



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 05:29 PM BST

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

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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

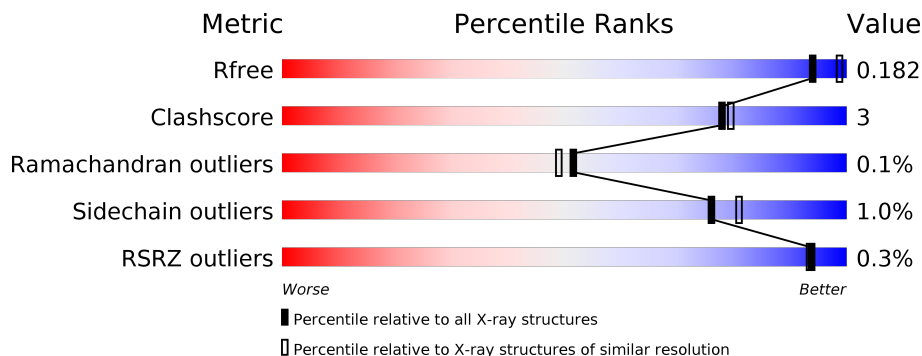
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	841	
1	B	841	
2	C	7	
2	J	7	
3	D	3	
3	G	3	

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Mol	Chain	Length	Quality of chain
3	L	3	 33% 67%
3	N	3	 100%
4	E	2	 50% 50%
5	F	10	 100%
5	M	10	 100%
6	H	7	 86% 14%
6	O	7	 71% 29%
7	I	7	 100%
8	K	6	 100%
9	P	8	 63% 38%
10	Q	2	 100%
10	R	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	MRD	A	943	-	-	X	-

2 Entry composition i

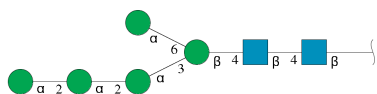
There are 13 unique types of molecules in this entry. The entry contains 15509 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-glucosidase 1.

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

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



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

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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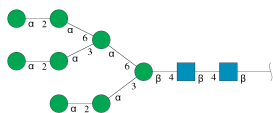
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



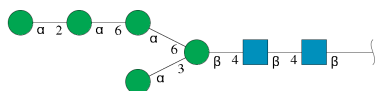
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



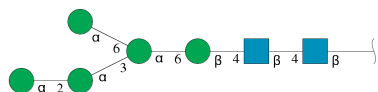
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	10	Total	C	N	O	0	0	0
			116	64	2	50			
5	M	10	Total	C	N	O	0	0	0
			116	64	2	50			

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



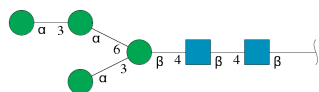
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	H	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



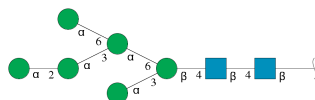
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

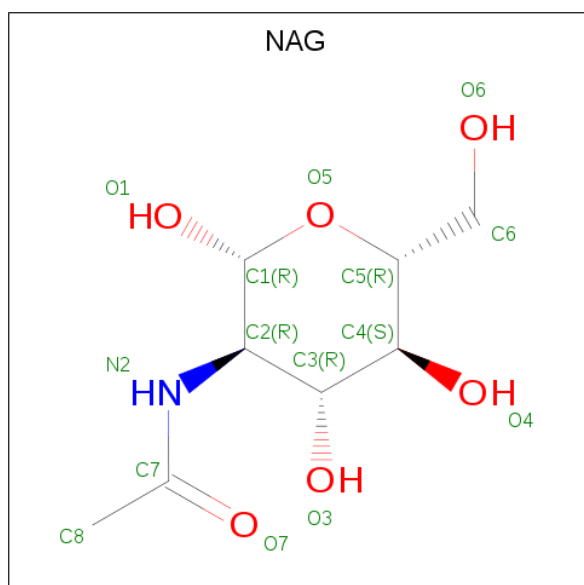


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	P	8	Total	C	N	O	0	0	0
			94	52	2	40			

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

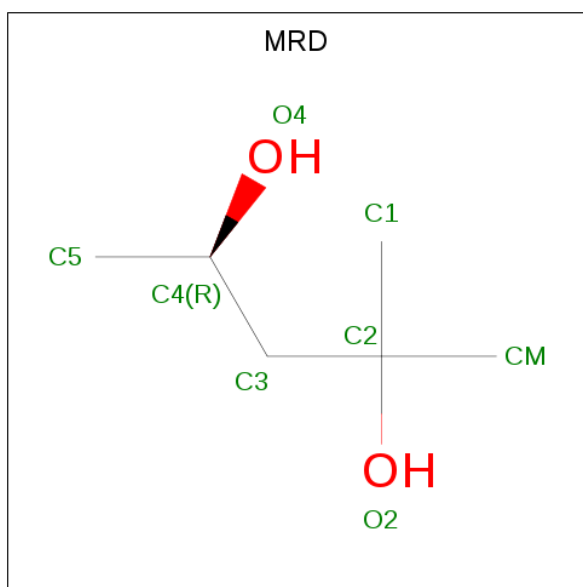
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
10	Q	2	23	12	10	1	0	0	0
10	R	2	23	12	10	1	0	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 12 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



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

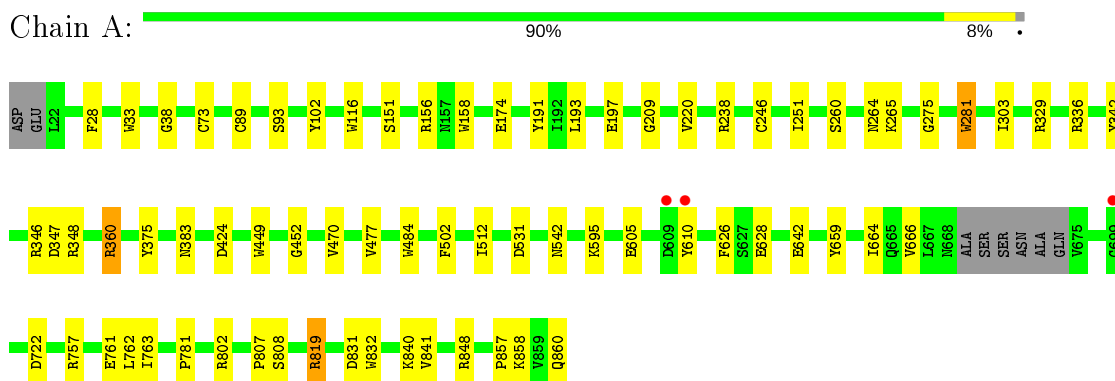
- Molecule 13 is water.

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

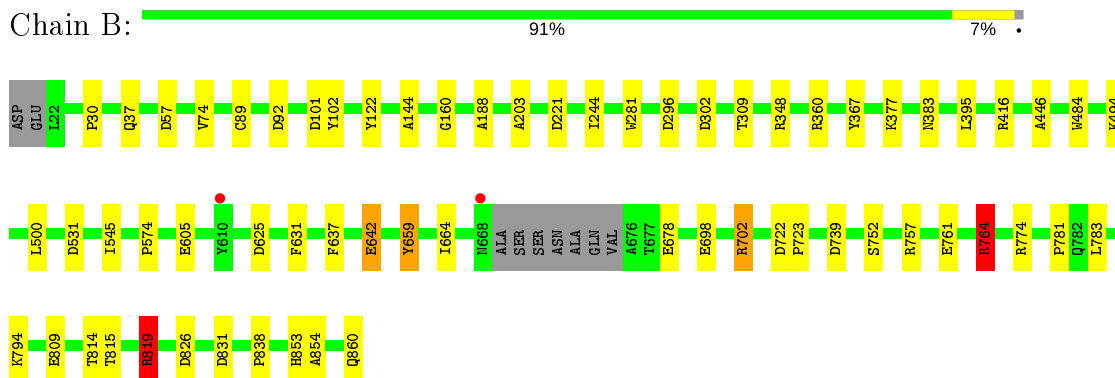
3 Residue-property plots [i](#)

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

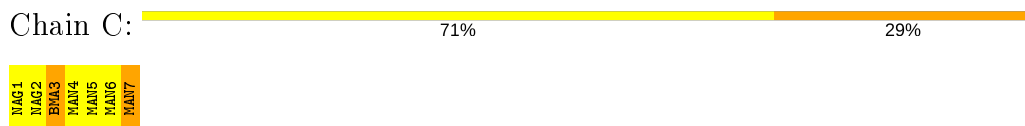
- Molecule 1: Beta-glucosidase 1



- Molecule 1: Beta-glucosidase 1




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



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

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

Chain J:  86% 14%

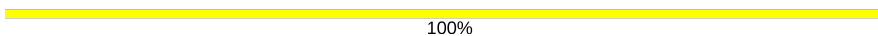
MAG1
MAG2
BOA3
MAN4
MAN5
MAN6
MAN7

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

Chain D:  67% 33%

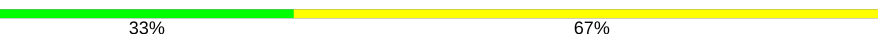
MAG1
MAG2
BOA3

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

Chain G:  100%

MAG1
MAG2
BOA3

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

Chain L:  33% 67%


MAG1
MAG2
BOA3

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

Chain N:  100%


MAG1
MAG2
BOA3

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

Chain E:  50% 50%

MAG1
MAG2

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

Chain F:  100%


MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

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

Chain M:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

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

Chain H:  86% 14%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

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

Chain O:  71% 29%


MAG1
MAG2
BMA3
MAN4
MAN5
MAN7

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

Chain I:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

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

Chain K:  100%

MAG1
MAG2
BMA3
MAN4
MAN6

- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  63% 38%


MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

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

Chain Q:  100%

SGC1
BGC2

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

Chain R:  50% 50%

SGC1
BGC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.08Å 122.39Å 221.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.07 – 2.00 41.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.07-2.00) 99.6 (41.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.28 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.140 , 0.181 0.141 , 0.182	Depositor DCC
R_{free} test set	7543 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15509	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NAG, BMA, MRD, SGC, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.29	11/6545 (0.2%)	1.07	18/8923 (0.2%)
1	B	1.35	10/6538 (0.2%)	1.11	24/8913 (0.3%)
All	All	1.32	21/13083 (0.2%)	1.09	42/17836 (0.2%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	642	GLU	CD-OE1	8.91	1.35	1.25
1	B	761	GLU	CD-OE2	-7.47	1.17	1.25
1	A	281	TRP	CB-CG	7.21	1.63	1.50
1	A	761	GLU	CD-OE2	-6.17	1.18	1.25
1	B	605	GLU	CG-CD	6.00	1.60	1.51

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	ARG	NE-CZ-NH2	-12.81	113.89	120.30
1	B	702	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	757	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	B	757	ARG	NE-CZ-NH1	-9.23	115.69	120.30
1	B	774	ARG	NE-CZ-NH2	-9.10	115.75	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	6382	0	6092	31	0
1	B	6375	0	6082	32	0
2	C	83	0	70	1	0
2	J	83	0	70	1	0
3	D	39	0	33	2	0
3	G	39	0	34	0	0
3	L	39	0	34	0	0
3	N	39	0	34	0	0
4	E	28	0	25	3	0
5	F	116	0	96	0	0
5	M	116	0	97	0	0
6	H	83	0	70	1	0
6	O	83	0	69	3	0
7	I	83	0	70	0	0
8	K	72	0	61	0	0
9	P	94	0	79	4	0
10	Q	23	0	21	0	0
10	R	23	0	21	4	0
11	A	28	0	26	0	0
11	B	42	0	39	0	0
12	A	16	0	28	9	0
12	B	16	0	28	4	0
13	A	748	0	0	3	0
13	B	859	0	0	11	0
All	All	15509	0	13179	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 79 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:ARG:HH12	1:A:860:GLN:C	1.51	1.12
1:B:815:THR:HG22	13:B:1525:HOH:O	1.70	0.89
1:A:819:ARG:NH1	1:A:860:GLN:C	2.31	0.84
12:A:942:MRD:H5C2	13:A:1191:HOH:O	1.77	0.84
4:E:2:NAG:H3	4:E:2:NAG:H83	1.63	0.81

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	829/841 (99%)	803 (97%)	25 (3%)	1 (0%)	51	49
1	B	828/841 (98%)	804 (97%)	24 (3%)	0	100	100
All	All	1657/1682 (98%)	1607 (97%)	49 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLY

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	671/677 (99%)	667 (99%)	4 (1%)	86	90
1	B	670/677 (99%)	660 (98%)	10 (2%)	65	69
All	All	1341/1354 (99%)	1327 (99%)	14 (1%)	76	81

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	281	TRP
1	B	302	ASP
1	B	764	ARG
1	B	92	ASP
1	B	698	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

