



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:48 PM UTC

PDB ID : 4IIC / pdb_00004iic
Title : Crystal structure of beta-glucosidase 1 from *Aspergillus aculeatus* in complex with isofagomine
Authors : Suzuki, K.; Sumitani, J.; Kawaguchi, T.; Fushinobu, S.
Deposited on : 2012-12-20
Resolution : 1.90 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

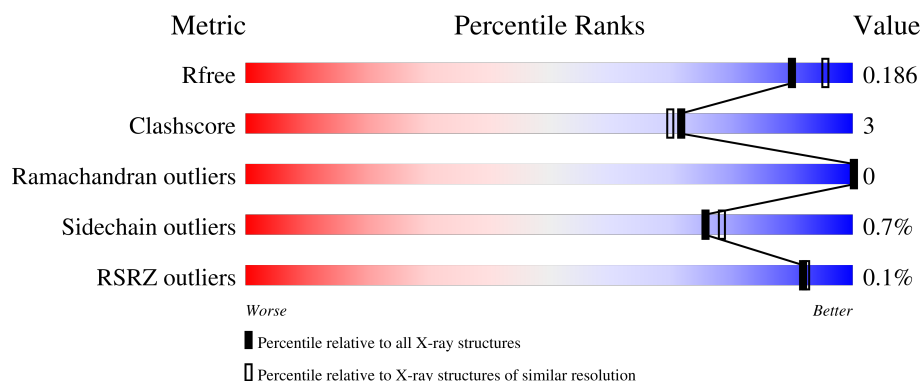
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

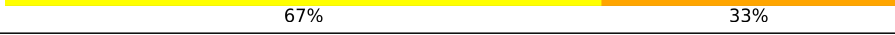
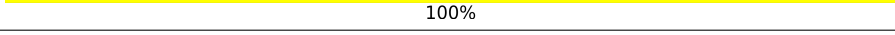
The reported resolution of this entry is 1.90 Å.

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.



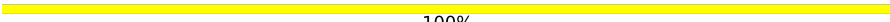
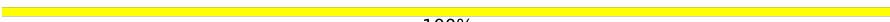
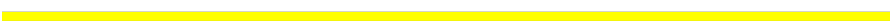
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	5	 80% 20%
3	D	3	 67% 33%
3	G	3	 100%

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Mol	Chain	Length	Quality of chain
3	L	3	 100%
3	N	3	 100%
4	E	2	 100%
5	F	10	 100%
5	M	10	 100%
6	H	7	 86% 14%
6	O	7	 86% 14%
7	I	7	 86% 14%
8	J	7	 86% 14%
9	K	4	 75% 25%
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
10	BMA	P	3	-	-	X	-
12	MRD	A	941	-	-	X	-
13	MPD	A	942	-	-	X	-

2 Entry composition [i](#)

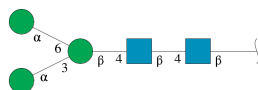
There are 16 unique types of molecules in this entry. The entry contains 15282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

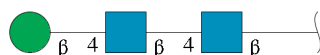
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6382	4028	1096	1240	18			
1	B	832	Total	C	N	O	S	0	0	0
			6375	4023	1095	1239	18			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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.



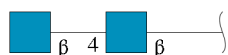
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

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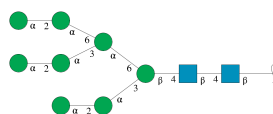
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



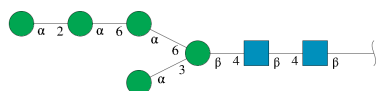
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



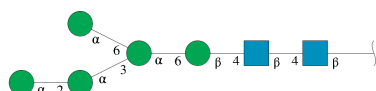
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	10	Total	C	N	O	0	0	0
			116	64	2	50			
5	M	10	Total	C	N	O	0	0	0
			116	64	2	50			

- 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.



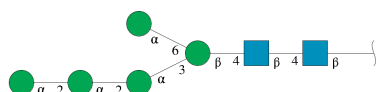
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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.



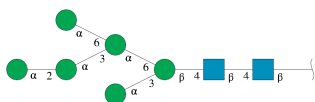
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



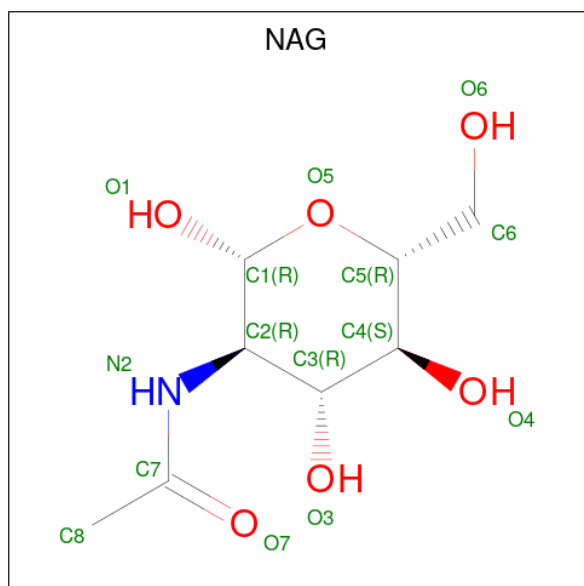
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



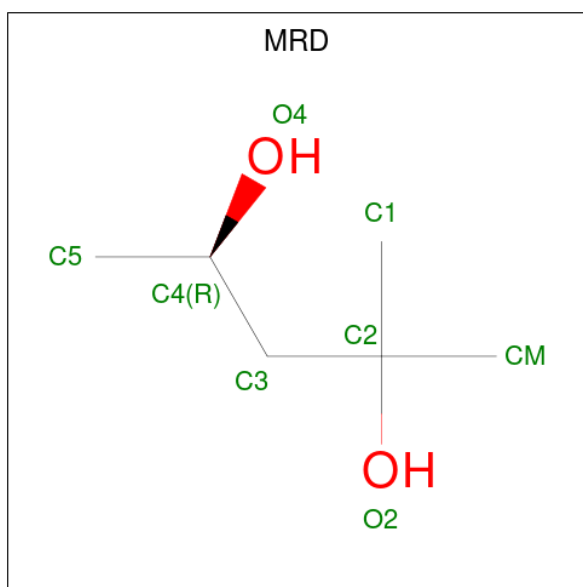
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

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



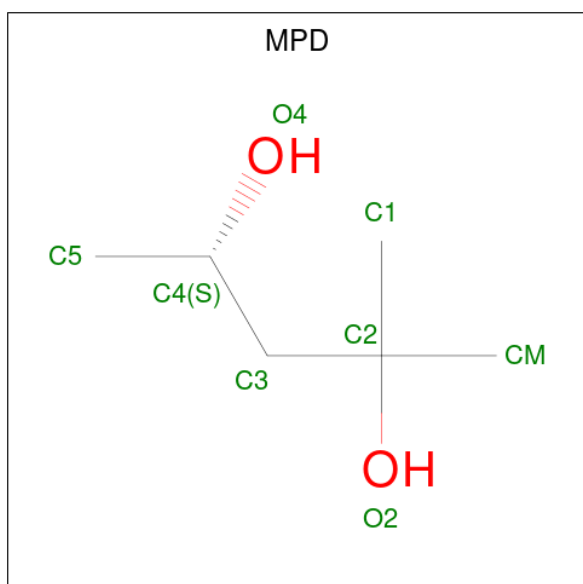
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			8	6	2		
12	A	1	Total	C	O	0	0
			8	6	2		
12	B	1	Total	C	O	0	0
			8	6	2		
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 (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).

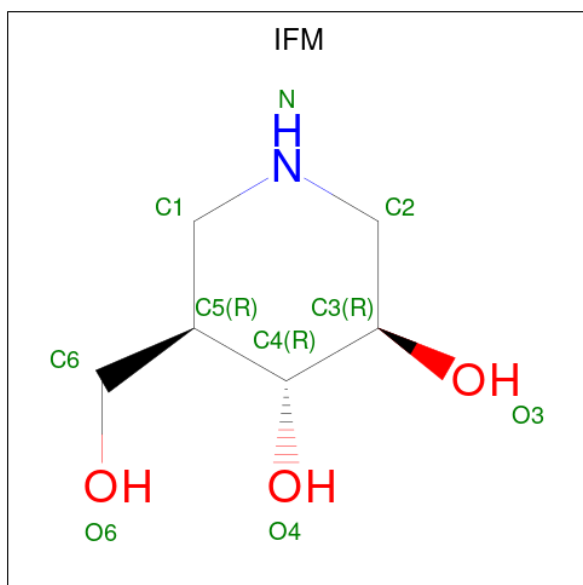


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 14 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 15 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (CCD ID: IFM) (formula: C₆H₁₃NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	N	O	0	0
			10	6	1	3		
15	B	1	Total	C	N	O	0	0
			10	6	1	3		

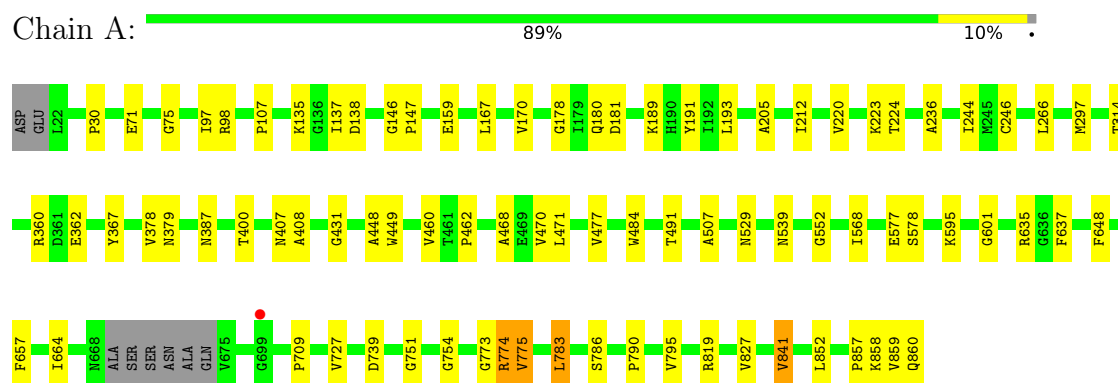
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	671	Total	O	0	0
			671	671		
16	B	761	Total	O	0	0
			761	761		

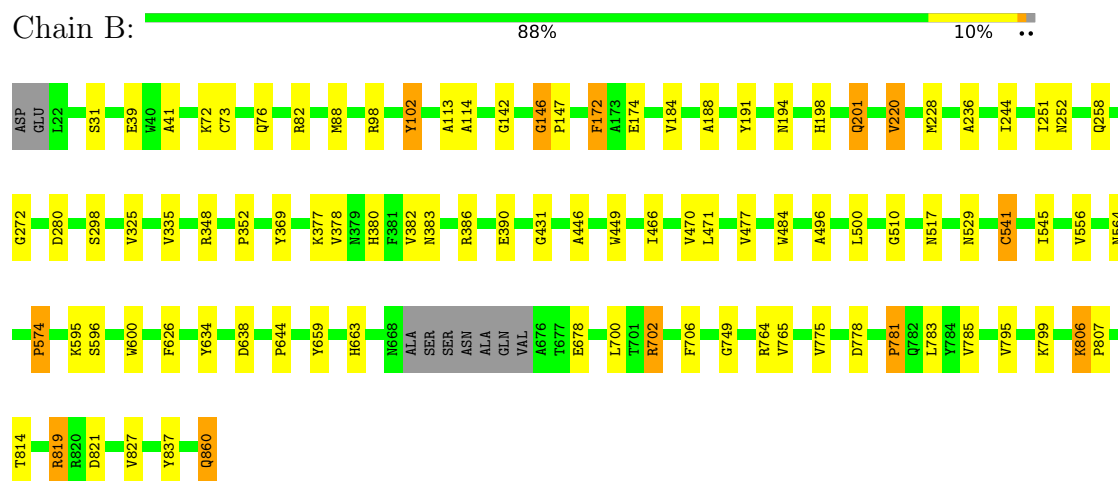
3 Residue-property plots [i](#)

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

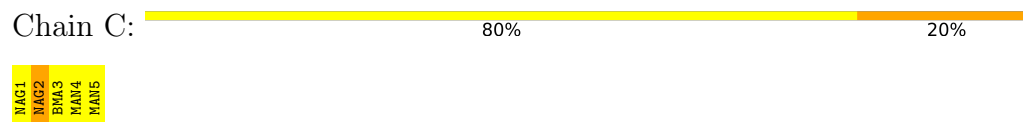
• Molecule 1: Beta-glucosidase 1



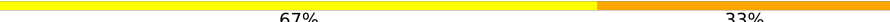
• Molecule 1: Beta-glucosidase 1



• Molecule 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

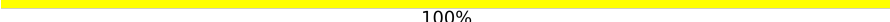


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  67% 33%

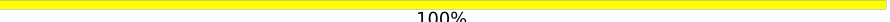
MAG1
MAG2
BMA3

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

Chain G:  100%

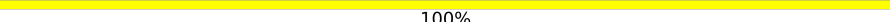
MAG1
MAG2
BMA3

- 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%

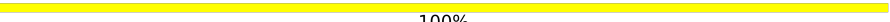
MAG1
MAG2
BMA3

- 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:  100%

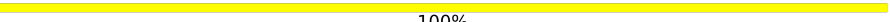
MAG1
MAG2
BMA3

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

Chain E:  100%

MAG1
MAG2

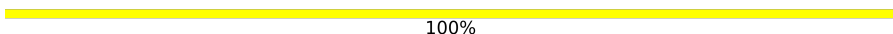
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:  86% 14%

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:  86% 14%

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:  86% 14%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

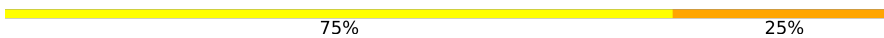
• Molecule 9: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 10: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[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 P:



NAG1
NAG2
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	82.14Å 122.48Å 222.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.23 – 1.90 37.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (37.23-1.90) 99.7 (37.23-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.145 , 0.184 0.147 , 0.186	Depositor DCC
R_{free} test set	8836 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.7	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	15282	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: MRD, BMA, MAN, IFM, NA, NAG, MPD

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	1.59	44/6545 (0.7%)	1.27	13/8923 (0.1%)
1	B	1.66	46/6538 (0.7%)	1.31	21/8913 (0.2%)
All	All	1.63	90/13083 (0.7%)	1.29	34/17836 (0.2%)

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	541	CYS	CA-CB	12.36	1.75	1.53
1	B	352	PRO	CA-C	11.31	1.58	1.51
1	B	775	VAL	N-CA	8.09	1.55	1.46
1	A	709	PRO	CA-C	8.01	1.61	1.52
1	A	471	LEU	N-CA	7.96	1.56	1.46
1	A	601	GLY	N-CA	7.65	1.54	1.45
1	B	174	GLU	N-CA	7.12	1.55	1.46
1	A	754	GLY	N-CA	7.02	1.51	1.45
1	A	181	ASP	N-CA	6.81	1.55	1.46
1	A	314	THR	N-CA	6.77	1.54	1.46
1	B	541	CYS	N-CA	6.72	1.54	1.46
1	A	635	ARG	N-CA	6.62	1.54	1.46
1	B	102	TYR	C-O	6.56	1.32	1.23
1	A	378	VAL	N-CA	6.56	1.53	1.46
1	A	224	THR	N-CA	6.48	1.54	1.46
1	A	71	GLU	CA-C	6.29	1.61	1.52
1	B	596	SER	C-N	6.19	1.38	1.33
1	A	751	GLY	N-CA	6.13	1.50	1.45
1	B	220	VAL	N-CA	6.11	1.53	1.46
1	B	795	VAL	N-CA	6.08	1.53	1.46
1	B	172	PHE	N-CA	6.07	1.53	1.46
1	B	369	TYR	CA-C	6.07	1.59	1.52
1	A	468	ALA	CA-C	6.07	1.60	1.52
1	A	751	GLY	C-O	-6.04	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	LEU	N-CA	6.02	1.53	1.46
1	B	634	TYR	N-CA	6.02	1.53	1.46
1	B	280	ASP	CA-C	6.01	1.61	1.53
1	A	431	GLY	N-CA	6.00	1.51	1.45
1	B	827	VAL	N-CA	5.99	1.54	1.46
1	A	852	LEU	N-CA	5.98	1.53	1.46
1	B	471	LEU	N-CA	5.96	1.53	1.46
1	B	574	PRO	N-CA	5.96	1.53	1.47
1	B	298	SER	N-CA	-5.94	1.38	1.46
1	B	765	VAL	CA-C	5.91	1.59	1.52
1	B	778	ASP	CA-C	-5.89	1.45	1.52
1	A	178	GLY	N-CA	5.88	1.53	1.45
1	A	297	MET	C-O	5.88	1.30	1.23
1	A	75	GLY	N-CA	5.85	1.52	1.45
1	B	807	PRO	C-O	5.82	1.30	1.23
1	B	702	ARG	CD-NE	-5.81	1.38	1.46
1	B	806	LYS	CA-C	5.77	1.60	1.52
1	B	201	GLN	CD-OE1	5.75	1.34	1.23
1	B	198	HIS	N-CA	5.70	1.53	1.46
1	A	407	ASN	CA-C	5.70	1.60	1.53
1	A	266	LEU	N-CA	5.70	1.53	1.46
1	B	644	PRO	C-O	5.69	1.30	1.23
1	A	841	VAL	N-CA	5.68	1.53	1.46
1	A	212	ILE	CA-C	-5.63	1.46	1.52
1	A	137	ILE	N-CA	5.61	1.53	1.46
1	B	194	ASN	CG-OD1	5.59	1.34	1.23
1	A	637	PHE	C-O	5.58	1.30	1.24
1	B	252	ASN	C-O	5.57	1.30	1.23
1	A	159	GLU	C-O	5.57	1.31	1.24
1	B	191	TYR	CA-C	5.54	1.60	1.53
1	A	107	PRO	CA-C	5.52	1.59	1.52
1	B	113	ALA	C-O	5.47	1.30	1.24
1	B	184	VAL	N-CA	5.46	1.52	1.46
1	B	781	PRO	C-O	5.46	1.30	1.23
1	A	212	ILE	N-CA	5.41	1.52	1.46
1	A	205	ALA	CA-C	5.36	1.59	1.52
1	A	460	VAL	N-CA	5.34	1.52	1.46
1	B	382	VAL	CA-C	5.32	1.58	1.52
1	A	773	GLY	C-O	-5.30	1.19	1.24
1	A	379	ASN	N-CA	5.29	1.52	1.46
1	A	568	ILE	N-CA	5.29	1.52	1.46
1	B	258	GLN	C-O	5.28	1.28	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	648	PHE	C-O	5.27	1.30	1.23
1	A	783	LEU	N-CA	5.26	1.52	1.46
1	B	41	ALA	N-CA	5.24	1.52	1.46
1	A	491	THR	N-CA	5.24	1.52	1.46
1	B	272	GLY	N-CA	5.21	1.52	1.45
1	B	749	GLY	N-CA	5.20	1.51	1.44
1	A	189	LYS	CA-C	5.20	1.59	1.52
1	A	223	LYS	CA-C	5.19	1.59	1.52
1	B	72	LYS	N-CA	5.18	1.52	1.46
1	B	236	ALA	N-CA	5.18	1.52	1.46
1	B	785	VAL	N-CA	5.16	1.51	1.46
1	B	325	VAL	N-CA	5.15	1.51	1.46
1	B	600	TRP	C-O	5.15	1.29	1.23
1	B	228	MET	N-CA	5.14	1.52	1.46
1	B	73	CYS	N-CA	5.14	1.51	1.45
1	A	138	ASP	N-CA	5.09	1.52	1.46
1	A	400	THR	CA-CB	5.09	1.59	1.53
1	B	496	ALA	N-CA	5.08	1.51	1.45
1	A	362	GLU	CA-C	5.07	1.59	1.52
1	A	657	PHE	C-O	-5.07	1.17	1.23
1	A	795	VAL	C-O	5.06	1.29	1.23
1	B	517	ASN	CA-CB	5.03	1.59	1.52
1	B	114	ALA	CA-CB	5.01	1.62	1.53
1	A	236	ALA	N-CA	5.01	1.52	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	CYS	N-CA-CB	9.95	127.53	110.81
1	A	727	VAL	N-CA-C	6.58	117.91	107.98
1	A	775	VAL	N-CA-CB	-6.54	100.72	111.44
1	A	790	PRO	CA-C-N	-6.33	113.17	122.86
1	A	790	PRO	C-N-CA	-6.33	113.17	122.86
1	B	638	ASP	N-CA-C	-6.21	104.59	111.36
1	B	702	ARG	NE-CZ-NH2	-5.97	113.83	119.20
1	B	510	GLY	N-CA-C	5.88	120.93	114.40
1	B	31	SER	CA-C-N	-5.81	113.80	119.78
1	B	31	SER	C-N-CA	-5.81	113.80	119.78
1	B	431	GLY	N-CA-C	-5.74	105.86	112.29
1	A	378	VAL	N-CA-C	-5.67	106.78	113.42
1	B	702	ARG	CB-CG-CD	-5.59	98.44	111.30
1	B	449	TRP	N-CA-C	5.58	118.79	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	ARG	N-CA-C	-5.54	105.39	111.82
1	B	541	CYS	N-CA-C	-5.52	98.91	108.69
1	B	142	GLY	N-CA-C	-5.45	101.22	112.34
1	B	146	GLY	N-CA-C	-5.44	101.24	112.34
1	A	170	VAL	CB-CA-C	-5.39	104.78	112.22
1	B	378	VAL	N-CA-C	-5.30	108.33	113.53
1	B	564	ASN	CA-C-N	-5.30	115.75	122.43
1	B	564	ASN	C-N-CA	-5.30	115.75	122.43
1	A	449	TRP	N-CA-C	5.29	118.34	110.14
1	A	180	GLN	CA-CB-CG	-5.26	103.58	114.10
1	B	335	VAL	N-CA-C	5.25	115.98	110.62
1	B	556	VAL	N-CA-C	-5.19	108.07	113.10
1	B	466	ILE	CA-C-N	-5.13	113.77	120.44
1	B	466	ILE	C-N-CA	-5.13	113.77	120.44
1	A	552	GLY	CA-C-N	-5.12	114.97	120.03
1	A	552	GLY	C-N-CA	-5.12	114.97	120.03
1	A	408	ALA	N-CA-C	-5.06	107.24	113.41
1	B	819	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	A	859	VAL	N-CA-C	-5.03	100.55	108.90
1	A	786	SER	N-CA-C	-5.02	100.22	108.41

