-C3-C4
12	B	949	MRD	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	942	MRD	3	0
12	B	948	MRD	2	0
12	B	949	MRD	2	0
12	A	943	MRD	6	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	833/841 (99%)	-0.90	4 (0%) 87 87	5, 12, 24, 50	0
1	B	832/841 (98%)	-1.03	3 (0%) 88 88	4, 9, 20, 52	0
All	All	1665/1682 (98%)	-0.96	7 (0%) 88 88	4, 10, 23, 52	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	610	TYR	3.6
1	B	610	TYR	3.5
1	B	609	ASP	3.1
1	A	609	ASP	3.1
1	A	699	GLY	2.9
1	B	698	GLU	2.0
1	A	860	GLN	2.0

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
6	MAN	O	7	11/12	0.65	0.16	56,65,71,77	0
6	MAN	H	7	11/12	0.71	0.15	52,58,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	C	3	11/12	0.71	0.17	35,60,65,67	0
9	MAN	P	8	11/12	0.72	0.15	51,60,65,66	0
9	MAN	P	7	11/12	0.73	0.17	48,54,66,71	0
3	BMA	G	3	11/12	0.73	0.17	45,66,75,79	0
2	MAN	C	4	11/12	0.74	0.15	52,58,63,65	0
2	MAN	C	5	11/12	0.75	0.16	55,60,62,63	0
2	MAN	C	7	11/12	0.76	0.15	45,53,59,60	0
7	MAN	I	7	11/12	0.76	0.16	49,53,62,70	0
3	BMA	L	3	11/12	0.77	0.16	45,59,70,74	0
9	MAN	P	6	11/12	0.78	0.16	44,50,62,64	0
3	BMA	N	3	11/12	0.78	0.16	42,51,62,68	0
3	NAG	G	2	14/15	0.78	0.16	40,48,59,62	0
10	SGC	R	1	12/12	0.79	0.17	40,53,60,60	0
3	BMA	D	3	11/12	0.81	0.12	25,34,40,46	0
8	MAN	K	6	11/12	0.82	0.13	37,42,50,51	0
7	MAN	I	6	11/12	0.84	0.12	36,39,46,47	0
2	MAN	C	6	11/12	0.85	0.14	32,38,48,51	0
8	MAN	K	5	11/12	0.86	0.12	37,39,46,54	0
10	SGC	Q	1	12/12	0.86	0.15	43,54,56,57	0
9	BMA	P	3	11/12	0.86	0.12	25,31,38,45	0
7	BMA	I	3	11/12	0.88	0.11	21,29,41,45	0
8	MAN	K	4	11/12	0.88	0.09	33,35,41,41	0
3	NAG	N	2	14/15	0.89	0.11	25,32,36,44	0
6	MAN	O	4	11/12	0.89	0.09	27,28,38,40	0
6	MAN	O	6	11/12	0.89	0.12	23,31,39,40	0
6	MAN	H	4	11/12	0.89	0.10	27,31,39,43	0
6	MAN	O	5	11/12	0.91	0.10	22,27,31,34	0
9	MAN	P	4	11/12	0.92	0.09	22,24,33,45	0
5	MAN	M	10	11/12	0.92	0.09	22,32,38,39	0
8	BMA	K	3	11/12	0.92	0.08	22,25,29,33	0
10	BGC	R	2	11/12	0.92	0.11	16,31,41,45	0
7	MAN	I	4	11/12	0.93	0.08	17,23,28,38	0
6	MAN	H	5	11/12	0.93	0.09	20,26,34,48	0
6	MAN	H	6	11/12	0.93	0.12	23,29,41,44	0
4	NAG	E	2	14/15	0.93	0.08	15,23,32,33	0
5	MAN	F	10	11/12	0.93	0.10	25,32,46,53	0
3	NAG	G	1	14/15	0.94	0.08	19,25,34,42	0
9	NAG	P	2	14/15	0.94	0.07	17,22,28,29	0
2	MAN	J	5	11/12	0.94	0.08	16,23,32,37	0
2	MAN	J	7	11/12	0.94	0.07	20,27,30,31	0
9	MAN	P	5	11/12	0.94	0.07	23,23,30,38	0
7	MAN	I	5	11/12	0.94	0.06	19,24,30,32	0

