



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2026 – 11:51 PM UTC

PDB ID : 7BYX / pdb_00007byx
Title : Crystal structure of exo-beta-1,3-galactanase from Phanerochaete chrysosporium Pc1,3Gal43A E208A with beta-1,3-galactotriose
Authors : Matsuyama, K.; Ishida, T.; Kishine, N.; Fujimoto, Z.; Igarashi, K.; Kaneko, S.
Deposited on : 2020-04-24
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

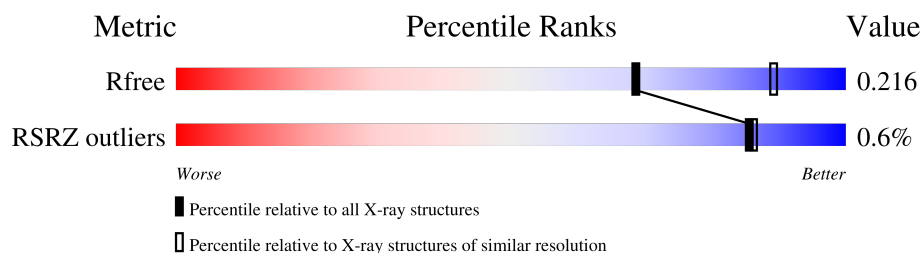
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14570 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.

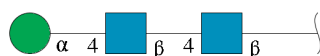
- Molecule 1 is a protein called Galactan 1,3-beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	2	0
			3222	2024	549	641	8			
1	B	427	Total	C	N	O	S	0	3	0
			3226	2026	550	642	8			
1	C	427	Total	C	N	O	S	0	2	0
			3224	2023	551	643	7			
1	D	427	Total	C	N	O	S	0	0	0
			3214	2017	549	641	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	ALA	GLU	engineered mutation	UNP Q50KB2
B	208	ALA	GLU	engineered mutation	UNP Q50KB2
C	208	ALA	GLU	engineered mutation	UNP Q50KB2
D	208	ALA	GLU	engineered mutation	UNP Q50KB2

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



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

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

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	3	Total	C	O		0	0	0
			34	18	16				
3	L	3	Total	C	O		0	0	0
			34	18	16				
3	P	3	Total	C	O		0	0	0
			34	18	16				
3	S	3	Total	C	O		0	0	0
			34	18	16				

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



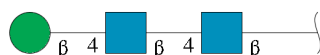
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	J	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	R	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 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.

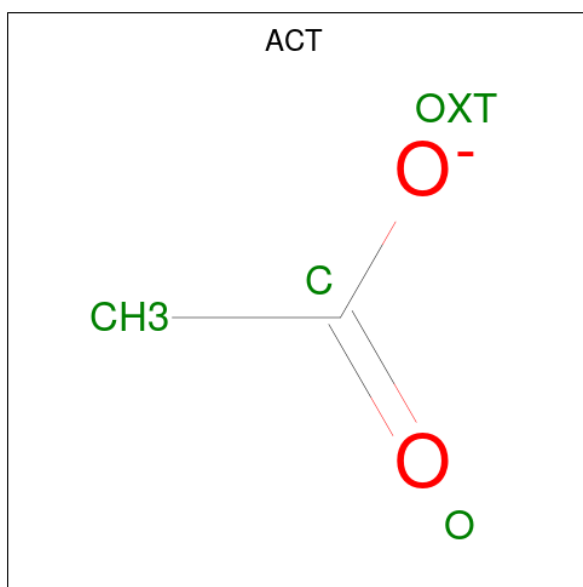


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

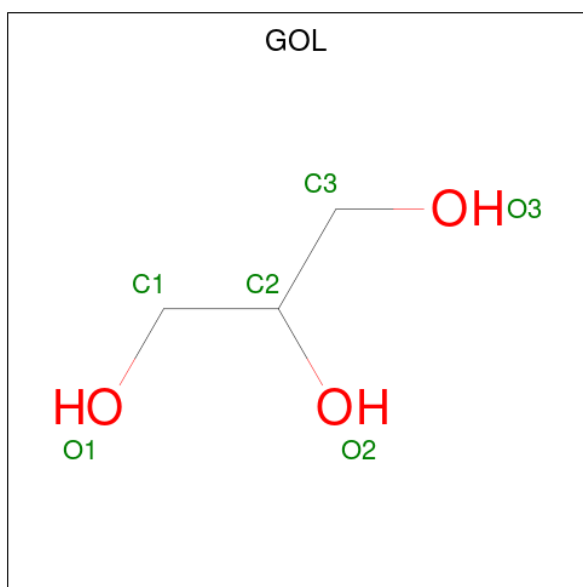
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	D	1	Total	Ca	0	0
			1	1		

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



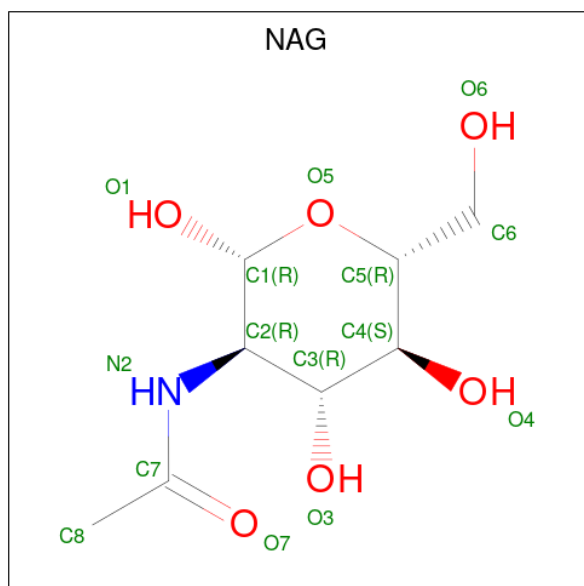
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	B	1	Total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

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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	338	Total	O	0	0
			338	338		
11	B	291	Total	O	0	0
			291	291		
11	C	181	Total	O	0	0
			181	181		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	196	Total 196	O 196	0	0

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3 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.74Å 156.74Å 147.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.14 – 2.30 31.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (31.14-2.30) 98.8 (31.14-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.16_3546, REFMAC 5.8.0158	Depositor
R, R_{free}	0.161 , 0.214 0.163 , 0.216	Depositor DCC
R_{free} test set	4569 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14570	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.34% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

40 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	1,2	14,14,15	1.92	3 (21%)	17,19,21	1.41	2 (11%)
2	NAG	E	2	2	14,14,15	1.96	3 (21%)	17,19,21	1.44	3 (17%)
2	MAN	E	3	2	11,11,12	0.88	0	15,15,17	1.30	1 (6%)
2	NAG	F	1	1,2	14,14,15	1.86	3 (21%)	17,19,21	1.83	3 (17%)
2	NAG	F	2	2	14,14,15	2.00	4 (28%)	17,19,21	1.15	2 (11%)
2	MAN	F	3	2	11,11,12	1.16	1 (9%)	15,15,17	1.14	2 (13%)
2	NAG	G	1	1,2	14,14,15	1.67	3 (21%)	17,19,21	1.32	1 (5%)
2	NAG	G	2	2	14,14,15	1.98	3 (21%)	17,19,21	1.12	0
2	MAN	G	3	2	11,11,12	1.08	0	15,15,17	1.18	2 (13%)
3	GAL	H	1	3	12,12,12	1.37	1 (8%)	17,17,17	1.30	2 (11%)
3	GAL	H	2	3	11,11,12	1.54	2 (18%)	15,15,17	0.83	0
3	GAL	H	3	3	11,11,12	1.49	2 (18%)	15,15,17	0.92	1 (6%)
4	NAG	I	1	4,1	14,14,15	1.95	4 (28%)	17,19,21	1.79	3 (17%)
4	NDG	I	2	4	14,14,15	0.89	1 (7%)	17,19,21	1.17	2 (11%)
5	NAG	J	1	5,1	14,14,15	1.88	3 (21%)	17,19,21	1.61	4 (23%)
5	NAG	J	2	5	14,14,15	2.11	5 (35%)	17,19,21	2.32	6 (35%)
2	NAG	K	1	1,2	14,14,15	1.84	3 (21%)	17,19,21	1.99	4 (23%)
2	NAG	K	2	2	14,14,15	2.04	4 (28%)	17,19,21	0.99	1 (5%)
2	MAN	K	3	2	11,11,12	1.21	1 (9%)	15,15,17	1.00	0
3	GAL	L	1	3	12,12,12	1.29	1 (8%)	17,17,17	0.57	0
3	GAL	L	2	3	11,11,12	1.78	3 (27%)	15,15,17	1.39	2 (13%)
3	GAL	L	3	3	11,11,12	1.65	2 (18%)	15,15,17	0.96	1 (6%)
6	NAG	M	1	1,6	14,14,15	1.82	4 (28%)	17,19,21	2.60	5 (29%)
6	NAG	M	2	6	14,14,15	2.01	4 (28%)	17,19,21	1.57	3 (17%)
6	BMA	M	3	6	11,11,12	1.63	1 (9%)	15,15,17	1.40	2 (13%)
4	NAG	N	1	4,1	14,14,15	2.00	5 (35%)	17,19,21	1.51	3 (17%)
4	NDG	N	2	4	14,14,15	0.98	1 (7%)	17,19,21	1.62	2 (11%)
5	NAG	O	1	5,1	14,14,15	1.99	4 (28%)	17,19,21	1.52	3 (17%)
5	NAG	O	2	5	14,14,15	2.28	4 (28%)	17,19,21	2.93	7 (41%)
3	GAL	P	1	3	12,12,12	1.39	1 (8%)	17,17,17	0.97	1 (5%)
3	GAL	P	2	3	11,11,12	1.84	4 (36%)	15,15,17	1.07	0
3	GAL	P	3	3	11,11,12	1.34	2 (18%)	15,15,17	1.40	1 (6%)
2	NAG	Q	1	1,2	14,14,15	2.03	5 (35%)	17,19,21	1.70	4 (23%)
2	NAG	Q	2	2	14,14,15	1.94	3 (21%)	17,19,21	1.26	2 (11%)
2	MAN	Q	3	2	11,11,12	1.05	1 (9%)	15,15,17	1.41	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	R	1	5,1	14,14,15	1.95	4 (28%)	17,19,21	1.45	2 (11%)
5	NAG	R	2	5	14,14,15	2.12	4 (28%)	17,19,21	1.30	2 (11%)
3	GAL	S	1	3	12,12,12	1.34	1 (8%)	17,17,17	1.01	1 (5%)
3	GAL	S	2	3	11,11,12	1.62	2 (18%)	15,15,17	0.71	0
3	GAL	S	3	3	11,11,12	1.71	3 (27%)	15,15,17	1.65	2 (13%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	4/6/23/26	0/1/1/1
3	GAL	P	1	3	-	0/2/22/22	0/1/1/1
3	GAL	P	2	3	-	2/2/19/22	0/1/1/1
3	GAL	P	3	3	-	0/2/19/22	0/1/1/1
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	3/6/23/26	0/1/1/1
2	MAN	Q	3	2	-	0/2/19/22	1/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
3	GAL	S	1	3	-	2/2/22/22	0/1/1/1
3	GAL	S	2	3	-	0/2/19/22	0/1/1/1
3	GAL	S	3	3	-	0/2/19/22	0/1/1/1

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	2	NAG	O5-C1	4.84	1.51	1.43
5	R	2	NAG	O5-C1	4.59	1.51	1.43
2	Q	1	NAG	O5-C1	4.55	1.51	1.43
4	I	1	NAG	O5-C1	4.54	1.51	1.43
2	K	2	NAG	O5-C1	4.53	1.51	1.43

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1	NAG	C1-O5-C5	-7.83	101.69	112.19
5	O	2	NAG	C2-N2-C7	7.36	132.76	122.90
5	O	2	NAG	C8-C7-N2	6.14	126.30	116.12
2	F	1	NAG	C2-N2-C7	-5.62	115.37	122.90
5	J	2	NAG	C2-N2-C7	-5.62	115.37	122.90

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	2	NAG	C3-C2-N2-C7
5	R	2	NAG	O5-C5-C6-O6
3	H	1	GAL	O5-C5-C6-O6
4	N	2	NDG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	P	2	GAL	O5-C5-C6-O6