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	26	0
1	B	6375	0	6082	37	0
2	C	61	0	52	1	0
3	D	39	0	34	1	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	0	0
5	F	116	0	96	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	116	0	96	0	0
6	H	83	0	70	1	0
6	O	83	0	70	1	0
7	I	83	0	69	1	0
8	J	83	0	70	1	0
9	K	50	0	43	1	0
10	P	94	0	77	6	0
11	A	28	0	26	0	0
11	B	42	0	39	0	0
12	A	16	0	28	7	0
12	B	24	0	42	8	0
13	A	8	0	14	9	0
14	A	1	0	0	0	0
14	B	1	0	0	0	0
15	A	10	0	13	0	0
15	B	10	0	13	0	0
16	A	671	0	0	6	0
16	B	761	0	0	14	0
All	All	15282	0	13153	89	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 (89) 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:B:541:CYS:CA	1:B:541:CYS:CB	1.75	1.64
13:A:942:MPD:H52	13:A:942:MPD:C1	1.66	1.23
13:A:942:MPD:H52	13:A:942:MPD:H11	1.08	1.05
1:B:678:GLU:HG2	16:B:1593:HOH:O	1.59	1.02
13:A:942:MPD:C1	13:A:942:MPD:C5	2.33	1.01
13:A:942:MPD:H11	13:A:942:MPD:C5	1.91	0.90
1:A:819:ARG:HH12	1:A:860:GLN:C	1.81	0.88
1:B:837:TYR:HE2	16:B:1541:HOH:O	1.56	0.87
12:B:947:MRD:C5	12:B:947:MRD:H1C2	2.02	0.83
1:A:360:ARG:HH11	12:A:941:MRD:HMC3	1.43	0.83
13:A:942:MPD:C5	13:A:942:MPD:H13	2.09	0.80
1:B:541:CYS:CB	1:B:541:CYS:C	2.55	0.79
12:B:947:MRD:H1C2	12:B:947:MRD:H5C3	1.65	0.78
13:A:942:MPD:H52	13:A:942:MPD:H13	1.63	0.78
1:B:819:ARG:HH12	1:B:860:GLN:C	1.93	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:ARG:NH1	1:A:860:GLN:C	2.44	0.76
1:A:664:ILE:HD11	1:A:841:VAL:HG11	1.70	0.72
12:A:941:MRD:HMC1	12:A:941:MRD:H5C3	1.71	0.72
12:A:941:MRD:HMC2	16:B:1147:HOH:O	1.89	0.72
1:A:98:ARG:HH22	13:A:942:MPD:H31	1.53	0.72
1:B:541:CYS:CB	1:B:541:CYS:HA	2.13	0.70
16:A:1390:HOH:O	7:I:6:MAN:H3	1.92	0.68
1:B:764:ARG:HD3	1:B:814:THR:HG21	1.78	0.66
1:B:201:GLN:HG3	16:B:1657:HOH:O	1.97	0.65
12:B:946:MRD:HMC2	16:B:1440:HOH:O	1.97	0.65
1:B:484:TRP:CE2	6:O:3:BMA:H62	2.32	0.64
12:B:948:MRD:O2	12:B:948:MRD:H5C3	2.00	0.61
1:B:764:ARG:HD3	1:B:814:THR:CG2	2.31	0.61
1:A:857:PRO:HD3	16:A:1230:HOH:O	2.01	0.60
1:A:484:TRP:CE2	6:H:3:BMA:H62	2.37	0.59
10:P:3:BMA:H62	10:P:4:MAN:H5	1.83	0.59
12:A:941:MRD:HMC1	12:A:941:MRD:C5	2.32	0.59
1:B:595:LYS:HE2	16:B:1396:HOH:O	2.02	0.59
12:B:948:MRD:O2	12:B:948:MRD:C5	2.50	0.58
1:B:98:ARG:HH12	12:B:946:MRD:HMC3	1.68	0.57
1:B:783:LEU:C	1:B:783:LEU:HD23	2.29	0.57
1:A:360:ARG:HH11	12:A:941:MRD:CM	2.18	0.56
10:P:3:BMA:H62	10:P:4:MAN:H3	1.89	0.54
1:A:470:VAL:HG11	1:A:477:VAL:HB	1.91	0.52
12:B:947:MRD:H5C3	12:B:947:MRD:C1	2.38	0.52
1:B:390:GLU:CG	16:B:1514:HOH:O	2.57	0.52
1:B:386:ARG:NH2	16:B:1738:HOH:O	2.34	0.51
1:B:663:HIS:HB3	16:B:1652:HOH:O	2.11	0.51
12:A:940:MRD:O2	12:A:940:MRD:H5C3	2.11	0.50
1:B:470:VAL:HG11	1:B:477:VAL:HB	1.95	0.49
1:B:172:PHE:CZ	1:B:188:ALA:HB1	2.48	0.49
1:A:827:VAL:HG11	3:D:2:NAG:O3	2.13	0.48
1:A:484:TRP:CZ2	1:A:529:ASN:HB2	2.49	0.47
10:P:3:BMA:C6	10:P:4:MAN:H3	2.43	0.47
1:B:390:GLU:HG3	16:B:1514:HOH:O	2.15	0.47
1:A:783:LEU:C	1:A:783:LEU:HD23	2.41	0.46
1:A:191:TYR:O	1:A:246:CYS:HA	2.15	0.46
1:B:799:LYS:NZ	1:B:821:ASP:OD2	2.47	0.46
1:A:193:LEU:HD13	1:A:220:VAL:HG21	1.97	0.45
1:B:76:GLN:HA	1:B:88:MET:O	2.17	0.45
1:B:484:TRP:CZ2	1:B:529:ASN:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ALA:HB3	1:B:244:ILE:HD13	1.98	0.45
1:A:577:GLU:O	1:A:578:SER:C	2.60	0.45
1:B:251:ILE:HG21	9:K:1:NAG:H82	1.99	0.45
1:A:360:ARG:HG2	12:A:941:MRD:HMC1	1.98	0.45
1:A:193:LEU:HD13	1:A:220:VAL:CG2	2.47	0.44
12:B:946:MRD:O4	12:B:946:MRD:O2	2.30	0.44
1:B:819:ARG:NH1	1:B:860:GLN:C	2.71	0.44
1:B:702:ARG:HD3	16:B:1082:HOH:O	2.18	0.43
1:B:146:GLY:HA2	1:B:147:PRO:C	2.43	0.43
1:B:659:TYR:HE1	1:B:781:PRO:HB3	1.81	0.43
16:B:1509:HOH:O	10:P:3:BMA:H61	2.18	0.43
10:P:3:BMA:H62	10:P:4:MAN:C3	2.49	0.43
13:A:942:MPD:H12	16:A:1406:HOH:O	2.19	0.43
13:A:942:MPD:H13	13:A:942:MPD:H53	1.99	0.43
1:B:172:PHE:HZ	1:B:188:ALA:HB1	1.82	0.43
1:A:387:ASN:HB2	16:A:1200:HOH:O	2.19	0.42
1:A:774:ARG:HE	1:A:774:ARG:HB3	1.45	0.42
1:A:539:ASN:HB2	16:A:1367:HOH:O	2.19	0.42
1:B:102:TYR:HB3	1:B:383:ASN:HA	2.02	0.42
10:P:3:BMA:C6	10:P:4:MAN:C3	2.98	0.42
1:A:448:ALA:HB1	1:A:507:ALA:O	2.20	0.42
1:B:595:LYS:HE3	16:B:1204:HOH:O	2.20	0.42
1:A:97:ILE:HD13	1:A:135:LYS:HG3	2.01	0.41
1:A:595:LYS:HE3	16:A:1155:HOH:O	2.19	0.41
1:B:220:VAL:HG22	1:B:626:PHE:CG	2.56	0.41
1:B:39:GLU:HG2	16:B:1324:HOH:O	2.21	0.41
1:B:706:PHE:CZ	8:J:2:NAG:H82	2.56	0.41
1:B:377:LYS:HD2	1:B:380:HIS:CE1	2.56	0.40
1:A:30:PRO:HG3	1:A:739:ASP:O	2.21	0.40
1:B:500:LEU:HD23	1:B:545:ILE:HB	2.04	0.40
1:A:146:GLY:HA2	1:A:147:PRO:C	2.46	0.40
1:A:367:TYR:CZ	2:C:2:NAG:H83	2.57	0.40
1:B:446:ALA:HA	1:B:574:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	829/841 (99%)	801 (97%)	28 (3%)	0	100	100
1	B	828/841 (98%)	806 (97%)	22 (3%)	0	100	100
All	All	1657/1682 (98%)	1607 (97%)	50 (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%)	666 (99%)	5 (1%)	76	78
1	B	670/677 (99%)	666 (99%)	4 (1%)	78	81
All	All	1341/1354 (99%)	1332 (99%)	9 (1%)	76	78

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

Mol	Chain	Res	Type
1	A	244	ILE
1	A	462	PRO
1	A	774	ARG
1	A	775	VAL
1	A	858	LYS
1	B	348	ARG
1	B	700	LEU
1	B	806	LYS

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Mol	Chain	Res	Type
1	B	860	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	126	GLN
1	A	219	ASN
1	A	860	GLN
1	B	219	ASN
1	B	253	ASN
1	B	623	GLN
1	B	791	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

79 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	1.41	2 (14%)	17,19,21	1.43	2 (11%)
2	NAG	C	2	2	14,14,15	1.02	1 (7%)	17,19,21	2.06	9 (52%)
2	BMA	C	3	2	11,11,12	1.14	0	15,15,17	2.35	6 (40%)
2	MAN	C	4	2	11,11,12	0.92	0	15,15,17	2.61	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	C	5	2	11,11,12	0.88	0	15,15,17	1.58	3 (20%)
3	NAG	D	1	1,3	14,14,15	1.17	1 (7%)	17,19,21	1.61	5 (29%)
3	NAG	D	2	3	14,14,15	1.25	2 (14%)	17,19,21	1.63	5 (29%)
3	BMA	D	3	3	11,11,12	1.02	0	15,15,17	2.94	6 (40%)
4	NAG	E	1	1,4	14,14,15	0.72	0	17,19,21	1.46	3 (17%)
4	NAG	E	2	4	14,14,15	1.01	1 (7%)	17,19,21	2.02	5 (29%)
5	NAG	F	1	1,5	14,14,15	1.54	3 (21%)	17,19,21	1.18	2 (11%)
5	MAN	F	10	5	11,11,12	1.12	1 (9%)	15,15,17	1.66	5 (33%)
5	NAG	F	2	5	14,14,15	1.25	2 (14%)	17,19,21	1.35	2 (11%)
5	BMA	F	3	5	11,11,12	0.86	0	15,15,17	1.33	2 (13%)
5	MAN	F	4	5	11,11,12	0.95	0	15,15,17	1.11	1 (6%)
5	MAN	F	5	5	11,11,12	0.76	0	15,15,17	1.77	3 (20%)
5	MAN	F	6	5	11,11,12	0.72	0	15,15,17	1.84	3 (20%)
5	MAN	F	7	5	11,11,12	1.40	2 (18%)	15,15,17	1.24	2 (13%)
5	MAN	F	8	5	11,11,12	1.07	0	15,15,17	1.51	3 (20%)
5	MAN	F	9	5	11,11,12	1.15	1 (9%)	15,15,17	1.38	3 (20%)
3	NAG	G	1	1,3	14,14,15	1.19	1 (7%)	17,19,21	1.85	4 (23%)
3	NAG	G	2	3	14,14,15	0.87	1 (7%)	17,19,21	1.60	2 (11%)
3	BMA	G	3	3	11,11,12	1.05	1 (9%)	15,15,17	3.00	6 (40%)
6	NAG	H	1	1,6	14,14,15	0.93	0	17,19,21	1.50	3 (17%)
6	NAG	H	2	6	14,14,15	0.77	0	17,19,21	1.85	6 (35%)
6	BMA	H	3	6	11,11,12	0.87	0	15,15,17	1.49	4 (26%)
6	MAN	H	4	6	11,11,12	0.82	0	15,15,17	1.62	6 (40%)
6	MAN	H	5	6	11,11,12	0.91	0	15,15,17	1.37	2 (13%)
6	MAN	H	6	6	11,11,12	1.22	1 (9%)	15,15,17	1.04	0
6	MAN	H	7	6	11,11,12	0.68	0	15,15,17	1.52	4 (26%)
7	NAG	I	1	1,14,7	14,14,15	1.25	1 (7%)	17,19,21	1.53	5 (29%)
7	NAG	I	2	7	14,14,15	1.37	1 (7%)	17,19,21	1.26	4 (23%)
7	BMA	I	3	7	11,11,12	0.86	1 (9%)	15,15,17	2.32	6 (40%)
7	MAN	I	4	7	11,11,12	1.16	1 (9%)	15,15,17	1.82	3 (20%)
7	MAN	I	5	7	11,11,12	0.80	0	15,15,17	2.22	6 (40%)
7	MAN	I	6	7	11,11,12	0.90	0	15,15,17	2.10	7 (46%)
7	MAN	I	7	7	11,11,12	0.73	0	15,15,17	1.71	4 (26%)
8	NAG	J	1	1,8	14,14,15	1.45	1 (7%)	17,19,21	2.73	7 (41%)
8	NAG	J	2	8	14,14,15	1.09	1 (7%)	17,19,21	1.95	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	J	3	8	11,11,12	1.33	1 (9%)	15,15,17	1.76	5 (33%)
8	MAN	J	4	8	11,11,12	0.56	0	15,15,17	1.74	5 (33%)
8	MAN	J	5	8	11,11,12	0.95	0	15,15,17	1.12	1 (6%)
8	MAN	J	6	8	11,11,12	0.86	0	15,15,17	1.41	2 (13%)
8	MAN	J	7	8	11,11,12	0.70	0	15,15,17	1.72	5 (33%)
9	NAG	K	1	1,9	14,14,15	1.13	1 (7%)	17,19,21	1.82	6 (35%)
9	NAG	K	2	9	14,14,15	1.68	5 (35%)	17,19,21	1.60	5 (29%)
9	BMA	K	3	9	11,11,12	0.71	0	15,15,17	1.82	2 (13%)
9	MAN	K	4	9	11,11,12	1.19	2 (18%)	15,15,17	2.02	6 (40%)
3	NAG	L	1	1,3	14,14,15	1.03	0	17,19,21	1.65	4 (23%)
3	NAG	L	2	3	14,14,15	0.67	0	17,19,21	1.69	3 (17%)
3	BMA	L	3	3	11,11,12	0.81	0	15,15,17	2.15	5 (33%)
5	NAG	M	1	1,5	14,14,15	1.29	2 (14%)	17,19,21	1.78	6 (35%)
5	MAN	M	10	5	11,11,12	1.15	1 (9%)	15,15,17	1.91	6 (40%)
5	NAG	M	2	5	14,14,15	1.29	1 (7%)	17,19,21	1.47	4 (23%)
5	BMA	M	3	5	11,11,12	1.14	1 (9%)	15,15,17	1.67	2 (13%)
5	MAN	M	4	5	11,11,12	0.90	0	15,15,17	1.64	5 (33%)
5	MAN	M	5	5	11,11,12	0.81	0	15,15,17	2.01	4 (26%)
5	MAN	M	6	5	11,11,12	1.04	0	15,15,17	1.33	1 (6%)
5	MAN	M	7	5	11,11,12	1.19	2 (18%)	15,15,17	2.19	5 (33%)
5	MAN	M	8	5	11,11,12	1.21	1 (9%)	15,15,17	1.74	3 (20%)
5	MAN	M	9	5	11,11,12	1.10	0	15,15,17	1.61	5 (33%)
3	NAG	N	1	1,3	14,14,15	0.72	0	17,19,21	1.06	1 (5%)
3	NAG	N	2	3	14,14,15	1.28	1 (7%)	17,19,21	1.43	2 (11%)
3	BMA	N	3	3	11,11,12	0.86	0	15,15,17	2.15	4 (26%)
6	NAG	O	1	1,6	14,14,15	0.99	0	17,19,21	1.31	1 (5%)
6	NAG	O	2	6	14,14,15	1.12	1 (7%)	17,19,21	1.93	5 (29%)
6	BMA	O	3	6	11,11,12	1.03	1 (9%)	15,15,17	1.15	1 (6%)
6	MAN	O	4	6	11,11,12	1.00	1 (9%)	15,15,17	1.88	7 (46%)
6	MAN	O	5	6	11,11,12	0.80	0	15,15,17	1.63	5 (33%)
6	MAN	O	6	6	11,11,12	0.76	0	15,15,17	1.66	5 (33%)
6	MAN	O	7	6	11,11,12	0.73	0	15,15,17	2.24	5 (33%)
10	NAG	P	1	1,14,10	14,14,15	1.43	2 (14%)	17,19,21	1.52	4 (23%)
10	NAG	P	2	10	14,14,15	0.94	0	17,19,21	1.43	3 (17%)
10	BMA	P	3	10	11,11,12	1.05	1 (9%)	15,15,17	3.65	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	P	4	10	11,11,12	0.95	0	15,15,17	1.69	4 (26%)
10	MAN	P	5	10	11,11,12	0.92	0	15,15,17	2.34	7 (46%)
10	MAN	P	6	10	11,11,12	0.84	0	15,15,17	2.19	5 (33%)
10	MAN	P	7	10	11,11,12	0.94	1 (9%)	15,15,17	1.68	3 (20%)
10	MAN	P	8	10	11,11,12	0.89	0	15,15,17	2.04	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
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	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	-	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	-	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	-	1/2/19/22	0/1/1/1
6	MAN	H	6	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	H	7	6	-	0/2/19/22	0/1/1/1
7	NAG	I	1	1,14,7	-	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	-	2/2/19/22	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	-	2/2/19/22	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
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
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	M	10	5	-	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	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	O	6	6	-	0/2/19/22	0/1/1/1
6	MAN	O	7	6	-	1/2/19/22	0/1/1/1
10	NAG	P	1	1,14,10	-	1/6/23/26	0/1/1/1
10	NAG	P	2	10	-	0/6/23/26	0/1/1/1
10	BMA	P	3	10	-	2/2/19/22	0/1/1/1
10	MAN	P	4	10	-	2/2/19/22	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	-	1/2/19/22	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	NAG	C1-C2	4.41	1.58	1.52
3	N	2	NAG	C1-C2	3.86	1.57	1.52
2	C	1	NAG	C1-C2	3.82	1.57	1.52
7	I	2	NAG	O5-C1	-3.75	1.37	1.43
10	P	1	NAG	C1-C2	-3.27	1.47	1.52
9	K	2	NAG	C3-C2	3.25	1.59	1.52
5	F	1	NAG	C1-C2	3.20	1.56	1.52
8	J	3	BMA	C2-C3	3.17	1.57	1.52
5	M	1	NAG	C1-C2	3.04	1.56	1.52
10	P	1	NAG	O7-C7	3.00	1.30	1.23
5	F	7	MAN	C4-C3	2.90	1.59	1.52
5	M	2	NAG	C4-C3	2.75	1.59	1.52
5	F	2	NAG	C1-C2	2.74	1.56	1.52
5	M	8	MAN	O5-C5	2.69	1.48	1.43
6	O	4	MAN	O2-C2	-2.68	1.37	1.43
9	K	2	NAG	C4-C5	2.65	1.58	1.53
5	M	3	BMA	O4-C4	-2.65	1.36	1.43
5	F	9	MAN	O4-C4	-2.63	1.36	1.43
3	G	1	NAG	C1-C2	2.61	1.55	1.52
6	O	2	NAG	C3-C2	2.58	1.57	1.52
9	K	2	NAG	O5-C1	-2.53	1.39	1.43
3	D	1	NAG	C1-C2	2.52	1.55	1.52
5	F	10	MAN	O5-C1	-2.49	1.39	1.43
2	C	2	NAG	C1-C2	2.47	1.55	1.52
8	J	2	NAG	C4-C5	2.46	1.58	1.53
5	F	1	NAG	C4-C3	2.44	1.58	1.52
4	E	2	NAG	O3-C3	-2.39	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	7	MAN	C2-C3	2.36	1.56	1.52
9	K	2	NAG	C1-C2	2.36	1.55	1.52
6	H	6	MAN	C4-C5	2.34	1.58	1.53
7	I	1	NAG	O5-C1	2.31	1.47	1.43
6	O	3	BMA	C1-C2	2.31	1.57	1.52
9	K	1	NAG	C1-C2	2.27	1.55	1.52
10	P	3	BMA	O5-C1	-2.27	1.39	1.43
5	M	10	MAN	O5-C1	-2.23	1.39	1.43
5	F	7	MAN	O5-C1	-2.23	1.40	1.43
3	G	2	NAG	O5-C1	-2.22	1.40	1.43
5	F	1	NAG	C2-N2	2.22	1.49	1.46
9	K	2	NAG	O7-C7	2.21	1.28	1.23
7	I	4	MAN	O5-C5	2.17	1.47	1.43
9	K	4	MAN	C4-C3	2.17	1.58	1.52
5	M	7	MAN	O3-C3	2.15	1.48	1.43
7	I	3	BMA	O2-C2	-2.14	1.38	1.43
5	M	1	NAG	C2-N2	2.13	1.49	1.46
5	M	7	MAN	C4-C3	2.12	1.57	1.52
3	D	2	NAG	O5-C1	-2.11	1.40	1.43
3	G	3	BMA	C1-C2	2.09	1.57	1.52
5	F	2	NAG	C6-C5	2.04	1.58	1.51
2	C	1	NAG	C8-C7	2.02	1.54	1.50
9	K	4	MAN	C2-C3	2.01	1.55	1.52
3	D	2	NAG	C4-C5	2.00	1.57	1.53