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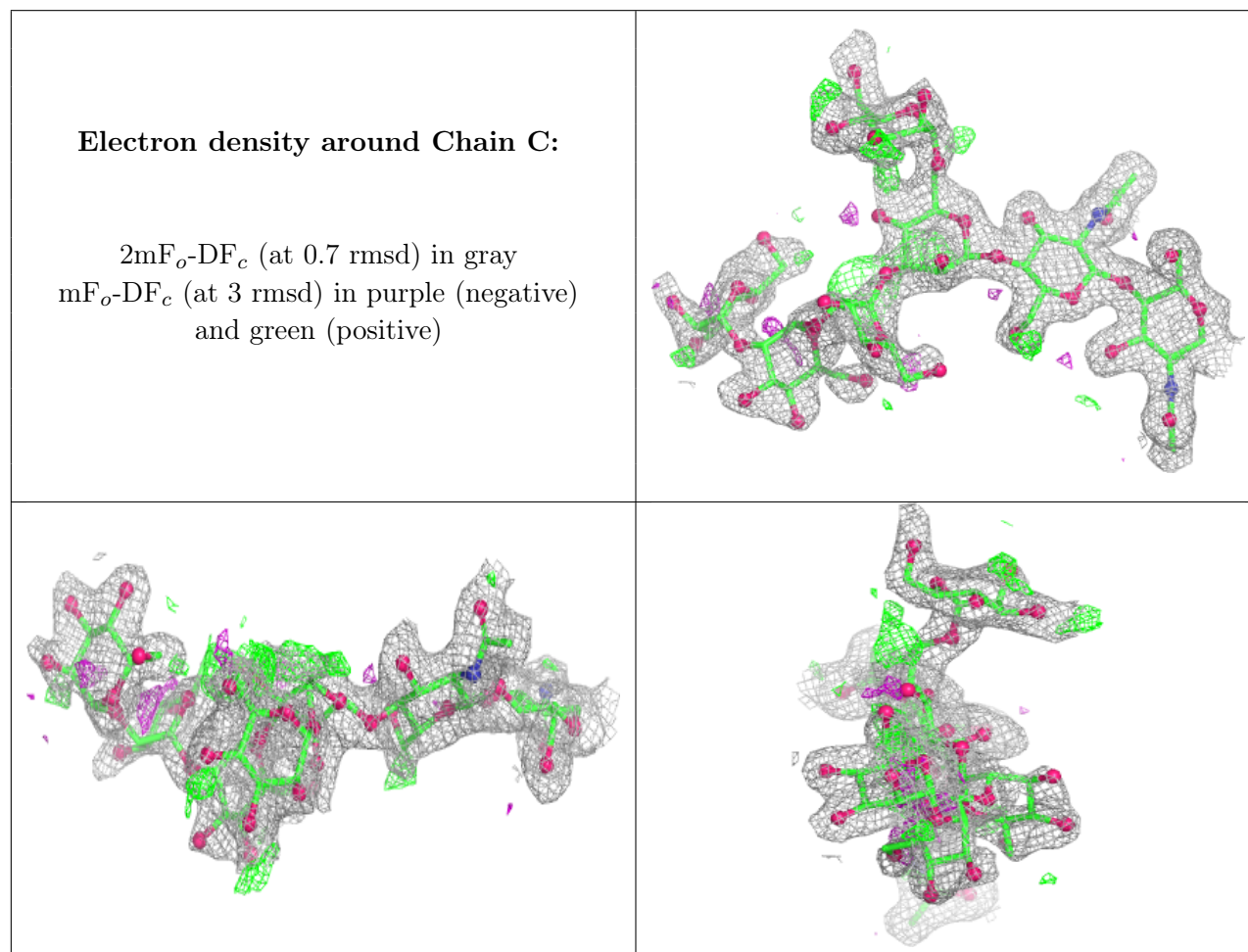
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	F	6	11/12	0.94	0.07	22,24,28,31	0
6	BMA	O	3	11/12	0.94	0.07	23,26,31,41	0
3	NAG	L	2	14/15	0.94	0.07	13,17,28,32	0
10	BGC	Q	2	11/12	0.94	0.10	23,36,44,46	0
2	MAN	J	4	11/12	0.94	0.07	18,25,31,32	0
6	BMA	H	3	11/12	0.94	0.07	20,24,31,40	0
2	MAN	J	6	11/12	0.95	0.07	15,17,21,28	0
5	MAN	F	9	11/12	0.95	0.06	16,18,23,24	0
2	NAG	C	2	14/15	0.95	0.07	15,22,31,33	0
3	NAG	D	2	14/15	0.95	0.07	16,21,23,29	0
6	NAG	H	2	14/15	0.95	0.06	15,19,23,26	0
5	MAN	F	5	11/12	0.96	0.06	17,19,24,31	0
5	MAN	M	5	11/12	0.96	0.05	12,14,18,24	0
8	NAG	K	1	14/15	0.96	0.06	10,12,13,14	0
5	MAN	M	6	11/12	0.96	0.06	19,21,25,26	0
3	NAG	N	1	14/15	0.96	0.06	16,20,30,32	0
7	NAG	I	2	14/15	0.96	0.06	14,18,24,29	0
6	NAG	H	1	14/15	0.96	0.07	12,16,35,39	0
6	NAG	O	2	14/15	0.96	0.06	14,17,23,24	0
2	BMA	J	3	11/12	0.96	0.06	12,17,19,20	0
9	NAG	P	1	14/15	0.97	0.04	12,14,15,16	0
8	NAG	K	2	14/15	0.97	0.06	12,16,24,25	0
3	NAG	D	1	14/15	0.97	0.05	13,14,16,16	0
2	NAG	C	1	14/15	0.97	0.05	13,14,15,15	0
6	NAG	O	1	14/15	0.97	0.06	12,15,29,30	0
5	NAG	F	1	14/15	0.97	0.05	15,17,20,21	0
5	MAN	F	8	11/12	0.98	0.04	13,14,15,19	0
7	NAG	I	1	14/15	0.98	0.05	13,15,17,18	0
5	NAG	F	2	14/15	0.98	0.04	12,13,14,14	0
5	BMA	F	3	11/12	0.98	0.04	14,15,17,18	0
5	NAG	M	1	14/15	0.98	0.05	9,11,14,15	0
5	NAG	M	2	14/15	0.98	0.05	8,9,10,11	0
5	MAN	M	4	11/12	0.98	0.04	9,9,10,12	0
5	MAN	F	4	11/12	0.98	0.04	13,14,16,18	0
2	NAG	J	2	14/15	0.98	0.04	9,12,15,21	0
5	MAN	M	7	11/12	0.98	0.04	9,10,11,11	0
5	MAN	M	9	11/12	0.98	0.04	12,14,18,19	0
4	NAG	E	1	14/15	0.98	0.04	12,13,17,18	0
5	MAN	F	7	11/12	0.98	0.04	12,13,15,15	0
5	BMA	M	3	11/12	0.99	0.03	10,11,12,13	0
3	NAG	L	1	14/15	0.99	0.03	8,10,11,12	0
5	MAN	M	8	11/12	0.99	0.04	11,11,14,17	0

