



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:11 PM UTC

PDB ID : 4IIE / pdb_00004iie
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with calystegine B(2)
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

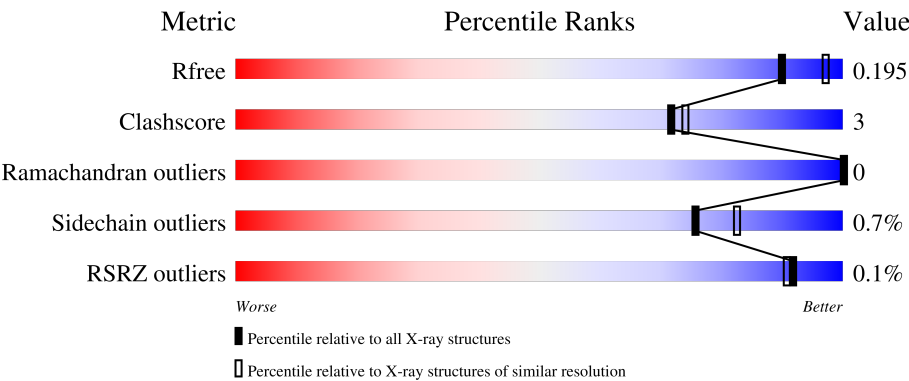
1 Overall quality at a glance i

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.



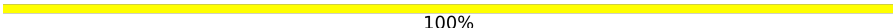
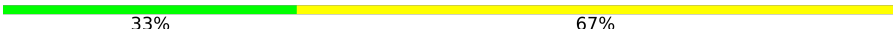
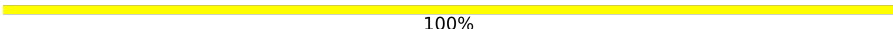
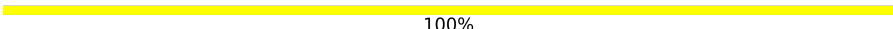
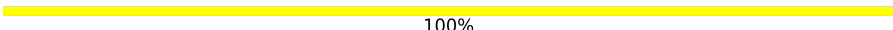
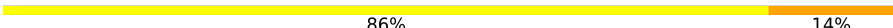
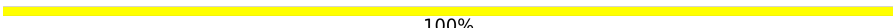
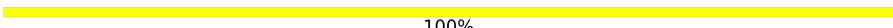
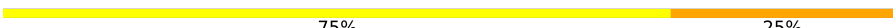
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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%11%
1	B	841	87%11%
2	C	4	75%25%
3	D	3	33%67%
3	G	3	100%

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Mol	Chain	Length	Quality of chain
3	L	3	 100%
3	N	3	 33% 67%
4	E	2	 100%
5	F	10	 100%
5	M	10	 100%
6	H	7	 86% 14%
6	O	7	 71% 29%
7	I	7	 100%
8	J	7	 100%
9	K	6	 83% 17%
10	P	8	 75% 25%

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	940	-	-	X	-
14	CGB	A	943	-	-	X	-
14	CGB	B	952	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 15193 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.

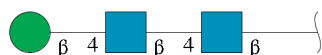
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	834	Total	C	N	O	S	0	0	0
			6387	4031	1097	1241	18			
1	B	832	Total	C	N	O	S	0	0	0
			6375	4023	1095	1239	18			

- 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.



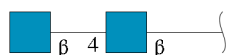
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

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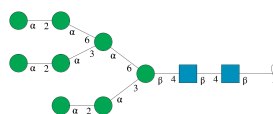
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



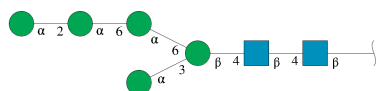
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



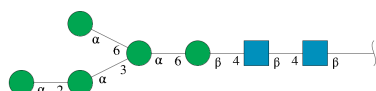
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	10	Total	C	N	O	0	0	0
			116	64	2	50			
5	M	10	Total	C	N	O	0	0	0
			116	64	2	50			

- 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.



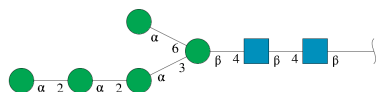
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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.



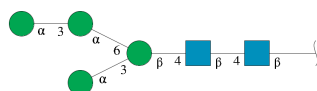
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



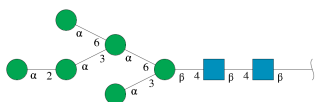
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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.



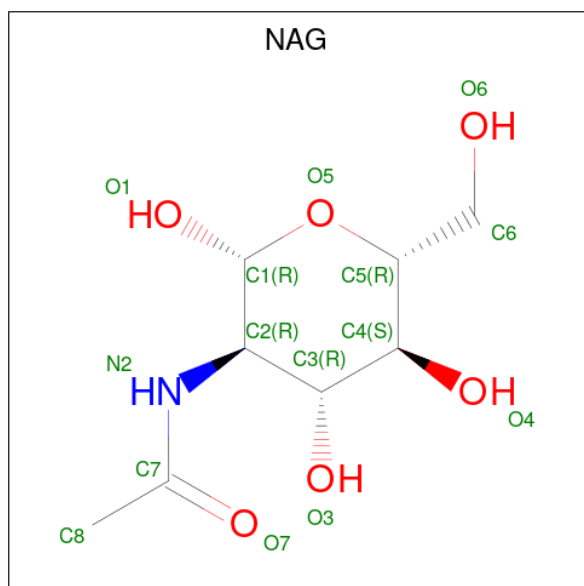
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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.



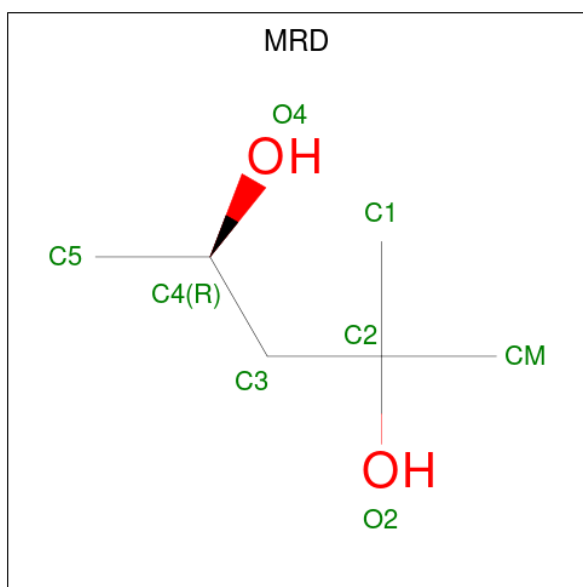
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

- 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: $C_6H_{14}O_2$).

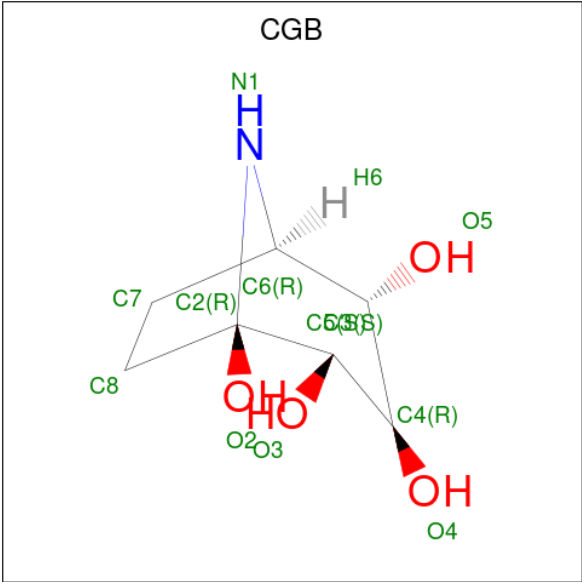


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 8 6 2	0	0
12	A	1	Total C O 8 6 2	0	0
12	A	1	Total C O 8 6 2	0	0
12	B	1	Total C O 8 6 2	0	0
12	B	1	Total C O 8 6 2	0	0
12	B	1	Total C O 8 6 2	0	0

- Molecule 13 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total Na 1 1	0	0
13	B	1	Total Na 1 1	0	0

- Molecule 14 is CALYSTEGINE B2 (CCD ID: CGB) (formula: C₇H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	N	O	0	0
			12	7	1	4		
14	B	1	Total	C	N	O	0	0
			12	7	1	4		

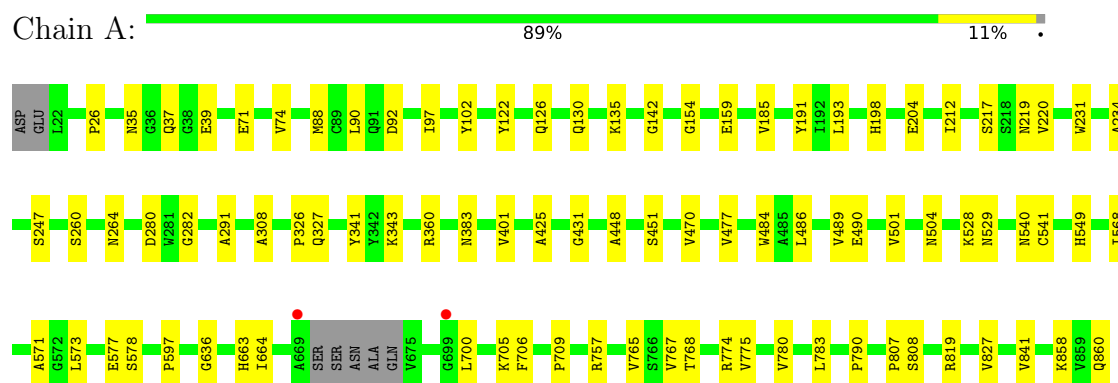
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	610	Total	O	0	0
			610	610		
15	B	713	Total	O	0	0
			713	713		

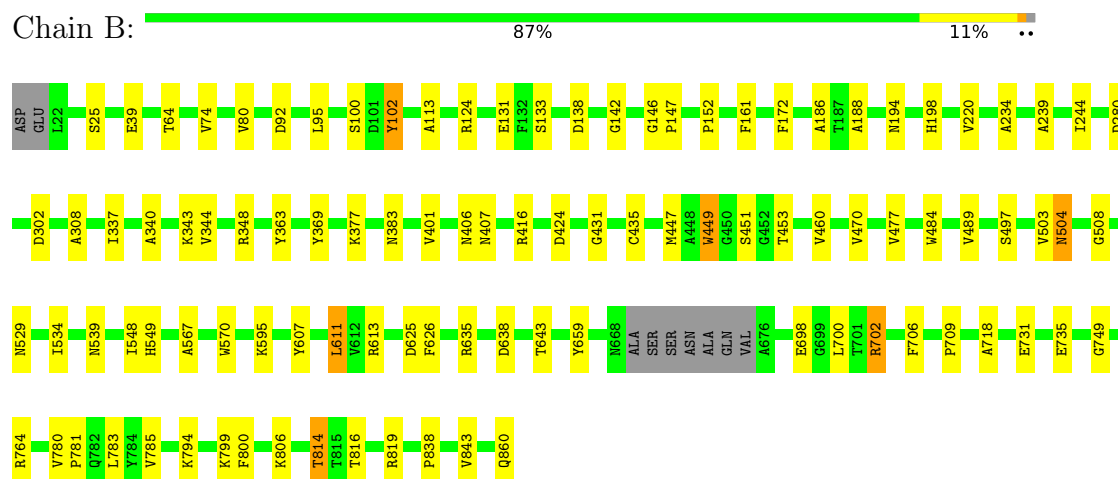
3 Residue-property plots

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.

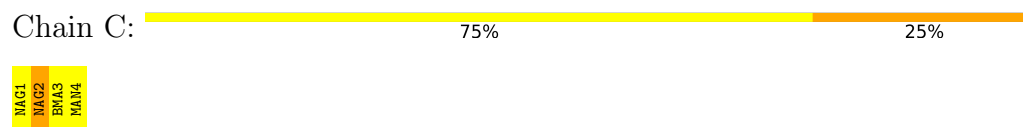
• Molecule 1: Beta-glucosidase 1



• 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

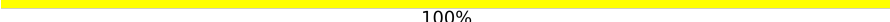


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  33% 67%

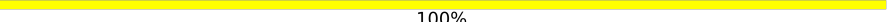
MAG1
MAG2
BMA3

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

Chain G:  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 L:  100%

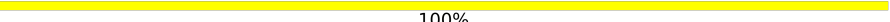
MAG1
MAG2
BMA3

- 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:  33% 67%

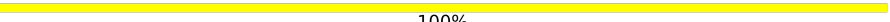
MAG1
MAG2
BMA3

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

Chain E:  100%

MAG1
MAG2

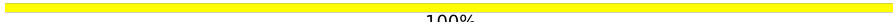
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

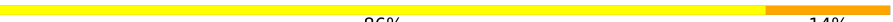
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(

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:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

• 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:  86% 14%

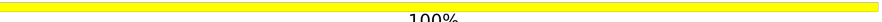
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

• 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:  71% 29%

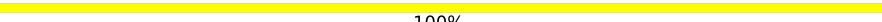
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

• 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%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

• 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:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

• Molecule 9: 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

Chain K:  83% 17%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

● 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-glucopyranos e



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	82.13Å 122.15Å 222.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.07 – 2.00 39.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.07-2.00) 99.5 (39.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.149 , 0.193 0.151 , 0.195	Depositor DCC
R_{free} test set	7631 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	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	15193	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MRD, BMA, CGB, NA, 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	1.51	33/6550 (0.5%)	1.24	13/8930 (0.1%)
1	B	1.61	41/6538 (0.6%)	1.28	24/8913 (0.3%)
All	All	1.56	74/13088 (0.6%)	1.26	37/17843 (0.2%)

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	503	VAL	C-O	8.18	1.32	1.23
1	B	447	MET	C-O	7.05	1.32	1.23
1	A	568	ILE	C-O	7.04	1.31	1.23
1	A	709	PRO	CA-C	6.88	1.60	1.52
1	B	131	GLU	N-CA	6.83	1.54	1.46
1	B	198	HIS	N-CA	6.58	1.54	1.46
1	B	401	VAL	C-O	6.45	1.31	1.24
1	B	570	TRP	C-O	6.44	1.31	1.24
1	B	113	ALA	C-O	6.26	1.31	1.24
1	A	541	CYS	CA-CB	6.21	1.64	1.53
1	B	453	THR	CA-CB	6.16	1.64	1.54
1	B	504	ASN	C-O	6.10	1.31	1.23
1	A	327	GLN	N-CA	-6.09	1.38	1.46
1	B	124	ARG	C-O	6.08	1.31	1.24
1	A	231	TRP	CA-C	6.03	1.60	1.52
1	A	448	ALA	N-CA	5.99	1.52	1.45
1	B	100	SER	C-O	5.97	1.29	1.24
1	B	534	ILE	CA-C	5.97	1.60	1.52
1	B	489	VAL	N-CA	5.97	1.53	1.46
1	B	133	SER	N-CA	-5.95	1.39	1.46
1	A	71	GLU	CA-C	5.88	1.60	1.52
1	B	548	ILE	CA-CB	5.87	1.61	1.54
1	B	709	PRO	CA-C	5.87	1.59	1.52
1	B	814	THR	CA-C	-5.87	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	ALA	C-O	5.86	1.30	1.24
1	B	308	ALA	CA-CB	5.85	1.62	1.53
1	A	597	PRO	CA-C	5.79	1.58	1.52
1	B	172	PHE	N-CA	5.78	1.53	1.46
1	A	212	ILE	N-CA	5.77	1.53	1.46
1	B	431	GLY	N-CA	5.73	1.51	1.45
1	B	843	VAL	C-O	5.68	1.29	1.24
1	B	161	PHE	CA-CB	5.67	1.63	1.53
1	A	90	LEU	N-CA	5.67	1.52	1.46
1	B	363	TYR	N-CA	5.57	1.52	1.45
1	B	706	PHE	N-CA	5.57	1.52	1.46
1	A	540	ASN	CA-C	5.54	1.60	1.52
1	A	401	VAL	CA-CB	5.53	1.60	1.54
1	A	217	SER	CA-CB	5.49	1.60	1.53
1	B	344	VAL	CA-CB	5.49	1.62	1.54
1	B	749	GLY	N-CA	5.44	1.51	1.44
1	A	191	TYR	CA-C	5.43	1.59	1.53
1	A	489	VAL	CA-CB	5.41	1.60	1.54
1	B	337	ILE	N-CA	-5.40	1.40	1.46
1	A	401	VAL	C-O	5.39	1.29	1.24
1	A	26	PRO	CA-C	5.39	1.54	1.51
1	B	348	ARG	CZ-NH1	5.37	1.40	1.32
1	B	435	CYS	CA-C	-5.36	1.46	1.52
1	A	159	GLU	C-O	5.36	1.30	1.24
1	A	154	GLY	N-CA	5.34	1.51	1.45
1	B	186	ALA	CA-C	5.32	1.59	1.52
1	B	460	VAL	CA-CB	5.31	1.59	1.53
1	A	198	HIS	N-CA	5.31	1.53	1.46
1	A	425	ALA	N-CA	5.30	1.53	1.46
1	B	194	ASN	C-O	5.28	1.29	1.23
1	B	64	THR	N-CA	5.26	1.52	1.46
1	A	185	VAL	N-CA	5.25	1.52	1.46
1	B	407	ASN	CA-C	5.24	1.59	1.53
1	A	219	ASN	CA-C	-5.24	1.46	1.52
1	A	234	ALA	CA-C	5.22	1.59	1.52
1	B	567	ALA	C-O	5.21	1.30	1.23
1	A	573	LEU	CA-C	5.20	1.58	1.52
1	B	548	ILE	C-O	5.20	1.29	1.24
1	A	204	GLU	C-O	5.19	1.30	1.24
1	A	636	GLY	N-CA	5.17	1.52	1.45
1	B	406	ASN	CA-CB	5.16	1.60	1.53
1	A	122	TYR	C-O	5.15	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	LYS	C-O	5.10	1.30	1.23
1	A	343	LYS	C-O	-5.09	1.18	1.24
1	B	102	TYR	C-O	5.07	1.30	1.23
1	A	501	VAL	C-O	5.06	1.29	1.24
1	B	800	PHE	CA-CB	5.05	1.62	1.53
1	A	571	ALA	CA-C	5.05	1.59	1.52
1	B	424	ASP	N-CA	5.00	1.52	1.46
1	B	785	VAL	C-O	5.00	1.29	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	CYS	N-CA-CB	8.13	123.78	110.69
1	A	540	ASN	N-CA-C	7.94	123.89	114.04
1	A	790	PRO	CA-C-N	-7.51	111.37	122.86
1	A	790	PRO	C-N-CA	-7.51	111.37	122.86
1	B	80	VAL	CA-C-N	-7.05	111.52	119.28
1	B	80	VAL	C-N-CA	-7.05	111.52	119.28
1	B	234	ALA	N-CA-C	-6.20	104.44	111.07
1	B	406	ASN	N-CA-C	-5.97	103.12	110.65
1	B	25	SER	CA-C-N	-5.90	114.31	120.38
1	B	25	SER	C-N-CA	-5.90	114.31	120.38
1	B	731	GLU	N-CA-C	-5.87	106.08	113.18
1	A	142	GLY	N-CA-C	-5.84	100.43	112.34
1	A	247	SER	N-CA-C	5.71	118.91	110.46
1	B	369	TYR	CA-C-N	-5.68	114.02	120.89
1	B	369	TYR	C-N-CA	-5.68	114.02	120.89
1	B	239	ALA	N-CA-C	-5.65	106.34	113.18
1	B	142	GLY	N-CA-C	-5.61	100.90	112.34
1	B	340	ALA	N-CA-C	-5.58	105.28	111.36
1	A	326	PRO	CB-CA-C	-5.53	104.32	111.46
1	B	497	SER	N-CA-C	-5.48	105.33	112.23
1	B	718	ALA	N-CA-C	-5.39	105.56	111.82
1	B	407	ASN	N-CA-CB	-5.37	104.02	112.13
1	B	780	VAL	CA-C-N	-5.36	114.44	119.85
1	B	780	VAL	C-N-CA	-5.36	114.44	119.85
1	A	700	LEU	N-CA-C	5.29	117.03	108.41
1	A	282	GLY	N-CA-C	-5.24	107.88	115.27
1	B	702	ARG	NE-CZ-NH2	-5.23	114.49	119.20
1	B	635	ARG	N-CA-C	-5.22	105.59	111.28
1	A	431	GLY	N-CA-C	-5.21	106.17	112.48
1	B	138	ASP	N-CA-C	-5.20	107.06	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	449	TRP	N-CA-C	5.17	118.14	110.14
1	B	643	THR	CB-CA-C	-5.11	104.02	109.85
1	B	611	LEU	N-CA-C	-5.08	103.33	110.50
1	B	534	ILE	N-CA-C	-5.04	105.63	110.72
1	A	775	VAL	N-CA-CB	-5.02	103.21	111.44
1	A	780	VAL	CA-C-N	-5.01	114.61	119.78
1	A	780	VAL	C-N-CA	-5.01	114.61	119.78