87 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	1.16	2 (14%)	17,19,21	1.50	3 (17%)
2	NAG	C	2	2	14,14,15	1.10	1 (7%)	17,19,21	1.42	3 (17%)
2	BMA	C	3	2	11,11,12	0.74	0	15,15,17	1.87	3 (20%)
2	MAN	C	4	2	11,11,12	0.99	1 (9%)	15,15,17	2.63	8 (53%)
2	MAN	C	5	2	11,11,12	0.90	1 (9%)	15,15,17	2.15	6 (40%)
2	MAN	C	6	2	11,11,12	1.04	1 (9%)	15,15,17	2.14	6 (40%)
2	MAN	C	7	2	11,11,12	0.87	0	15,15,17	1.08	1 (6%)
3	NAG	D	1	1,3	14,14,15	1.04	0	17,19,21	1.41	3 (17%)
3	NAG	D	2	3	14,14,15	1.48	2 (14%)	17,19,21	2.04	7 (41%)
3	BMA	D	3	3	11,11,12	1.29	1 (9%)	15,15,17	2.75	8 (53%)
4	NAG	E	1	1,4	14,14,15	1.27	2 (14%)	17,19,21	1.84	4 (23%)
4	NAG	E	2	4	14,14,15	1.08	2 (14%)	17,19,21	1.87	7 (41%)
5	NAG	F	1	1,5	14,14,15	1.49	3 (21%)	17,19,21	1.28	3 (17%)
5	MAN	F	10	5	11,11,12	1.27	2 (18%)	15,15,17	2.45	6 (40%)
5	NAG	F	2	5	14,14,15	1.05	0	17,19,21	1.54	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	F	3	5	11,11,12	0.68	0	15,15,17	1.30	3 (20%)
5	MAN	F	4	5	11,11,12	0.81	1 (9%)	15,15,17	1.04	2 (13%)
5	MAN	F	5	5	11,11,12	1.32	3 (27%)	15,15,17	1.26	3 (20%)
5	MAN	F	6	5	11,11,12	0.85	0	15,15,17	1.56	3 (20%)
5	MAN	F	7	5	11,11,12	1.47	3 (27%)	15,15,17	1.56	2 (13%)
5	MAN	F	8	5	11,11,12	0.91	0	15,15,17	0.98	1 (6%)
5	MAN	F	9	5	11,11,12	1.57	4 (36%)	15,15,17	2.01	7 (46%)
3	NAG	G	1	1,3	14,14,15	1.04	1 (7%)	17,19,21	2.03	5 (29%)
3	NAG	G	2	3	14,14,15	0.83	0	17,19,21	1.91	4 (23%)
3	BMA	G	3	3	11,11,12	1.29	2 (18%)	15,15,17	2.15	5 (33%)
6	NAG	H	1	1,6	14,14,15	1.15	1 (7%)	17,19,21	1.50	4 (23%)
6	NAG	H	2	6	14,14,15	0.82	0	17,19,21	1.42	3 (17%)
6	BMA	H	3	6	11,11,12	1.33	1 (9%)	15,15,17	1.71	3 (20%)
6	MAN	H	4	6	11,11,12	0.67	0	15,15,17	1.54	2 (13%)
6	MAN	H	5	6	11,11,12	0.84	0	15,15,17	2.17	5 (33%)
6	MAN	H	6	6	11,11,12	1.62	2 (18%)	15,15,17	1.68	4 (26%)
6	MAN	H	7	6	11,11,12	0.82	0	15,15,17	1.83	4 (26%)
7	NAG	I	1	1,7	14,14,15	1.04	0	17,19,21	1.47	2 (11%)
7	NAG	I	2	7	14,14,15	1.34	2 (14%)	17,19,21	1.44	3 (17%)
7	BMA	I	3	7	11,11,12	1.49	1 (9%)	15,15,17	1.82	3 (20%)
7	MAN	I	4	7	11,11,12	1.25	1 (9%)	15,15,17	1.26	1 (6%)
7	MAN	I	5	7	11,11,12	1.26	0	15,15,17	2.38	7 (46%)
7	MAN	I	6	7	11,11,12	0.98	1 (9%)	15,15,17	1.87	4 (26%)
7	MAN	I	7	7	11,11,12	1.99	2 (18%)	15,15,17	1.24	1 (6%)
2	NAG	J	1	1,2	14,14,15	1.41	3 (21%)	17,19,21	2.20	6 (35%)
2	NAG	J	2	2	14,14,15	0.93	0	17,19,21	2.01	6 (35%)
2	BMA	J	3	2	11,11,12	1.81	2 (18%)	15,15,17	1.83	5 (33%)
2	MAN	J	4	2	11,11,12	0.71	0	15,15,17	1.76	4 (26%)
2	MAN	J	5	2	11,11,12	1.10	1 (9%)	15,15,17	1.15	1 (6%)
2	MAN	J	6	2	11,11,12	0.90	0	15,15,17	1.42	3 (20%)
2	MAN	J	7	2	11,11,12	0.70	0	15,15,17	1.93	5 (33%)
8	NAG	K	1	1,8	14,14,15	0.91	0	17,19,21	1.69	3 (17%)
8	NAG	K	2	8	14,14,15	1.65	5 (35%)	17,19,21	1.87	6 (35%)
8	BMA	K	3	8	11,11,12	1.14	2 (18%)	15,15,17	1.91	5 (33%)
8	MAN	K	4	8	11,11,12	0.83	0	15,15,17	1.91	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	K	5	8	11,11,12	0.86	0	15,15,17	2.09	4 (26%)
8	MAN	K	6	8	11,11,12	1.24	1 (9%)	15,15,17	1.41	3 (20%)
3	NAG	L	1	1,3	14,14,15	0.88	0	17,19,21	0.95	0
3	NAG	L	2	3	14,14,15	0.79	0	17,19,21	1.88	6 (35%)
3	BMA	L	3	3	11,11,12	0.93	0	15,15,17	1.98	5 (33%)
5	NAG	M	1	1,5	14,14,15	1.27	1 (7%)	17,19,21	1.58	3 (17%)
5	MAN	M	10	5	11,11,12	1.17	1 (9%)	15,15,17	2.32	4 (26%)
5	NAG	M	2	5	14,14,15	1.53	2 (14%)	17,19,21	1.52	3 (17%)
5	BMA	M	3	5	11,11,12	1.21	1 (9%)	15,15,17	1.35	2 (13%)
5	MAN	M	4	5	11,11,12	0.89	0	15,15,17	1.34	3 (20%)
5	MAN	M	5	5	11,11,12	0.98	0	15,15,17	2.03	5 (33%)
5	MAN	M	6	5	11,11,12	1.18	0	15,15,17	2.12	6 (40%)
5	MAN	M	7	5	11,11,12	0.83	0	15,15,17	2.01	4 (26%)
5	MAN	M	8	5	11,11,12	1.22	1 (9%)	15,15,17	1.52	2 (13%)
5	MAN	M	9	5	11,11,12	0.93	1 (9%)	15,15,17	2.36	7 (46%)
3	NAG	N	1	1,3	14,14,15	1.15	1 (7%)	17,19,21	1.47	5 (29%)
3	NAG	N	2	3	14,14,15	1.38	3 (21%)	17,19,21	2.82	7 (41%)
3	BMA	N	3	3	11,11,12	1.37	2 (18%)	15,15,17	3.03	9 (60%)
6	NAG	O	1	1,6	14,14,15	1.06	1 (7%)	17,19,21	0.92	0
6	NAG	O	2	6	14,14,15	1.17	1 (7%)	17,19,21	1.92	6 (35%)
6	BMA	O	3	6	11,11,12	1.35	2 (18%)	15,15,17	2.07	4 (26%)
6	MAN	O	4	6	11,11,12	0.89	0	15,15,17	1.78	5 (33%)
6	MAN	O	5	6	11,11,12	1.27	1 (9%)	15,15,17	1.78	5 (33%)
6	MAN	O	6	6	11,11,12	0.99	0	15,15,17	1.74	6 (40%)
6	MAN	O	7	6	11,11,12	1.24	2 (18%)	15,15,17	2.46	6 (40%)
9	NAG	P	1	1,9	14,14,15	0.95	1 (7%)	17,19,21	1.97	5 (29%)
9	NAG	P	2	9	14,14,15	0.82	0	17,19,21	1.13	1 (5%)
9	BMA	P	3	9	11,11,12	1.32	2 (18%)	15,15,17	3.44	7 (46%)
9	MAN	P	4	9	11,11,12	1.08	1 (9%)	15,15,17	2.08	5 (33%)
9	MAN	P	5	9	11,11,12	1.11	0	15,15,17	1.83	3 (20%)
9	MAN	P	6	9	11,11,12	0.87	0	15,15,17	3.57	7 (46%)
9	MAN	P	7	9	11,11,12	0.98	1 (9%)	15,15,17	2.85	8 (53%)
9	MAN	P	8	9	11,11,12	1.09	1 (9%)	15,15,17	2.16	6 (40%)
10	SGC	Q	1	10	11,12,12	2.71	2 (18%)	13,17,17	1.99	6 (46%)
10	BGC	Q	2	10	11,11,12	1.52	3 (27%)	15,15,17	1.83	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	SGC	R	1	10	11,12,12	3.19	4 (36%)	13,17,17	2.13	3 (23%)
10	BGC	R	2	10	11,11,12	2.00	2 (18%)	15,15,17	3.06	6 (40%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	I	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
7	MAN	I	4	7	-	2/2/19/22	0/1/1/1
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
7	MAN	I	6	7	-	2/2/19/22	0/1/1/1
7	MAN	I	7	7	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	BMA	J	3	2	-	0/2/19/22	0/1/1/1
2	MAN	J	4	2	-	1/2/19/22	0/1/1/1
2	MAN	J	5	2	-	2/2/19/22	0/1/1/1
2	MAN	J	6	2	-	1/2/19/22	0/1/1/1
2	MAN	J	7	2	-	0/2/19/22	0/1/1/1
8	NAG	K	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	0/6/23/26	0/1/1/1
8	BMA	K	3	8	-	0/2/19/22	0/1/1/1
8	MAN	K	4	8	-	0/2/19/22	0/1/1/1
8	MAN	K	5	8	-	1/2/19/22	0/1/1/1
8	MAN	K	6	8	-	0/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	M	10	5	-	2/2/19/22	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
5	MAN	M	6	5	-	0/2/19/22	0/1/1/1
5	MAN	M	7	5	-	0/2/19/22	0/1/1/1
5	MAN	M	8	5	-	0/2/19/22	0/1/1/1
5	MAN	M	9	5	-	0/2/19/22	0/1/1/1
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
6	NAG	O	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
6	MAN	O	4	6	-	0/2/19/22	0/1/1/1
6	MAN	O	5	6	-	0/2/19/22	0/1/1/1

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

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	R	1	SGC	C5-C4	8.77	1.60	1.53
10	Q	1	SGC	C5-C4	7.43	1.59	1.53
10	R	2	BGC	O5-C1	5.15	1.51	1.43
7	I	7	MAN	O5-C1	-5.13	1.35	1.43
2	J	3	BMA	C2-C3	4.45	1.59	1.52

The worst 5 of 370 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	6	MAN	C1-O5-C5	10.39	126.27	112.19
9	P	3	BMA	C1-O5-C5	8.38	123.54	112.19
3	N	2	NAG	C1-O5-C5	-8.08	101.25	112.19
9	P	3	BMA	C6-C5-C4	-7.76	94.84	113.00
10	R	2	BGC	C1-O5-C5	7.02	121.71	112.19

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	MAN	C4-C5-C6-O6
2	J	5	MAN	O5-C5-C6-O6
7	I	6	MAN	O5-C5-C6-O6
9	P	7	MAN	O5-C5-C6-O6

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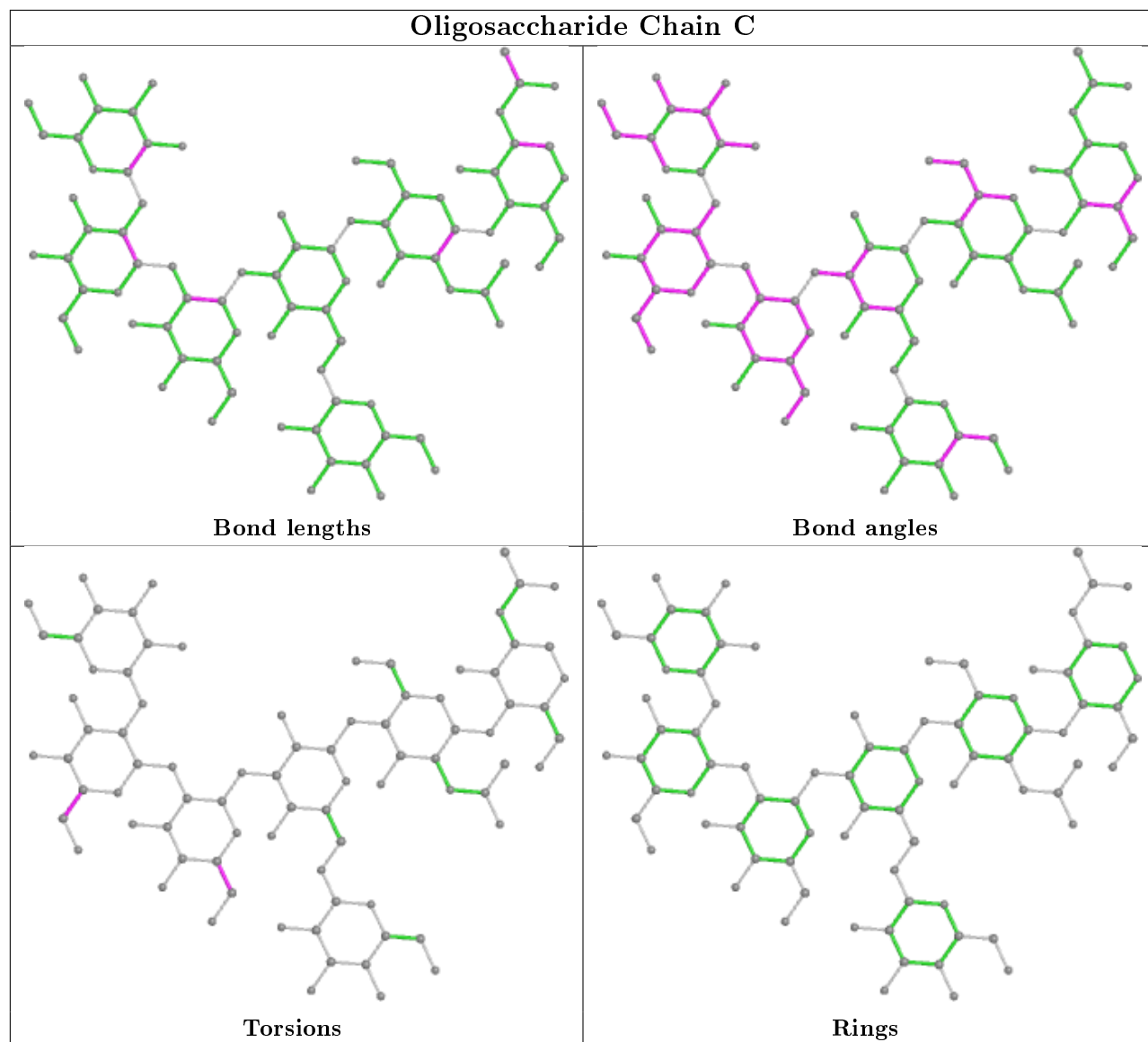
Mol	Chain	Res	Type	Atoms
7	I	4	MAN	O5-C5-C6-O6

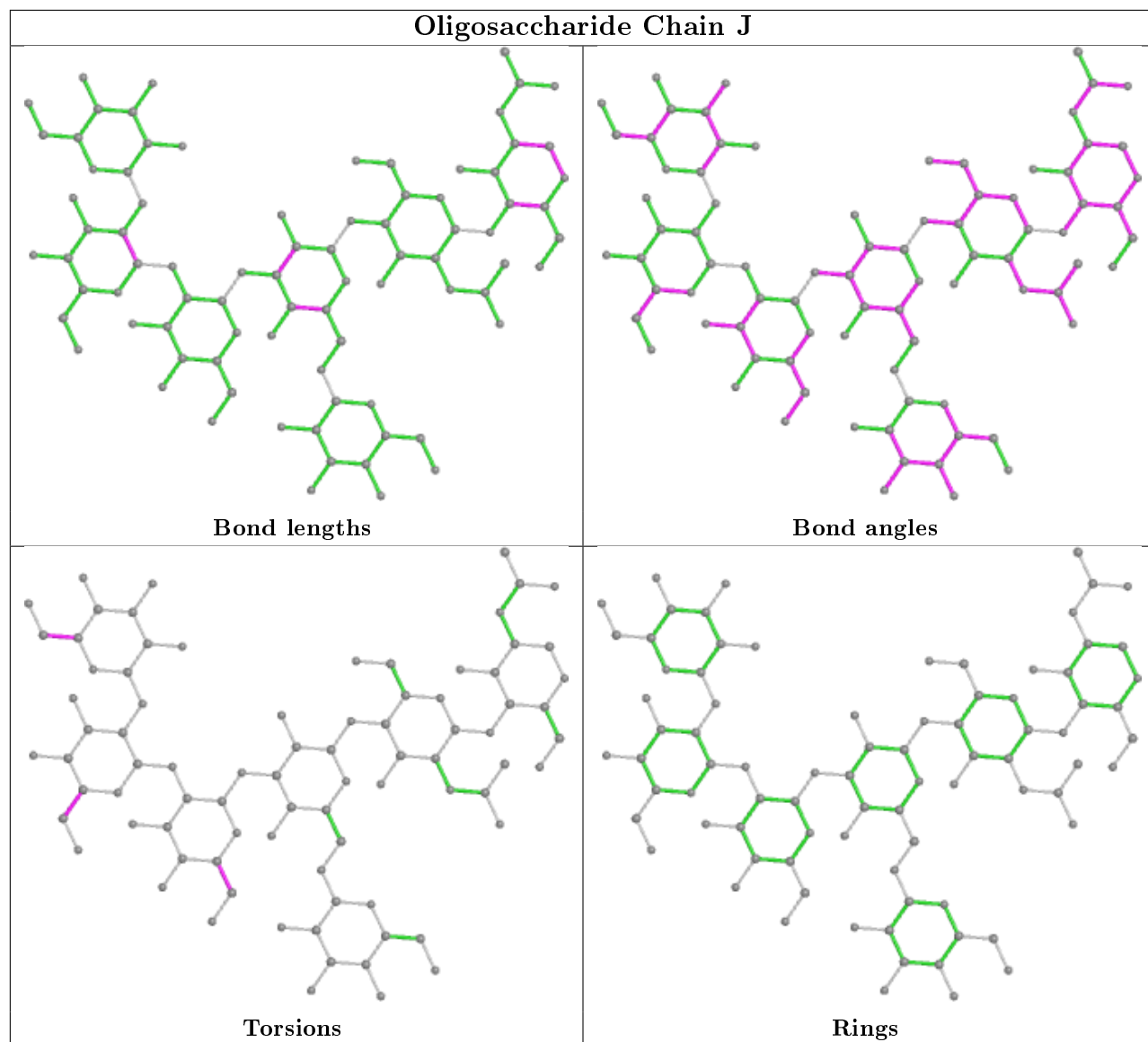
There are no ring outliers.

