



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:42 AM BST

PDB ID : 5NBS
Title : Structural studies of a Glycoside Hydrolase Family 3 beta-glucosidase from the Model Fungus *Neurospora crassa*
Authors : Gudmundsson, M.; Karkehabadi, S.; Kaper, T.; Sandgren, M.
Deposited on : 2017-03-02
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

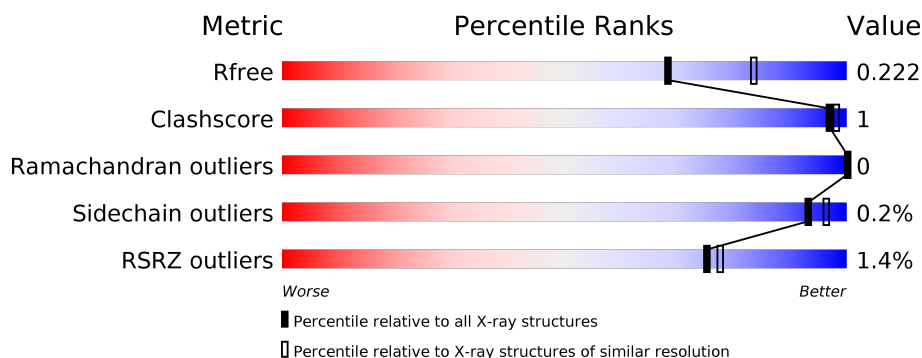
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.








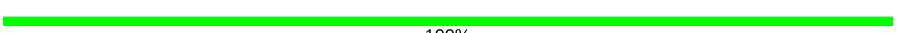




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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	857	<div> <div style="width: 95%;"></div> <div>95%</div> </div>
1	B	857	<div> <div style="width: 96%;"></div> <div>96%</div> </div>
2	C	6	<div> <div style="width: 83%;"></div> <div>83%</div> </div>
2	J	6	<div> <div style="width: 67%;"></div> <div>67%</div> </div>
3	D	8	<div> <div style="width: 63%;"></div> <div>63%</div> </div>
3	F	8	<div> <div style="width: 63%;"></div> <div>63%</div> </div>

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Mol	Chain	Length	Quality of chain
3	M	8	
3	N	8	
4	E	4	
4	L	4	
5	G	2	
5	O	2	
5	P	2	
6	H	9	
7	I	3	
8	K	5	

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
6	MAN	H	9	-	-	-	X

2 Entry composition [i](#)

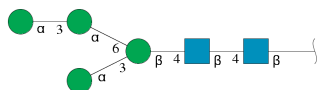
There are 10 unique types of molecules in this entry. The entry contains 15111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

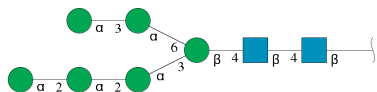
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	13	0
			6613	4184	1123	1279	27			
1	B	841	Total	C	N	O	S	0	4	0
			6523	4131	1102	1264	26			

- Molecule 2 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
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	J	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
3	D	8	Total	C	N	O	0	0	0
			94	52	2	40			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	8	Total	C	N	O	0	0	0
			94	52	2	40			
3	M	8	Total	C	N	O	0	0	0
			94	52	2	40			
3	N	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 4 is an oligosaccharide called 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.



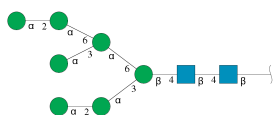
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 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
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 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
6	H	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 7 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
7	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called 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
8	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

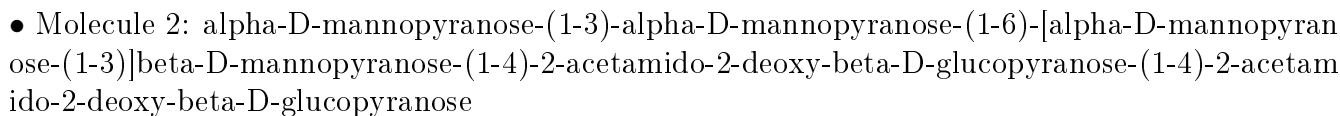
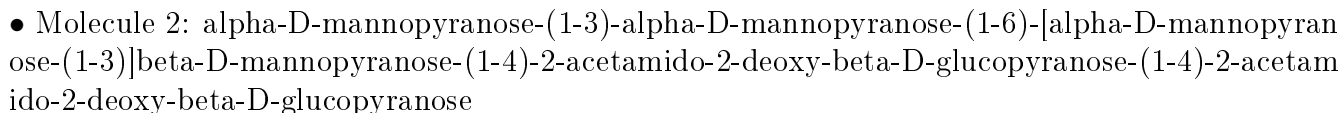


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	625	Total	O	0	0
			625	625		
10	B	329	Total	O	0	0
			329	329		

- Molecule 1: Beta-glucosidase



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



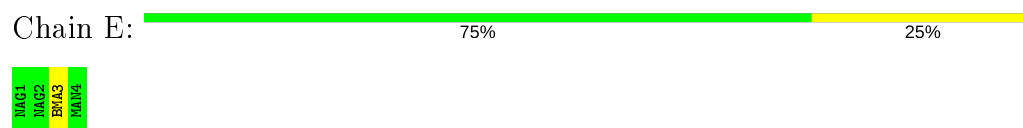
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 4: 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



- Molecule 4: 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%



MAG1

MAG2

MAG3

MAG4

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%



MAG1

MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



MAG1

MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose


Chain P:  50% 50%



MAG1

MAG2

- Molecule 6: 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:  33% 67%



MAG1

MAG2

MAG3

MAG4

MAG5

MAG6

MAG7

MAG8

MAG9

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

Chain I:  100%



MAG1

MAG2

MAG3

- Molecule 8: 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 K:



HA01
HA02
HA03
HA04
HA05

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.93Å 286.84Å 58.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 2.25 47.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.00-2.25) 99.2 (47.00-2.25)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.30 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.180 , 0.220 0.185 , 0.222	Depositor DCC
R_{free} test set	5627 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15111	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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: BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/6793	0.65	2/9246 (0.0%)
1	B	0.41	0/6703	0.61	1/9131 (0.0%)
All	All	0.43	0/13496	0.63	3/18377 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	325	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	325	ARG	NE-CZ-NH1	5.52	123.06	120.30

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	6613	0	6320	18	0
1	B	6523	0	6230	10	0
2	C	72	0	61	0	0
2	J	72	0	61	1	0
3	D	94	0	79	0	0
3	F	94	0	79	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	94	0	79	0	0
3	N	94	0	79	0	0
4	E	50	0	43	0	0
4	L	50	0	43	0	0
5	G	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	0	0
6	H	105	0	88	0	0
7	I	39	0	34	0	0
8	K	61	0	52	0	0
9	A	70	0	65	0	0
9	B	42	0	39	0	0
10	A	625	0	0	0	0
10	B	329	0	0	1	0
All	All	15111	0	13427	26	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 1.

All (26) 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:337:PHE:CE1	1:B:342:GLN:HG2	2.29	0.68
1:A:802[A]:ARG:HH11	1:A:802[A]:ARG:HG2	1.60	0.64
1:A:802[A]:ARG:NH1	1:A:802[A]:ARG:HG2	2.13	0.64
1:A:471:ARG:HH22	1:A:490:GLN:HE22	1.50	0.59
1:A:249:ASN:HD21	1:A:619:GLN:HE22	1.52	0.58
1:A:224[A]:MET:SD	1:A:631:ARG:NH1	2.82	0.52
1:B:141:ALA:HB2	1:B:168:MET:SD	2.51	0.51
1:A:769:ILE:HD11	1:A:781:PRO:HB3	1.91	0.51
1:A:459[B]:GLN:HG2	1:B:459:GLN:HG2	1.96	0.48
1:A:233:ILE:HD11	1:A:263:LEU:HD12	1.97	0.46
1:A:444:TRP:CZ3	1:A:510:ILE:HD12	2.51	0.45
1:A:135:VAL:HG22	1:A:181:VAL:HB	1.99	0.44
1:A:783:LEU:HD11	1:A:841:VAL:HG13	1.98	0.44
1:B:704:PHE:CZ	2:J:2:NAG:H82	2.53	0.44
1:A:113:ASP:OD2	1:A:802[A]:ARG:NH1	2.51	0.43
1:B:769:ILE:HD11	1:B:781:PRO:HB3	1.99	0.43
1:B:342:GLN:NE2	10:B:1202:HOH:O	2.51	0.42
1:A:783:LEU:CD1	1:A:841:VAL:HG13	2.49	0.42
1:A:802[A]:ARG:CG	1:A:802[A]:ARG:HH11	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:CYS:SG	1:B:275:SER:HA	2.60	0.41
1:B:727:ALA:HB1	1:B:731:LEU:HD12	2.02	0.41
1:B:471:ARG:HH22	1:B:490:GLN:HE22	1.69	0.41
1:A:390:GLU:OE2	1:A:394[B]:ARG:NH1	2.54	0.41
1:A:545:HIS:CD2	1:A:567:ALA:HB3	2.56	0.41
1:A:491:GLN:CG	1:B:359:THR:OG1	2.69	0.41
1:A:444:TRP:CD1	1:A:508:ILE:HB	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	853/857 (100%)	827 (97%)	26 (3%)	0	100	100
1	B	843/857 (98%)	818 (97%)	25 (3%)	0	100	100
All	All	1696/1714 (99%)	1645 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	699/700 (100%)	696 (100%)	3 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	689/700 (98%)	688 (100%)	1 (0%)	93	96
All	All	1388/1400 (99%)	1384 (100%)	4 (0%)	93	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	TRP
1	A	674[A]	GLN
1	A	674[B]	GLN
1	B	277	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	261	ASN
1	A	302	ASN
1	A	433	ASN
1	A	462	GLN
1	A	467	GLN
1	A	490	GLN
1	A	491	GLN
1	A	619	GLN
1	A	703	GLN
1	B	126	GLN
1	B	186	HIS
1	B	207	ASN
1	B	261	ASN
1	B	433	ASN
1	B	450	ASN
1	B	462	GLN
1	B	479	HIS
1	B	490	GLN
1	B	725	GLN

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 ⓘ

75 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	0.36	0	17,19,21	0.62	0
2	NAG	C	2	2	14,14,15	0.36	0	17,19,21	0.87	1 (5%)
2	BMA	C	3	2	11,11,12	0.39	0	15,15,17	0.60	0
2	MAN	C	4	2	11,11,12	0.36	0	15,15,17	0.81	0
2	MAN	C	5	2	11,11,12	0.53	0	15,15,17	0.79	0
2	MAN	C	6	2	11,11,12	0.55	0	15,15,17	0.59	0
3	NAG	D	1	1,3	14,14,15	0.31	0	17,19,21	0.89	0
3	NAG	D	2	3	14,14,15	0.39	0	17,19,21	1.01	0
3	BMA	D	3	3	11,11,12	0.24	0	15,15,17	1.07	2 (13%)
3	MAN	D	4	3	11,11,12	0.30	0	15,15,17	0.96	0
3	MAN	D	5	3	11,11,12	0.32	0	15,15,17	1.05	1 (6%)
3	MAN	D	6	3	11,11,12	0.52	0	15,15,17	0.74	0
3	MAN	D	7	3	11,11,12	0.65	0	15,15,17	0.88	1 (6%)
3	MAN	D	8	3	11,11,12	0.54	0	15,15,17	0.95	0
4	NAG	E	1	1,4	14,14,15	0.42	0	17,19,21	1.06	0
4	NAG	E	2	4	14,14,15	0.26	0	17,19,21	0.79	0
4	BMA	E	3	4	11,11,12	0.49	0	15,15,17	1.48	4 (26%)
4	MAN	E	4	4	11,11,12	0.48	0	15,15,17	0.82	0
3	NAG	F	1	1,3	14,14,15	0.36	0	17,19,21	0.97	1 (5%)
3	NAG	F	2	3	14,14,15	0.49	0	17,19,21	0.80	0
3	BMA	F	3	3	11,11,12	0.33	0	15,15,17	1.01	1 (6%)
3	MAN	F	4	3	11,11,12	0.47	0	15,15,17	1.13	1 (6%)
3	MAN	F	5	3	11,11,12	0.40	0	15,15,17	0.86	0
3	MAN	F	6	3	11,11,12	0.46	0	15,15,17	0.77	0
3	MAN	F	7	3	11,11,12	0.36	0	15,15,17	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	F	8	3	11,11,12	0.58	0	15,15,17	0.93	0
5	NAG	G	1	1,5	14,14,15	0.47	0	17,19,21	0.95	0
5	NAG	G	2	5	14,14,15	0.50	0	17,19,21	1.13	1 (5%)
6	NAG	H	1	1,6	14,14,15	0.30	0	17,19,21	0.96	1 (5%)
6	NAG	H	2	6	14,14,15	0.37	0	17,19,21	1.14	1 (5%)
6	BMA	H	3	6	11,11,12	0.44	0	15,15,17	0.73	0
6	MAN	H	4	6	11,11,12	0.44	0	15,15,17	1.12	1 (6%)
6	MAN	H	5	6	11,11,12	0.46	0	15,15,17	1.10	2 (13%)
6	MAN	H	6	6	11,11,12	0.43	0	15,15,17	0.83	0
6	MAN	H	7	6	11,11,12	0.58	0	15,15,17	0.83	0
6	MAN	H	8	6	11,11,12	0.43	0	15,15,17	0.96	1 (6%)
6	MAN	H	9	6	11,11,12	0.80	0	15,15,17	1.28	2 (13%)
7	NAG	I	1	1,7	14,14,15	0.34	0	17,19,21	0.90	1 (5%)
7	NAG	I	2	7	14,14,15	0.39	0	17,19,21	1.14	1 (5%)
7	BMA	I	3	7	11,11,12	0.40	0	15,15,17	1.09	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.40	0	17,19,21	0.81	0
2	NAG	J	2	2	14,14,15	0.29	0	17,19,21	0.95	1 (5%)
2	BMA	J	3	2	11,11,12	0.27	0	15,15,17	0.58	0
2	MAN	J	4	2	11,11,12	0.34	0	15,15,17	1.12	1 (6%)
2	MAN	J	5	2	11,11,12	0.42	0	15,15,17	0.79	0
2	MAN	J	6	2	11,11,12	0.63	0	15,15,17	0.72	0
8	NAG	K	1	1,8	14,14,15	0.34	0	17,19,21	0.89	1 (5%)
8	NAG	K	2	8	14,14,15	0.31	0	17,19,21	0.75	0
8	BMA	K	3	8	11,11,12	0.34	0	15,15,17	0.80	1 (6%)
8	MAN	K	4	8	11,11,12	0.48	0	15,15,17	1.18	3 (20%)
8	MAN	K	5	8	11,11,12	0.50	0	15,15,17	0.84	0
4	NAG	L	1	1,4	14,14,15	0.33	0	17,19,21	1.09	1 (5%)
4	NAG	L	2	4	14,14,15	0.34	0	17,19,21	1.17	1 (5%)
4	BMA	L	3	4	11,11,12	0.36	0	15,15,17	0.51	0
4	MAN	L	4	4	11,11,12	0.37	0	15,15,17	0.85	0
3	NAG	M	1	1,3	14,14,15	0.33	0	17,19,21	0.99	1 (5%)
3	NAG	M	2	3	14,14,15	0.49	0	17,19,21	0.84	0
3	BMA	M	3	3	11,11,12	0.35	0	15,15,17	0.68	0
3	MAN	M	4	3	11,11,12	0.38	0	15,15,17	1.03	1 (6%)
3	MAN	M	5	3	11,11,12	0.47	0	15,15,17	0.75	0
3	MAN	M	6	3	11,11,12	0.41	0	15,15,17	0.82	0
3	MAN	M	7	3	11,11,12	0.36	0	15,15,17	0.91	0
3	MAN	M	8	3	11,11,12	0.39	0	15,15,17	1.08	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	1	1,3	14,14,15	0.37	0	17,19,21	0.60	0
3	NAG	N	2	3	14,14,15	0.41	0	17,19,21	1.05	2 (11%)
3	BMA	N	3	3	11,11,12	0.59	0	15,15,17	0.76	0
3	MAN	N	4	3	11,11,12	0.39	0	15,15,17	0.83	0
3	MAN	N	5	3	11,11,12	0.36	0	15,15,17	0.80	1 (6%)
3	MAN	N	6	3	11,11,12	0.35	0	15,15,17	0.84	0
3	MAN	N	7	3	11,11,12	0.33	0	15,15,17	0.88	1 (6%)
3	MAN	N	8	3	11,11,12	0.50	0	15,15,17	0.80	0
5	NAG	O	1	1,5	14,14,15	0.41	0	17,19,21	0.82	0
5	NAG	O	2	5	14,14,15	0.49	0	17,19,21	0.82	0
5	NAG	P	1	1,5	14,14,15	0.34	0	17,19,21	1.05	2 (11%)
5	NAG	P	2	5	14,14,15	0.51	0	17,19,21	0.81	0