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	6097	38	0
1	B	6375	0	6082	36	0
2	C	50	0	43	1	0
3	D	39	0	34	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	24	0	0
5	F	116	0	97	0	0
5	M	116	0	97	0	0
6	H	83	0	70	2	0
6	O	83	0	69	2	0
7	I	83	0	69	0	0
8	J	83	0	70	0	0
9	K	72	0	61	2	0
10	P	94	0	78	1	0
11	A	28	0	26	0	0
11	B	42	0	39	0	0
12	A	24	0	42	8	0
12	B	24	0	42	5	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	12	0	13	8	0
14	B	12	0	12	7	0
15	A	610	0	0	4	0
15	B	713	0	0	7	0
All	All	15193	0	13167	88	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 (88) 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:92:ASP:OD2	14:A:943:CGB:H7C1	1.71	0.90
1:A:819:ARG:HH12	1:A:860:GLN:C	1.82	0.86
1:B:92:ASP:OD2	14:B:952:CGB:H7C1	1.75	0.86
1:A:280:ASP:OD1	14:A:943:CGB:H3	1.78	0.82
1:A:360:ARG:HH11	12:A:940:MRD:HMC3	1.44	0.82
1:B:280:ASP:OD1	14:B:952:CGB:H3	1.85	0.76
12:A:940:MRD:HMC2	15:B:1104:HOH:O	1.86	0.75
1:A:819:ARG:NH1	1:A:860:GLN:C	2.48	0.72
1:B:539:ASN:HB2	15:B:1702:HOH:O	1.91	0.70
1:B:764:ARG:HD2	1:B:814:THR:CG2	2.25	0.66
1:A:451:SER:OG	14:A:943:CGB:H8C2	1.94	0.66
10:P:3:BMA:H62	10:P:4:MAN:H5	1.78	0.66
1:B:702:ARG:HD3	15:B:1174:HOH:O	1.97	0.65
12:A:939:MRD:H5C2	15:A:1190:HOH:O	1.98	0.64
1:B:451:SER:CB	14:B:952:CGB:C8	2.77	0.62
1:A:819:ARG:NH1	1:A:860:GLN:O	2.21	0.62
1:B:451:SER:OG	14:B:952:CGB:H8C2	2.00	0.61
1:B:764:ARG:HD2	1:B:814:THR:HG21	1.82	0.60
1:B:449:TRP:CD1	1:B:508:GLY:HA3	2.37	0.60
1:A:451:SER:CB	14:A:943:CGB:C8	2.80	0.59
1:A:484:TRP:CE2	6:H:3:BMA:H62	2.38	0.59
1:B:625:ASP:HB3	12:B:950:MRD:HMC2	1.84	0.59
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.83	0.58
1:B:484:TRP:CZ2	1:B:529:ASN:HB2	2.39	0.58
12:A:940:MRD:HMC1	12:A:940:MRD:H5C3	1.84	0.58
12:A:940:MRD:HMC1	12:A:940:MRD:C5	2.36	0.55
12:A:939:MRD:O2	12:A:939:MRD:H5C3	2.08	0.54
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.90	0.53
1:B:451:SER:CB	14:B:952:CGB:H8C2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:838:PRO:HD2	15:B:1586:HOH:O	2.09	0.53
1:B:416:ARG:HG3	15:B:1113:HOH:O	2.08	0.51
1:A:451:SER:CB	14:A:943:CGB:H8C2	2.41	0.51
1:B:595:LYS:HE3	15:B:1003:HOH:O	2.11	0.50
1:A:484:TRP:CZ2	1:A:529:ASN:HB2	2.48	0.48
1:B:613:ARG:NH1	15:B:1055:HOH:O	2.37	0.48
1:A:39:GLU:HG2	15:A:1223:HOH:O	2.13	0.48
1:A:484:TRP:CZ2	6:H:3:BMA:H62	2.48	0.47
1:A:35:ASN:OD1	1:A:37:GLN:HB2	2.13	0.47
1:A:757:ARG:NH1	15:A:1153:HOH:O	2.38	0.47
1:B:764:ARG:CD	1:B:814:THR:CG2	2.91	0.47
14:B:952:CGB:H4	14:B:952:CGB:H7C2	1.07	0.47
1:B:220:VAL:HG22	1:B:626:PHE:CG	2.49	0.47
1:B:783:LEU:C	1:B:783:LEU:HD23	2.40	0.47
1:A:504:ASN:HA	1:A:549:HIS:O	2.14	0.47
1:B:146:GLY:HA2	1:B:147:PRO:C	2.40	0.47
1:B:470:VAL:HG11	1:B:477:VAL:HB	1.97	0.46
1:A:767:VAL:HG22	1:A:768:THR:N	2.30	0.46
1:B:484:TRP:CE2	6:O:3:BMA:H62	2.50	0.46
1:B:659:TYR:HE1	1:B:781:PRO:HB3	1.81	0.46
1:A:360:ARG:HG2	12:A:940:MRD:HMC1	1.98	0.46
1:A:663:HIS:O	1:A:664:ILE:HD13	2.16	0.45
1:A:827:VAL:HG11	3:D:2:NAG:O3	2.15	0.45
1:B:611:LEU:HD12	1:B:613:ARG:NH2	2.32	0.45
1:A:126:GLN:O	1:A:130:GLN:HG3	2.17	0.45
1:A:308:ALA:HB2	1:A:705:LYS:HA	1.98	0.45
12:B:949:MRD:H4	12:B:949:MRD:H1C2	1.19	0.44
1:B:102:TYR:HB3	1:B:383:ASN:HA	1.99	0.44
1:A:807:PRO:O	1:A:808:SER:HB2	2.18	0.44
12:B:950:MRD:H5C1	9:K:1:NAG:H62	2.00	0.44
1:B:819:ARG:HH12	1:B:860:GLN:C	2.26	0.44
1:A:486:LEU:O	1:A:490:GLU:HG3	2.18	0.43
1:A:470:VAL:HG11	1:A:477:VAL:HB	2.00	0.43
1:B:152:PRO:HG3	1:B:607:TYR:CG	2.54	0.43
1:B:799:LYS:HE3	1:B:816:THR:O	2.19	0.43
1:B:806:LYS:HZ3	1:B:806:LYS:HG3	1.52	0.43
1:A:451:SER:OG	14:A:943:CGB:C8	2.65	0.42
1:A:706:PHE:CZ	2:C:2:NAG:H82	2.54	0.42
1:B:451:SER:OG	14:B:952:CGB:C8	2.68	0.42
12:B:948:MRD:H4	12:B:948:MRD:H1C3	1.73	0.42
1:A:360:ARG:HH11	12:A:940:MRD:CM	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLU:HG3	1:B:343:LYS:HE2	2.00	0.42
15:A:1590:HOH:O	3:D:3:BMA:H3	2.19	0.42
1:A:97:ILE:HD13	1:A:135:LYS:HG3	2.01	0.42
1:A:664:ILE:HD12	1:A:765:VAL:HG22	2.01	0.42
1:B:819:ARG:NH1	1:B:860:GLN:C	2.78	0.41
1:A:92:ASP:CG	14:A:943:CGB:H7C1	2.43	0.41
1:A:193:LEU:HD13	1:A:220:VAL:HG21	2.02	0.41
1:A:783:LEU:C	1:A:783:LEU:HD23	2.46	0.41
1:A:88:MET:HE2	1:A:341:TYR:CD1	2.56	0.41
1:A:260:SER:O	1:A:264:ASN:HB2	2.20	0.41
14:A:943:CGB:H7C2	14:A:943:CGB:H4	1.21	0.41
1:B:95:LEU:C	1:B:95:LEU:HD12	2.45	0.41
12:B:950:MRD:H5C1	9:K:1:NAG:C6	2.49	0.41
1:B:504:ASN:HA	1:B:549:HIS:O	2.21	0.41
1:A:577:GLU:O	1:A:578:SER:C	2.64	0.41
1:B:638:ASP:O	1:B:794:LYS:HE3	2.21	0.41
6:O:3:BMA:H61	6:O:4:MAN:H5	2.02	0.40
1:A:102:TYR:HB3	1:A:383:ASN:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	830/841 (99%)	798 (96%)	32 (4%)	0	100	100
1	B	828/841 (98%)	803 (97%)	25 (3%)	0	100	100
All	All	1658/1682 (99%)	1601 (97%)	57 (3%)	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%)	668 (100%)	3 (0%)	84	89
1	B	670/677 (99%)	664 (99%)	6 (1%)	70	78
All	All	1341/1354 (99%)	1332 (99%)	9 (1%)	76	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	774	ARG
1	A	858	LYS
1	B	74	VAL
1	B	302	ASP
1	B	377	LYS
1	B	698	GLU
1	B	700	LEU
1	B	735	GLU

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	126	GLN
1	A	157	ASN
1	A	219	ASN
1	A	253	ASN
1	A	623	GLN
1	A	860	GLN
1	B	219	ASN
1	B	253	ASN
1	B	371	GLN
1	B	540	ASN
1	B	623	GLN
1	B	663	HIS

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 ⓘ

80 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	1.14	1 (7%)	17,19,21	1.57	4 (23%)
2	NAG	C	2	2	14,14,15	0.91	1 (7%)	17,19,21	2.02	5 (29%)
2	BMA	C	3	2	11,11,12	1.25	1 (9%)	15,15,17	1.82	5 (33%)
2	MAN	C	4	2	11,11,12	0.96	0	15,15,17	2.42	6 (40%)
3	NAG	D	1	1,3	14,14,15	1.03	1 (7%)	17,19,21	1.44	3 (17%)
3	NAG	D	2	3	14,14,15	1.15	1 (7%)	17,19,21	1.34	2 (11%)
3	BMA	D	3	3	11,11,12	1.11	0	15,15,17	2.56	9 (60%)
4	NAG	E	1	1,4	14,14,15	0.99	0	17,19,21	1.68	4 (23%)
4	NAG	E	2	4	14,14,15	1.01	1 (7%)	17,19,21	2.40	5 (29%)
5	NAG	F	1	1,5	14,14,15	1.59	3 (21%)	17,19,21	1.67	4 (23%)
5	MAN	F	10	5	11,11,12	1.46	3 (27%)	15,15,17	2.28	5 (33%)
5	NAG	F	2	5	14,14,15	1.00	1 (7%)	17,19,21	0.96	0
5	BMA	F	3	5	11,11,12	1.09	1 (9%)	15,15,17	1.15	1 (6%)
5	MAN	F	4	5	11,11,12	0.59	0	15,15,17	1.53	5 (33%)
5	MAN	F	5	5	11,11,12	1.22	1 (9%)	15,15,17	1.28	2 (13%)
5	MAN	F	6	5	11,11,12	0.82	0	15,15,17	1.47	2 (13%)
5	MAN	F	7	5	11,11,12	1.00	1 (9%)	15,15,17	1.22	1 (6%)
5	MAN	F	8	5	11,11,12	1.11	1 (9%)	15,15,17	1.75	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	F	9	5	11,11,12	1.06	1 (9%)	15,15,17	1.60	3 (20%)
3	NAG	G	1	1,3	14,14,15	0.95	0	17,19,21	1.37	1 (5%)
3	NAG	G	2	3	14,14,15	0.93	1 (7%)	17,19,21	1.47	4 (23%)
3	BMA	G	3	3	11,11,12	1.01	1 (9%)	15,15,17	2.31	3 (20%)
6	NAG	H	1	1,6	14,14,15	0.91	0	17,19,21	1.54	4 (23%)
6	NAG	H	2	6	14,14,15	0.90	0	17,19,21	2.12	5 (29%)
6	BMA	H	3	6	11,11,12	0.91	0	15,15,17	1.15	1 (6%)
6	MAN	H	4	6	11,11,12	0.69	0	15,15,17	1.49	3 (20%)
6	MAN	H	5	6	11,11,12	1.35	2 (18%)	15,15,17	1.98	5 (33%)
6	MAN	H	6	6	11,11,12	1.17	1 (9%)	15,15,17	1.28	2 (13%)
6	MAN	H	7	6	11,11,12	0.84	1 (9%)	15,15,17	1.97	5 (33%)
7	NAG	I	1	1,7,13	14,14,15	1.13	0	17,19,21	1.64	3 (17%)
7	NAG	I	2	7	14,14,15	1.18	2 (14%)	17,19,21	1.48	3 (17%)
7	BMA	I	3	7	11,11,12	0.84	0	15,15,17	2.07	3 (20%)
7	MAN	I	4	7	11,11,12	1.16	1 (9%)	15,15,17	1.30	1 (6%)
7	MAN	I	5	7	11,11,12	1.33	1 (9%)	15,15,17	2.17	5 (33%)
7	MAN	I	6	7	11,11,12	0.82	0	15,15,17	1.75	5 (33%)
7	MAN	I	7	7	11,11,12	1.06	1 (9%)	15,15,17	2.36	7 (46%)
8	NAG	J	1	1,8	14,14,15	1.65	1 (7%)	17,19,21	1.46	5 (29%)
8	NAG	J	2	8	14,14,15	1.07	2 (14%)	17,19,21	1.54	2 (11%)
8	BMA	J	3	8	11,11,12	1.14	1 (9%)	15,15,17	2.06	6 (40%)
8	MAN	J	4	8	11,11,12	0.63	0	15,15,17	1.89	6 (40%)
8	MAN	J	5	8	11,11,12	1.06	1 (9%)	15,15,17	1.62	3 (20%)
8	MAN	J	6	8	11,11,12	0.95	0	15,15,17	1.54	2 (13%)
8	MAN	J	7	8	11,11,12	0.69	0	15,15,17	1.89	5 (33%)
9	NAG	K	1	1,9	14,14,15	1.17	1 (7%)	17,19,21	1.49	3 (17%)
9	NAG	K	2	9	14,14,15	1.21	2 (14%)	17,19,21	1.58	4 (23%)
9	BMA	K	3	9	11,11,12	0.75	0	15,15,17	1.64	3 (20%)
9	MAN	K	4	9	11,11,12	0.66	0	15,15,17	1.61	6 (40%)
9	MAN	K	5	9	11,11,12	0.69	0	15,15,17	1.37	3 (20%)
9	MAN	K	6	9	11,11,12	1.60	1 (9%)	15,15,17	2.28	5 (33%)
3	NAG	L	1	1,3	14,14,15	0.66	0	17,19,21	1.76	4 (23%)
3	NAG	L	2	3	14,14,15	0.55	0	17,19,21	1.62	4 (23%)
3	BMA	L	3	3	11,11,12	0.83	0	15,15,17	1.74	5 (33%)
5	NAG	M	1	1,5	14,14,15	1.16	2 (14%)	17,19,21	1.92	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	M	10	5	11,11,12	1.05	0	15,15,17	1.77	5 (33%)
5	NAG	M	2	5	14,14,15	1.38	3 (21%)	17,19,21	1.36	3 (17%)
5	BMA	M	3	5	11,11,12	1.06	1 (9%)	15,15,17	1.71	4 (26%)
5	MAN	M	4	5	11,11,12	0.79	0	15,15,17	1.73	5 (33%)
5	MAN	M	5	5	11,11,12	0.75	0	15,15,17	2.45	6 (40%)
5	MAN	M	6	5	11,11,12	0.74	0	15,15,17	1.30	2 (13%)
5	MAN	M	7	5	11,11,12	1.27	1 (9%)	15,15,17	2.27	2 (13%)
5	MAN	M	8	5	11,11,12	1.34	1 (9%)	15,15,17	1.94	4 (26%)
5	MAN	M	9	5	11,11,12	0.81	0	15,15,17	1.42	2 (13%)
3	NAG	N	1	1,3	14,14,15	0.61	0	17,19,21	1.31	2 (11%)
3	NAG	N	2	3	14,14,15	0.86	0	17,19,21	1.20	0
3	BMA	N	3	3	11,11,12	0.89	0	15,15,17	1.25	2 (13%)
6	NAG	O	1	1,6	14,14,15	1.10	2 (14%)	17,19,21	2.11	5 (29%)
6	NAG	O	2	6	14,14,15	1.08	0	17,19,21	1.81	6 (35%)
6	BMA	O	3	6	11,11,12	1.06	0	15,15,17	1.72	3 (20%)
6	MAN	O	4	6	11,11,12	1.03	1 (9%)	15,15,17	1.42	3 (20%)
6	MAN	O	5	6	11,11,12	1.21	1 (9%)	15,15,17	2.05	6 (40%)
6	MAN	O	6	6	11,11,12	0.78	0	15,15,17	1.62	3 (20%)
6	MAN	O	7	6	11,11,12	0.89	0	15,15,17	1.90	5 (33%)
10	NAG	P	1	1,10,13	14,14,15	1.23	1 (7%)	17,19,21	1.54	4 (23%)
10	NAG	P	2	10	14,14,15	0.77	0	17,19,21	1.46	3 (17%)
10	BMA	P	3	10	11,11,12	1.36	2 (18%)	15,15,17	4.18	9 (60%)
10	MAN	P	4	10	11,11,12	1.02	1 (9%)	15,15,17	1.72	4 (26%)
10	MAN	P	5	10	11,11,12	1.02	0	15,15,17	1.77	3 (20%)
10	MAN	P	6	10	11,11,12	0.64	0	15,15,17	2.58	6 (40%)
10	MAN	P	7	10	11,11,12	0.91	1 (9%)	15,15,17	1.61	1 (6%)
10	MAN	P	8	10	11,11,12	0.92	0	15,15,17	1.92	5 (33%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	C	4	2	-	1/2/19/22	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	-	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	-	1/2/19/22	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	-	0/2/19/22	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	-	2/2/19/22	0/1/1/1
6	MAN	H	6	6	-	2/2/19/22	0/1/1/1
6	MAN	H	7	6	-	2/2/19/22	0/1/1/1
7	NAG	I	1	1,7,13	-	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	-	1/2/19/22	0/1/1/1
8	NAG	J	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	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	-	0/2/19/22	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/2/19/22	0/1/1/1
9	MAN	K	5	9	-	1/2/19/22	0/1/1/1
9	MAN	K	6	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	-	1/6/23/26	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	-	3/6/23/26	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	-	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
10	NAG	P	1	1,10,13	-	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	-	2/2/19/22	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	-	2/2/19/22	0/1/1/1
10	MAN	P	8	10	-	2/2/19/22	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	NAG	C1-C2	4.94	1.59	1.52
9	K	6	MAN	C2-C3	4.07	1.58	1.52
5	F	1	NAG	C2-N2	3.91	1.52	1.46
10	P	1	NAG	C2-N2	3.12	1.51	1.46
10	P	3	BMA	C2-C3	3.07	1.57	1.52
5	F	5	MAN	O5-C1	-3.03	1.38	1.43
7	I	2	NAG	O5-C1	-3.02	1.38	1.43
5	M	8	MAN	C2-C3	2.97	1.57	1.52
5	M	7	MAN	O5-C1	-2.96	1.38	1.43
2	C	1	NAG	C1-C2	2.88	1.56	1.52
9	K	1	NAG	C1-C2	2.87	1.56	1.52
6	H	5	MAN	O2-C2	-2.86	1.37	1.43
5	F	10	MAN	O5-C1	-2.78	1.39	1.43
5	M	2	NAG	C1-C2	2.78	1.56	1.52
4	E	2	NAG	O3-C3	-2.74	1.36	1.43
7	I	7	MAN	C2-C3	2.72	1.56	1.52
5	F	10	MAN	C2-C3	2.65	1.56	1.52
3	G	2	NAG	O5-C1	-2.62	1.39	1.43
6	O	5	MAN	O3-C3	-2.62	1.36	1.43
5	M	2	NAG	C4-C3	2.61	1.59	1.52
5	M	1	NAG	C1-C2	2.54	1.55	1.52
3	D	1	NAG	C1-C2	2.49	1.55	1.52
5	M	1	NAG	O5-C1	-2.44	1.39	1.43
10	P	7	MAN	C2-C3	2.44	1.56	1.52
5	F	8	MAN	O2-C2	-2.43	1.38	1.43
7	I	4	MAN	O5-C5	2.42	1.48	1.43
5	M	3	BMA	O4-C4	-2.39	1.37	1.43
10	P	3	BMA	O5-C1	-2.33	1.39	1.43
8	J	3	BMA	O5-C5	-2.31	1.38	1.43
5	F	9	MAN	O3-C3	-2.25	1.37	1.43
9	K	2	NAG	C3-C2	2.22	1.57	1.52
8	J	5	MAN	C1-C2	2.21	1.57	1.52
9	K	2	NAG	O5-C1	-2.21	1.40	1.43
6	H	6	MAN	O5-C5	2.20	1.47	1.43
7	I	5	MAN	C2-C3	-2.17	1.49	1.52
2	C	3	BMA	C4-C5	2.17	1.57	1.53
8	J	2	NAG	C4-C3	2.15	1.57	1.52
2	C	2	NAG	O5-C1	-2.14	1.40	1.43
3	G	3	BMA	C1-C2	2.14	1.57	1.52
7	I	2	NAG	O3-C3	-2.14	1.37	1.43
3	D	2	NAG	C4-C5	2.13	1.57	1.53
5	M	2	NAG	C4-C5	2.12	1.57	1.53
5	F	1	NAG	C4-C3	2.10	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	7	MAN	O3-C3	-2.08	1.37	1.43
6	O	4	MAN	O2-C2	-2.07	1.39	1.43
5	F	1	NAG	O5-C5	-2.06	1.39	1.43
5	F	3	BMA	C4-C5	2.05	1.57	1.53
8	J	2	NAG	C1-C2	2.05	1.55	1.52
5	F	2	NAG	O4-C4	-2.04	1.37	1.43
5	F	10	MAN	O3-C3	-2.03	1.37	1.43
10	P	4	MAN	O4-C4	-2.03	1.37	1.43
5	F	7	MAN	C4-C3	2.03	1.57	1.52
6	O	1	NAG	O5-C1	-2.02	1.40	1.43
6	H	5	MAN	C1-C2	2.02	1.57	1.52
6	O	1	NAG	O5-C5	-2.01	1.39	1.43