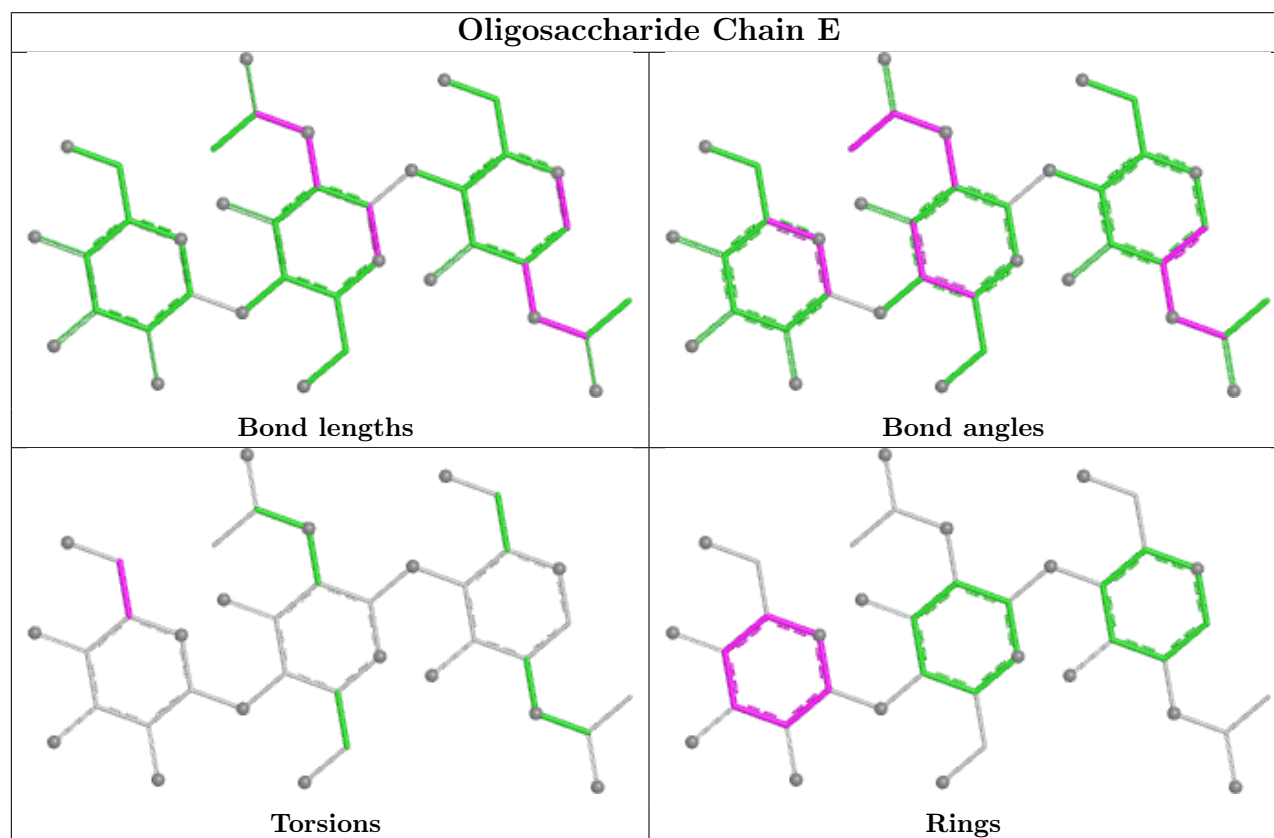
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	3	MAN	C1-C2-C3-C4-C5-O5
2	E	3	MAN	C1-C2-C3-C4-C5-O5

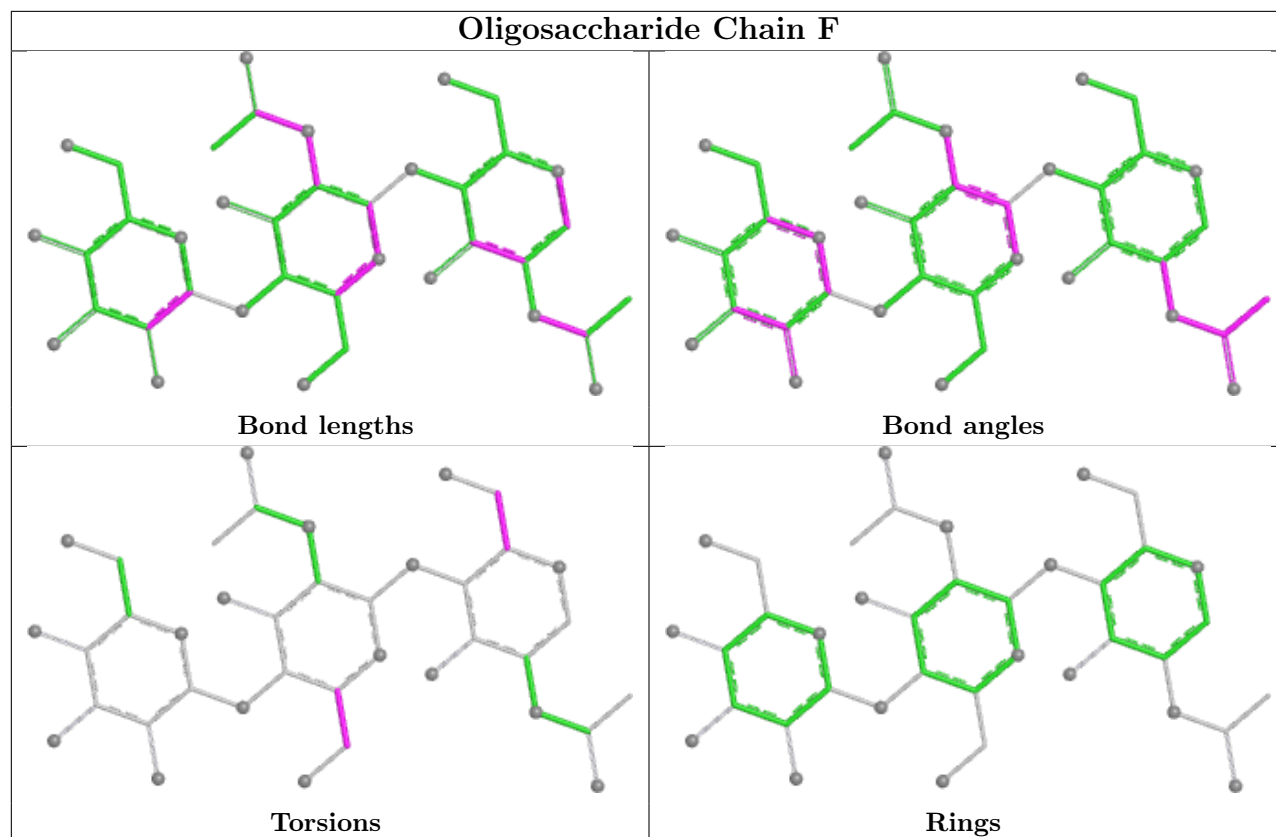
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	MAN	0	1

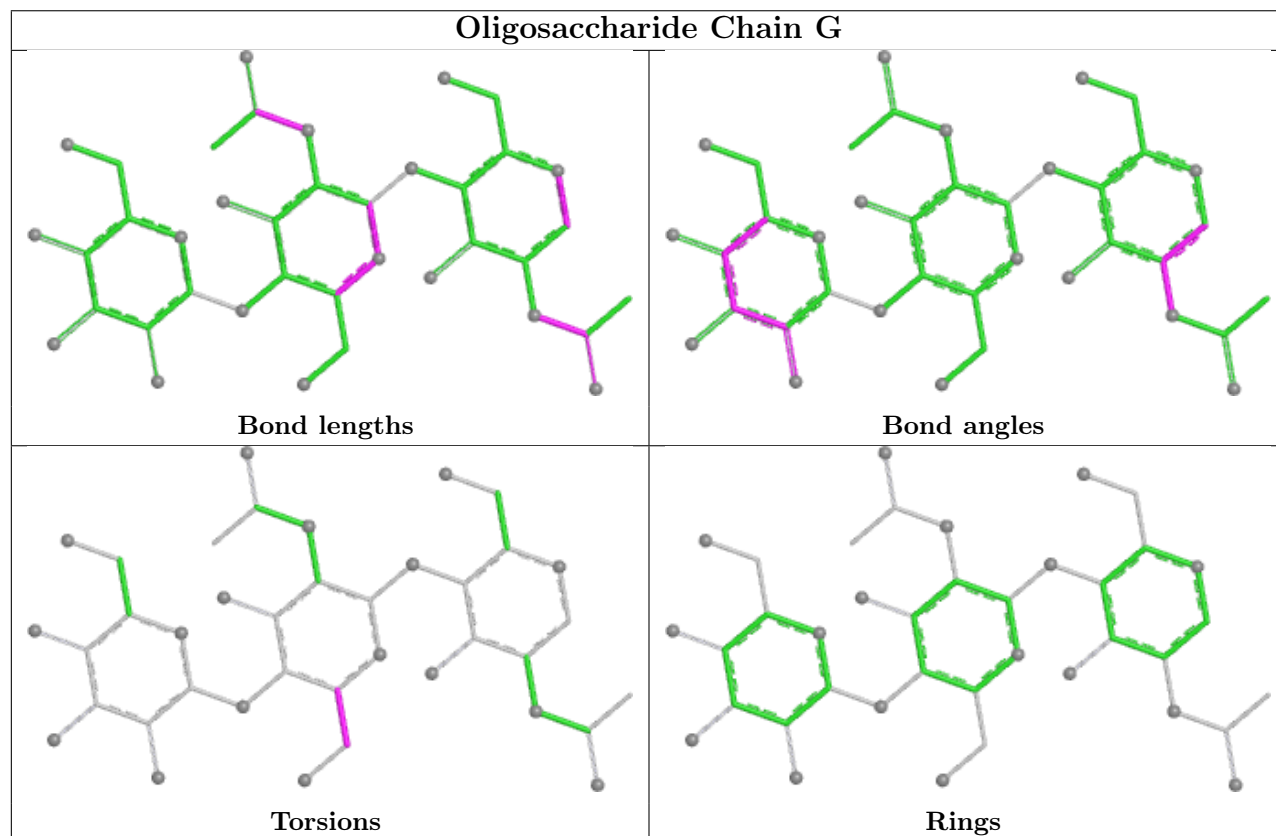
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