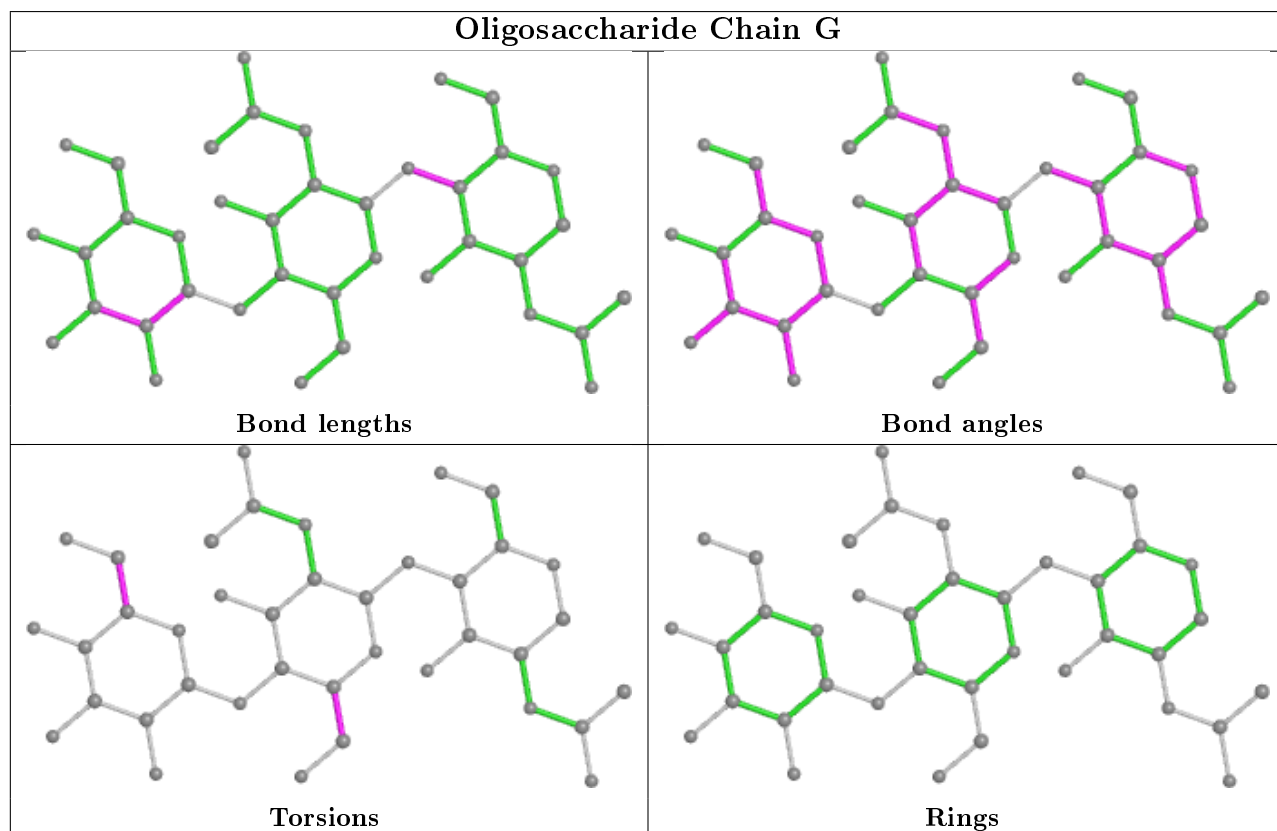
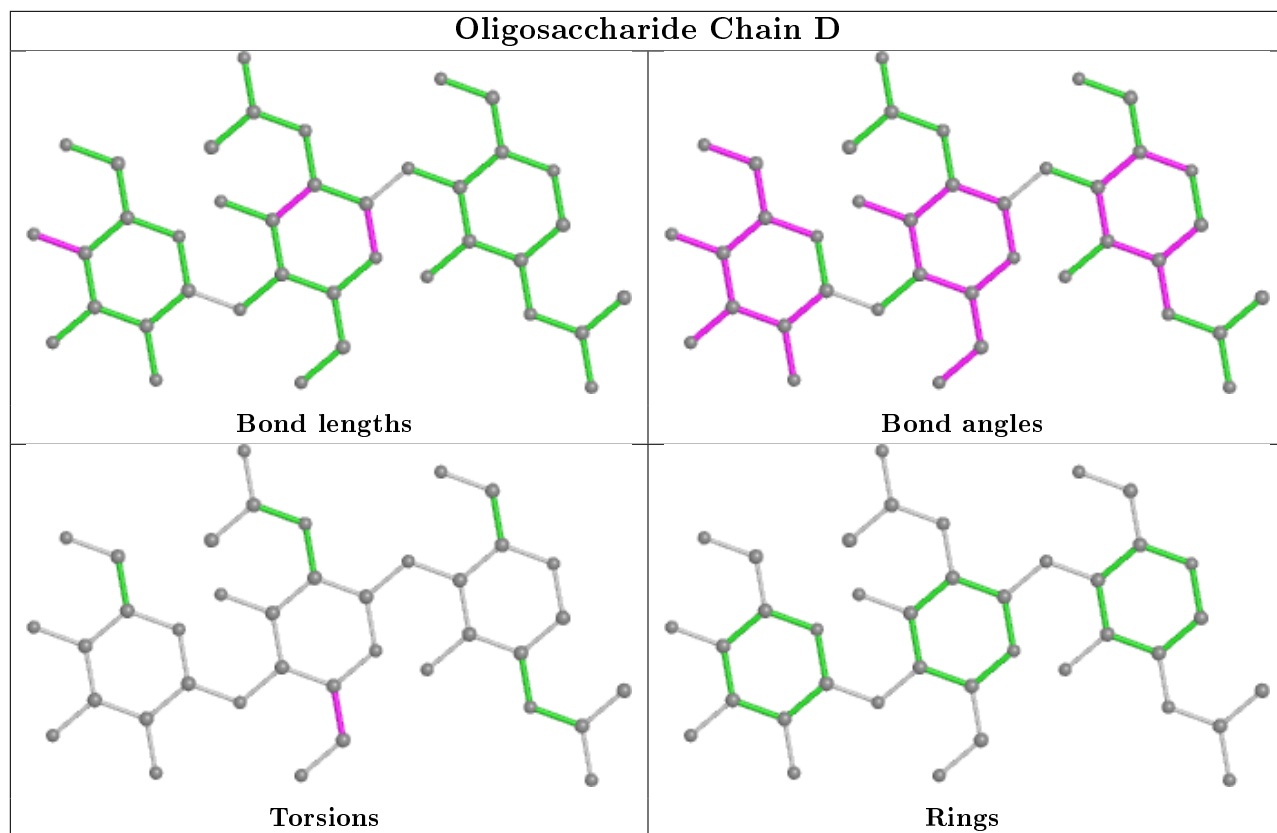
12 monomers are involved in 19 short contacts:

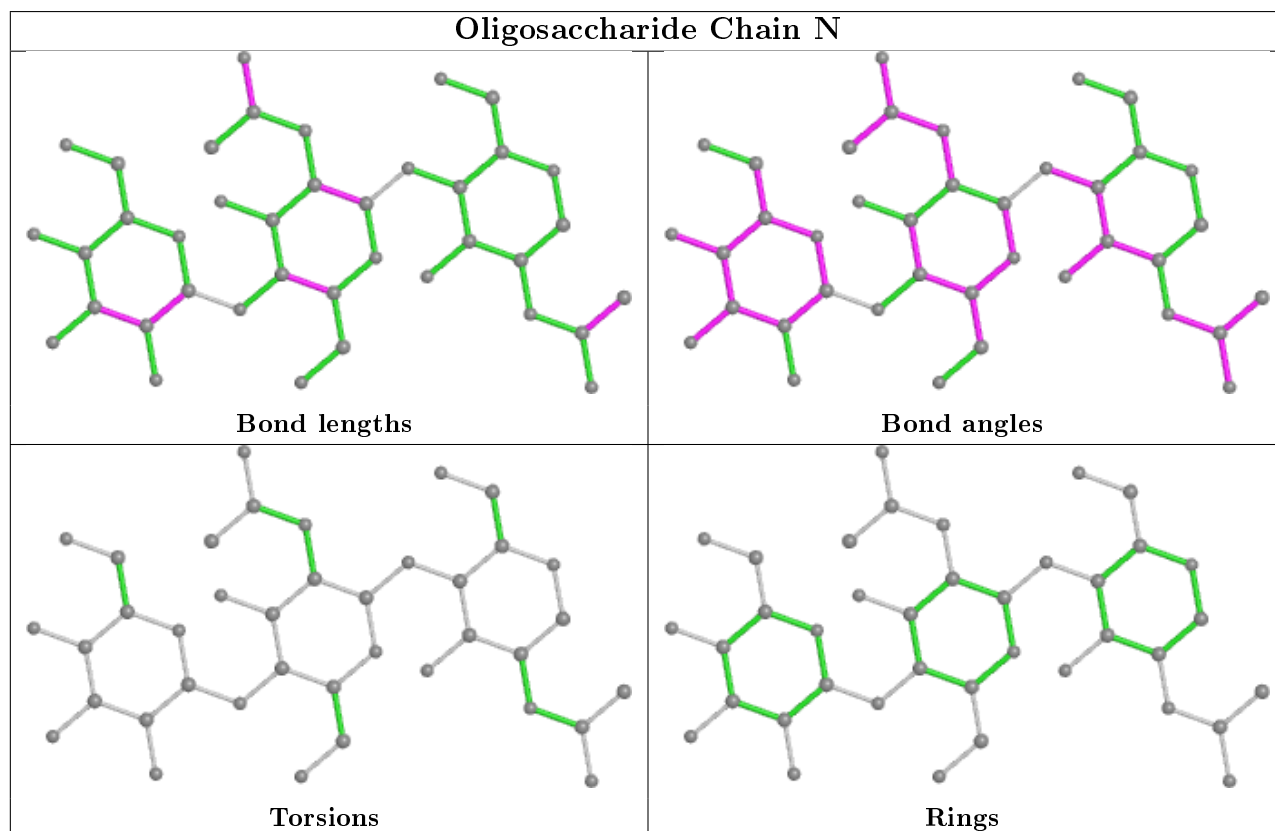
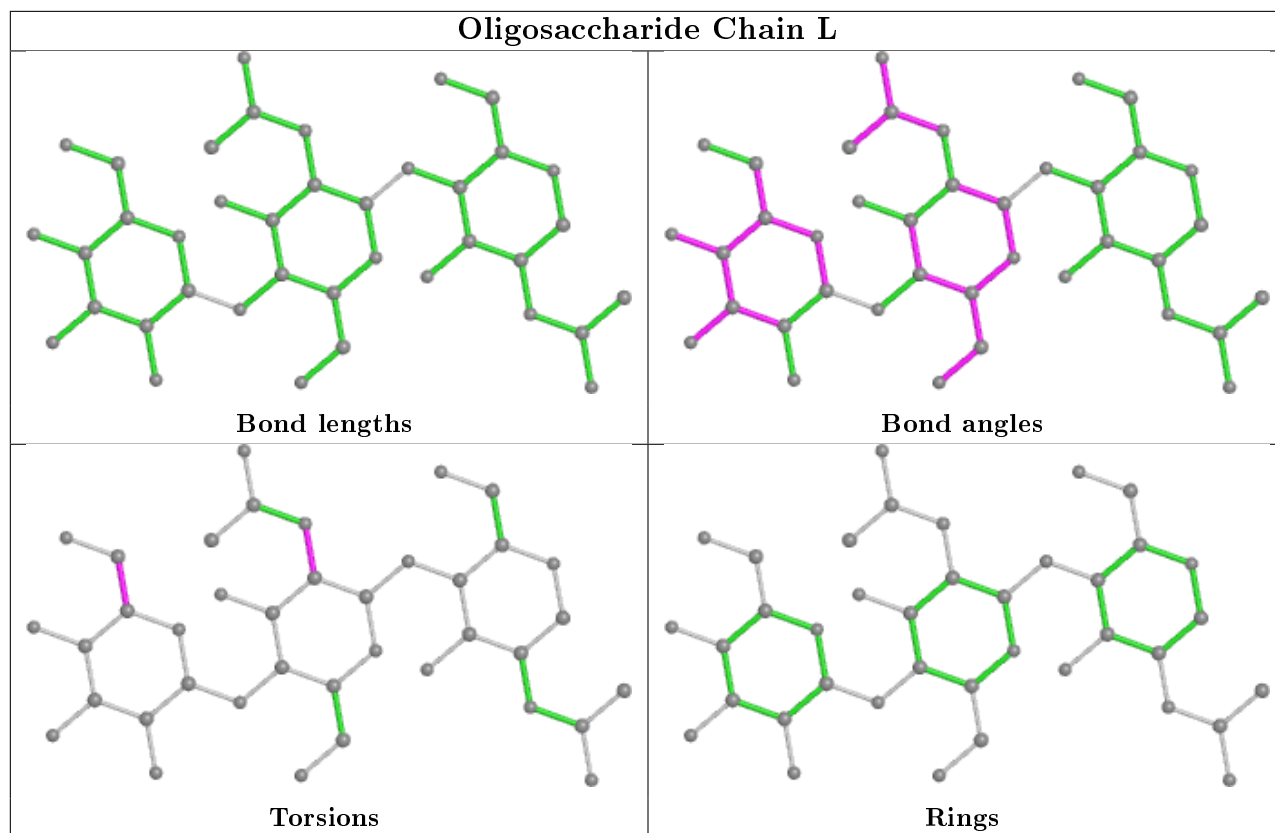
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	R	2	BGC	4	0
9	P	7	MAN	1	0
6	O	4	MAN	1	0
9	P	3	BMA	3	0
2	C	7	MAN	1	0
2	J	2	NAG	1	0
6	O	3	BMA	3	0
3	D	1	NAG	2	0
9	P	4	MAN	2	0
4	E	2	NAG	3	0
2	C	3	BMA	1	0
6	H	3	BMA	1	0

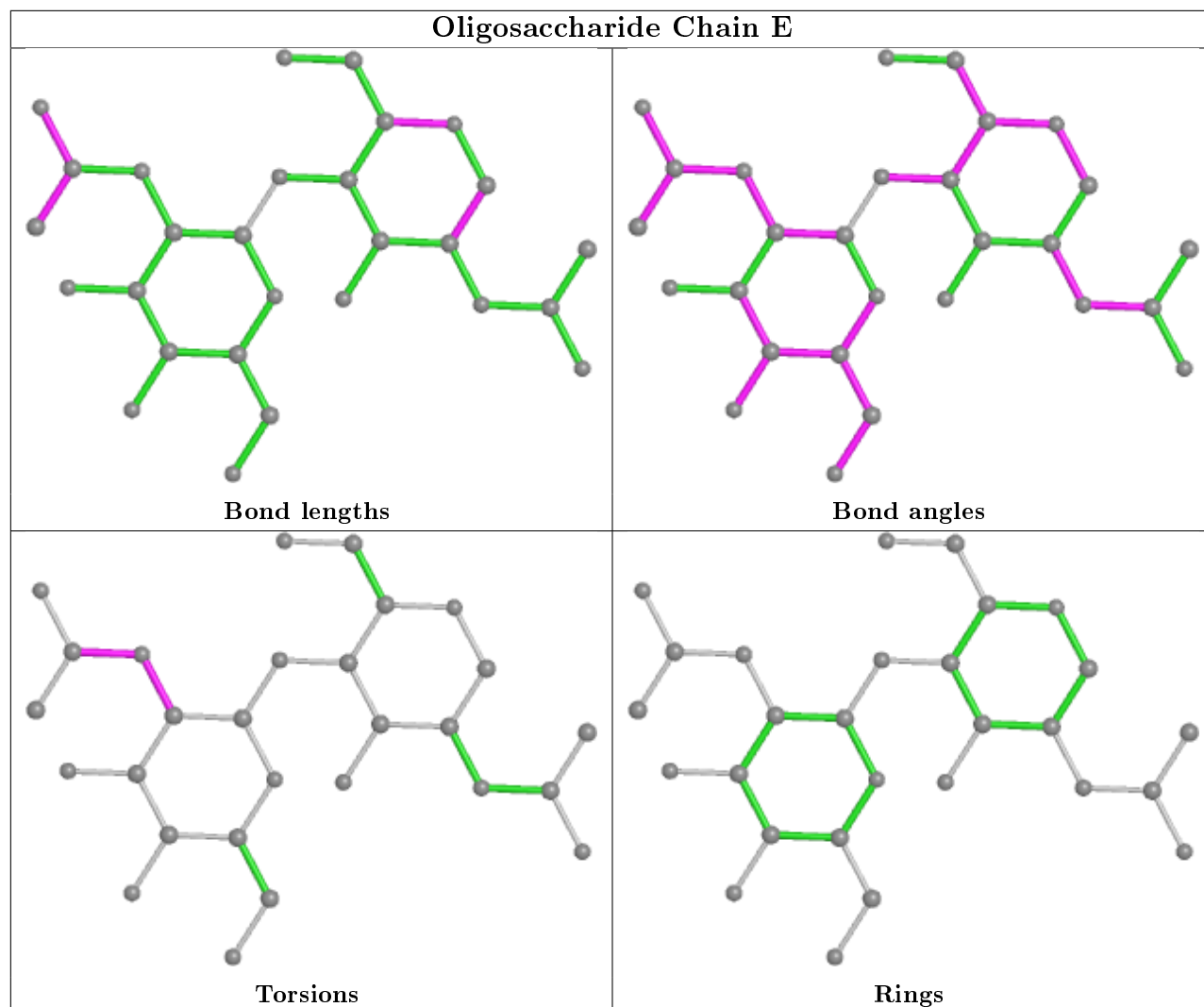
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