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	3	BMA	C1-O5-C5	9.95	125.53	112.19
10	P	3	BMA	C6-C5-C4	-8.02	93.32	113.02
4	E	2	NAG	C3-C4-C5	-6.95	97.63	110.23
3	G	3	BMA	C1-O5-C5	6.72	121.19	112.19
5	M	7	MAN	C1-O5-C5	6.55	120.96	112.19
7	I	3	BMA	C1-O5-C5	6.17	120.45	112.19
10	P	3	BMA	O2-C2-C3	5.87	122.31	110.15
2	C	4	MAN	O5-C5-C6	5.82	118.99	107.66
5	M	5	MAN	O6-C6-C5	-5.75	91.74	111.33
5	F	10	MAN	O2-C2-C3	5.59	121.73	110.15
6	H	2	NAG	C2-N2-C7	-5.50	115.52	122.90
10	P	6	MAN	O3-C3-C4	5.40	123.10	110.38
9	K	6	MAN	O2-C2-C3	5.14	120.80	110.15
2	C	2	NAG	C2-N2-C7	4.92	129.50	122.90
6	O	1	NAG	C1-O5-C5	4.70	118.48	112.19
8	J	7	MAN	O5-C5-C6	4.48	116.39	107.66
9	K	6	MAN	O5-C5-C6	4.47	116.36	107.66
7	I	7	MAN	O2-C2-C3	4.46	119.39	110.15
10	P	6	MAN	O4-C4-C3	4.40	120.74	110.38
5	M	7	MAN	O2-C2-C3	-4.39	101.06	110.15
5	M	8	MAN	C1-O5-C5	4.38	118.05	112.19
6	H	7	MAN	O4-C4-C3	-4.36	100.09	110.38
10	P	2	NAG	C1-O5-C5	4.33	117.98	112.19
7	I	7	MAN	C1-O5-C5	4.32	117.97	112.19
8	J	3	BMA	C1-C2-C3	-4.32	103.36	109.64
7	I	1	NAG	C1-O5-C5	4.29	117.94	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	4	MAN	O2-C2-C1	-4.29	99.41	109.22
10	P	3	BMA	O3-C3-C2	4.28	118.79	110.05
4	E	2	NAG	O5-C5-C6	4.25	115.94	107.66
3	L	1	NAG	O4-C4-C5	-4.17	99.05	109.32
6	O	3	BMA	O5-C5-C6	4.11	115.66	107.66
7	I	5	MAN	C3-C4-C5	-4.09	102.81	110.23
5	M	1	NAG	O4-C4-C5	-4.08	99.26	109.32
10	P	6	MAN	C3-C4-C5	-4.08	102.83	110.23
5	F	6	MAN	O5-C5-C6	4.08	115.61	107.66
7	I	5	MAN	O2-C2-C3	-4.06	101.74	110.15
3	G	1	NAG	C1-C2-N2	-4.05	104.06	110.43
5	F	9	MAN	O5-C5-C6	4.04	115.53	107.66
10	P	5	MAN	C3-C4-C5	-4.01	102.97	110.23
3	D	3	BMA	O3-C3-C2	-4.00	101.88	110.05
5	M	3	BMA	O5-C5-C4	-4.00	101.11	110.83
6	O	5	MAN	C6-C5-C4	-3.98	103.26	113.02
3	D	3	BMA	C3-C4-C5	3.97	117.42	110.23
4	E	1	NAG	C1-O5-C5	3.96	117.49	112.19
7	I	4	MAN	O5-C5-C6	3.95	115.36	107.66
8	J	5	MAN	C6-C5-C4	-3.94	103.35	113.02
5	M	5	MAN	C1-O5-C5	3.92	117.44	112.19
5	M	5	MAN	C6-C5-C4	-3.89	103.47	113.02
8	J	2	NAG	O6-C6-C5	-3.86	98.20	111.33
6	H	7	MAN	C1-C2-C3	-3.80	104.12	109.64
8	J	6	MAN	C6-C5-C4	-3.77	103.75	113.02
6	O	6	MAN	C1-O5-C5	3.76	117.22	112.19
6	O	7	MAN	C1-O5-C5	-3.75	107.17	112.19
3	G	3	BMA	O2-C2-C1	3.74	117.80	109.22
5	F	10	MAN	C1-O5-C5	3.74	117.20	112.19
9	K	3	BMA	C1-O5-C5	3.73	117.18	112.19
8	J	4	MAN	O5-C5-C6	3.68	114.82	107.66
6	H	5	MAN	O5-C5-C6	3.67	114.81	107.66
5	M	8	MAN	O3-C3-C4	-3.66	101.76	110.38
5	F	10	MAN	O3-C3-C4	-3.63	101.82	110.38
8	J	3	BMA	O5-C5-C4	-3.62	102.02	110.83
2	C	4	MAN	C1-C2-C3	3.58	114.86	109.64
7	I	5	MAN	O6-C6-C5	-3.55	99.24	111.33
3	D	3	BMA	O5-C5-C6	3.54	114.56	107.66
3	L	2	NAG	O6-C6-C5	-3.50	99.42	111.33
3	N	1	NAG	C1-C2-N2	-3.48	104.95	110.43
2	C	4	MAN	C1-O5-C5	3.47	116.84	112.19
3	D	3	BMA	O6-C6-C5	3.46	123.12	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	9	MAN	O2-C2-C3	-3.45	103.00	110.15
6	O	1	NAG	O4-C4-C5	-3.44	100.85	109.32
6	H	6	MAN	O5-C5-C6	3.42	114.33	107.66
10	P	7	MAN	O5-C5-C6	3.42	114.32	107.66
5	M	5	MAN	O3-C3-C4	-3.41	102.33	110.38
6	H	1	NAG	C1-C2-N2	-3.41	105.06	110.43
2	C	3	BMA	C3-C4-C5	3.40	116.39	110.23
9	K	5	MAN	C1-O5-C5	3.38	116.71	112.19
6	H	5	MAN	O2-C2-C3	-3.38	103.16	110.15
6	O	5	MAN	C1-O5-C5	3.34	116.66	112.19
5	M	4	MAN	O6-C6-C5	-3.32	100.03	111.33
5	M	1	NAG	C4-C3-C2	3.29	115.85	111.02
5	F	8	MAN	O3-C3-C4	-3.29	102.62	110.38
6	H	2	NAG	O6-C6-C5	-3.29	100.14	111.33
6	H	2	NAG	C4-C3-C2	3.28	115.83	111.02
6	O	1	NAG	C1-C2-N2	-3.26	105.30	110.43
3	G	2	NAG	C4-C3-C2	3.26	115.79	111.02
10	P	6	MAN	O5-C5-C6	3.25	113.99	107.66
5	F	1	NAG	O5-C5-C6	-3.25	101.35	107.66
9	K	6	MAN	C2-C3-C4	3.22	116.53	110.86
7	I	7	MAN	O5-C5-C6	3.21	113.91	107.66
8	J	7	MAN	O3-C3-C2	3.19	116.57	110.05
5	F	8	MAN	C3-C4-C5	3.18	116.00	110.23
6	H	5	MAN	C6-C5-C4	-3.18	105.22	113.02
3	N	3	BMA	O5-C5-C6	3.17	113.83	107.66
3	D	3	BMA	O3-C3-C4	3.16	117.83	110.38
8	J	4	MAN	C2-C3-C4	-3.16	105.30	110.86
3	L	2	NAG	C2-N2-C7	3.16	127.13	122.90
10	P	3	BMA	O6-C6-C5	-3.15	100.60	111.33
8	J	3	BMA	O6-C6-C5	-3.14	100.63	111.33
10	P	5	MAN	O2-C2-C3	-3.14	103.65	110.15
5	F	5	MAN	O6-C6-C5	-3.14	100.65	111.33
3	D	3	BMA	C1-C2-C3	3.13	114.20	109.64
5	M	4	MAN	C1-O5-C5	3.13	116.38	112.19
6	O	5	MAN	O2-C2-C1	3.12	116.38	109.22
5	M	10	MAN	O6-C6-C5	-3.12	100.70	111.33
9	K	6	MAN	O3-C3-C2	3.09	116.36	110.05
2	C	1	NAG	O3-C3-C2	-3.08	103.01	109.40
7	I	7	MAN	C1-C2-C3	-3.07	105.18	109.64
2	C	2	NAG	C3-C4-C5	-3.06	104.68	110.23
4	E	1	NAG	O4-C4-C5	-3.06	101.79	109.32
6	H	2	NAG	O4-C4-C3	-3.03	103.23	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	C1-O5-C5	3.03	116.24	112.19
9	K	4	MAN	O5-C5-C6	3.03	113.55	107.66
10	P	3	BMA	C2-C3-C4	3.01	116.16	110.86
10	P	3	BMA	O3-C3-C4	-3.00	103.31	110.38
4	E	1	NAG	O5-C5-C6	2.98	113.46	107.66
6	O	1	NAG	O5-C1-C2	-2.97	106.70	111.29
2	C	4	MAN	C6-C5-C4	-2.95	105.77	113.02
4	E	2	NAG	C1-C2-N2	2.95	115.08	110.43
2	C	3	BMA	C2-C3-C4	-2.95	105.67	110.86
8	J	5	MAN	O5-C5-C6	2.95	113.40	107.66
7	I	2	NAG	C1-O5-C5	2.94	116.12	112.19
5	F	6	MAN	O3-C3-C2	2.93	116.03	110.05
10	P	1	NAG	O6-C6-C5	-2.92	101.39	111.33
3	L	3	BMA	C2-C3-C4	2.90	115.96	110.86
3	L	3	BMA	C3-C4-C5	2.89	115.47	110.23
6	O	3	BMA	O2-C2-C1	-2.89	102.61	109.22
5	M	1	NAG	O3-C3-C2	2.89	115.40	109.40
10	P	1	NAG	C1-O5-C5	2.88	116.05	112.19
7	I	6	MAN	O2-C2-C1	2.87	115.80	109.22
2	C	4	MAN	C2-C3-C4	-2.87	105.81	110.86
6	O	7	MAN	C3-C4-C5	2.87	115.44	110.23
8	J	3	BMA	O2-C2-C3	-2.87	104.21	110.15
6	O	2	NAG	O7-C7-N2	-2.87	116.92	121.98
8	J	5	MAN	O2-C2-C3	-2.86	104.22	110.15
8	J	7	MAN	O4-C4-C3	-2.86	103.63	110.38
3	L	1	NAG	C3-C4-C5	2.86	115.41	110.23
6	H	2	NAG	C3-C4-C5	-2.85	105.07	110.23
5	F	4	MAN	O6-C6-C5	-2.84	101.66	111.33
6	O	2	NAG	O5-C1-C2	-2.83	106.92	111.29
10	P	8	MAN	C2-C3-C4	2.81	115.81	110.86
9	K	4	MAN	C3-C4-C5	-2.81	105.13	110.23
7	I	5	MAN	C6-C5-C4	2.81	119.91	113.02
6	O	5	MAN	C1-C2-C3	-2.80	105.56	109.64
10	P	8	MAN	O5-C5-C6	2.80	113.11	107.66
7	I	6	MAN	O3-C3-C4	2.79	116.94	110.38
7	I	6	MAN	O6-C6-C5	-2.78	101.85	111.33
3	L	2	NAG	C3-C4-C5	-2.76	105.23	110.23
5	F	1	NAG	C8-C7-N2	2.74	120.66	116.12
6	O	7	MAN	C2-C3-C4	2.74	115.67	110.86
5	F	1	NAG	C1-O5-C5	2.74	115.85	112.19
10	P	8	MAN	C1-C2-C3	2.73	113.62	109.64
5	M	10	MAN	O3-C3-C4	-2.72	103.97	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	3	BMA	O5-C5-C4	-2.71	104.23	110.83
3	D	2	NAG	C6-C5-C4	2.71	119.67	113.02
6	H	1	NAG	C3-C4-C5	2.71	115.14	110.23
6	O	6	MAN	O4-C4-C5	-2.70	102.67	109.32
6	O	1	NAG	O7-C7-C8	2.69	126.85	122.05
5	M	2	NAG	C1-C2-N2	-2.69	106.19	110.43
6	O	4	MAN	C1-C2-C3	2.69	113.56	109.64
7	I	3	BMA	O3-C3-C4	2.69	116.71	110.38
3	G	2	NAG	C1-O5-C5	2.68	115.78	112.19
9	K	2	NAG	O6-C6-C5	-2.68	102.22	111.33
7	I	5	MAN	O4-C4-C3	-2.67	104.09	110.38
5	M	10	MAN	C6-C5-C4	-2.67	106.47	113.02
10	P	8	MAN	C1-O5-C5	2.66	115.75	112.19
7	I	7	MAN	C6-C5-C4	-2.66	106.48	113.02
5	M	10	MAN	C1-O5-C5	2.65	115.74	112.19
10	P	6	MAN	O4-C4-C5	-2.65	102.80	109.32
10	P	8	MAN	O4-C4-C5	-2.64	102.81	109.32
6	H	4	MAN	O3-C3-C4	2.64	116.59	110.38
6	O	3	BMA	O3-C3-C2	2.63	115.42	110.05
9	K	1	NAG	C4-C3-C2	-2.62	107.17	111.02
9	K	1	NAG	O6-C6-C5	-2.61	102.43	111.33
7	I	1	NAG	C4-C3-C2	2.61	114.85	111.02
10	P	3	BMA	O5-C5-C4	2.61	117.18	110.83
5	M	6	MAN	C1-C2-C3	-2.61	105.85	109.64
7	I	2	NAG	O3-C3-C4	-2.61	104.23	110.38
6	O	7	MAN	O2-C2-C1	2.60	115.17	109.22
6	H	4	MAN	O4-C4-C5	-2.60	102.93	109.32
5	M	1	NAG	C1-C2-N2	-2.59	106.35	110.43
8	J	3	BMA	O3-C3-C4	-2.59	104.27	110.38
6	H	1	NAG	O3-C3-C2	-2.59	104.02	109.40
2	C	3	BMA	C1-C2-C3	2.59	113.41	109.64
5	F	5	MAN	C1-O5-C5	2.59	115.65	112.19
3	D	1	NAG	O4-C4-C5	-2.58	102.98	109.32
5	M	4	MAN	O3-C3-C4	-2.57	104.33	110.38
5	F	7	MAN	O3-C3-C4	-2.57	104.33	110.38
3	L	3	BMA	O4-C4-C3	-2.56	104.35	110.38
5	F	8	MAN	C1-O5-C5	2.54	115.59	112.19
10	P	6	MAN	C2-C3-C4	-2.54	106.40	110.86
7	I	2	NAG	O5-C1-C2	-2.53	107.38	111.29
6	O	4	MAN	C1-O5-C5	2.52	115.56	112.19
5	M	3	BMA	C2-C3-C4	-2.51	106.45	110.86
8	J	7	MAN	O6-C6-C5	2.50	119.84	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	7	MAN	O4-C4-C3	2.49	116.25	110.38
10	P	4	MAN	O4-C4-C3	-2.48	104.52	110.38
5	F	4	MAN	C1-C2-C3	-2.48	106.03	109.64
6	H	7	MAN	C3-C4-C5	-2.47	105.75	110.23
10	P	4	MAN	C1-C2-C3	2.46	113.23	109.64
8	J	2	NAG	O4-C4-C5	-2.46	103.26	109.32
10	P	3	BMA	O5-C5-C6	-2.45	102.90	107.66
3	D	3	BMA	O2-C2-C3	-2.45	105.08	110.15
9	K	5	MAN	C3-C4-C5	2.43	114.64	110.23
5	F	10	MAN	C2-C3-C4	2.42	115.12	110.86
9	K	3	BMA	C6-C5-C4	-2.42	107.08	113.02
2	C	1	NAG	O5-C5-C4	-2.41	104.95	110.83
3	G	2	NAG	C1-C2-N2	-2.40	106.65	110.43
3	L	1	NAG	O5-C5-C6	2.39	112.31	107.66
8	J	1	NAG	O7-C7-C8	-2.39	117.80	122.05
3	G	2	NAG	O4-C4-C5	-2.38	103.45	109.32
8	J	1	NAG	O4-C4-C3	-2.38	104.77	110.38
9	K	2	NAG	O5-C5-C4	-2.38	105.05	110.83
9	K	2	NAG	O7-C7-N2	-2.37	117.79	121.98
3	L	3	BMA	O5-C1-C2	-2.37	105.13	110.79
6	O	5	MAN	O6-C6-C5	-2.37	103.26	111.33
10	P	4	MAN	O5-C1-C2	2.36	116.41	110.79
5	F	1	NAG	C6-C5-C4	2.35	118.79	113.02
5	F	9	MAN	O3-C3-C2	-2.35	105.26	110.05
3	D	1	NAG	C1-C2-N2	2.35	114.13	110.43
5	M	2	NAG	O4-C4-C3	-2.34	104.86	110.38
5	F	4	MAN	O5-C5-C6	2.32	112.18	107.66
4	E	1	NAG	C2-N2-C7	2.31	126.00	122.90
6	H	3	BMA	O2-C2-C1	-2.31	103.93	109.22
5	F	9	MAN	C3-C4-C5	-2.31	106.05	110.23
6	H	4	MAN	C1-O5-C5	2.31	115.28	112.19
3	D	3	BMA	O4-C4-C5	-2.31	103.64	109.32
8	J	6	MAN	C1-O5-C5	2.30	115.26	112.19
9	K	1	NAG	C1-C2-N2	2.28	114.03	110.43
5	M	5	MAN	O2-C2-C1	2.28	114.44	109.22
6	H	5	MAN	C2-C3-C4	-2.27	106.86	110.86
5	M	3	BMA	O5-C5-C6	2.27	112.08	107.66
5	F	10	MAN	O2-C2-C1	2.26	114.40	109.22
10	P	5	MAN	C6-C5-C4	2.26	118.56	113.02
6	H	5	MAN	O3-C3-C2	2.25	114.65	110.05
9	K	5	MAN	O5-C5-C6	2.25	112.04	107.66
5	M	4	MAN	C1-C2-C3	-2.25	106.37	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	4	MAN	O3-C3-C2	-2.25	105.47	110.05
7	I	1	NAG	O6-C6-C5	-2.24	103.69	111.33
4	E	2	NAG	C4-C3-C2	2.24	114.31	111.02
3	L	1	NAG	C1-O5-C5	2.24	115.19	112.19
5	M	10	MAN	O2-C2-C1	2.24	114.35	109.22
5	F	3	BMA	O6-C6-C5	-2.24	103.72	111.33
2	C	3	BMA	O3-C3-C4	2.23	115.64	110.38
9	K	4	MAN	C1-C2-C3	2.23	112.90	109.64
3	D	1	NAG	O7-C7-C8	-2.23	118.08	122.05
6	H	1	NAG	O5-C1-C2	2.23	114.74	111.29
5	M	8	MAN	O6-C6-C5	-2.22	103.77	111.33
5	F	4	MAN	O2-C2-C1	2.21	114.28	109.22
8	J	1	NAG	O5-C1-C2	-2.21	107.88	111.29
6	O	6	MAN	C6-C5-C4	-2.20	107.61	113.02
2	C	2	NAG	O4-C4-C5	-2.20	103.90	109.32
8	J	1	NAG	C4-C3-C2	-2.19	107.80	111.02
9	K	6	MAN	C1-C2-C3	-2.19	106.45	109.64
5	M	1	NAG	O6-C6-C5	-2.19	103.88	111.33
5	F	4	MAN	O4-C4-C5	2.19	114.71	109.32
3	N	1	NAG	O3-C3-C2	-2.19	104.86	109.40
5	M	5	MAN	O2-C2-C3	-2.19	105.62	110.15
10	P	2	NAG	O5-C5-C6	2.18	111.91	107.66
5	M	8	MAN	C1-C2-C3	2.18	112.82	109.64
9	K	3	BMA	O6-C6-C5	-2.17	103.95	111.33
2	C	2	NAG	O3-C3-C2	-2.16	104.91	109.40
3	D	2	NAG	O6-C6-C5	-2.16	103.97	111.33
6	O	5	MAN	O2-C2-C3	-2.16	105.67	110.15
3	G	3	BMA	C2-C3-C4	-2.16	107.06	110.86
6	O	7	MAN	O5-C5-C6	2.15	111.85	107.66
5	M	6	MAN	C1-O5-C5	2.14	115.06	112.19
2	C	1	NAG	O5-C1-C2	-2.14	107.98	111.29
3	L	3	BMA	O4-C4-C5	2.13	114.58	109.32
6	H	7	MAN	O6-C6-C5	-2.13	104.09	111.33
9	K	2	NAG	C6-C5-C4	2.13	118.24	113.02
10	P	1	NAG	O5-C5-C6	2.12	111.80	107.66
7	I	7	MAN	O5-C5-C4	-2.12	105.67	110.83
6	H	6	MAN	O4-C4-C3	-2.11	105.40	110.38
3	N	3	BMA	O3-C3-C2	2.11	114.36	110.05
8	J	4	MAN	C6-C5-C4	-2.11	107.84	113.02
8	J	4	MAN	O6-C6-C5	-2.11	104.16	111.33
6	O	4	MAN	O6-C6-C5	-2.09	104.22	111.33
2	C	3	BMA	O5-C1-C2	2.08	115.75	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	7	MAN	C1-C2-C3	2.08	112.67	109.64
6	H	7	MAN	O3-C3-C2	2.08	114.29	110.05
10	P	1	NAG	C4-C3-C2	2.07	114.06	111.02
2	C	2	NAG	O5-C5-C6	2.07	111.70	107.66
5	M	3	BMA	O2-C2-C3	2.07	114.44	110.15
8	J	4	MAN	O2-C2-C3	-2.07	105.87	110.15
7	I	6	MAN	C6-C5-C4	2.06	118.09	113.02
6	O	2	NAG	O5-C5-C4	-2.06	105.81	110.83
6	O	2	NAG	O6-C6-C5	-2.06	104.31	111.33
10	P	2	NAG	O3-C3-C2	-2.06	105.12	109.40
9	K	4	MAN	C6-C5-C4	2.06	118.06	113.02
6	O	2	NAG	O4-C4-C3	-2.05	105.53	110.38
8	J	3	BMA	C1-O5-C5	2.05	114.94	112.19
6	O	2	NAG	C1-C2-N2	-2.05	107.20	110.43
5	M	9	MAN	C1-C2-C3	2.05	112.62	109.64
8	J	1	NAG	O7-C7-N2	2.04	125.59	121.98
3	L	2	NAG	O4-C4-C3	-2.04	105.57	110.38
2	C	4	MAN	O3-C3-C2	2.04	114.21	110.05
5	M	4	MAN	O3-C3-C2	2.03	114.21	110.05
9	K	4	MAN	C1-O5-C5	2.03	114.91	112.19
4	E	2	NAG	O6-C6-C5	-2.03	104.43	111.33
5	M	2	NAG	O7-C7-C8	-2.01	118.48	122.05
7	I	6	MAN	O5-C5-C6	-2.01	103.76	107.66
2	C	1	NAG	C8-C7-N2	-2.00	112.79	116.12
9	K	4	MAN	O5-C5-C4	-2.00	105.96	110.83