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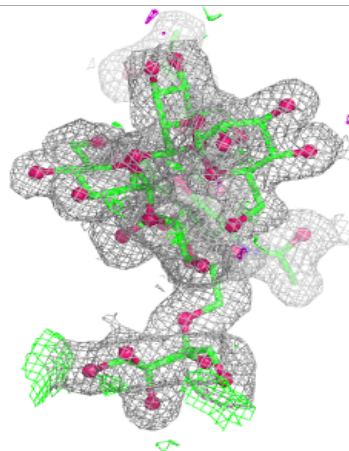
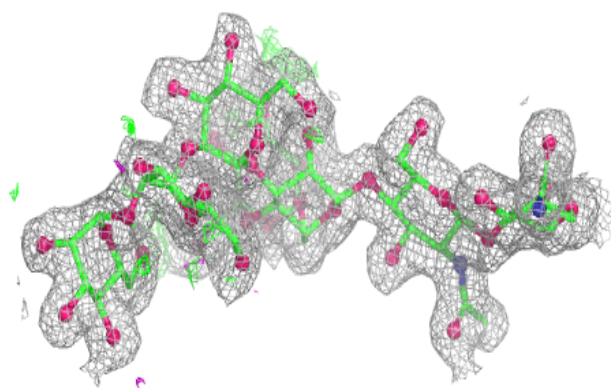
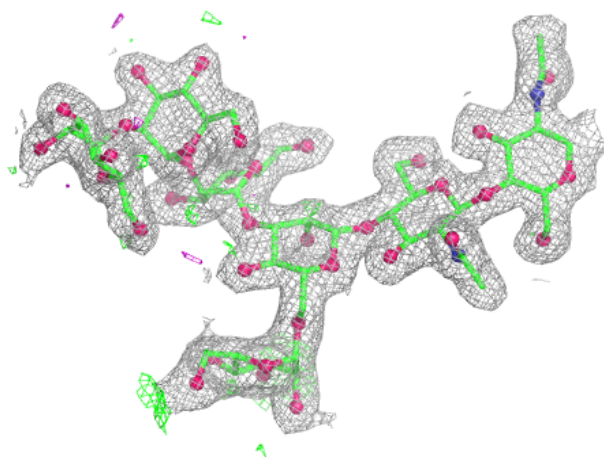
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	J	1	14/15	0.99	0.03	8,9,10,10	0

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.



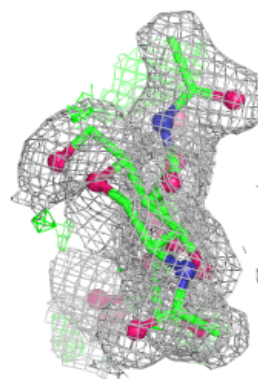
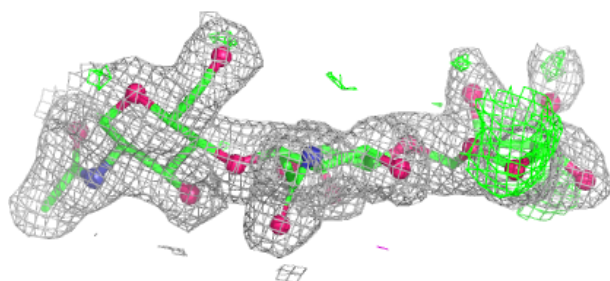
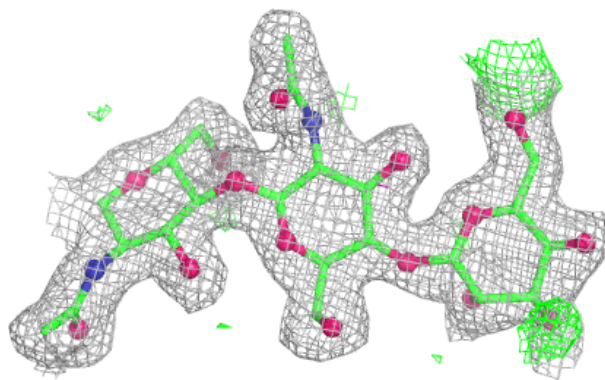
Electron density around Chain J:

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

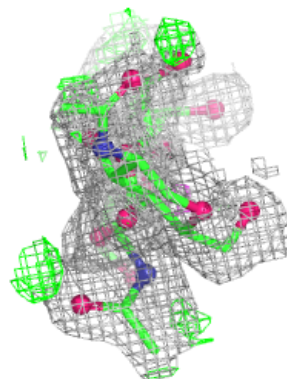
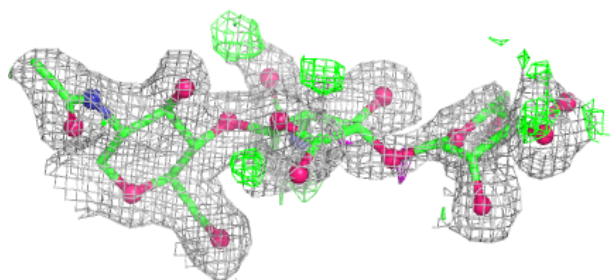
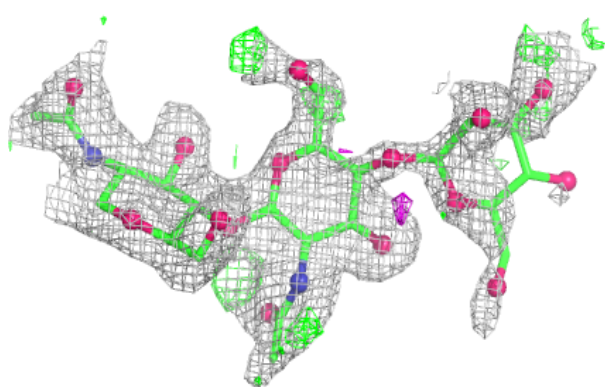


Electron density around Chain D:

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

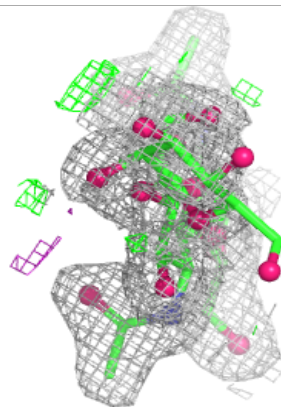
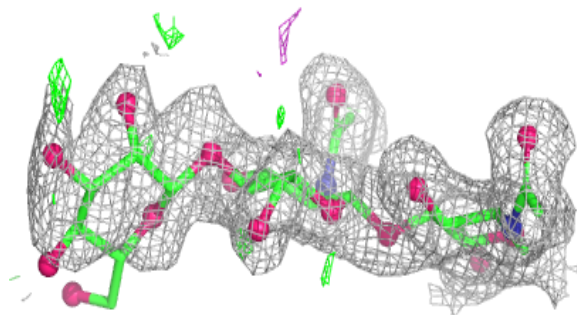
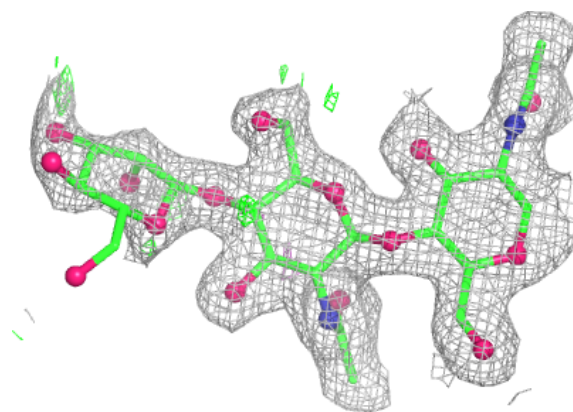
**Electron density around Chain G:**

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



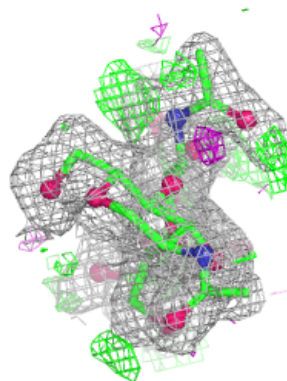
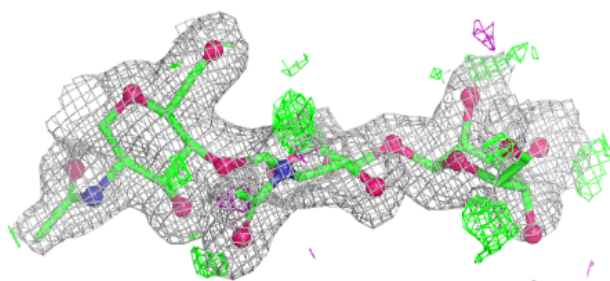
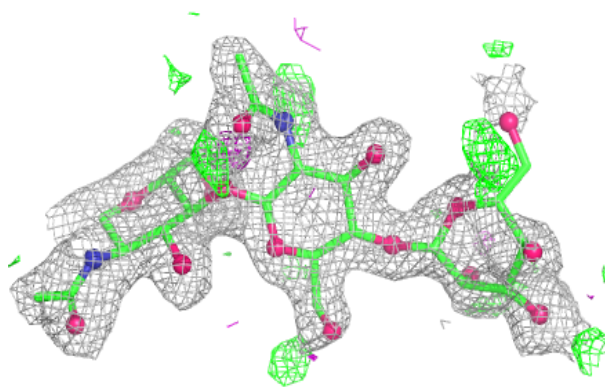
Electron density around Chain L:

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



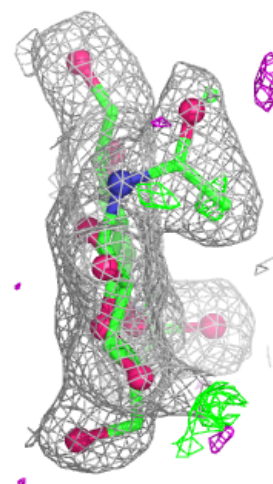
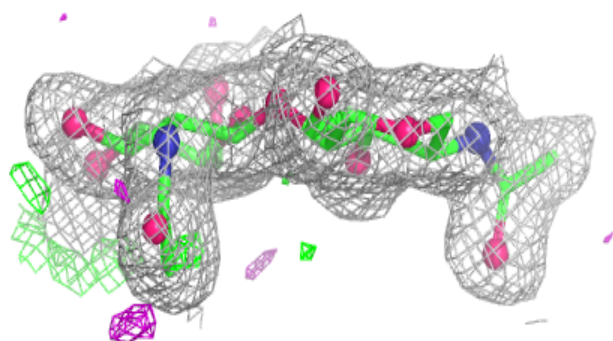
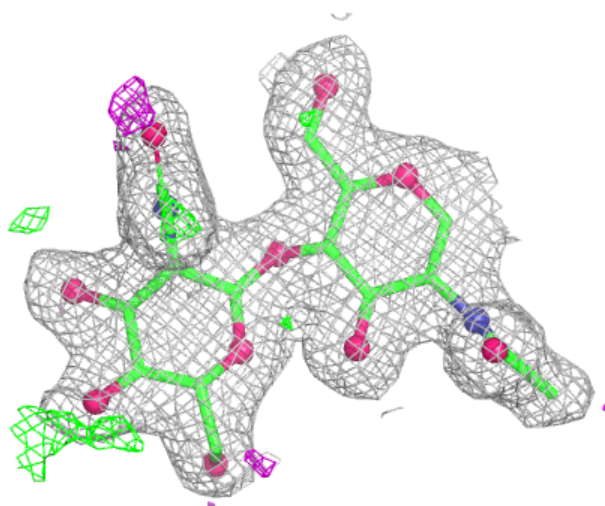
Electron density around Chain N:

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and green (positive)