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	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	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	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1
3	MAN	D	8	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	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

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

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

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	4	MAN	O5-C1-C2	-3.28	105.71	110.77
3	D	5	MAN	O5-C5-C6	3.13	112.11	107.20
6	H	9	MAN	O5-C1-C2	-3.09	106.00	110.77
3	M	1	NAG	O4-C4-C5	-3.05	101.72	109.30
6	H	4	MAN	O5-C5-C6	2.89	111.74	107.20
5	P	1	NAG	C1-O5-C5	2.69	115.84	112.19
6	H	1	NAG	C1-C2-N2	2.68	115.06	110.49
7	I	2	NAG	O4-C4-C3	-2.68	104.16	110.35
3	F	1	NAG	O4-C4-C5	-2.65	102.72	109.30
6	H	2	NAG	O4-C4-C3	-2.62	104.29	110.35
5	G	2	NAG	C1-O5-C5	2.61	115.73	112.19
5	P	1	NAG	O5-C1-C2	-2.61	107.16	111.29
4	E	3	BMA	C6-C5-C4	-2.56	107.01	113.00
4	L	2	NAG	C1-O5-C5	2.46	115.52	112.19
2	J	2	NAG	C1-O5-C5	2.44	115.50	112.19
6	H	5	MAN	O5-C5-C6	2.42	110.99	107.20
3	N	2	NAG	C2-N2-C7	2.41	126.33	122.90
4	L	1	NAG	C1-O5-C5	2.40	115.44	112.19
7	I	3	BMA	O5-C5-C6	2.38	110.93	107.20
8	K	4	MAN	O2-C2-C1	-2.37	104.31	109.15
3	N	2	NAG	O4-C4-C3	-2.30	105.02	110.35
3	N	7	MAN	O5-C1-C2	-2.29	107.23	110.77
4	E	3	BMA	C3-C4-C5	2.29	114.32	110.24
6	H	5	MAN	O5-C1-C2	-2.27	107.27	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	8	MAN	O5-C1-C2	-2.26	107.28	110.77
2	C	2	NAG	O5-C5-C6	2.23	110.69	107.20
6	H	9	MAN	C1-O5-C5	2.22	115.20	112.19
4	E	3	BMA	O5-C5-C6	2.19	110.63	107.20
8	K	4	MAN	O5-C1-C2	-2.13	107.48	110.77
8	K	1	NAG	C4-C3-C2	-2.13	107.89	111.02
3	F	3	BMA	O3-C3-C4	-2.13	105.43	110.35
3	F	4	MAN	O6-C6-C5	-2.12	104.01	111.29
3	N	5	MAN	O5-C1-C2	-2.11	107.51	110.77
7	I	1	NAG	C2-N2-C7	2.07	125.86	122.90
8	K	3	BMA	O5-C5-C6	2.04	110.40	107.20
3	D	7	MAN	O5-C5-C6	2.04	110.40	107.20
3	D	3	BMA	O5-C1-C2	-2.03	107.63	110.77
8	K	4	MAN	O5-C5-C6	2.02	110.37	107.20
3	M	4	MAN	O6-C6-C5	-2.01	104.39	111.29
3	D	3	BMA	O3-C3-C4	-2.01	105.71	110.35
3	M	8	MAN	O5-C1-C2	-2.01	107.68	110.77
4	E	3	BMA	O4-C4-C3	-2.00	105.71	110.35

There are no chirality outliers.

All (28) torsion outliers are listed below:

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

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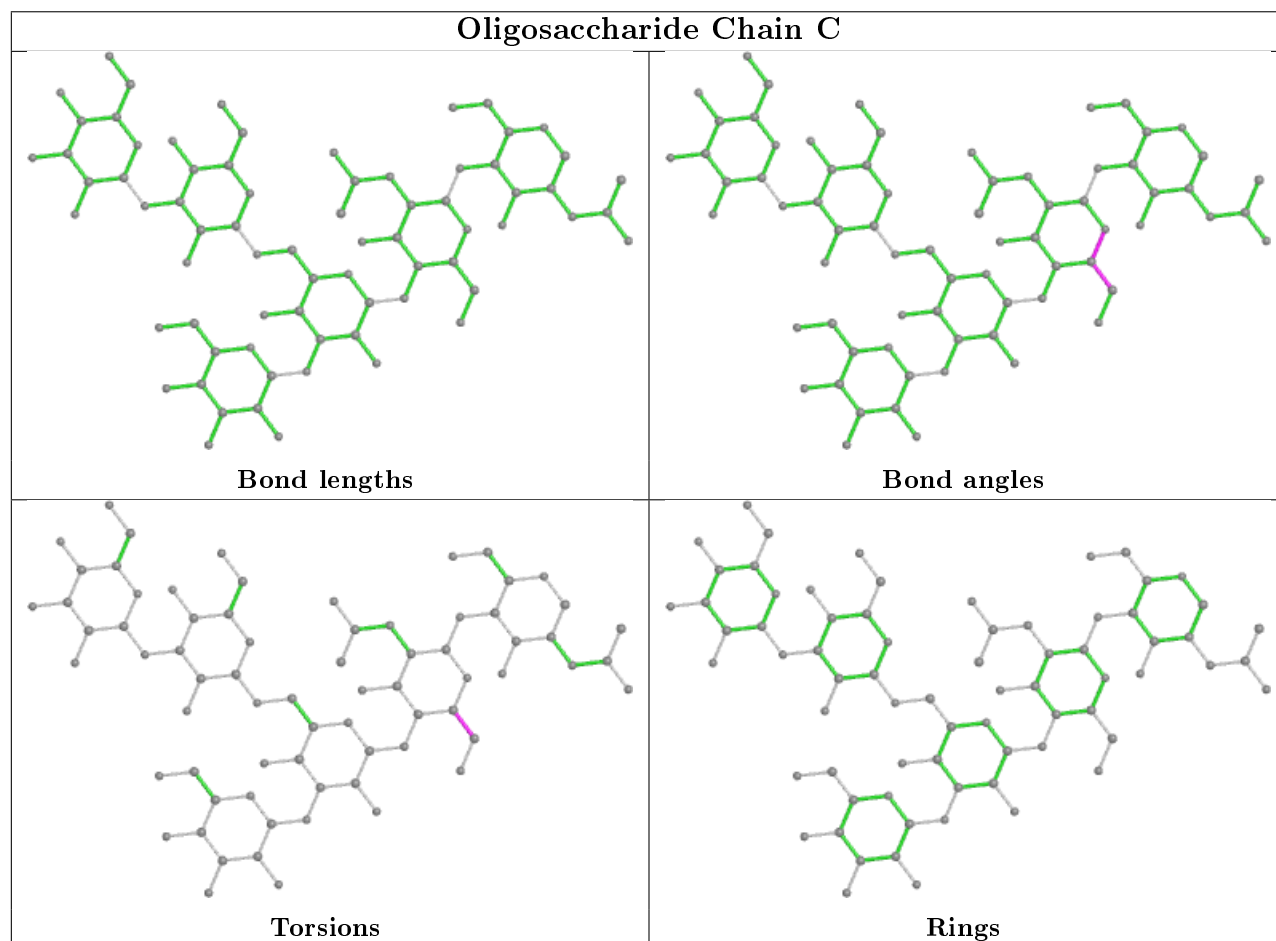
Mol	Chain	Res	Type	Atoms
3	D	4	MAN	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
3	N	6	MAN	O5-C5-C6-O6
3	F	8	MAN	O5-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
2	J	5	MAN	O5-C5-C6-O6
4	L	3	BMA	C4-C5-C6-O6

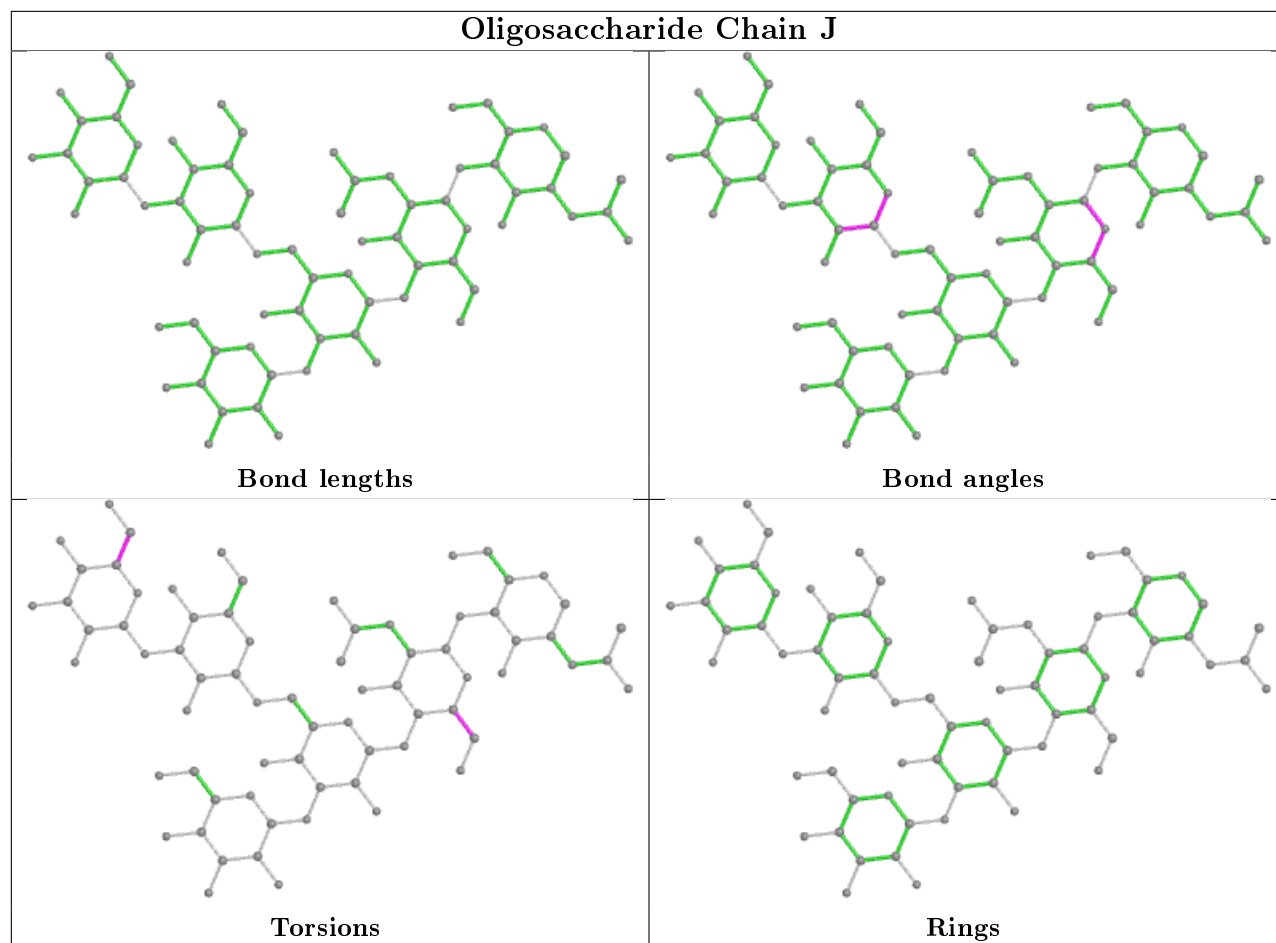
There are no ring outliers.