All (323) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BMA	C1-O5-C5	9.27	124.61	112.19
10	P	3	BMA	C1-O5-C5	8.55	123.65	112.19
10	P	3	BMA	C6-C5-C4	-6.94	95.98	113.02
2	C	4	MAN	C1-O5-C5	6.55	120.96	112.19
7	I	3	BMA	C1-O5-C5	5.86	120.04	112.19
8	J	1	NAG	O5-C1-C2	-5.56	102.68	111.29
5	M	7	MAN	C1-O5-C5	5.47	119.52	112.19
7	I	4	MAN	O5-C5-C6	5.34	118.05	107.66
3	L	3	BMA	C1-O5-C5	5.23	119.20	112.19
9	K	3	BMA	C1-O5-C5	5.19	119.14	112.19
3	D	3	BMA	O5-C5-C6	5.17	117.72	107.66
6	O	7	MAN	C1-C2-C3	-5.11	102.20	109.64
3	D	3	BMA	C3-C4-C5	5.10	119.47	110.23
3	N	3	BMA	C1-O5-C5	5.09	119.01	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	O6-C6-C5	5.08	128.62	111.33
10	P	3	BMA	O6-C6-C5	-4.76	95.14	111.33
7	I	5	MAN	C3-C4-C5	-4.75	101.61	110.23
5	M	5	MAN	O6-C6-C5	-4.74	95.19	111.33
2	C	3	BMA	C1-C2-C3	4.71	116.50	109.64
9	K	1	NAG	C4-C3-C2	-4.68	104.15	111.02
10	P	5	MAN	C6-C5-C4	-4.67	101.55	113.02
5	F	5	MAN	O6-C6-C5	-4.57	95.76	111.33
8	J	1	NAG	C1-O5-C5	-4.55	106.09	112.19
10	P	8	MAN	C2-C3-C4	4.53	118.83	110.86
8	J	1	NAG	C4-C3-C2	-4.50	104.43	111.02
5	M	8	MAN	O3-C3-C4	-4.49	99.80	110.38
4	E	2	NAG	C3-C4-C5	-4.47	102.12	110.23
8	J	2	NAG	O7-C7-C8	-4.40	114.22	122.05
3	L	2	NAG	C3-C4-C5	-4.40	102.25	110.23
8	J	1	NAG	O7-C7-N2	4.25	129.48	121.98
3	G	2	NAG	C1-C2-N2	-4.24	103.75	110.43
10	P	3	BMA	O2-C2-C3	4.21	118.88	110.15
8	J	1	NAG	C8-C7-N2	-4.15	109.24	116.12
3	G	1	NAG	C1-C2-N2	-4.09	103.98	110.43
2	C	4	MAN	C3-C4-C5	4.04	117.56	110.23
10	P	6	MAN	O5-C5-C6	4.04	115.53	107.66
9	K	4	MAN	O5-C5-C6	4.01	115.46	107.66
10	P	6	MAN	O3-C3-C4	3.95	119.68	110.38
2	C	2	NAG	O6-C6-C5	-3.93	97.94	111.33
5	M	5	MAN	C1-O5-C5	3.92	117.44	112.19
2	C	1	NAG	O5-C1-C2	-3.90	105.25	111.29
7	I	6	MAN	C1-O5-C5	3.90	117.41	112.19
2	C	3	BMA	O2-C2-C3	-3.89	102.09	110.15
3	D	3	BMA	O3-C3-C2	-3.89	102.12	110.05
5	M	1	NAG	O4-C4-C5	-3.87	99.78	109.32
10	P	5	MAN	C1-O5-C5	3.87	117.38	112.19
3	G	1	NAG	C2-N2-C7	3.86	128.08	122.90
5	F	6	MAN	O3-C3-C2	3.85	117.91	110.05
7	I	5	MAN	O2-C2-C3	-3.83	102.21	110.15
10	P	7	MAN	O5-C5-C6	3.82	115.11	107.66
3	N	3	BMA	O5-C5-C6	3.81	115.08	107.66
4	E	2	NAG	O6-C6-C5	-3.78	98.47	111.33
6	H	1	NAG	C1-C2-N2	-3.78	104.48	110.43
5	F	6	MAN	O5-C5-C6	3.76	114.97	107.66
5	M	3	BMA	C2-C3-C4	-3.75	104.27	110.86
2	C	4	MAN	C1-C2-C3	3.72	115.06	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	3	BMA	C6-C5-C4	-3.72	103.89	113.02
8	J	4	MAN	O5-C5-C6	3.71	114.89	107.66
9	K	4	MAN	O3-C3-C4	3.70	119.09	110.38
7	I	7	MAN	C1-O5-C5	3.69	117.14	112.19
3	L	3	BMA	O4-C4-C3	-3.69	101.68	110.38
5	M	7	MAN	O2-C2-C3	-3.69	102.51	110.15
5	M	6	MAN	O5-C5-C6	3.68	114.83	107.66
2	C	3	BMA	C2-C3-C4	-3.66	104.43	110.86
6	O	7	MAN	O4-C4-C3	-3.65	101.77	110.38
10	P	4	MAN	O2-C2-C1	-3.63	100.92	109.22
8	J	3	BMA	O5-C5-C4	-3.63	102.00	110.83
8	J	7	MAN	O3-C3-C2	3.62	117.44	110.05
7	I	6	MAN	O3-C3-C4	3.60	118.86	110.38
7	I	3	BMA	O3-C3-C4	-3.59	101.91	110.38
3	G	3	BMA	O2-C2-C1	3.58	117.43	109.22
8	J	2	NAG	O6-C6-C5	-3.58	99.14	111.33
10	P	5	MAN	O2-C2-C3	-3.53	102.83	110.15
3	D	3	BMA	C1-O5-C5	3.52	116.90	112.19
3	L	1	NAG	O4-C4-C5	-3.48	100.74	109.32
3	N	2	NAG	O7-C7-C8	-3.48	115.85	122.05
6	H	2	NAG	O4-C4-C3	-3.42	102.31	110.38
5	F	6	MAN	O2-C2-C1	-3.40	101.45	109.22
6	H	2	NAG	C2-N2-C7	-3.39	118.36	122.90
3	L	1	NAG	C3-C4-C5	3.37	116.34	110.23
4	E	1	NAG	O4-C4-C5	-3.37	101.03	109.32
5	M	2	NAG	C1-C2-N2	-3.35	105.15	110.43
10	P	3	BMA	O5-C5-C4	3.34	118.94	110.83
3	G	3	BMA	O3-C3-C4	3.32	118.21	110.38
10	P	8	MAN	C1-C2-C3	3.32	114.48	109.64
5	M	10	MAN	O2-C2-C1	3.32	116.83	109.22
5	F	8	MAN	C3-C4-C5	3.30	116.22	110.23
5	M	3	BMA	O5-C5-C4	-3.30	102.80	110.83
6	O	6	MAN	C1-O5-C5	3.30	116.61	112.19
3	D	3	BMA	C1-C2-C3	3.29	114.44	109.64
6	O	4	MAN	C1-C2-C3	3.27	114.40	109.64
8	J	3	BMA	O6-C6-C5	-3.25	100.26	111.33
3	N	3	BMA	C3-C4-C5	3.24	116.11	110.23
10	P	4	MAN	O4-C4-C3	-3.24	102.74	110.38
6	O	2	NAG	O4-C4-C3	-3.23	102.75	110.38
10	P	3	BMA	C3-C4-C5	3.21	116.06	110.23
6	H	3	BMA	C6-C5-C4	-3.21	105.15	113.02
3	G	1	NAG	C4-C3-C2	-3.21	106.32	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	8	MAN	O3-C3-C4	-3.20	102.82	110.38
10	P	6	MAN	O4-C4-C5	-3.19	101.47	109.32
9	K	4	MAN	C1-C2-C3	3.17	114.26	109.64
6	O	7	MAN	O2-C2-C3	3.16	116.69	110.15
8	J	7	MAN	C1-O5-C5	-3.15	107.96	112.19
2	C	3	BMA	O3-C3-C4	3.13	117.76	110.38
8	J	2	NAG	O7-C7-N2	3.13	127.51	121.98
5	M	10	MAN	O6-C6-C5	-3.08	100.84	111.33
3	L	3	BMA	C3-C4-C5	3.08	115.81	110.23
3	L	2	NAG	O6-C6-C5	-3.07	100.88	111.33
9	K	2	NAG	C6-C5-C4	3.06	120.54	113.02
5	M	1	NAG	C1-C2-N2	-3.04	105.64	110.43
10	P	6	MAN	C3-C4-C5	-3.02	104.75	110.23
6	O	4	MAN	O3-C3-C4	3.02	117.49	110.38
8	J	6	MAN	C1-O5-C5	3.01	116.22	112.19
3	D	1	NAG	O5-C5-C4	-3.00	103.52	110.83
5	M	2	NAG	O6-C6-C5	-3.00	101.13	111.33
5	F	5	MAN	C1-O5-C5	2.99	116.19	112.19
7	I	6	MAN	O2-C2-C1	2.99	116.06	109.22
5	F	7	MAN	C2-C3-C4	-2.97	105.64	110.86
4	E	2	NAG	C1-C2-N2	2.94	115.07	110.43
10	P	6	MAN	C1-O5-C5	2.93	116.12	112.19
3	D	1	NAG	C1-C2-N2	2.93	115.06	110.43
5	F	4	MAN	O6-C6-C5	-2.93	101.37	111.33
5	M	9	MAN	C1-C2-C3	2.92	113.89	109.64
3	D	2	NAG	C1-O5-C5	-2.91	108.28	112.19
6	O	4	MAN	O2-C2-C3	-2.91	104.13	110.15
5	M	4	MAN	C1-O5-C5	2.91	116.08	112.19
7	I	5	MAN	C1-O5-C5	2.90	116.08	112.19
7	I	4	MAN	O4-C4-C3	-2.90	103.55	110.38
5	F	10	MAN	C2-C3-C4	2.90	115.95	110.86
8	J	5	MAN	O5-C5-C6	2.87	113.25	107.66
2	C	5	MAN	C6-C5-C4	2.86	120.03	113.02
10	P	7	MAN	C1-C2-C3	-2.85	105.49	109.64
9	K	2	NAG	O6-C6-C5	-2.84	101.65	111.33
6	O	7	MAN	O3-C3-C2	2.84	115.85	110.05
6	H	7	MAN	O4-C4-C3	-2.84	103.68	110.38
5	M	8	MAN	O5-C5-C6	2.84	113.19	107.66
2	C	5	MAN	O3-C3-C4	2.82	117.02	110.38
7	I	6	MAN	O5-C5-C4	2.81	117.65	110.83
10	P	8	MAN	C3-C4-C5	2.80	115.31	110.23
7	I	1	NAG	C2-N2-C7	-2.80	119.15	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	6	MAN	C6-C5-C4	-2.79	106.17	113.02
6	O	7	MAN	O5-C1-C2	-2.79	104.14	110.79
6	H	3	BMA	C1-O5-C5	-2.79	108.45	112.19
10	P	5	MAN	O5-C5-C6	2.78	113.08	107.66
6	O	2	NAG	C6-C5-C4	2.78	119.85	113.02
5	F	5	MAN	C6-C5-C4	-2.77	106.22	113.02
6	O	2	NAG	O3-C3-C2	-2.76	103.66	109.40
3	N	3	BMA	C6-C5-C4	-2.76	106.25	113.02
5	M	9	MAN	O3-C3-C2	-2.75	104.44	110.05
5	M	4	MAN	O2-C2-C3	2.74	115.83	110.15
3	L	3	BMA	O3-C3-C2	2.74	115.64	110.05
2	C	2	NAG	O7-C7-C8	-2.73	117.19	122.05
8	J	1	NAG	O5-C5-C4	-2.73	104.19	110.83
2	C	4	MAN	O5-C5-C6	-2.72	102.37	107.66
7	I	7	MAN	C1-C2-C3	-2.72	105.69	109.64
2	C	2	NAG	O4-C4-C5	-2.71	102.65	109.32
5	M	4	MAN	O6-C6-C5	-2.70	102.14	111.33
3	D	2	NAG	C6-C5-C4	2.69	119.64	113.02
7	I	2	NAG	C1-O5-C5	2.69	115.80	112.19
6	O	6	MAN	C1-C2-C3	-2.69	105.73	109.64
7	I	5	MAN	O2-C2-C1	2.68	115.37	109.22
7	I	5	MAN	C6-C5-C4	2.67	119.57	113.02
10	P	1	NAG	O7-C7-C8	2.67	126.80	122.05
6	O	2	NAG	C3-C4-C5	-2.66	105.40	110.23
3	D	1	NAG	C4-C3-C2	-2.66	107.12	111.02
6	H	2	NAG	C4-C3-C2	2.66	114.92	111.02
6	H	7	MAN	O5-C1-C2	-2.65	104.48	110.79
7	I	6	MAN	C6-C5-C4	-2.64	106.54	113.02
3	L	2	NAG	C2-N2-C7	2.63	126.43	122.90
3	G	1	NAG	O3-C3-C2	-2.63	103.93	109.40
6	H	4	MAN	C6-C5-C4	2.63	119.48	113.02
6	O	5	MAN	C6-C5-C4	-2.62	106.58	113.02
7	I	2	NAG	O5-C1-C2	-2.62	107.23	111.29
3	N	1	NAG	C1-O5-C5	-2.62	108.67	112.19
3	G	3	BMA	C3-C4-C5	2.61	114.96	110.23
6	H	4	MAN	O6-C6-C5	-2.60	102.47	111.33
7	I	1	NAG	O6-C6-C5	-2.60	102.49	111.33
5	M	1	NAG	O5-C5-C6	-2.60	102.61	107.66
2	C	5	MAN	C1-O5-C5	2.60	115.66	112.19
3	G	3	BMA	O4-C4-C5	-2.59	102.94	109.32
2	C	3	BMA	C3-C4-C5	2.58	114.91	110.23
8	J	4	MAN	C6-C5-C4	-2.58	106.69	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	5	MAN	O2-C2-C3	-2.57	104.82	110.15
6	H	2	NAG	O6-C6-C5	-2.57	102.58	111.33
5	F	9	MAN	O4-C4-C3	-2.57	104.32	110.38
5	F	10	MAN	O2-C2-C3	2.56	115.44	110.15
6	H	5	MAN	C3-C4-C5	-2.54	105.62	110.23
3	D	2	NAG	O3-C3-C2	-2.54	104.12	109.40
5	M	5	MAN	O3-C3-C4	-2.53	104.41	110.38
5	M	7	MAN	O6-C6-C5	-2.53	102.73	111.33
5	M	7	MAN	O5-C5-C4	-2.52	104.69	110.83
6	O	5	MAN	O6-C6-C5	-2.52	102.75	111.33
7	I	5	MAN	O4-C4-C3	-2.51	104.45	110.38
2	C	2	NAG	C6-C5-C4	2.51	119.18	113.02
10	P	2	NAG	C8-C7-N2	2.51	120.27	116.12
5	M	2	NAG	O4-C4-C3	-2.51	104.47	110.38
5	M	4	MAN	C2-C3-C4	-2.50	106.47	110.86
7	I	7	MAN	O5-C5-C6	2.49	112.52	107.66
10	P	4	MAN	O3-C3-C4	-2.49	104.50	110.38
4	E	2	NAG	O5-C5-C6	2.49	112.51	107.66
5	M	9	MAN	O2-C2-C3	-2.48	105.00	110.15
5	F	3	BMA	C1-C2-C3	2.48	113.25	109.64
6	H	3	BMA	O5-C5-C4	-2.46	104.83	110.83
7	I	7	MAN	O2-C2-C3	2.45	115.23	110.15
10	P	1	NAG	C1-O5-C5	2.43	115.44	112.19
3	D	1	NAG	C2-N2-C7	-2.43	119.65	122.90
2	C	2	NAG	O5-C5-C4	-2.43	104.92	110.83
10	P	5	MAN	O6-C6-C5	-2.42	103.08	111.33
3	N	2	NAG	C2-N2-C7	-2.42	119.65	122.90
8	J	3	BMA	C1-C2-C3	-2.42	106.12	109.64
5	M	10	MAN	C1-C2-C3	-2.42	106.12	109.64
6	O	5	MAN	O5-C5-C6	2.42	112.37	107.66
5	F	10	MAN	O3-C3-C4	-2.42	104.68	110.38
6	O	3	BMA	O4-C4-C5	-2.41	103.39	109.32
9	K	2	NAG	O4-C4-C5	-2.41	103.39	109.32
10	P	7	MAN	O4-C4-C5	-2.40	103.41	109.32
7	I	1	NAG	C6-C5-C4	-2.40	107.13	113.02
8	J	7	MAN	O4-C4-C3	-2.39	104.74	110.38
6	O	4	MAN	O4-C4-C5	-2.38	103.46	109.32
6	O	1	NAG	C1-O5-C5	2.38	115.38	112.19
6	O	6	MAN	O6-C6-C5	-2.38	103.23	111.33
2	C	4	MAN	C2-C3-C4	2.37	115.03	110.86
6	O	5	MAN	O4-C4-C3	-2.37	104.79	110.38
10	P	5	MAN	O3-C3-C4	-2.37	104.80	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O3-C3-C4	2.36	115.95	110.38
6	H	2	NAG	C3-C4-C5	-2.36	105.95	110.23
7	I	1	NAG	C1-O5-C5	2.36	115.35	112.19
6	H	1	NAG	O5-C5-C4	-2.35	105.10	110.83
10	P	3	BMA	O4-C4-C5	-2.35	103.53	109.32
7	I	6	MAN	C2-C3-C4	-2.35	106.73	110.86
8	J	2	NAG	O4-C4-C5	-2.35	103.54	109.32
9	K	1	NAG	C1-C2-N2	2.33	114.10	110.43
6	H	3	BMA	O2-C2-C1	-2.33	103.89	109.22
10	P	2	NAG	O5-C1-C2	-2.33	107.69	111.29
5	F	2	NAG	O5-C1-C2	-2.32	107.69	111.29
5	M	5	MAN	C6-C5-C4	-2.31	107.33	113.02
5	F	9	MAN	O3-C3-C2	-2.31	105.33	110.05
2	C	2	NAG	O3-C3-C2	-2.31	104.61	109.40
3	D	2	NAG	O5-C1-C2	-2.30	107.73	111.29
3	G	2	NAG	C4-C3-C2	2.30	114.39	111.02
7	I	3	BMA	O2-C2-C3	2.30	114.91	110.15
2	C	2	NAG	C2-N2-C7	2.29	125.97	122.90
2	C	2	NAG	O7-C7-N2	2.29	126.03	121.98
9	K	2	NAG	C1-O5-C5	-2.29	109.12	112.19
5	M	10	MAN	O5-C5-C6	-2.28	103.22	107.66
5	F	10	MAN	C1-O5-C5	2.28	115.24	112.19
10	P	4	MAN	O5-C1-C2	2.28	116.23	110.79
8	J	7	MAN	O5-C5-C6	2.28	112.10	107.66
5	M	7	MAN	O5-C5-C6	2.27	112.08	107.66
9	K	4	MAN	C6-C5-C4	2.26	118.56	113.02
5	M	10	MAN	C1-O5-C5	2.25	115.21	112.19
6	H	7	MAN	C1-C2-C3	-2.25	106.37	109.64
5	F	7	MAN	O5-C1-C2	-2.25	105.43	110.79
7	I	1	NAG	C1-C2-N2	-2.24	106.90	110.43
5	M	10	MAN	O2-C2-C3	2.24	114.80	110.15
6	O	2	NAG	O6-C6-C5	-2.24	103.72	111.33
2	C	3	BMA	O3-C3-C2	-2.23	105.51	110.05
5	M	1	NAG	O5-C5-C4	-2.23	105.41	110.83
2	C	1	NAG	O5-C5-C6	2.22	111.99	107.66
9	K	4	MAN	O4-C4-C5	-2.22	103.85	109.32
3	D	1	NAG	O6-C6-C5	-2.22	103.77	111.33
5	M	8	MAN	C1-O5-C5	2.22	115.16	112.19
5	F	8	MAN	O4-C4-C5	2.22	114.79	109.32
7	I	3	BMA	C1-C2-C3	2.22	112.87	109.64
2	C	4	MAN	O5-C1-C2	2.21	116.06	110.79
3	D	2	NAG	O6-C6-C5	-2.20	103.84	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	7	MAN	C2-C3-C4	-2.19	107.00	110.86
3	L	1	NAG	C6-C5-C4	-2.19	107.64	113.02
3	L	1	NAG	O5-C5-C6	2.19	111.92	107.66
5	M	9	MAN	O5-C5-C6	-2.18	103.41	107.66
7	I	6	MAN	O6-C6-C5	-2.18	103.90	111.33
8	J	3	BMA	O3-C3-C4	-2.18	105.23	110.38
9	K	1	NAG	O3-C3-C2	-2.18	104.88	109.40
10	P	2	NAG	O6-C6-C5	-2.18	103.92	111.33
10	P	8	MAN	O2-C2-C1	2.16	114.17	109.22
5	F	1	NAG	C3-C4-C5	2.16	114.15	110.23
6	H	4	MAN	O4-C4-C3	-2.16	105.29	110.38
6	O	4	MAN	C1-O5-C5	2.16	115.08	112.19
5	M	4	MAN	O5-C5-C4	-2.15	105.59	110.83
6	H	4	MAN	O5-C1-C2	2.15	115.91	110.79
7	I	2	NAG	C6-C5-C4	-2.14	107.75	113.02
8	J	4	MAN	O2-C2-C3	-2.14	105.72	110.15
6	O	4	MAN	O2-C2-C1	2.14	114.12	109.22
8	J	1	NAG	O4-C4-C3	-2.13	105.35	110.38
5	M	9	MAN	C1-O5-C5	2.13	115.04	112.19
5	M	1	NAG	O5-C1-C2	-2.12	108.01	111.29
6	H	7	MAN	O6-C6-C5	-2.12	104.12	111.33
6	O	5	MAN	C1-O5-C5	2.11	115.01	112.19
6	O	6	MAN	O4-C4-C3	-2.11	105.41	110.38
8	J	4	MAN	O6-C6-C5	-2.10	104.18	111.33
8	J	3	BMA	C3-C4-C5	2.10	114.04	110.23
5	F	9	MAN	C1-O5-C5	2.10	115.00	112.19
5	M	2	NAG	C2-N2-C7	-2.09	120.10	122.90
6	O	4	MAN	O6-C6-C5	-2.09	104.22	111.33
10	P	1	NAG	O3-C3-C2	-2.09	105.07	109.40
3	L	3	BMA	O5-C5-C4	2.08	115.89	110.83
5	M	1	NAG	C4-C3-C2	2.08	114.07	111.02
9	K	1	NAG	O5-C5-C4	-2.08	105.76	110.83
4	E	2	NAG	O5-C5-C4	-2.08	105.77	110.83
4	E	1	NAG	C1-O5-C5	2.08	114.97	112.19
6	H	1	NAG	C8-C7-N2	2.08	119.56	116.12
7	I	4	MAN	O4-C4-C5	2.07	114.43	109.32
6	H	4	MAN	C1-O5-C5	2.07	114.96	112.19
9	K	2	NAG	C1-C2-N2	2.07	113.69	110.43
9	K	1	NAG	O6-C6-C5	-2.06	104.30	111.33
10	P	5	MAN	C1-C2-C3	2.04	112.62	109.64
6	O	6	MAN	C6-C5-C4	-2.04	108.01	113.02
5	F	3	BMA	C2-C3-C4	-2.04	107.27	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	4	MAN	C1-O5-C5	-2.04	109.45	112.19
9	K	1	NAG	O7-C7-N2	2.03	125.58	121.98
6	H	2	NAG	O5-C1-C2	-2.03	108.14	111.29
5	F	10	MAN	O4-C4-C3	-2.03	105.58	110.38
9	K	3	BMA	O3-C3-C2	2.03	114.20	110.05
3	G	3	BMA	O5-C5-C4	2.03	115.77	110.83
5	F	8	MAN	O2-C2-C1	-2.03	104.58	109.22
4	E	1	NAG	C1-C2-N2	-2.03	107.24	110.43
10	P	1	NAG	O5-C5-C6	2.02	111.60	107.66
5	F	2	NAG	O6-C6-C5	-2.02	104.45	111.33
6	H	4	MAN	O3-C3-C2	2.02	114.17	110.05
7	I	2	NAG	O3-C3-C2	-2.02	105.21	109.40
5	F	1	NAG	O5-C5-C6	-2.01	103.75	107.66
7	I	3	BMA	O6-C6-C5	-2.01	104.49	111.33
9	K	4	MAN	O4-C4-C3	2.00	115.10	110.38