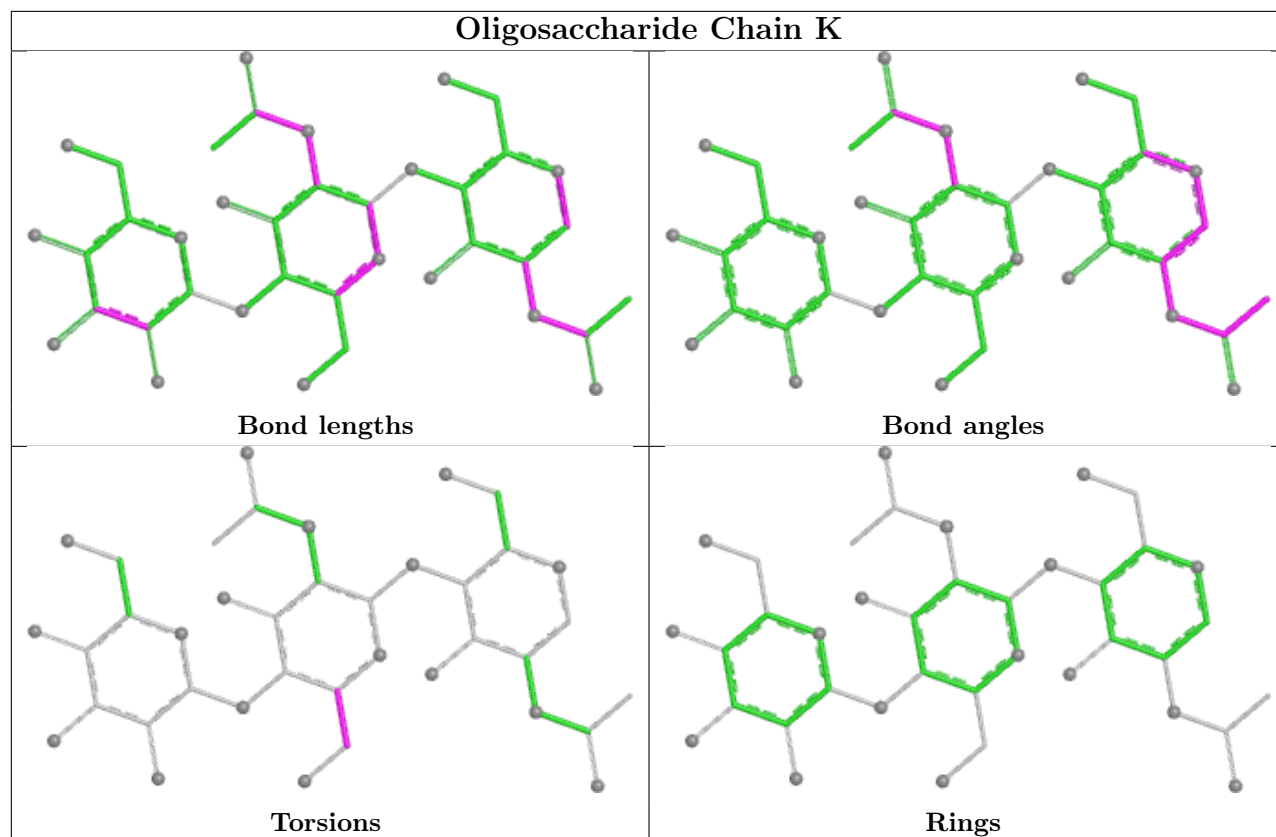
Oligosaccharide Chain F



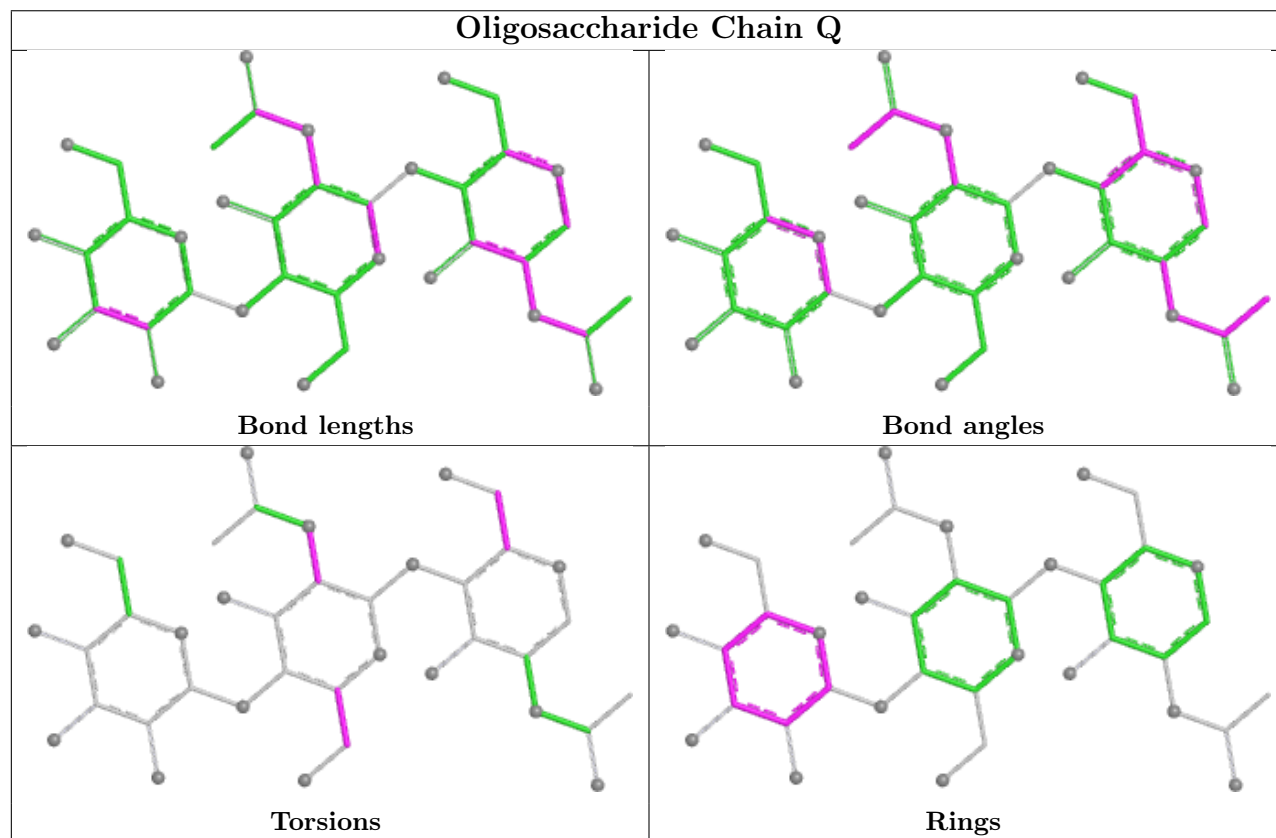
Oligosaccharide Chain G

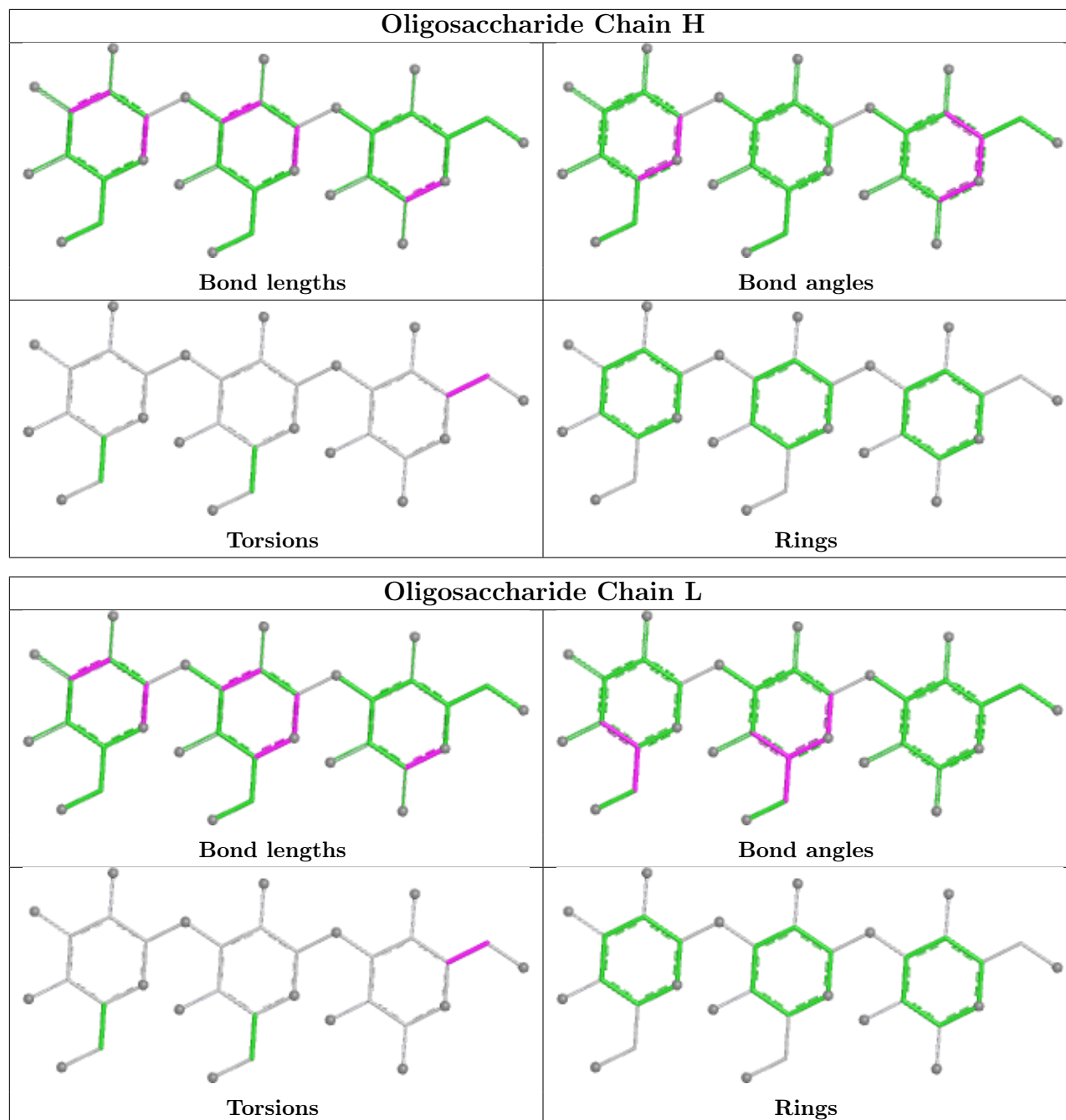


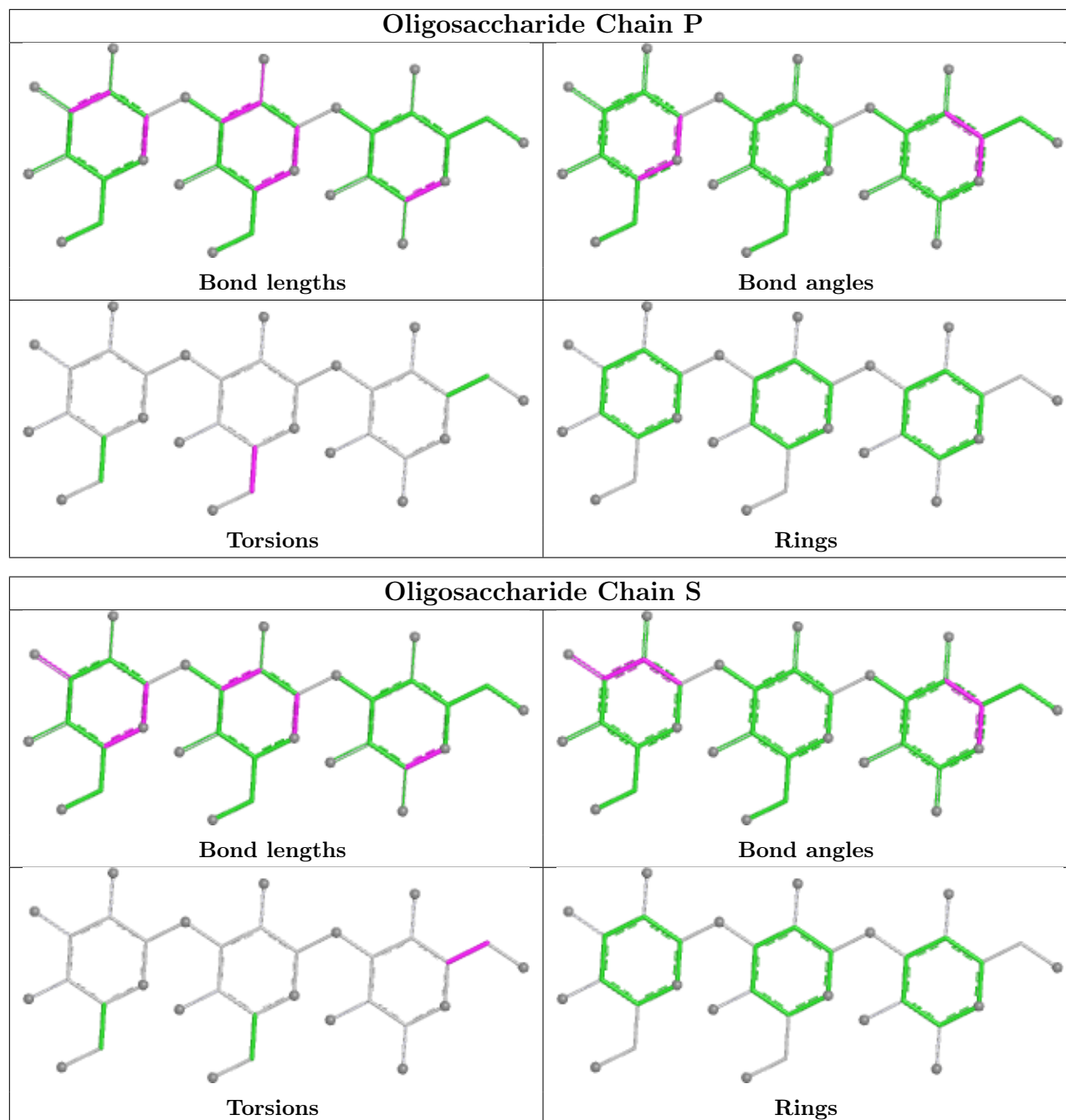
Oligosaccharide Chain K

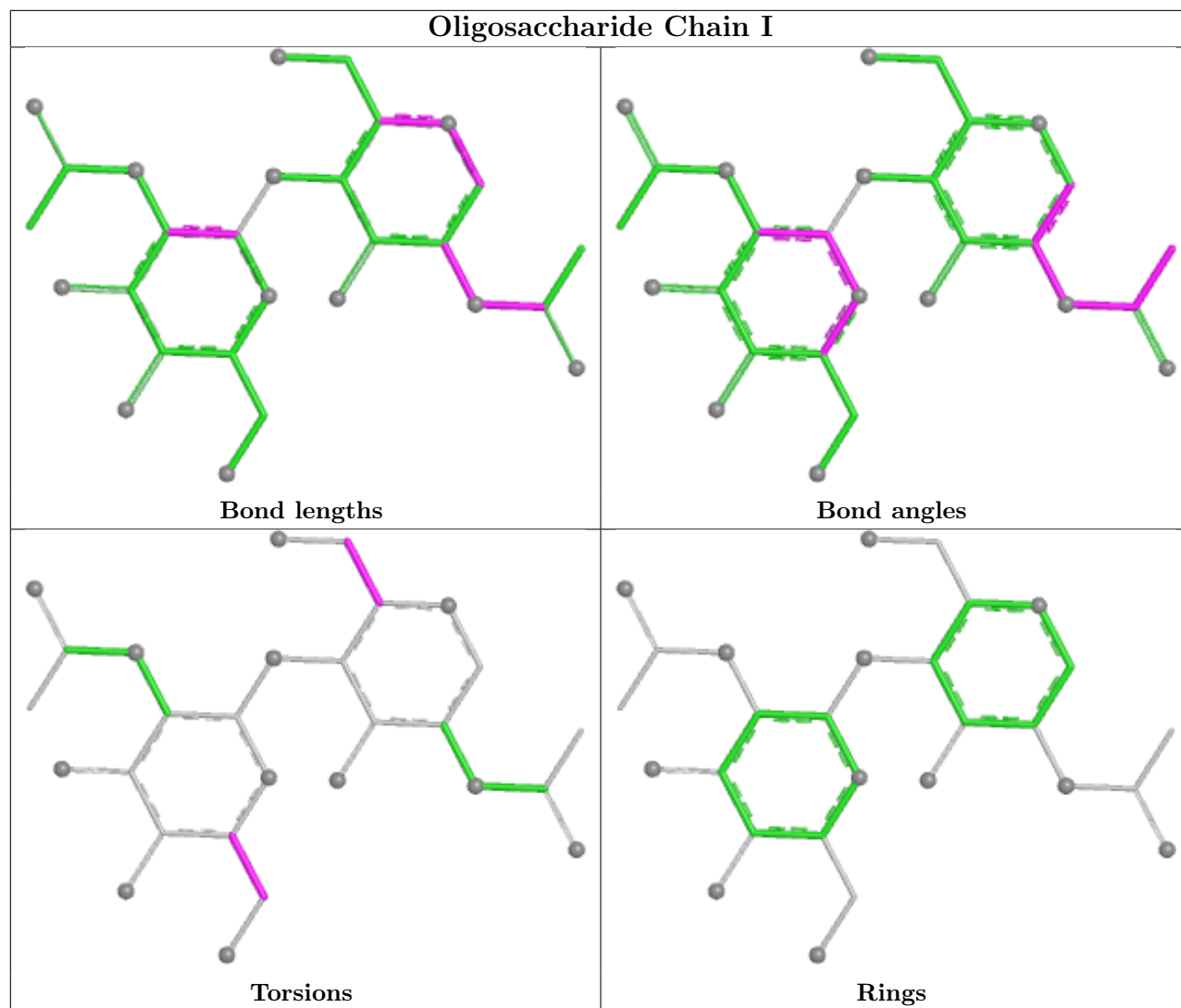


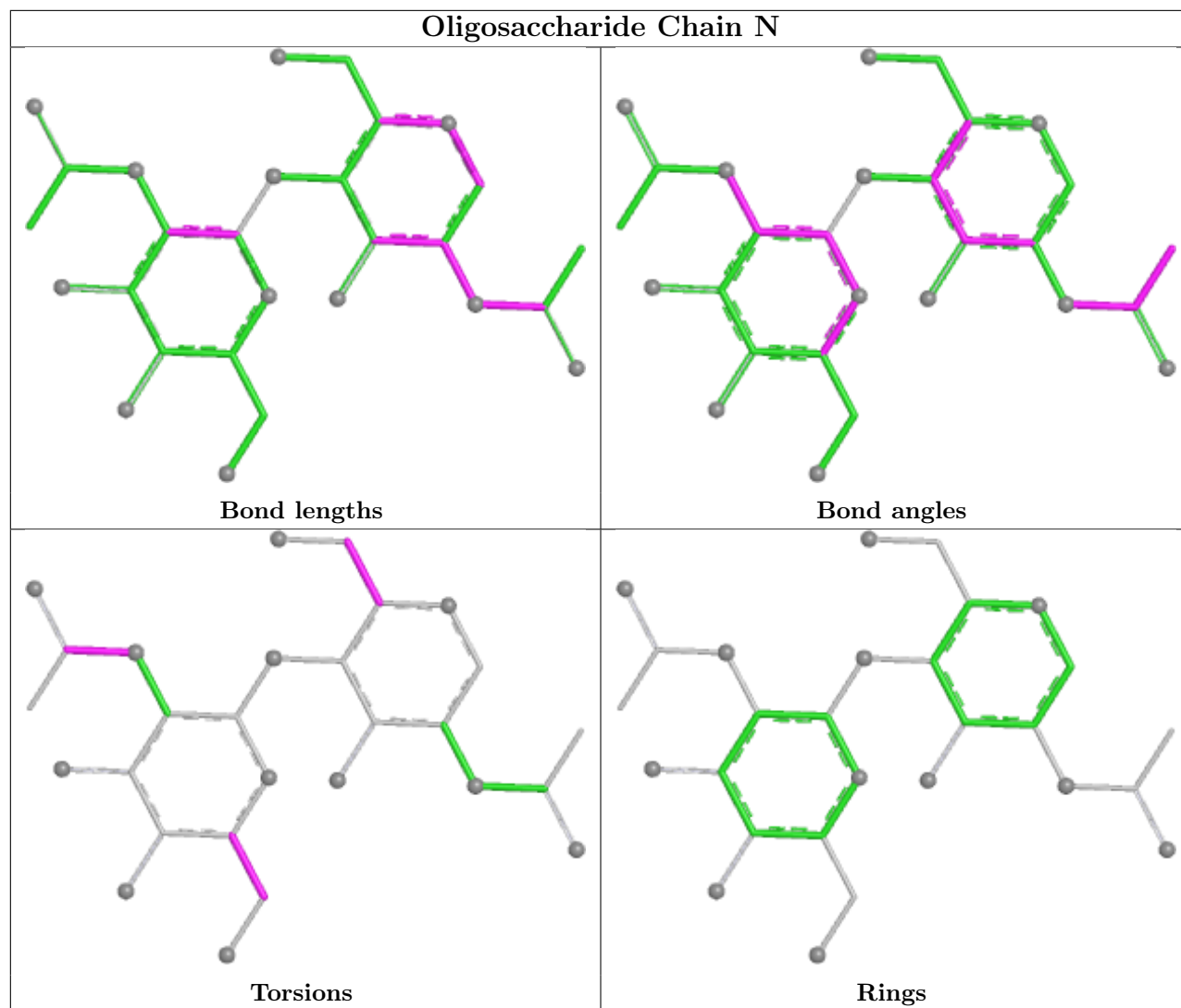
Oligosaccharide Chain Q

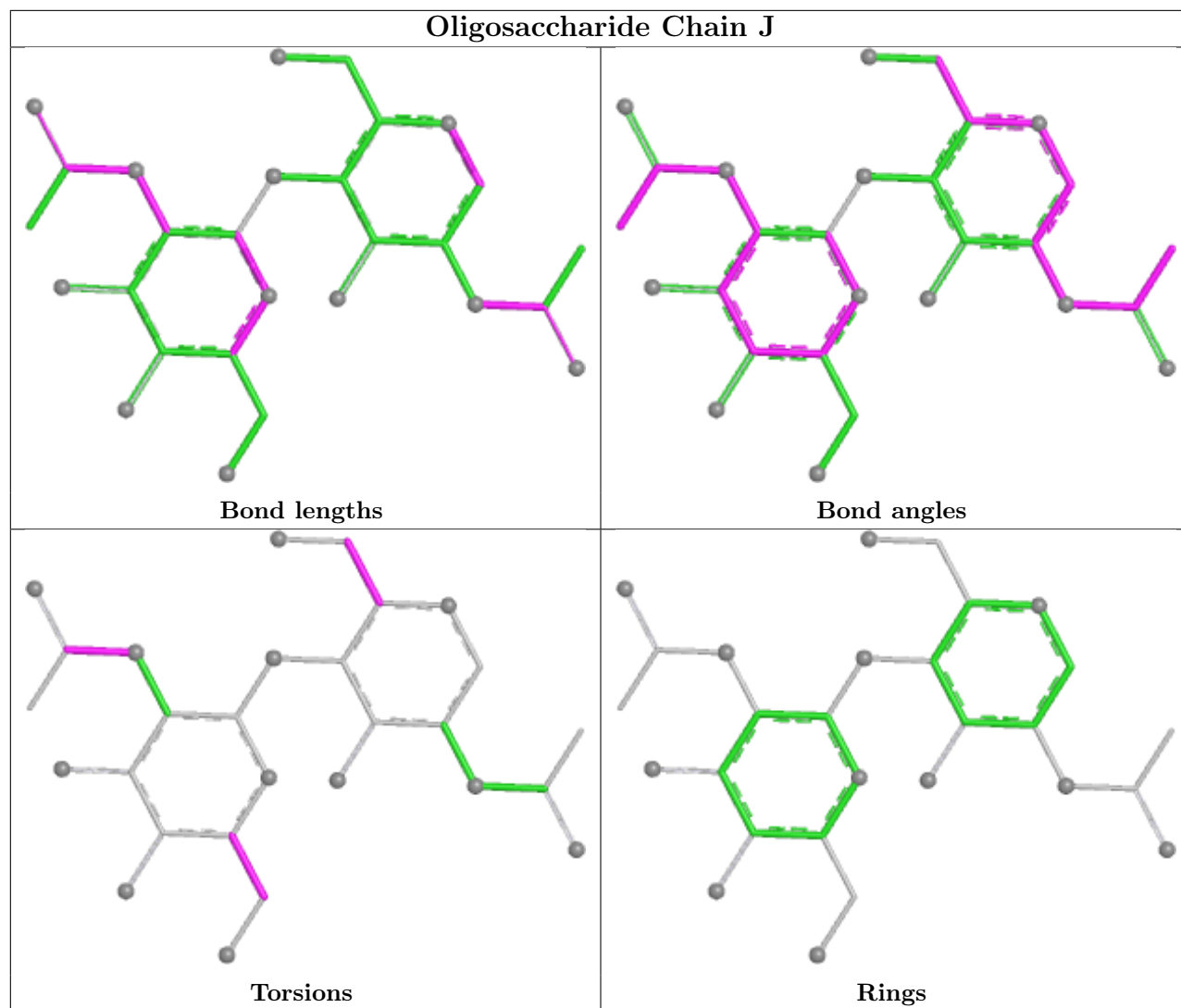


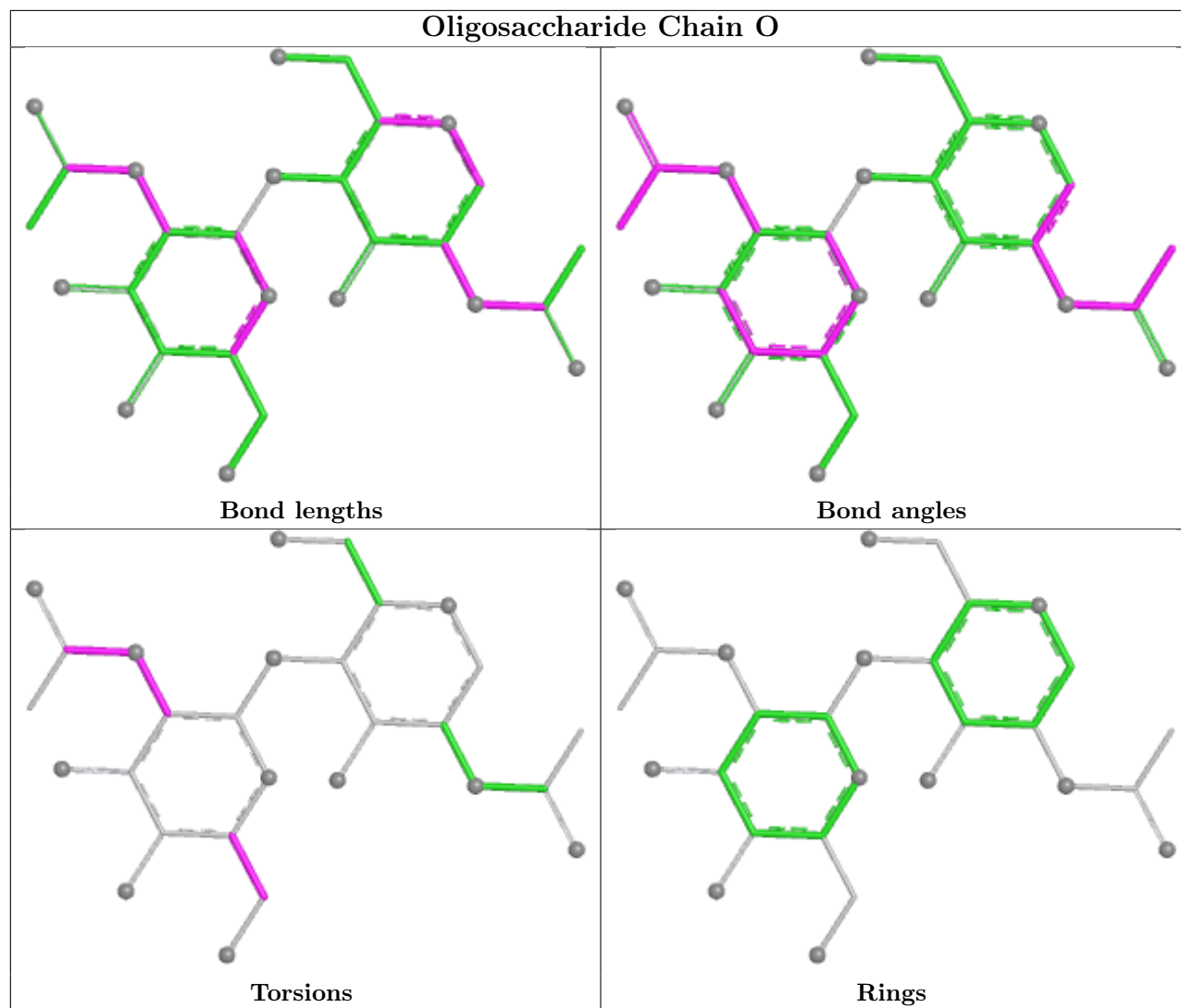


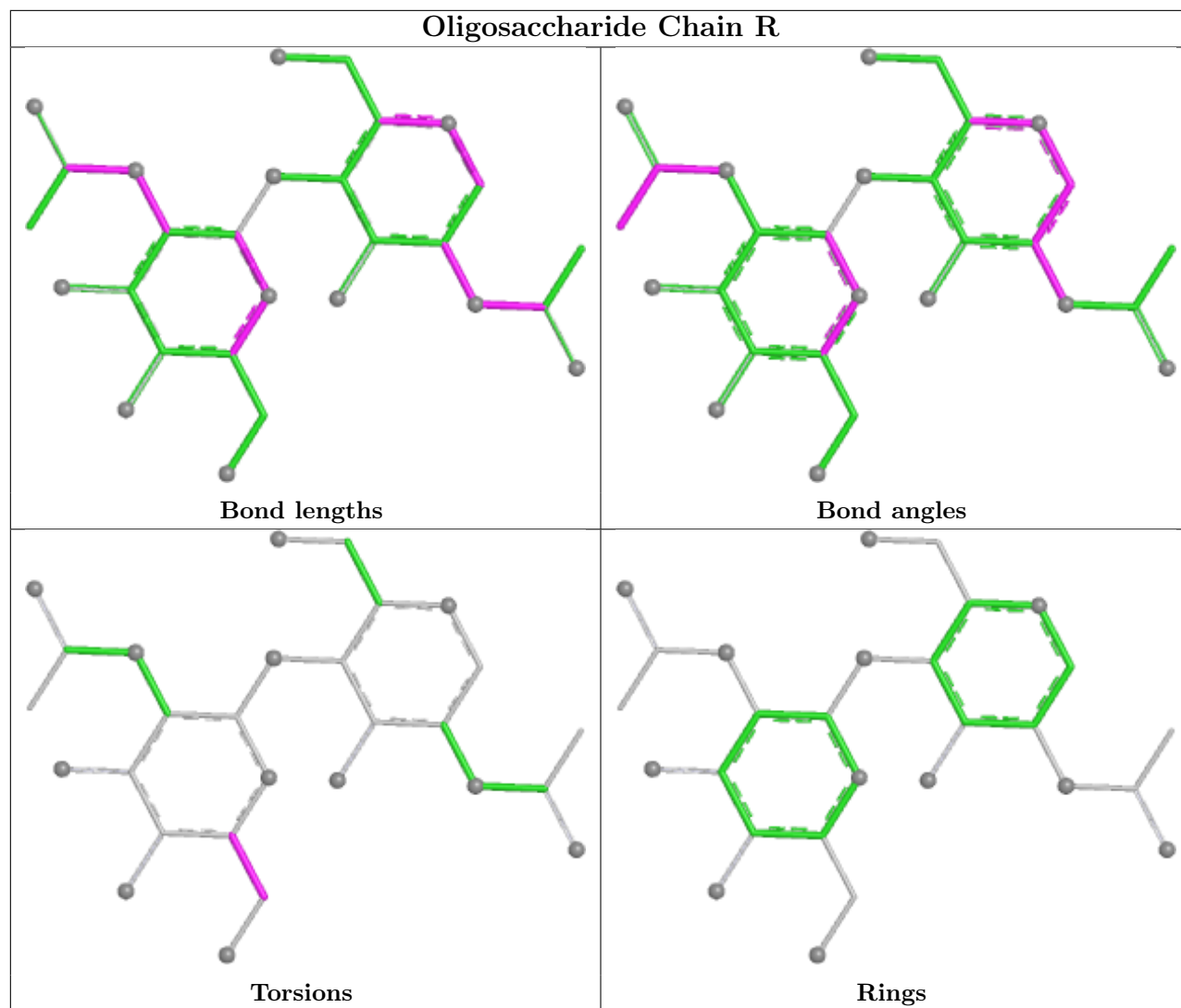


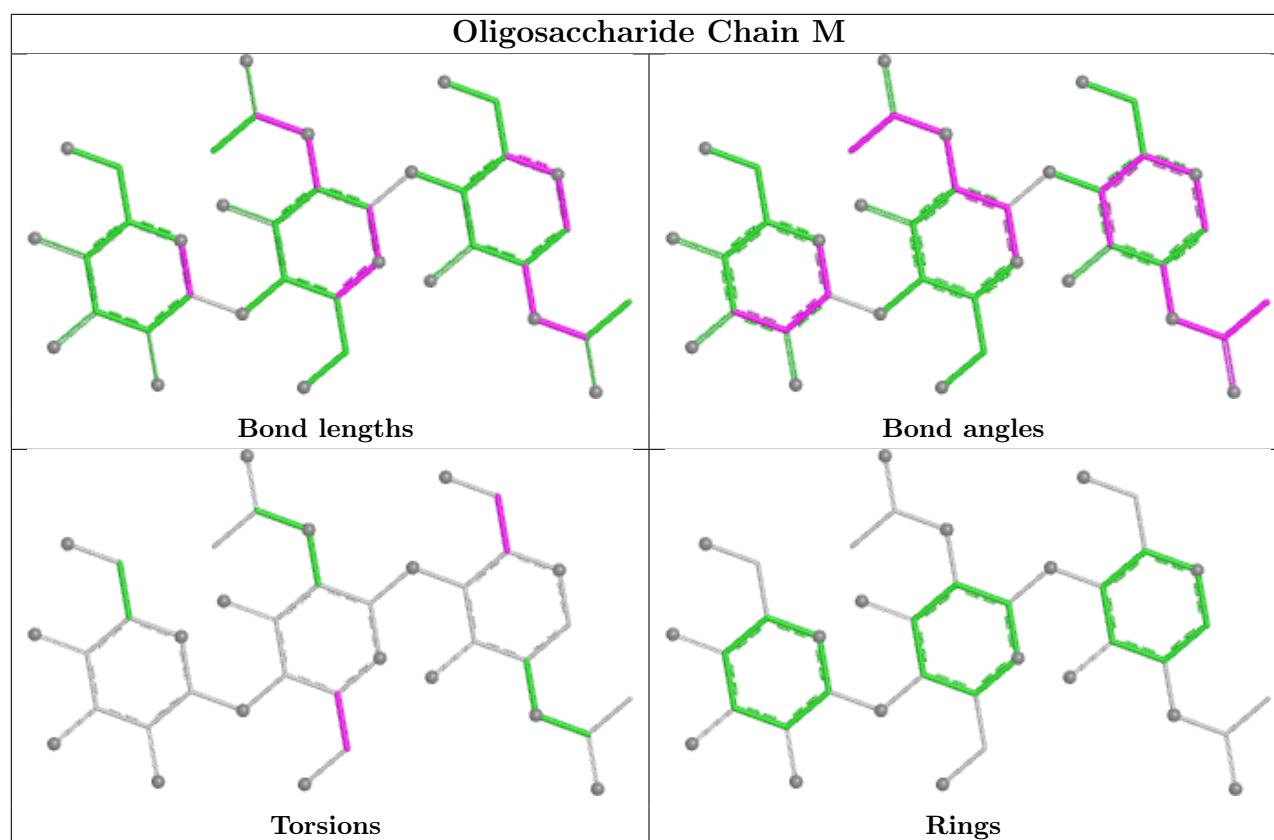












4.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 4 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	ACT	D	508	-	3,3,3	0.91	0	3,3,3	0.60	0
9	GOL	A	507	-	5,5,5	0.96	0	5,5,5	0.96	0
8	ACT	B	502	-	3,3,3	1.06	0	3,3,3	1.00	0
8	ACT	C	503	-	3,3,3	1.13	0	3,3,3	0.69	0
9	GOL	A	511	-	5,5,5	1.06	0	5,5,5	0.90	0
9	GOL	D	505	-	5,5,5	0.82	0	5,5,5	1.01	0
9	GOL	A	510	-	5,5,5	0.99	0	5,5,5	1.08	0
9	GOL	C	502	-	5,5,5	1.25	1 (20%)	5,5,5	0.93	0