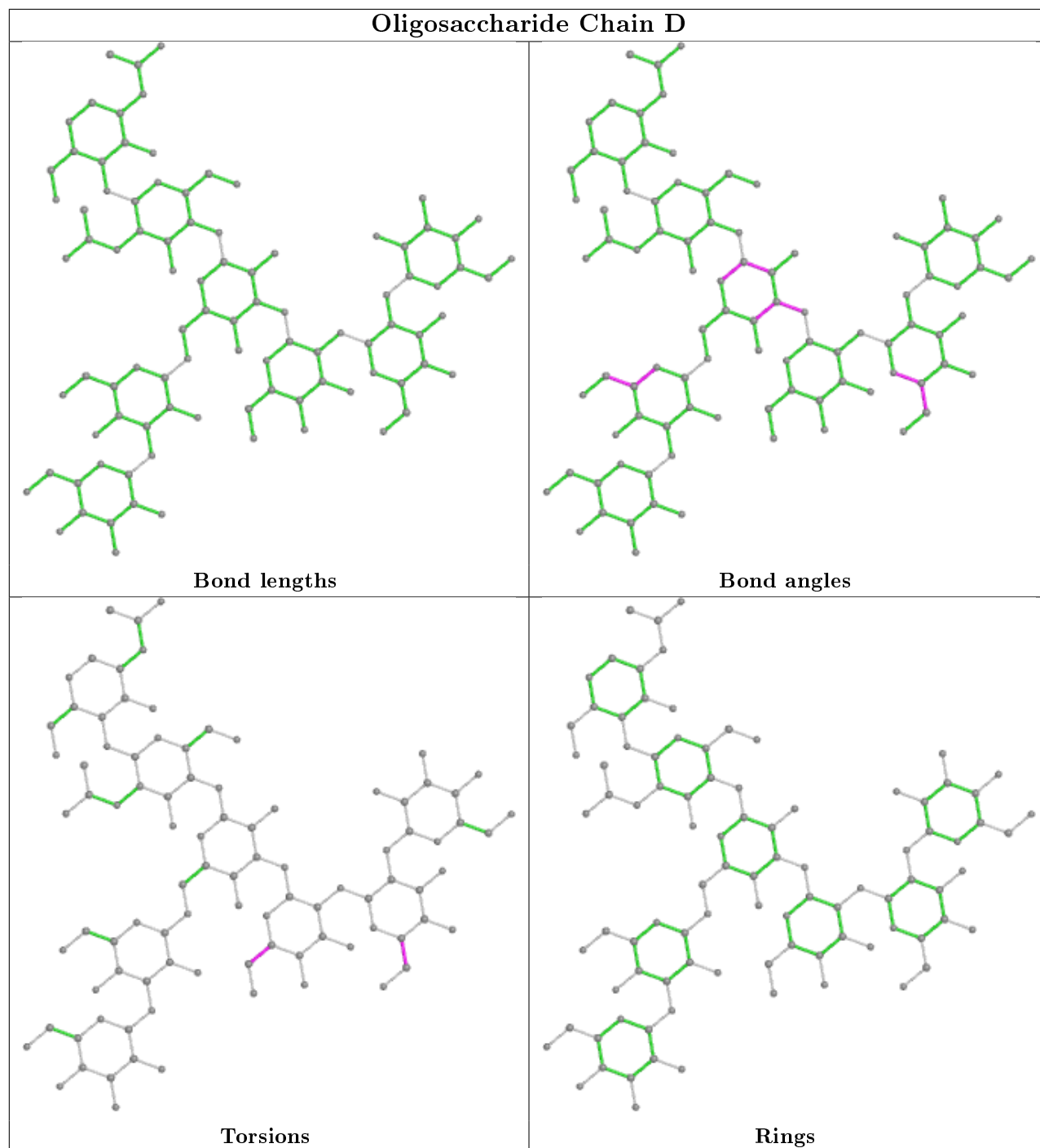
1 monomer is involved in 1 short contact:

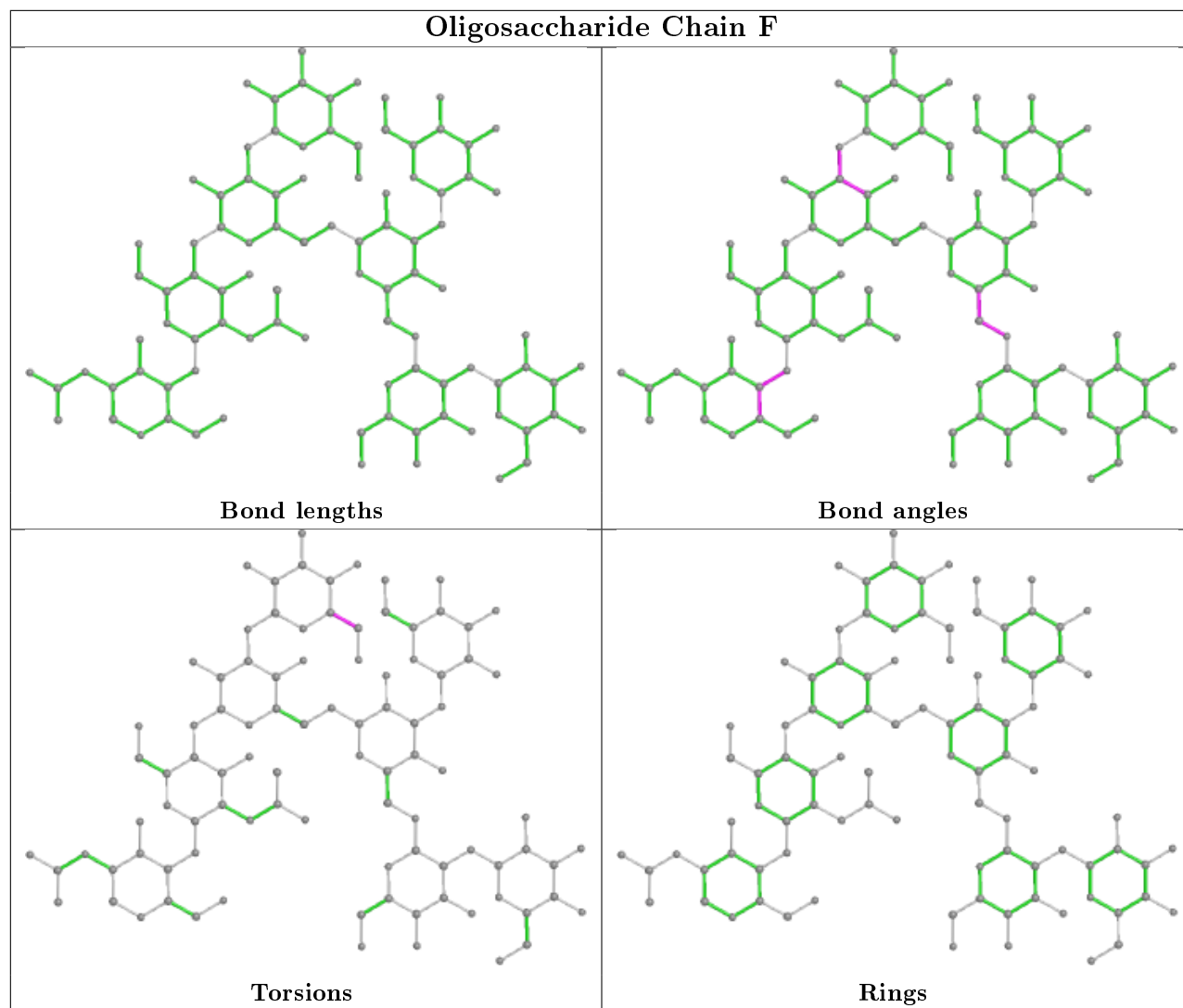
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2	NAG	1	0

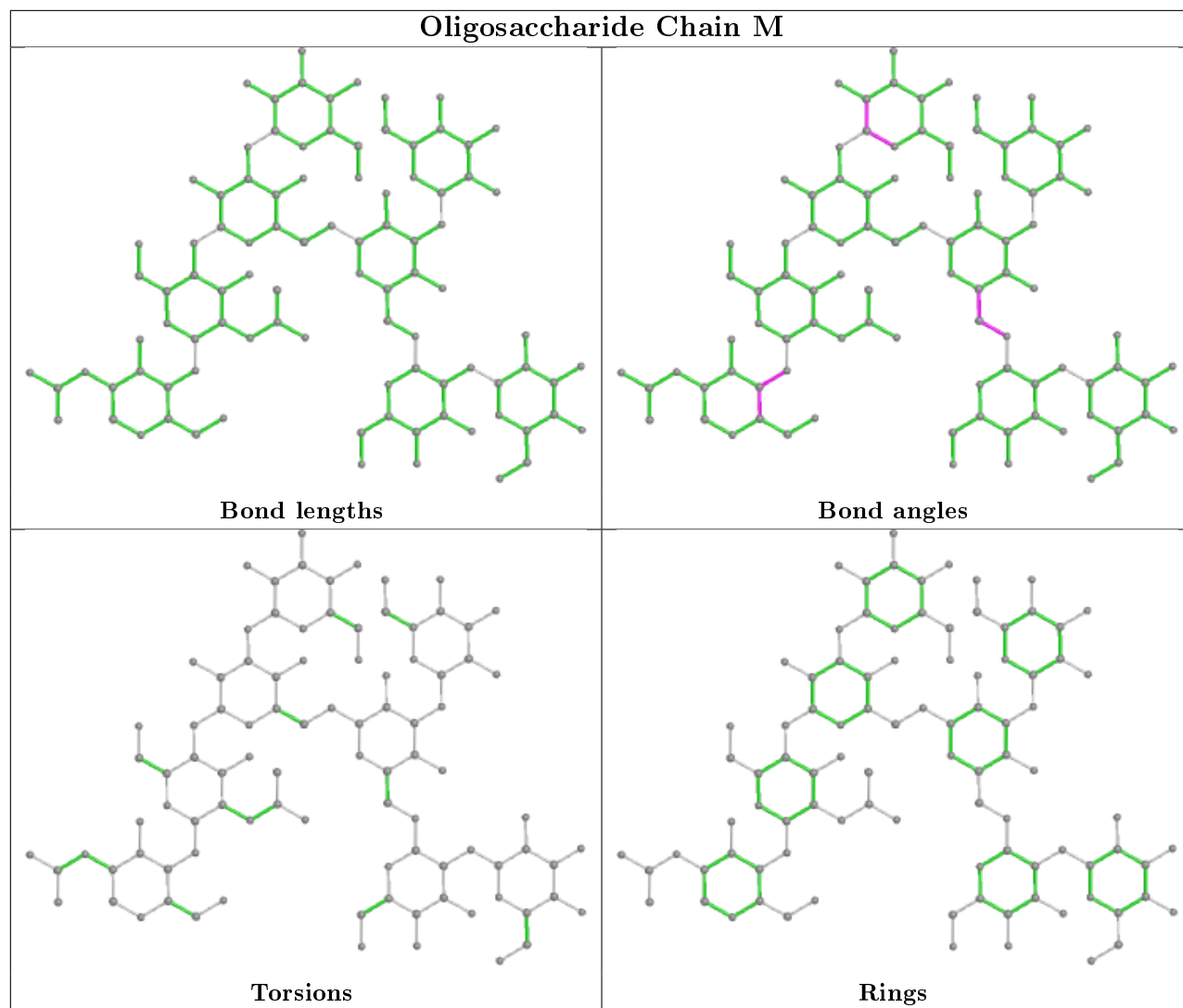
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