There are no chirality outliers.

All (38) torsion outliers are listed below:

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

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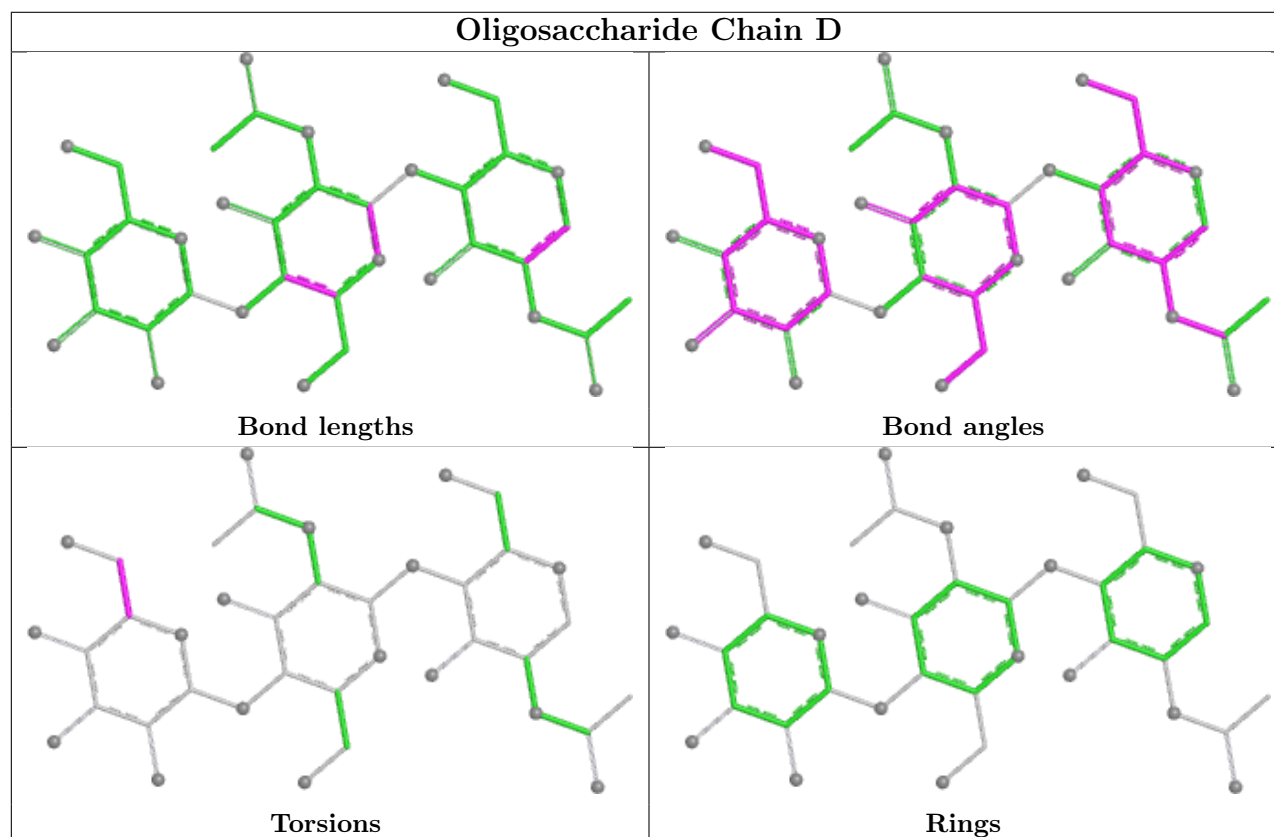
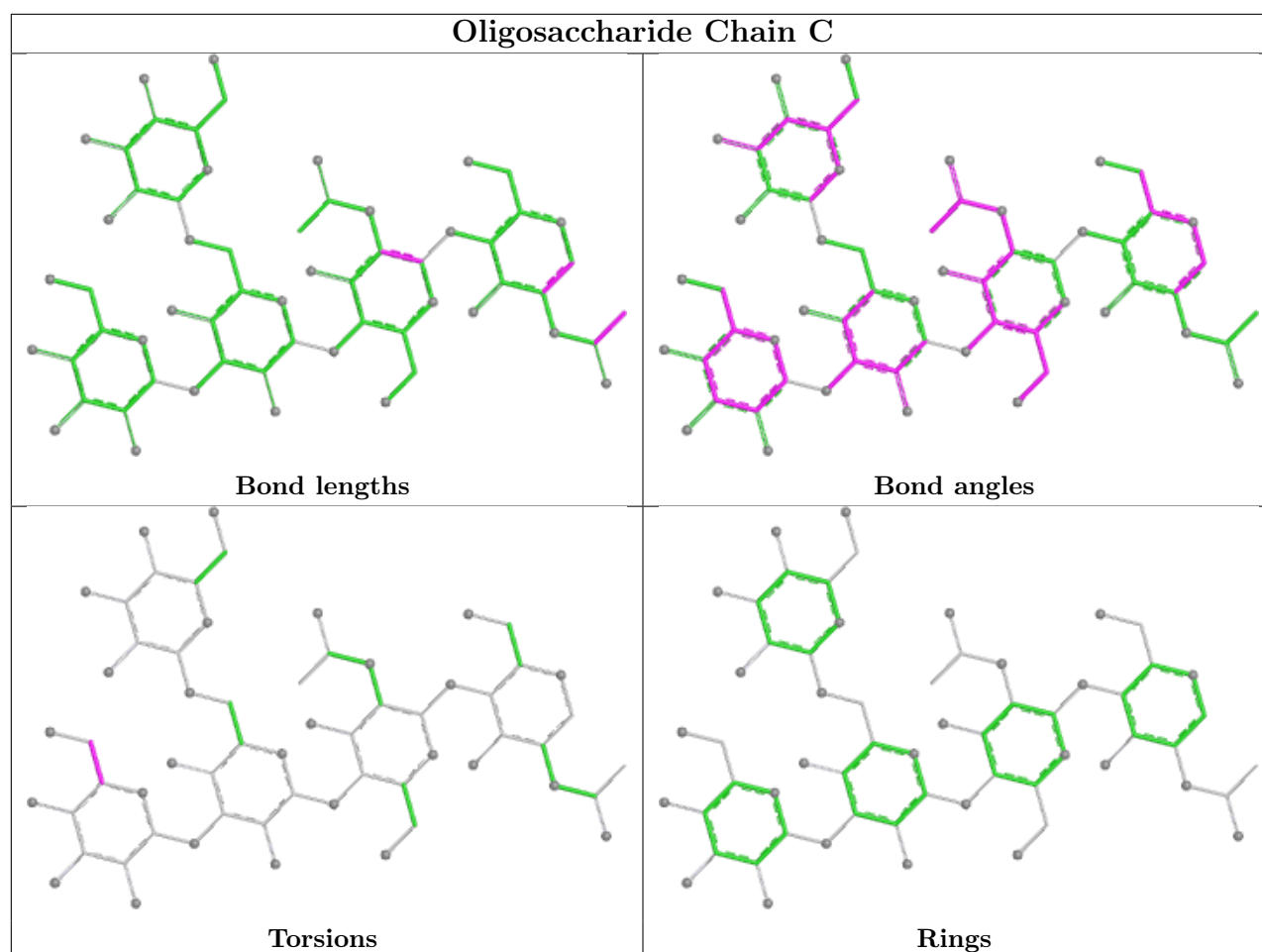
Mol	Chain	Res	Type	Atoms
10	P	3	BMA	O5-C5-C6-O6
3	D	3	BMA	O5-C5-C6-O6
10	P	6	MAN	C4-C5-C6-O6
10	P	6	MAN	O5-C5-C6-O6
7	I	7	MAN	C4-C5-C6-O6
10	P	8	MAN	O5-C5-C6-O6
7	I	7	MAN	O5-C5-C6-O6
6	O	7	MAN	C4-C5-C6-O6
7	I	6	MAN	C4-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C3-C2-N2-C7
3	L	2	NAG	C1-C2-N2-C7
4	E	2	NAG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

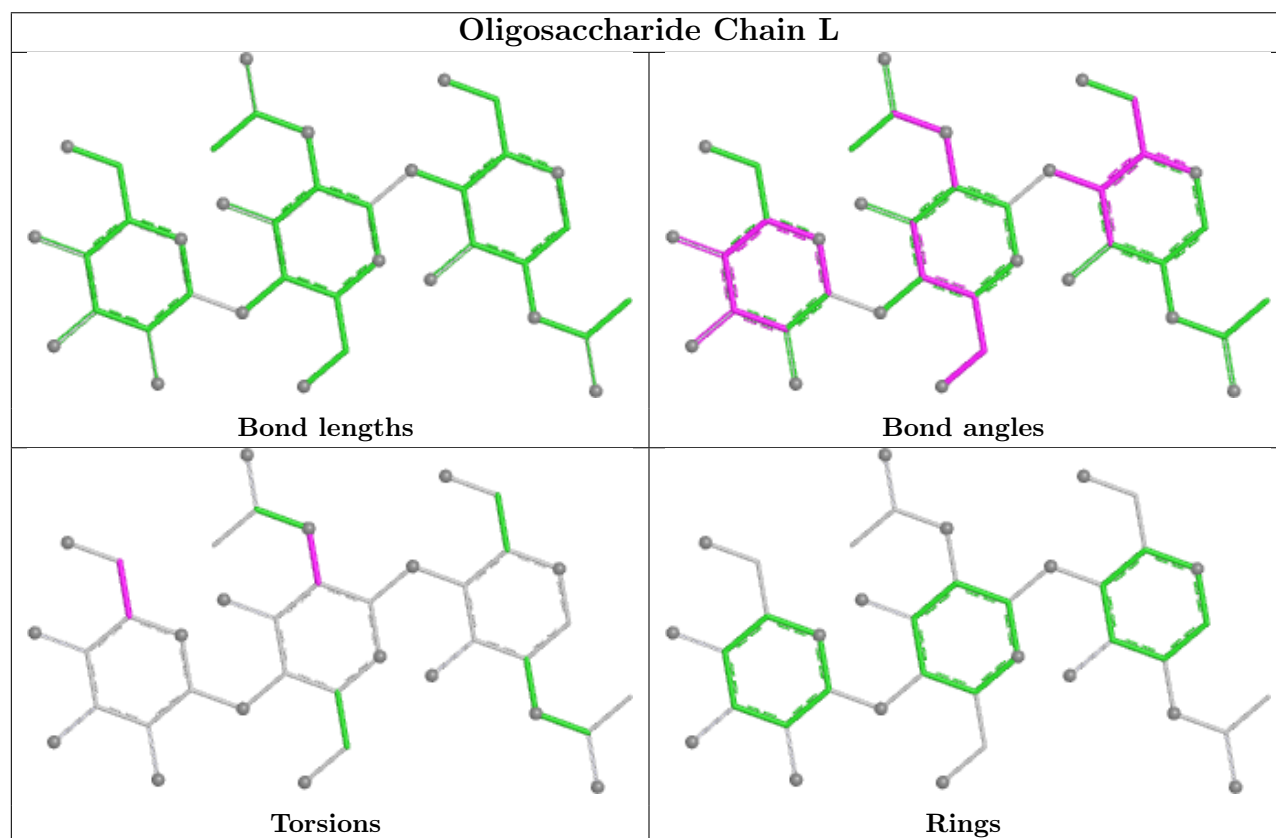
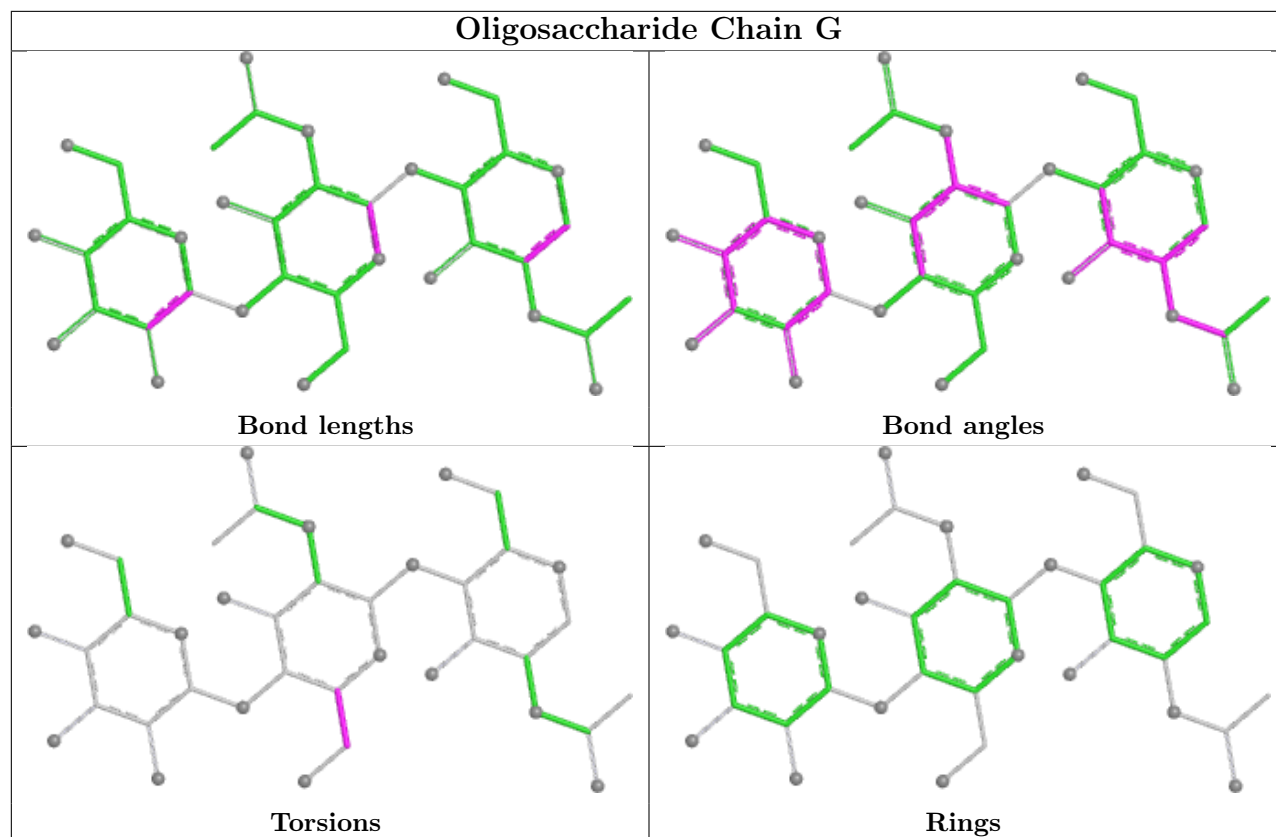
There are no ring outliers.