9	GOL	C	504	-	5,5,5	1.17	0	5,5,5	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	D	503	-	5,5,5	1.06	1 (20%)	5,5,5	1.33	1 (20%)
9	GOL	A	503	-	5,5,5	1.12	0	5,5,5	1.05	0
8	ACT	D	506	-	3,3,3	1.14	0	3,3,3	1.23	0
8	ACT	A	502	-	3,3,3	1.02	0	3,3,3	1.05	0
9	GOL	A	509	-	5,5,5	0.96	0	5,5,5	1.06	0
9	GOL	C	506	-	5,5,5	1.25	1 (20%)	5,5,5	1.05	0
9	GOL	A	504	-	5,5,5	1.09	1 (20%)	5,5,5	1.15	1 (20%)
8	ACT	C	505	-	3,3,3	0.95	0	3,3,3	0.98	0
8	ACT	A	505	-	3,3,3	1.05	0	3,3,3	0.84	0
9	GOL	A	508	-	5,5,5	1.39	1 (20%)	5,5,5	0.83	0
9	GOL	A	506	-	5,5,5	1.39	1 (20%)	5,5,5	1.18	0
9	GOL	B	504	-	5,5,5	1.25	0	5,5,5	0.91	0
8	ACT	B	505	-	3,3,3	1.09	0	3,3,3	0.91	0
9	GOL	B	503	-	5,5,5	1.00	0	5,5,5	1.14	0
9	GOL	C	507	-	5,5,5	0.98	0	5,5,5	1.04	0
10	NAG	D	501	1	14,14,15	2.08	3 (21%)	17,19,21	1.50	3 (17%)
9	GOL	D	507	-	5,5,5	0.91	0	5,5,5	1.10	0
9	GOL	A	512	-	5,5,5	1.09	0	5,5,5	0.99	0
9	GOL	D	504	-	5,5,5	1.40	2 (40%)	5,5,5	1.38	1 (20%)
8	ACT	D	509	-	3,3,3	1.05	0	3,3,3	0.92	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	GOL	A	507	-	-	0/4/4/4	-