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	6	MAN	C4-C5-C6-O6
6	H	5	MAN	O5-C5-C6-O6
7	I	4	MAN	O5-C5-C6-O6
6	O	7	MAN	O5-C5-C6-O6
6	H	6	MAN	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
7	I	6	MAN	O5-C5-C6-O6
7	I	4	MAN	C4-C5-C6-O6
10	P	8	MAN	O5-C5-C6-O6
3	L	3	BMA	O5-C5-C6-O6

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

There are no ring outliers.

9 monomers are involved in 10 short contacts:

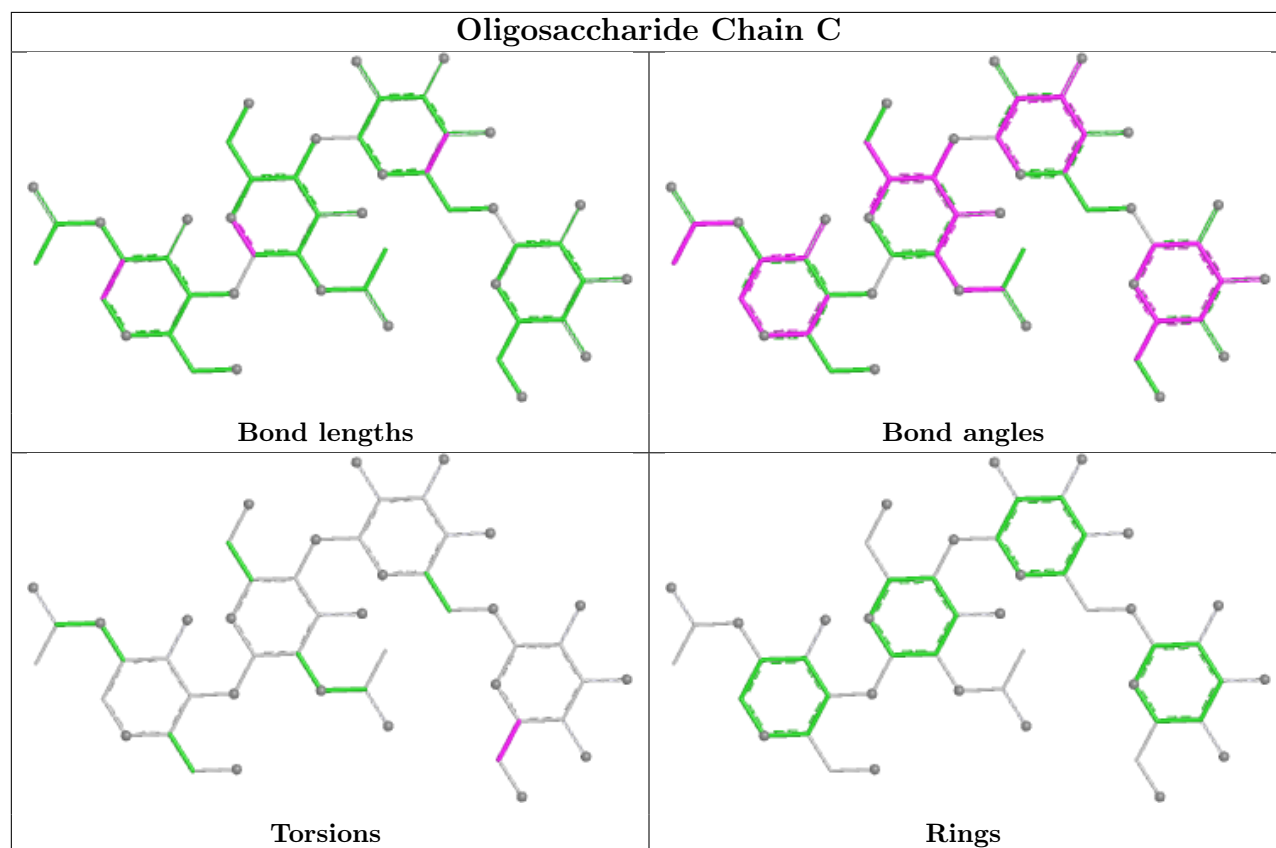
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	P	4	MAN	1	0
6	H	3	BMA	2	0
3	D	2	NAG	1	0

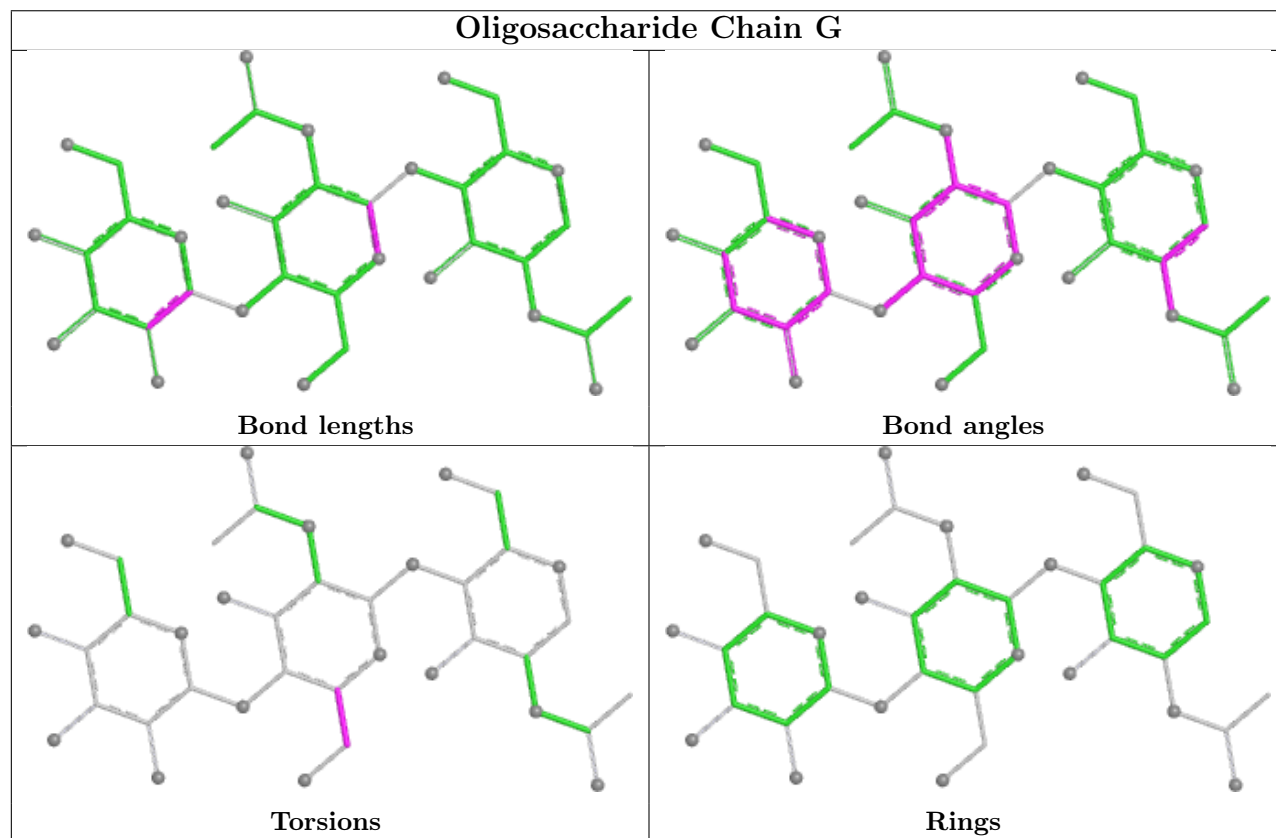
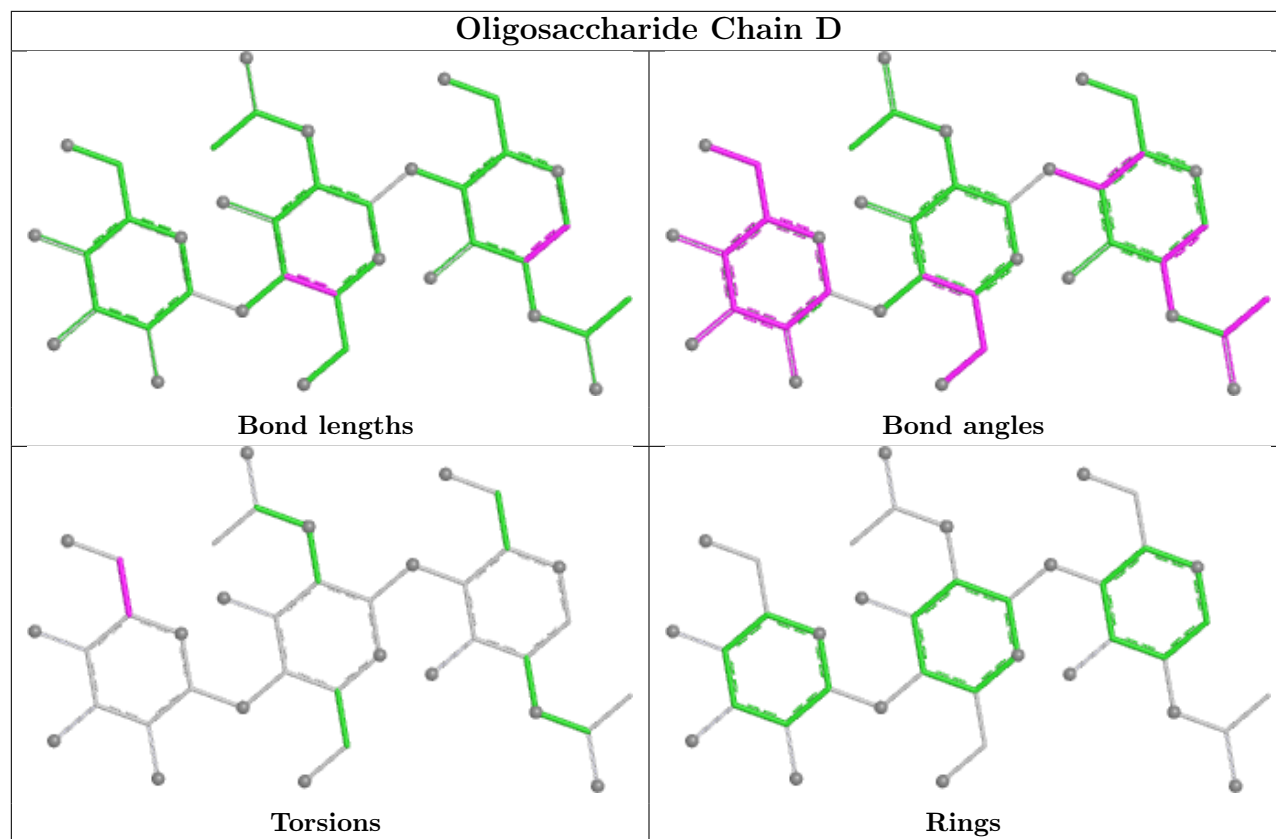
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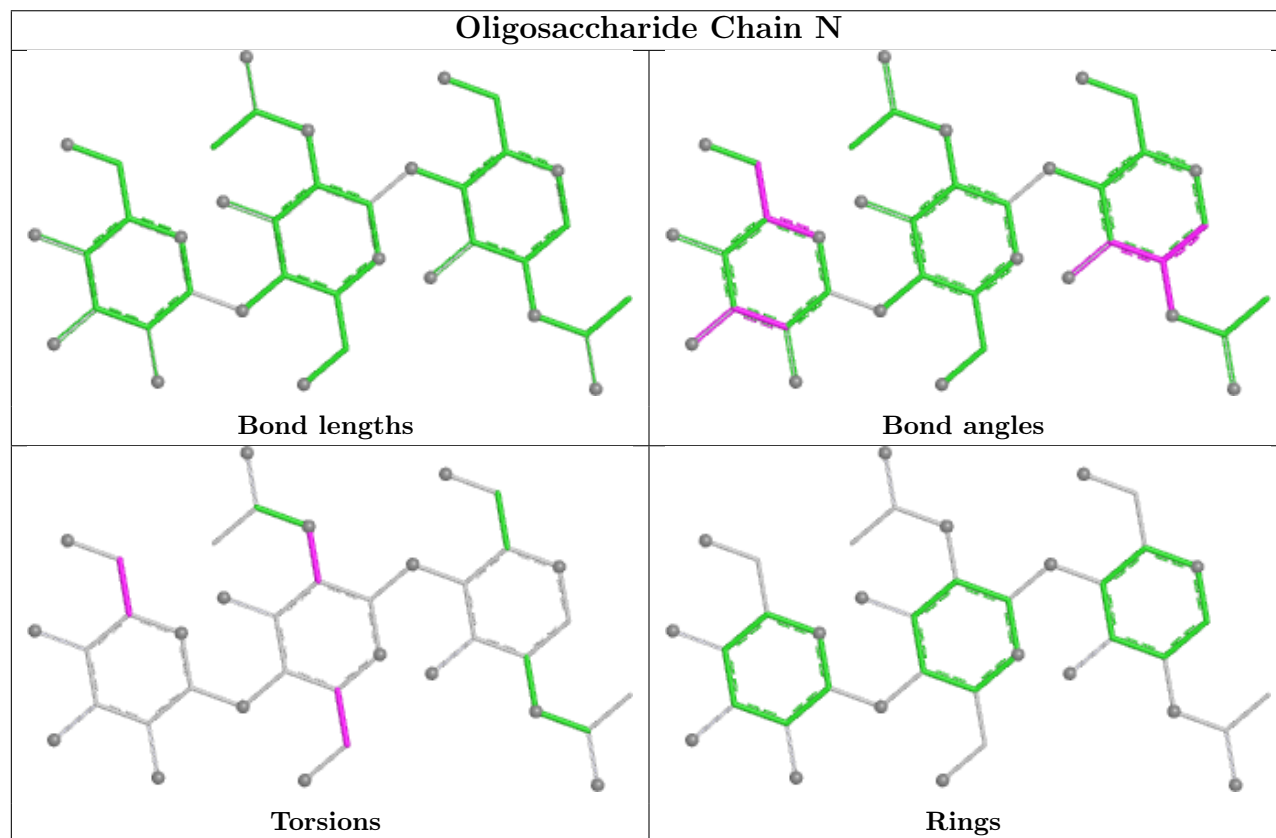
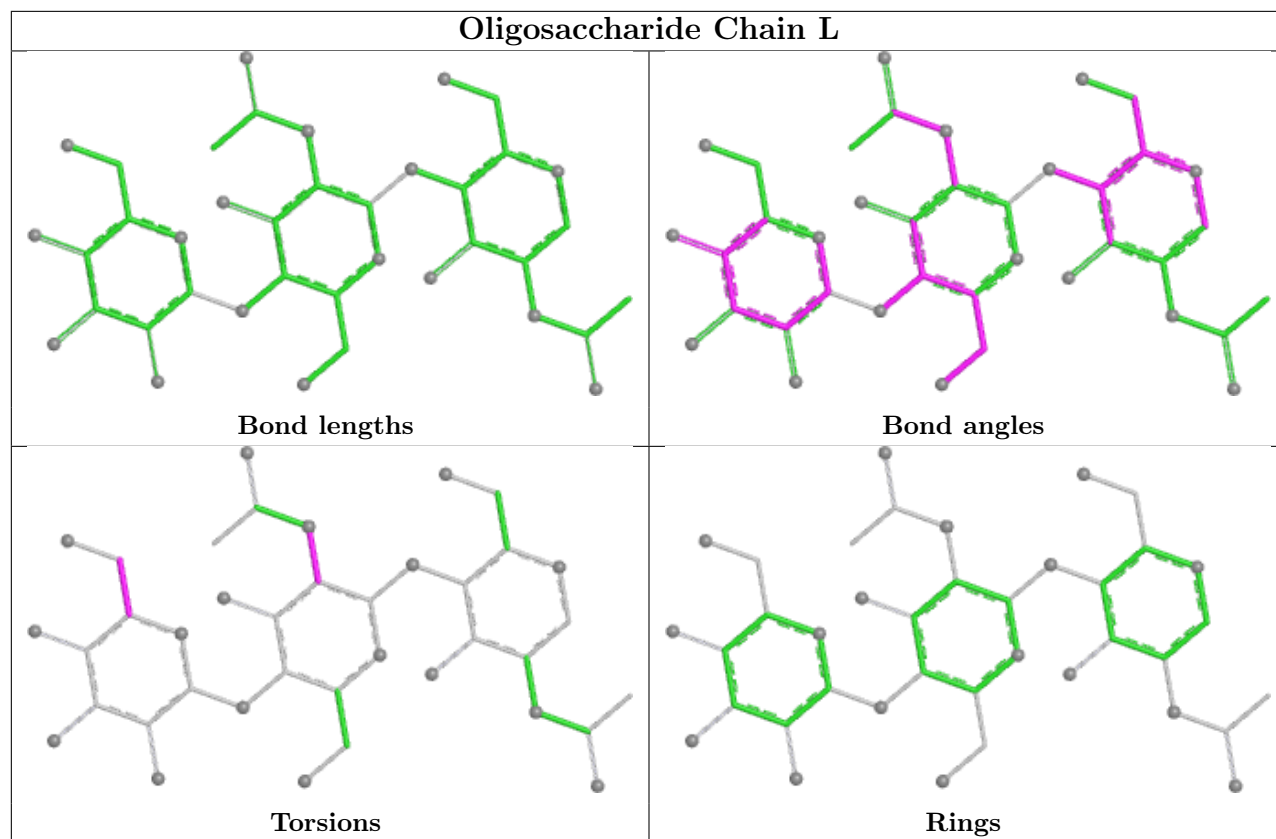
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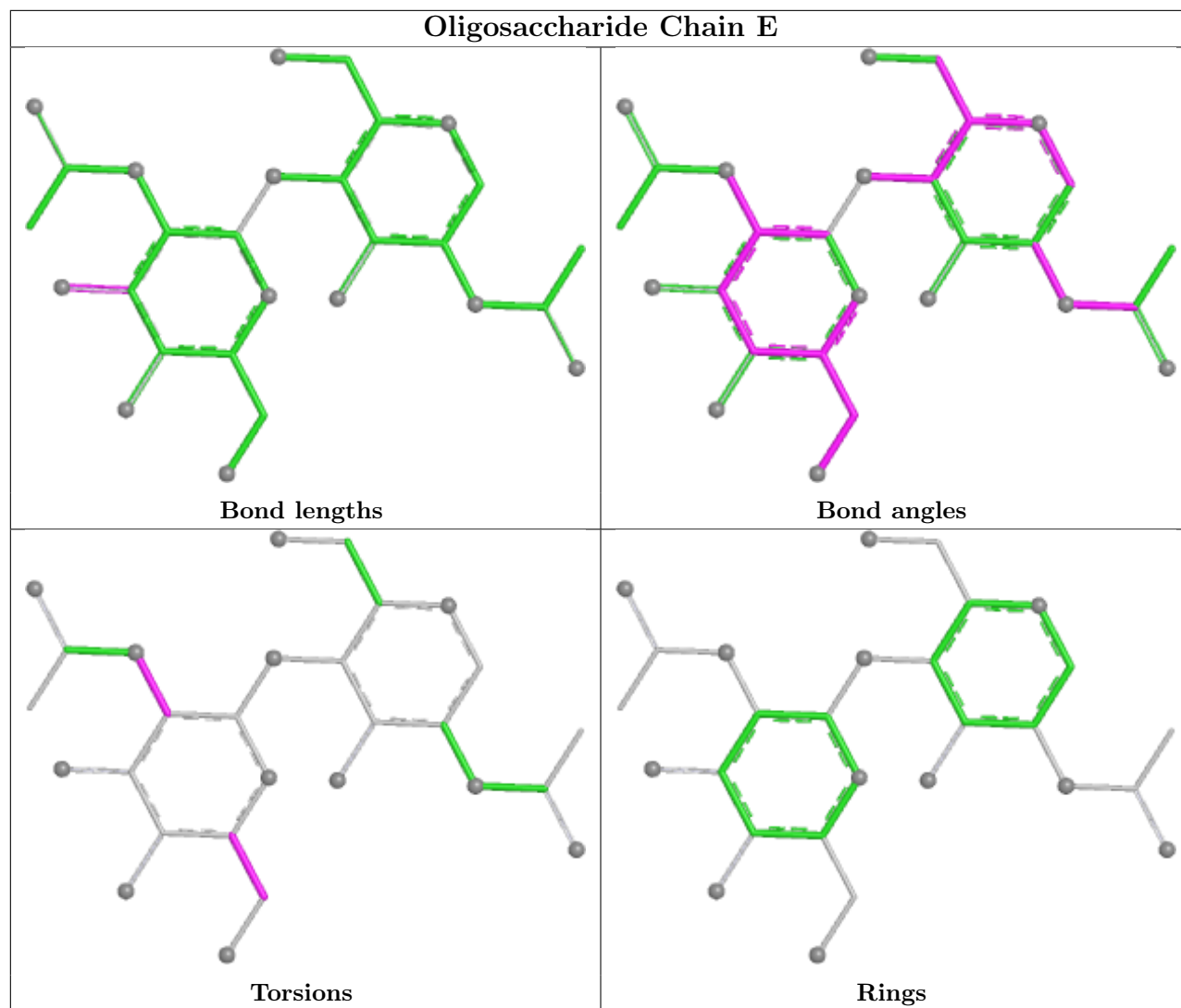
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	3	BMA	2	0
9	K	1	NAG	2	0
6	O	4	MAN	1	0
10	P	3	BMA	1	0
2	C	2	NAG	1	0
3	D	3	BMA	1	0