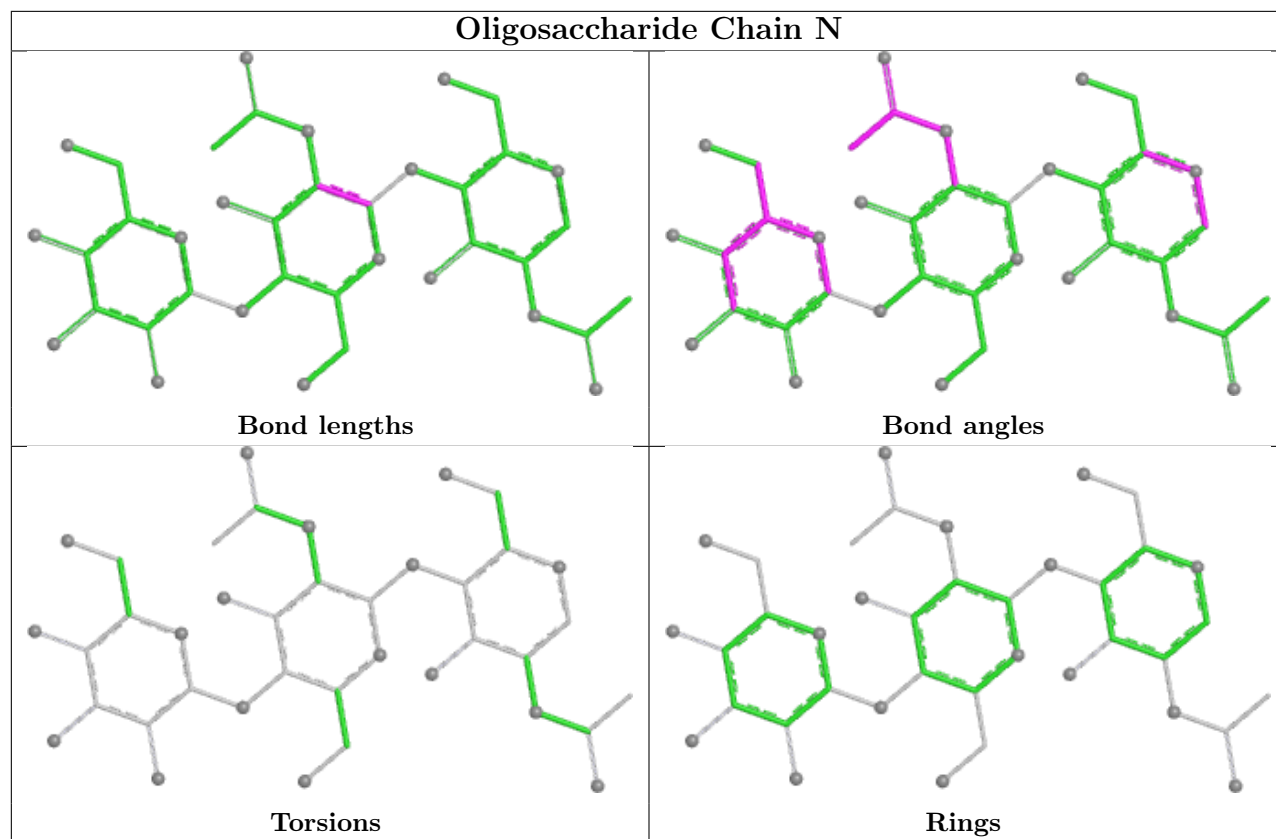
9 monomers are involved in 13 short contacts:

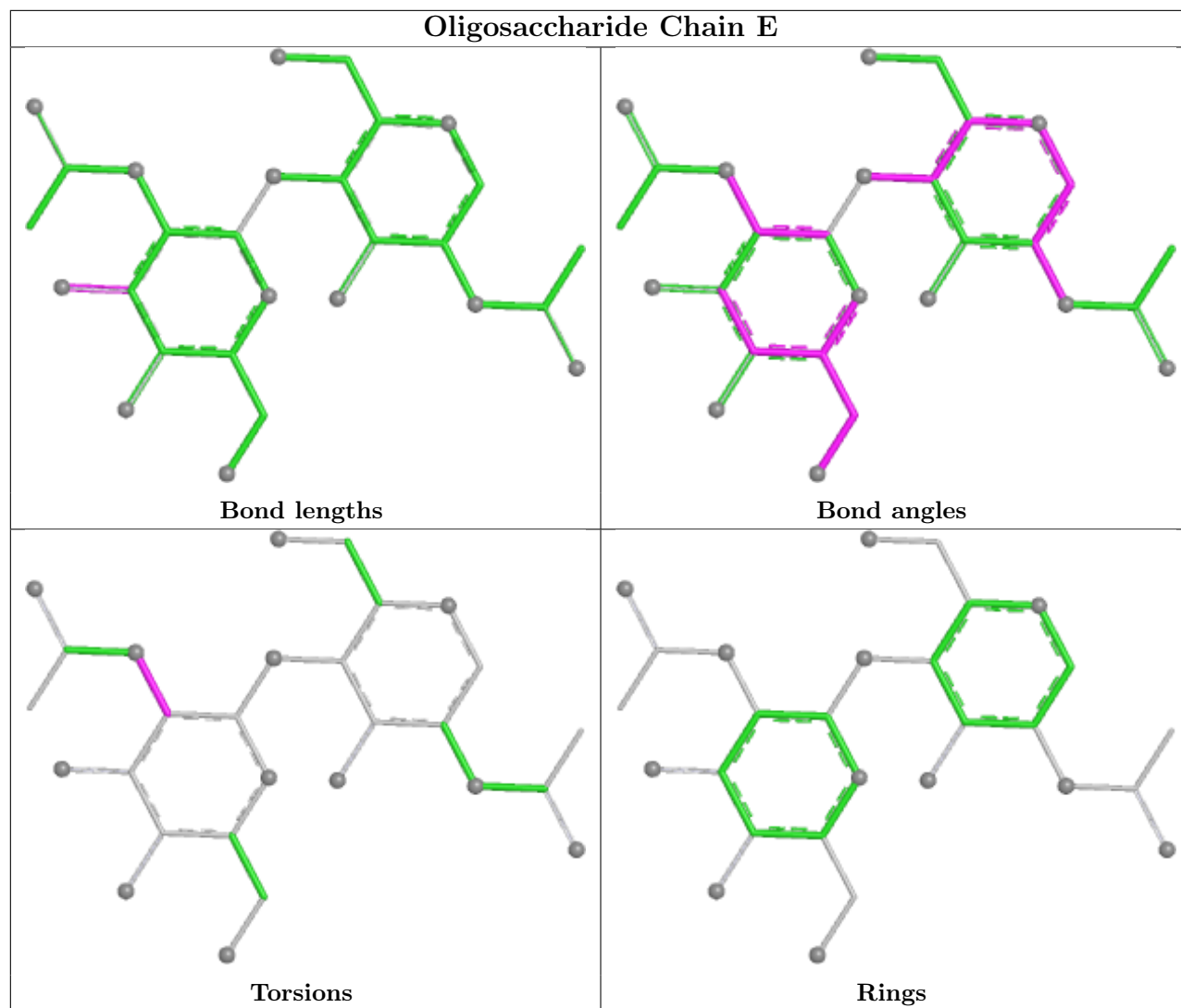
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	3	BMA	1	0
3	D	2	NAG	1	0
10	P	4	MAN	5	0
6	O	3	BMA	1	0
7	I	6	MAN	1	0
10	P	3	BMA	6	0
2	C	2	NAG	1	0
8	J	2	NAG	1	0
9	K	1	NAG	1	0

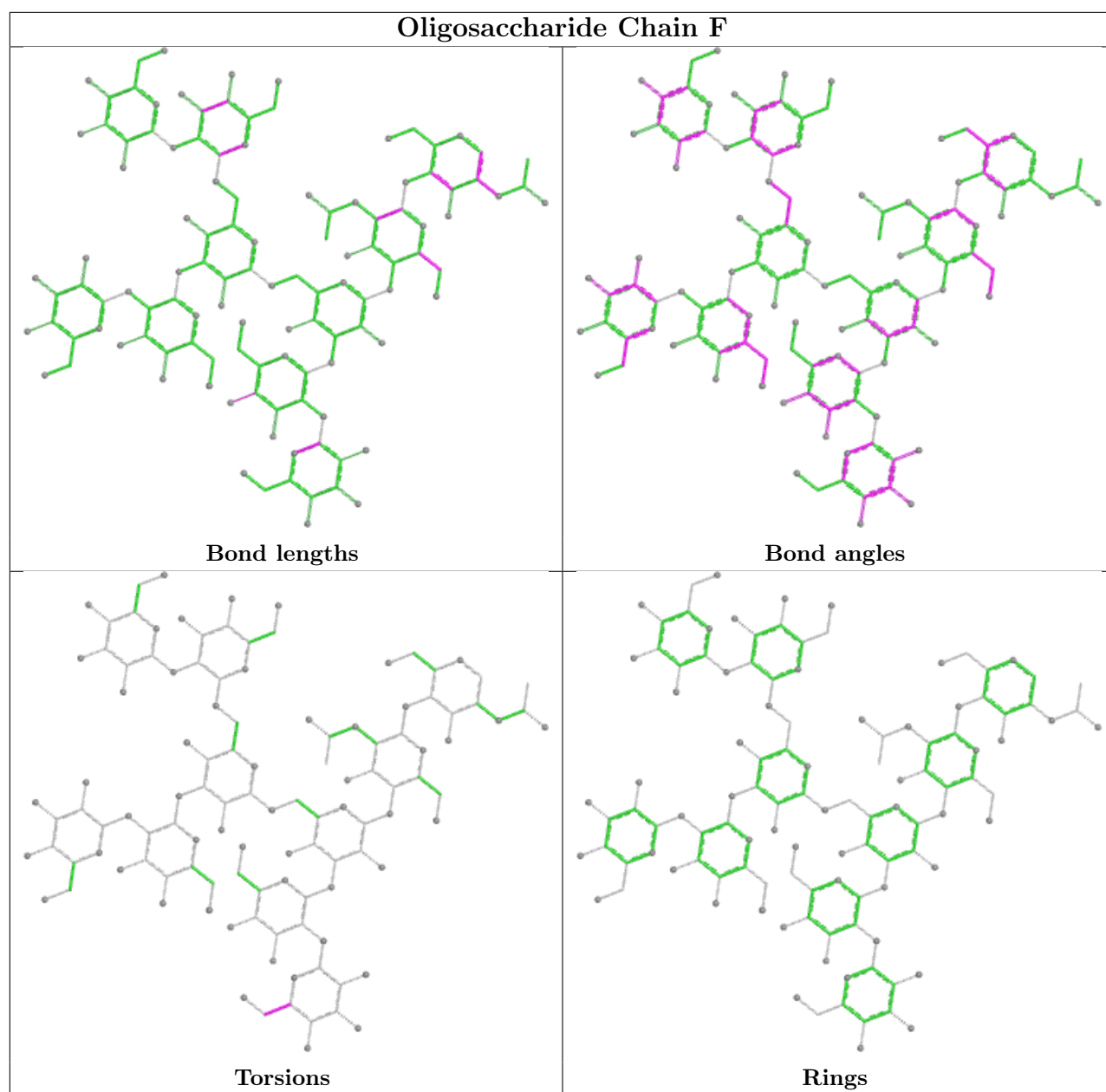
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