9	GOL	D	505	-	-	3/4/4/4	-
9	GOL	A	511	-	-	0/4/4/4	-
9	GOL	A	510	-	-	2/4/4/4	-
9	GOL	C	502	-	-	3/4/4/4	-
9	GOL	C	504	-	-	2/4/4/4	-
9	GOL	D	503	-	-	2/4/4/4	-
9	GOL	A	503	-	-	3/4/4/4	-
9	GOL	A	509	-	-	3/4/4/4	-
9	GOL	C	506	-	-	2/4/4/4	-
9	GOL	A	504	-	-	0/4/4/4	-
9	GOL	A	508	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	A	506	-	-	4/4/4/4	-
9	GOL	B	504	-	-	2/4/4/4	-
9	GOL	B	503	-	-	1/4/4/4	-
9	GOL	C	507	-	-	2/4/4/4	-
10	NAG	D	501	1	-	2/6/23/26	0/1/1/1
9	GOL	D	507	-	-	0/4/4/4	-
9	GOL	A	512	-	-	2/4/4/4	-
9	GOL	D	504	-	-	1/4/4/4	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	501	NAG	O5-C1	4.49	1.51	1.43
10	D	501	NAG	C7-N2	4.11	1.47	1.34
10	D	501	NAG	C2-N2	2.92	1.51	1.46
9	D	504	GOL	C1-C2	2.33	1.60	1.51
9	A	506	GOL	C1-C2	2.17	1.60	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	501	NAG	C8-C7-N2	3.20	121.42	116.12
10	D	501	NAG	C1-C2-N2	-2.83	105.97	110.43
9	D	504	GOL	C3-C2-C1	-2.62	102.20	111.80
10	D	501	NAG	O5-C1-C2	2.39	115.00	111.29
9	A	504	GOL	C3-C2-C1	-2.24	103.58	111.80

