



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:59 AM UTC

PDB ID : 8IDP / pdb_00008idp
Title : Crystal structure of reducing-end xylose-releasing exoxylanase in GH30 from *Talaromyces cellulolyticus*
Authors : Nakamichi, Y.; Watanabe, M.; Fujii, T.; Inoue, H.; Morita, T.
Deposited on : 2023-02-14
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

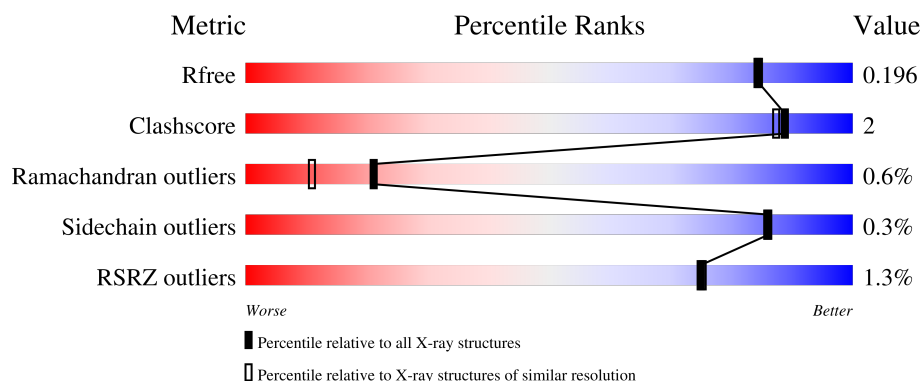
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.



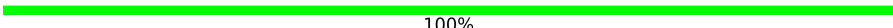
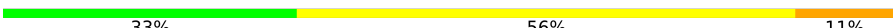
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	462	2% 93% 5% 0%
1	B	462	92% 5% 0%
1	C	462	2% 93% 5% 0%
1	D	462	0% 92% 5% 0%
2	E	11	45% 45% 9%

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Mol	Chain	Length	Quality of chain
2	K	11	 45%55%
3	F	6	 50%50%
3	L	6	 50%50%
4	G	2	 50%50%
4	I	2	 50%50%
4	M	2	 100%
4	O	2	 50%50%
5	H	9	 22%67%11%
6	J	5	 60%40%
6	P	5	 60%40%
7	N	9	 33%56%11%

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
9	GOL	C	1908	-	-	X	-

2 Entry composition [i](#)

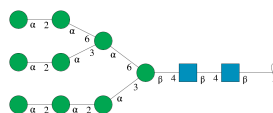
There are 12 unique types of molecules in this entry. The entry contains 16663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Reducing-end xylose-releasing exoxylanase Xyn30A.

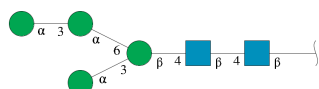
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	6	0
			3531	2234	591	690	16			
1	C	446	Total	C	N	O	S	0	4	0
			3512	2222	587	687	16			
1	B	446	Total	C	N	O	S	0	3	0
			3507	2221	586	684	16			
1	D	445	Total	C	N	O	S	0	3	0
			3498	2214	586	682	16			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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
2	E	11	Total	C	N	O	0	0	0
			127	70	2	55			
2	K	11	Total	C	N	O	0	0	0
			127	70	2	55			

- Molecule 3 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.



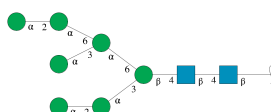
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	6	Total	C	N	O	0	0	0
			72	40	2	30			
3	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



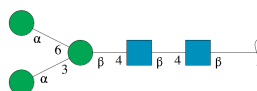
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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.



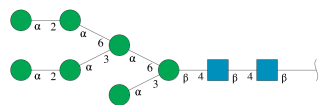
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 6 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.



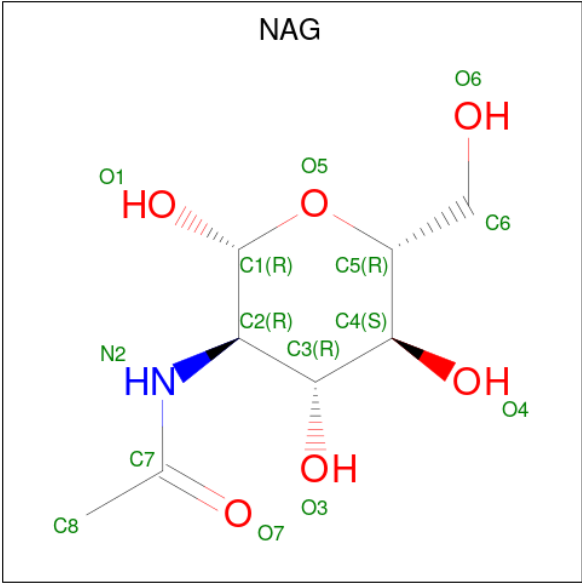
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 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-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	N	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



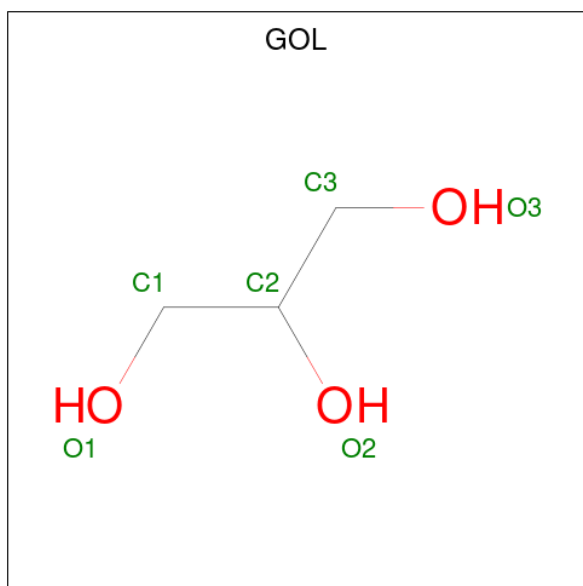
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



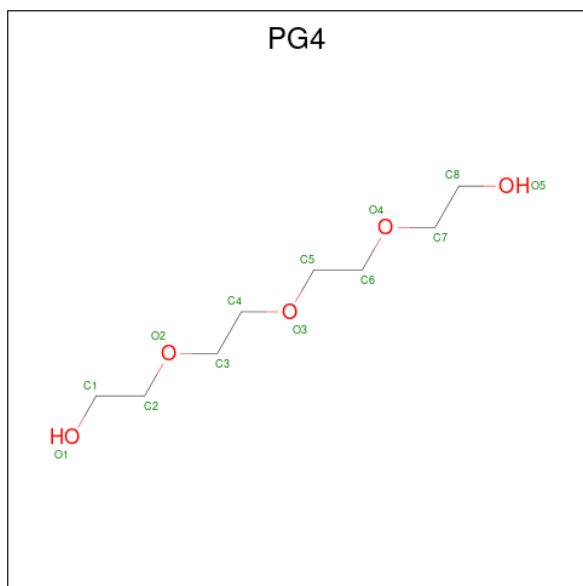
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	1
			12	6	6		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	1
			12	6	6		
9	C	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	1
			12	6	6		
9	D	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



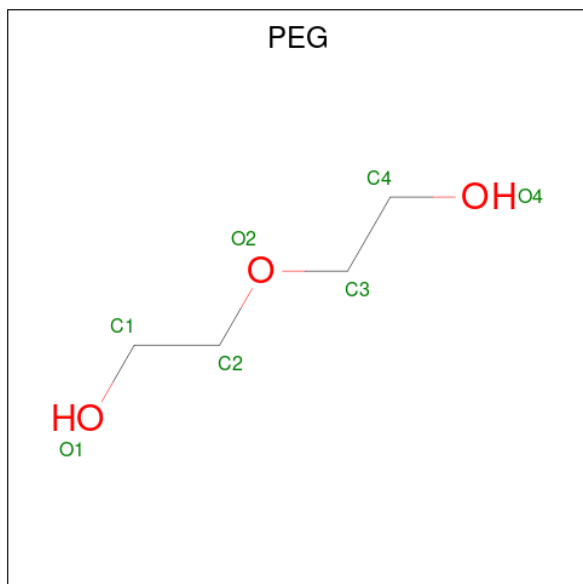
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			13	8	5		
10	C	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	366	Total	O	0	0
			366	366		
12	C	363	Total	O	0	0
			363	363		
12	B	412	Total	O	0	0
			412	412		
12	D	380	Total	O	0	0
			380	380		

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.

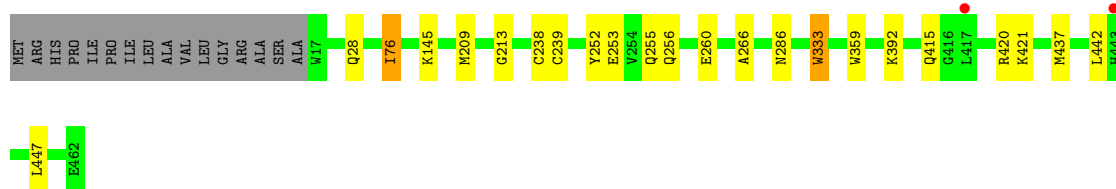
- Molecule 1: Reducing-end xylose-releasing exoxylanase Xyn30A



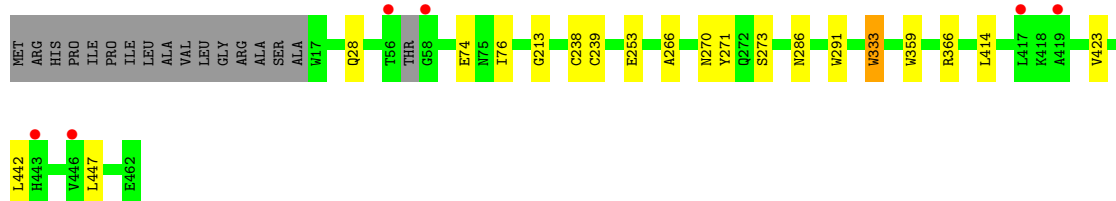
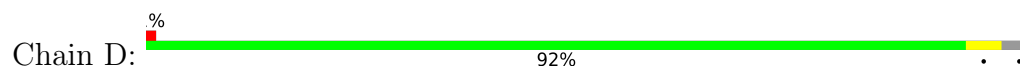
- Molecule 1: Reducing-end xylose-releasing exoxylanase Xyn30A



- Molecule 1: Reducing-end xylose-releasing exoxylanase Xyn30A



- Molecule 1: Reducing-end xylose-releasing exoxylanase Xyn30A



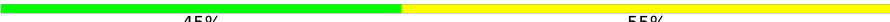
- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-

(1-2)-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 E:  45% 45% 9%



• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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 K:  45% 55%



• Molecule 3: 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 F:  50% 50%



• Molecule 3: 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 L:  50% 50%



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

Chain G:  50% 50%

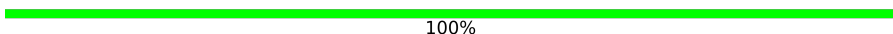


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%



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

Chain M:  100%

GLU1
GLU2

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

Chain O:  50% 50%

GLU1
GLU2

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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 H:  22% 67% 11%

GLU1
GLU2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 6: 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:  60% 40%

GLU1
GLU2
MAN3
MAN5

- Molecule 6: 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 P:  60% 40%

GLU1
GLU2
MAN3
MAN4
MAN5

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

Chain N:  33% 56% 11%

MAG1
MAG2
BM/A3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	138.46Å 120.07Å 122.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.94 – 1.80 40.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.94-1.80) 99.5 (40.94-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.12	Depositor
R, R_{free}	0.165 , 0.195 0.165 , 0.196	Depositor DCC
R_{free} test set	9422 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.054 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16663	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1297e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PEG, PG4, NAG, GOL, MAN, BMA

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	0.31	0/3631	0.52	0/4957
1	B	0.33	0/3607	0.53	0/4925
1	C	0.33	0/3612	0.53	0/4931
1	D	0.33	0/3597	0.54	0/4909
All	All	0.32	0/14447	0.53	0/19722

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3531	0	3283	9	0
1	B	3507	0	3264	14	0
1	C	3512	0	3264	14	0
1	D	3498	0	3252	11	0
2	E	127	0	106	1	0
2	K	127	0	106	0	0
3	F	72	0	61	0	0
3	L	72	0	61	0	0
4	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	28	0	25	0	0
4	M	28	0	25	0	0
4	O	28	0	25	0	0
5	H	105	0	88	1	0
6	J	61	0	52	0	0
6	P	61	0	52	0	0
7	N	105	0	88	1	0
8	A	14	0	13	0	0
8	B	28	0	26	0	0
8	C	28	0	26	0	0
8	D	28	0	26	0	0
9	A	24	0	32	2	0
9	B	18	0	24	2	0
9	C	42	0	56	8	0
9	D	24	0	31	3	0
10	A	13	0	18	2	0
10	C	13	0	18	2	0
10	D	13	0	18	1	0
11	B	7	0	10	0	0
12	A	366	0	0	1	0
12	B	412	0	0	0	0
12	C	363	0	0	3	0
12	D	380	0	0	2	0
All	All	16663	0	14075	56	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 2.