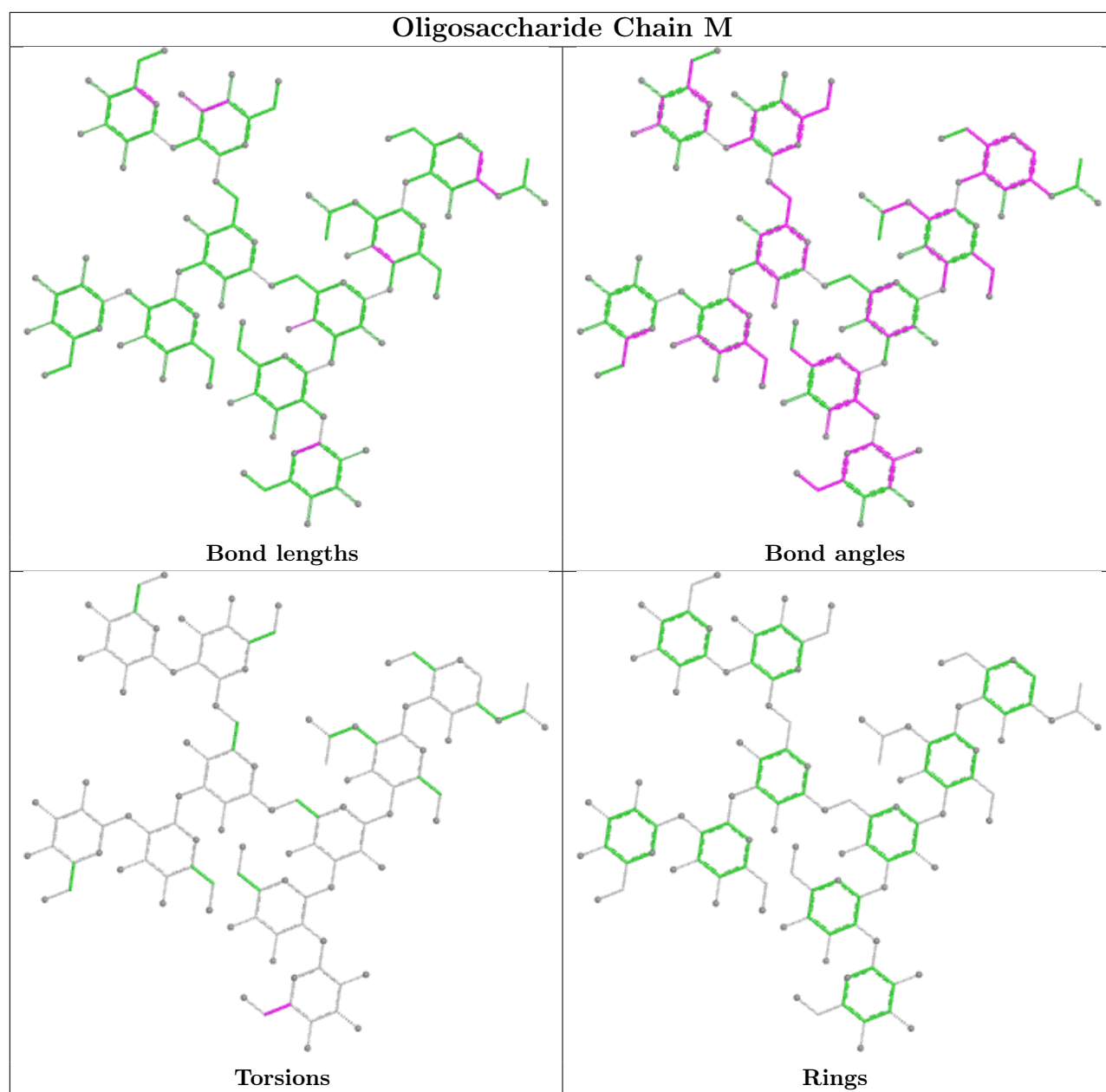


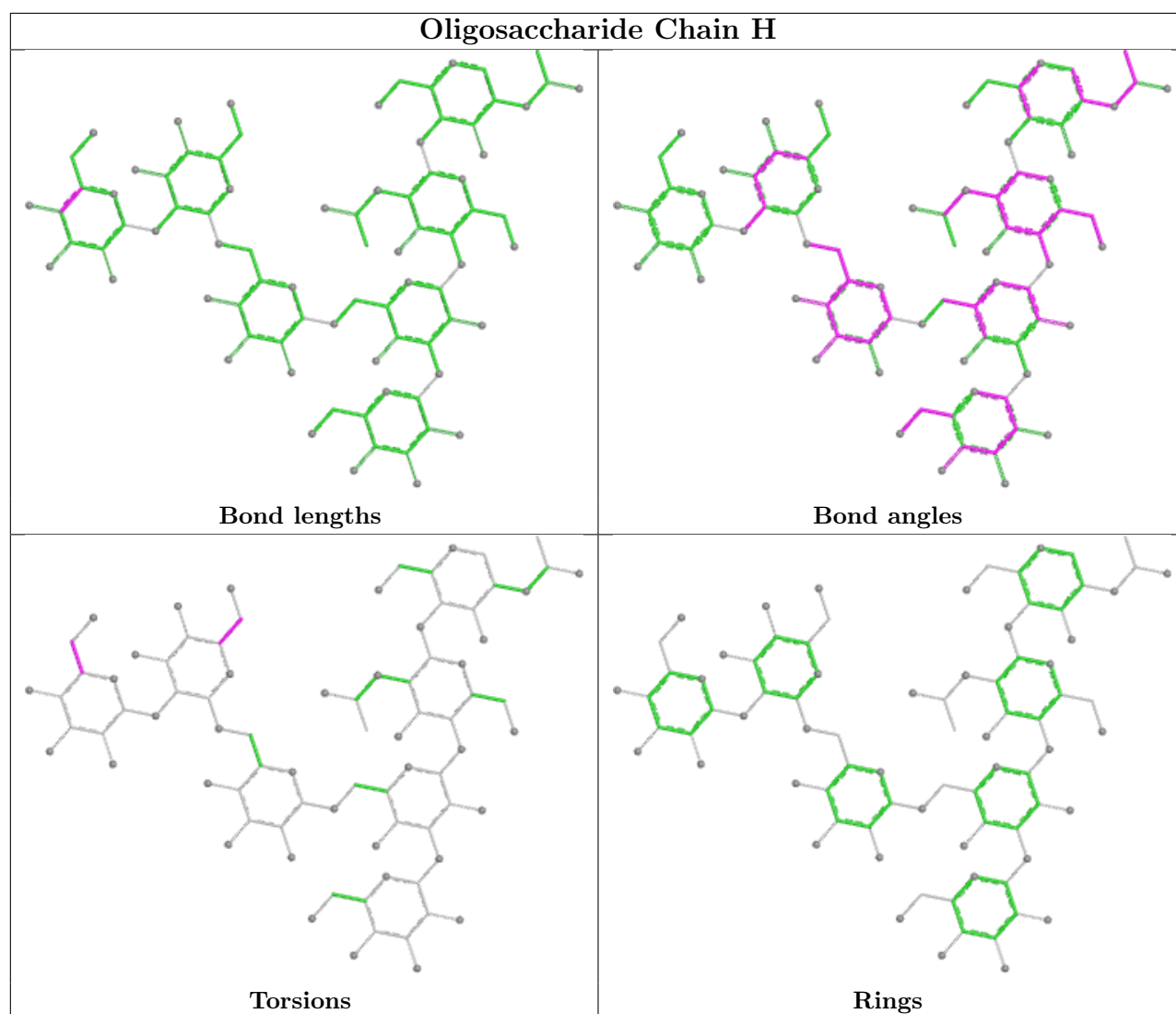


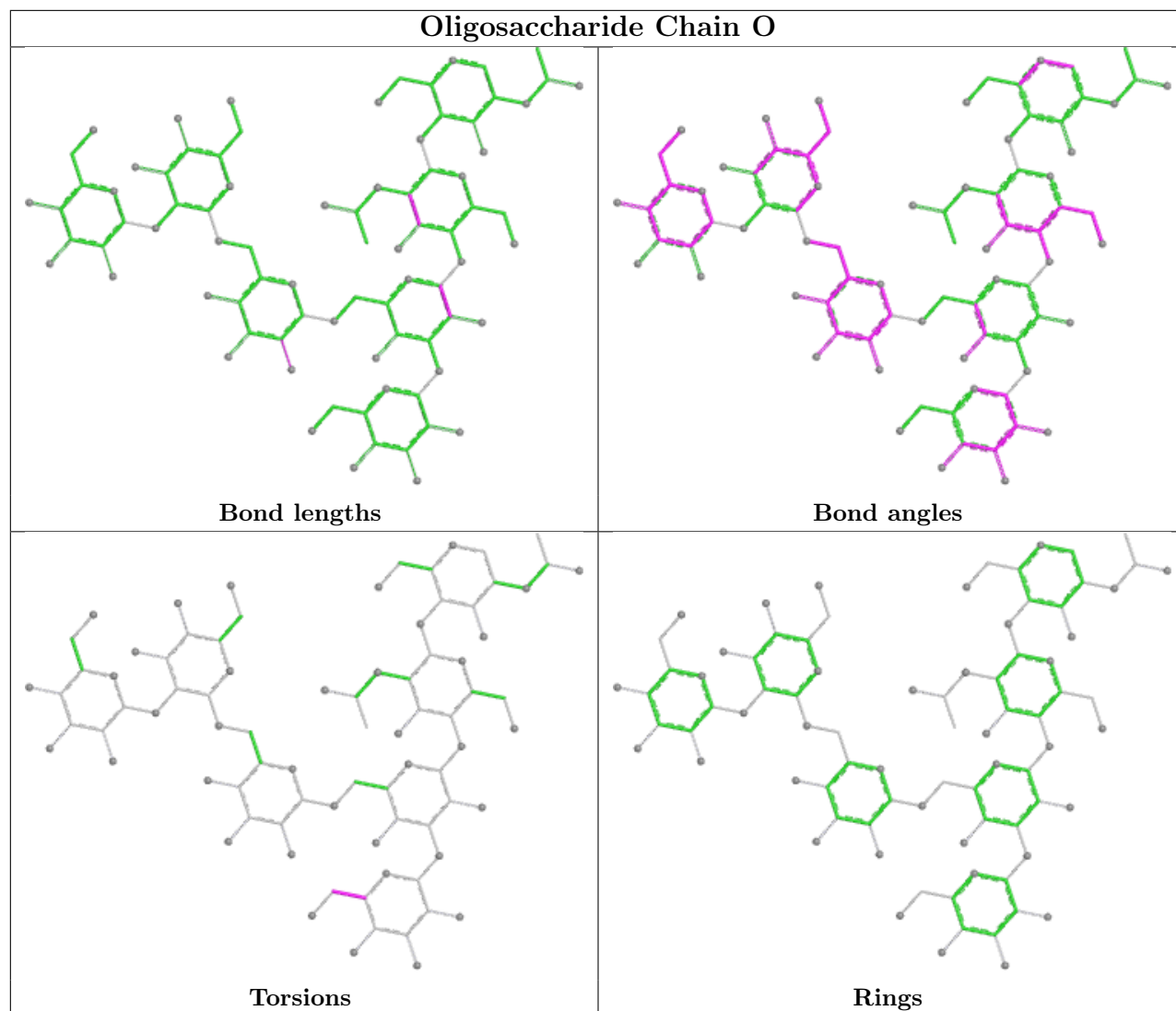


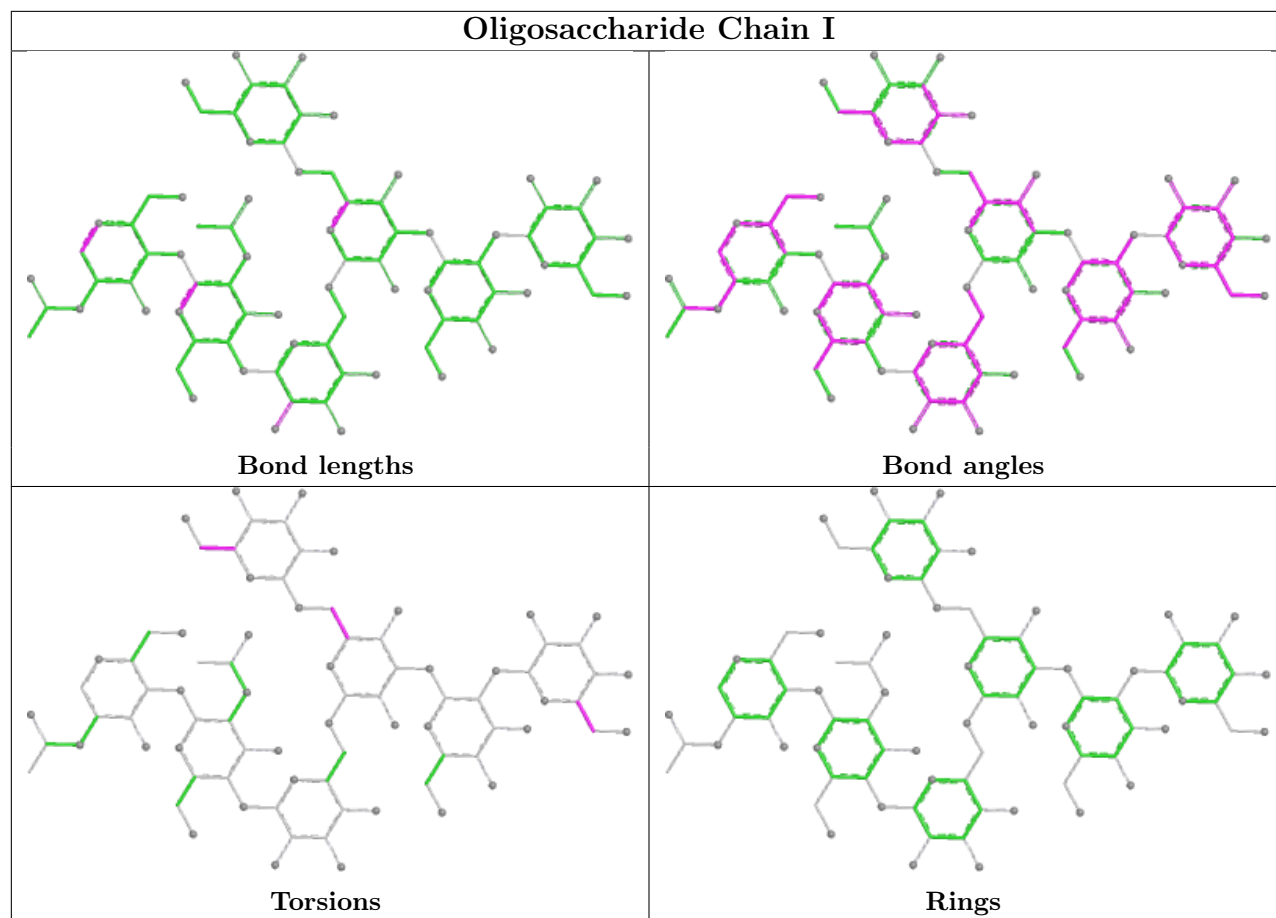


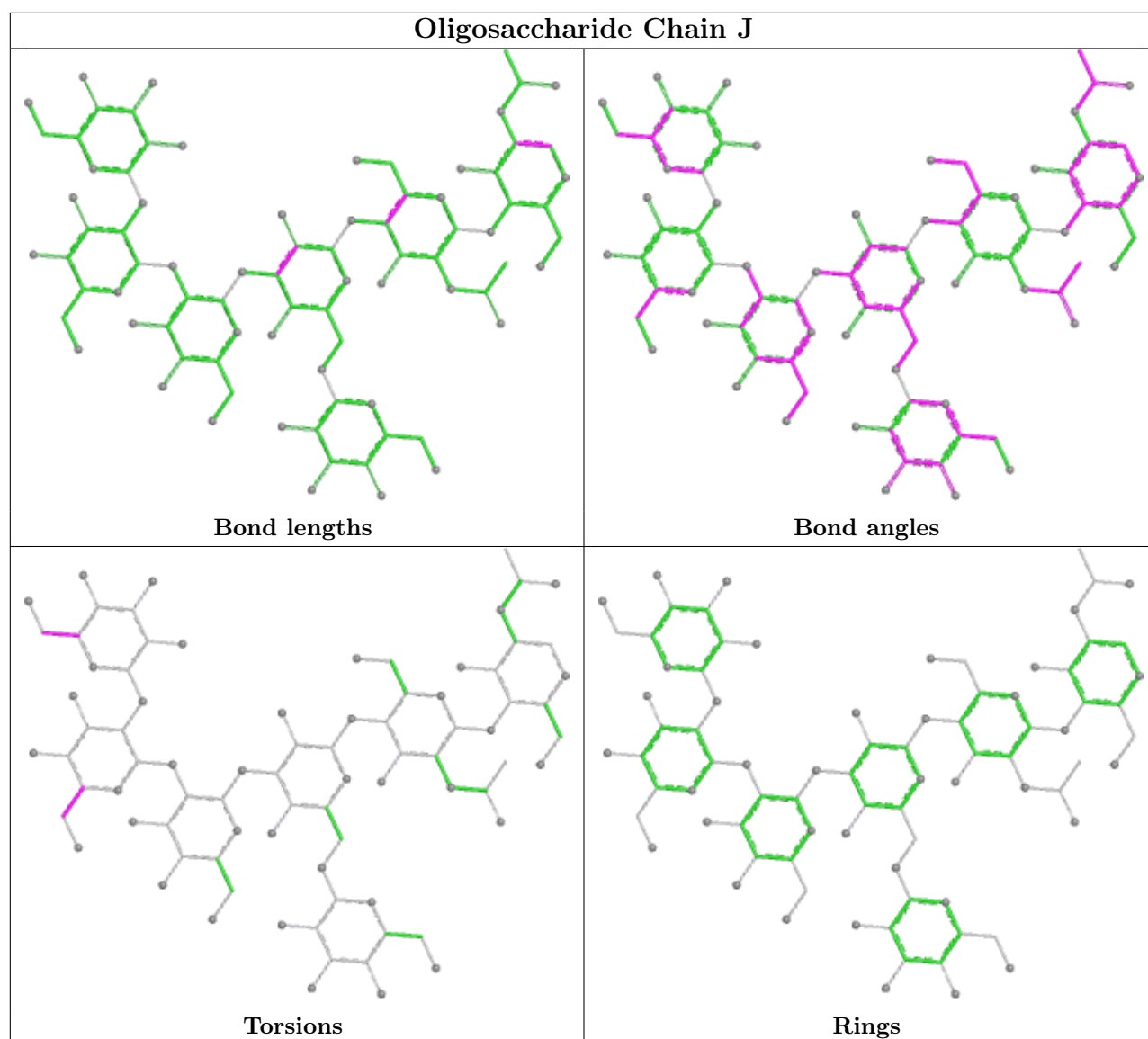


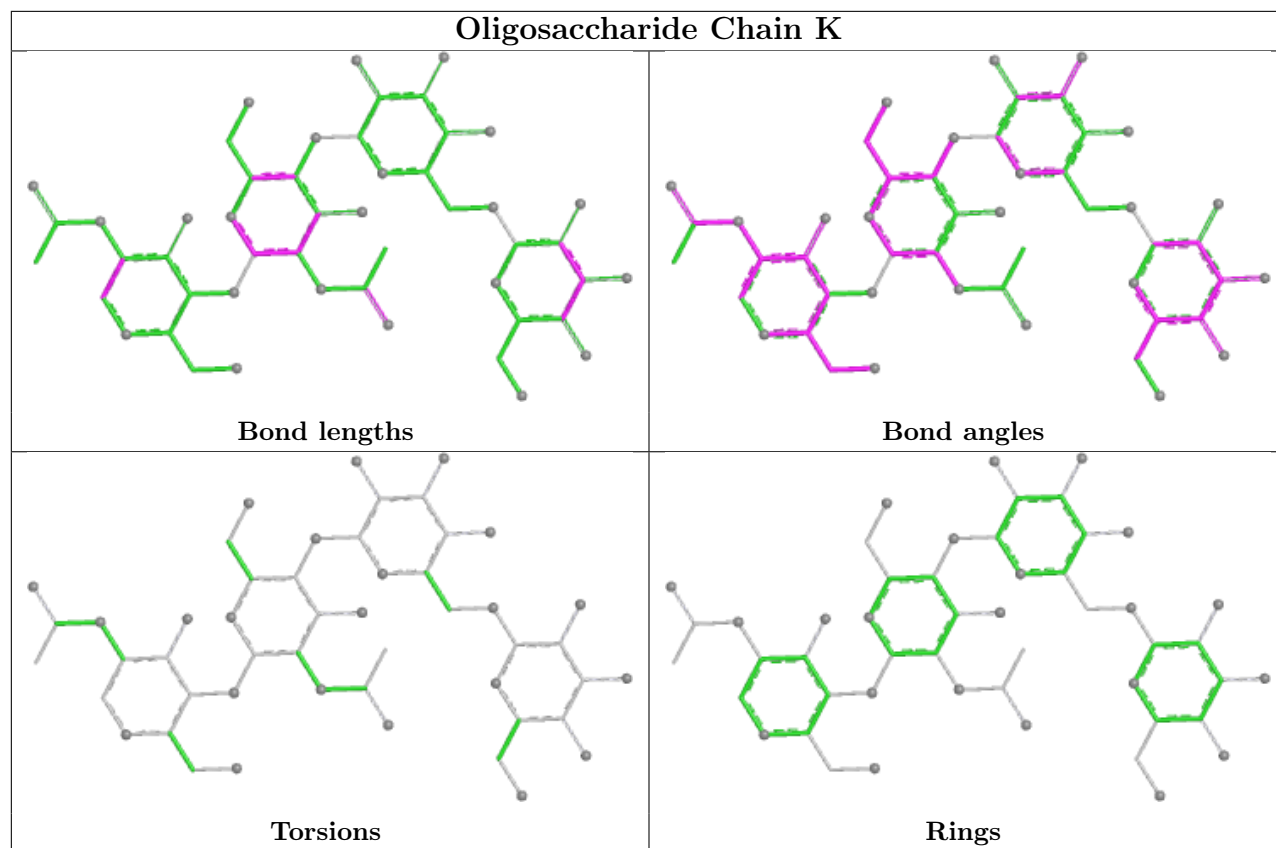


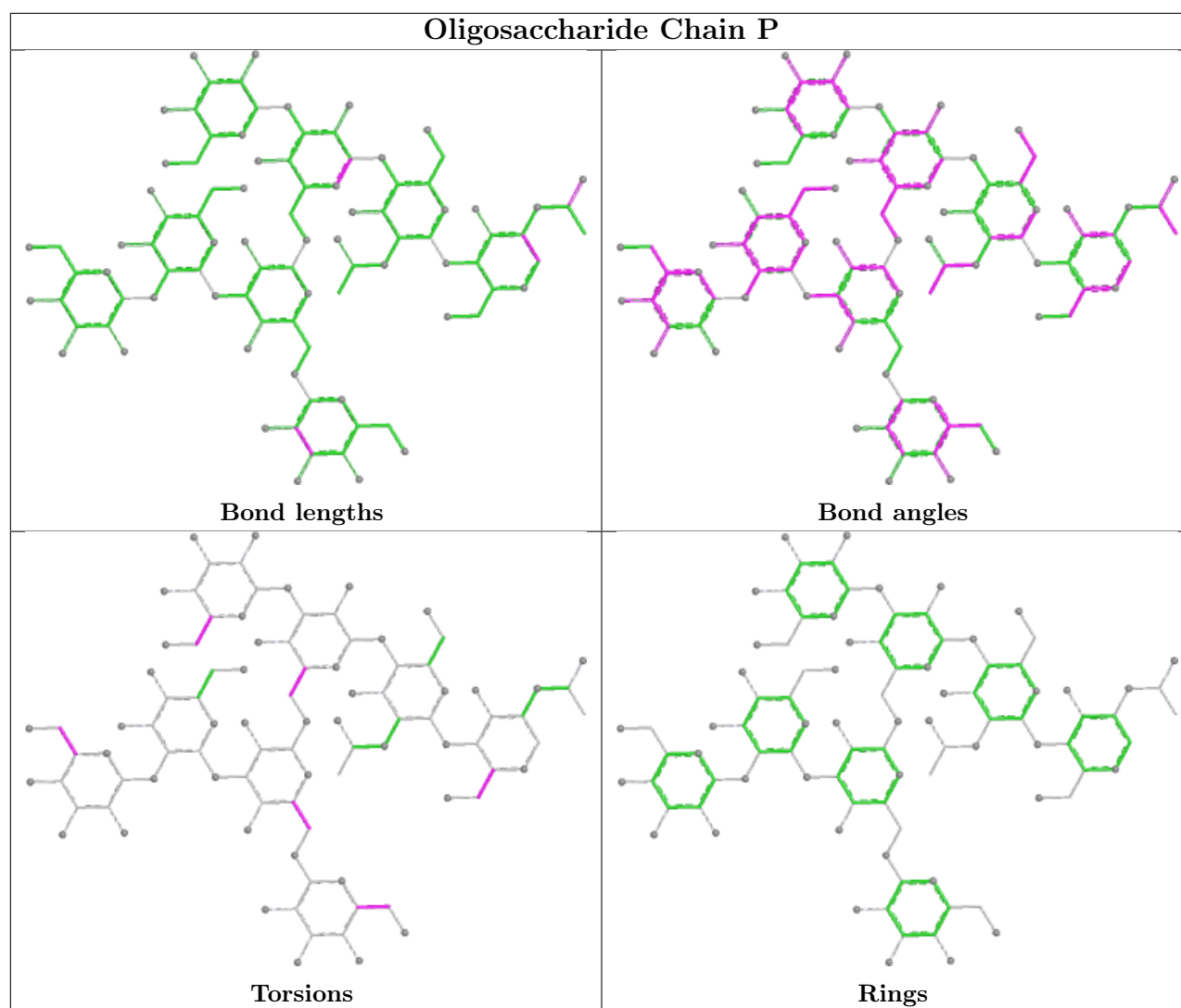












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
12	MRD	A	940	-	7,7,7	1.34	0	9,10,10	0.49	0
15	IFM	B	950	-	10,10,10	2.69	3 (30%)	9,13,13	1.29	2 (22%)
13	MPD	A	942	-	7,7,7	0.76	0	9,10,10	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	B	908	1	14,14,15	0.91	1 (7%)	17,19,21	2.86	8 (47%)
11	NAG	B	944	1	14,14,15	0.76	0	17,19,21	2.21	4 (23%)
11	NAG	A	939	1	14,14,15	1.07	1 (7%)	17,19,21	2.12	8 (47%)
12	MRD	B	946	-	7,7,7	1.32	0	9,10,10	0.60	0
11	NAG	A	906	1	14,14,15	0.84	0	17,19,21	1.77	3 (17%)
15	IFM	A	944	-	10,10,10	2.90	4 (40%)	9,13,13	1.47	1 (11%)
12	MRD	B	948	-	7,7,7	1.15	1 (14%)	9,10,10	0.53	0
12	MRD	A	941	-	7,7,7	1.44	0	9,10,10	1.28	1 (11%)
12	MRD	B	947	-	7,7,7	1.15	1 (14%)	9,10,10	1.50	3 (33%)
11	NAG	B	945	1	14,14,15	0.79	0	17,19,21	1.68	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MRD	A	940	-	-	0/5/5/5	-
15	IFM	B	950	-	-	0/2/16/16	0/1/1/1
13	MPD	A	942	-	-	2/5/5/5	-
11	NAG	B	908	1	-	6/6/23/26	0/1/1/1
11	NAG	B	944	1	-	4/6/23/26	0/1/1/1
11	NAG	A	939	1	-	0/6/23/26	0/1/1/1
12	MRD	B	946	-	-	4/5/5/5	-
11	NAG	A	906	1	-	0/6/23/26	0/1/1/1
15	IFM	A	944	-	-	0/2/16/16	0/1/1/1
12	MRD	B	948	-	-	4/5/5/5	-
12	MRD	A	941	-	-	4/5/5/5	-
12	MRD	B	947	-	-	3/5/5/5	-
11	NAG	B	945	1	-	1/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	944	IFM	C2-C3	7.35	1.59	1.52
15	B	950	IFM	C2-C3	5.21	1.57	1.52
15	B	950	IFM	C1-C5	5.13	1.58	1.52
15	A	944	IFM	C6-C5	3.08	1.58	1.52
12	B	948	MRD	O2-C2	-2.54	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	944	IFM	C5-C4	2.52	1.60	1.53
11	B	908	NAG	O5-C1	-2.50	1.39	1.43
12	B	947	MRD	C3-C2	-2.46	1.46	1.54
15	A	944	IFM	C1-N	2.41	1.53	1.47
11	A	939	NAG	O3-C3	-2.23	1.37	1.43
15	B	950	IFM	C6-C5	2.10	1.56	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	908	NAG	C8-C7-N2	6.11	126.26	116.12
11	B	908	NAG	C2-N2-C7	5.67	130.50	122.90
11	A	906	NAG	C1-C2-N2	5.12	118.50	110.43
11	B	944	NAG	C8-C7-N2	4.86	124.18	116.12
11	B	944	NAG	O5-C1-C2	-4.34	104.58	111.29
11	A	939	NAG	C2-N2-C7	-3.87	117.72	122.90
11	B	908	NAG	O5-C1-C2	-3.73	105.53	111.29
11	B	908	NAG	O5-C5-C6	3.70	114.86	107.66
11	B	944	NAG	O7-C7-C8	-3.62	115.61	122.05
11	B	908	NAG	O7-C7-N2	-3.25	116.24	121.98
11	A	939	NAG	C1-O5-C5	3.16	116.42	112.19
12	B	947	MRD	O4-C4-C3	-3.09	99.05	111.35
11	B	908	NAG	O3-C3-C4	-3.07	103.14	110.38
11	B	945	NAG	C3-C4-C5	-3.07	104.67	110.23
11	A	939	NAG	C8-C7-N2	3.03	121.14	116.12
15	A	944	IFM	C1-C5-C6	-2.91	105.20	110.99
11	B	908	NAG	C1-C2-N2	-2.75	106.11	110.43
11	B	945	NAG	C1-O5-C5	-2.72	108.55	112.19
15	B	950	IFM	C2-C3-C4	-2.64	107.02	110.25
11	A	939	NAG	O5-C5-C4	-2.62	104.45	110.83
11	A	939	NAG	O5-C1-C2	2.58	115.28	111.29
11	B	908	NAG	O7-C7-C8	-2.56	117.49	122.05
11	B	945	NAG	O5-C5-C4	-2.53	104.67	110.83
12	A	941	MRD	O4-C4-C3	-2.52	101.33	111.35
11	A	939	NAG	O3-C3-C4	-2.46	104.58	110.38
11	A	906	NAG	C2-N2-C7	-2.35	119.75	122.90
12	B	947	MRD	C1-C2-C3	-2.30	100.29	110.20
12	B	947	MRD	O2-C2-C1	2.24	114.98	107.99
11	A	939	NAG	C4-C3-C2	-2.23	107.75	111.02
11	A	939	NAG	C3-C4-C5	-2.14	106.35	110.23
11	B	944	NAG	O6-C6-C5	-2.06	104.32	111.33
11	B	945	NAG	O7-C7-C8	-2.06	118.39	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	906	NAG	O7-C7-C8	-2.04	118.42	122.05
15	B	950	IFM	O4-C4-C3	-2.03	105.92	110.05

