



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:07 PM UTC

PDB ID : 8PO9 / pdb_00008po9
Title : Polyethylene oxidation hexamerin PEase Cibeles (XP_026756460) from *Galleria mellonella*
Authors : Illanes-Vicioso, R.; Ruiz-Lopez, E.; Sola, M.; Bertocchini, F.; Palomo, E.A.
Deposited on : 2023-07-03
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

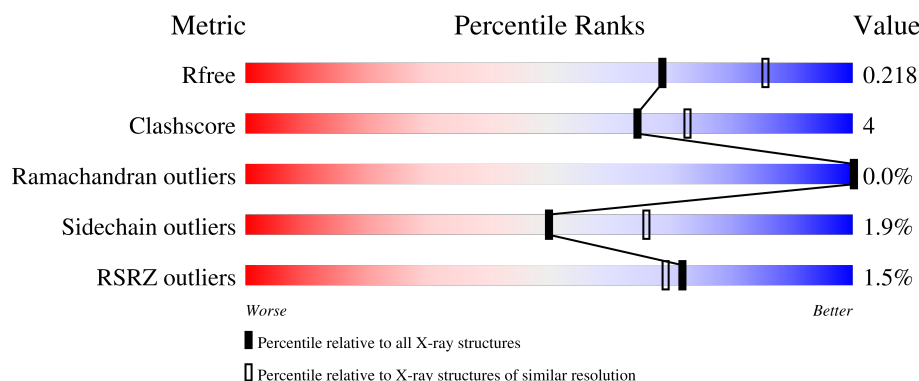
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	702	0% 86% 10% .
1	B	702	2% 86% 9% . .
1	C	702	0% 85% 11% .
1	D	702	2% 86% 9% . .
1	E	702	2% 84% 11% . .

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Mol	Chain	Length	Quality of chain
1	F	702	
2	G	6	
3	H	5	
3	K	5	
3	M	5	
3	N	5	
3	O	5	
3	P	5	
3	R	5	
4	I	3	
4	L	3	
5	J	9	
6	Q	6	

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	GOL	E	908	-	X	-	-
13	GLY	D	912	-	X	-	-
13	GLY	E	909	-	X	-	-

2 Entry composition [i](#)

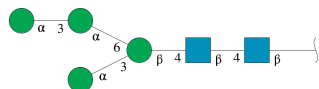
There are 15 unique types of molecules in this entry. The entry contains 37172 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Arylphorin.

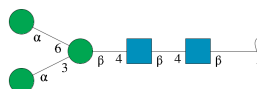
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	679	Total	C	N	O	S	0	1	0
			5796	3812	912	1065	7			
1	B	672	Total	C	N	O	S	0	1	0
			5734	3771	903	1053	7			
1	C	678	Total	C	N	O	S	0	1	0
			5783	3802	910	1064	7			
1	D	677	Total	C	N	O	S	0	0	0
			5775	3797	909	1062	7			
1	E	671	Total	C	N	O	S	0	0	0
			5711	3752	901	1051	7			
1	F	678	Total	C	N	O	S	0	1	0
			5792	3810	911	1064	7			

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



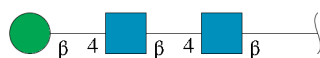
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



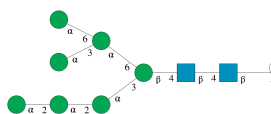
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	N	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	O	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	P	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 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
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

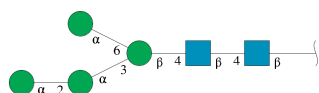
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is an oligosaccharide called 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
6	Q	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cu	0	0
			1	1		
7	B	1	Total	Cu	0	0
			1	1		
7	C	1	Total	Cu	0	0
			1	1		
7	D	1	Total	Cu	0	0
			1	1		
7	E	1	Total	Cu	0	0
			1	1		
7	F	1	Total	Cu	0	0
			1	1		

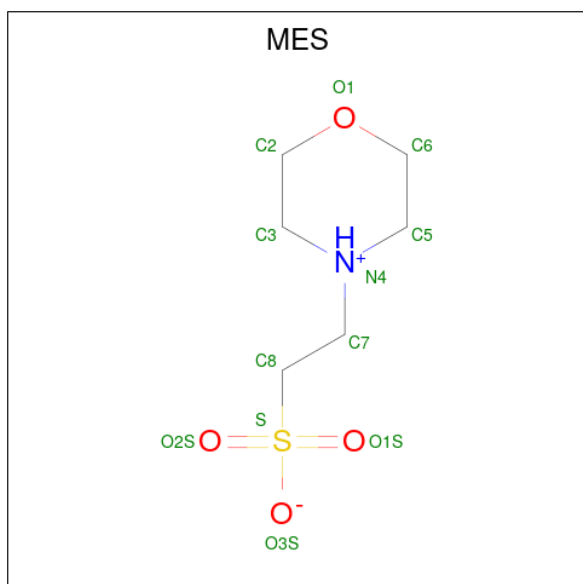
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	E	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