The worst 5 of 56 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:C:163:ASN:HA	9:C:1904:GOL:H31	1.73	0.71
1:A:417:LEU:HA	1:A:420:ARG:HH21	1.61	0.65
9:C:1908:GOL:H12	10:C:1909:PG4:H42	1.82	0.62
9:C:1908:GOL:C1	10:C:1909:PG4:H42	2.29	0.62
1:D:28:GLN:NE2	12:D:1201:HOH:O	2.33	0.62

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	450/462 (97%)	432 (96%)	15 (3%)	3 (1%)	18	8
1	B	447/462 (97%)	430 (96%)	15 (3%)	2 (0%)	30	19
1	C	448/462 (97%)	429 (96%)	16 (4%)	3 (1%)	18	8
1	D	444/462 (96%)	429 (97%)	12 (3%)	3 (1%)	18	8
All	All	1789/1848 (97%)	1720 (96%)	58 (3%)	11 (1%)	21	11

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	273	SER
1	A	273	SER
1	C	273	SER
1	C	333	TRP
1	B	333	TRP

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	377/383 (98%)	376 (100%)	1 (0%)	86	86
1	B	374/383 (98%)	373 (100%)	1 (0%)	86	86
1	C	375/383 (98%)	373 (100%)	2 (0%)	81	80
1	D	373/383 (97%)	372 (100%)	1 (0%)	86	86
All	All	1499/1532 (98%)	1494 (100%)	5 (0%)	86	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	333	TRP
1	C	57	THR
1	C	333	TRP
1	B	333	TRP
1	D	333	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	255	GLN
1	D	28	GLN
1	B	415	GLN
1	C	320	ASN
1	B	249	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 ⓘ

70 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	E	1	1,2	14,14,15	0.59	0	17,19,21	0.61	0
2	MAN	E	10	2	11,11,12	0.69	0	15,15,17	1.06	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	E	11	2	11,11,12	0.87	1 (9%)	15,15,17	0.96	2 (13%)
2	NAG	E	2	2	14,14,15	0.22	0	17,19,21	0.56	0
2	BMA	E	3	2	11,11,12	0.79	0	15,15,17	0.85	0
2	MAN	E	4	2	11,11,12	0.84	0	15,15,17	1.06	2 (13%)
2	MAN	E	5	2	11,11,12	0.84	0	15,15,17	0.94	1 (6%)
2	MAN	E	6	2	11,11,12	0.93	0	15,15,17	0.84	0
2	MAN	E	7	2	11,11,12	0.68	0	15,15,17	1.12	2 (13%)
2	MAN	E	8	2	11,11,12	1.05	0	15,15,17	0.86	0
2	MAN	E	9	2	11,11,12	1.05	0	15,15,17	1.13	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.14	0	17,19,21	0.65	0
3	NAG	F	2	3	14,14,15	0.46	0	17,19,21	0.46	0
3	BMA	F	3	3	11,11,12	0.74	0	15,15,17	0.84	0
3	MAN	F	4	3	11,11,12	0.85	0	15,15,17	0.98	2 (13%)
3	MAN	F	5	3	11,11,12	1.06	1 (9%)	15,15,17	0.99	1 (6%)
3	MAN	F	6	3	11,11,12	0.88	1 (9%)	15,15,17	1.02	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.31	0	17,19,21	0.76	1 (5%)
4	NAG	G	2	4	14,14,15	0.32	0	17,19,21	0.51	0
5	NAG	H	1	1,5	14,14,15	0.44	0	17,19,21	0.62	0
5	NAG	H	2	5	14,14,15	0.37	0	17,19,21	0.56	0
5	BMA	H	3	5	11,11,12	0.71	0	15,15,17	0.86	1 (6%)
5	MAN	H	4	5	11,11,12	0.78	0	15,15,17	1.37	2 (13%)
5	MAN	H	5	5	11,11,12	0.60	0	15,15,17	1.22	2 (13%)
5	MAN	H	6	5	11,11,12	0.71	0	15,15,17	1.10	2 (13%)
5	MAN	H	7	5	11,11,12	1.06	1 (9%)	15,15,17	1.35	2 (13%)
5	MAN	H	8	5	11,11,12	0.64	0	15,15,17	1.03	2 (13%)
5	MAN	H	9	5	11,11,12	0.91	0	15,15,17	0.93	1 (6%)
4	NAG	I	1	1,4	14,14,15	0.27	0	17,19,21	0.57	0
4	NAG	I	2	4	14,14,15	0.25	0	17,19,21	0.66	1 (5%)
6	NAG	J	1	1,6	14,14,15	0.20	0	17,19,21	0.63	0
6	NAG	J	2	6	14,14,15	0.44	0	17,19,21	0.61	0
6	BMA	J	3	6	11,11,12	0.78	0	15,15,17	0.80	0
6	MAN	J	4	6	11,11,12	0.85	0	15,15,17	1.03	2 (13%)
6	MAN	J	5	6	11,11,12	0.86	0	15,15,17	1.00	1 (6%)
2	NAG	K	1	1,2	14,14,15	0.56	0	17,19,21	0.57	0
2	MAN	K	10	2	11,11,12	0.76	0	15,15,17	1.18	2 (13%)
2	MAN	K	11	2	11,11,12	0.90	0	15,15,17	1.15	2 (13%)
2	NAG	K	2	2	14,14,15	0.37	0	17,19,21	0.58	0
2	BMA	K	3	2	11,11,12	0.64	0	15,15,17	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	K	4	2	11,11,12	0.79	0	15,15,17	0.89	0
2	MAN	K	5	2	11,11,12	0.77	0	15,15,17	1.45	2 (13%)
2	MAN	K	6	2	11,11,12	0.84	0	15,15,17	1.04	1 (6%)
2	MAN	K	7	2	11,11,12	0.73	0	15,15,17	1.10	1 (6%)
2	MAN	K	8	2	11,11,12	0.83	0	15,15,17	0.86	0
2	MAN	K	9	2	11,11,12	0.81	1 (9%)	15,15,17	1.05	1 (6%)
3	NAG	L	1	3,1	14,14,15	0.18	0	17,19,21	0.61	0
3	NAG	L	2	3	14,14,15	0.56	0	17,19,21	0.58	0
3	BMA	L	3	3	11,11,12	0.67	0	15,15,17	0.81	0
3	MAN	L	4	3	11,11,12	0.81	0	15,15,17	1.07	2 (13%)
3	MAN	L	5	3	11,11,12	0.95	0	15,15,17	1.19	1 (6%)
3	MAN	L	6	3	11,11,12	1.01	1 (9%)	15,15,17	0.92	1 (6%)
4	NAG	M	1	1,4	14,14,15	0.26	0	17,19,21	0.64	0
4	NAG	M	2	4	14,14,15	0.51	0	17,19,21	0.56	0
7	NAG	N	1	1,7	14,14,15	0.52	0	17,19,21	0.68	0
7	NAG	N	2	7	14,14,15	0.28	0	17,19,21	0.56	0
7	BMA	N	3	7	11,11,12	0.70	0	15,15,17	0.72	0
7	MAN	N	4	7	11,11,12	0.93	1 (9%)	15,15,17	1.14	1 (6%)
7	MAN	N	5	7	11,11,12	1.15	1 (9%)	15,15,17	1.15	2 (13%)
7	MAN	N	6	7	11,11,12	0.85	0	15,15,17	0.84	1 (6%)
7	MAN	N	7	7	11,11,12	0.90	0	15,15,17	1.22	2 (13%)
7	MAN	N	8	7	11,11,12	0.53	0	15,15,17	0.96	2 (13%)
7	MAN	N	9	7	11,11,12	0.78	0	15,15,17	0.93	1 (6%)
4	NAG	O	1	1,4	14,14,15	0.33	0	17,19,21	0.63	0
4	NAG	O	2	4	14,14,15	0.40	0	17,19,21	0.63	1 (5%)
6	NAG	P	1	1,6	14,14,15	0.20	0	17,19,21	0.59	0
6	NAG	P	2	6	14,14,15	0.36	0	17,19,21	0.45	0
6	BMA	P	3	6	11,11,12	0.69	0	15,15,17	0.72	0
6	MAN	P	4	6	11,11,12	1.22	2 (18%)	15,15,17	0.84	0
6	MAN	P	5	6	11,11,12	0.75	0	15,15,17	1.21	1 (6%)

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	E	1	1,2	-	0/6/23/26	0/1/1/1
2	MAN	E	10	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	E	11	2	-	0/2/19/22	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	2/2/19/22	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	0/1/1/1
2	MAN	E	7	2	-	0/2/19/22	0/1/1/1
2	MAN	E	8	2	-	1/2/19/22	0/1/1/1
2	MAN	E	9	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	1/2/19/22	0/1/1/1
3	MAN	F	6	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	MAN	H	6	5	-	0/2/19/22	0/1/1/1
5	MAN	H	7	5	-	2/2/19/22	0/1/1/1
5	MAN	H	8	5	-	0/2/19/22	0/1/1/1
5	MAN	H	9	5	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	1/2/19/22	0/1/1/1
6	MAN	J	5	6	-	2/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	MAN	K	10	2	-	0/2/19/22	0/1/1/1
2	MAN	K	11	2	-	0/2/19/22	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	MAN	K	5	2	-	2/2/19/22	0/1/1/1
2	MAN	K	6	2	-	0/2/19/22	0/1/1/1

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	5	MAN	O5-C5	2.43	1.48	1.43
3	F	5	MAN	C2-C3	2.35	1.56	1.52
6	P	4	MAN	O5-C1	-2.29	1.39	1.43
2	E	11	MAN	O5-C5	2.29	1.47	1.43
5	H	7	MAN	O5-C5	2.19	1.47	1.43

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	5	MAN	C1-O5-C5	3.85	117.35	112.19
5	H	5	MAN	C1-O5-C5	3.75	117.21	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	5	MAN	C1-O5-C5	3.71	117.16	112.19
6	P	5	MAN	C1-O5-C5	3.66	117.09	112.19
7	N	7	MAN	C1-O5-C5	3.62	117.04	112.19

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

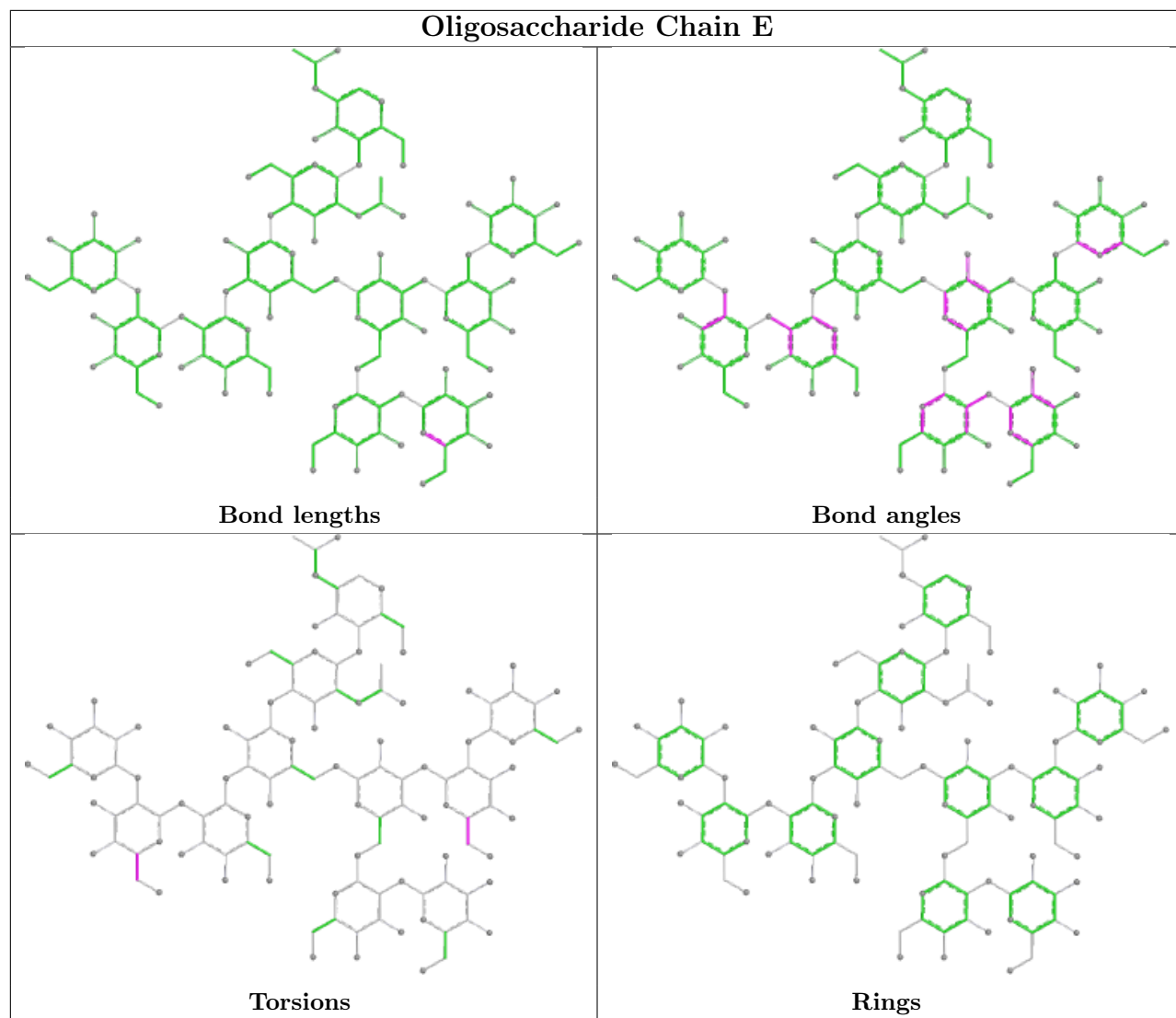
Mol	Chain	Res	Type	Atoms
6	J	5	MAN	C4-C5-C6-O6
6	J	5	MAN	O5-C5-C6-O6
3	L	4	MAN	C4-C5-C6-O6
3	L	4	MAN	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6