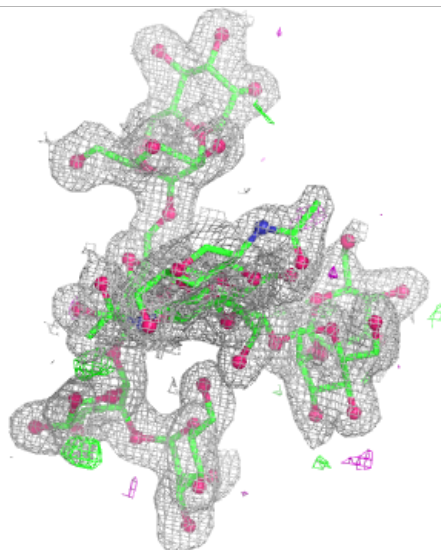
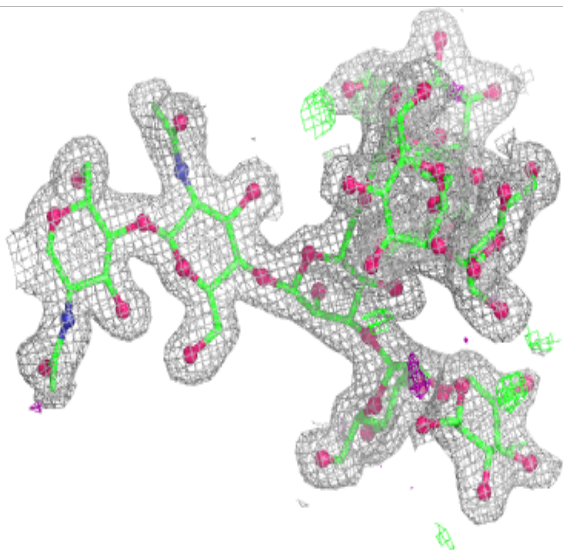
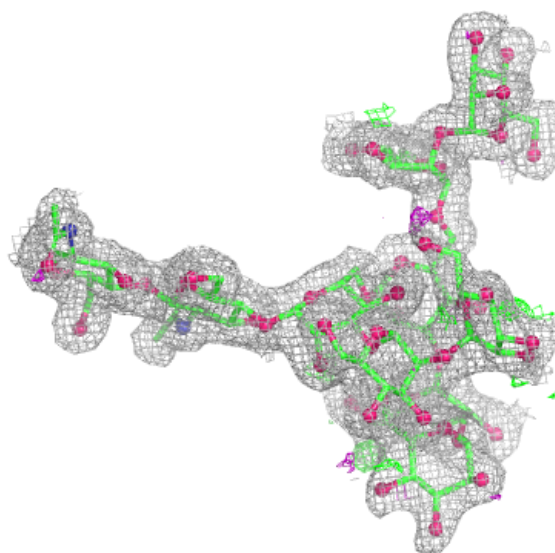
Electron density around Chain E:

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



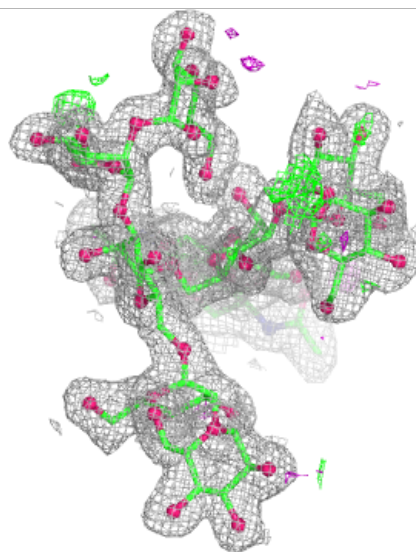
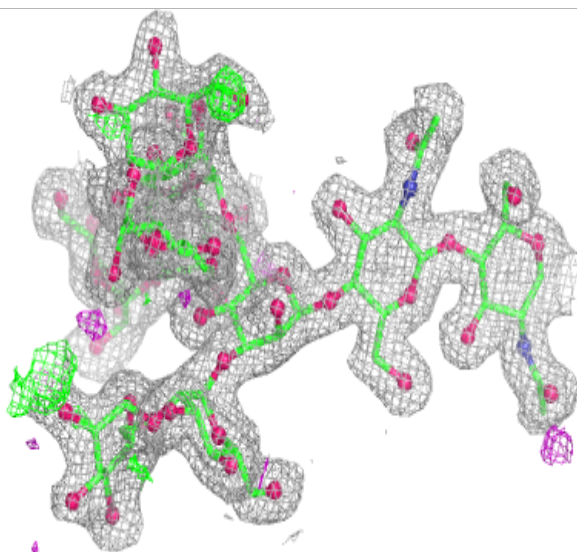
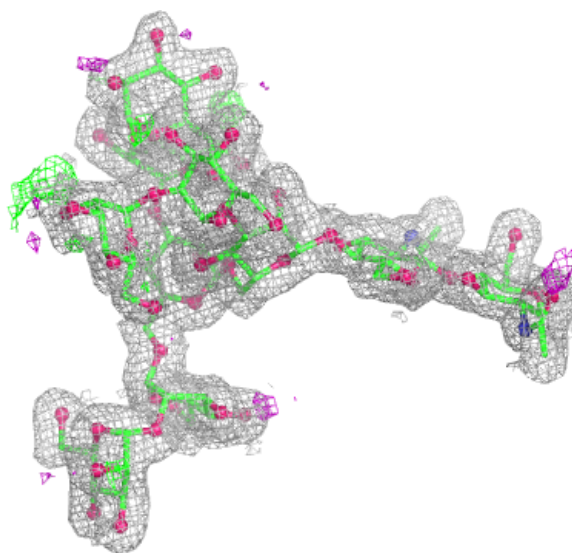
Electron density around Chain F:

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



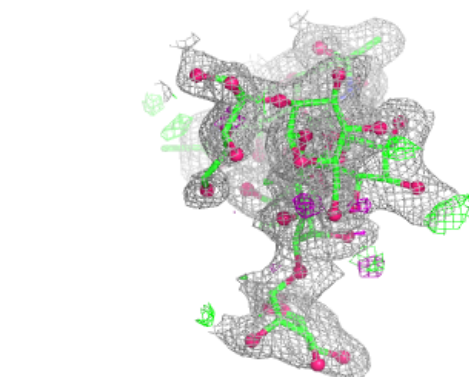
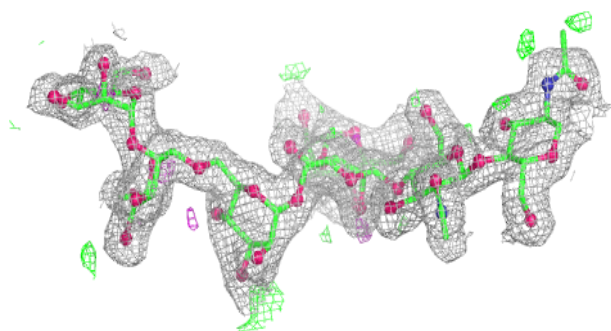
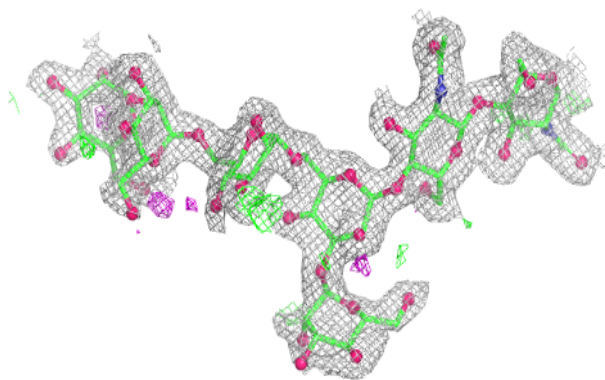
Electron density around Chain M:

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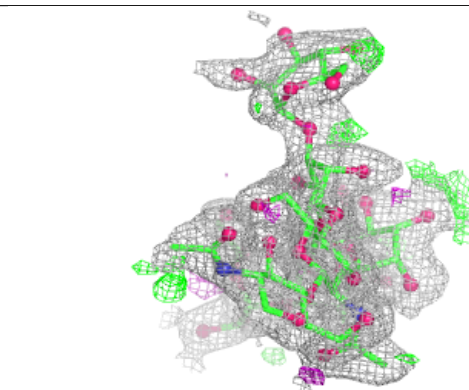
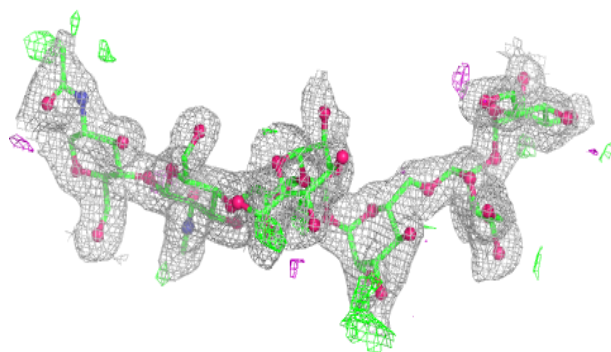
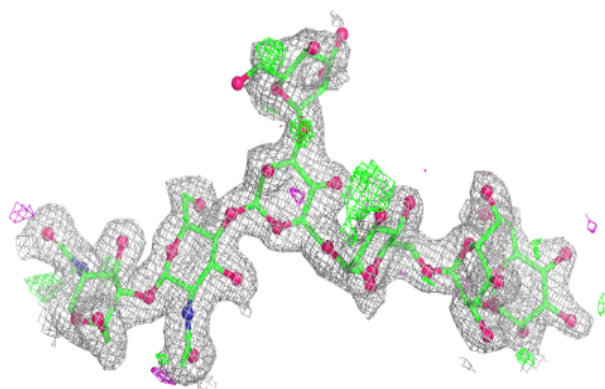


Electron density around Chain H:

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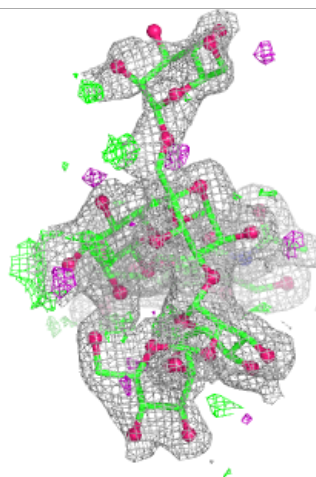
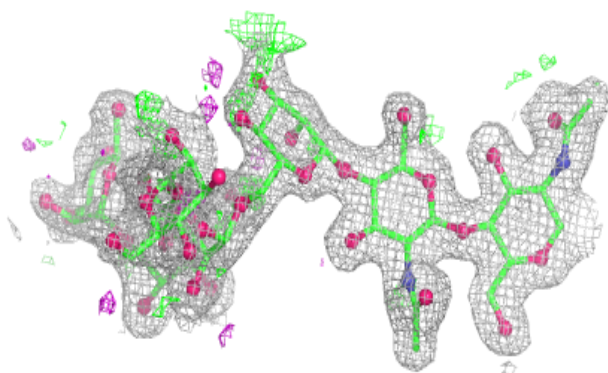
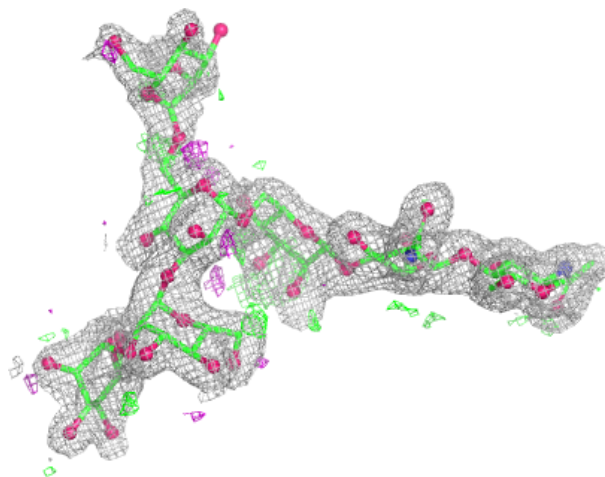
**Electron density around Chain O:**