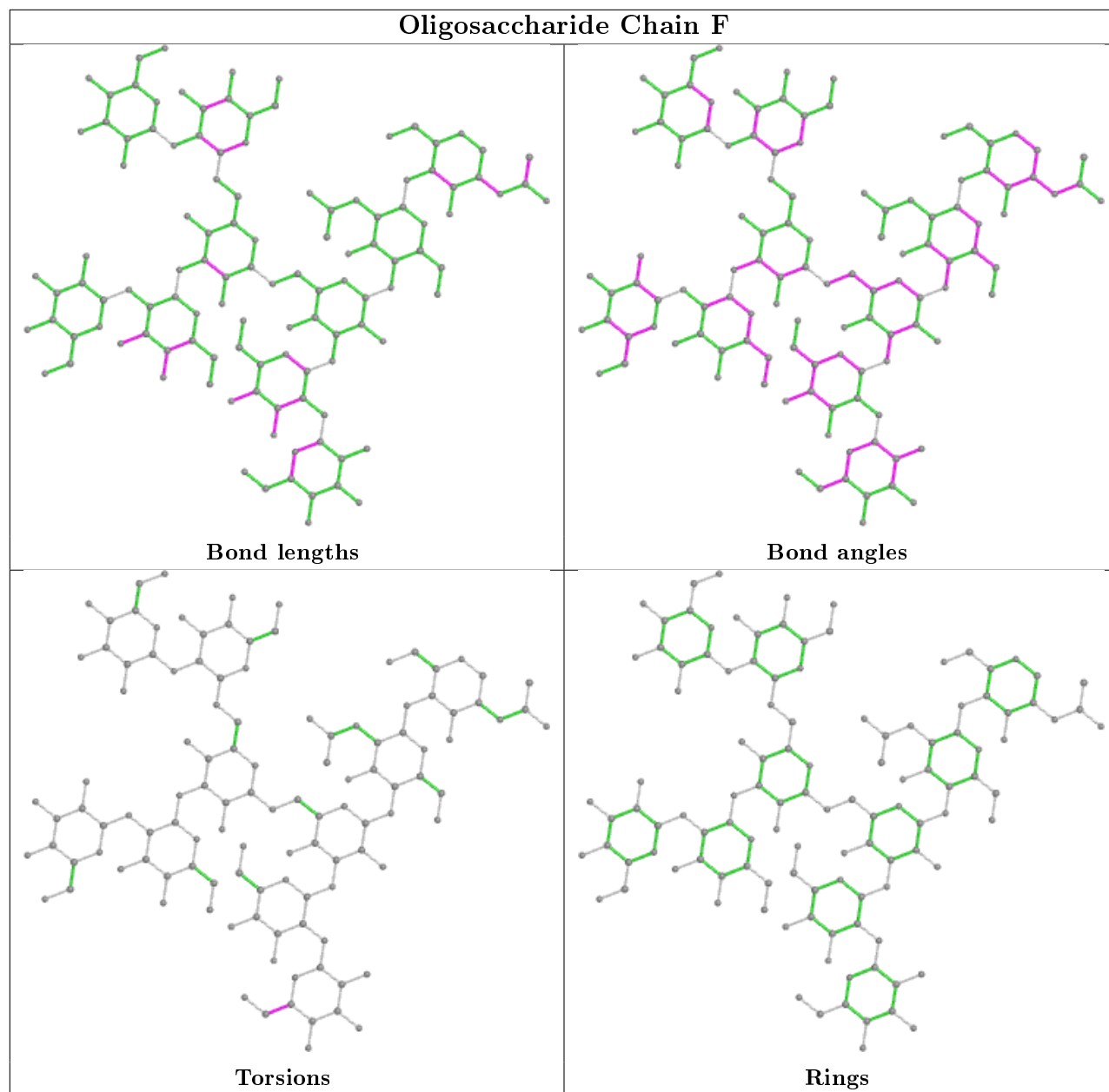


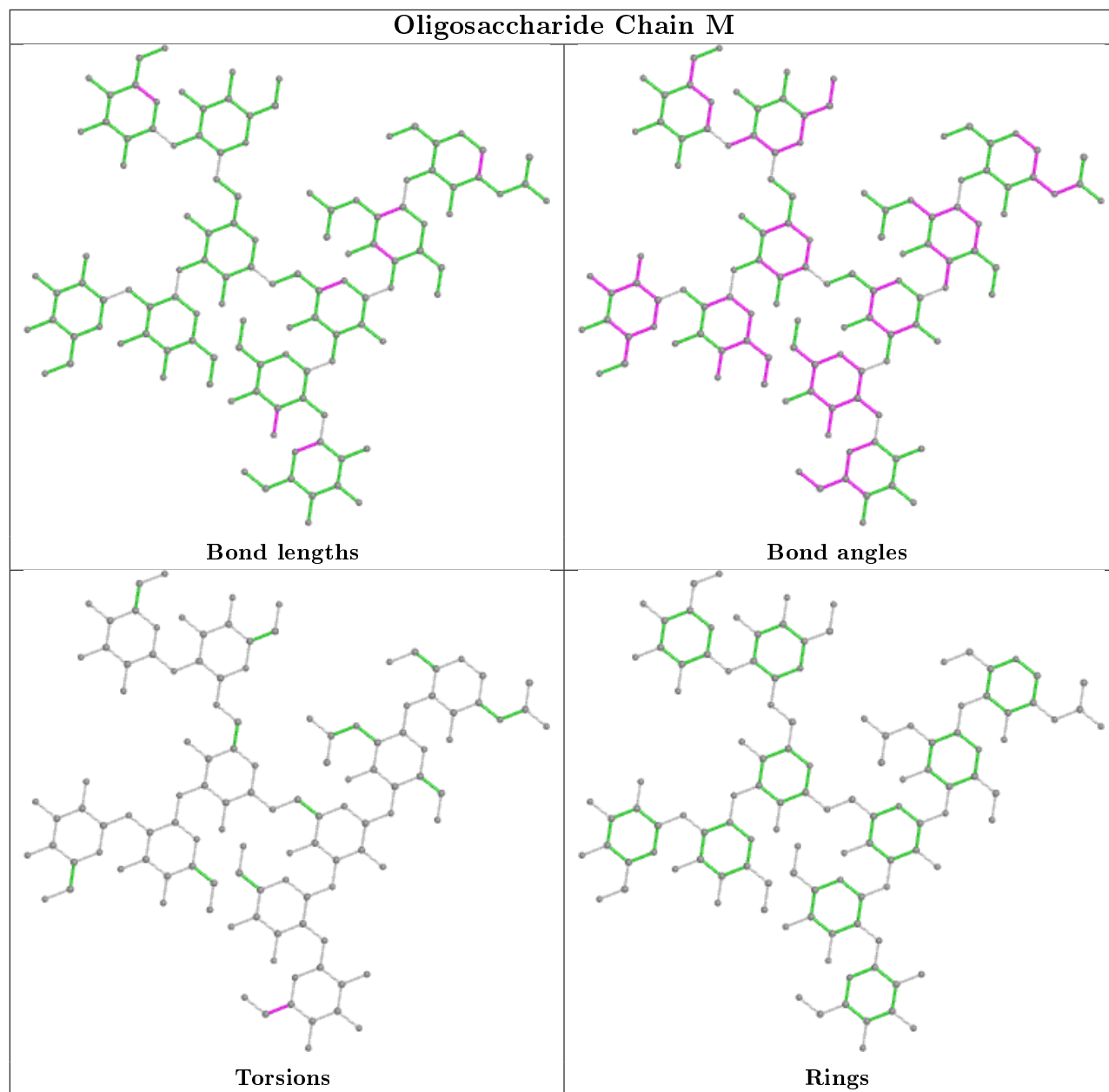


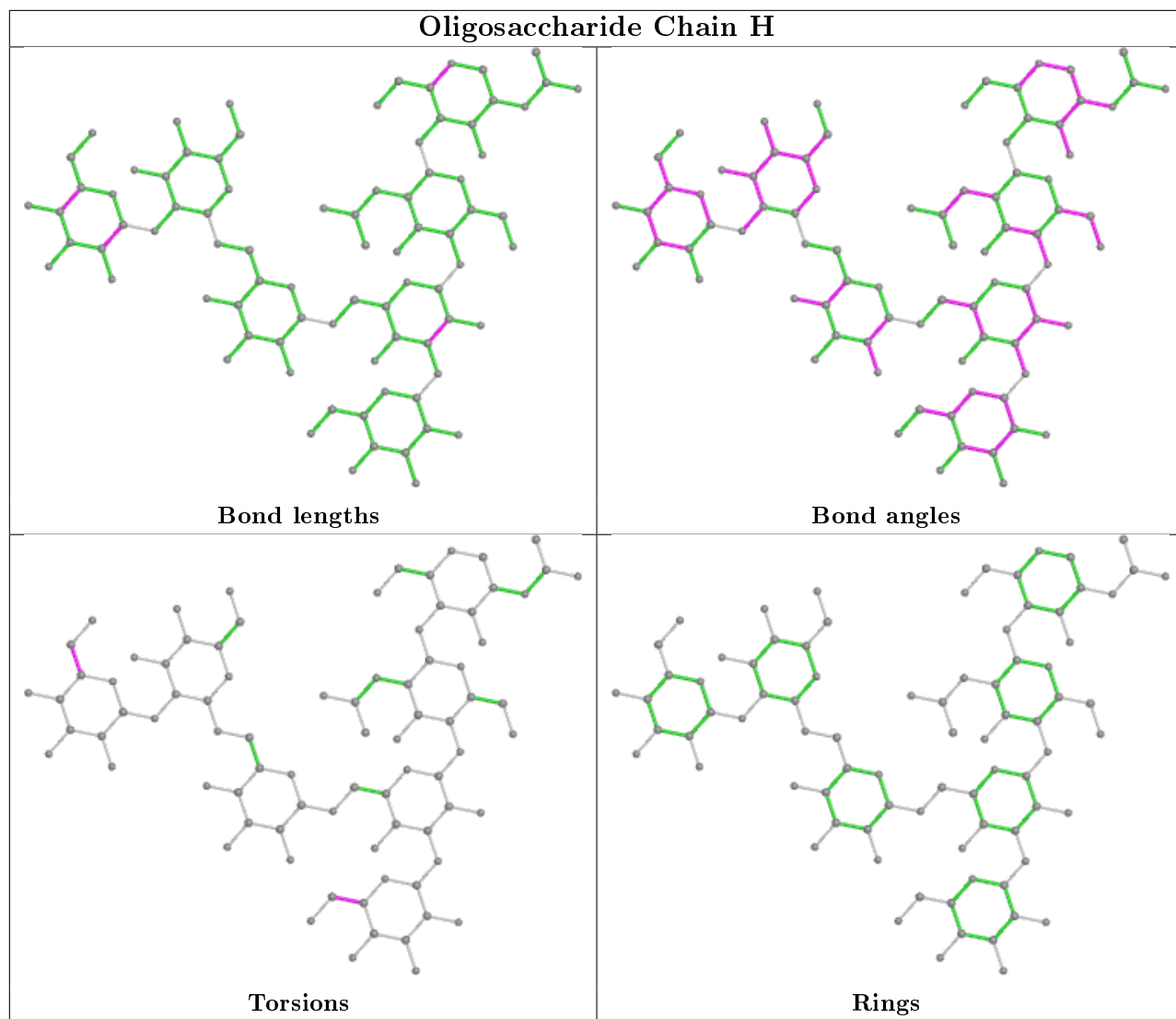


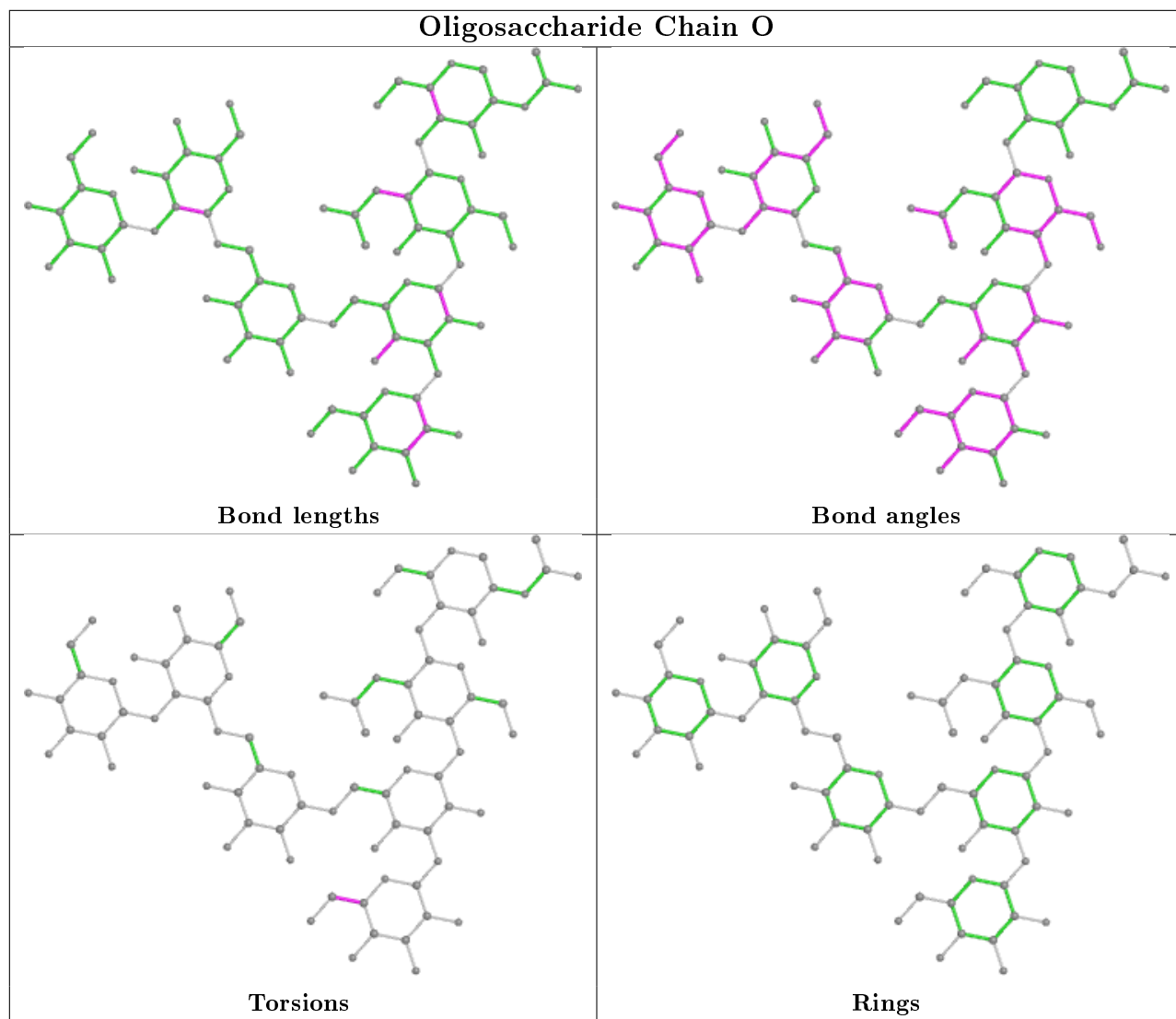


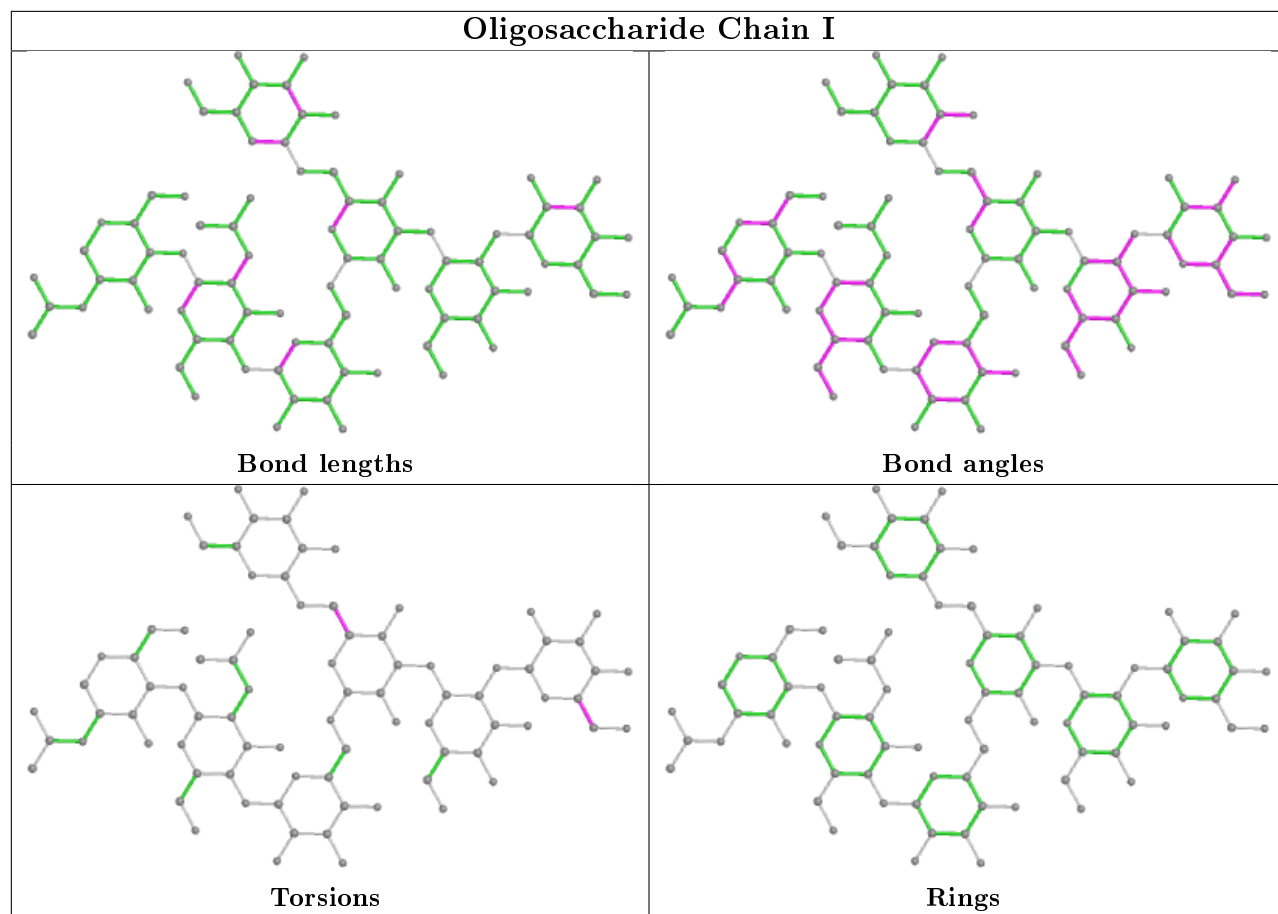


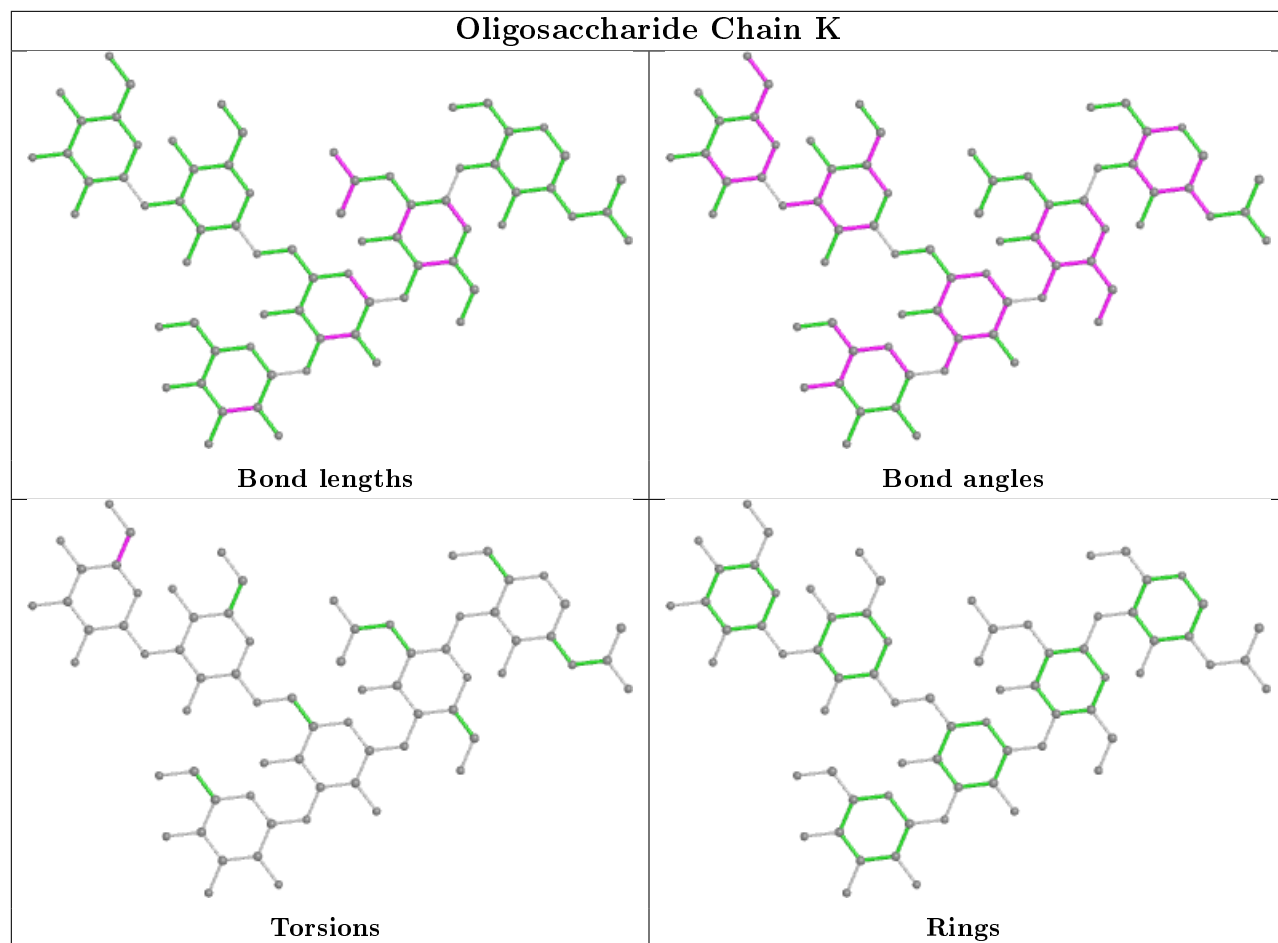


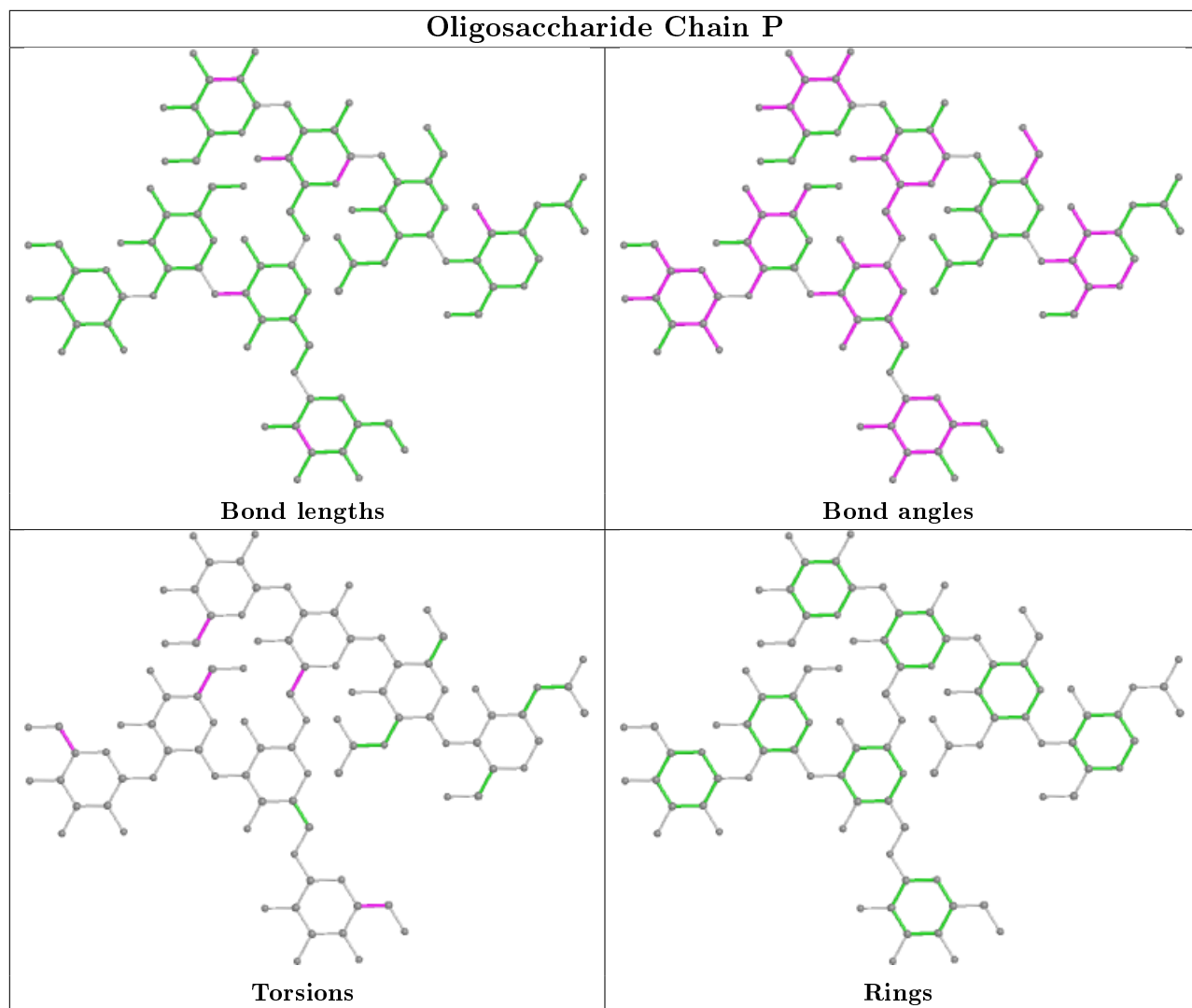


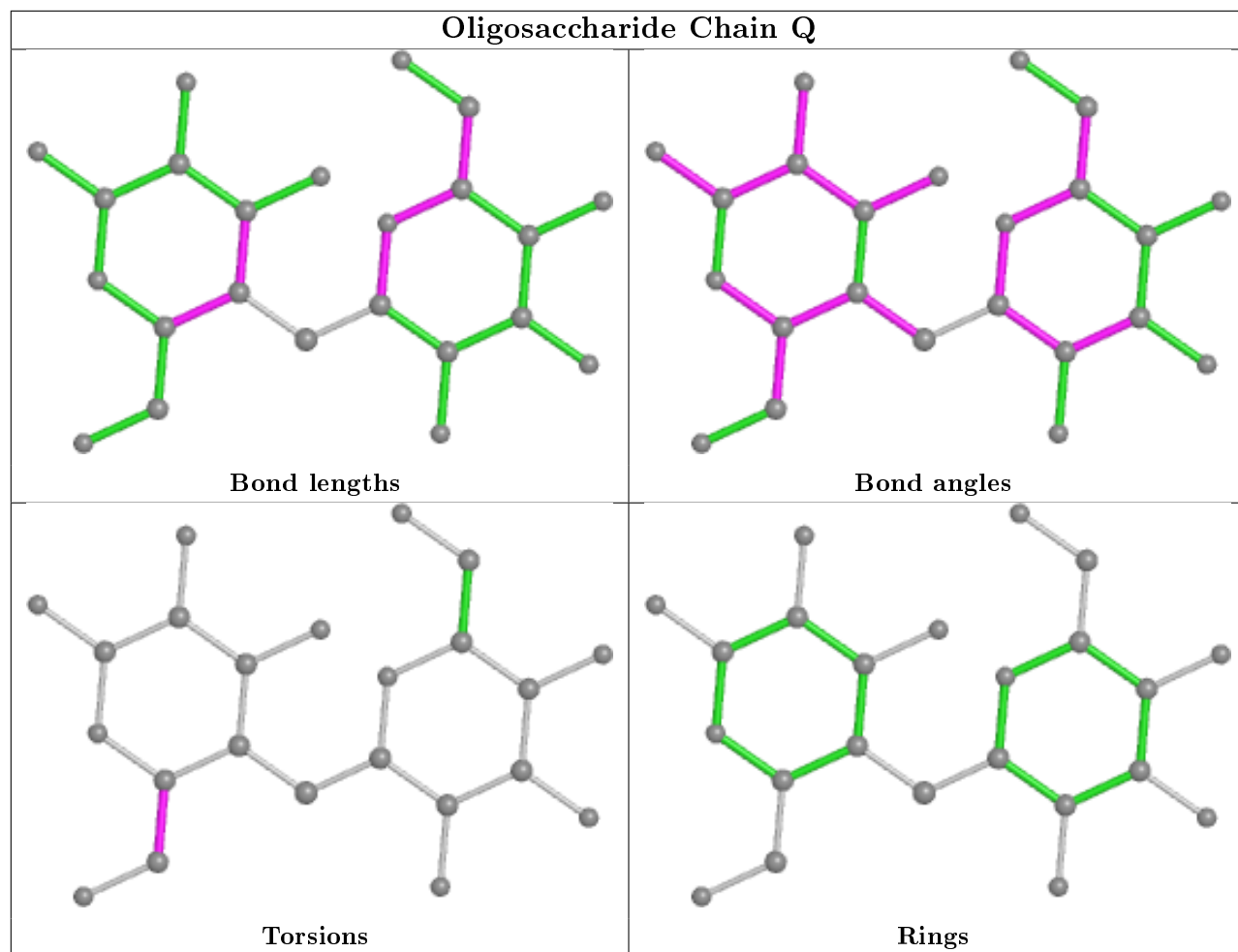


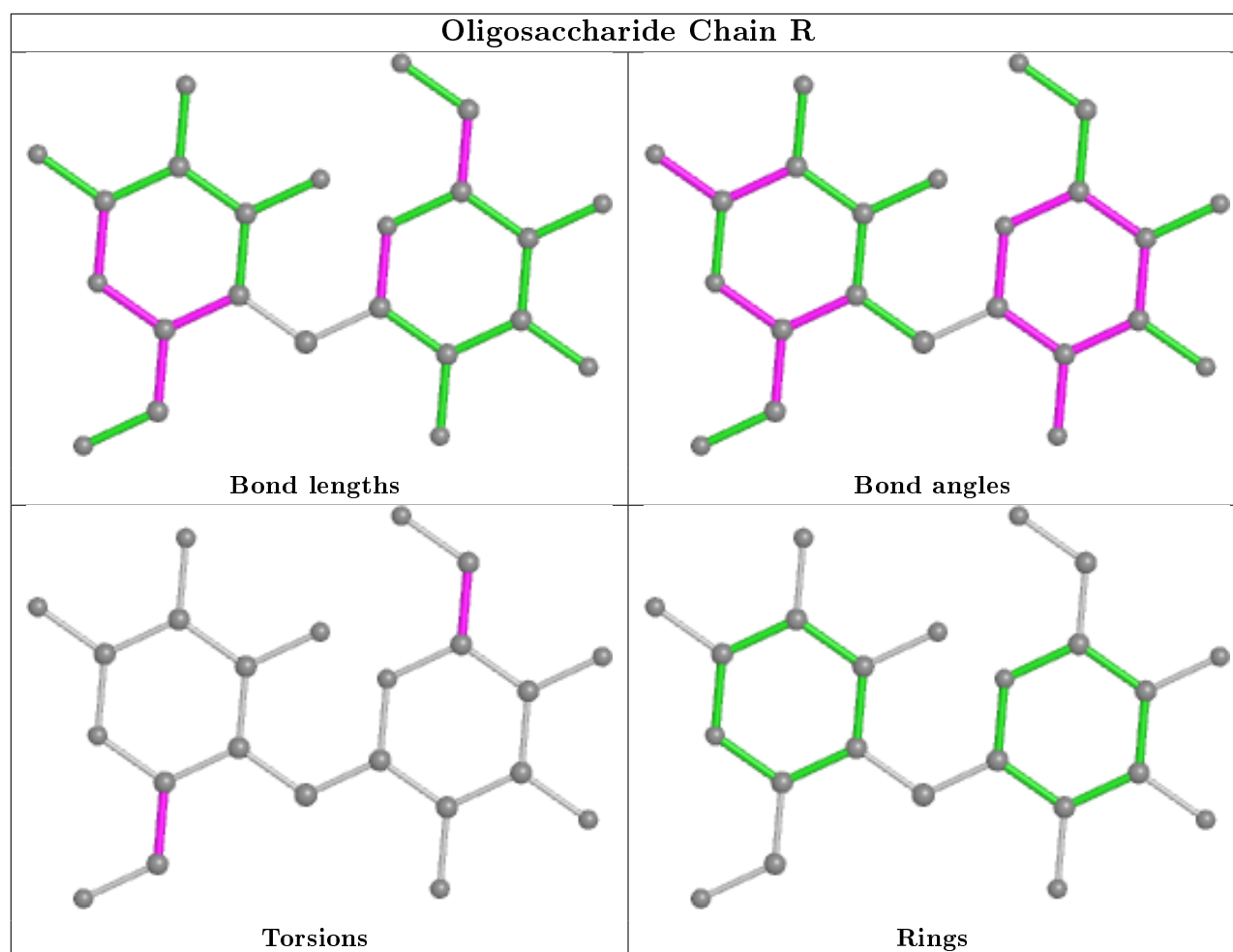












5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	NAG	B	947	1	14,14,15	0.85	0	17,19,21	1.23	0
12	MRD	B	948	-	7,7,7	0.74	0	9,10,10	1.30	1 (11%)
11	NAG	B	908	1	14,14,15	1.15	2 (14%)	17,19,21	3.53	9 (52%)
11	NAG	A	941	1	14,14,15	0.90	1 (7%)	17,19,21	2.20	8 (47%)
11	NAG	B	946	1	14,14,15	1.18	3 (21%)	17,19,21	1.94	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	A	908	1	14,14,15	1.16	1 (7%)	17,19,21	1.52	4 (23%)
12	MRD	A	942	-	7,7,7	1.52	2 (28%)	9,10,10	1.20	1 (11%)
12	MRD	B	949	-	7,7,7	1.08	1 (14%)	9,10,10	0.89	0
12	MRD	A	943	-	7,7,7	0.87	0	9,10,10	1.31	2 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	B	947	1	-	0/6/23/26	0/1/1/1
12	MRD	B	948	-	-	1/5/5/5	-
11	NAG	B	908	1	-	1/6/23/26	0/1/1/1
11	NAG	A	941	1	-	0/6/23/26	0/1/1/1
11	NAG	B	946	1	-	2/6/23/26	0/1/1/1
11	NAG	A	908	1	-	0/6/23/26	0/1/1/1
12	MRD	A	942	-	-	1/5/5/5	-
12	MRD	B	949	-	-	3/5/5/5	-
12	MRD	A	943	-	-	3/5/5/5	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	908	NAG	O5-C1	-3.10	1.38	1.43
11	B	908	NAG	O5-C1	-2.91	1.39	1.43
12	A	942	MRD	C3-C2	2.54	1.60	1.53
12	B	949	MRD	O2-C2	-2.48	1.38	1.44
11	B	946	NAG	O5-C5	-2.40	1.38	1.43

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	908	NAG	C4-C3-C2	-7.33	100.27	111.02
11	B	908	NAG	O5-C1-C2	-6.57	100.92	111.29
11	B	908	NAG	C2-N2-C7	5.83	131.20	122.90
11	B	908	NAG	C6-C5-C4	-4.20	103.17	113.00
11	B	946	NAG	O5-C5-C4	-3.85	101.46	110.83

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	948	MRD	C2-C3-C4-O4
12	B	949	MRD	C2-C3-C4-O4
12	B	949	MRD	C2-C3-C4-C5
11	B	946	NAG	O5-C5-C6-O6
11	B	946	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	948	MRD	2	0
12	A	942	MRD	3	0
12	B	949	MRD	2	0