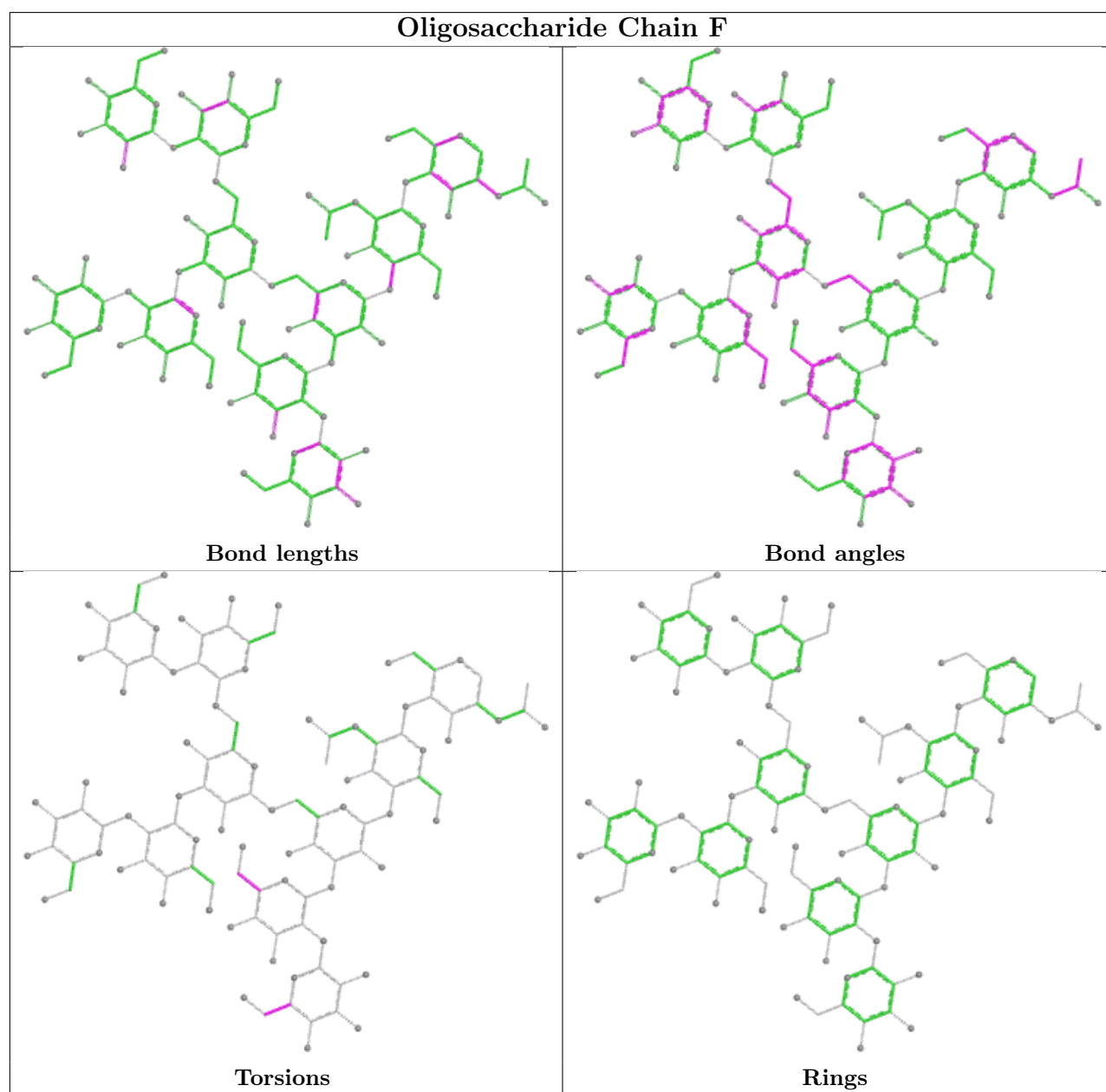
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