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	506	GOL	C1-C2-C3-O3
9	A	508	GOL	O1-C1-C2-O2
9	A	508	GOL	O1-C1-C2-C3
9	A	508	GOL	C1-C2-C3-O3
9	A	508	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

5.1 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	427/427 (100%)	-0.69	0 100 100	13, 25, 35, 61	2 (0%)
1	B	427/427 (100%)	-0.57	0 100 100	15, 27, 39, 50	3 (0%)
1	C	427/427 (100%)	-0.17	5 (1%) 76 77	19, 34, 60, 68	2 (0%)
1	D	427/427 (100%)	-0.18	5 (1%) 76 77	19, 34, 61, 71	0
All	All	1708/1708 (100%)	-0.40	10 (0%) 85 86	13, 30, 55, 71	7 (0%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	357	GLY	2.7
1	C	359	GLY	2.4
1	C	389	ASN	2.4
1	D	22	ASN	2.3
1	D	353	VAL	2.3

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

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

5.3 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
4	NDG	N	2	14/15	0.36	0.21	82,88,94,102	0
6	BMA	M	3	11/12	0.45	0.14	88,91,94,96	0

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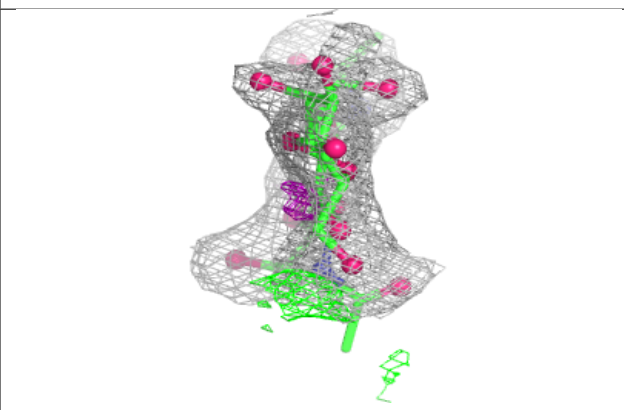
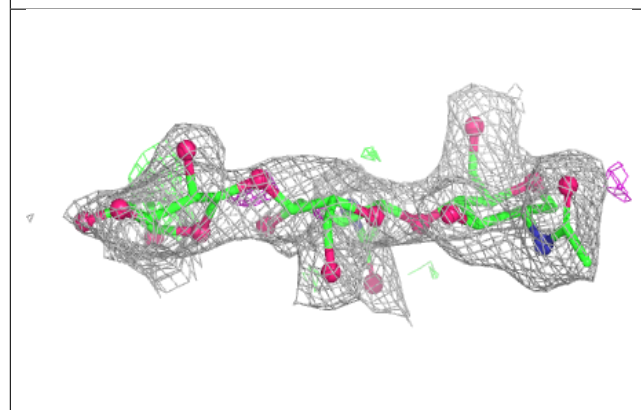
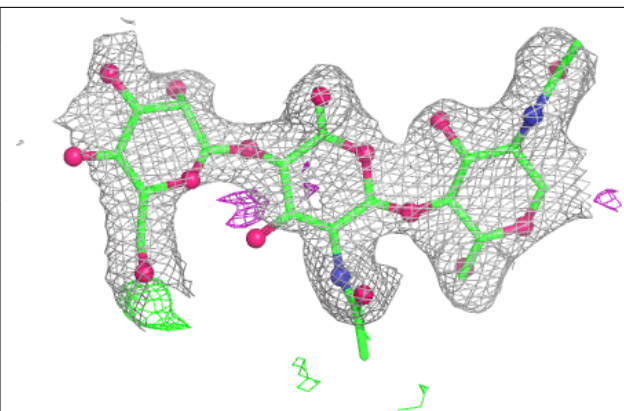
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	F	3	11/12	0.47	0.17	78,88,92,92	0
2	MAN	Q	3	11/12	0.52	0.14	72,86,89,91	0
2	MAN	G	3	11/12	0.54	0.14	71,79,84,87	0
2	MAN	K	3	11/12	0.58	0.15	76,80,86,86	0
2	MAN	E	3	11/12	0.58	0.14	68,78,80,83	0
5	NAG	R	2	14/15	0.59	0.16	63,82,90,94	0
4	NDG	I	2	14/15	0.64	0.17	56,70,77,77	0
5	NAG	O	2	14/15	0.69	0.14	69,79,88,89	0
5	NAG	J	2	14/15	0.70	0.15	51,60,69,70	0
2	NAG	E	2	14/15	0.75	0.15	63,71,77,81	0
6	NAG	M	2	14/15	0.81	0.11	59,72,82,89	0
4	NAG	N	1	14/15	0.81	0.12	45,60,75,78	0
2	NAG	Q	2	14/15	0.82	0.11	57,65,77,78	0
2	NAG	G	2	14/15	0.84	0.11	38,49,62,73	0
5	NAG	O	1	14/15	0.84	0.11	50,56,69,73	0
2	NAG	F	2	14/15	0.84	0.13	41,56,71,79	0
3	GAL	P	1	12/12	0.86	0.10	54,58,63,70	0
3	GAL	S	1	12/12	0.86	0.12	57,63,67,72	0
3	GAL	S	3	11/12	0.86	0.12	53,60,66,67	0
2	NAG	E	1	14/15	0.86	0.11	44,49,56,66	0
2	NAG	K	2	14/15	0.88	0.09	38,49,59,67	0
3	GAL	P	2	11/12	0.89	0.13	45,51,57,83	0
6	NAG	M	1	14/15	0.89	0.10	41,52,57,59	0
3	GAL	S	2	11/12	0.89	0.12	49,57,60,63	0
5	NAG	J	1	14/15	0.89	0.09	34,45,58,59	0
3	GAL	P	3	11/12	0.90	0.10	42,50,52,53	0
5	NAG	R	1	14/15	0.90	0.08	45,53,61,65	0
2	NAG	F	1	14/15	0.90	0.08	32,39,48,55	0
2	NAG	Q	1	14/15	0.91	0.08	42,48,51,56	0
3	GAL	H	1	12/12	0.92	0.09	27,37,54,58	0
4	NAG	I	1	14/15	0.92	0.09	47,53,61,62	0
2	NAG	K	1	14/15	0.94	0.07	29,32,42,42	0
3	GAL	L	2	11/12	0.95	0.07	25,27,31,33	0
2	NAG	G	1	14/15	0.96	0.06	26,33,36,37	0
3	GAL	H	2	11/12	0.96	0.07	20,26,31,37	0
3	GAL	H	3	11/12	0.96	0.06	23,26,30,34	0
3	GAL	L	1	12/12	0.96	0.07	27,35,44,45	0
3	GAL	L	3	11/12	0.97	0.05	22,27,30,37	0

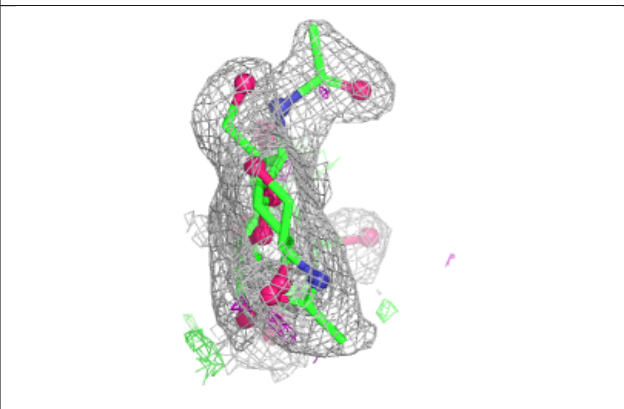
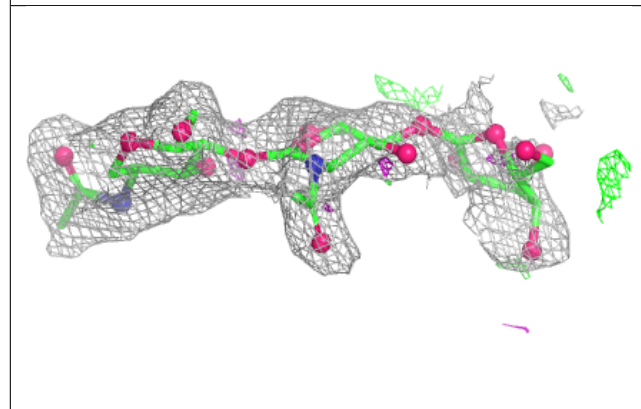
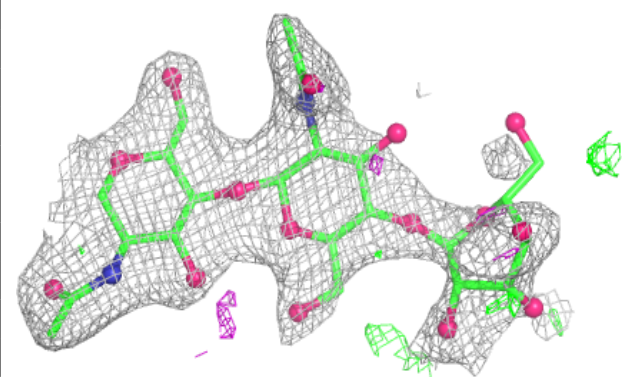
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

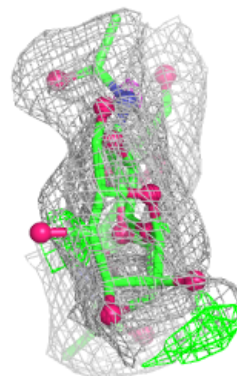
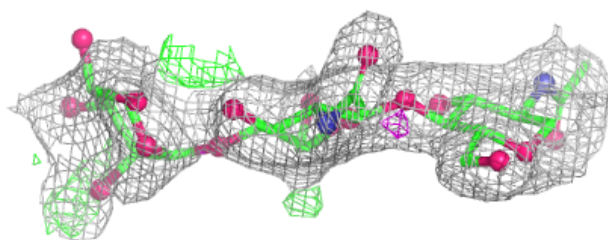
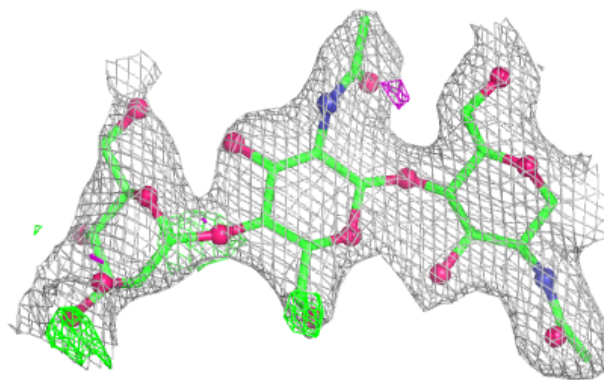
**Electron density around Chain F:**