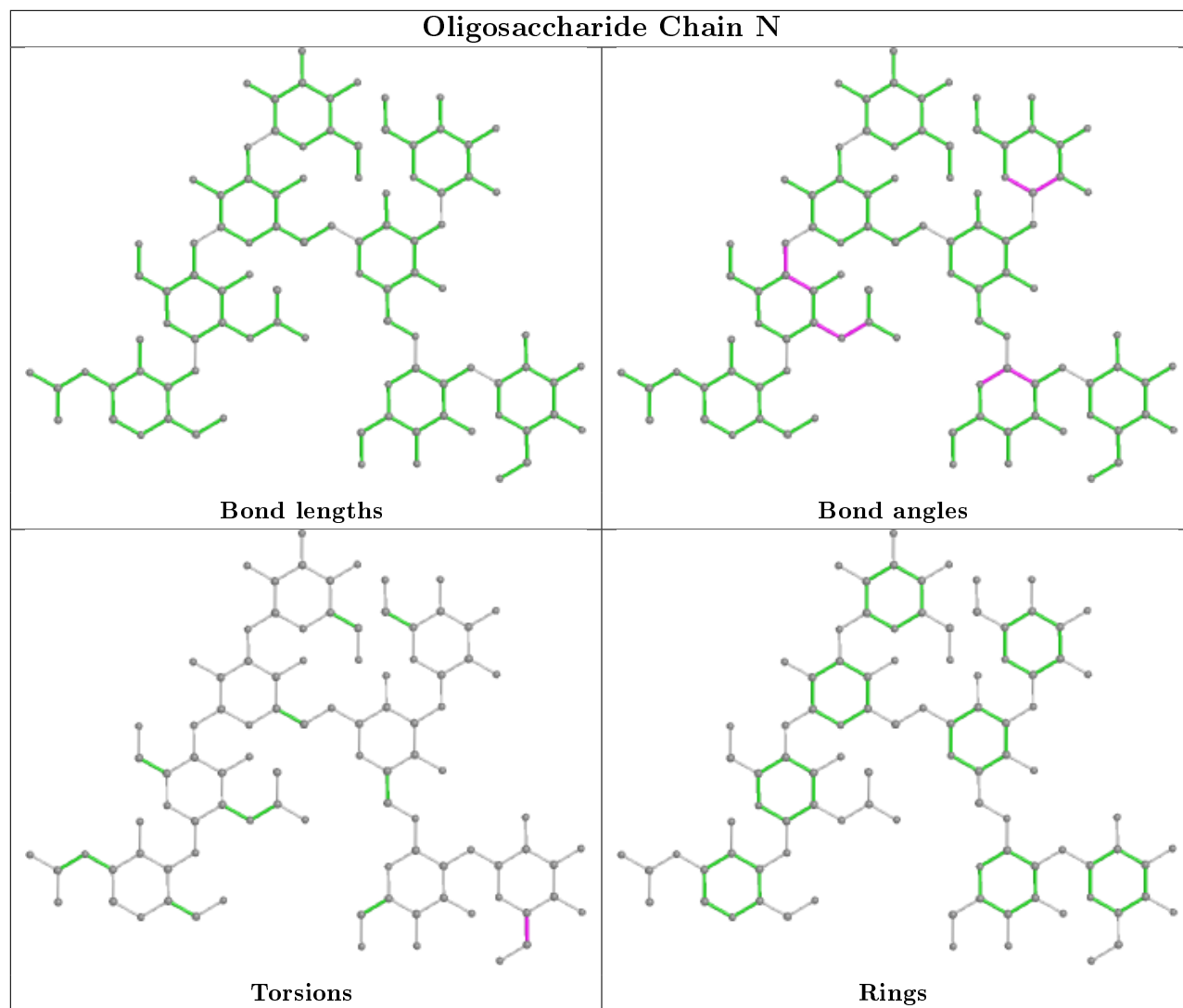


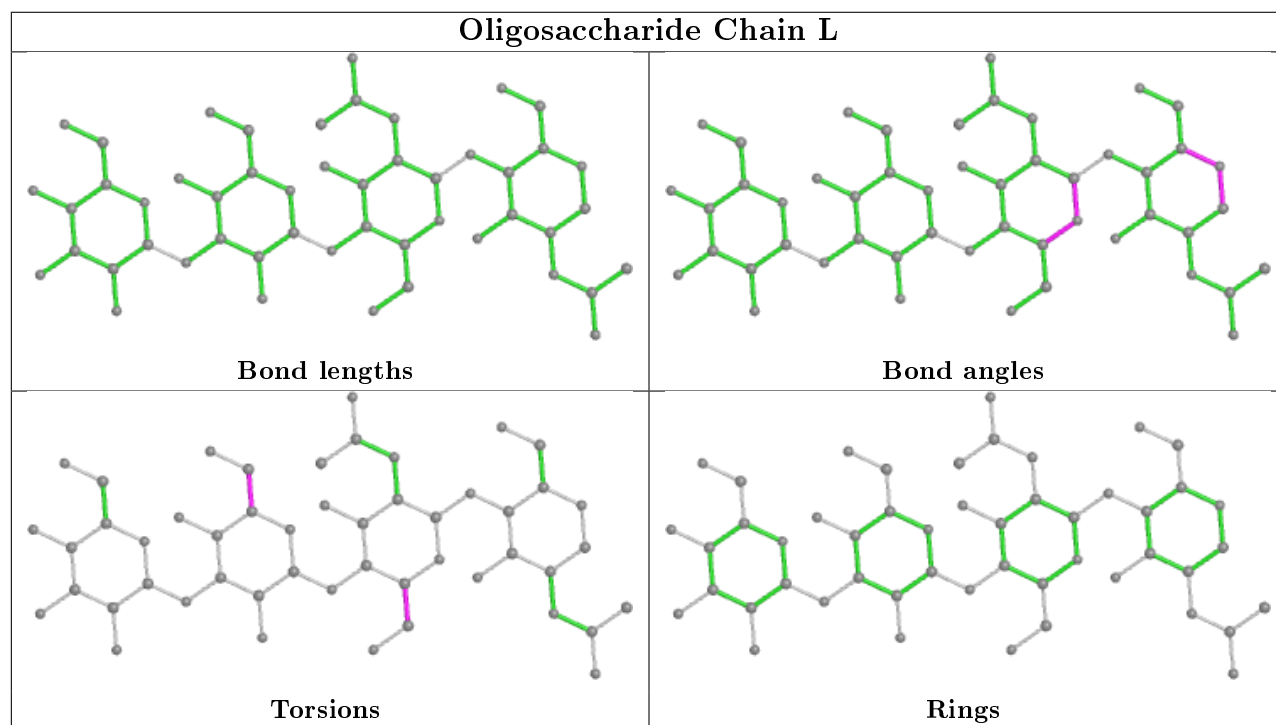
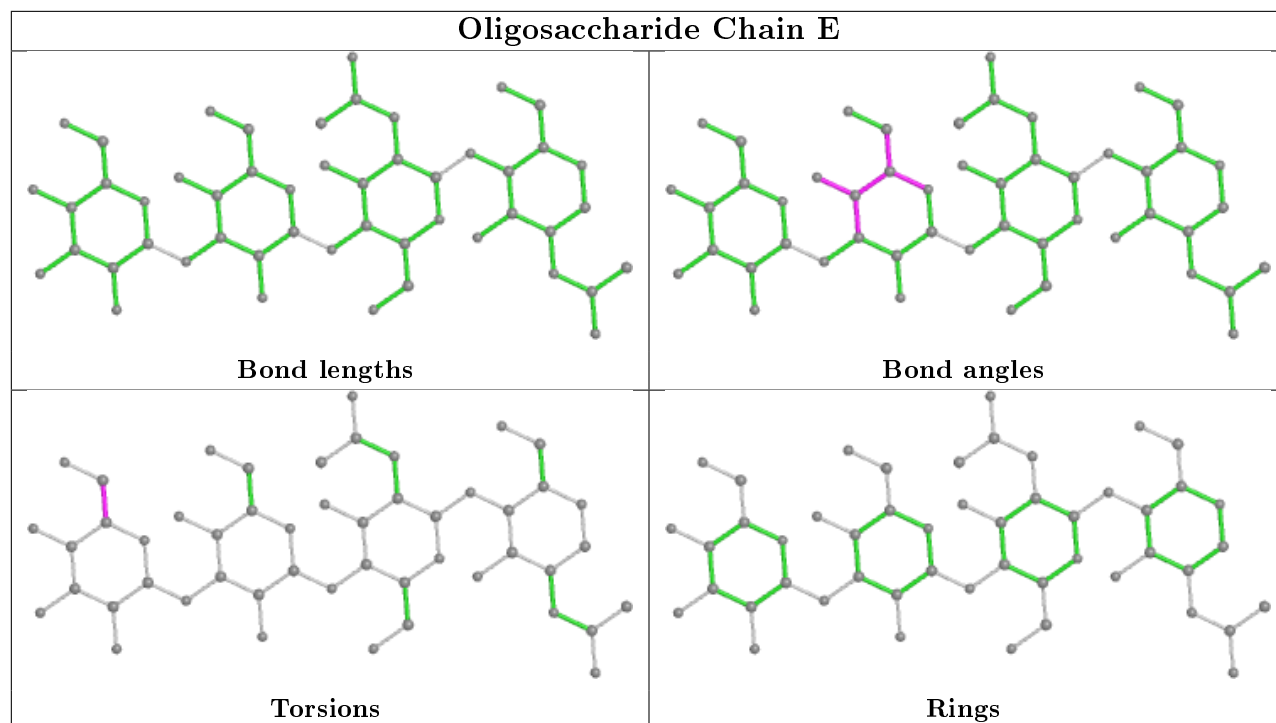