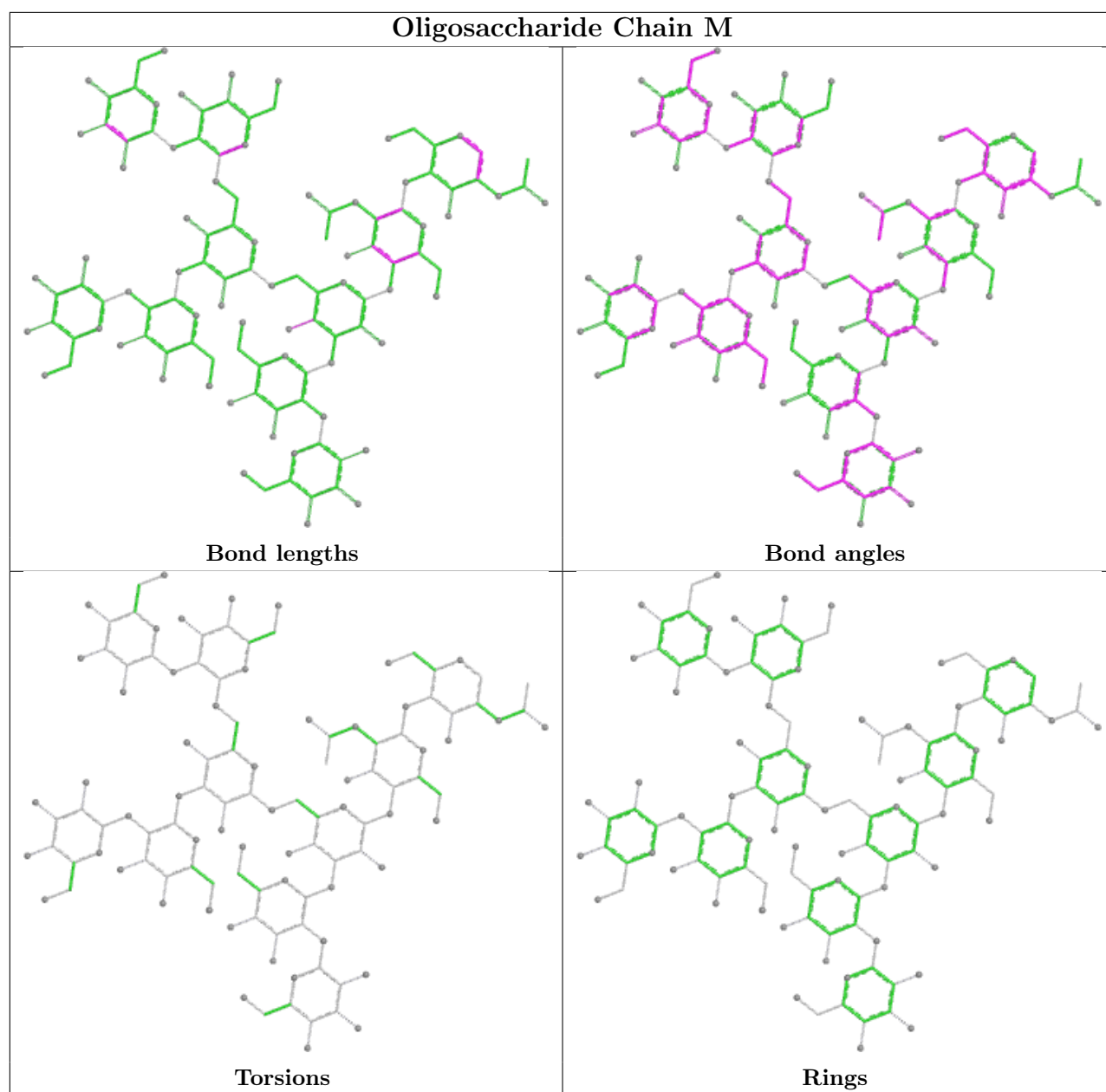


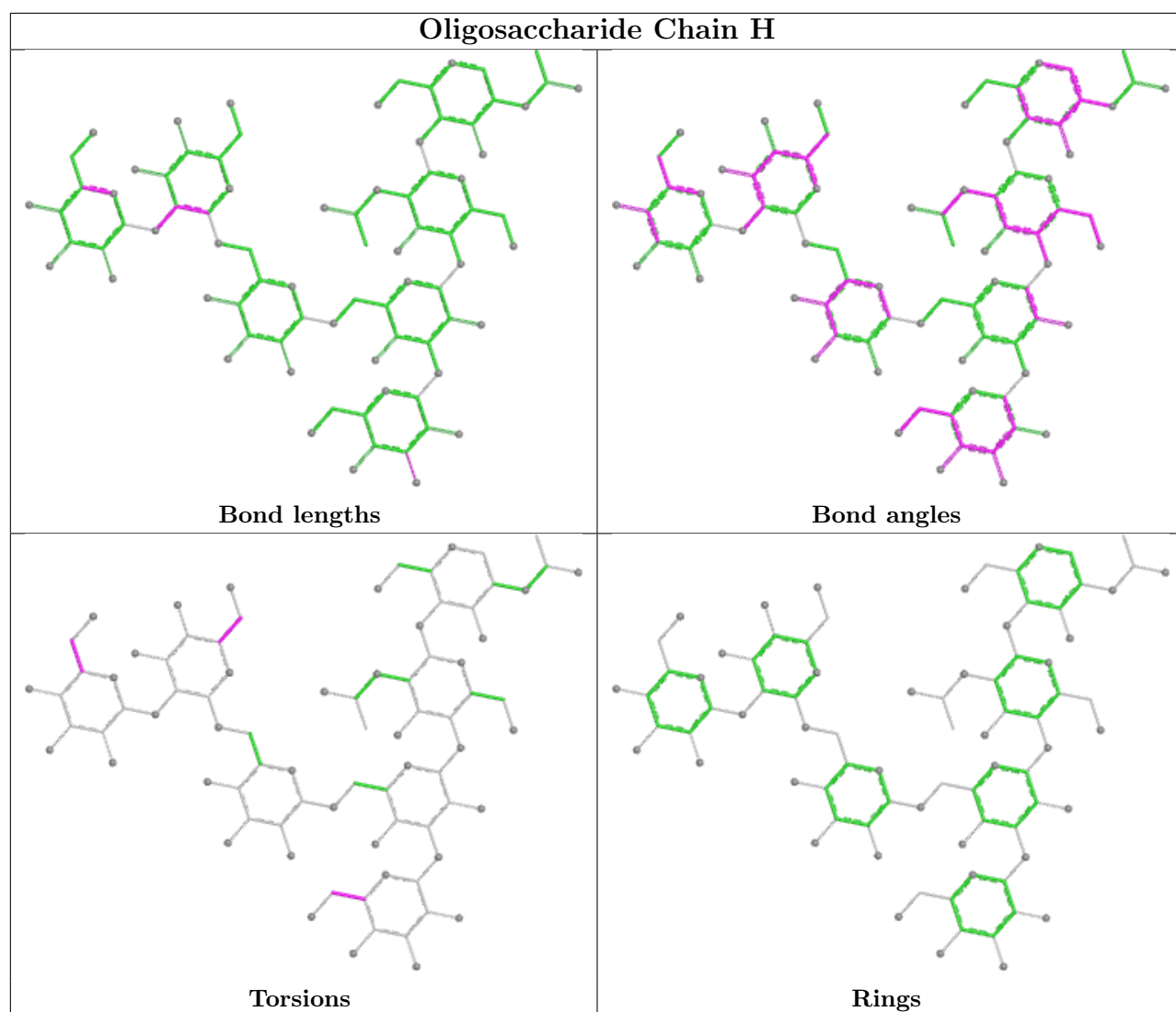


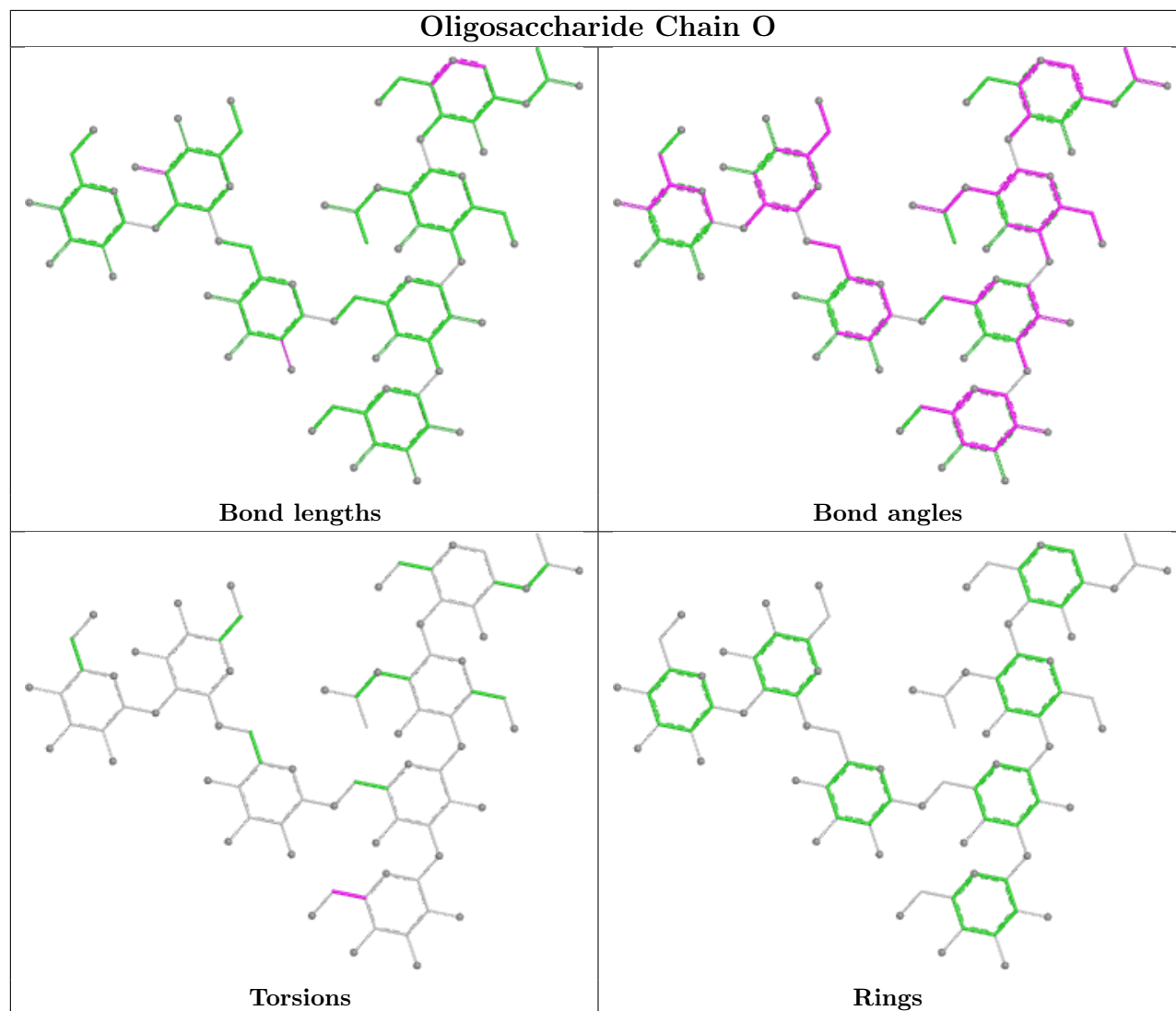


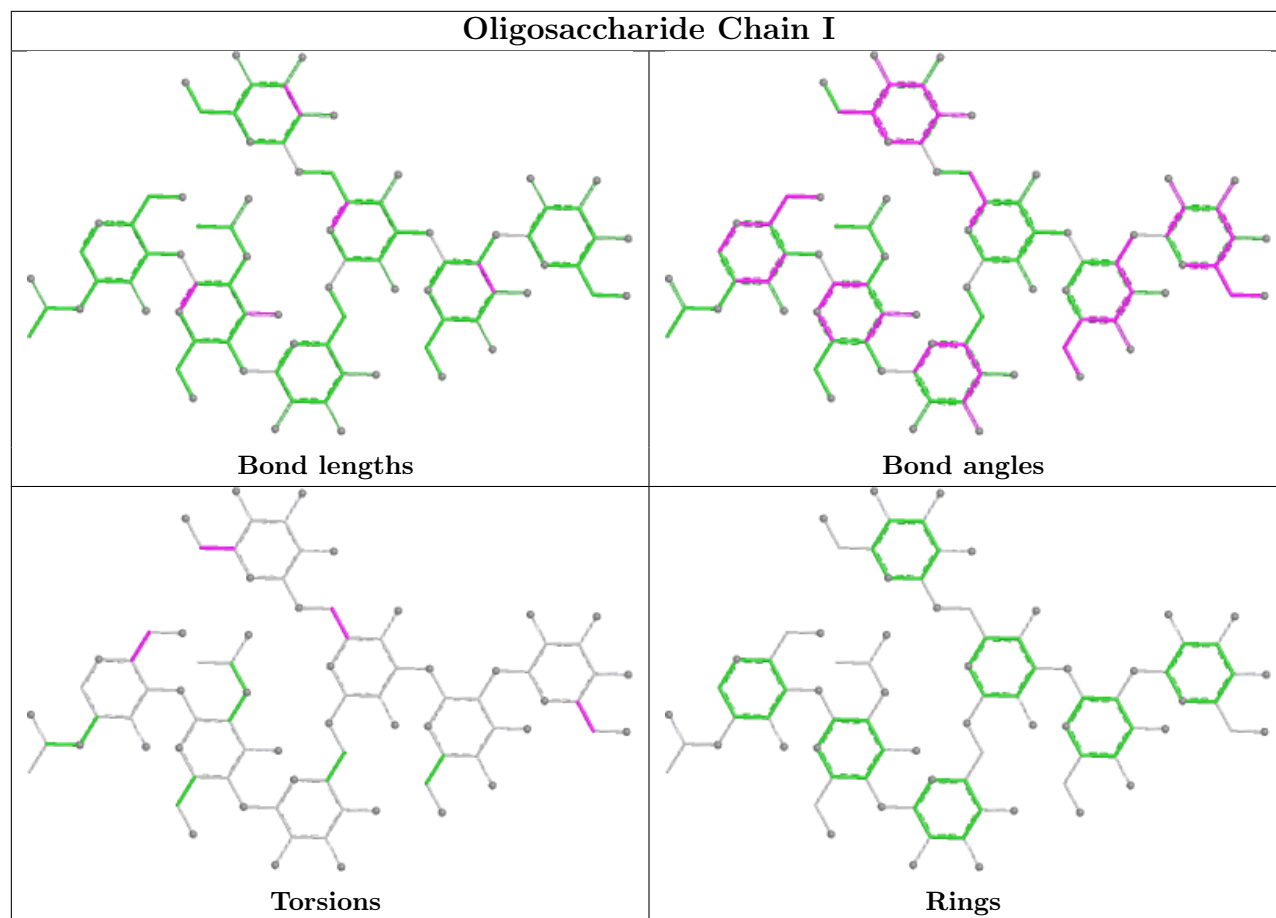




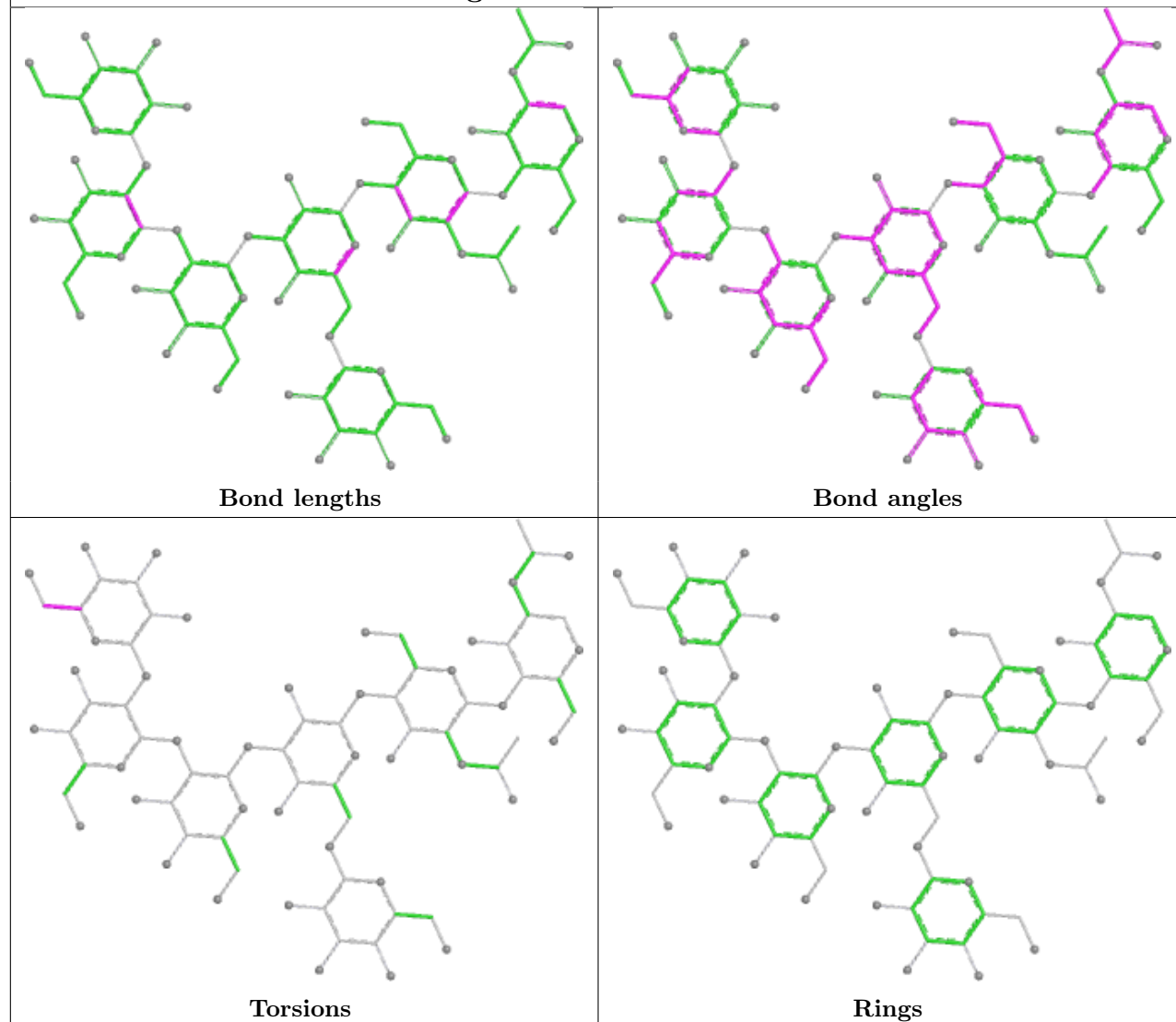


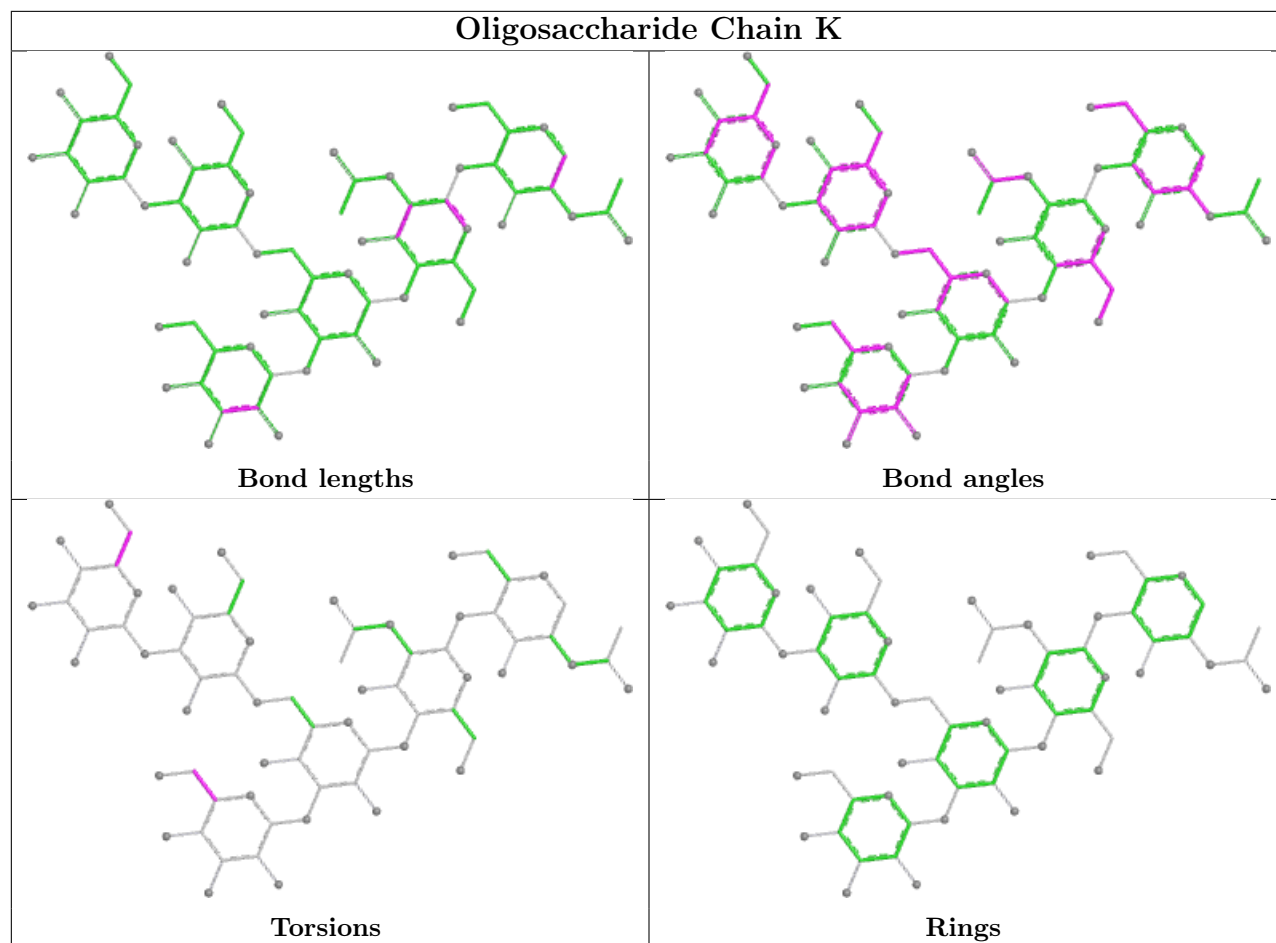


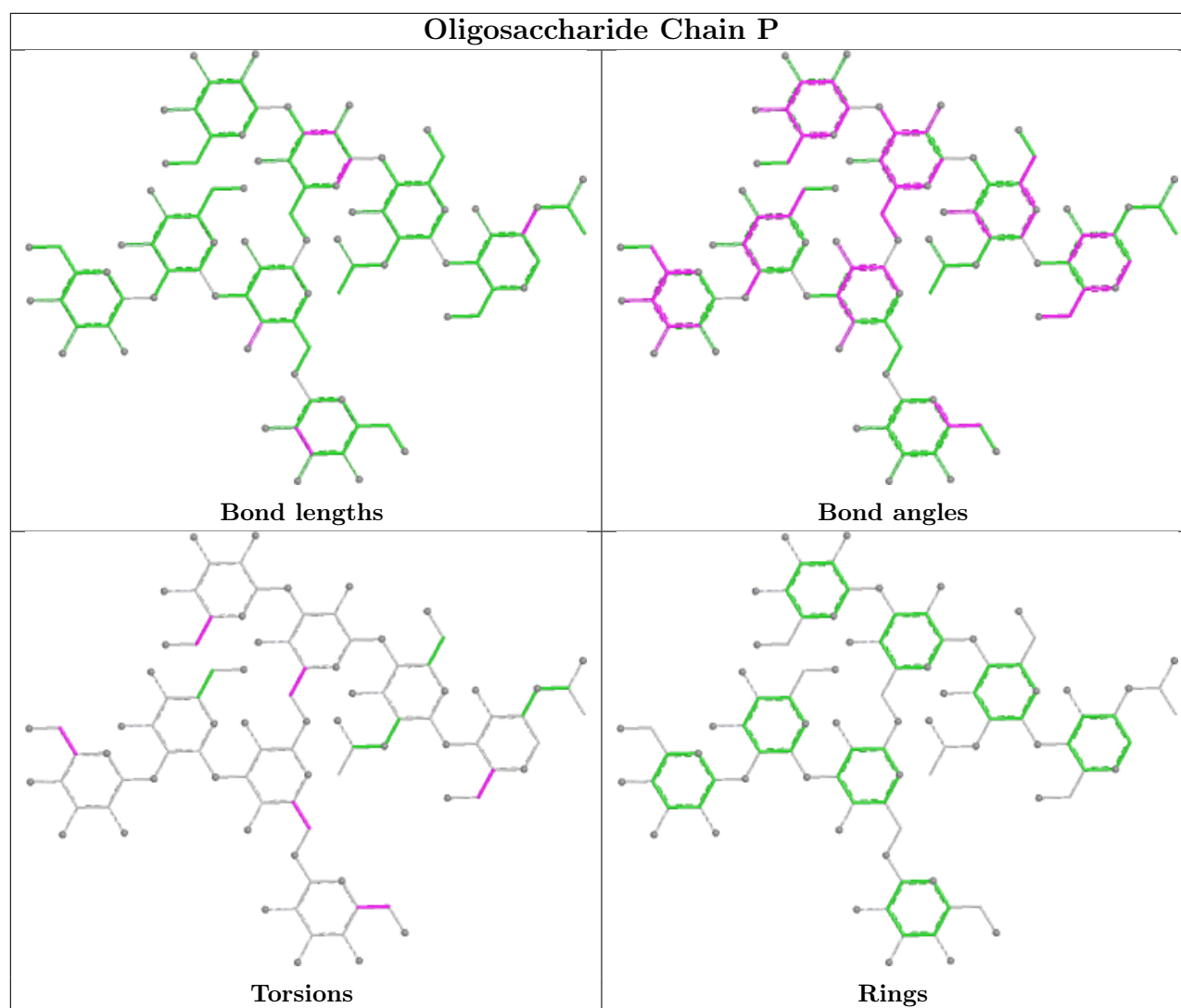




Oligosaccharide Chain J







5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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	938	1	14,14,15	0.80	1 (7%)	17,19,21	2.14	7 (41%)
14	CGB	B	952	-	11,13,13	2.70	4 (36%)	12,21,21	8.72	9 (75%)
12	MRD	B	950	-	7,7,7	1.02	1 (14%)	9,10,10	0.97	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MRD	B	949	-	7,7,7	1.01	0	9,10,10	1.57	2 (22%)
14	CGB	A	943	-	11,13,13	2.33	3 (27%)	12,21,21	7.63	10 (83%)
11	NAG	B	908	1	14,14,15	0.92	0	17,19,21	2.48	7 (41%)
12	MRD	B	948	-	7,7,7	1.60	1 (14%)	9,10,10	3.23	7 (77%)
12	MRD	A	939	-	7,7,7	1.29	0	9,10,10	0.60	0
11	NAG	B	946	1	14,14,15	1.04	0	17,19,21	1.88	5 (29%)
12	MRD	A	941	-	7,7,7	1.20	1 (14%)	9,10,10	1.15	1 (11%)
11	NAG	B	947	1	14,14,15	1.04	0	17,19,21	2.01	5 (29%)
12	MRD	A	940	-	7,7,7	1.47	2 (28%)	9,10,10	1.34	2 (22%)
11	NAG	A	905	1	14,14,15	0.97	1 (7%)	17,19,21	1.31	2 (11%)

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	938	1	-	0/6/23/26	0/1/1/1
14	CGB	B	952	-	-	-	0/3/2/2
12	MRD	B	950	-	-	0/5/5/5	-
12	MRD	B	949	-	-	4/5/5/5	-
14	CGB	A	943	-	-	-	0/3/2/2
11	NAG	B	908	1	-	6/6/23/26	0/1/1/1
12	MRD	B	948	-	-	0/5/5/5	-
12	MRD	A	939	-	-	0/5/5/5	-
11	NAG	B	946	1	-	0/6/23/26	0/1/1/1
12	MRD	A	941	-	-	0/5/5/5	-
11	NAG	B	947	1	-	2/6/23/26	0/1/1/1
12	MRD	A	940	-	-	3/5/5/5	-
11	NAG	A	905	1	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	952	CGB	C8-C2	-5.99	1.45	1.53
14	A	943	CGB	C8-C2	-5.96	1.45	1.53
14	B	952	CGB	C6-N1	4.18	1.51	1.47
12	B	948	MRD	C3-C2	3.00	1.62	1.54
14	B	952	CGB	O4-C4	-2.99	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	952	CGB	O3-C3	2.89	1.48	1.42
14	A	943	CGB	C4-C3	-2.88	1.48	1.53
14	A	943	CGB	O3-C3	2.75	1.48	1.42
12	A	940	MRD	CM-C2	-2.24	1.45	1.52
12	B	950	MRD	O2-C2	-2.21	1.39	1.44
12	A	941	MRD	CM-C2	2.14	1.58	1.52
11	A	905	NAG	O5-C1	-2.07	1.40	1.43
11	A	938	NAG	O3-C3	-2.03	1.37	1.43
12	A	940	MRD	O2-C2	-2.03	1.39	1.44

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	952	CGB	C7-C6-C5	-27.93	87.84	113.30
14	A	943	CGB	C7-C6-C5	-23.28	92.07	113.30
14	A	943	CGB	O4-C4-C5	7.16	127.25	110.38
14	B	952	CGB	O4-C4-C5	5.43	123.18	110.38
14	A	943	CGB	O3-C3-C2	5.24	123.14	109.92
11	B	947	NAG	C1-O5-C5	-5.16	105.27	112.19
11	B	908	NAG	C8-C7-N2	5.16	124.68	116.12
14	B	952	CGB	C4-C5-C6	-4.91	103.81	111.02
14	B	952	CGB	O3-C3-C2	4.87	122.21	109.92
11	B	908	NAG	C2-N2-C7	4.83	129.38	122.90
12	B	948	MRD	O2-C2-C1	4.53	122.11	107.99
12	B	948	MRD	O2-C2-C3	-4.26	93.32	109.27
14	B	952	CGB	O4-C4-C3	4.24	118.62	109.77
11	A	938	NAG	C2-N2-C7	-4.22	117.24	122.90
14	A	943	CGB	C8-C2-C3	4.13	118.31	111.29
14	A	943	CGB	O4-C4-C3	3.95	118.00	109.77
11	B	946	NAG	O7-C7-C8	-3.84	115.22	122.05
12	B	948	MRD	C1-C2-C3	-3.82	93.73	110.20
12	B	948	MRD	O2-C2-CM	3.81	119.85	107.99
14	B	952	CGB	C8-C2-C3	3.67	117.53	111.29
11	B	946	NAG	O5-C5-C6	3.58	114.64	107.66
11	A	938	NAG	C8-C7-N2	3.52	121.95	116.12
11	A	938	NAG	O5-C1-C2	3.48	116.68	111.29
11	B	908	NAG	C4-C3-C2	-3.39	106.05	111.02
14	A	943	CGB	O5-C5-C6	-3.36	102.42	109.40
14	A	943	CGB	C4-C5-C6	-3.36	106.10	111.02
11	B	908	NAG	O7-C7-N2	-3.27	116.20	121.98
12	B	948	MRD	CM-C2-C3	-3.27	96.10	110.20
11	B	908	NAG	O5-C1-C2	-3.17	106.38	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	952	CGB	O3-C3-C4	3.12	117.05	110.00
12	B	949	MRD	O4-C4-C3	-3.10	99.01	111.35
11	A	905	NAG	C1-C2-N2	3.02	115.19	110.43
11	A	938	NAG	C1-O5-C5	2.96	116.16	112.19
11	B	946	NAG	O3-C3-C4	-2.78	103.82	110.38
12	B	948	MRD	O4-C4-C5	-2.68	97.90	109.45
14	B	952	CGB	C5-C4-C3	2.60	114.89	111.18
12	A	941	MRD	O2-C2-CM	2.60	116.08	107.99
14	A	943	CGB	O3-C3-C4	2.58	115.83	110.00
12	B	948	MRD	CM-C2-C1	2.55	116.33	110.63
11	B	947	NAG	O4-C4-C3	-2.53	104.42	110.38
11	B	947	NAG	C3-C4-C5	-2.53	105.65	110.23
12	B	949	MRD	O2-C2-C1	2.53	115.86	107.99
12	A	940	MRD	O2-C2-C3	-2.52	99.86	109.27
14	A	943	CGB	C7-C6-N1	-2.51	98.60	103.19
11	A	938	NAG	O7-C7-N2	-2.33	117.87	121.98
12	B	950	MRD	O4-C4-C3	-2.29	102.24	111.35
11	B	908	NAG	O5-C5-C6	2.28	112.10	107.66
11	A	938	NAG	O3-C3-C4	-2.27	105.02	110.38
11	A	938	NAG	O6-C6-C5	-2.25	103.68	111.33
14	A	943	CGB	O5-C5-C4	-2.23	105.13	110.38
14	B	952	CGB	C7-C6-N1	-2.19	99.19	103.19
11	A	905	NAG	O7-C7-C8	-2.18	118.17	122.05
12	A	940	MRD	O4-C4-C3	-2.17	102.72	111.35
11	B	946	NAG	C1-C2-N2	2.12	113.78	110.43
11	B	947	NAG	O3-C3-C4	-2.11	105.39	110.38
11	B	947	NAG	O5-C5-C6	2.11	111.76	107.66
11	B	946	NAG	C4-C3-C2	2.08	114.07	111.02
11	B	908	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	908	NAG	C1-C2-N2-C7
12	B	949	MRD	C2-C3-C4-O4
12	B	949	MRD	C2-C3-C4-C5
11	B	908	NAG	C8-C7-N2-C2
11	B	908	NAG	O7-C7-N2-C2
11	B	947	NAG	O5-C5-C6-O6
11	B	947	NAG	C4-C5-C6-O6
11	B	908	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	B	908	NAG	O5-C5-C6-O6
12	B	949	MRD	C1-C2-C3-C4
12	A	940	MRD	C2-C3-C4-C5
11	B	908	NAG	C3-C2-N2-C7
12	A	940	MRD	C1-C2-C3-C4
12	A	940	MRD	CM-C2-C3-C4
12	B	949	MRD	CM-C2-C3-C4

There are no ring outliers.