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

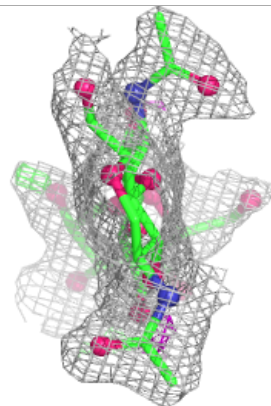
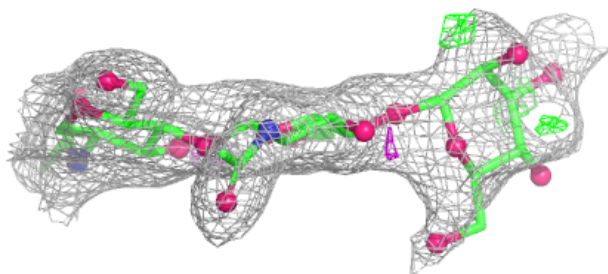
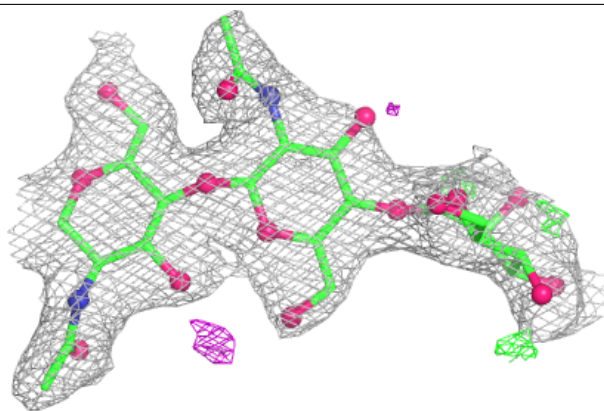


Electron density around Chain G:

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

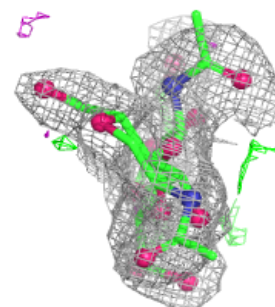
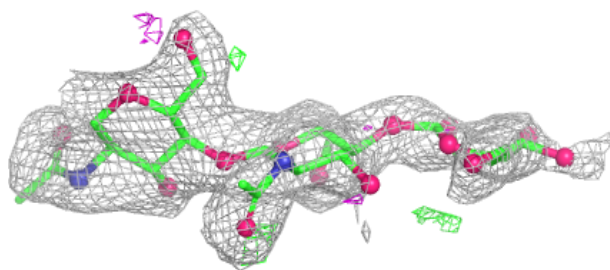
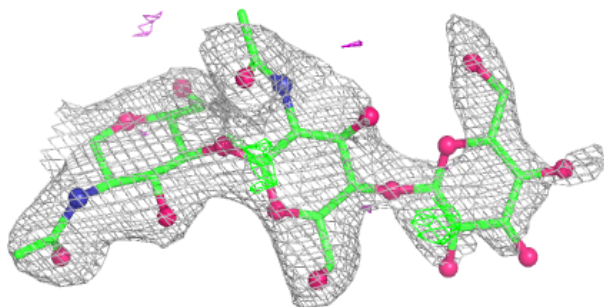
**Electron density around Chain K:**

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

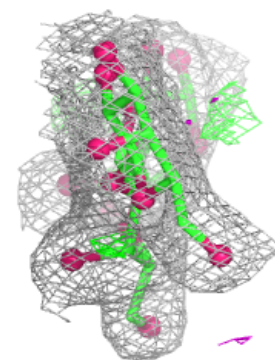
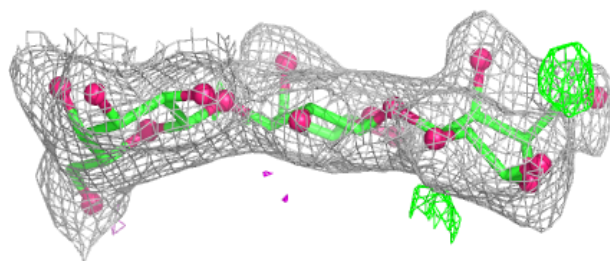
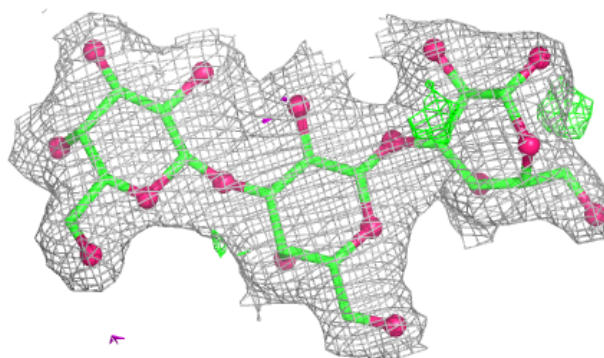


Electron density around Chain Q:

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and green (positive)

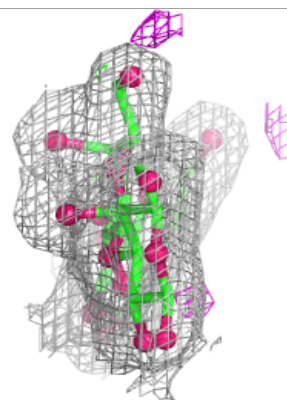
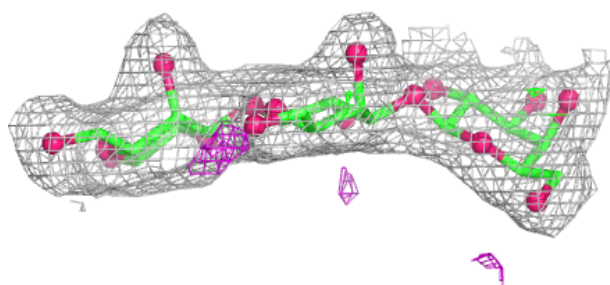
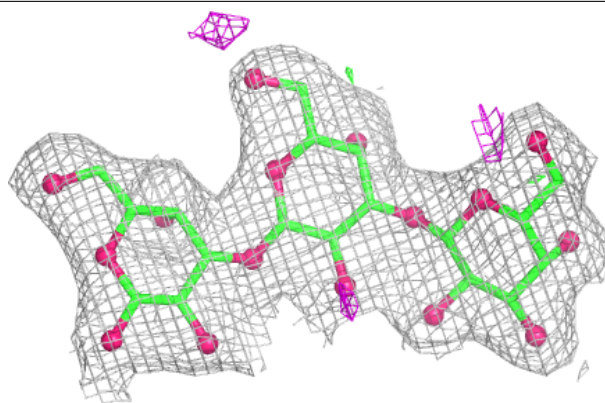
**Electron density around Chain H:**

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and green (positive)

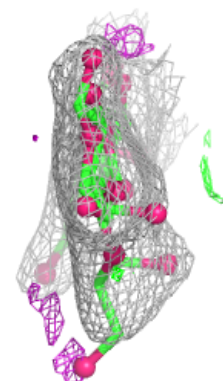
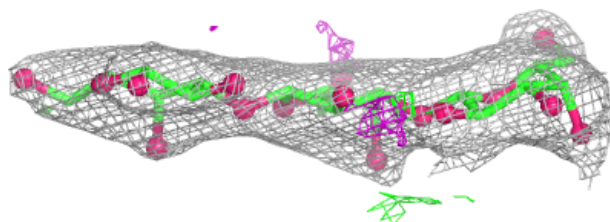
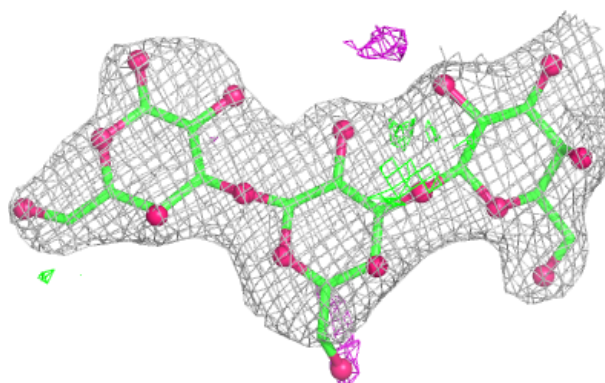


Electron density around Chain L:

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

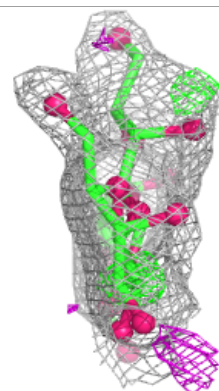
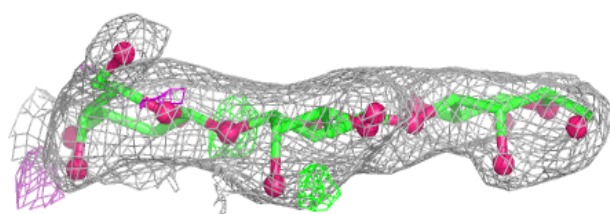
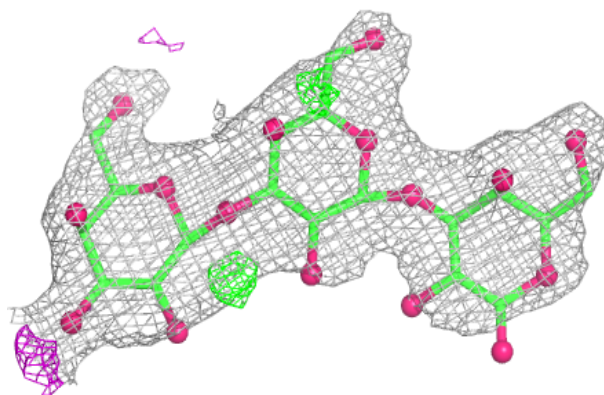
**Electron density around Chain P:**

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

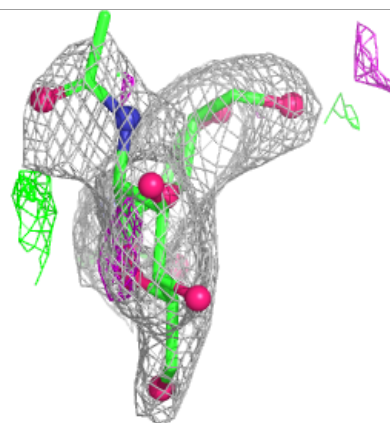
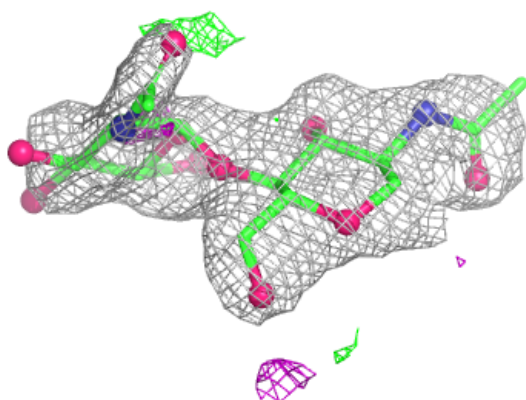
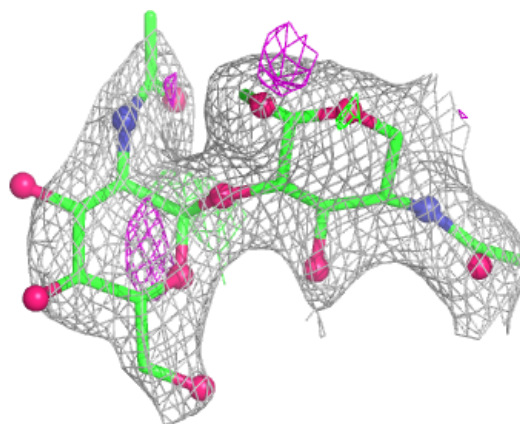


Electron density around Chain S:

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

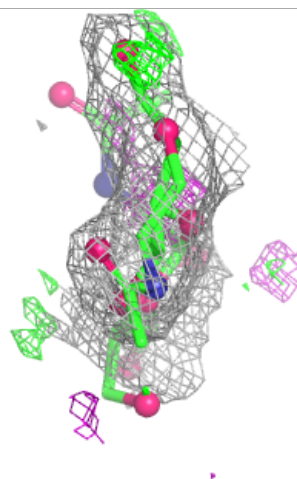
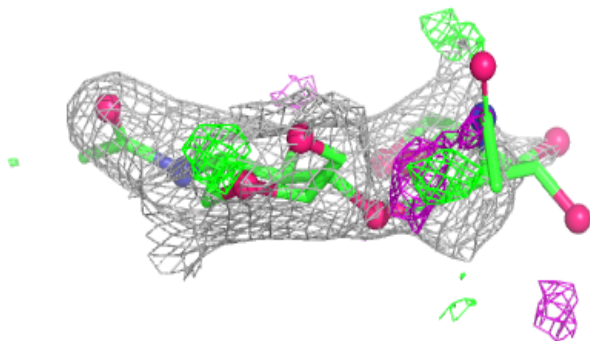
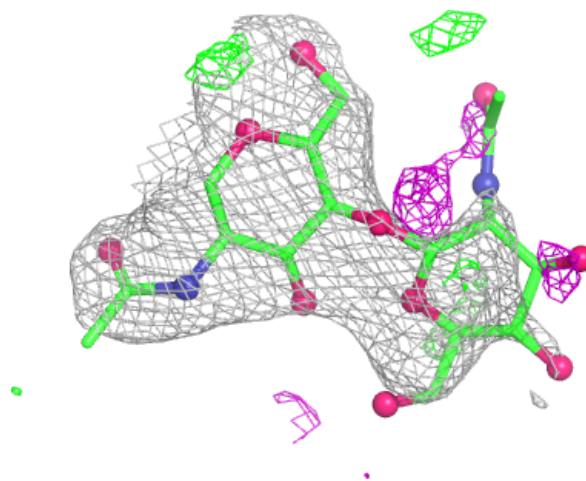
**Electron density around Chain I:**