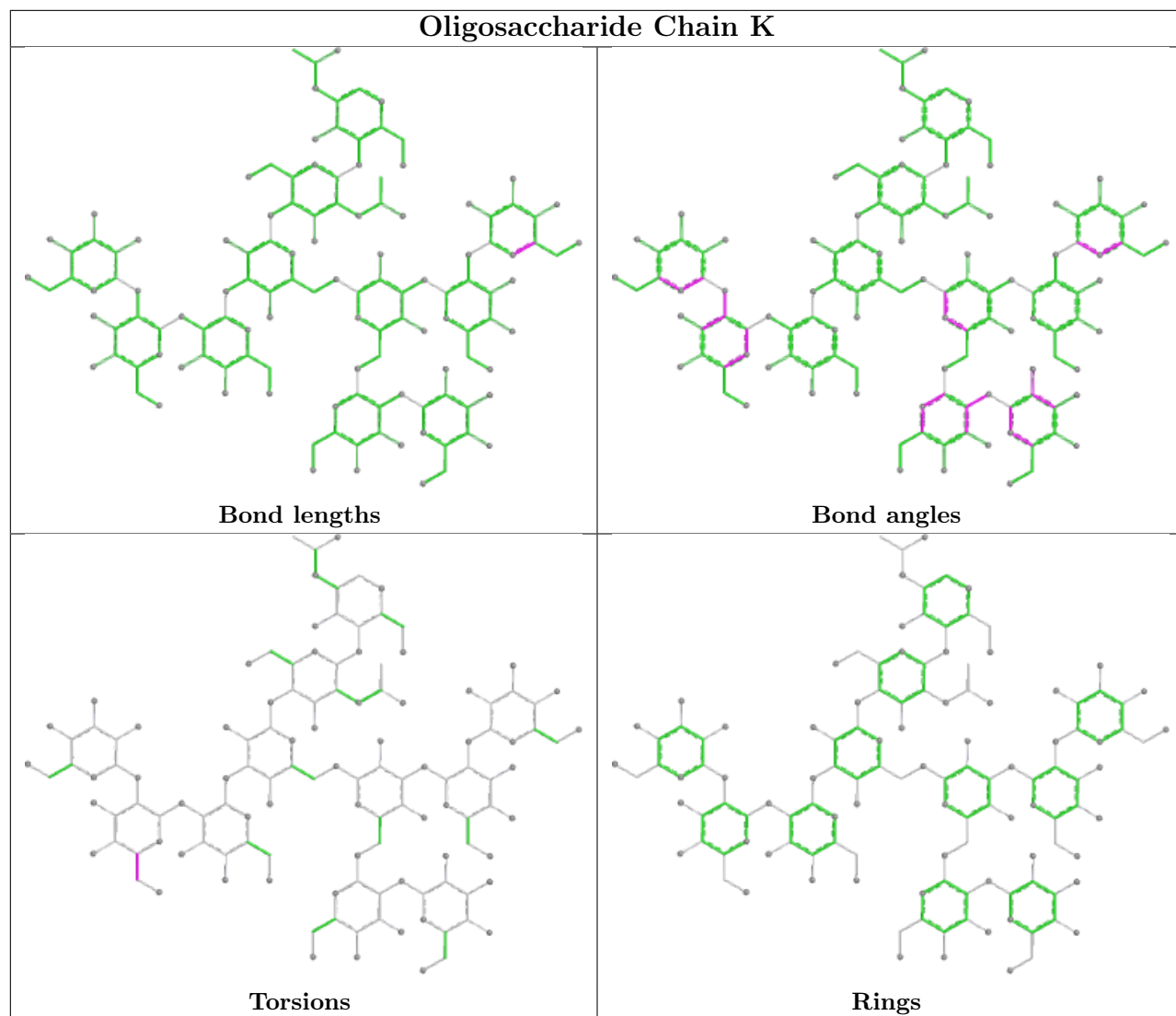
There are no ring outliers.

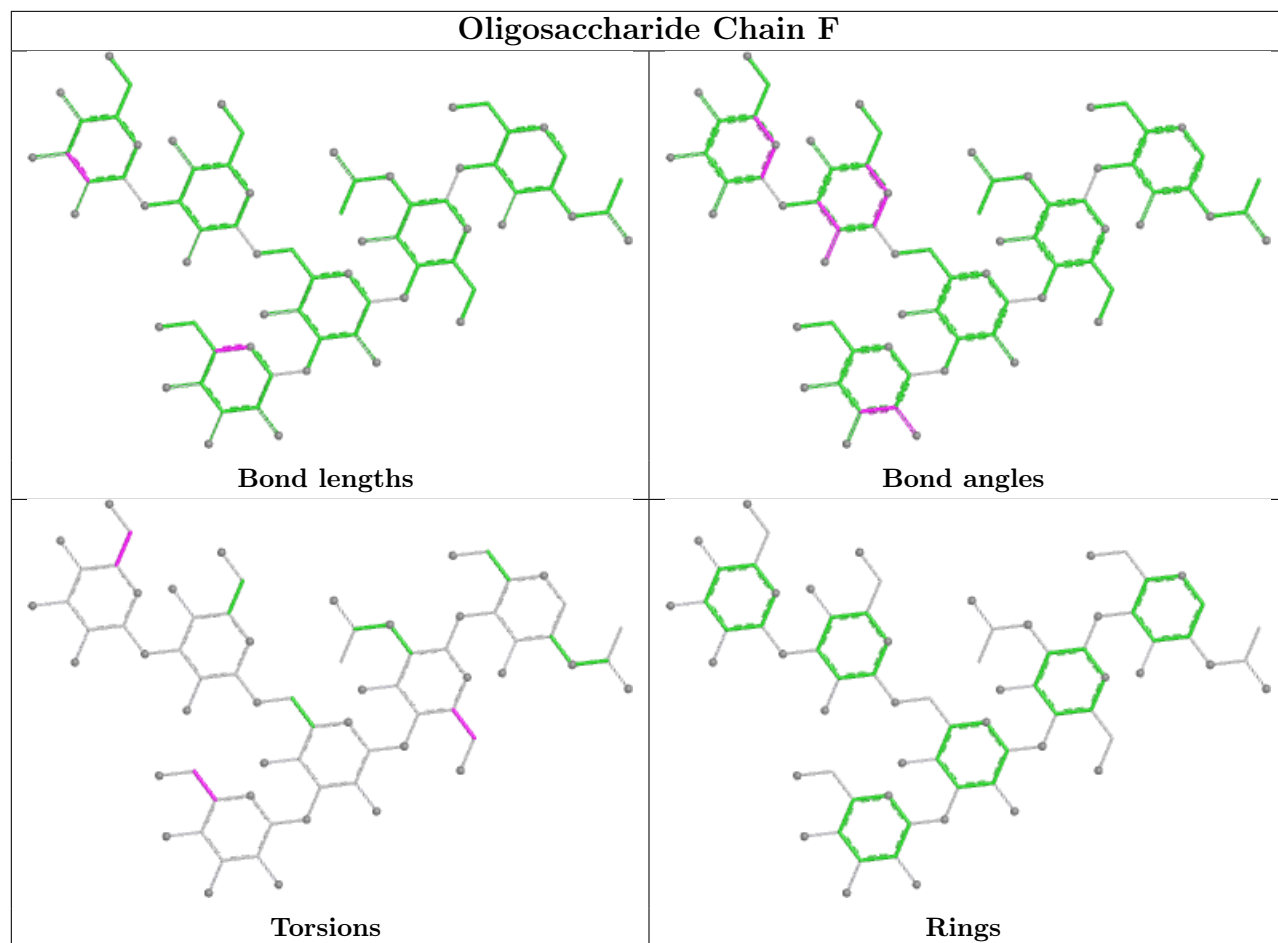
3 monomers are involved in 3 short contacts:

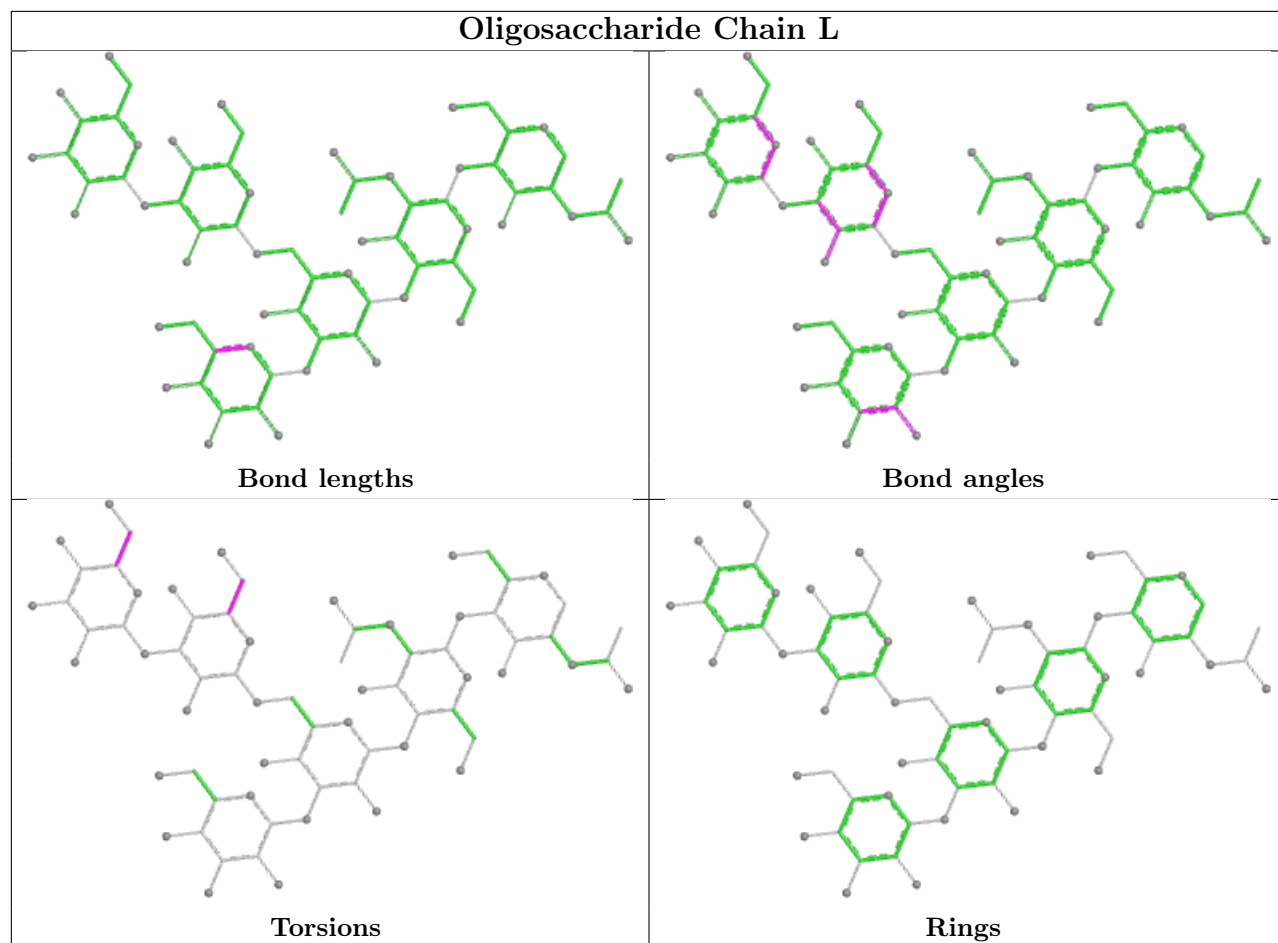
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	5	MAN	1	0
2	E	9	MAN	1	0
5	H	7	MAN	1	0

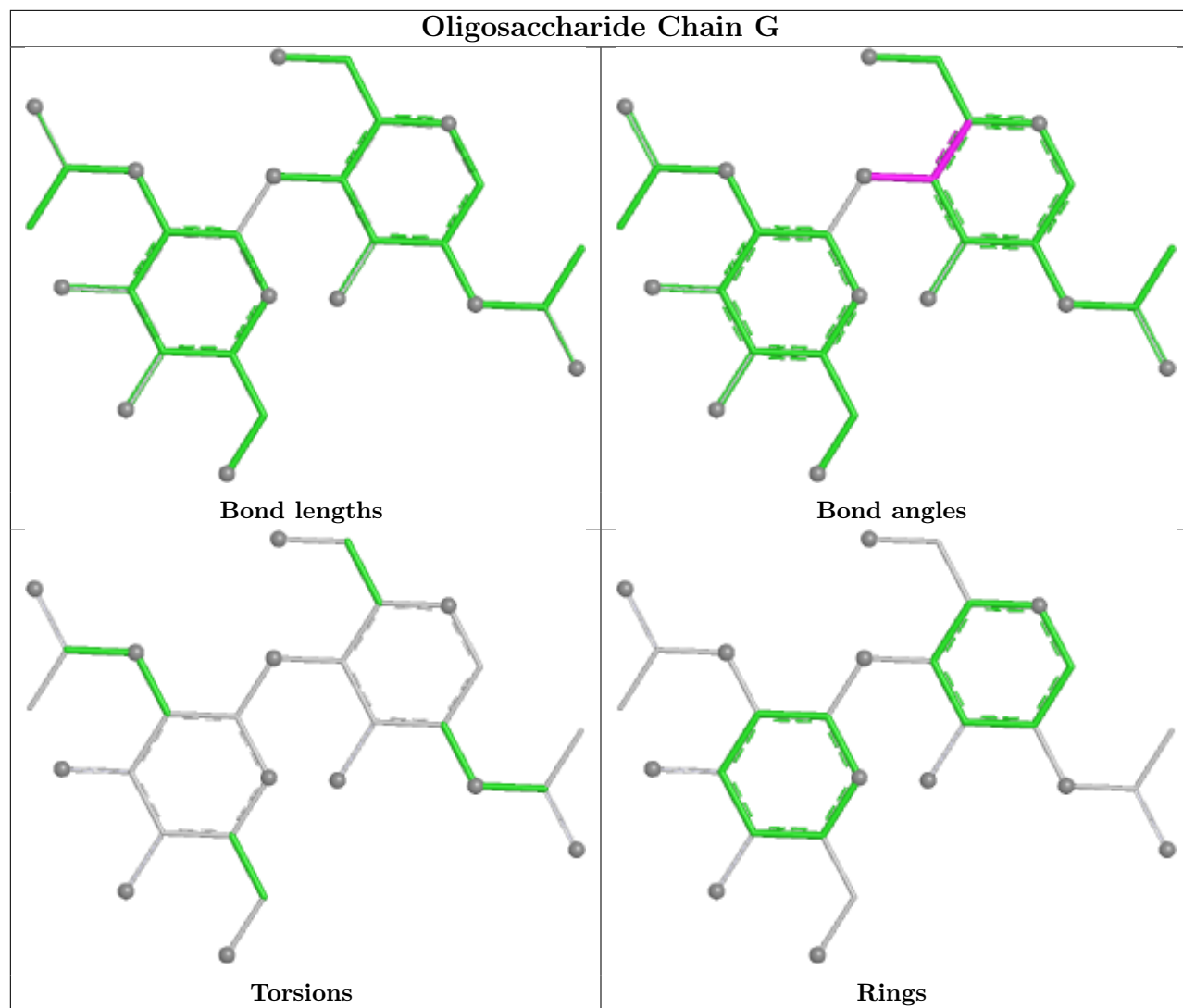
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