7 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	952	CGB	7	0
12	B	950	MRD	3	0
12	B	949	MRD	1	0
14	A	943	CGB	8	0
12	B	948	MRD	1	0
12	A	939	MRD	2	0
12	A	940	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	834/841 (99%)	-0.71	2 (0%) 91 90	11, 20, 34, 63	0
1	B	832/841 (98%)	-0.90	0 100 100	9, 16, 28, 53	0
All	All	1666/1682 (99%)	-0.80	2 (0%) 92 91	9, 17, 31, 63	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	669	ALA	3.7
1	A	699	GLY	2.4

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	MAN	P	8	11/12	0.66	0.18	58,71,82,84	0
9	MAN	K	6	11/12	0.69	0.18	57,62,68,68	0
7	MAN	I	7	11/12	0.76	0.15	50,54,60,73	0
3	BMA	G	3	11/12	0.76	0.15	46,60,73,77	0
10	MAN	P	7	11/12	0.76	0.16	47,56,66,68	0
3	BMA	L	3	11/12	0.76	0.13	55,65,76,80	0
6	MAN	H	7	11/12	0.77	0.14	54,60,65,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	O	7	11/12	0.77	0.14	62,71,74,79	0
7	MAN	I	6	11/12	0.78	0.17	54,58,62,66	0
2	MAN	C	4	11/12	0.78	0.12	45,52,65,71	0
9	MAN	K	5	11/12	0.78	0.16	68,74,76,85	0
3	BMA	D	3	11/12	0.79	0.11	42,48,57,62	0
10	MAN	P	6	11/12	0.80	0.14	49,52,56,61	0
9	MAN	K	4	11/12	0.81	0.13	56,66,70,70	0
10	BMA	P	3	11/12	0.83	0.15	37,41,54,60	0
2	BMA	C	3	11/12	0.84	0.11	36,44,48,53	0
7	BMA	I	3	11/12	0.85	0.13	30,41,52,63	0
3	NAG	G	2	14/15	0.85	0.14	42,50,61,69	0
3	BMA	N	3	11/12	0.86	0.11	43,52,60,62	0
8	MAN	J	7	11/12	0.89	0.09	27,31,36,38	0
10	MAN	P	4	11/12	0.90	0.11	31,34,43,48	0
5	MAN	M	10	11/12	0.90	0.09	30,37,41,42	0
5	MAN	F	10	11/12	0.91	0.10	39,40,50,51	0
9	BMA	K	3	11/12	0.91	0.08	40,44,54,60	0
10	NAG	P	2	14/15	0.92	0.09	26,30,37,39	0
7	MAN	I	4	11/12	0.92	0.09	24,30,38,45	0
6	MAN	H	4	11/12	0.92	0.08	27,30,40,43	0
8	MAN	J	6	11/12	0.93	0.09	26,30,35,42	0
5	MAN	F	5	11/12	0.93	0.07	23,30,33,42	0
7	MAN	I	5	11/12	0.93	0.08	28,34,44,44	0
10	MAN	P	5	11/12	0.93	0.09	28,35,42,47	0
6	NAG	H	2	14/15	0.93	0.07	20,26,32,40	0
4	NAG	E	2	14/15	0.93	0.07	30,33,48,53	0
8	MAN	J	5	11/12	0.93	0.08	28,34,42,49	0
7	NAG	I	2	14/15	0.94	0.07	23,27,36,42	0
3	NAG	N	2	14/15	0.94	0.09	31,33,46,48	0
3	NAG	D	2	14/15	0.94	0.07	25,29,34,37	0
6	BMA	O	3	11/12	0.94	0.07	23,27,34,46	0
6	MAN	O	4	11/12	0.94	0.07	25,27,37,39	0
5	MAN	F	6	11/12	0.94	0.07	33,38,43,44	0
8	MAN	J	4	11/12	0.94	0.06	27,32,39,43	0
7	NAG	I	1	14/15	0.95	0.06	21,23,25,26	0
5	MAN	F	9	11/12	0.95	0.06	27,31,34,36	0
6	MAN	H	5	11/12	0.95	0.07	21,24,34,41	0
2	NAG	C	2	14/15	0.95	0.07	24,32,43,48	0
9	NAG	K	2	14/15	0.95	0.07	20,27,31,35	0
3	NAG	G	1	14/15	0.95	0.07	25,29,36,38	0
6	NAG	H	1	14/15	0.95	0.07	20,22,41,47	0
3	NAG	L	2	14/15	0.95	0.07	19,26,41,45	0

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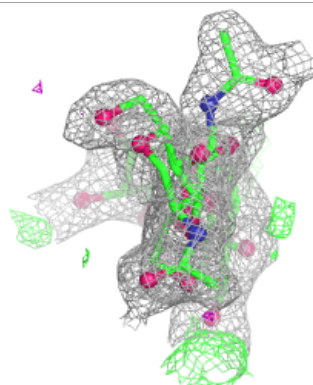
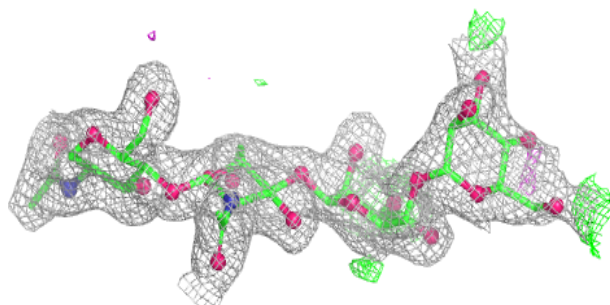
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	H	6	11/12	0.96	0.06	21,24,37,43	0
5	NAG	F	1	14/15	0.96	0.07	26,28,33,35	0
6	NAG	O	1	14/15	0.96	0.07	16,21,36,38	0
6	NAG	O	2	14/15	0.96	0.06	19,24,32,33	0
10	NAG	P	1	14/15	0.96	0.06	19,21,23,24	0
5	BMA	F	3	11/12	0.96	0.07	24,26,29,32	0
8	BMA	J	3	11/12	0.96	0.05	20,24,26,27	0
3	NAG	D	1	14/15	0.96	0.05	22,25,27,27	0
6	MAN	O	6	11/12	0.96	0.06	20,24,30,34	0
6	BMA	H	3	11/12	0.96	0.06	23,27,34,43	0
5	MAN	M	5	11/12	0.96	0.05	18,22,25,33	0
5	MAN	M	6	11/12	0.96	0.07	24,29,33,36	0
5	MAN	M	8	11/12	0.97	0.05	17,19,20,24	0
3	NAG	N	1	14/15	0.97	0.06	22,28,32,33	0
5	MAN	F	8	11/12	0.97	0.05	23,24,26,26	0
5	NAG	F	2	14/15	0.97	0.05	21,23,27,27	0
8	NAG	J	2	14/15	0.97	0.05	15,18,23,29	0
6	MAN	O	5	11/12	0.97	0.05	21,22,29,34	0
4	NAG	E	1	14/15	0.97	0.05	19,23,27,28	0
5	NAG	M	1	14/15	0.97	0.05	16,17,24,24	0
5	NAG	M	2	14/15	0.97	0.05	12,16,18,18	0
5	MAN	F	4	11/12	0.97	0.05	20,24,26,28	0
9	NAG	K	1	14/15	0.97	0.05	17,20,22,24	0
2	NAG	C	1	14/15	0.97	0.06	17,23,26,27	0
8	NAG	J	1	14/15	0.98	0.04	14,16,18,19	0
5	BMA	M	3	11/12	0.98	0.04	17,18,19,20	0
5	MAN	M	9	11/12	0.98	0.04	19,21,25,29	0
5	MAN	M	4	11/12	0.98	0.04	16,18,19,19	0
5	MAN	F	7	11/12	0.98	0.04	20,22,25,26	0
3	NAG	L	1	14/15	0.98	0.04	13,17,21,21	0
5	MAN	M	7	11/12	0.98	0.04	16,18,18,19	0

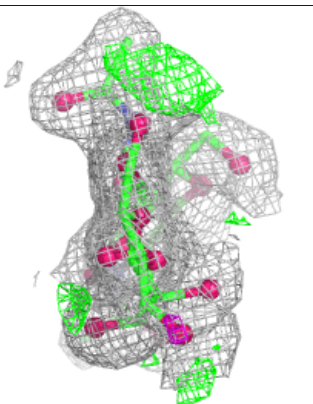
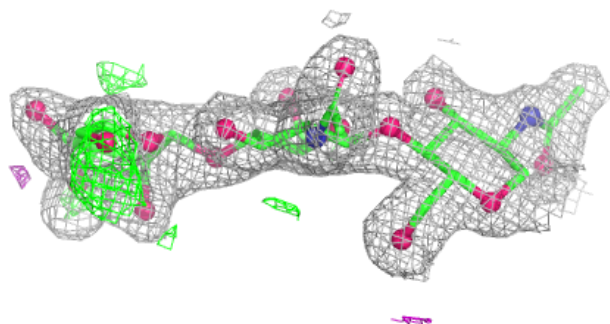
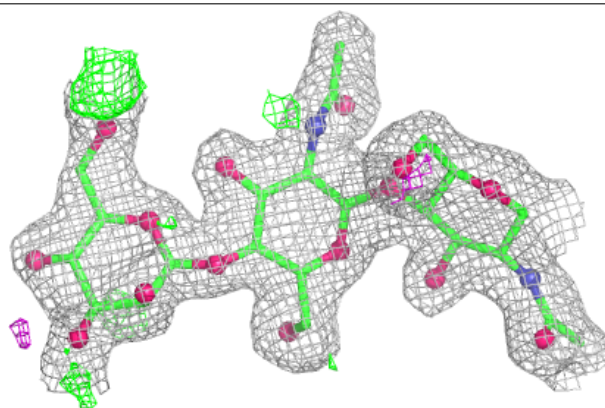
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

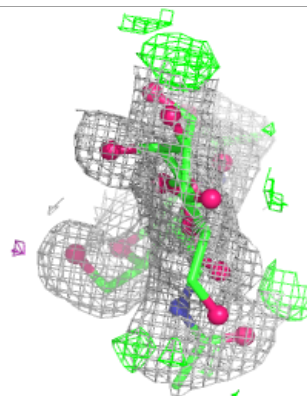
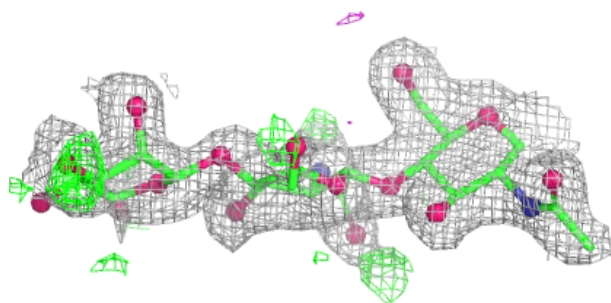
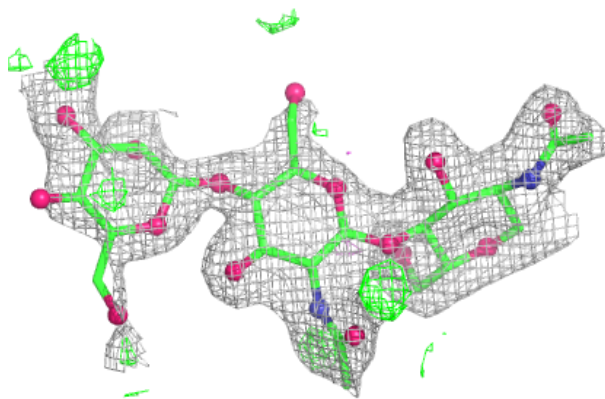
**Electron density around Chain D:**

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



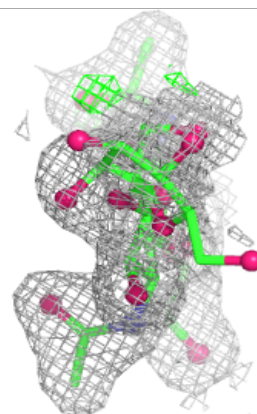
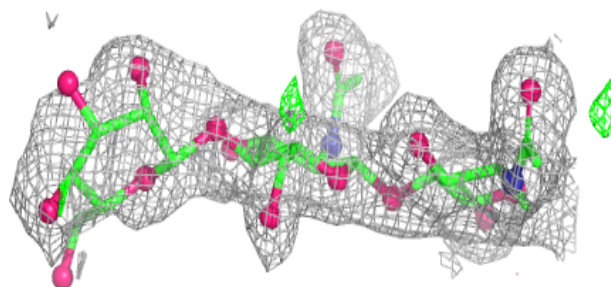
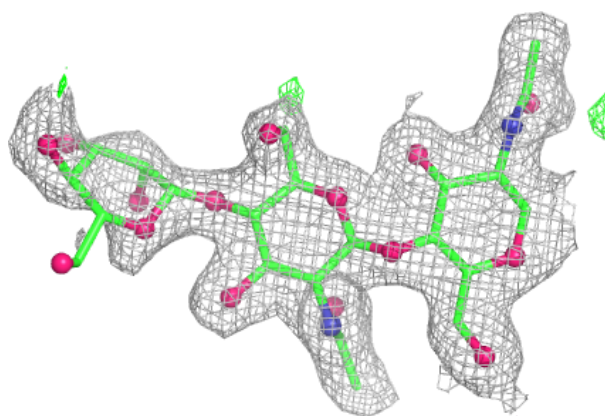
Electron density around Chain G:

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



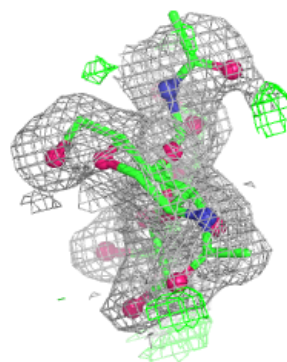
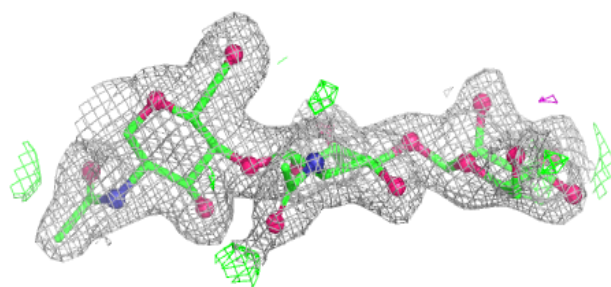
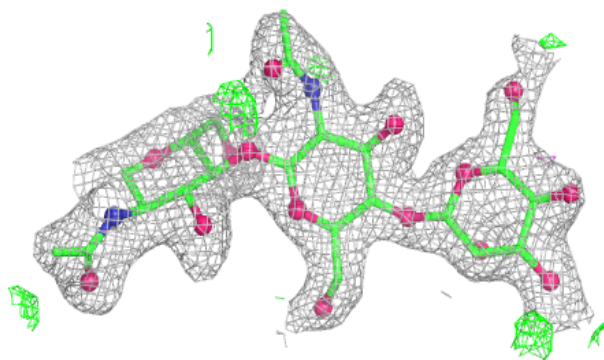
Electron density around Chain L:

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



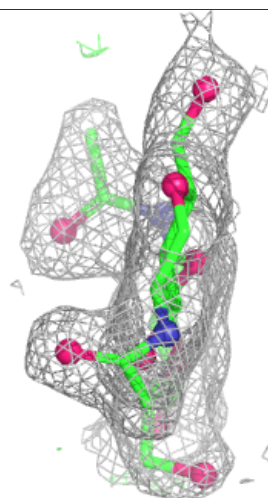
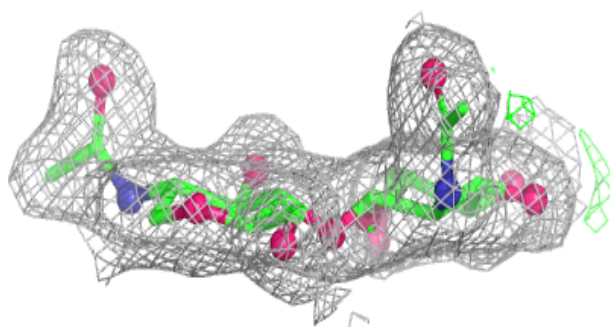
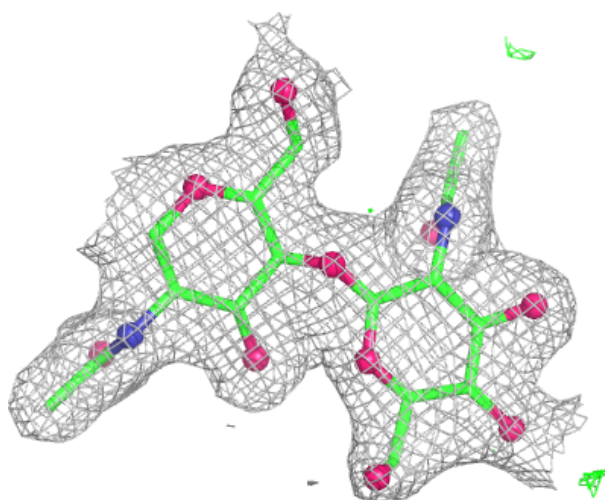
Electron density around Chain N:

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



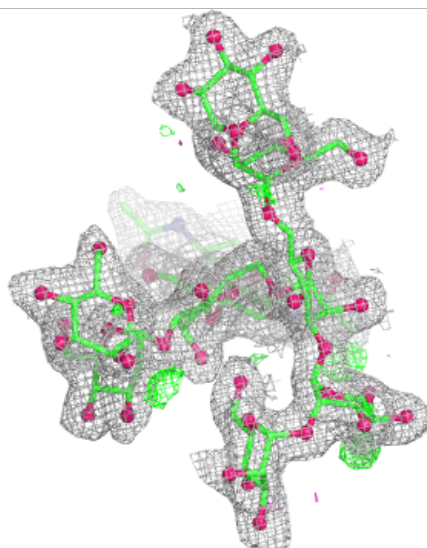
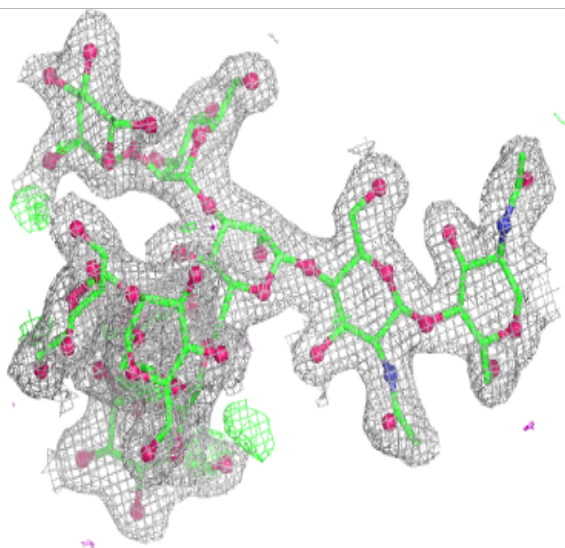
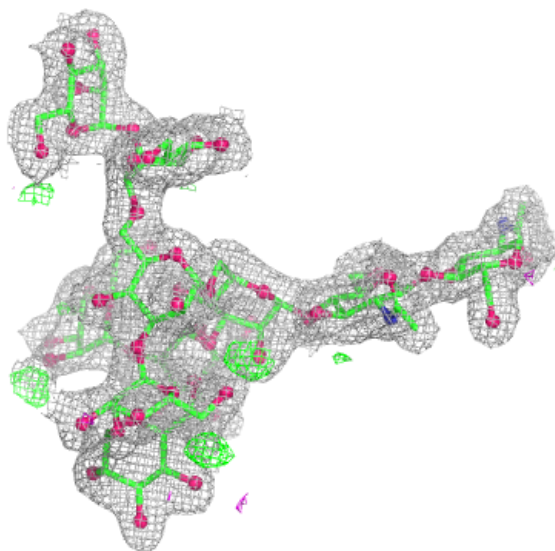
Electron density around Chain E:

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



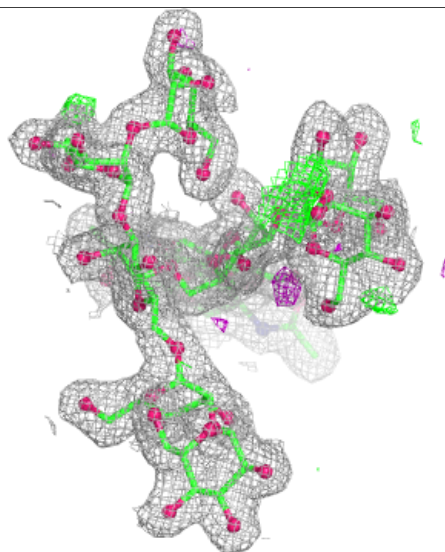
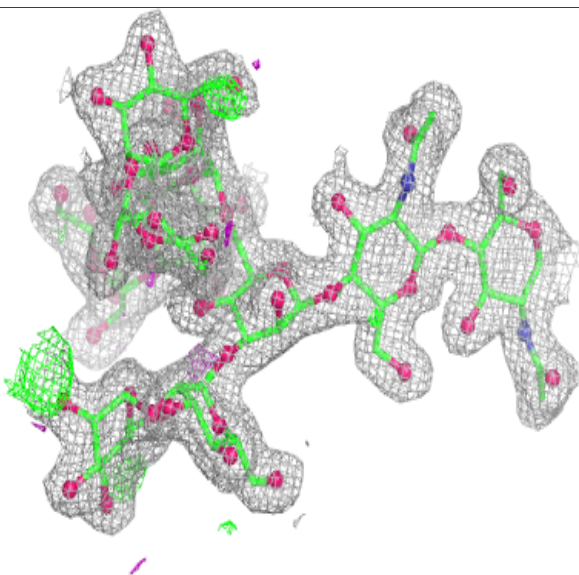
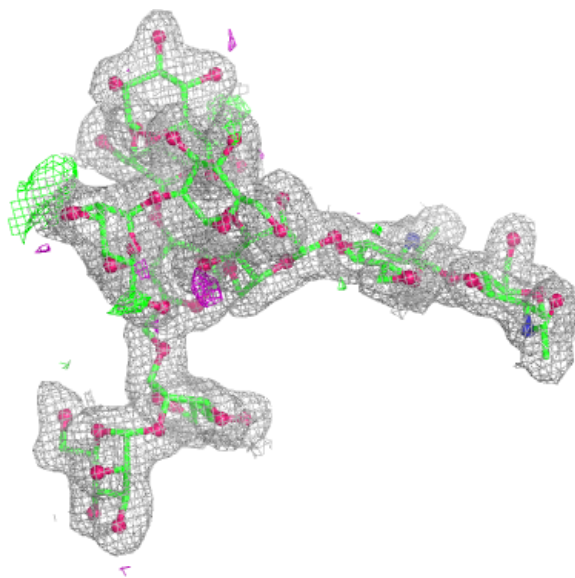
Electron density around Chain F:

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



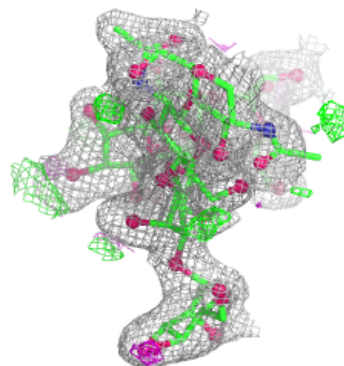
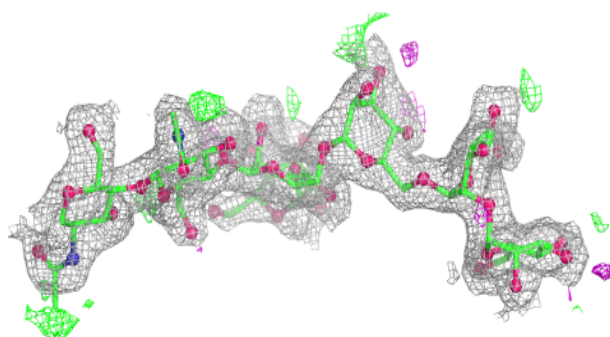
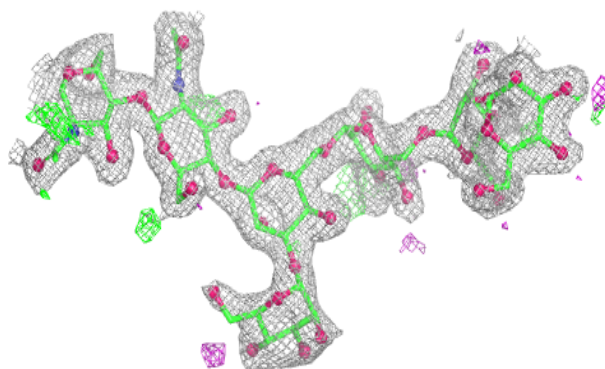
Electron density around Chain M:

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and green (positive)

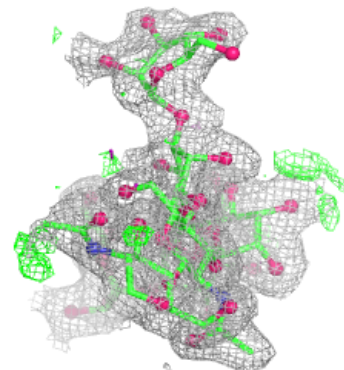
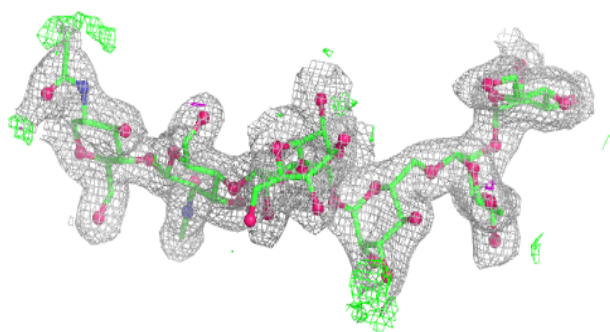
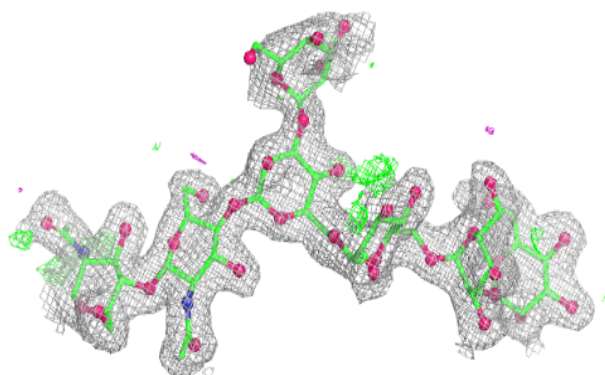


Electron density around Chain H:

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

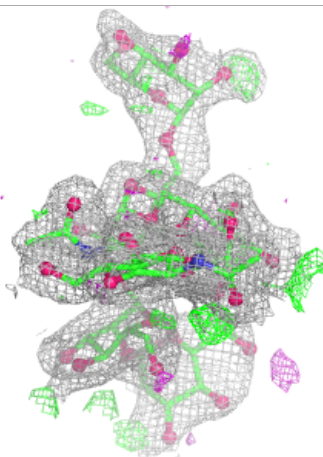
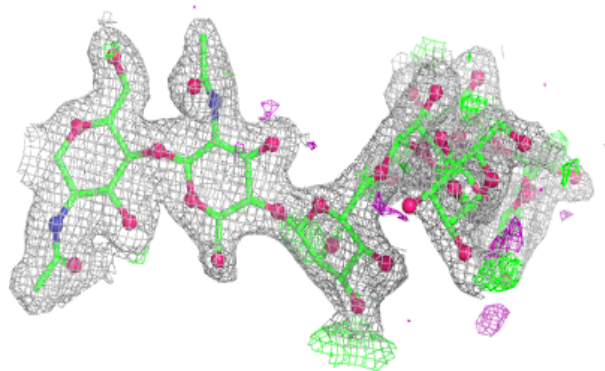
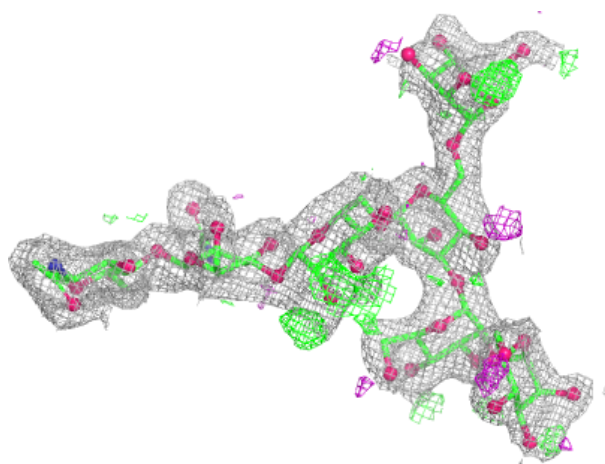
**Electron density around Chain O:**

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



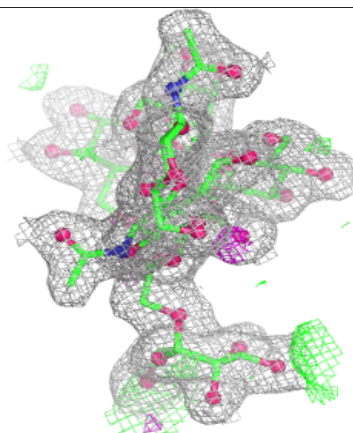
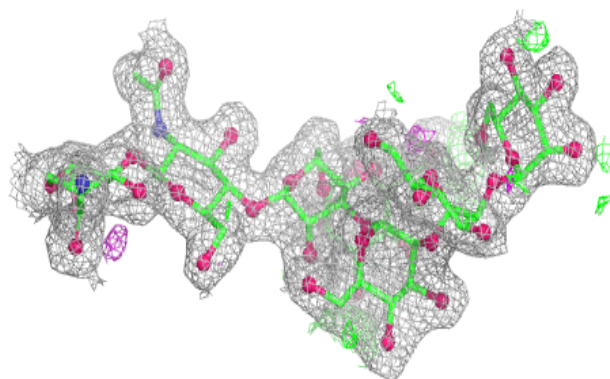
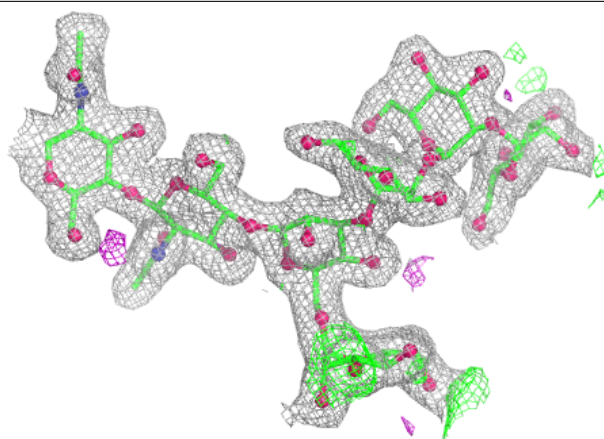
Electron density around Chain I:

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



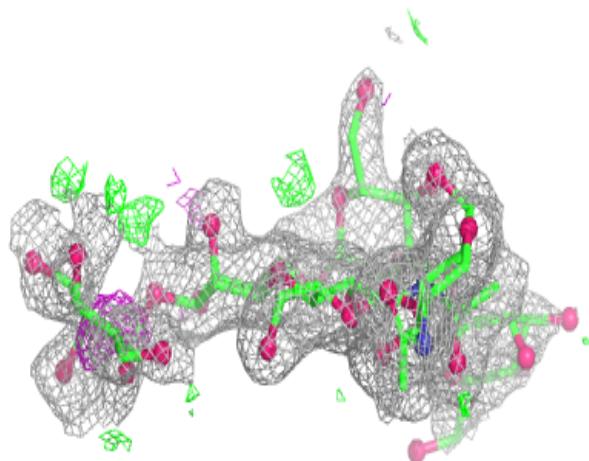
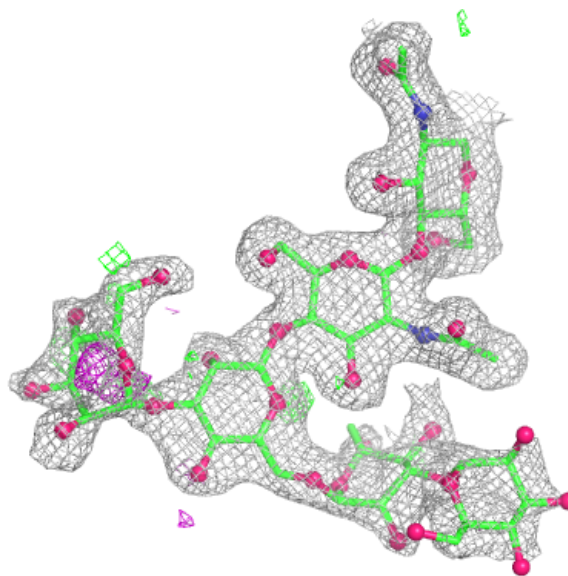
Electron density around Chain J:

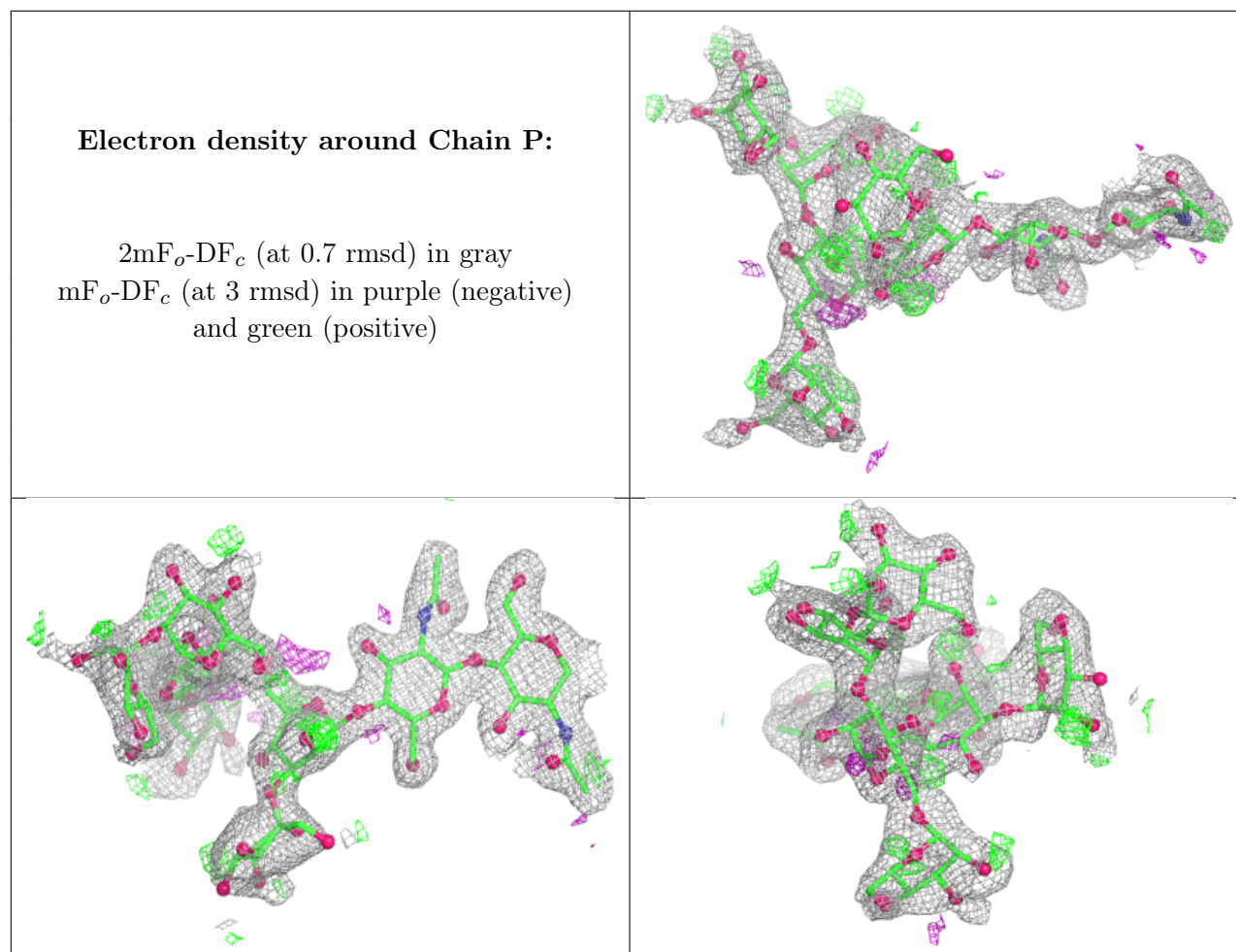
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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	B	908	14/15	0.74	0.15	43,53,59,63	0
11	NAG	A	905	14/15	0.80	0.13	51,58,69,75	0
12	MRD	A	941	8/8	0.82	0.18	34,40,45,47	0
12	MRD	A	940	8/8	0.85	0.14	21,29,41,43	0
11	NAG	B	946	14/15	0.85	0.11	38,50,53,55	0
12	MRD	B	948	8/8	0.85	0.17	31,44,52,53	0
12	MRD	B	949	8/8	0.88	0.11	21,28,35,39	0
12	MRD	B	950	8/8	0.91	0.12	33,43,45,48	0
13	NA	B	951	1/1	0.91	0.08	32,32,32,32	0
14	CGB	A	943	12/12	0.91	0.10	21,28,33,34	0
11	NAG	A	938	14/15	0.92	0.09	33,42,49,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CGB	B	952	12/12	0.94	0.08	15,23,29,29	0
12	MRD	A	939	8/8	0.95	0.07	20,25,29,31	0
11	NAG	B	947	14/15	0.95	0.06	25,31,36,38	0
13	NA	A	942	1/1	0.95	0.06	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.