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



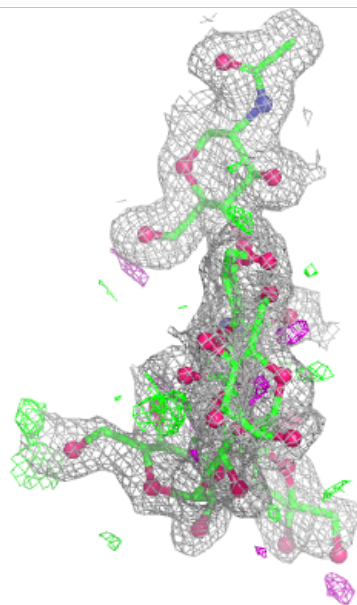
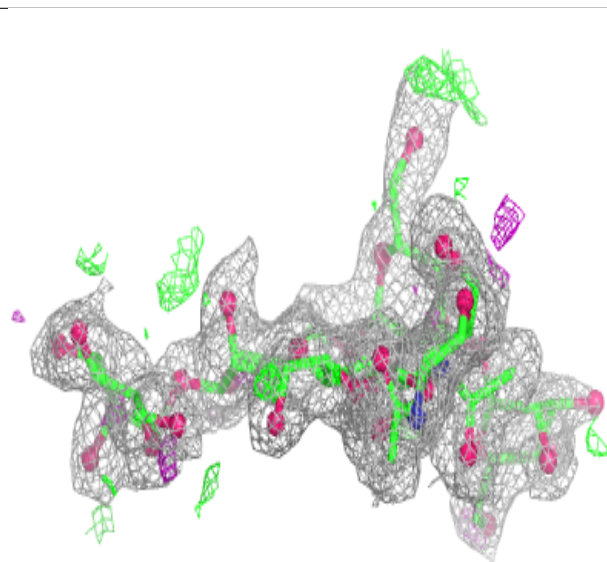
Electron density around Chain I:

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



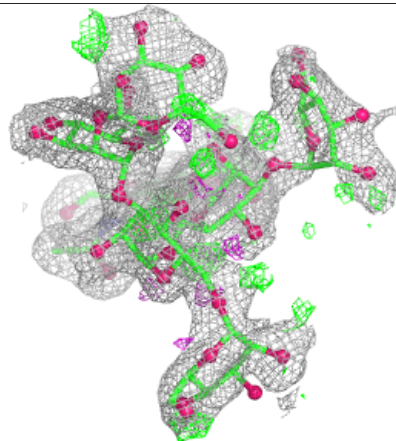
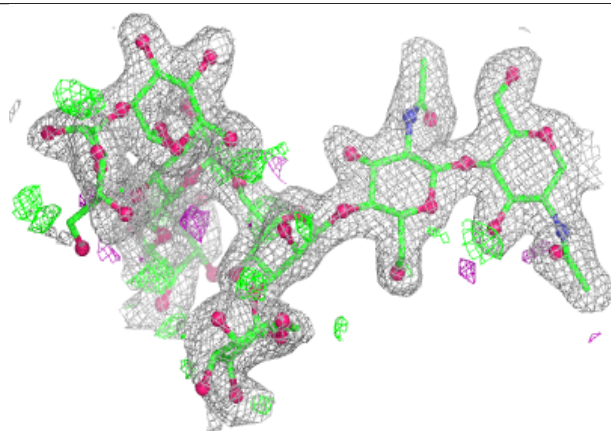
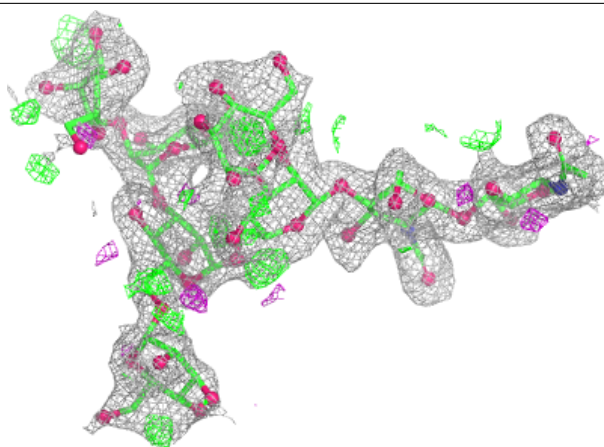
Electron density around Chain K:

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



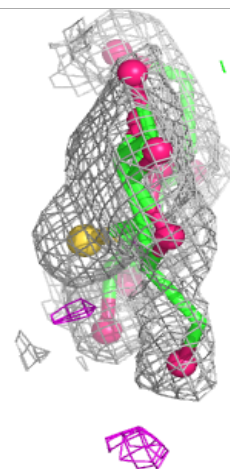
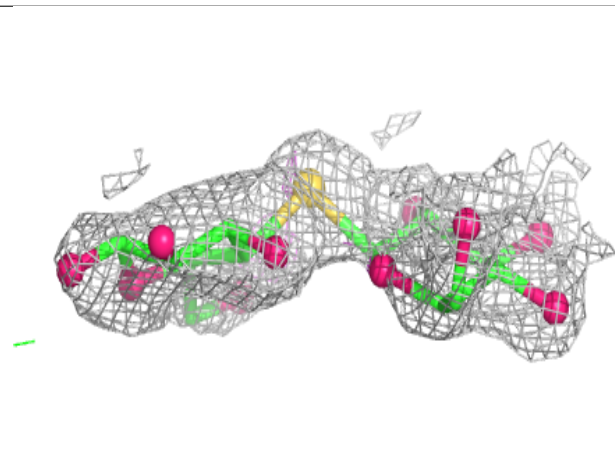
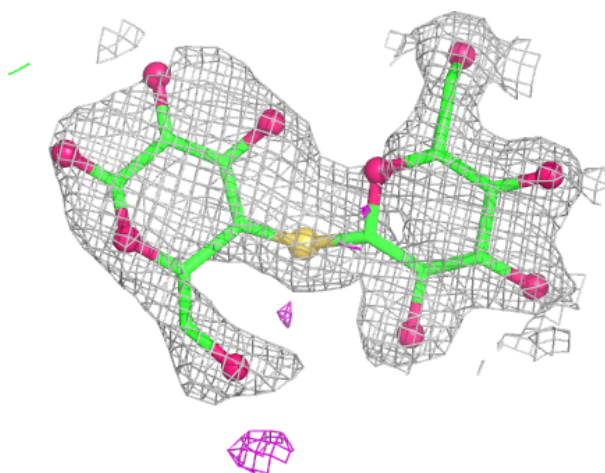
Electron density around Chain P:

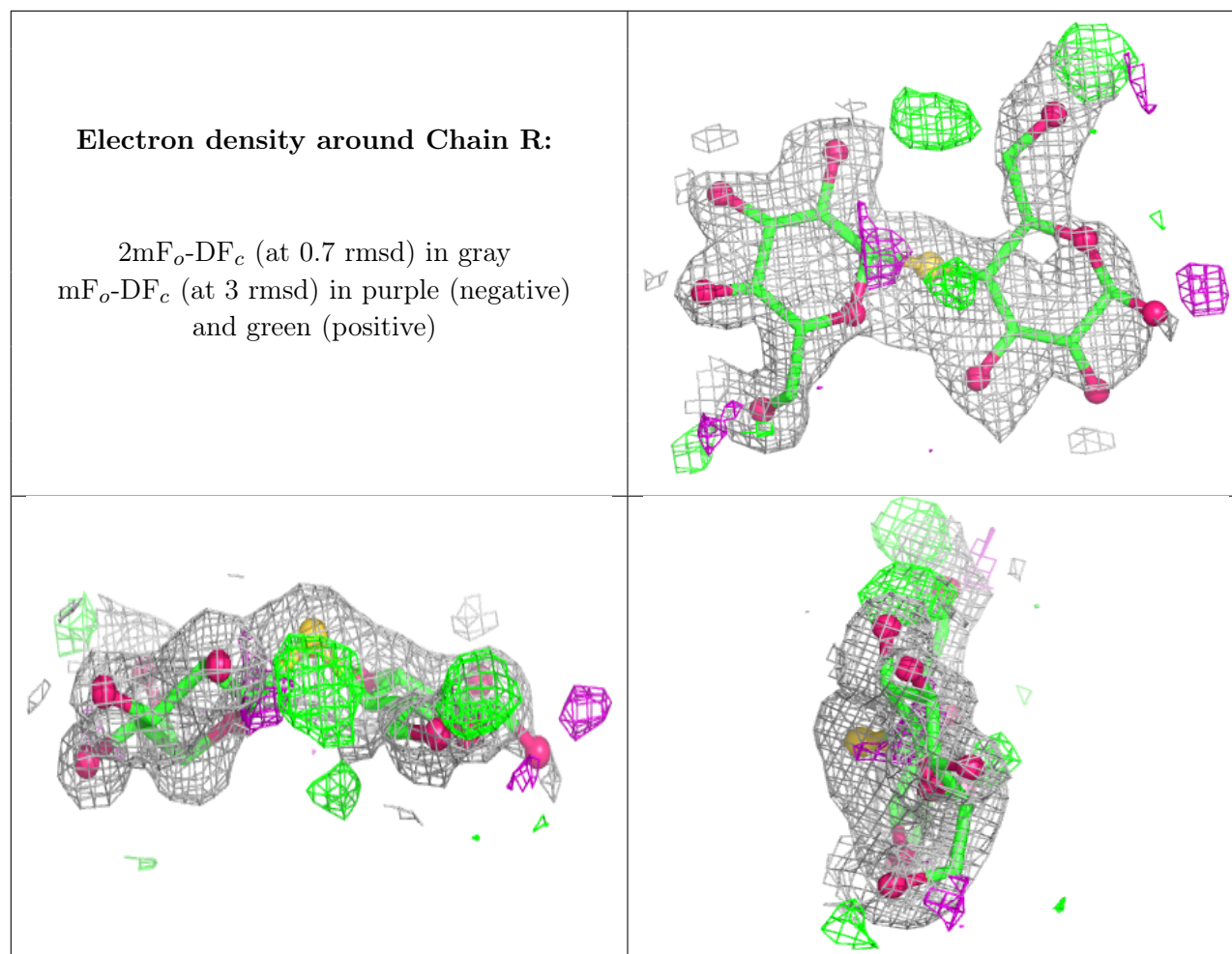
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	MRD	A	943	8/8	0.80	0.17	15,26,33,39	0
11	NAG	A	908	14/15	0.81	0.14	39,53,62,67	0
11	NAG	B	908	14/15	0.85	0.12	34,39,46,46	0
11	NAG	B	946	14/15	0.87	0.12	34,50,55,57	0
12	MRD	B	949	8/8	0.87	0.15	35,39,42,43	0
11	NAG	A	941	14/15	0.92	0.08	24,32,36,36	0
12	MRD	B	948	8/8	0.93	0.10	15,19,33,35	0
12	MRD	A	942	8/8	0.94	0.08	16,17,20,27	0
11	NAG	B	947	14/15	0.95	0.06	22,24,28,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.