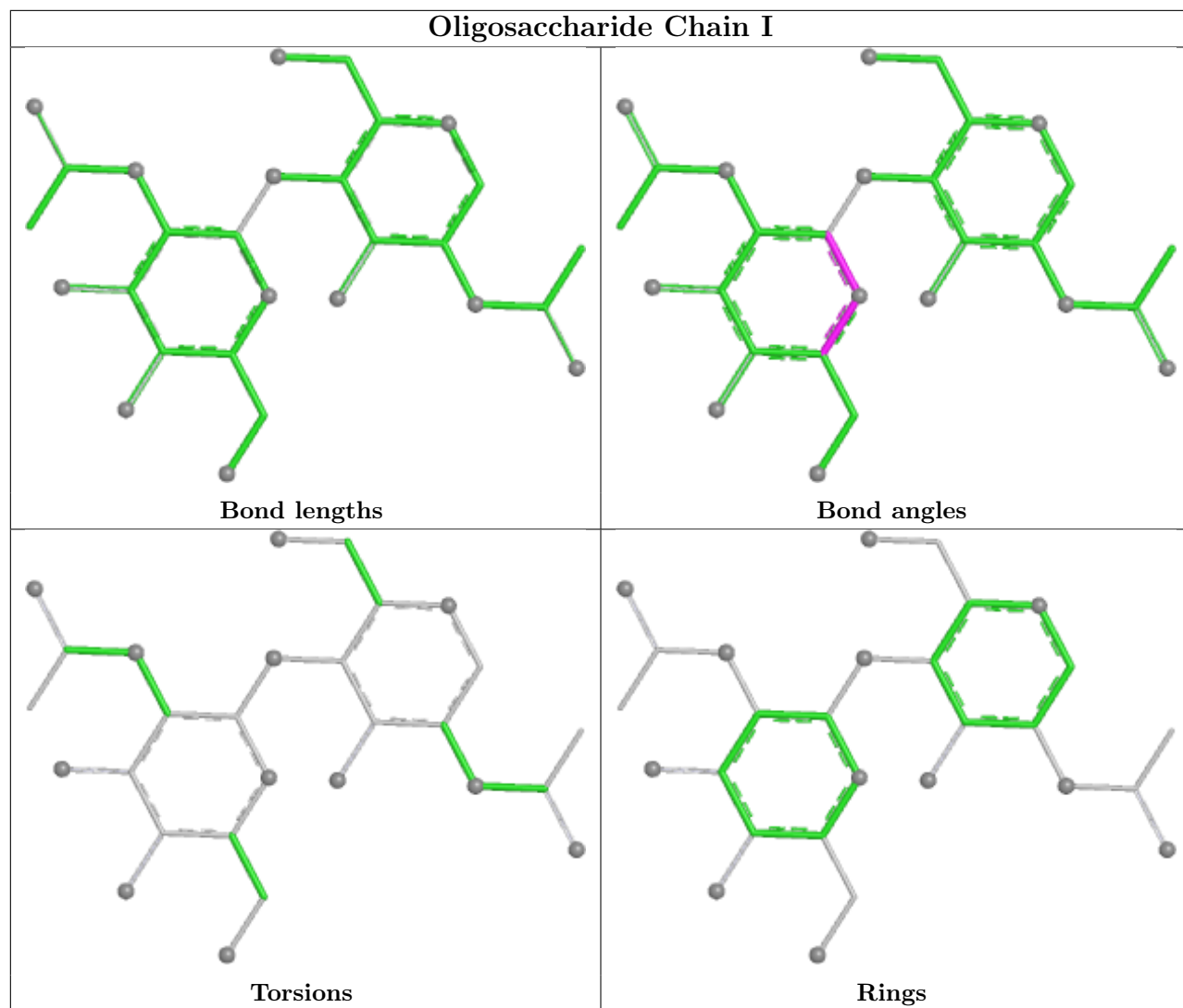


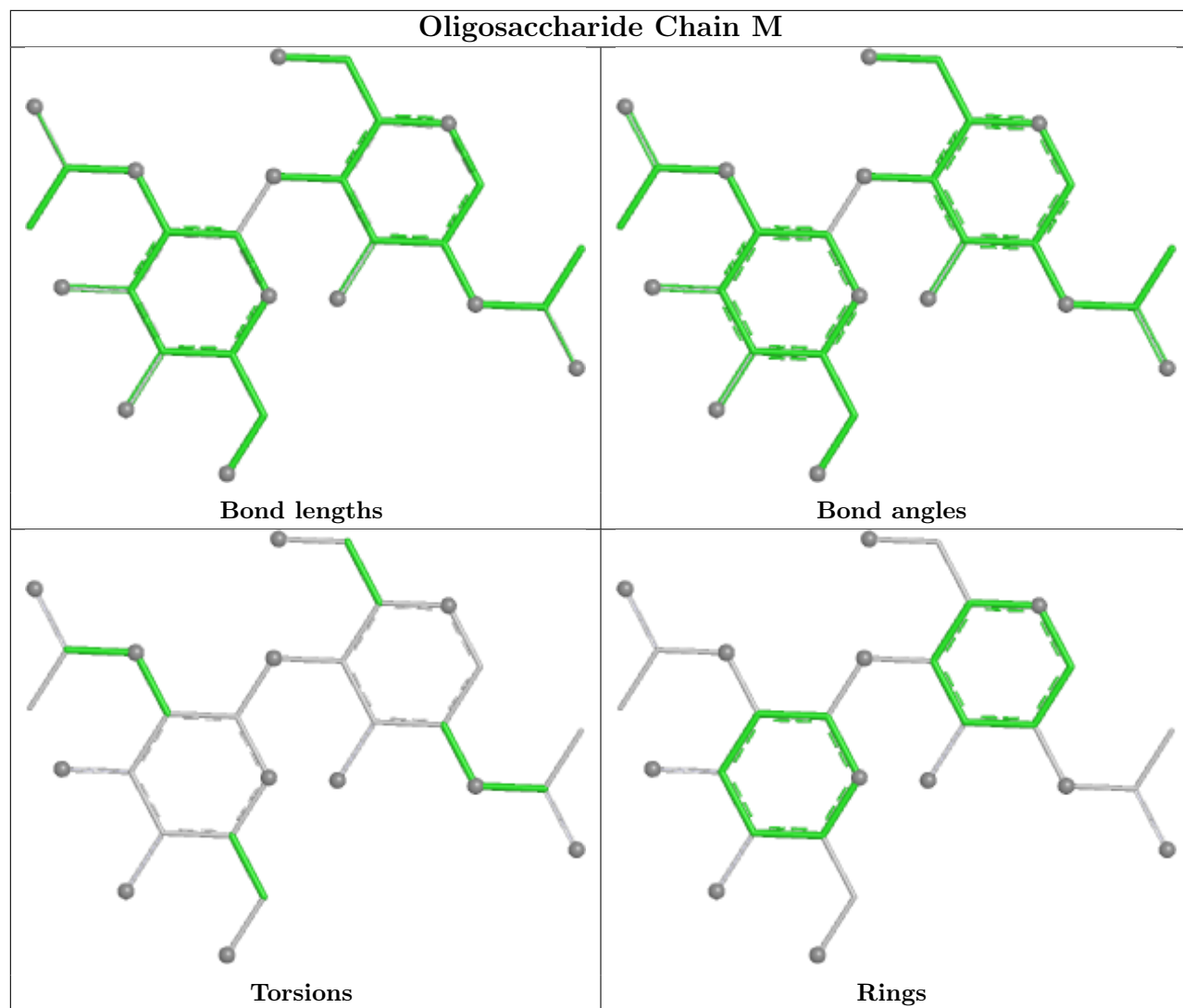


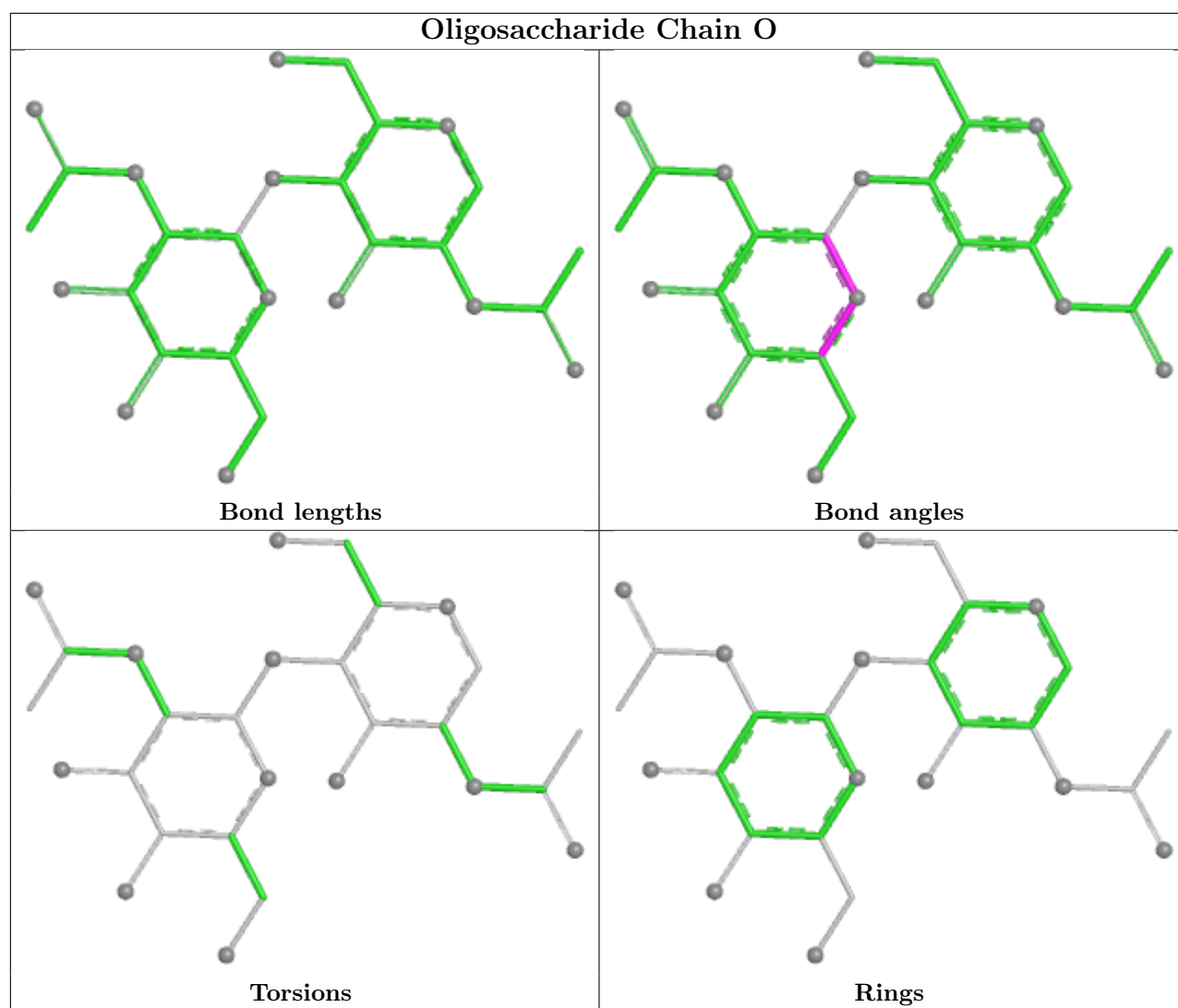


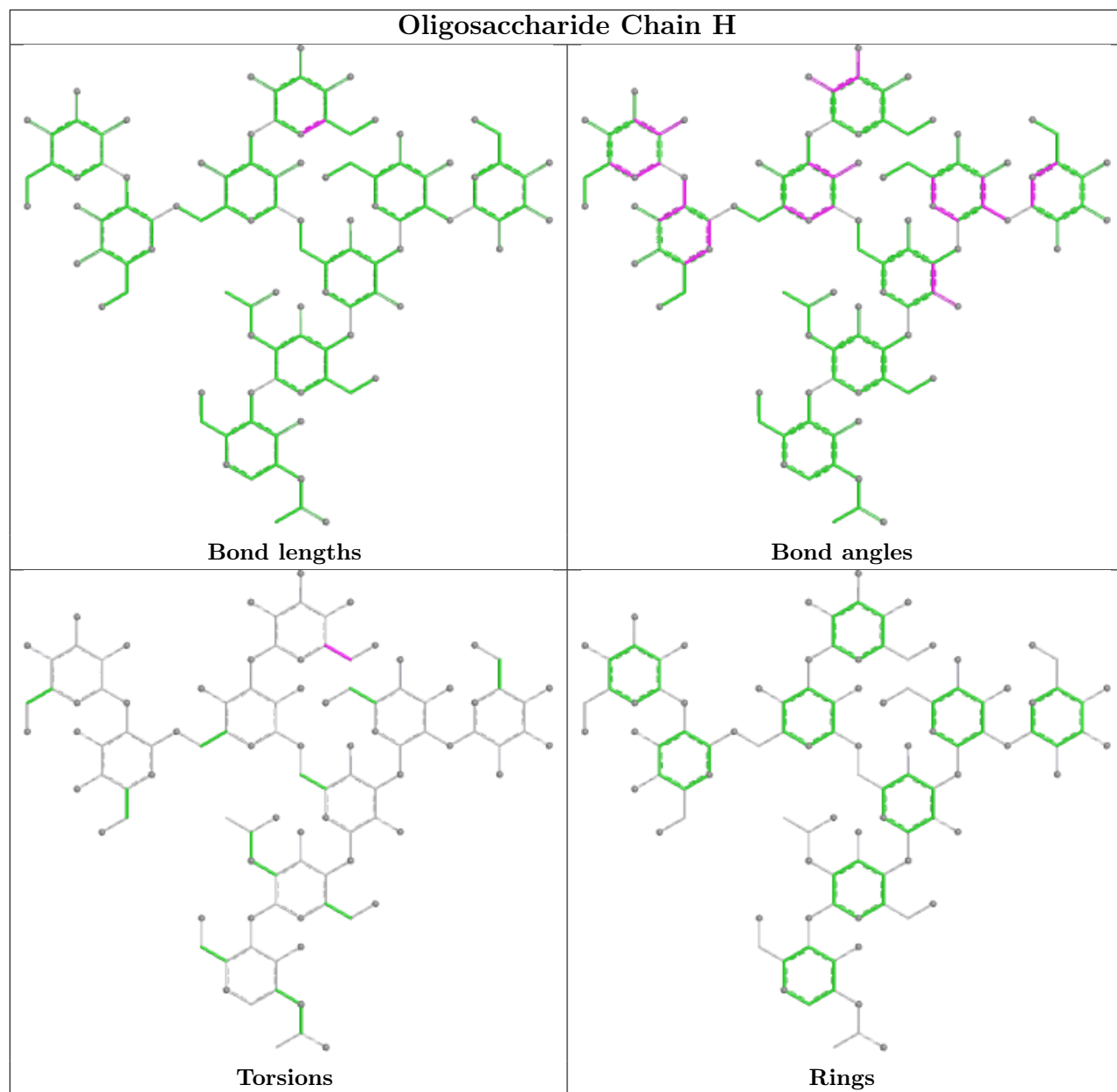


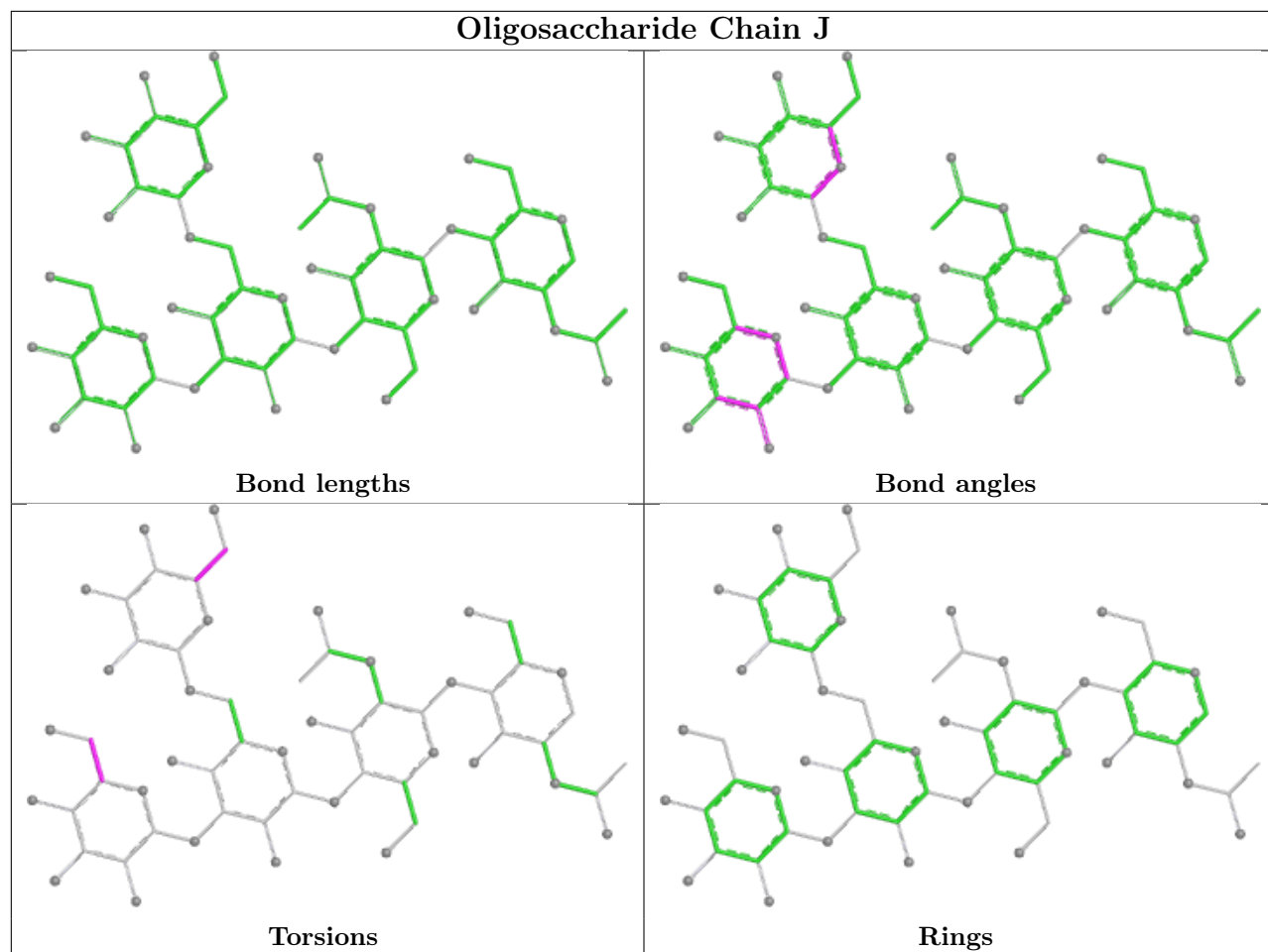


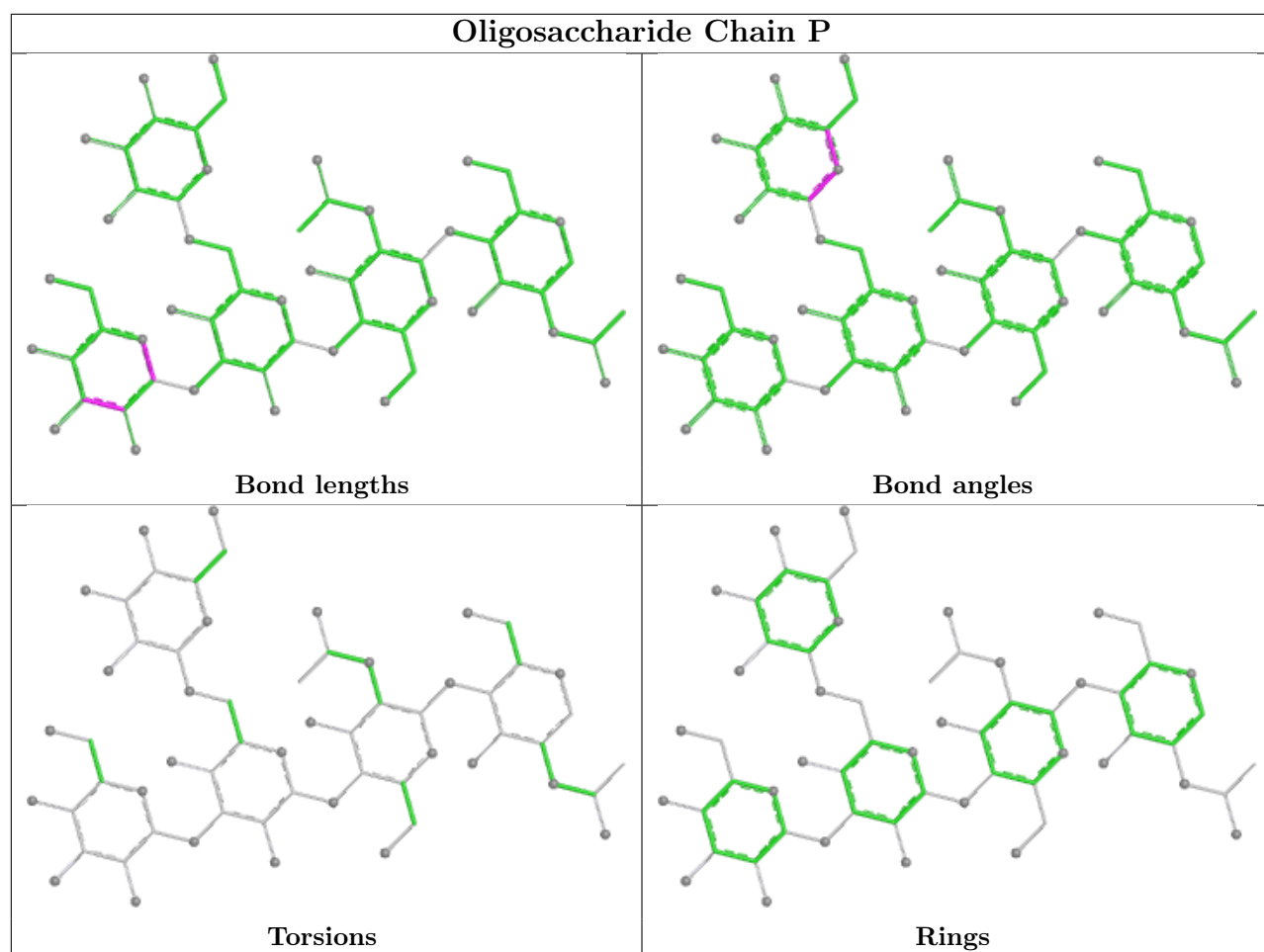


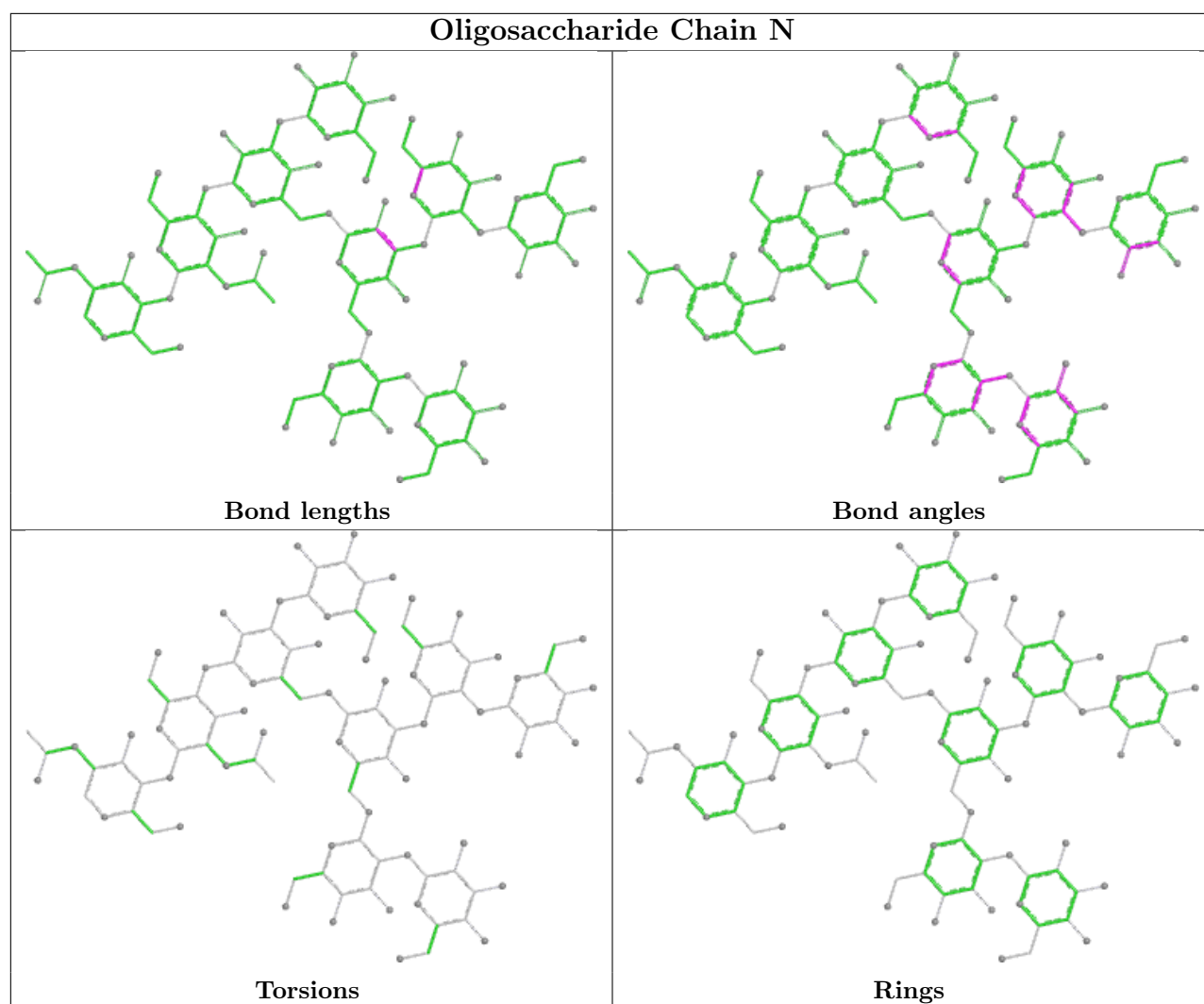












5.6 Ligand geometry [i](#)

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	GOL	C	1904	-	5,5,5	0.96	0	5,5,5	1.29	1 (20%)
9	GOL	B	2103[B]	-	5,5,5	0.69	0	5,5,5	1.18	0
8	NAG	D	1101	1	14,14,15	0.61	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	C	1901[A]	-	5,5,5	0.67	0	5,5,5	1.28	1 (20%)
9	GOL	A	502[B]	-	5,5,5	0.93	0	5,5,5	1.06	0
9	GOL	D	1105	-	5,5,5	0.65	0	5,5,5	1.09	0
10	PG4	C	1909	-	12,12,12	0.14	0	11,11,11	0.79	1 (9%)
8	NAG	C	1903	1	14,14,15	0.42	0	17,19,21	0.50	0
9	GOL	C	1907	-	5,5,5	1.18	0	5,5,5	0.91	0
9	GOL	D	1104	-	5,5,5	0.82	0	5,5,5	1.32	1 (20%)
8	NAG	D	1103	1	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
9	GOL	B	2103[A]	-	5,5,5	0.84	0	5,5,5	1.13	0
9	GOL	A	502[A]	-	5,5,5	0.72	0	5,5,5	1.23	1 (20%)
9	GOL	D	1102	-	5,5,5	1.10	0	5,5,5	1.03	0
8	NAG	B	2101	1	14,14,15	0.33	0	17,19,21	0.66	0
10	PG4	D	1107	-	12,12,12	0.17	0	11,11,11	0.56	0
9	GOL	C	1905	-	5,5,5	0.83	0	5,5,5	1.30	1 (20%)
9	GOL	A	503	-	5,5,5	0.81	0	5,5,5	1.01	0
10	PG4	A	505	-	12,12,12	0.16	0	11,11,11	0.59	0
9	GOL	D	1106	-	5,5,5	1.01	0	5,5,5	0.83	0
8	NAG	C	1902	1	14,14,15	0.29	0	17,19,21	0.49	0
9	GOL	C	1906	-	5,5,5	0.96	0	5,5,5	1.10	0
9	GOL	C	1908	-	5,5,5	1.00	0	5,5,5	1.02	0
9	GOL	B	2102	-	5,5,5	1.01	0	5,5,5	0.90	0
9	GOL	A	504	-	5,5,5	0.71	0	5,5,5	1.28	1 (20%)
9	GOL	C	1901[B]	-	5,5,5	0.81	0	5,5,5	1.07	0
11	PEG	B	2105	-	6,6,6	0.16	0	5,5,5	0.08	0
8	NAG	B	2104	1	14,14,15	0.20	0	17,19,21	0.51	0
8	NAG	A	501	1	14,14,15	0.41	0	17,19,21	0.93	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	C	1904	-	-	4/4/4/4	-
9	GOL	B	2103[B]	-	-	2/4/4/4	-
8	NAG	D	1101	1	-	0/6/23/26	0/1/1/1
9	GOL	C	1901[A]	-	-	0/4/4/4	-
9	GOL	A	502[B]	-	-	2/4/4/4	-
9	GOL	D	1105	-	-	2/4/4/4	-
10	PG4	C	1909	-	-	8/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	C	1903	1	-	0/6/23/26	0/1/1/1
9	GOL	C	1907	-	-	3/4/4/4	-
9	GOL	D	1104	-	-	2/4/4/4	-
8	NAG	D	1103	1	-	1/6/23/26	0/1/1/1
9	GOL	B	2103[A]	-	-	1/4/4/4	-
9	GOL	A	502[A]	-	-	2/4/4/4	-
9	GOL	D	1102	-	-	0/4/4/4	-
8	NAG	B	2101	1	-	0/6/23/26	0/1/1/1
10	PG4	D	1107	-	-	2/10/10/10	-
9	GOL	C	1905	-	-	4/4/4/4	-