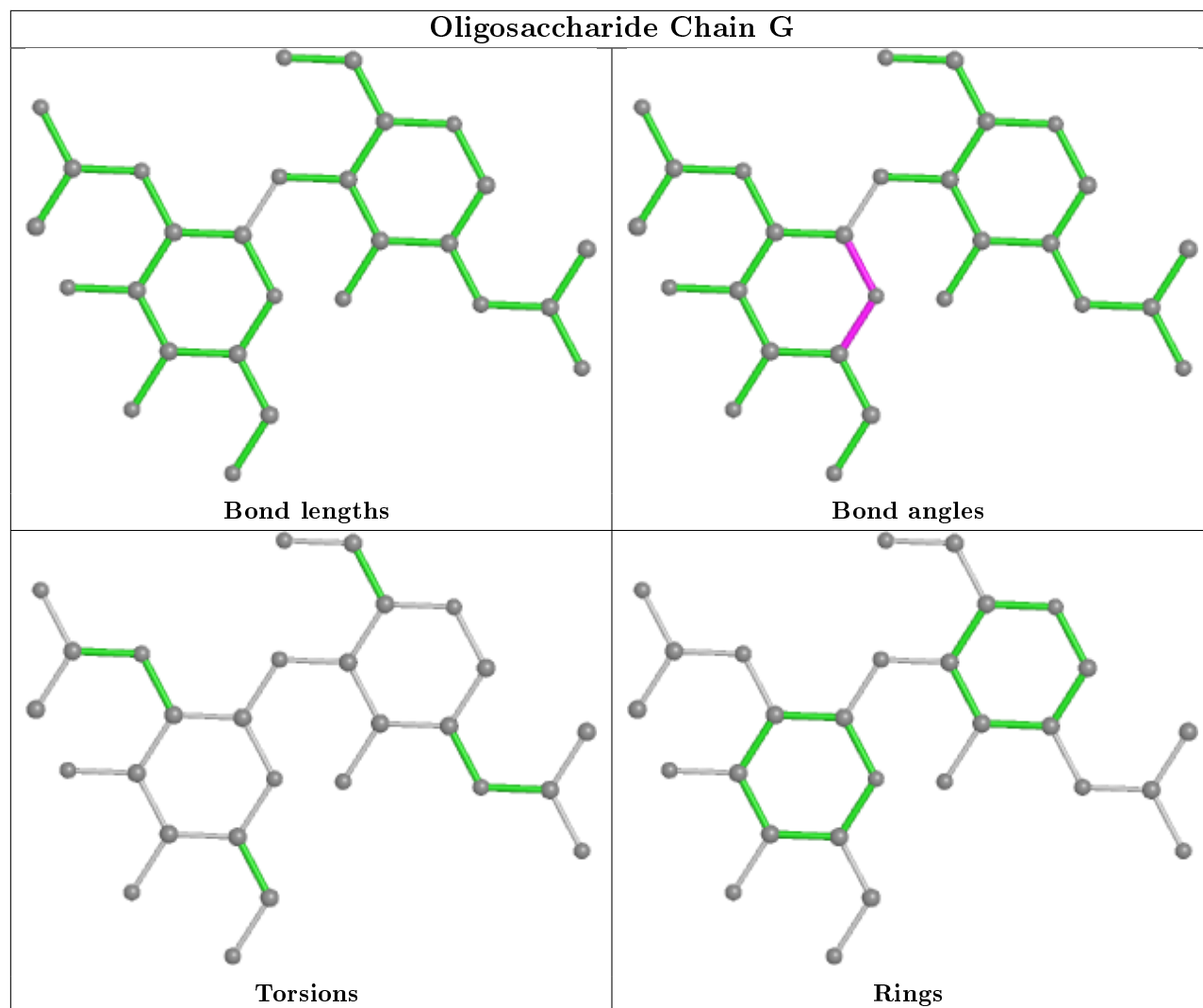


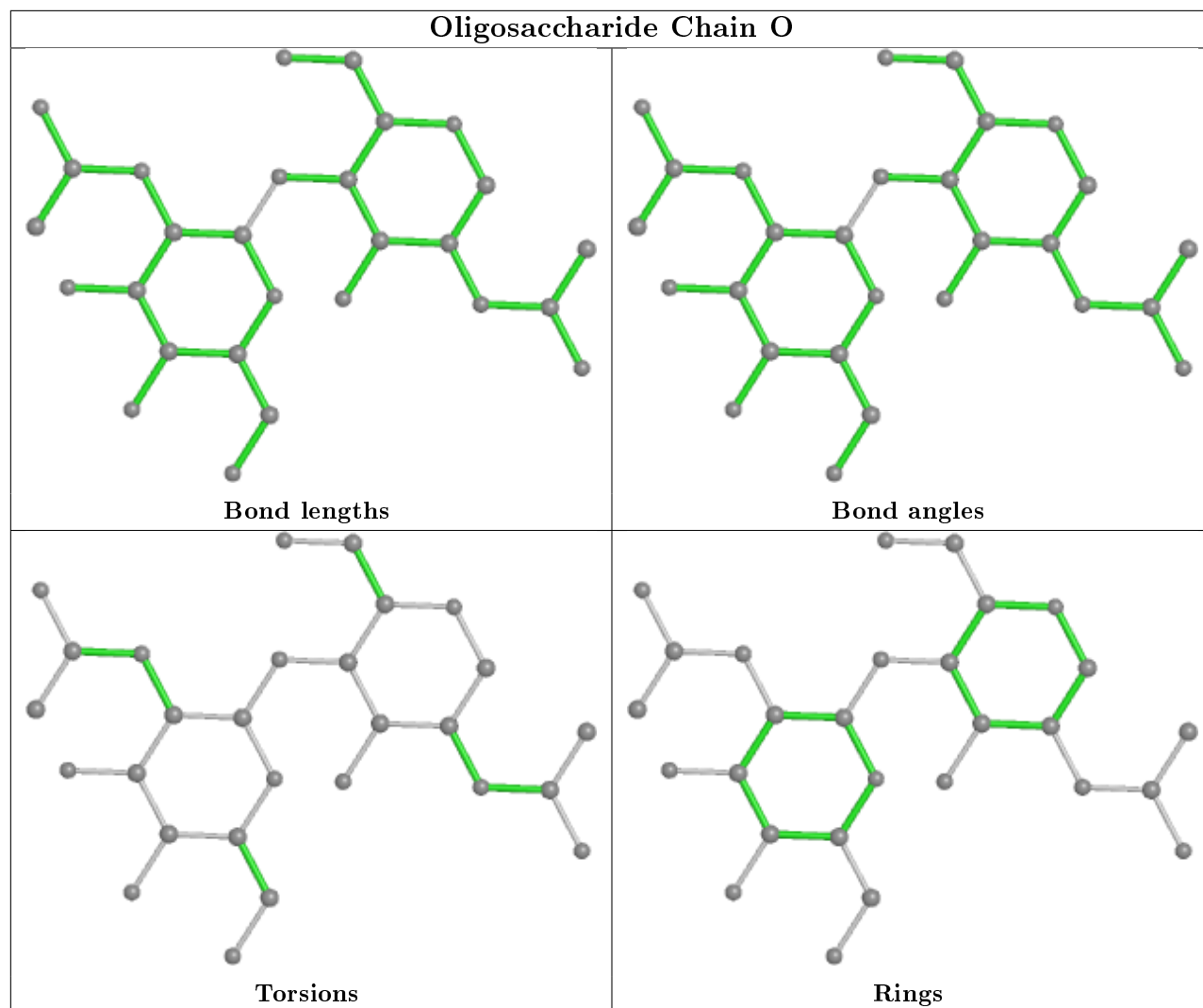


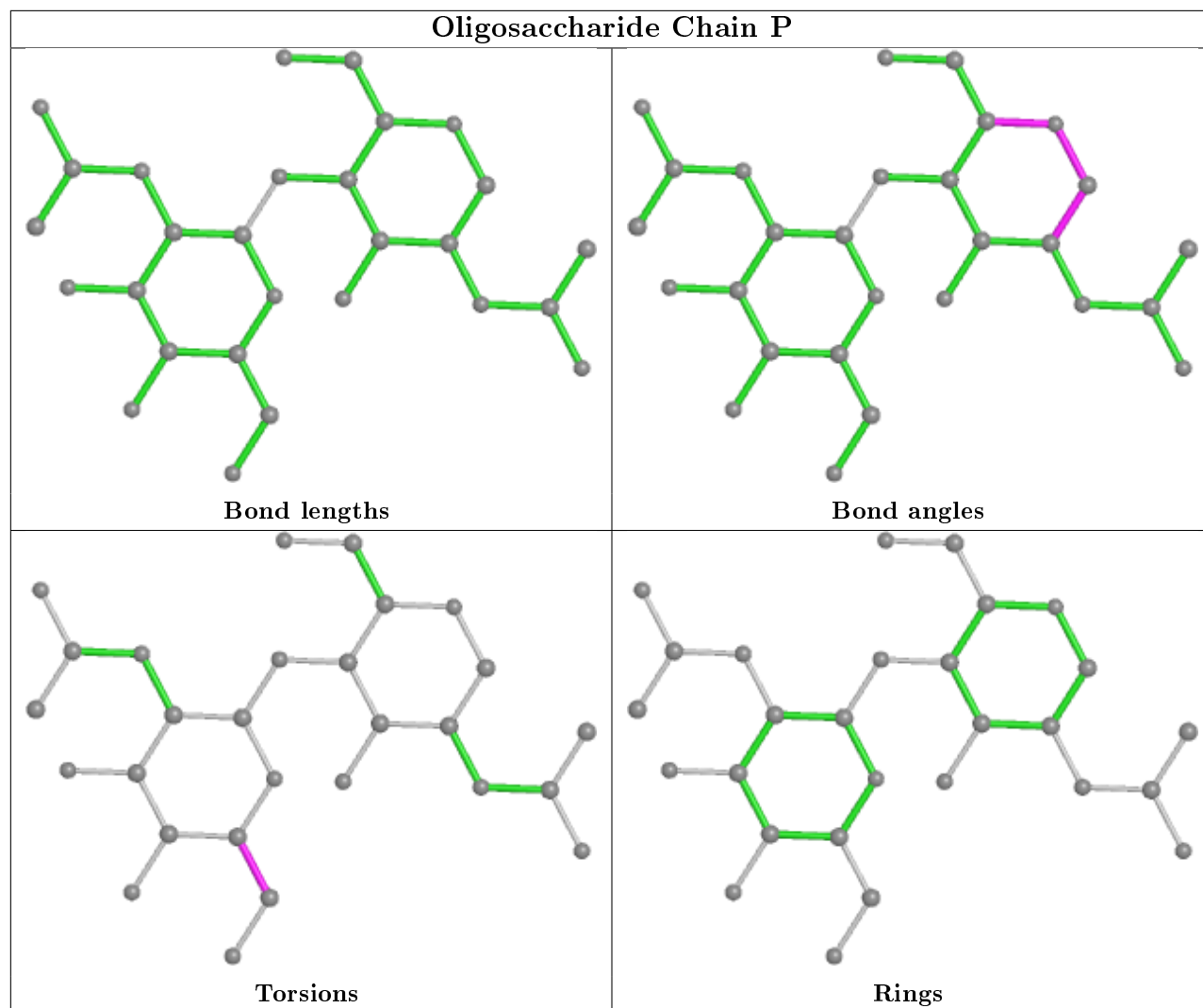


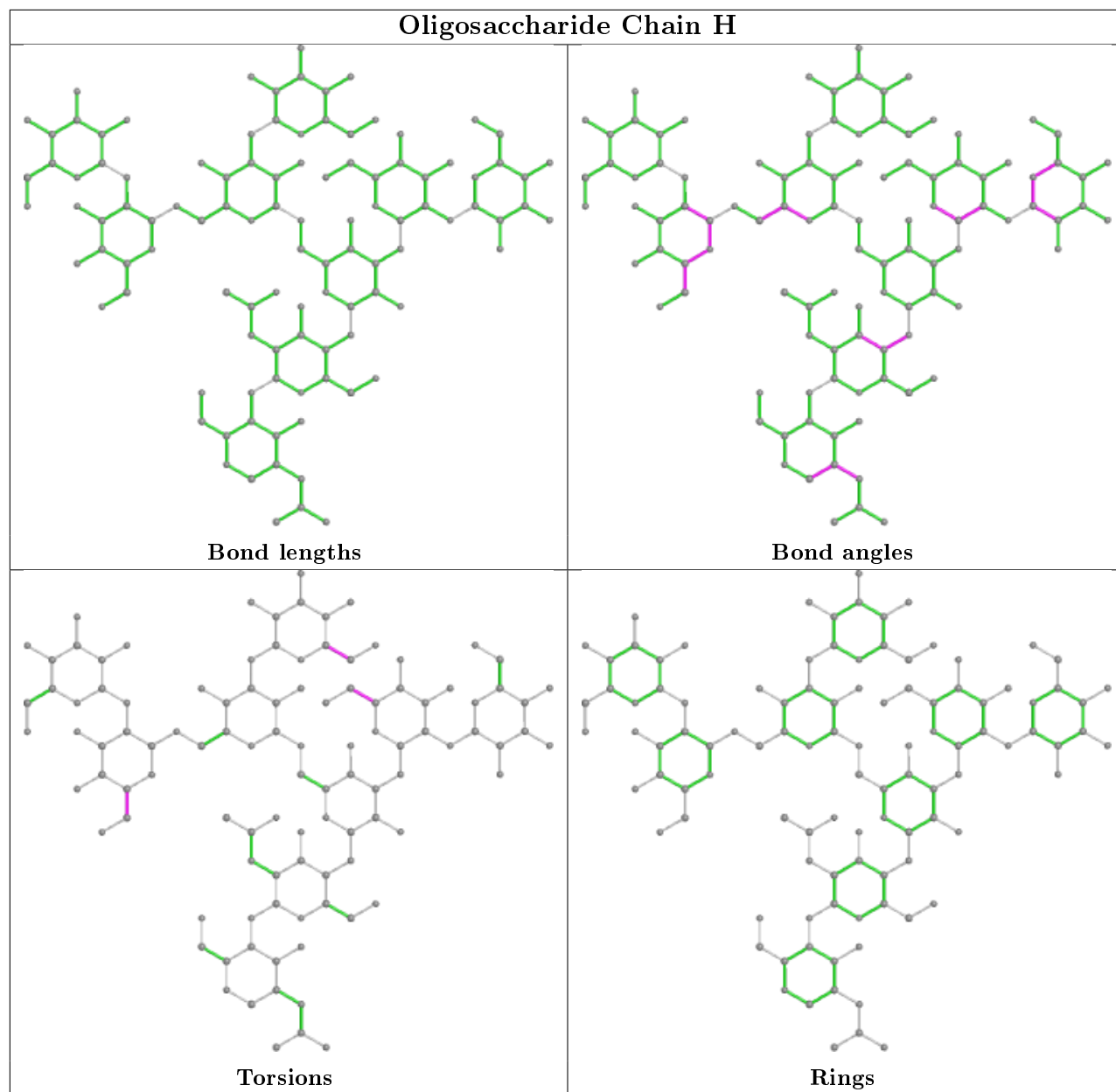


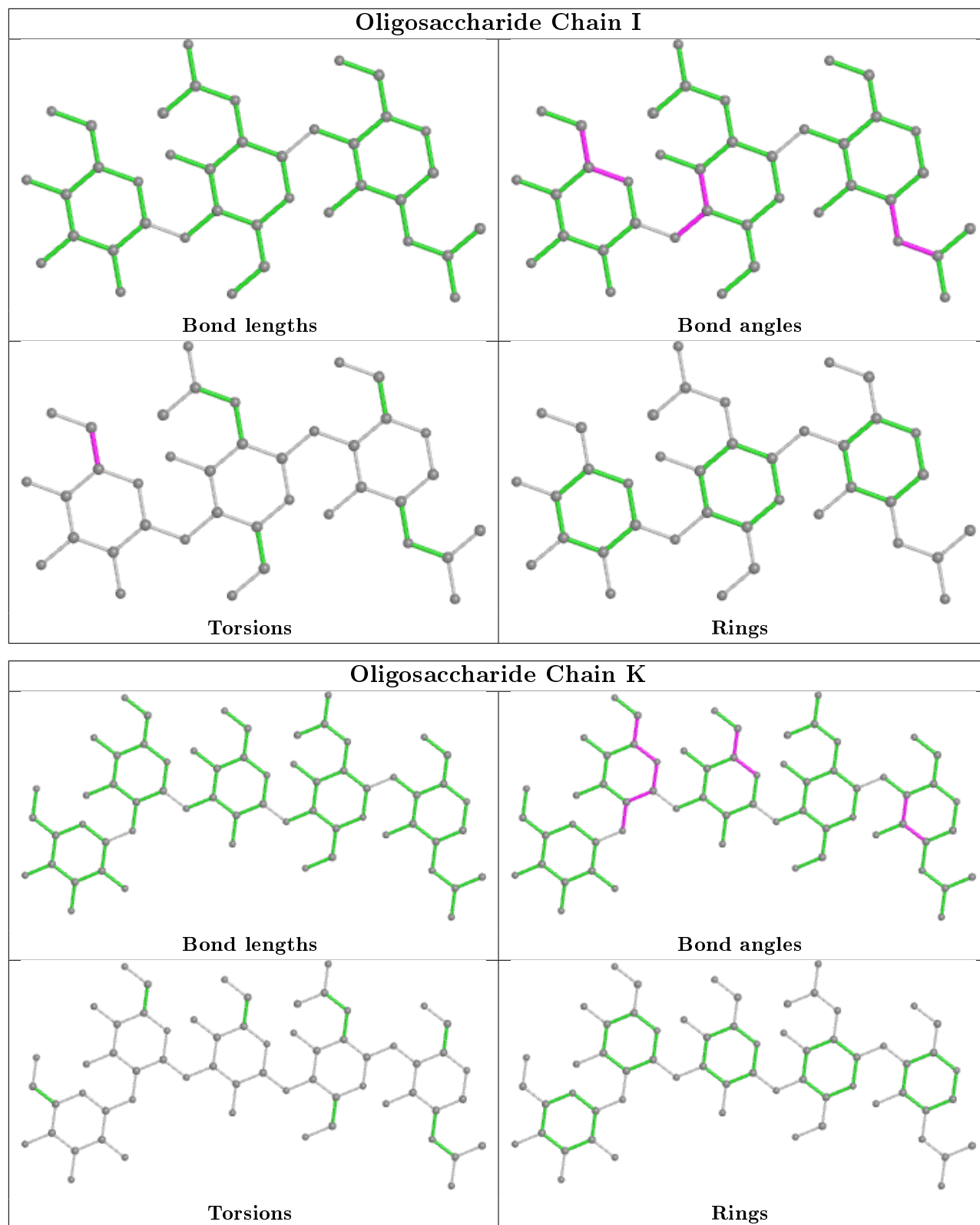












5.6 Ligand geometry ⓘ

8 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	NAG	A	1129	1	14,14,15	0.65	0	17,19,21	1.22	2 (11%)
9	NAG	A	1108	1	14,14,15	0.55	0	17,19,21	1.58	3 (17%)
9	NAG	A	1145	1	14,14,15	0.33	0	17,19,21	1.12	1 (5%)
9	NAG	B	1134	1	14,14,15	0.50	0	17,19,21	1.40	2 (11%)
9	NAG	A	1107	1	14,14,15	0.29	0	17,19,21	0.73	0
9	NAG	A	1141	1	14,14,15	0.56	0	17,19,21	1.05	0
9	NAG	B	1124	1	14,14,15	0.49	0	17,19,21	1.05	0
9	NAG	B	1125	1	14,14,15	0.35	0	17,19,21	0.65	0