12	A	943	MRD	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	833/841 (99%)	-0.77	3 (0%) 92 92	5, 12, 24, 50	0
1	B	832/841 (98%)	-0.93	2 (0%) 95 94	4, 9, 20, 52	0
All	All	1665/1682 (98%)	-0.85	5 (0%) 94 93	4, 10, 23, 52	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	GLY	3.0
1	A	610	TYR	2.5
1	B	668	ASN	2.4
1	A	609	ASP	2.3
1	B	610	TYR	2.2

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
3	BMA	G	3	11/12	0.61	0.32	45,66,75,79	0
6	MAN	O	7	11/12	0.73	0.25	56,65,71,77	0
9	MAN	P	7	11/12	0.76	0.22	48,54,66,71	0
7	MAN	I	7	11/12	0.78	0.26	49,53,62,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MAN	H	7	11/12	0.79	0.31	52,58,67,68	0
3	BMA	N	3	11/12	0.79	0.20	42,51,62,68	0
2	MAN	C	7	11/12	0.80	0.14	45,53,59,60	0
3	NAG	G	2	14/15	0.80	0.18	40,48,59,62	0
9	MAN	P	6	11/12	0.80	0.23	44,50,62,64	0
8	MAN	K	6	11/12	0.80	0.21	37,42,50,51	0
2	MAN	C	5	11/12	0.80	0.26	55,60,62,63	0
3	BMA	L	3	11/12	0.81	0.23	45,59,70,74	0
3	BMA	D	3	11/12	0.82	0.17	25,34,40,46	0
9	MAN	P	8	11/12	0.82	0.22	51,60,65,66	0
2	MAN	C	4	11/12	0.83	0.27	52,58,63,65	0
10	SGC	R	1	12/12	0.83	0.16	40,53,60,60	0
10	SGC	Q	1	12/12	0.85	0.14	43,54,56,57	0
2	MAN	C	6	11/12	0.85	0.20	32,38,48,51	0
2	BMA	C	3	11/12	0.85	0.17	35,60,65,67	0
7	MAN	I	6	11/12	0.85	0.24	36,39,46,47	0
9	BMA	P	3	11/12	0.87	0.12	25,31,38,45	0
10	BGC	Q	2	11/12	0.91	0.13	23,36,44,46	0
6	MAN	O	6	11/12	0.91	0.17	23,31,39,40	0
6	MAN	H	6	11/12	0.91	0.26	23,29,41,44	0
10	BGC	R	2	11/12	0.91	0.13	16,31,41,45	0
8	MAN	K	4	11/12	0.91	0.17	33,35,41,41	0
8	MAN	K	5	11/12	0.91	0.21	37,39,46,54	0
3	NAG	N	2	14/15	0.91	0.15	25,32,36,44	0
9	MAN	P	4	11/12	0.92	0.13	22,24,33,45	0
6	MAN	H	4	11/12	0.92	0.14	27,31,39,43	0
6	MAN	O	5	11/12	0.92	0.14	22,27,31,34	0
8	BMA	K	3	11/12	0.93	0.12	22,25,29,33	0
6	NAG	O	2	14/15	0.93	0.11	14,17,23,24	0
6	MAN	O	4	11/12	0.93	0.12	27,28,38,40	0
7	BMA	I	3	11/12	0.93	0.16	21,29,41,45	0
7	MAN	I	4	11/12	0.94	0.11	17,23,28,38	0
6	MAN	H	5	11/12	0.94	0.16	20,26,34,48	0
6	BMA	H	3	11/12	0.94	0.17	20,24,31,40	0
6	NAG	H	2	14/15	0.94	0.12	15,19,23,26	0
3	NAG	L	2	14/15	0.94	0.09	13,17,28,32	0
4	NAG	E	2	14/15	0.94	0.12	15,23,32,33	0
8	NAG	K	1	14/15	0.94	0.09	10,12,13,14	0