9	GOL	A	503	-	-	4/4/4/4	-
10	PG4	A	505	-	-	7/10/10/10	-
9	GOL	D	1106	-	-	2/4/4/4	-
8	NAG	C	1902	1	-	2/6/23/26	0/1/1/1
9	GOL	C	1906	-	-	1/4/4/4	-
9	GOL	C	1908	-	-	0/4/4/4	-
9	GOL	B	2102	-	-	2/4/4/4	-
9	GOL	A	504	-	-	2/4/4/4	-
9	GOL	C	1901[B]	-	-	2/4/4/4	-
11	PEG	B	2105	-	-	3/4/4/4	-
8	NAG	B	2104	1	-	2/6/23/26	0/1/1/1
8	NAG	A	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	501	NAG	C1-O5-C5	3.22	116.51	112.19
9	D	1104	GOL	C3-C2-C1	-2.52	102.55	111.80
9	C	1904	GOL	C3-C2-C1	-2.39	103.04	111.80
9	A	502[A]	GOL	C3-C2-C1	-2.38	103.07	111.80
8	D	1103	NAG	C1-O5-C5	2.29	115.25	112.19

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	502[A]	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
9	A	502[A]	GOL	O2-C2-C3-O3
9	A	503	GOL	O1-C1-C2-C3
9	C	1901[B]	GOL	C1-C2-C3-O3
9	C	1904	GOL	O1-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1904	GOL	3	0
10	C	1909	PG4	2	0
9	D	1104	GOL	1	0
9	D	1102	GOL	1	0
10	D	1107	PG4	1	0
9	A	503	GOL	1	0
10	A	505	PG4	2	0
9	D	1106	GOL	1	0
9	C	1906	GOL	1	0
9	C	1908	GOL	4	0
9	B	2102	GOL	2	0
9	A	504	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	446/462 (96%)	0.02	8 (1%) 67 68	10, 20, 34, 62	6 (1%)
1	B	446/462 (96%)	-0.11	2 (0%) 88 89	10, 19, 33, 60	3 (0%)
1	C	446/462 (96%)	-0.01	8 (1%) 67 68	10, 19, 37, 57	4 (0%)
1	D	445/462 (96%)	-0.06	6 (1%) 75 75	10, 19, 34, 58	3 (0%)
All	All	1783/1848 (96%)	-0.04	24 (1%) 75 75	10, 19, 35, 62	16 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	56	THR	6.2
1	A	184[A]	GLN	4.0
1	D	56	THR	3.9
1	A	417	LEU	3.4
1	C	417	LEU	3.2

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MAN	J	5	11/12	0.63	0.15	44,50,57,59	0
2	MAN	E	6	11/12	0.67	0.15	43,51,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	L	5	11/12	0.68	0.14	38,47,54,55	0
6	MAN	J	4	11/12	0.68	0.13	47,55,59,63	0
3	MAN	F	6	11/12	0.68	0.15	36,42,47,49	0
6	MAN	P	4	11/12	0.71	0.14	37,44,48,51	0
6	MAN	P	5	11/12	0.73	0.12	44,47,53,59	0
3	MAN	F	5	11/12	0.74	0.13	42,47,55,56	0
3	MAN	F	4	11/12	0.75	0.13	41,45,53,55	0
4	NAG	O	2	14/15	0.75	0.13	34,39,43,43	0
4	NAG	I	2	14/15	0.77	0.12	31,39,48,52	0
3	MAN	L	6	11/12	0.78	0.12	38,40,46,46	0
2	MAN	E	5	11/12	0.79	0.11	34,41,44,44	0
2	MAN	K	5	11/12	0.80	0.13	38,43,51,53	0
5	MAN	H	7	11/12	0.80	0.14	34,36,39,45	0
2	MAN	K	6	11/12	0.81	0.12	40,44,49,49	0
4	NAG	G	2	14/15	0.82	0.12	32,36,44,49	0
4	NAG	M	2	14/15	0.82	0.12	29,35,45,48	0