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	NAG	A	1129	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1108	1	-	2/6/23/26	0/1/1/1
9	NAG	A	1145	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1134	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1107	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1141	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1124	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1125	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1108	NAG	C2-N2-C7	3.98	128.56	122.90
9	B	1134	NAG	C1-O5-C5	3.80	117.34	112.19
9	A	1129	NAG	C1-O5-C5	3.35	116.73	112.19
9	B	1134	NAG	O5-C1-C2	-3.09	106.41	111.29
9	A	1145	NAG	C1-O5-C5	2.98	116.23	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1108	NAG	C8-C7-N2	2.64	120.57	116.10
9	A	1129	NAG	C2-N2-C7	2.41	126.33	122.90
9	A	1108	NAG	O7-C7-C8	-2.09	118.17	122.06

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1141	NAG	O5-C5-C6-O6
9	A	1141	NAG	C4-C5-C6-O6
9	A	1108	NAG	C8-C7-N2-C2
9	A	1108	NAG	O7-C7-N2-C2
9	B	1124	NAG	O5-C5-C6-O6
9	B	1124	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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	842/857 (98%)	-0.32	5 (0%) 89 89	17, 26, 39, 55	0
1	B	841/857 (98%)	-0.12	19 (2%) 60 63	25, 42, 62, 81	0
All	All	1683/1714 (98%)	-0.22	24 (1%) 75 77	17, 33, 57, 81	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	17	LEU	4.2
1	B	774	LYS	4.0
1	B	775	VAL	3.2
1	B	761	ILE	3.2
1	B	666	GLY	3.2
1	B	665	VAL	3.0
1	B	667	GLU	2.9
1	B	807	PRO	2.9
1	B	638	ALA	2.9
1	B	664	GLN	2.8
1	A	346	ASP	2.6
1	B	663	HIS	2.5
1	B	368	ARG	2.3
1	B	636	ALA	2.3
1	A	696	ALA	2.3
1	B	662	LYS	2.2
1	B	80	GLY	2.2
1	B	661	GLU	2.2
1	B	140	VAL	2.2
1	A	664	GLN	2.1
1	A	666	GLY	2.1
1	B	511	ASP	2.1
1	B	19	TYR	2.1
1	A	137	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

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
4	MAN	E	4	11/12	0.74	0.23	61,63,65,65	0
2	MAN	C	6	11/12	0.79	0.22	65,68,69,70	0
6	MAN	H	9	11/12	0.79	0.41	64,66,67,67	0
3	MAN	D	6	11/12	0.80	0.24	60,63,65,65	0
3	MAN	D	7	11/12	0.81	0.26	50,51,53,54	0
4	BMA	E	3	11/12	0.82	0.19	48,53,55,57	0
7	BMA	I	3	11/12	0.82	0.22	50,53,55,56	0
2	MAN	J	6	11/12	0.83	0.34	67,70,72,73	0
8	MAN	K	5	11/12	0.83	0.16	64,66,68,69	0
6	MAN	H	7	11/12	0.84	0.33	54,55,57,58	0
5	NAG	O	2	14/15	0.84	0.23	57,59,62,62	0
4	BMA	L	3	11/12	0.85	0.17	68,73,76,76	0
5	NAG	G	2	14/15	0.86	0.29	44,48,49,50	0
3	MAN	N	8	11/12	0.86	0.39	65,68,69,70	0
3	MAN	N	6	11/12	0.86	0.20	47,50,50,50	0
2	MAN	C	5	11/12	0.86	0.31	63,64,66,66	0
3	BMA	N	3	11/12	0.87	0.27	53,55,57,61	0
8	MAN	K	4	11/12	0.87	0.24	61,63,64,64	0
3	MAN	D	8	11/12	0.87	0.33	56,58,58,59	0
5	NAG	P	2	14/15	0.88	0.34	73,75,76,77	0
3	MAN	N	5	11/12	0.88	0.30	51,54,56,57	0
2	MAN	C	4	11/12	0.88	0.20	62,65,67,68	0
2	MAN	J	5	11/12	0.88	0.30	57,58,59,59	0
8	BMA	K	3	11/12	0.88	0.19	60,62,63,63	0
6	MAN	H	5	11/12	0.88	0.18	46,47,50,50	0
6	MAN	H	8	11/12	0.89	0.32	52,55,57,59	0
4	MAN	L	4	11/12	0.89	0.22	78,79,80,80	0
8	NAG	K	1	14/15	0.90	0.13	49,51,55,56	0
3	NAG	N	1	14/15	0.90	0.24	44,46,49,50	0
3	NAG	M	1	14/15	0.90	0.13	46,48,50,51	0
5	NAG	O	1	14/15	0.90	0.11	46,47,50,54	0
5	NAG	P	1	14/15	0.90	0.22	64,66,67,70	0

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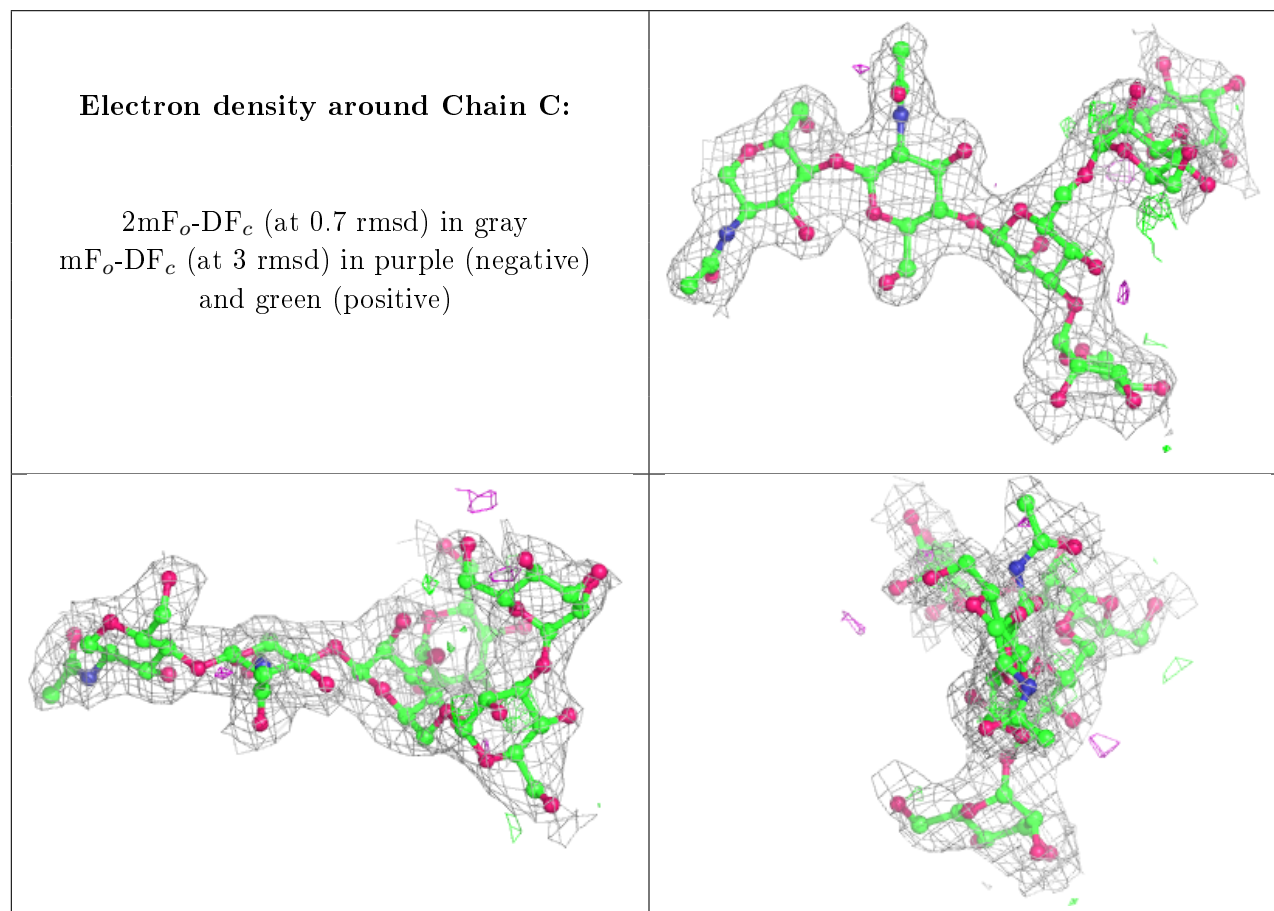
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MAN	M	5	11/12	0.91	0.14	46,48,49,49	0
3	MAN	N	4	11/12	0.91	0.21	54,56,58,62	0
3	MAN	N	7	11/12	0.91	0.40	66,68,69,69	0
8	NAG	K	2	14/15	0.92	0.14	55,56,58,58	0
3	MAN	M	6	11/12	0.92	0.16	49,49,51,51	0
2	MAN	J	4	11/12	0.92	0.24	56,57,59,60	0
3	MAN	D	5	11/12	0.92	0.15	48,49,51,56	0
6	MAN	H	6	11/12	0.92	0.16	44,45,46,46	0
3	MAN	M	8	11/12	0.92	0.18	57,59,60,60	0
2	BMA	J	3	11/12	0.92	0.15	54,56,58,63	0
3	NAG	M	2	14/15	0.92	0.14	48,49,51,51	0
6	BMA	H	3	11/12	0.92	0.15	37,39,42,46	0
5	NAG	G	1	14/15	0.92	0.10	32,33,36,40	0
3	BMA	M	3	11/12	0.93	0.14	50,52,53,55	0
3	MAN	F	8	11/12	0.93	0.13	33,35,36,36	0
3	NAG	N	2	14/15	0.93	0.20	46,47,50,51	0
2	BMA	C	3	11/12	0.93	0.14	54,58,61,63	0
3	BMA	D	3	11/12	0.93	0.15	36,39,43,46	0
2	NAG	J	2	14/15	0.94	0.12	43,46,49,51	0
3	MAN	M	4	11/12	0.94	0.13	49,50,51,52	0
4	NAG	E	2	14/15	0.94	0.12	36,38,40,44	0
3	MAN	M	7	11/12	0.94	0.12	50,51,51,51	0
6	MAN	H	4	11/12	0.94	0.16	44,46,47,51	0
2	NAG	C	2	14/15	0.94	0.12	40,42,44,49	0
7	NAG	I	2	14/15	0.94	0.15	35,37,40,45	0
3	MAN	F	6	11/12	0.95	0.09	25,25,26,26	0
4	NAG	L	2	14/15	0.95	0.16	55,58,60,63	0
3	NAG	F	1	14/15	0.96	0.09	27,28,29,30	0
3	NAG	F	2	14/15	0.96	0.08	27,28,29,29	0
7	NAG	I	1	14/15	0.96	0.09	27,27,29,32	0
3	MAN	D	4	11/12	0.96	0.10	41,42,43,45	0
6	NAG	H	2	14/15	0.96	0.10	28,29,31,34	0
6	NAG	H	1	14/15	0.96	0.09	24,25,26,26	0
2	NAG	C	1	14/15	0.96	0.10	33,34,35,37	0
4	NAG	L	1	14/15	0.96	0.11	47,48,50,53	0
2	NAG	J	1	14/15	0.96	0.12	41,42,42,43	0
3	BMA	F	3	11/12	0.97	0.07	27,29,30,32	0
3	MAN	F	5	11/12	0.97	0.07	25,26,26,26	0
3	MAN	F	4	11/12	0.97	0.09	26,27,27,27	0
3	NAG	D	1	14/15	0.97	0.09	24,25,26,27	0
4	NAG	E	1	14/15	0.97	0.09	30,31,32,35	0
3	MAN	F	7	11/12	0.97	0.07	27,28,28,28	0