6	BMA	O	3	11/12	0.95	0.11	23,26,31,41	0
5	MAN	M	10	11/12	0.95	0.11	22,32,38,39	0
5	MAN	F	10	11/12	0.95	0.12	25,32,46,53	0
6	NAG	H	1	14/15	0.95	0.10	12,16,35,39	0

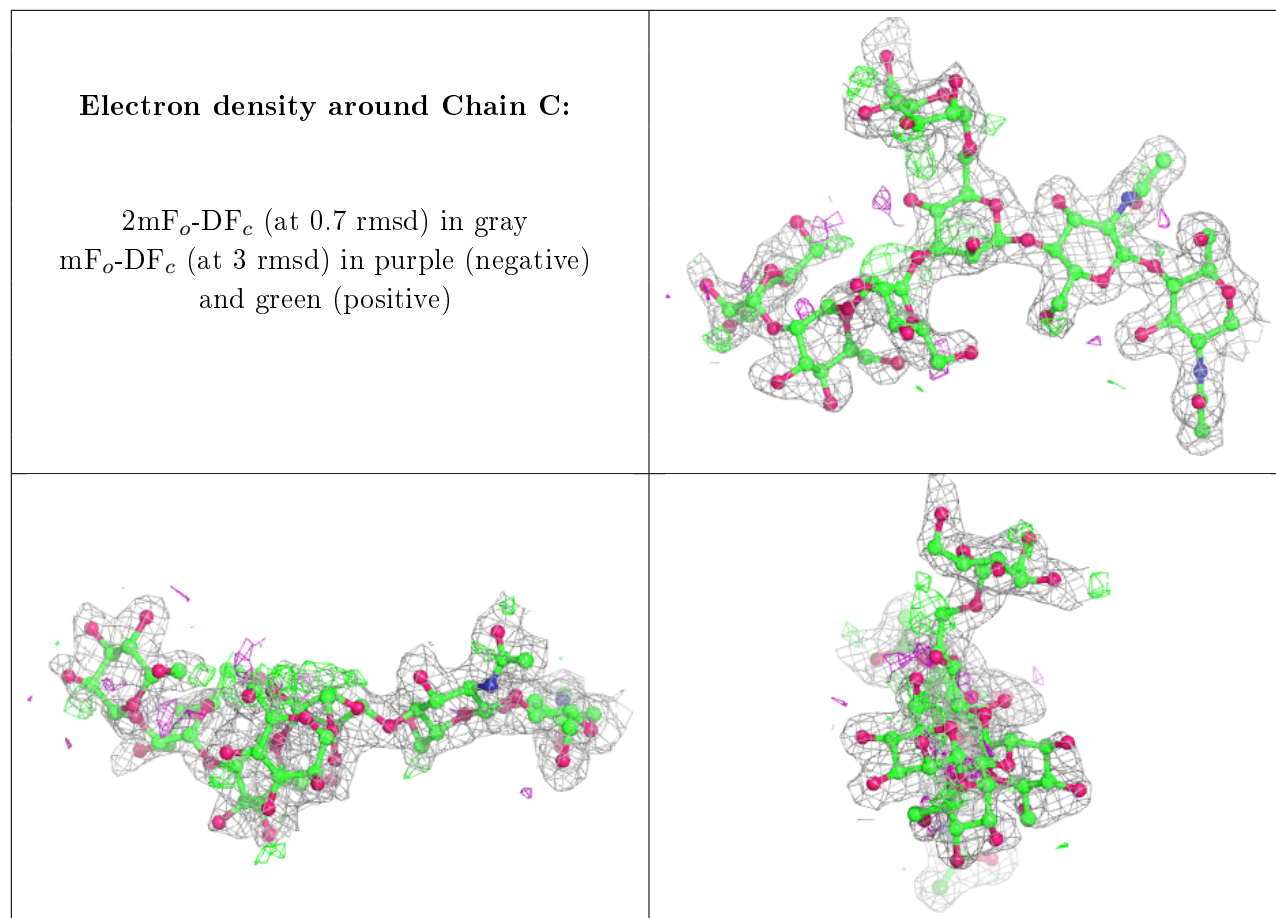
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	F	6	11/12	0.95	0.13	22,24,28,31	0
2	MAN	J	7	11/12	0.95	0.09	20,27,30,31	0
9	MAN	P	5	11/12	0.95	0.10	23,23,30,38	0
2	BMA	J	3	11/12	0.96	0.07	12,17,19,20	0
2	NAG	C	2	14/15	0.96	0.07	15,22,31,33	0
6	NAG	O	1	14/15	0.96	0.07	12,15,29,30	0
2	MAN	J	5	11/12	0.96	0.09	16,23,32,37	0
5	MAN	M	6	11/12	0.96	0.08	19,21,25,26	0
9	NAG	P	2	14/15	0.96	0.10	17,22,28,29	0
5	MAN	F	5	11/12	0.96	0.06	17,19,24,31	0
2	MAN	J	6	11/12	0.96	0.10	15,17,21,28	0
7	MAN	I	5	11/12	0.96	0.12	19,24,30,32	0
3	NAG	G	1	14/15	0.96	0.07	19,25,34,42	0
2	MAN	J	4	11/12	0.96	0.10	18,25,31,32	0
3	NAG	D	2	14/15	0.96	0.13	16,21,23,29	0
7	NAG	I	2	14/15	0.97	0.10	14,18,24,29	0
5	NAG	F	1	14/15	0.97	0.10	15,17,20,21	0
5	MAN	M	5	11/12	0.97	0.06	12,14,18,24	0
3	NAG	D	1	14/15	0.97	0.07	13,14,16,16	0
5	MAN	F	9	11/12	0.97	0.10	16,18,23,24	0
8	NAG	K	2	14/15	0.97	0.07	12,16,24,25	0
3	NAG	N	1	14/15	0.97	0.06	16,20,30,32	0
5	NAG	M	2	14/15	0.97	0.06	8,9,10,11	0
5	MAN	F	4	11/12	0.98	0.05	13,14,16,18	0
7	NAG	I	1	14/15	0.98	0.05	13,15,17,18	0
5	MAN	M	7	11/12	0.98	0.06	9,10,11,11	0
5	MAN	M	9	11/12	0.98	0.04	12,14,18,19	0
5	MAN	F	7	11/12	0.98	0.05	12,13,15,15	0
4	NAG	E	1	14/15	0.98	0.06	12,13,17,18	0
5	NAG	F	2	14/15	0.98	0.06	12,13,14,14	0
9	NAG	P	1	14/15	0.98	0.06	12,14,15,16	0
2	NAG	J	1	14/15	0.98	0.05	8,9,10,10	0
5	BMA	F	3	11/12	0.98	0.05	14,15,17,18	0
2	NAG	C	1	14/15	0.98	0.06	13,14,15,15	0
5	NAG	M	1	14/15	0.98	0.05	9,11,14,15	0
2	NAG	J	2	14/15	0.98	0.04	9,12,15,21	0
5	MAN	F	8	11/12	0.99	0.05	13,14,15,19	0
5	BMA	M	3	11/12	0.99	0.04	10,11,12,13	0
5	MAN	M	4	11/12	0.99	0.06	9,9,10,12	0
3	NAG	L	1	14/15	0.99	0.05	8,10,11,12	0
5	MAN	M	8	11/12	0.99	0.05	11,11,14,17	0

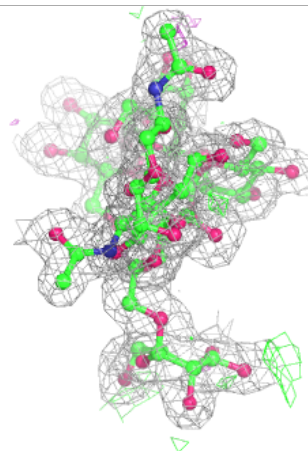
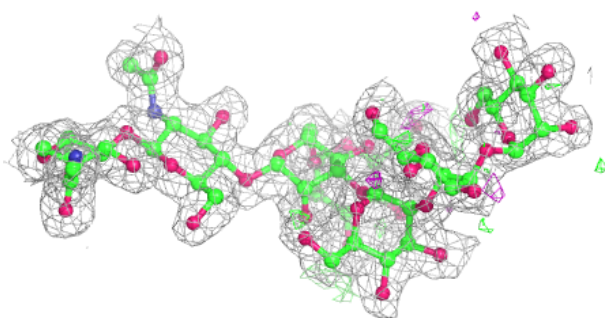
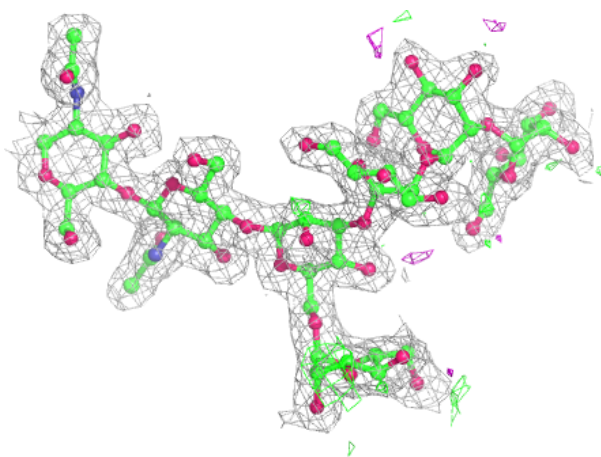
The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.