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



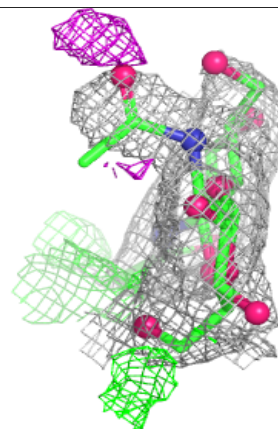
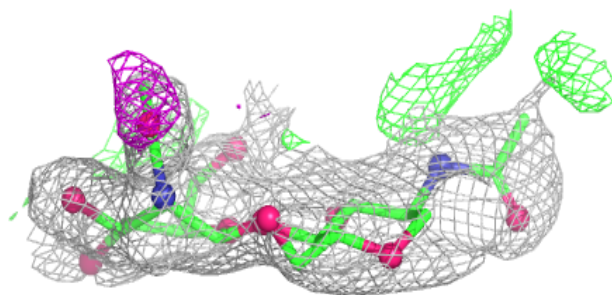
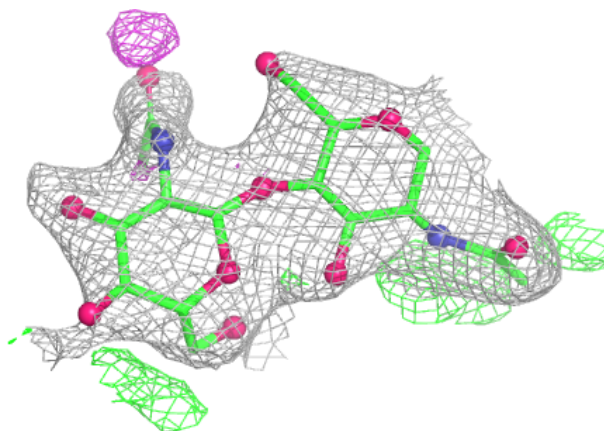
Electron density around Chain N:

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



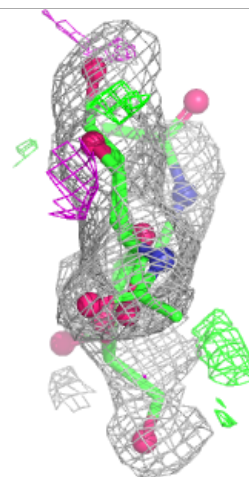
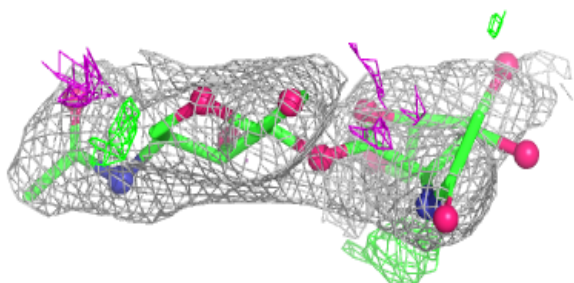
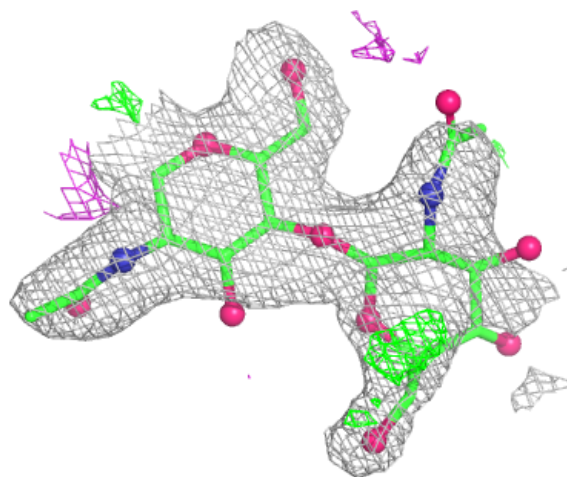
Electron density around Chain J:

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



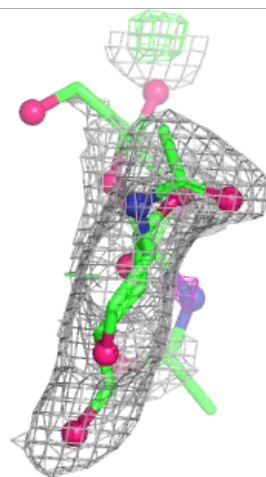
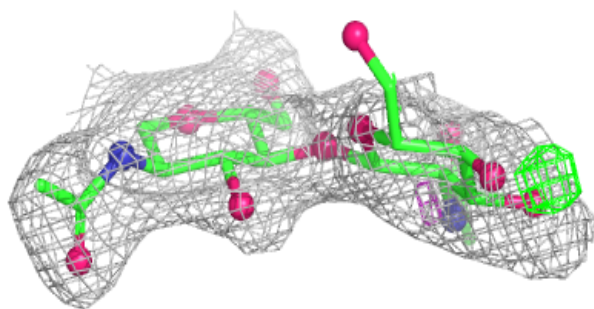
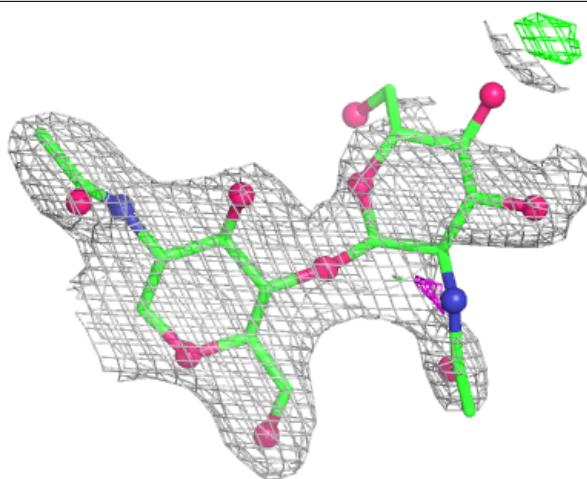
Electron density around Chain O:

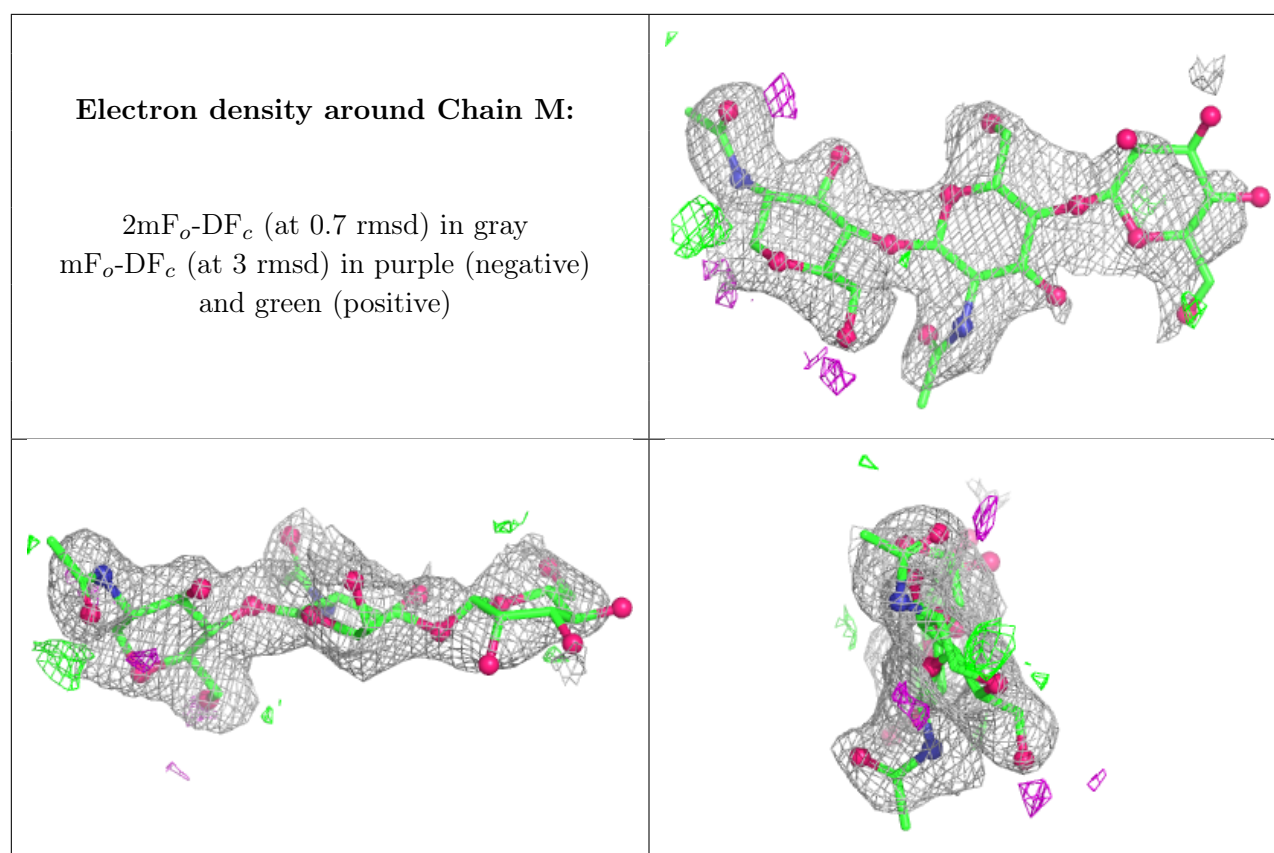
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain R:

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





5.4 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
8	ACT	A	505	4/4	0.64	0.19	49,55,57,60	0
8	ACT	C	503	4/4	0.68	0.27	48,50,54,63	0
9	GOL	A	507	6/6	0.68	0.16	54,64,67,68	0
9	GOL	D	507	6/6	0.69	0.21	50,59,63,64	0
9	GOL	C	507	6/6	0.70	0.20	58,62,63,64	0
9	GOL	A	509	6/6	0.72	0.20	50,55,61,63	0
9	GOL	D	503	6/6	0.73	0.20	45,48,52,53	0
10	NAG	D	501	14/15	0.73	0.13	55,63,71,75	0
8	ACT	C	505	4/4	0.74	0.17	48,49,55,61	0
8	ACT	D	509	4/4	0.74	0.15	37,47,54,55	0
9	GOL	A	512	6/6	0.78	0.20	43,49,58,61	0
9	GOL	A	506	6/6	0.79	0.15	39,47,56,57	0
8	ACT	A	502	4/4	0.79	0.20	37,44,52,70	0
9	GOL	A	510	6/6	0.80	0.17	48,51,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	GOL	C	502	6/6	0.81	0.16	40,45,47,55	0
9	GOL	D	505	6/6	0.83	0.13	45,50,55,58	0
8	ACT	D	506	4/4	0.83	0.13	23,29,30,42	0
8	ACT	B	505	4/4	0.83	0.17	36,42,46,51	0
9	GOL	A	511	6/6	0.84	0.16	39,48,55,55	0
9	GOL	A	508	6/6	0.84	0.16	39,45,58,63	0
9	GOL	D	504	6/6	0.85	0.16	29,37,42,46	0
8	ACT	B	502	4/4	0.86	0.22	25,36,45,65	0
9	GOL	A	504	6/6	0.86	0.18	33,39,42,45	0
9	GOL	C	506	6/6	0.86	0.17	42,44,47,48	0
8	ACT	D	508	4/4	0.87	0.14	40,45,47,51	0
9	GOL	B	503	6/6	0.89	0.11	32,36,39,45	0
9	GOL	C	504	6/6	0.90	0.14	40,41,45,50	0
9	GOL	B	504	6/6	0.91	0.12	38,42,44,45	0
9	GOL	A	503	6/6	0.91	0.15	27,38,38,39	0
7	CA	D	502	1/1	0.99	0.02	42,42,42,42	0
7	CA	C	501	1/1	0.99	0.02	40,40,40,40	0
7	CA	B	501	1/1	1.00	0.01	20,20,20,20	0
7	CA	A	501	1/1	1.00	0.01	18,18,18,18	0

5.5 Other polymers [i](#)

There are no such residues in this entry.