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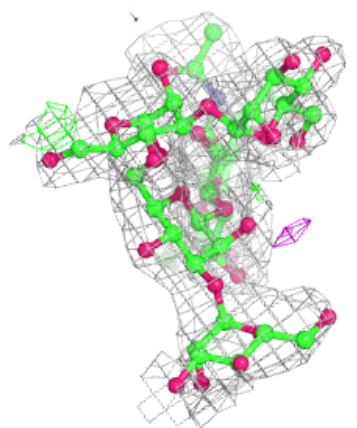
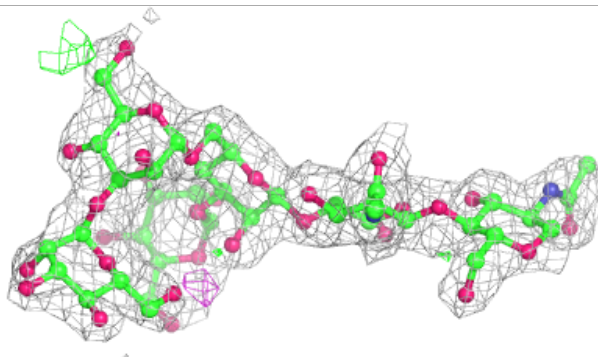
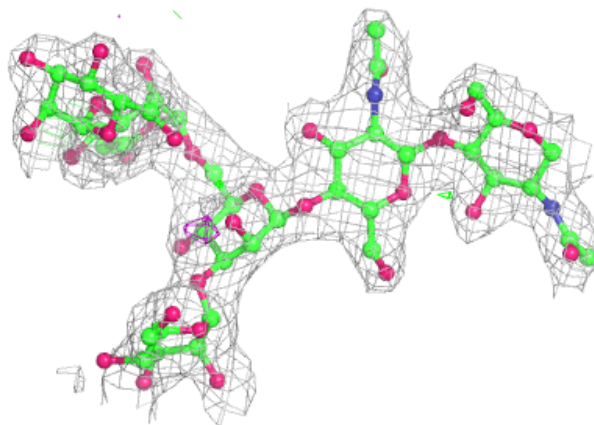
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	D	2	14/15	0.98	0.09	29,30,31,33	0

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



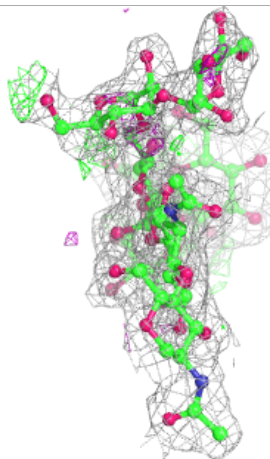
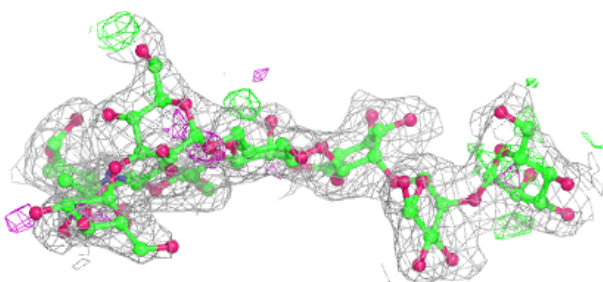
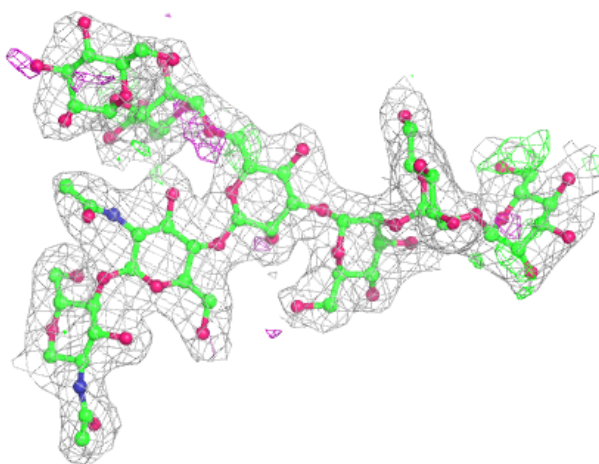
Electron density around Chain J:

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



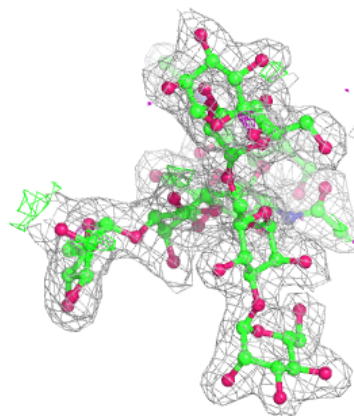
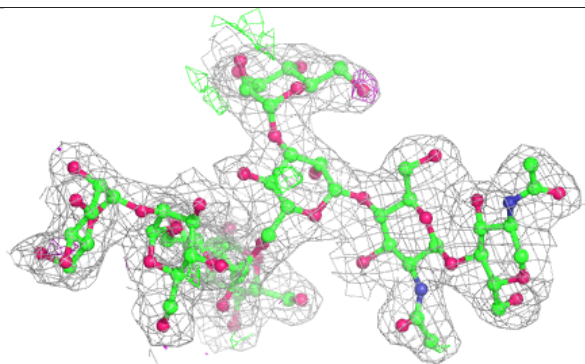
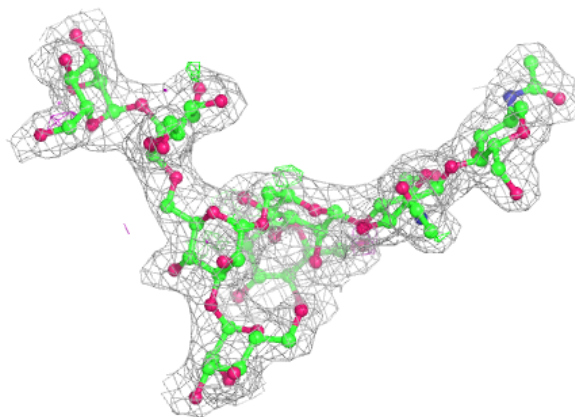
Electron density around Chain D:

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



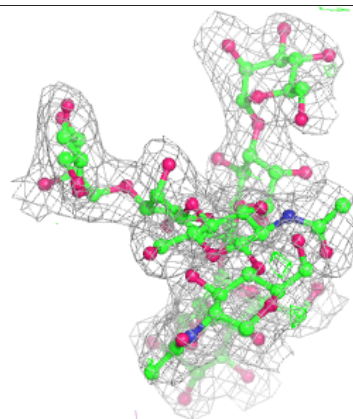
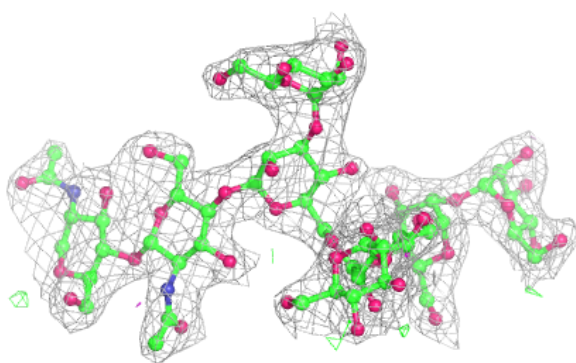
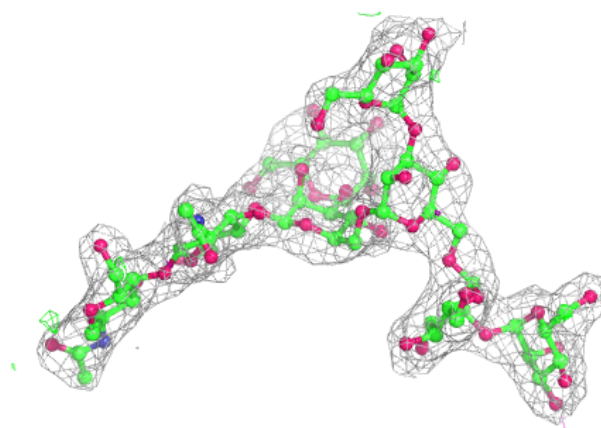
Electron density around Chain F:

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

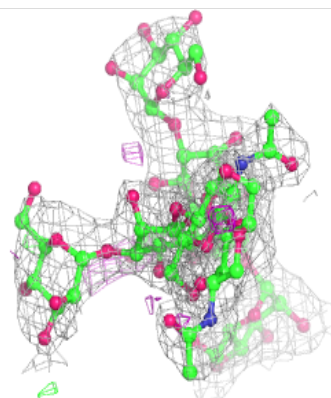
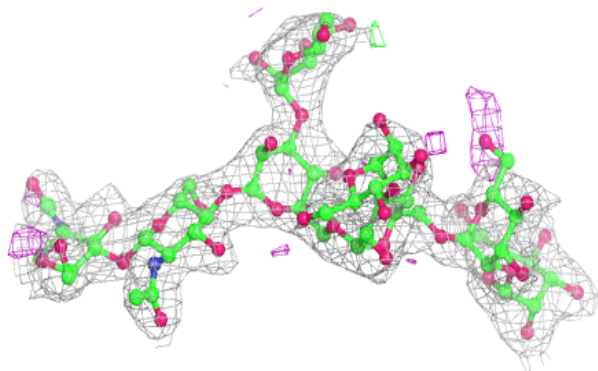
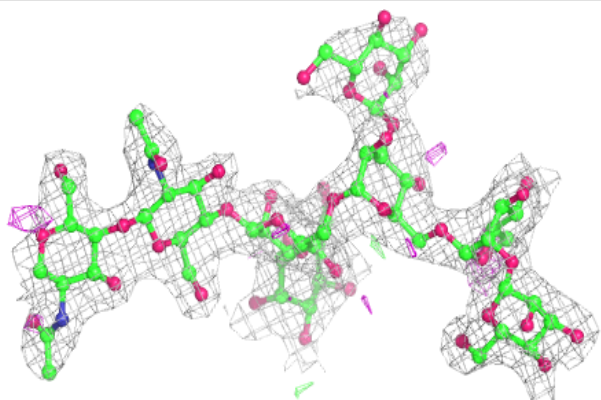


Electron density around Chain M:

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

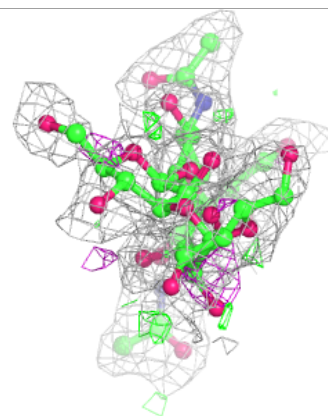
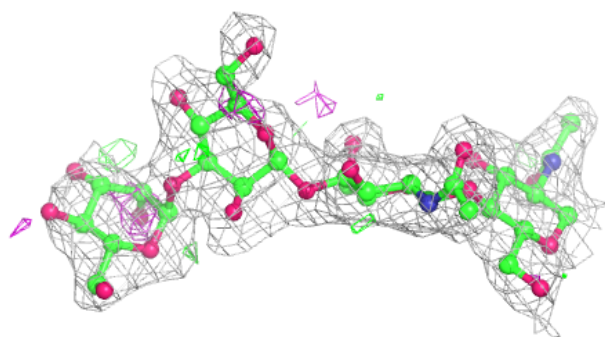
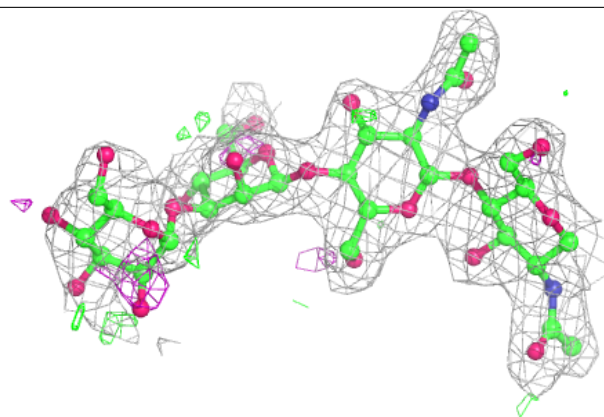
**Electron density around Chain N:**

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

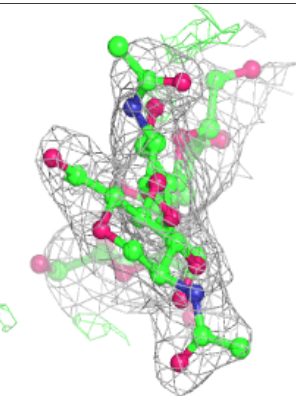
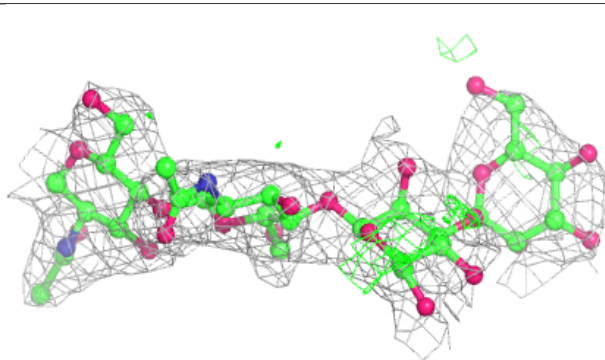
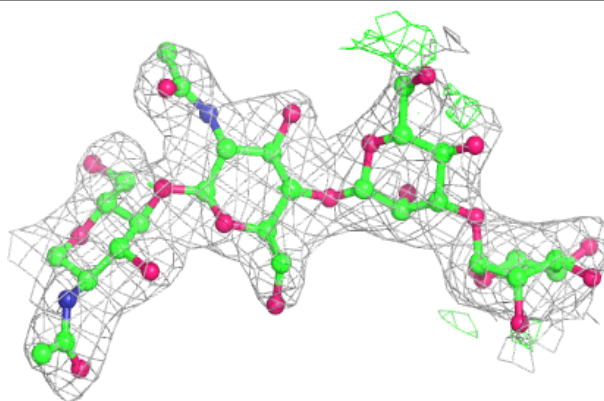