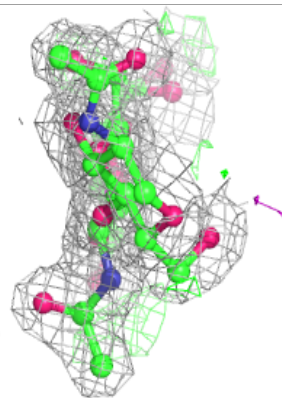
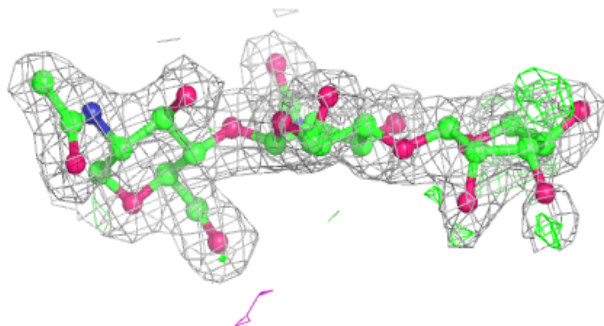
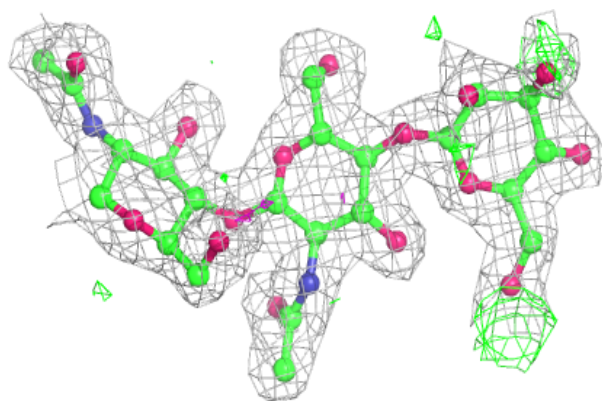
Electron density around Chain J:

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

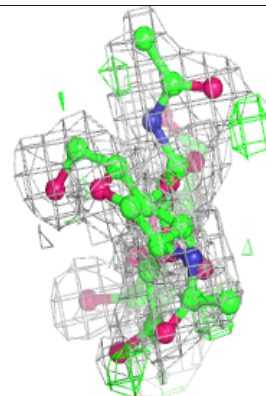
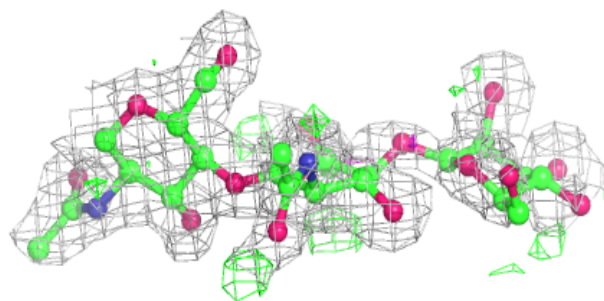
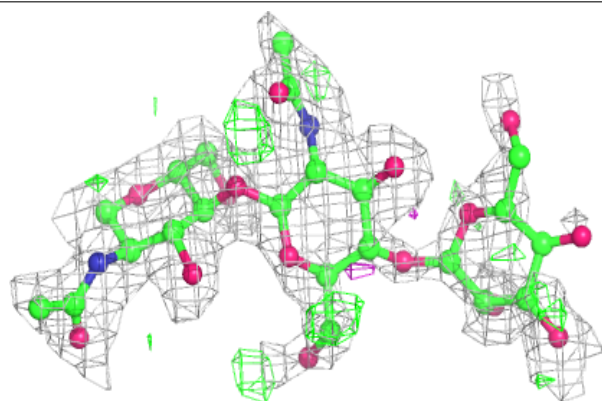


Electron density around Chain D:

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

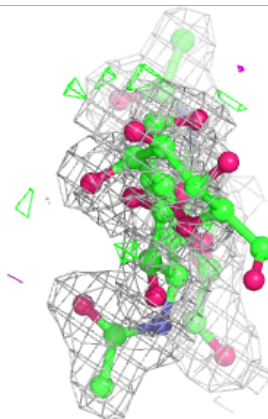
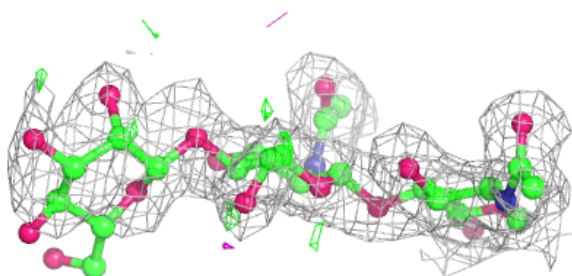
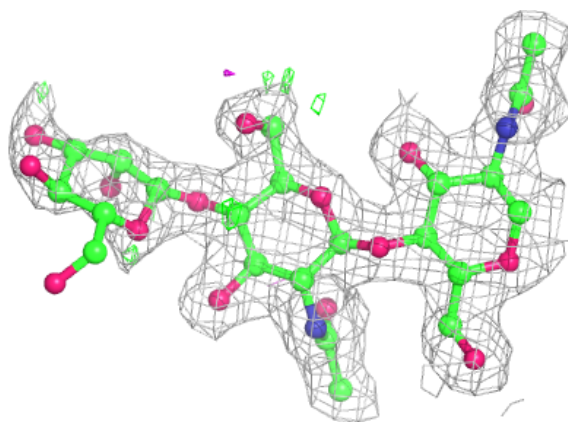
**Electron density around Chain G:**

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



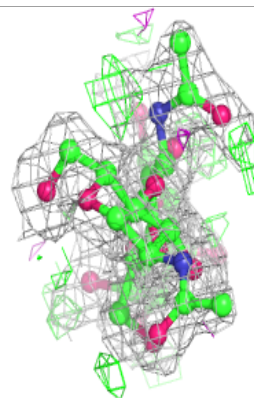
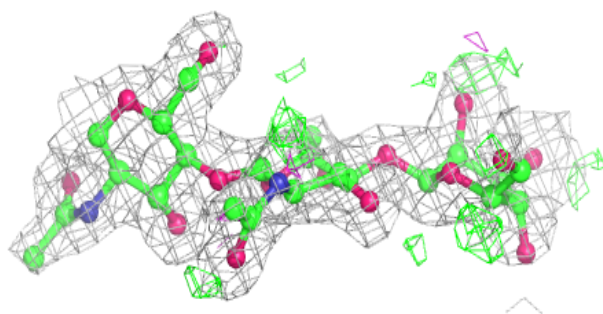
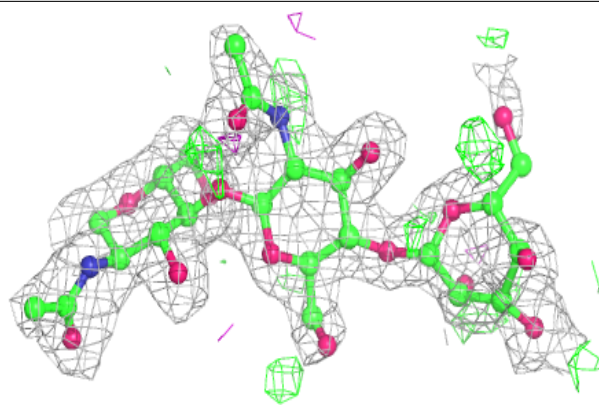
Electron density around Chain L:

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



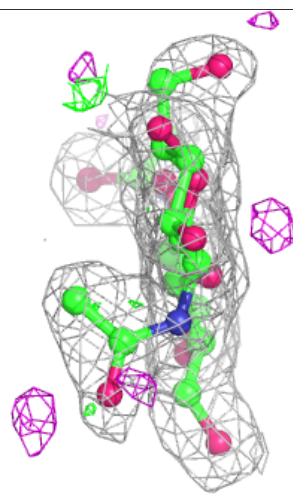
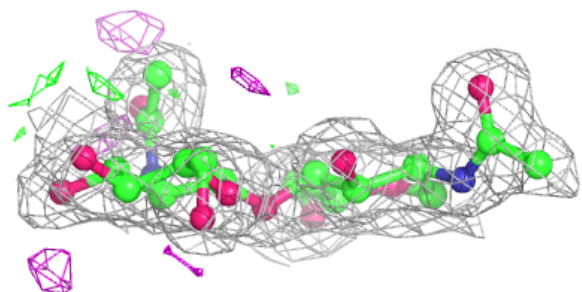
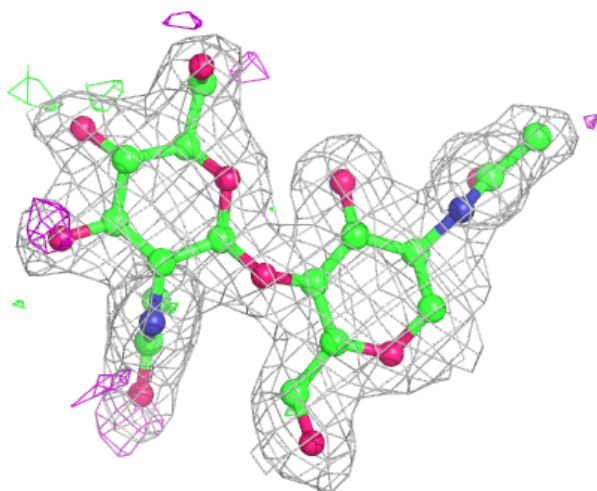
Electron density around Chain N:

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



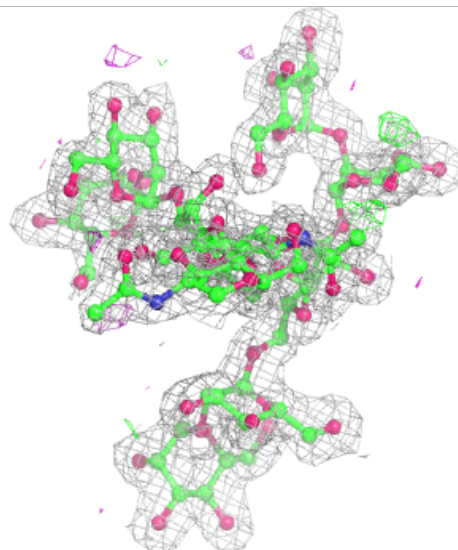
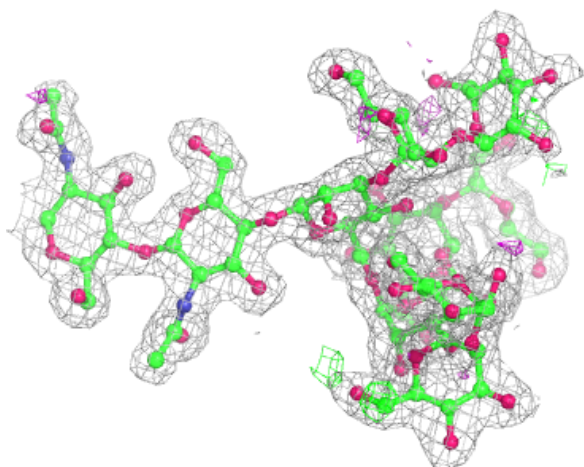
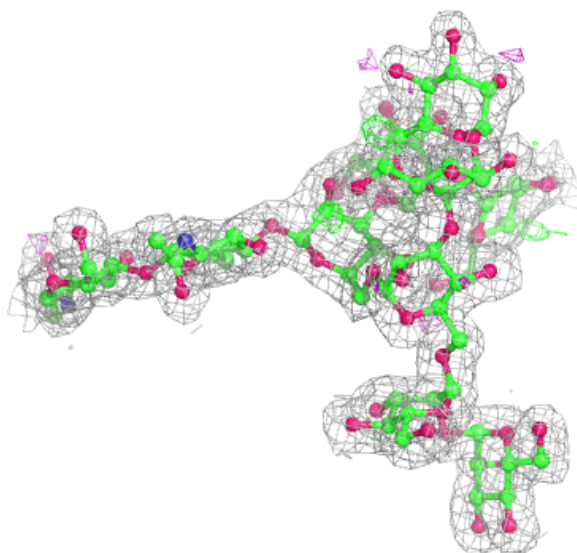
Electron density around Chain E:

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



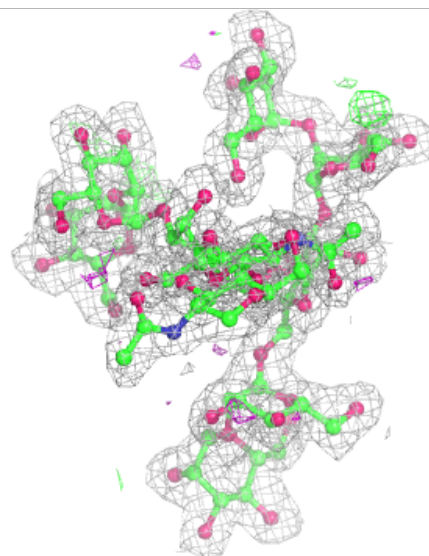
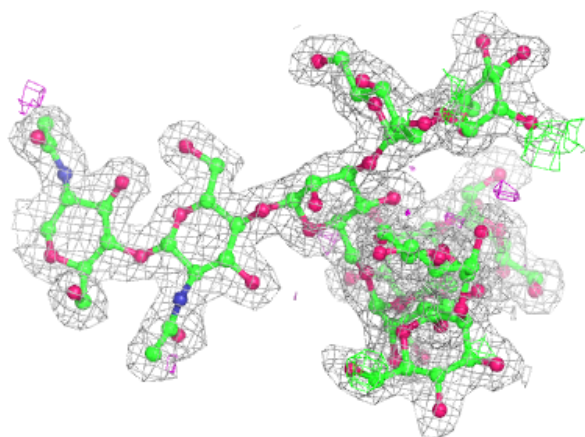
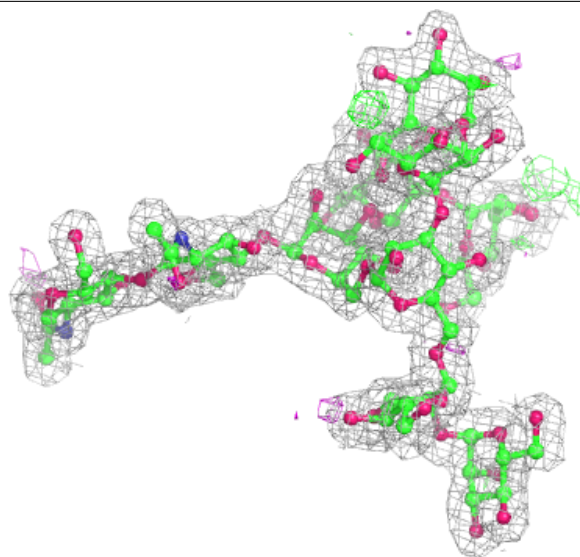
Electron density around Chain F:

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



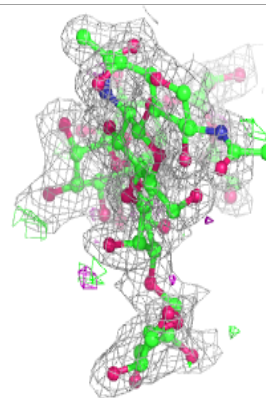
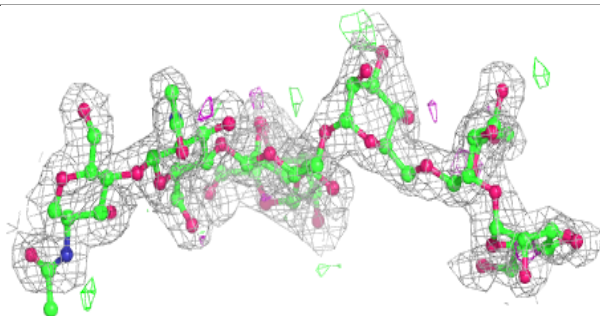
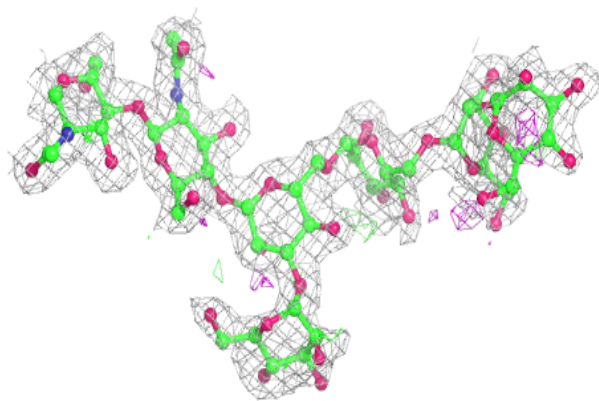
Electron density around Chain M:

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

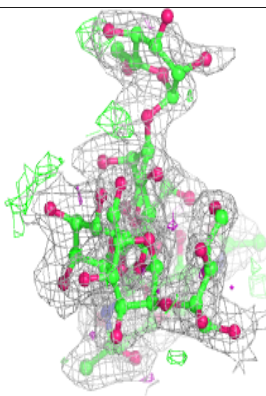
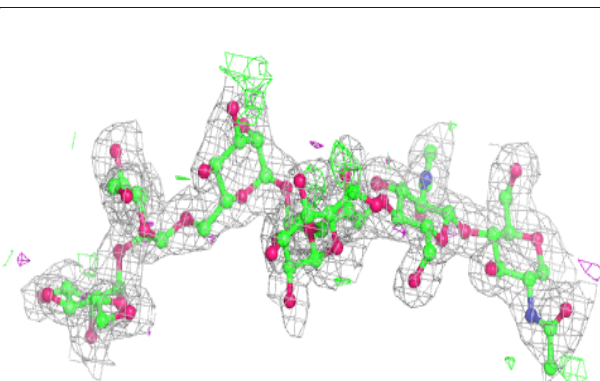
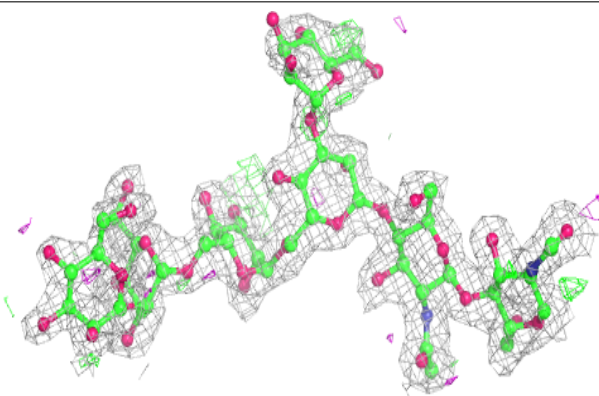


Electron density around Chain H:

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

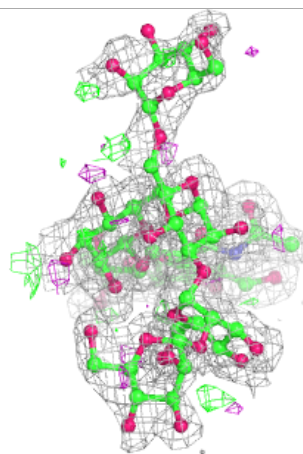
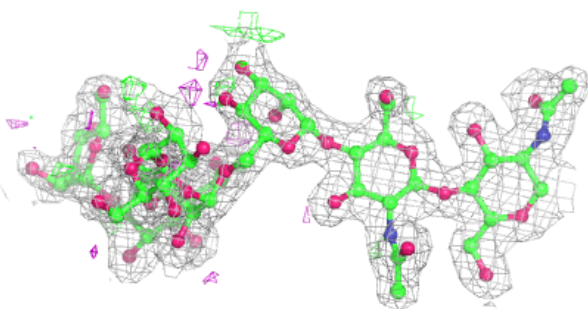
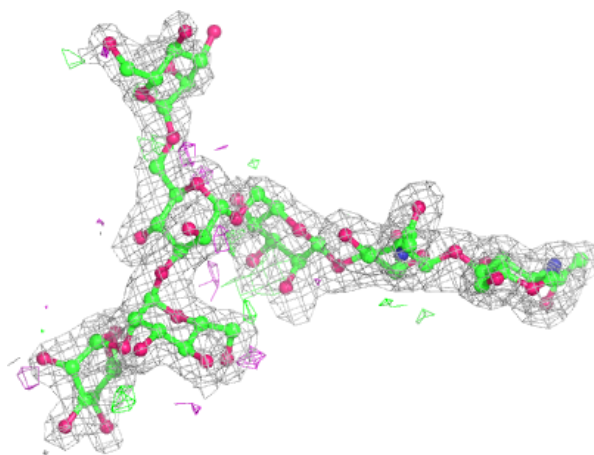
**Electron density around Chain O:**

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



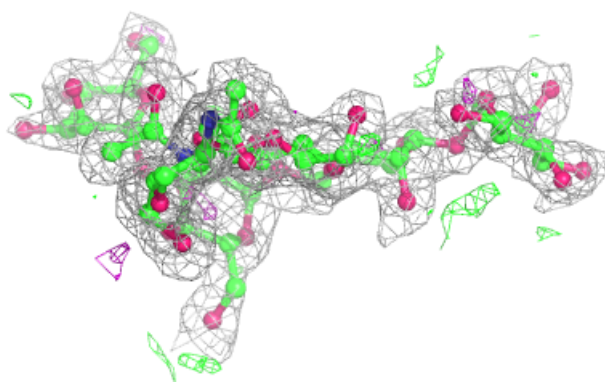
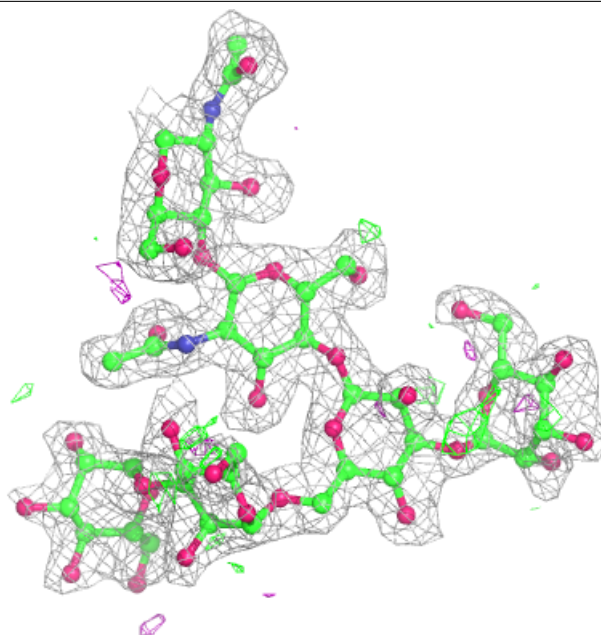
Electron density around Chain I:

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



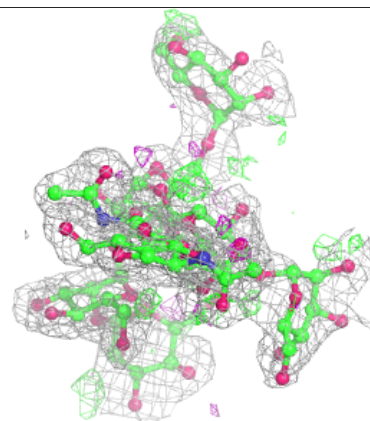
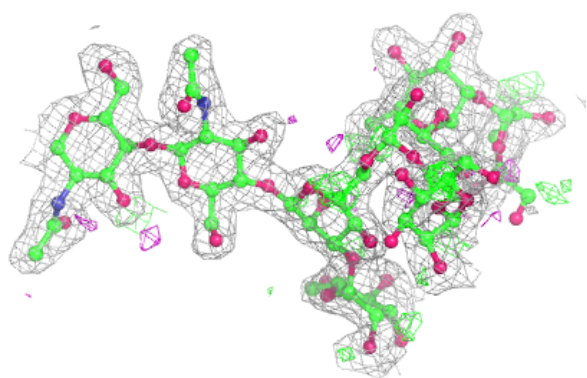
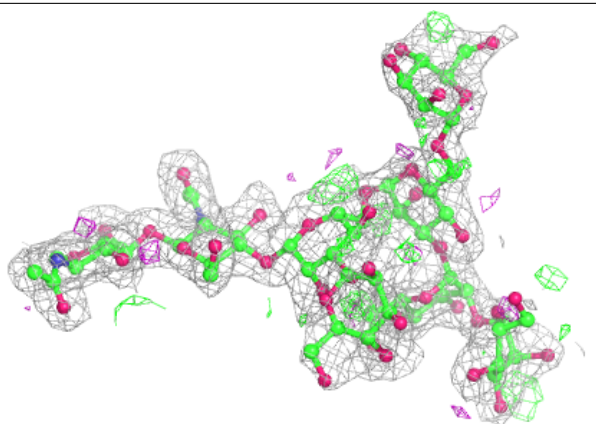
Electron density around Chain K:

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



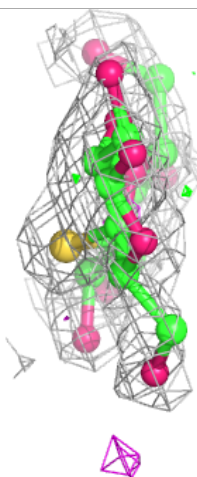
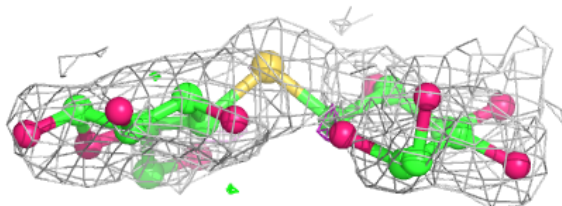
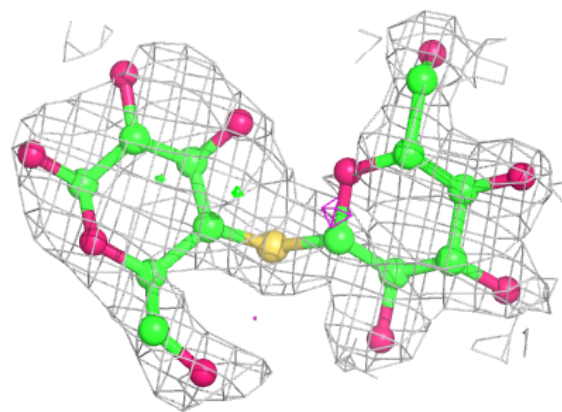
Electron density around Chain P:

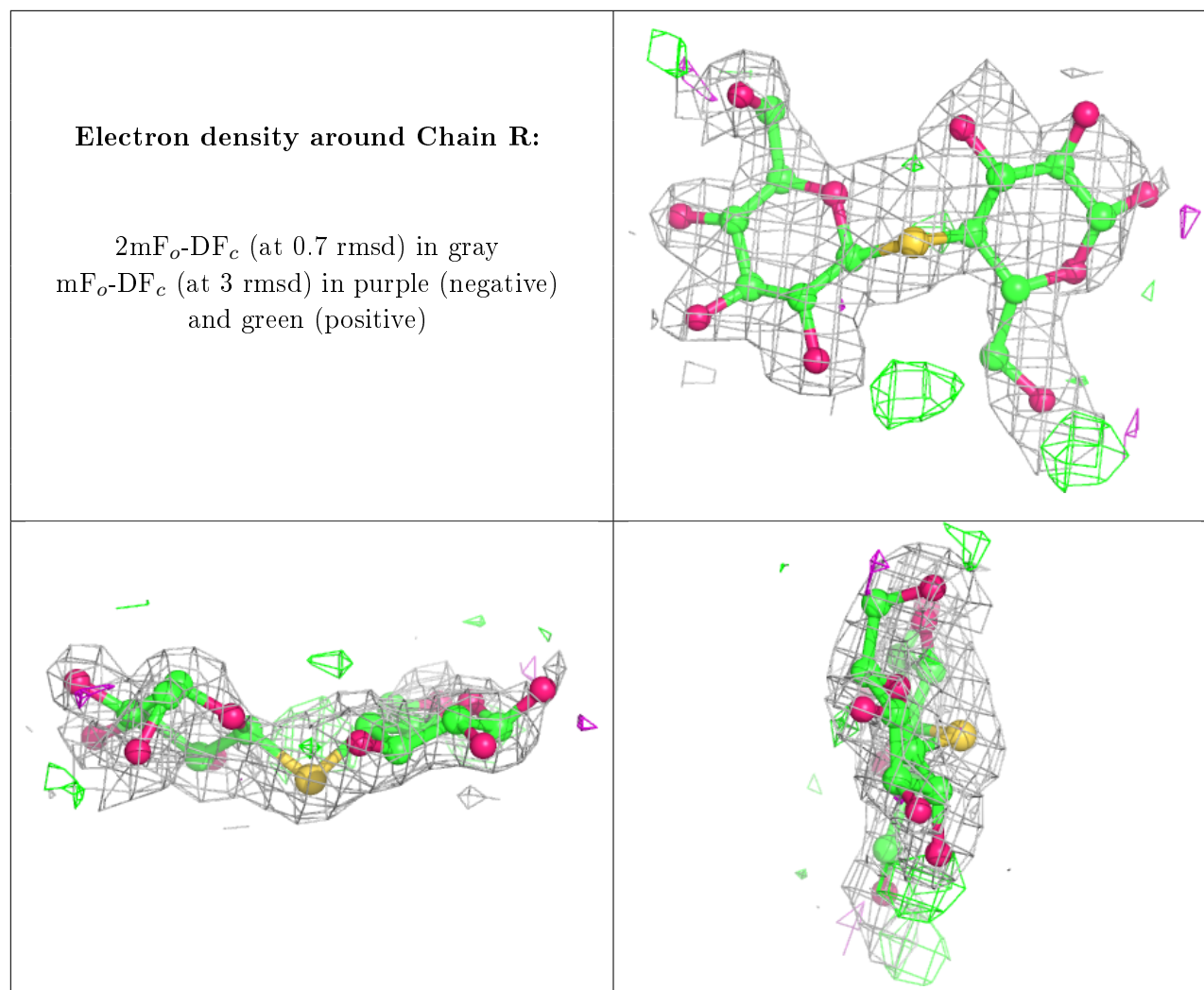
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain Q:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	MRD	A	943	8/8	0.82	0.20	15,26,33,39	0
11	NAG	A	908	14/15	0.83	0.38	39,53,62,67	0
11	NAG	B	946	14/15	0.90	0.20	34,50,55,57	0
11	NAG	B	908	14/15	0.90	0.21	34,39,46,46	0
12	MRD	B	949	8/8	0.92	0.17	35,39,42,43	0
11	NAG	A	941	14/15	0.94	0.15	24,32,36,36	0
12	MRD	A	942	8/8	0.94	0.09	16,17,20,27	0
12	MRD	B	948	8/8	0.94	0.13	15,19,33,35	0
11	NAG	B	947	14/15	0.96	0.13	22,24,28,31	0

6.5 Other polymers

There are no such residues in this entry.