5	MAN	H	9	11/12	0.83	0.10	37,42,49,50	0
7	MAN	N	9	11/12	0.83	0.13	34,38,40,42	0
3	MAN	L	4	11/12	0.84	0.11	42,46,52,54	0
2	MAN	E	9	11/12	0.84	0.12	33,36,39,39	0
2	MAN	E	8	11/12	0.85	0.11	26,31,33,34	0
3	NAG	F	2	14/15	0.87	0.10	24,26,30,37	0
2	MAN	K	8	11/12	0.87	0.10	30,33,37,38	0
6	BMA	J	3	11/12	0.88	0.10	29,34,41,42	0
2	MAN	K	9	11/12	0.88	0.09	29,34,38,41	0
2	MAN	E	7	11/12	0.89	0.10	25,30,31,32	0
3	BMA	F	3	11/12	0.89	0.09	27,33,35,36	0
5	MAN	H	4	11/12	0.89	0.10	29,32,41,41	0
5	MAN	H	6	11/12	0.89	0.10	26,31,37,38	0
2	MAN	K	4	11/12	0.90	0.09	31,35,36,40	0
2	MAN	K	10	11/12	0.90	0.10	24,26,28,29	0
6	BMA	P	3	11/12	0.90	0.08	27,33,38,39	0
2	MAN	E	10	11/12	0.90	0.10	28,29,35,37	0
6	NAG	J	2	14/15	0.90	0.09	24,30,33,39	0
5	MAN	H	5	11/12	0.90	0.11	27,33,37,39	0
5	BMA	H	3	11/12	0.91	0.09	23,27,30,31	0
2	NAG	E	1	14/15	0.91	0.10	22,26,29,30	0
6	NAG	P	1	14/15	0.91	0.09	19,26,29,30	0
7	MAN	N	6	11/12	0.91	0.09	29,32,36,37	0
7	MAN	N	7	11/12	0.91	0.08	24,26,28,28	0
6	NAG	P	2	14/15	0.91	0.08	23,27,31,37	0
2	MAN	E	4	11/12	0.92	0.08	28,29,32,32	0

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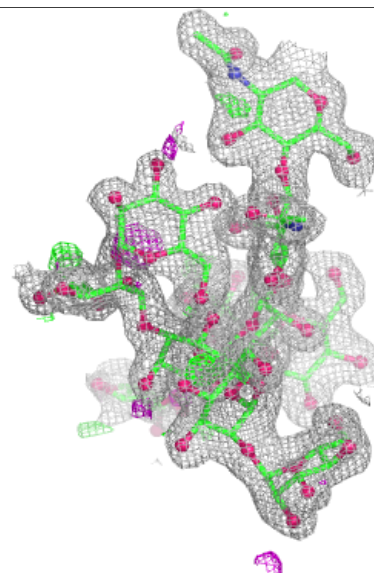
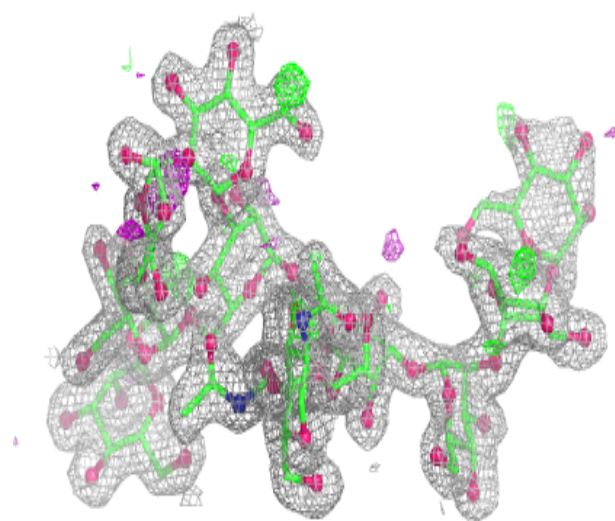
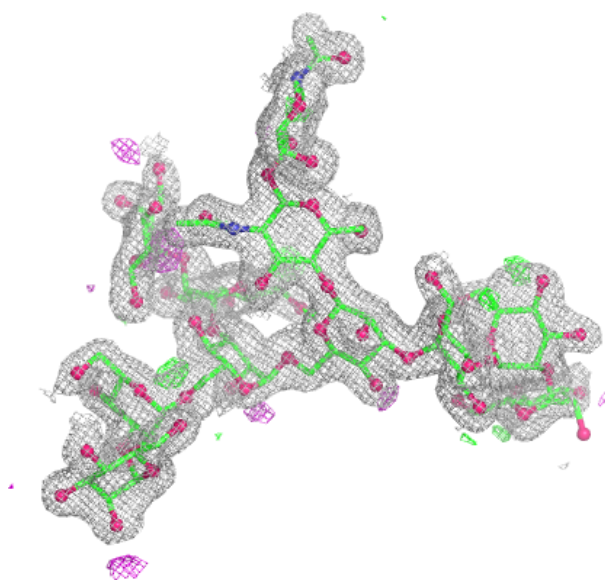
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	K	3	11/12	0.92	0.08	24,26,30,31	0
6	NAG	J	1	14/15	0.92	0.08	22,27,32,33	0
5	NAG	H	2	14/15	0.93	0.08	23,27,29,30	0
3	NAG	L	2	14/15	0.93	0.07	23,26,31,37	0
3	BMA	L	3	11/12	0.93	0.07	25,31,37,40	0
2	NAG	E	2	14/15	0.93	0.08	22,25,29,31	0
2	MAN	K	11	11/12	0.93	0.08	25,27,32,33	0
2	MAN	E	11	11/12	0.93	0.07	26,31,35,39	0
2	NAG	K	1	14/15	0.93	0.10	20,24,29,29	0
2	MAN	K	7	11/12	0.93	0.08	23,27,29,29	0
2	NAG	K	2	14/15	0.93	0.09	22,25,28,28	0
7	MAN	N	8	11/12	0.93	0.08	23,28,32,33	0
2	BMA	E	3	11/12	0.93	0.07	23,26,27,28	0
5	NAG	H	1	14/15	0.94	0.08	25,27,29,29	0
4	NAG	I	1	14/15	0.94	0.06	17,18,24,25	0
7	MAN	N	4	11/12	0.94	0.07	23,24,25,26	0
5	MAN	H	8	11/12	0.94	0.07	29,31,34,34	0
3	NAG	F	1	14/15	0.94	0.08	20,24,33,36	0
4	NAG	G	1	14/15	0.94	0.08	16,18,23,24	0
3	NAG	L	1	14/15	0.94	0.08	20,25,31,34	0
4	NAG	O	1	14/15	0.95	0.07	16,20,23,26	0
7	NAG	N	1	14/15	0.95	0.07	20,25,32,34	0
7	NAG	N	2	14/15	0.95	0.07	22,25,27,28	0
4	NAG	M	1	14/15	0.95	0.07	15,19,21,23	0
7	BMA	N	3	11/12	0.96	0.06	23,25,29,30	0
7	MAN	N	5	11/12	0.96	0.07	23,26,27,29	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.