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	941	MRD	C2-C3-C4-C5
12	B	948	MRD	C2-C3-C4-O4
12	B	948	MRD	C2-C3-C4-C5
11	B	908	NAG	C4-C5-C6-O6
11	B	908	NAG	O5-C5-C6-O6
11	B	908	NAG	C8-C7-N2-C2
11	B	908	NAG	O7-C7-N2-C2
11	B	944	NAG	C8-C7-N2-C2
11	B	944	NAG	O7-C7-N2-C2
11	B	944	NAG	C4-C5-C6-O6
11	B	908	NAG	C1-C2-N2-C7
12	B	946	MRD	C1-C2-C3-C4
12	B	946	MRD	CM-C2-C3-C4
12	B	947	MRD	C1-C2-C3-C4
12	B	947	MRD	C2-C3-C4-C5
11	B	945	NAG	O5-C5-C6-O6
11	B	944	NAG	O5-C5-C6-O6
11	B	908	NAG	C3-C2-N2-C7
12	B	946	MRD	O2-C2-C3-C4
12	A	941	MRD	C2-C3-C4-O4
12	B	946	MRD	C2-C3-C4-O4
12	A	941	MRD	C1-C2-C3-C4
12	A	941	MRD	CM-C2-C3-C4
12	B	947	MRD	CM-C2-C3-C4
12	B	948	MRD	C1-C2-C3-C4
12	B	948	MRD	CM-C2-C3-C4
13	A	942	MPD	C1-C2-C3-C4
13	A	942	MPD	CM-C2-C3-C4

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	940	MRD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	942	MPD	9	0
12	B	946	MRD	3	0
12	B	948	MRD	2	0
12	A	941	MRD	6	0
12	B	947	MRD	3	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%)	-0.67	1 (0%) 92 92	10, 17, 30, 53	0
1	B	832/841 (98%)	-0.83	0 100 100	9, 14, 26, 53	0
All	All	1665/1682 (98%)	-0.75	1 (0%) 92 92	9, 15, 29, 53	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	GLY	2.3

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
2	MAN	C	4	11/12	0.50	0.23	60,74,81,87	0
3	BMA	L	3	11/12	0.65	0.17	56,73,91,97	0
9	MAN	K	4	11/12	0.70	0.16	53,60,64,65	0
10	MAN	P	8	11/12	0.70	0.16	59,67,77,86	0
6	MAN	O	7	11/12	0.74	0.15	58,63,67,71	0
6	MAN	H	7	11/12	0.76	0.14	52,62,64,67	0
7	MAN	I	7	11/12	0.76	0.16	50,55,60,72	0
10	MAN	P	7	11/12	0.77	0.17	42,50,57,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	G	3	11/12	0.78	0.14	41,51,62,72	0
10	BMA	P	3	11/12	0.82	0.14	35,38,46,58	0
2	MAN	C	5	11/12	0.82	0.13	41,50,56,62	0
3	NAG	G	2	14/15	0.82	0.14	36,43,52,56	0
3	BMA	D	3	11/12	0.83	0.12	34,42,51,57	0
10	MAN	P	6	11/12	0.83	0.14	47,52,60,63	0
7	MAN	I	6	11/12	0.84	0.14	40,51,55,66	0
7	BMA	I	3	11/12	0.86	0.12	30,37,47,51	0
2	BMA	C	3	11/12	0.86	0.12	33,46,53,57	0
3	BMA	N	3	11/12	0.87	0.11	35,42,55,67	0
10	MAN	P	4	11/12	0.90	0.11	27,31,39,42	0
5	MAN	F	10	11/12	0.91	0.11	31,37,44,57	0
6	MAN	O	4	11/12	0.92	0.09	23,28,38,43	0
9	BMA	K	3	11/12	0.92	0.08	32,38,48,49	0
7	MAN	I	4	11/12	0.92	0.09	22,29,39,50	0
5	MAN	M	10	11/12	0.92	0.10	27,36,41,43	0
5	MAN	F	5	11/12	0.93	0.07	20,24,30,34	0
7	MAN	I	5	11/12	0.93	0.09	24,31,40,43	0
10	NAG	P	2	14/15	0.93	0.08	24,29,35,36	0
8	MAN	J	7	11/12	0.93	0.07	22,29,34,34	0
3	NAG	G	1	14/15	0.94	0.08	19,25,35,38	0
6	MAN	H	4	11/12	0.94	0.08	24,26,38,39	0
4	NAG	E	2	14/15	0.94	0.07	25,30,47,49	0
6	BMA	O	3	11/12	0.94	0.07	24,28,34,45	0
10	MAN	P	5	11/12	0.94	0.07	24,31,35,42	0
2	NAG	C	2	14/15	0.94	0.07	20,28,38,42	0
3	NAG	N	2	14/15	0.94	0.08	24,29,41,41	0
7	NAG	I	2	14/15	0.94	0.07	22,27,32,37	0
8	MAN	J	6	11/12	0.95	0.07	22,26,29,37	0
5	MAN	M	6	11/12	0.95	0.07	25,28,34,35	0
9	NAG	K	2	14/15	0.95	0.06	17,23,31,31	0
3	NAG	D	2	14/15	0.95	0.06	23,27,34,37	0
6	NAG	H	2	14/15	0.95	0.07	17,23,28,34	0
6	BMA	H	3	11/12	0.95	0.07	21,25,32,43	0
5	MAN	F	6	11/12	0.95	0.07	27,29,34,40	0
5	MAN	F	9	11/12	0.95	0.06	24,25,32,33	0
6	NAG	O	2	14/15	0.95	0.07	18,23,32,33	0
3	NAG	L	2	14/15	0.95	0.07	18,23,42,43	0
8	MAN	J	4	11/12	0.95	0.07	24,31,40,41	0
8	MAN	J	5	11/12	0.95	0.07	23,30,37,47	0
6	NAG	O	1	14/15	0.96	0.07	16,20,39,43	0
5	MAN	M	5	11/12	0.96	0.05	18,21,22,33	0

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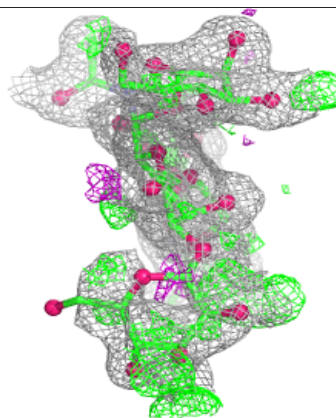
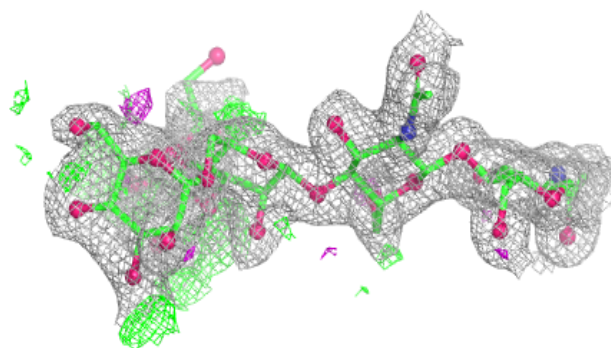
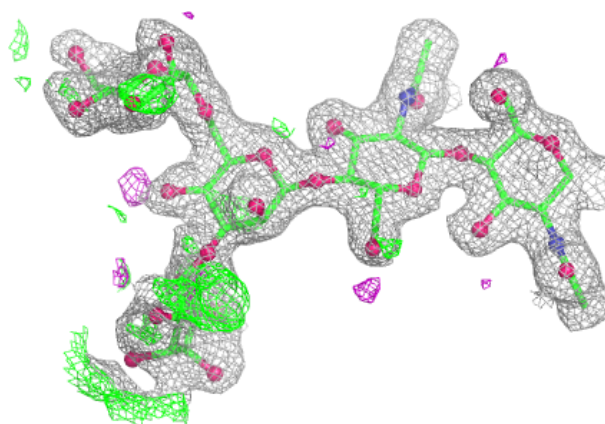
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	F	1	14/15	0.96	0.06	20,23,26,29	0
10	NAG	P	1	14/15	0.96	0.05	15,18,21,22	0
5	BMA	F	3	11/12	0.96	0.06	19,21,26,27	0
6	MAN	O	5	11/12	0.96	0.06	21,23,29,34	0
8	BMA	J	3	11/12	0.96	0.06	19,21,22,24	0
6	MAN	O	6	11/12	0.96	0.06	18,22,29,32	0
6	MAN	H	6	11/12	0.96	0.07	18,22,33,38	0
7	NAG	I	1	14/15	0.96	0.06	17,20,23,24	0
6	NAG	H	1	14/15	0.96	0.07	15,18,39,42	0
9	NAG	K	1	14/15	0.97	0.05	16,18,20,21	0
6	MAN	H	5	11/12	0.97	0.06	19,22,34,37	0
5	NAG	M	2	14/15	0.97	0.05	12,15,15,16	0
2	NAG	C	1	14/15	0.97	0.06	16,19,21,23	0
4	NAG	E	1	14/15	0.97	0.05	16,19,23,25	0
5	MAN	M	8	11/12	0.97	0.05	16,17,19,21	0
5	MAN	M	9	11/12	0.97	0.05	18,20,24,26	0
3	NAG	N	1	14/15	0.97	0.06	18,23,32,33	0
5	MAN	F	8	11/12	0.97	0.05	18,20,21,22	0
3	NAG	D	1	14/15	0.97	0.05	17,20,22,24	0
5	NAG	F	2	14/15	0.97	0.05	17,19,20,22	0
5	NAG	M	1	14/15	0.97	0.05	12,14,19,22	0
5	MAN	F	7	11/12	0.98	0.04	16,18,21,22	0
3	NAG	L	1	14/15	0.98	0.04	14,16,19,19	0
8	NAG	J	1	14/15	0.98	0.04	12,14,17,18	0
8	NAG	J	2	14/15	0.98	0.05	14,16,20,28	0
5	MAN	M	7	11/12	0.98	0.05	13,14,16,16	0
5	MAN	F	4	11/12	0.98	0.05	17,20,22,23	0
5	BMA	M	3	11/12	0.98	0.04	14,16,18,18	0
5	MAN	M	4	11/12	0.99	0.04	14,15,15,16	0

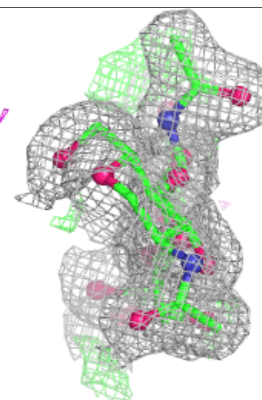
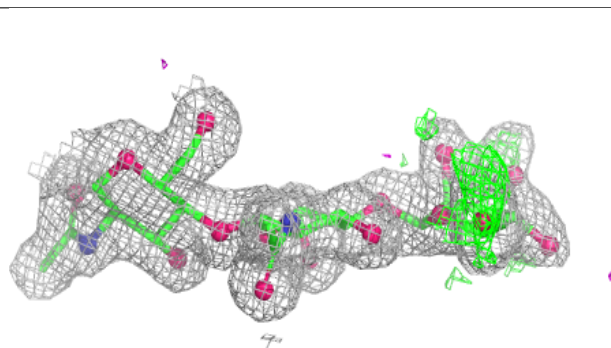
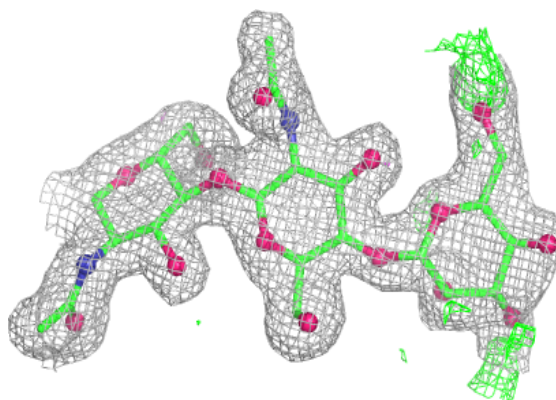
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

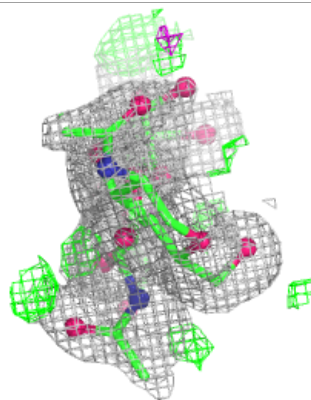
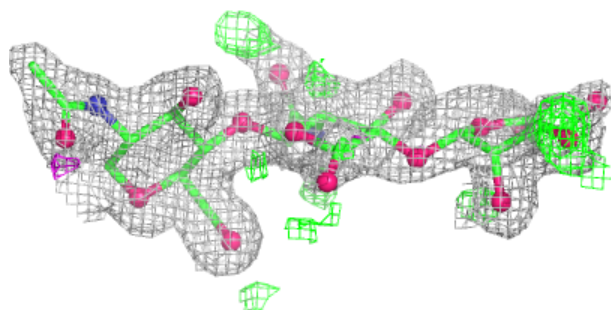
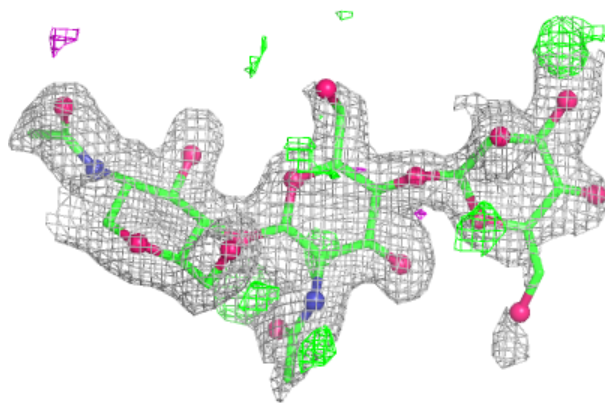
**Electron density around Chain D:**

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

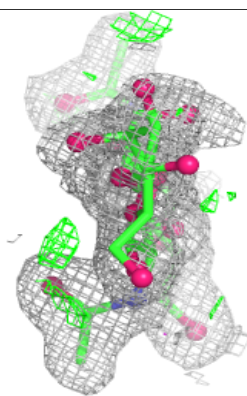
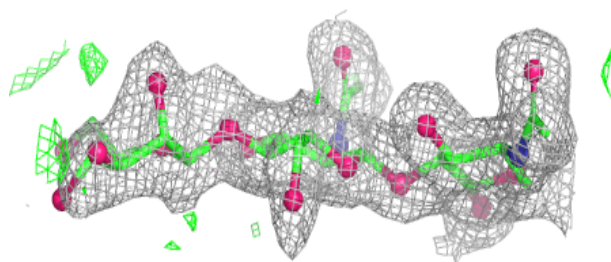
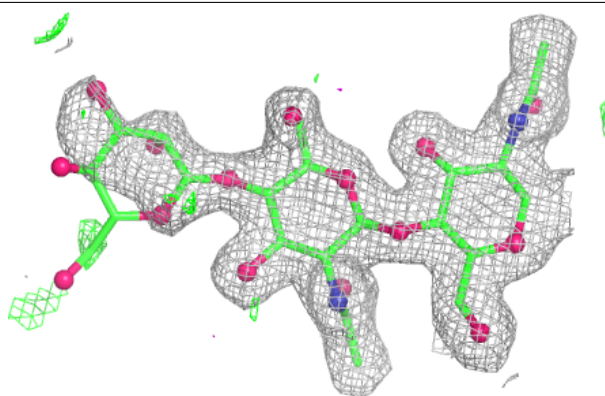


Electron density around Chain G:

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

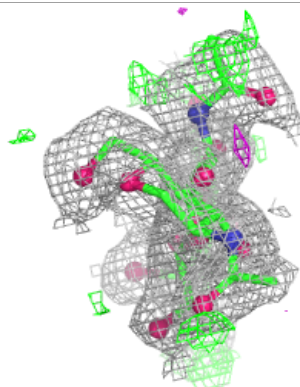
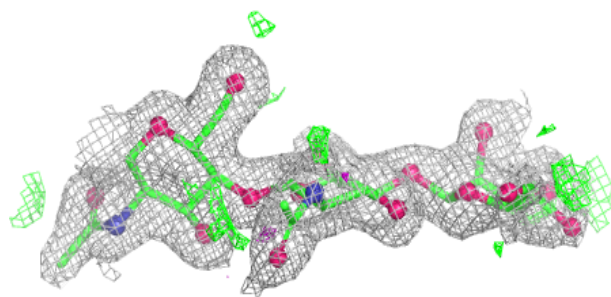
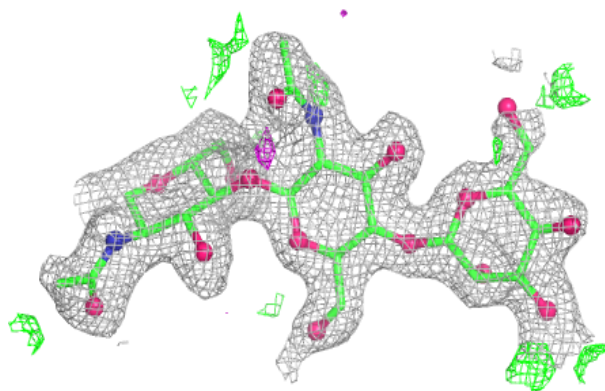
**Electron density around Chain L:**

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



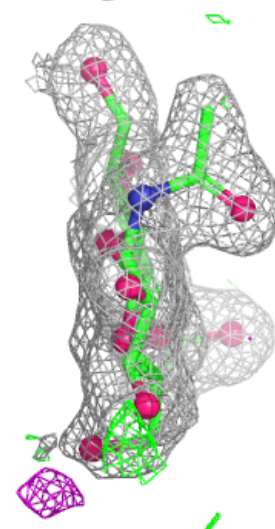
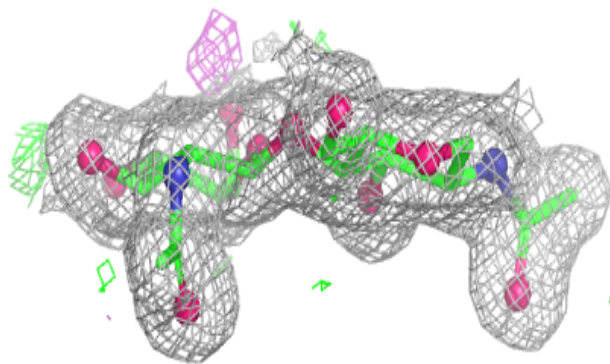
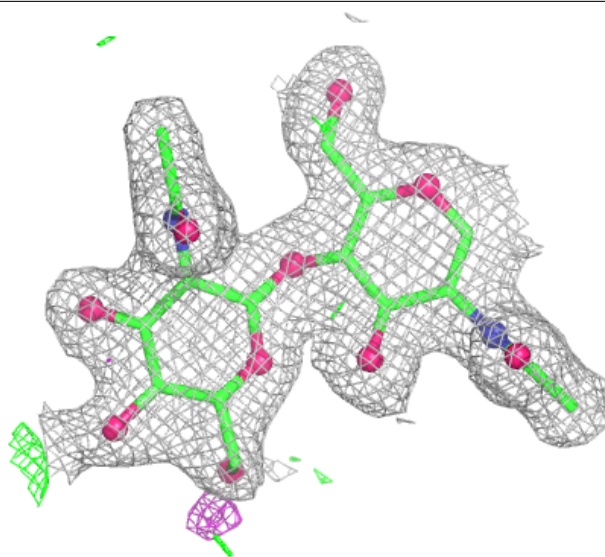
Electron density around Chain N:

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



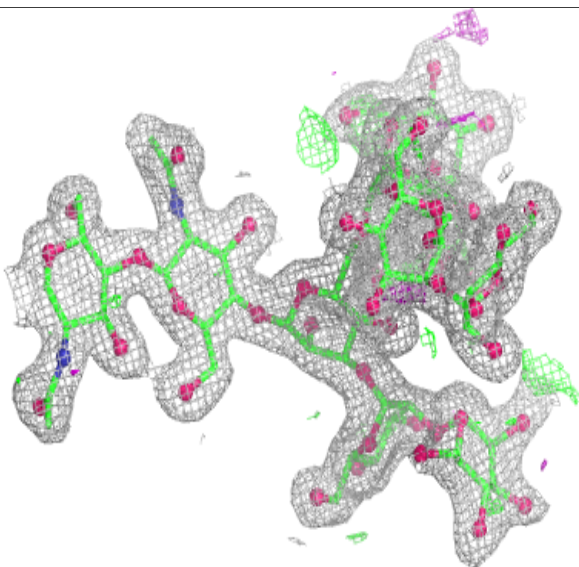
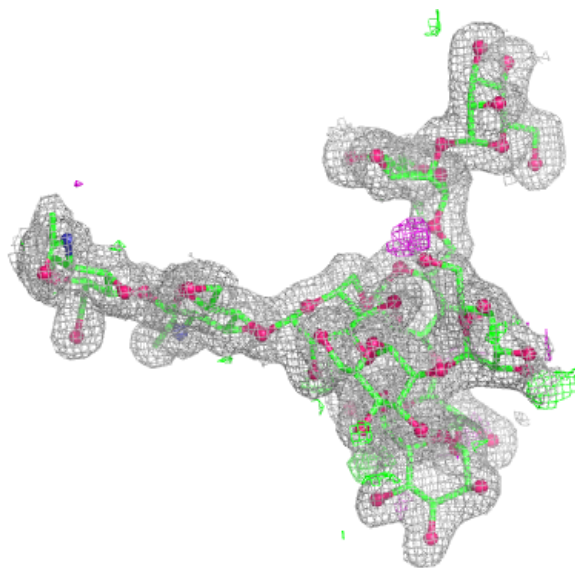
Electron density around Chain E:

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and green (positive)



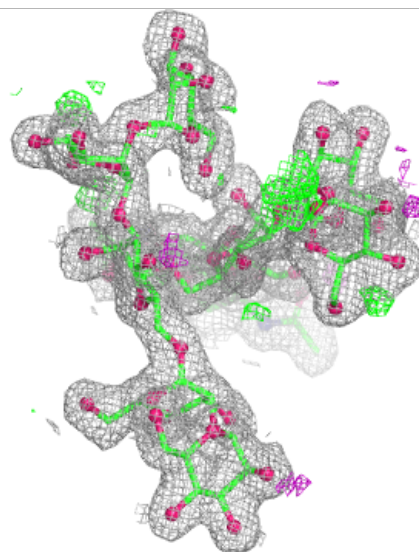
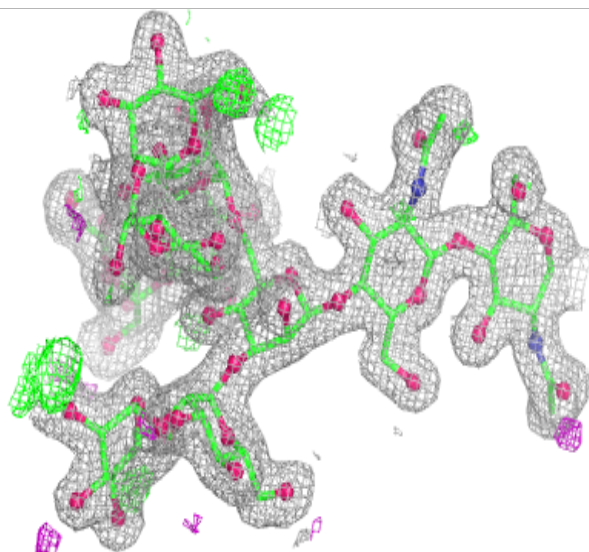
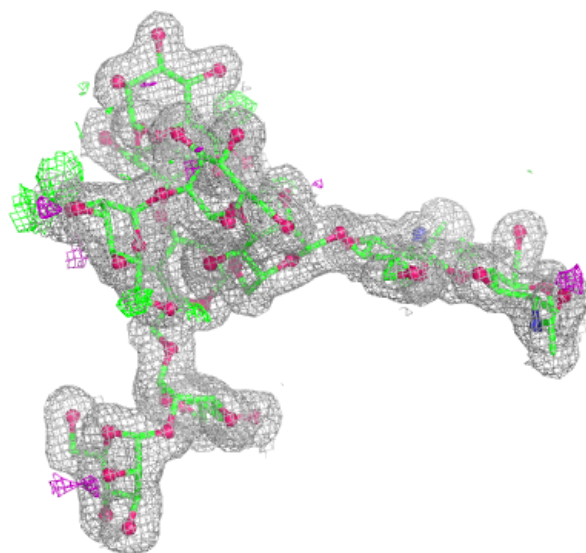
Electron density around Chain F:

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



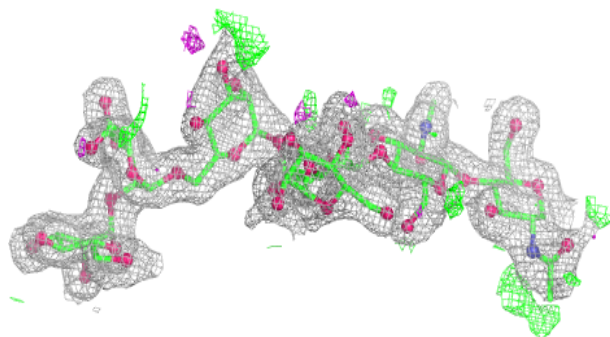
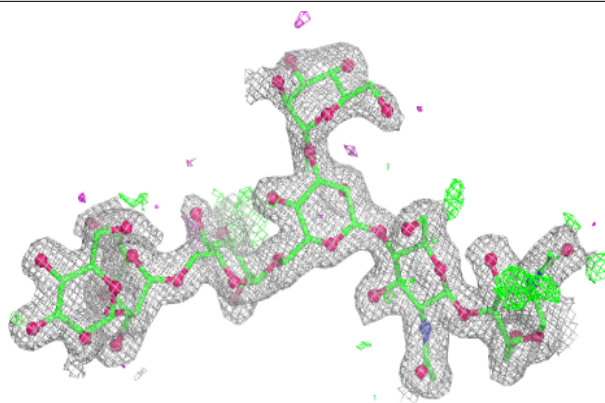
Electron density around Chain M:

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

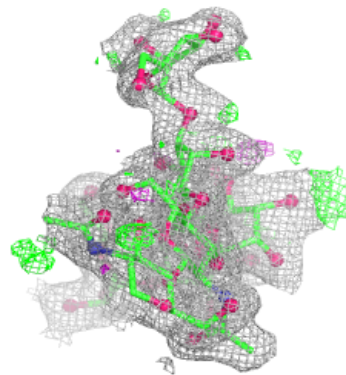
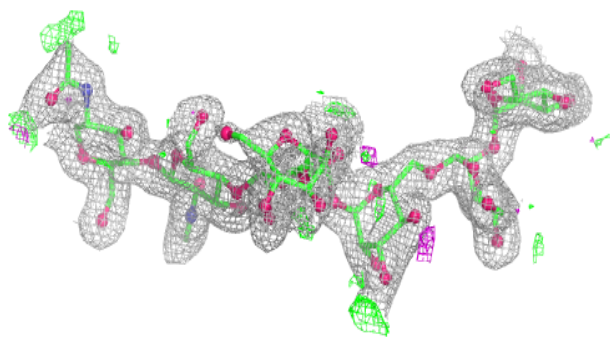
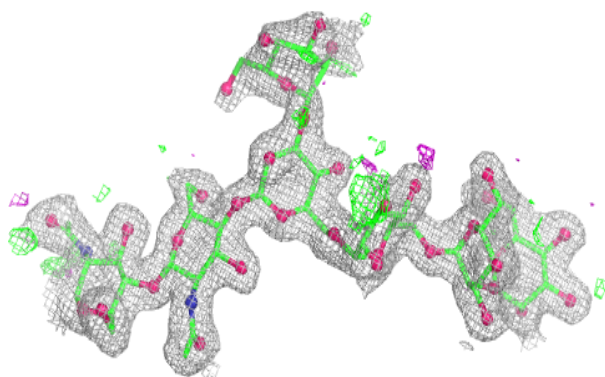


Electron density around Chain H:

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

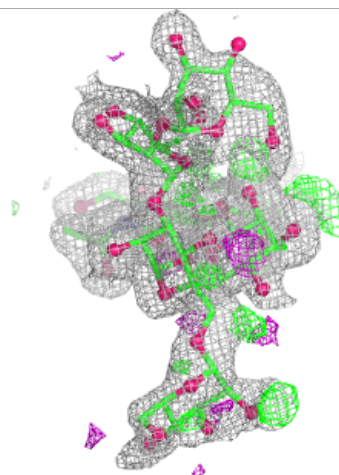
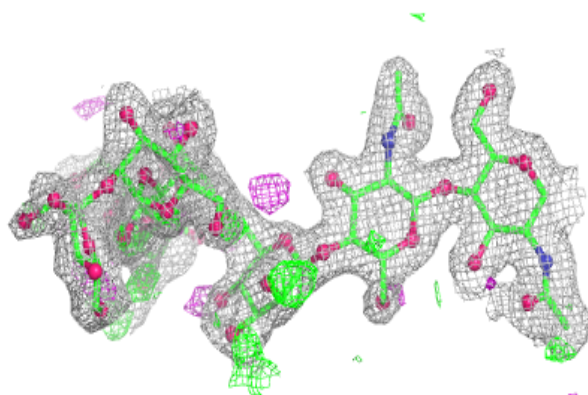
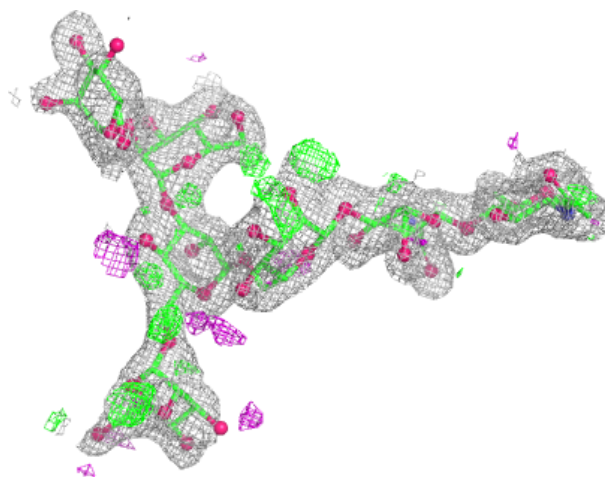
**Electron density around Chain O:**

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



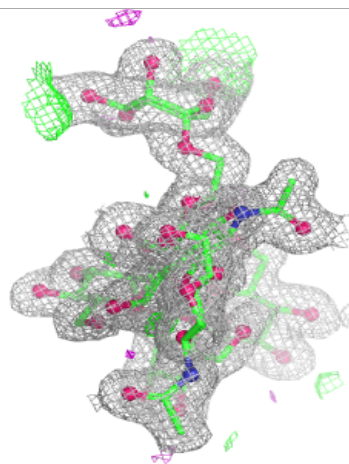
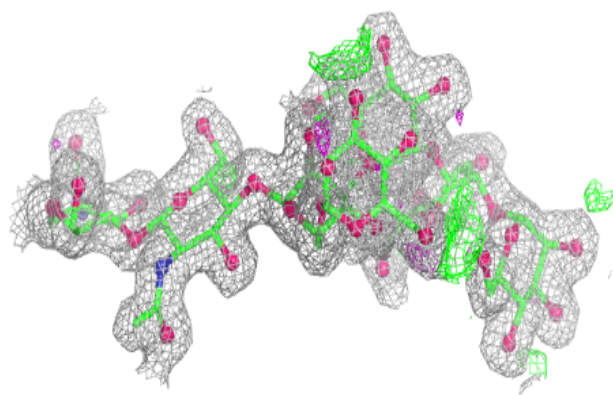
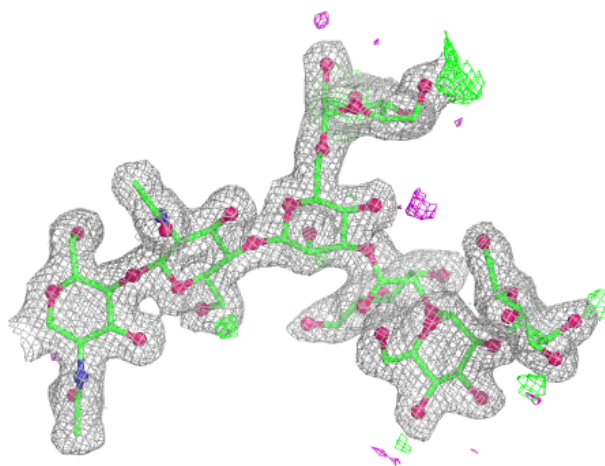
Electron density around Chain I:

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



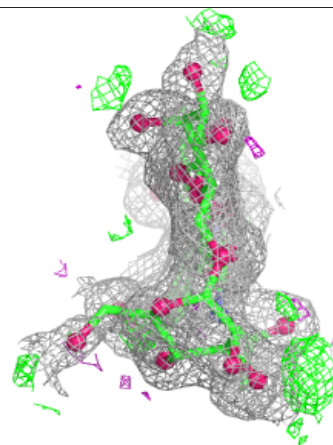
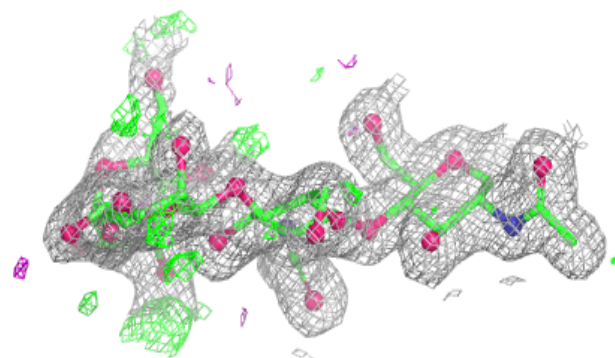
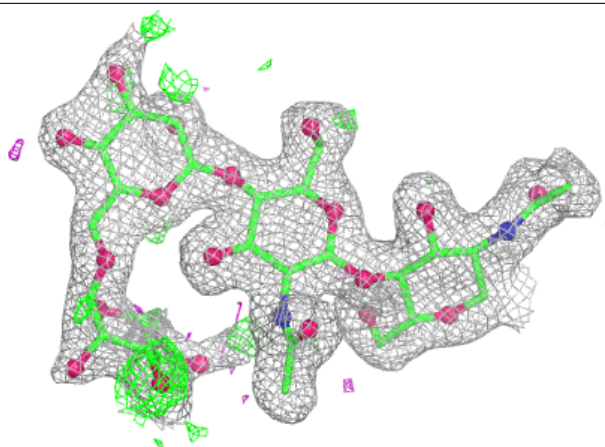
Electron density around Chain J:

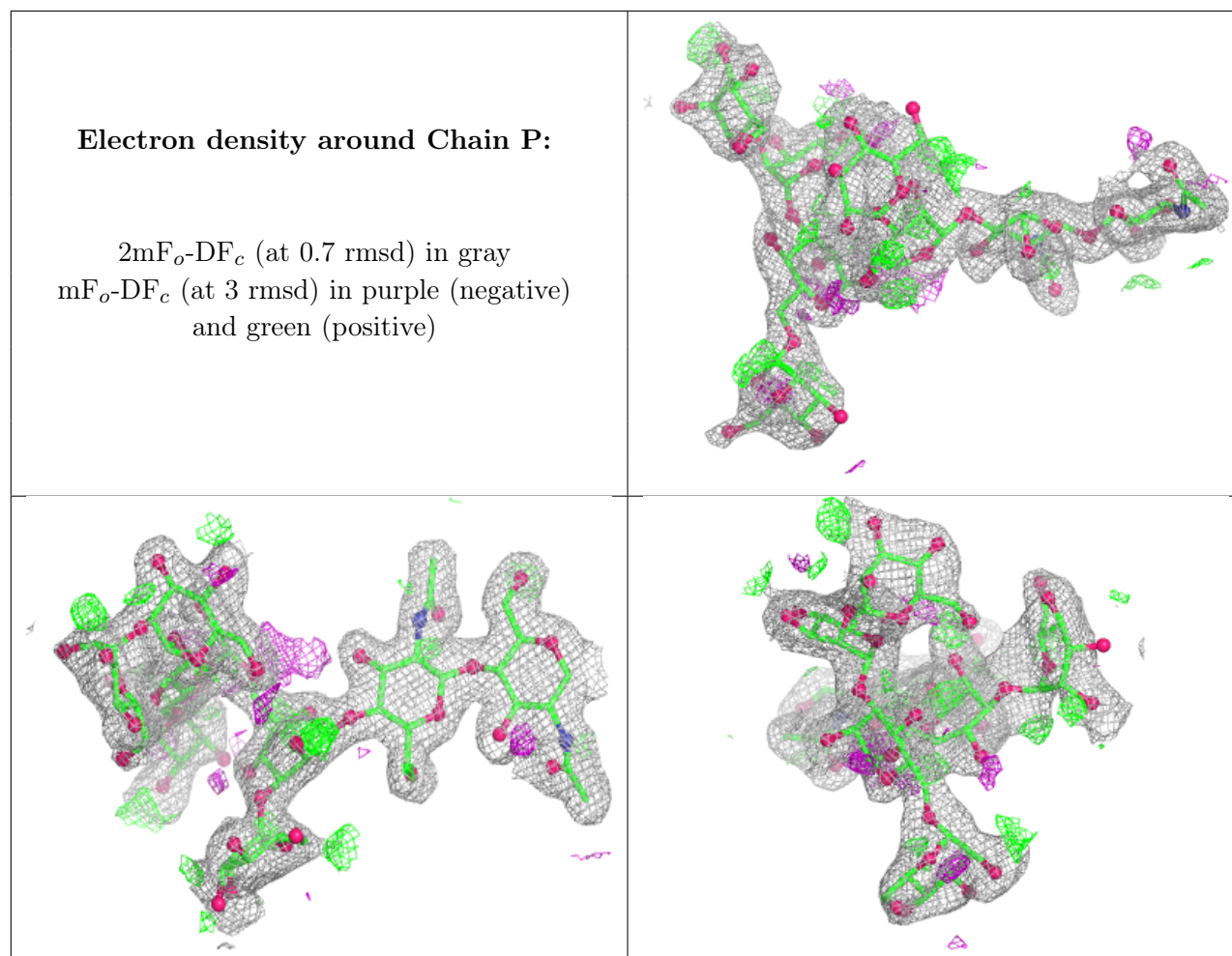
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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	0.77	0.15	39,48,52,53	0
11	NAG	B	944	14/15	0.83	0.12	36,50,55,59	0
11	NAG	A	906	14/15	0.84	0.12	42,52,57,58	0
12	MRD	A	941	8/8	0.84	0.14	18,30,41,43	0
13	MPD	A	942	8/8	0.84	0.18	37,39,45,48	0
12	MRD	B	948	8/8	0.89	0.12	32,41,42,43	0
12	MRD	B	946	8/8	0.89	0.14	19,32,40,43	0
11	NAG	A	939	14/15	0.92	0.09	35,38,42,46	0
12	MRD	B	947	8/8	0.92	0.09	20,25,37,37	0
14	NA	B	949	1/1	0.93	0.09	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	B	945	14/15	0.95	0.06	26,29,33,34	0
12	MRD	A	940	8/8	0.95	0.07	20,22,25,26	0
14	NA	A	943	1/1	0.97	0.08	26,26,26,26	0
15	IFM	A	944	10/10	0.98	0.04	12,13,14,15	0
15	IFM	B	950	10/10	0.99	0.03	10,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.