Electron density around Chain E:

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

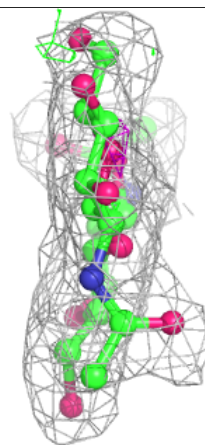
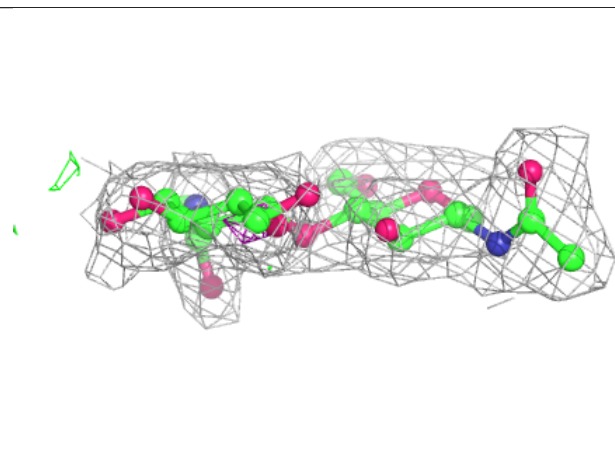
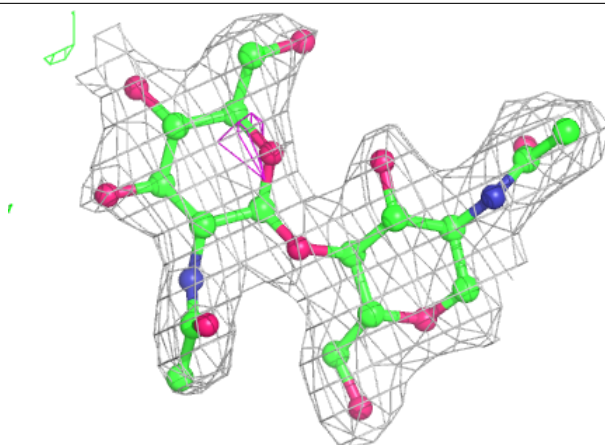
**Electron density around Chain L:**

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



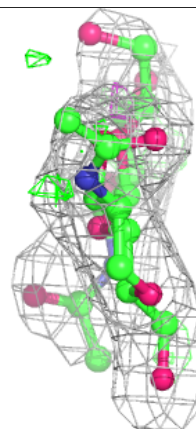
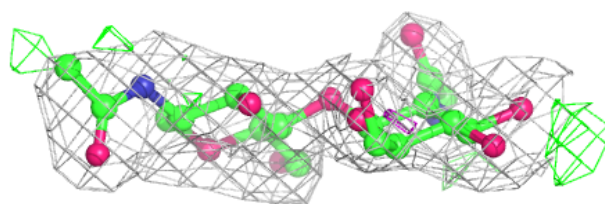
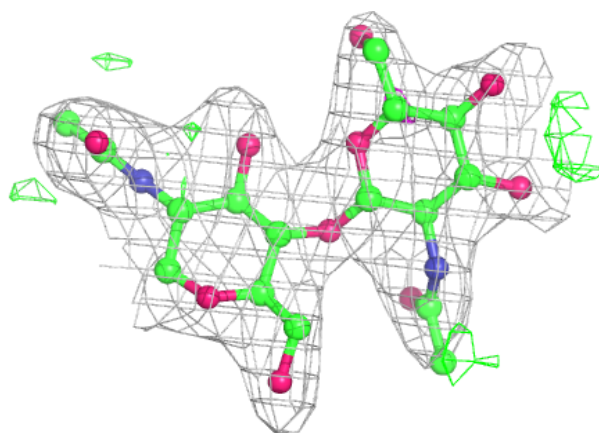
Electron density around Chain G:

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



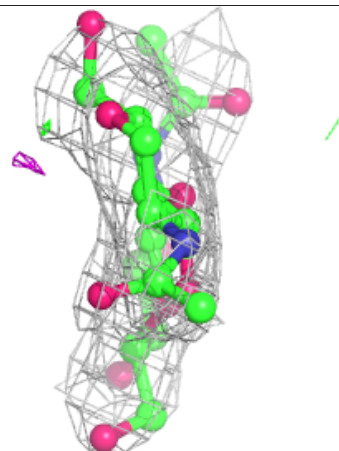
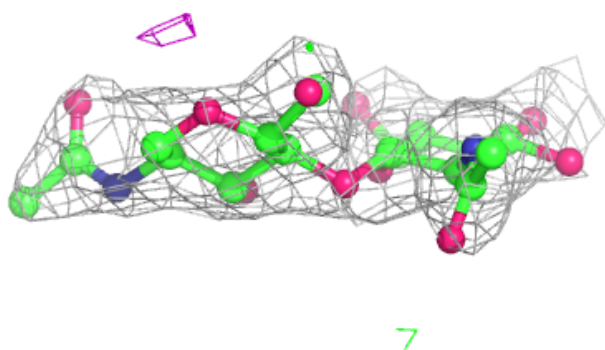
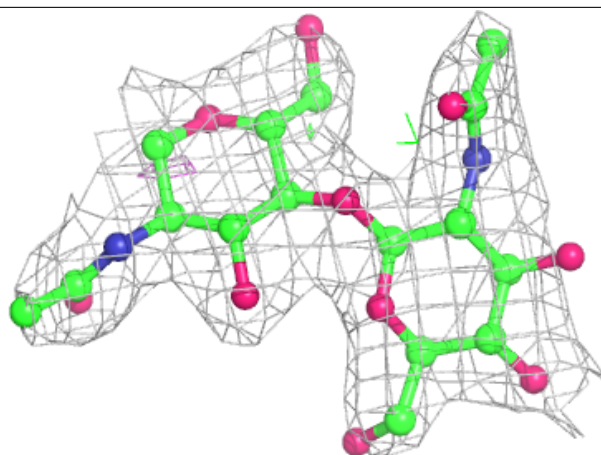
Electron density around Chain O:

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



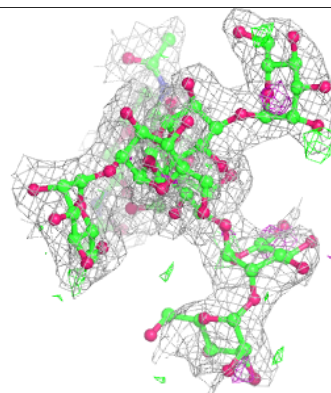
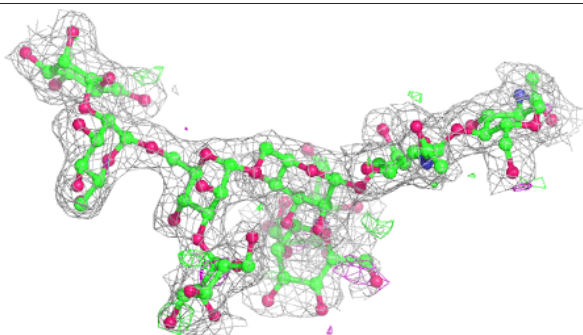
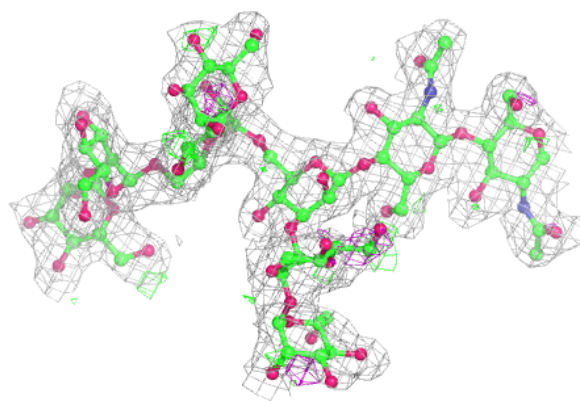
Electron density around Chain P:

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

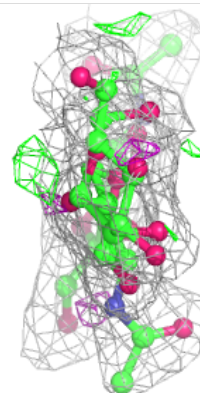
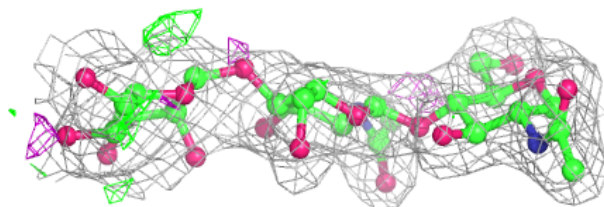
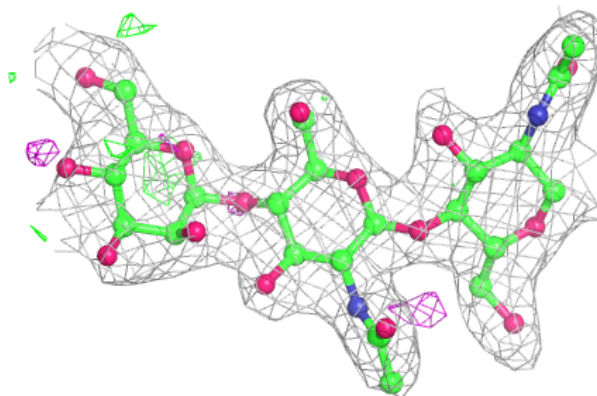


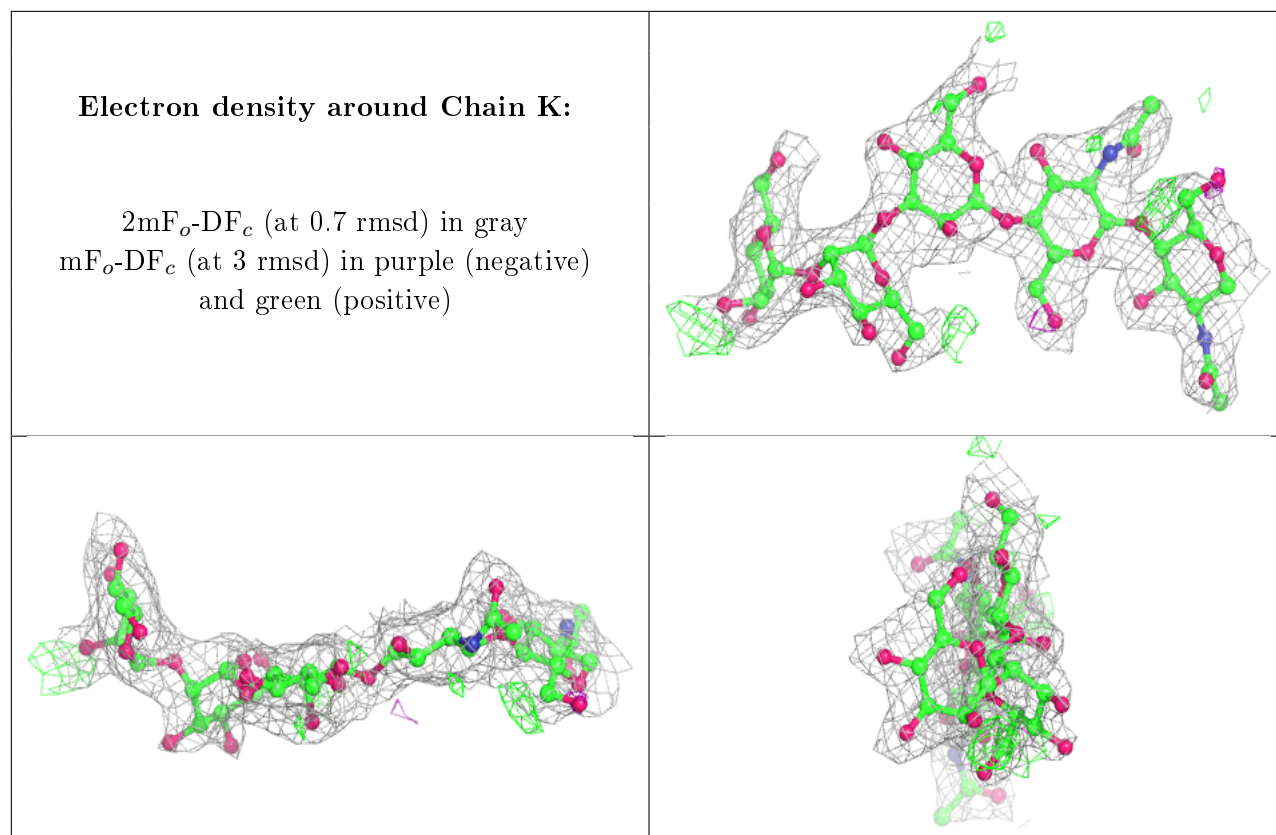
Electron density around Chain H:

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

**Electron density around Chain I:**

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
9	NAG	A	1129	14/15	0.81	0.23	41,44,47,47	0
9	NAG	B	1134	14/15	0.82	0.20	47,49,52,53	0
9	NAG	B	1124	14/15	0.87	0.18	51,53,55,55	0
9	NAG	A	1107	14/15	0.89	0.21	50,54,56,56	0
9	NAG	A	1141	14/15	0.91	0.20	30,31,33,33	0
9	NAG	A	1145	14/15	0.91	0.20	41,42,45,45	0
9	NAG	B	1125	14/15	0.91	0.12	49,51,51,53	0
9	NAG	A	1108	14/15	0.94	0.13	22,22,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.