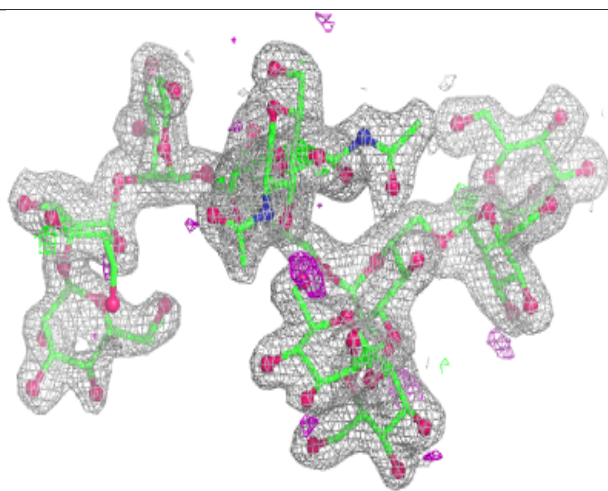
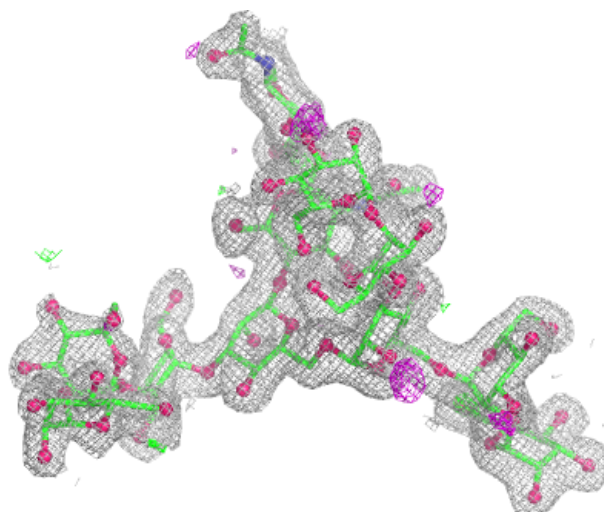
Electron density around Chain E:

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



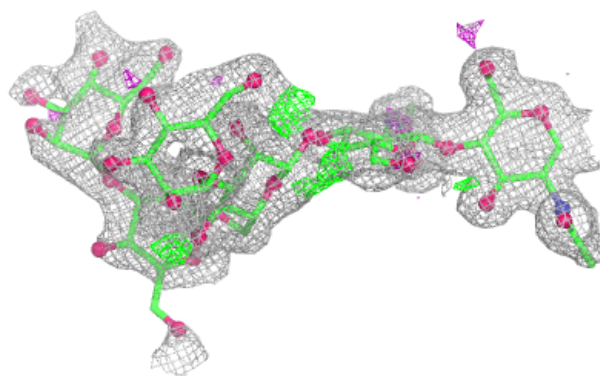
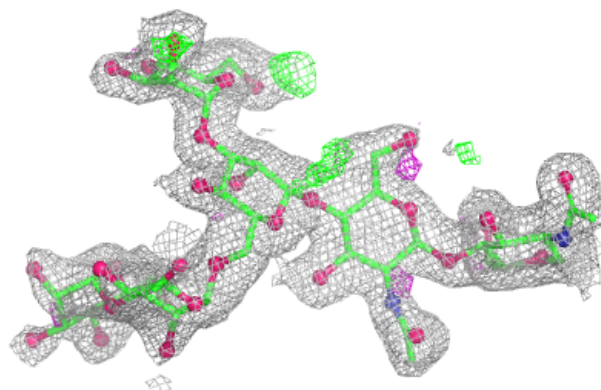
Electron density around Chain K:

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

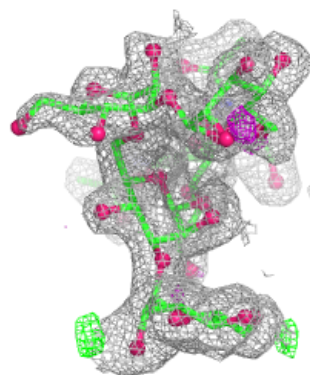
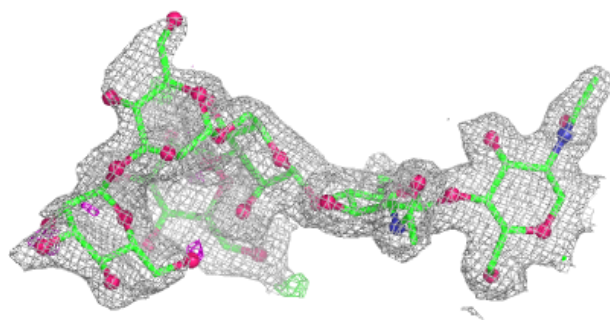
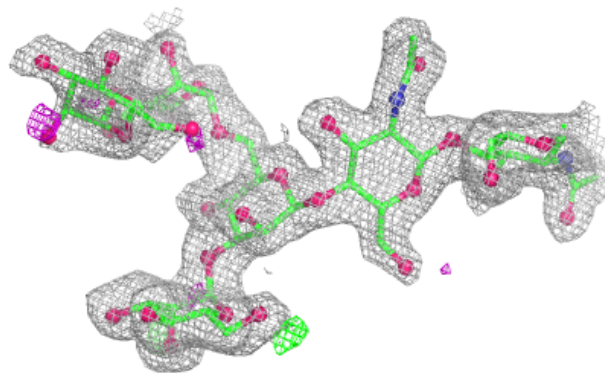


Electron density around Chain F:

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

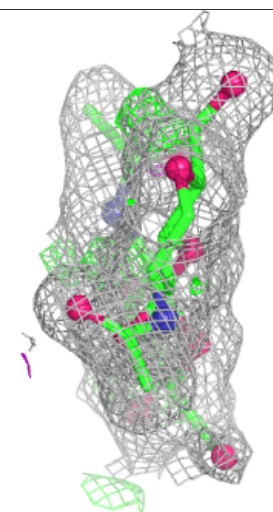
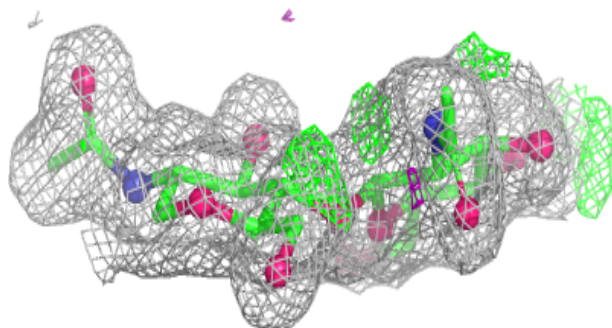
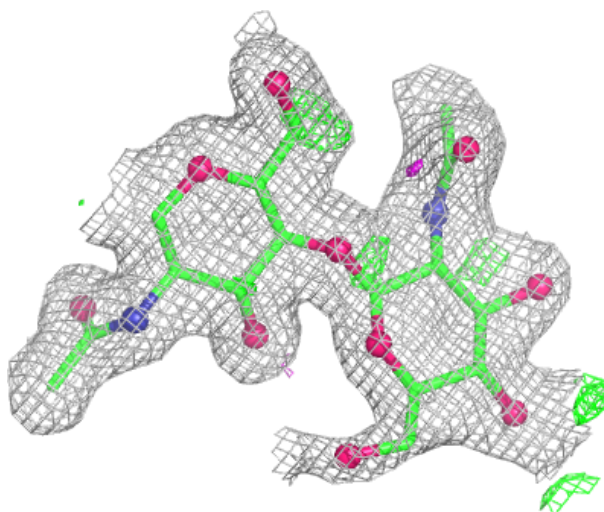
**Electron density around Chain L:**

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



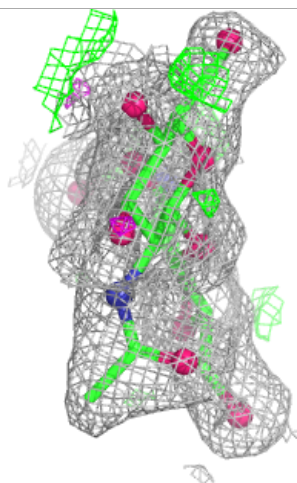
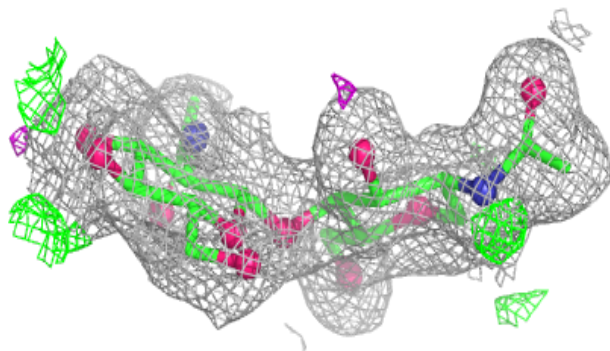
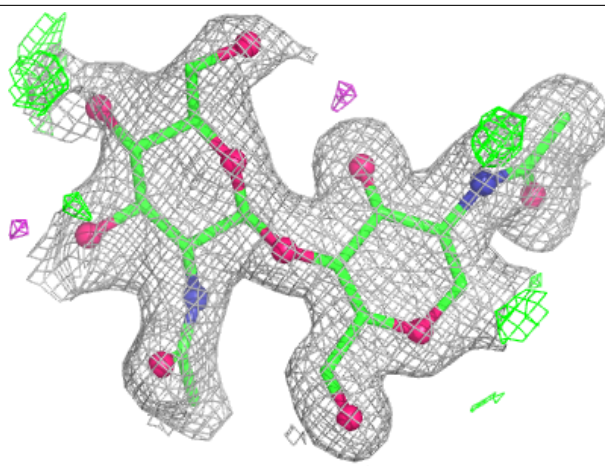
Electron density around Chain G:

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



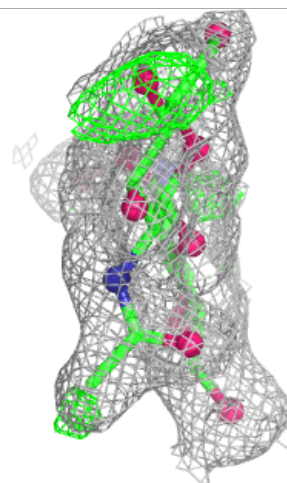
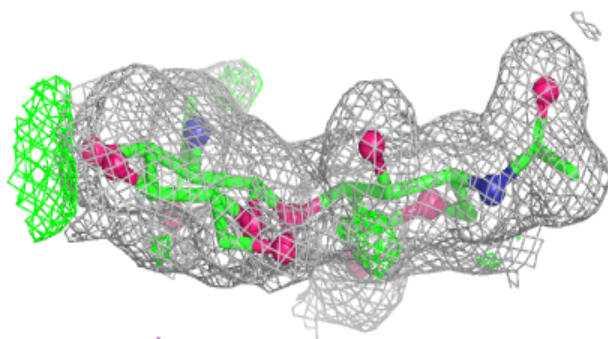
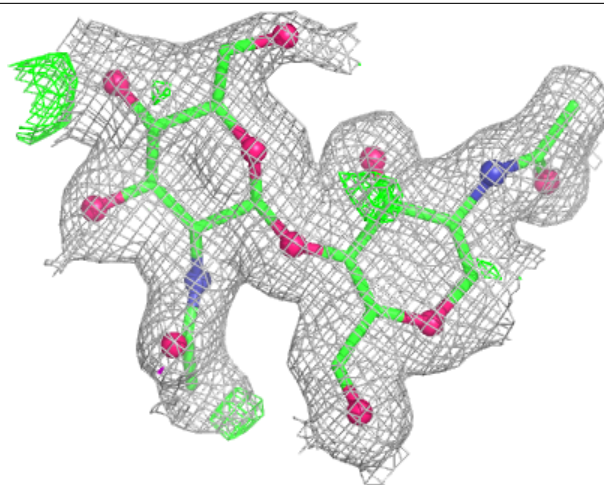
Electron density around Chain I:

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



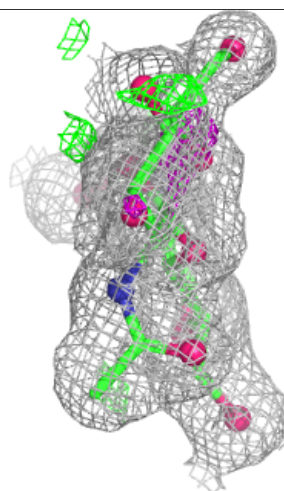
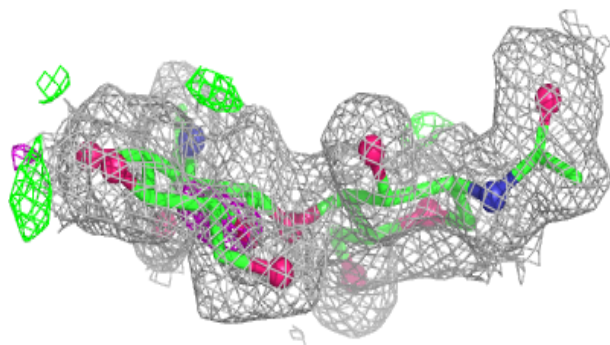
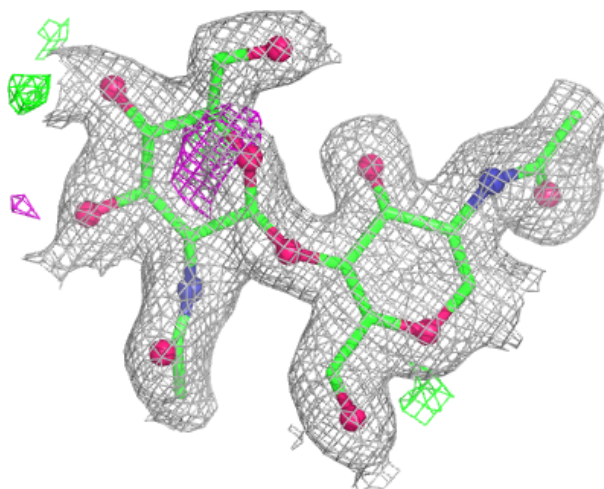
Electron density around Chain M:

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



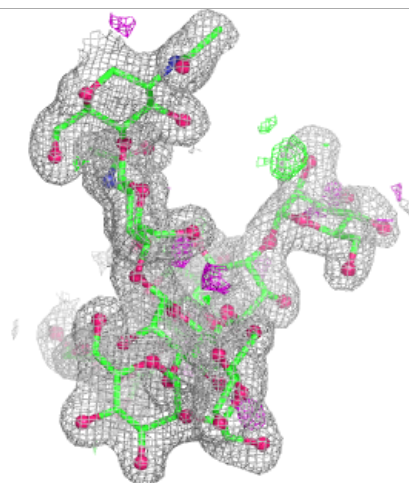
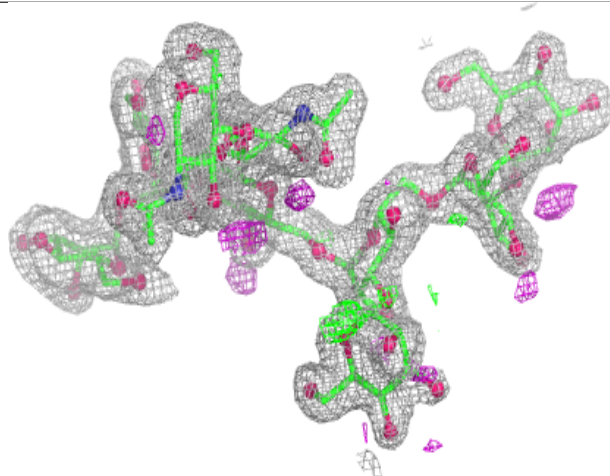
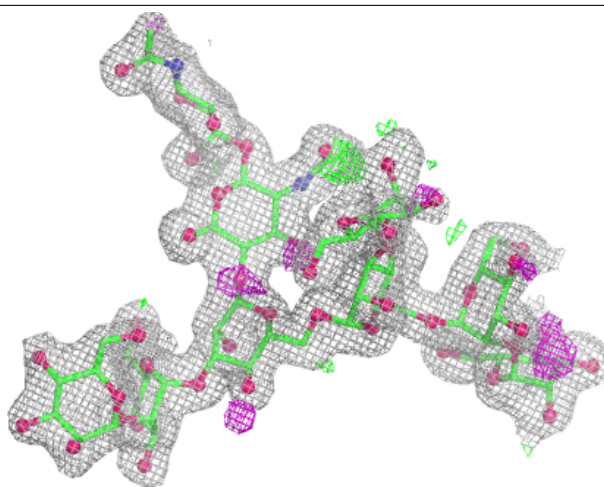
Electron density around Chain O:

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



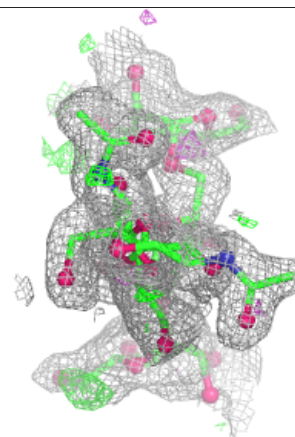
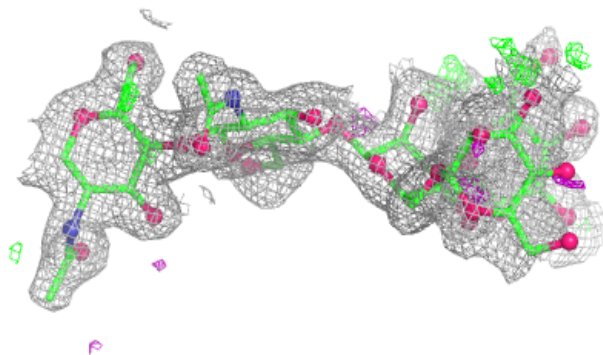
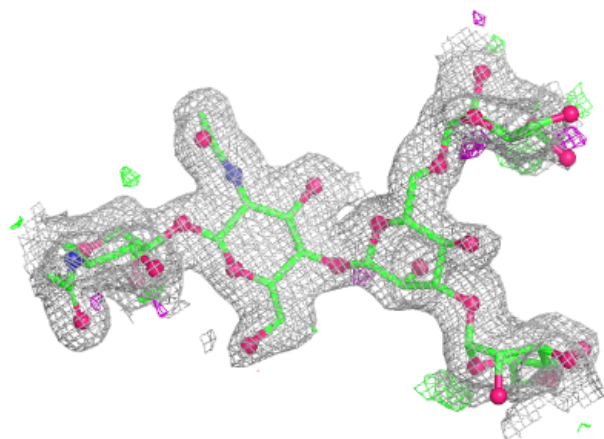
Electron density around Chain H:

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

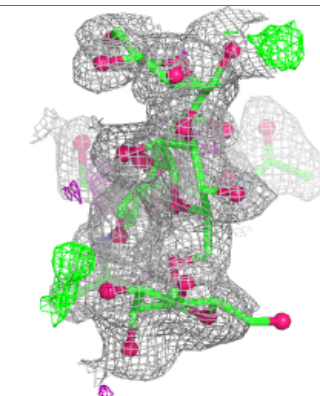
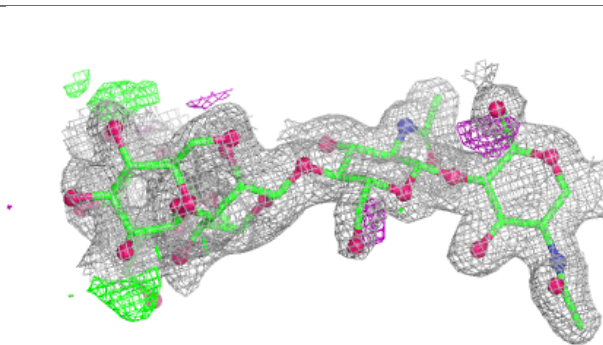
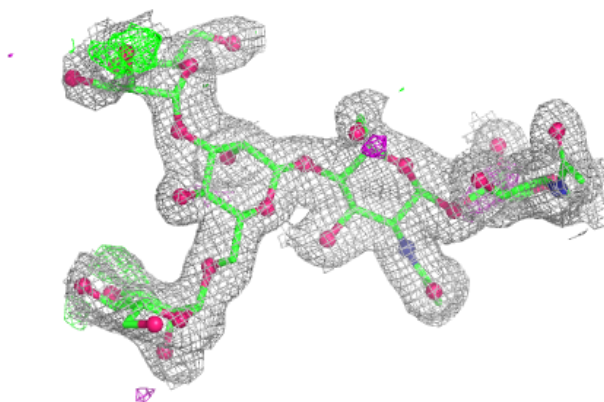


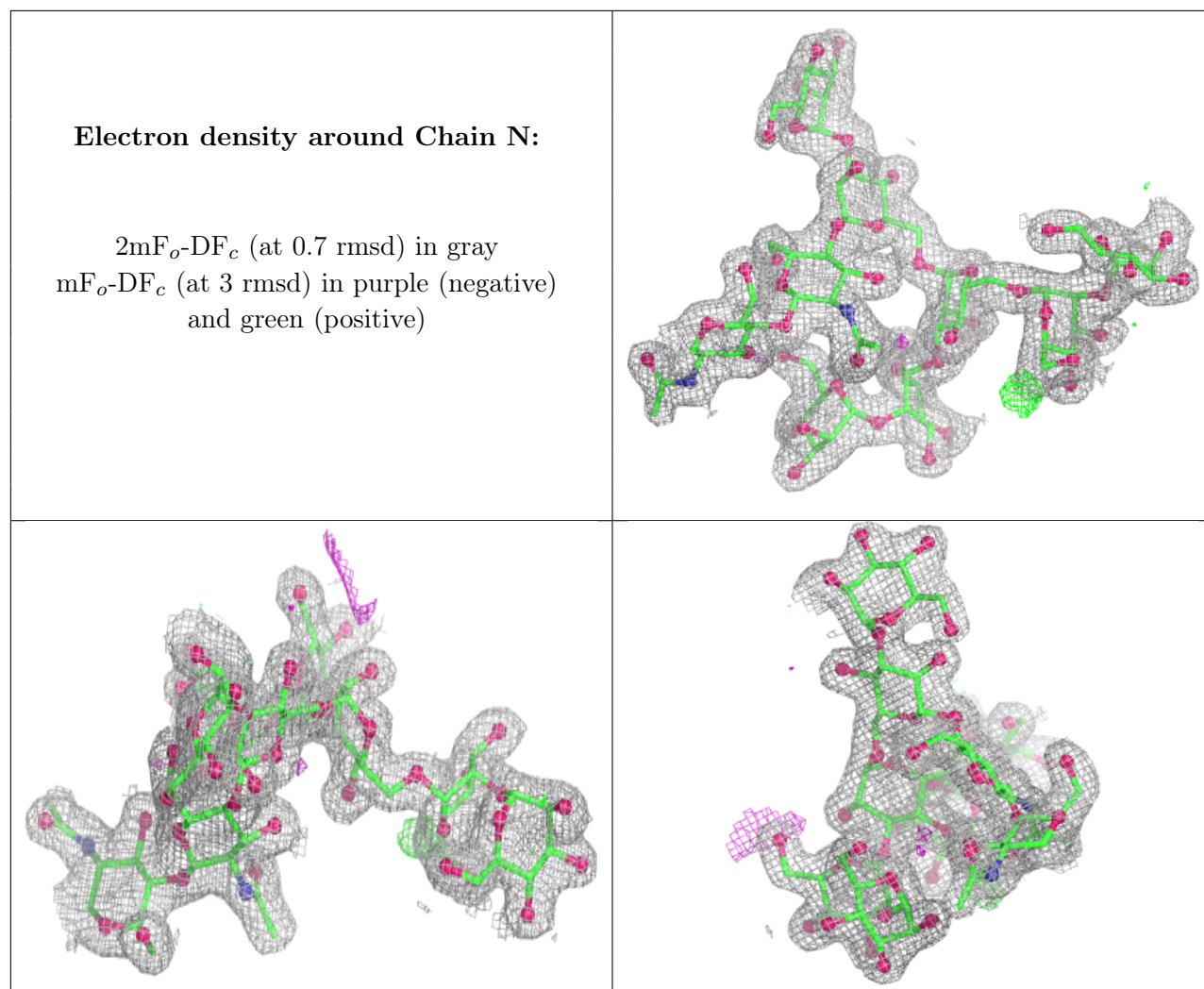
Electron density around Chain J:

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

**Electron density around Chain P:**

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





6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	A	501	14/15	0.68	0.14	44,51,57,59	0
8	NAG	C	1902	14/15	0.72	0.15	41,47,50,52	0
8	NAG	B	2104	14/15	0.73	0.13	40,44,51,52	0
10	PG4	C	1909	13/13	0.73	0.16	32,37,43,49	0
10	PG4	D	1107	13/13	0.76	0.16	29,35,46,47	0
9	GOL	C	1905	6/6	0.77	0.14	31,32,36,42	0
9	GOL	A	502[A]	6/6	0.78	0.16	24,25,28,28	6
9	GOL	A	502[B]	6/6	0.78	0.16	24,27,29,29	6
9	GOL	A	504	6/6	0.78	0.13	26,34,36,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	GOL	C	1906	6/6	0.79	0.14	39,39,42,43	0
11	PEG	B	2105	7/7	0.79	0.15	29,35,37,44	0
9	GOL	D	1104	6/6	0.80	0.17	26,28,33,35	0
8	NAG	D	1103	14/15	0.81	0.12	39,46,50,54	0
9	GOL	C	1908	6/6	0.82	0.13	30,35,38,39	0
9	GOL	C	1904	6/6	0.82	0.16	24,32,34,38	0
10	PG4	A	505	13/13	0.82	0.14	31,36,40,46	0
9	GOL	C	1901[B]	6/6	0.83	0.11	21,25,28,28	6
9	GOL	C	1901[A]	6/6	0.83	0.11	22,26,27,28	6
9	GOL	C	1907	6/6	0.85	0.17	19,30,37,39	0
9	GOL	B	2103[A]	6/6	0.87	0.11	20,26,27,30	6
9	GOL	B	2103[B]	6/6	0.87	0.11	23,25,27,30	6
9	GOL	A	503	6/6	0.87	0.11	28,31,38,44	0
9	GOL	D	1106	6/6	0.87	0.12	32,33,35,37	0
8	NAG	C	1903	14/15	0.88	0.10	21,25,29,32	0
9	GOL	D	1105	6/6	0.90	0.09	25,30,33,42	0
8	NAG	B	2101	14/15	0.92	0.08	20,22,27,34	0
8	NAG	D	1101	14/15	0.93	0.08	19,23,30,31	0
9	GOL	D	1102	6/6	0.94	0.11	20,28,29,29	0
9	GOL	B	2102	6/6	0.94	0.08	18,27,28,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.