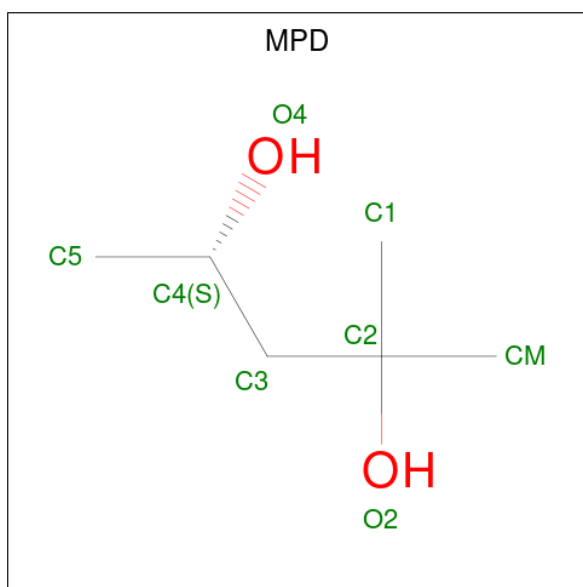
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		
9	B	4	Total	Cl	0	0
			4	4		
9	C	5	Total	Cl	0	0
			5	5		
9	D	7	Total	Cl	0	0
			7	7		
9	E	3	Total	Cl	0	0
			3	3		
9	F	2	Total	Cl	0	0
			2	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



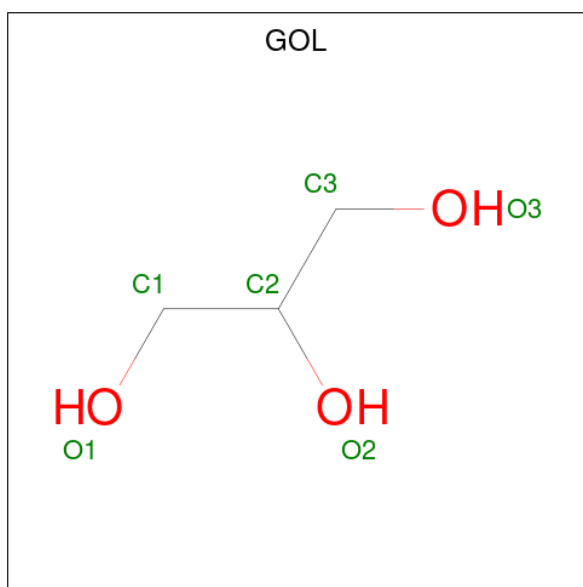
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



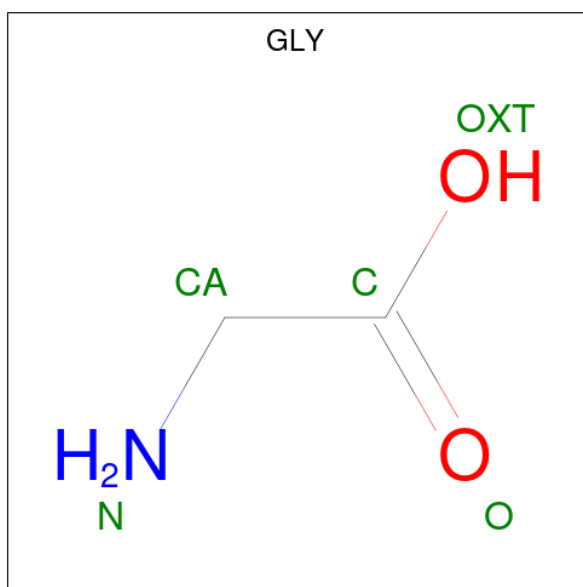
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			8	6	2		
11	A	1	Total	C	O	0	0
			8	6	2		
11	A	1	Total	C	O	0	0
			8	6	2		
11	A	1	Total	C	O	0	0
			8	6	2		
11	B	1	Total	C	O	0	0
			8	6	2		
11	B	1	Total	C	O	0	0
			8	6	2		
11	C	1	Total	C	O	0	0
			8	6	2		
11	D	1	Total	C	O	0	0
			8	6	2		
11	D	1	Total	C	O	0	0
			8	6	2		
11	E	1	Total	C	O	0	0
			8	6	2		
11	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 12 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



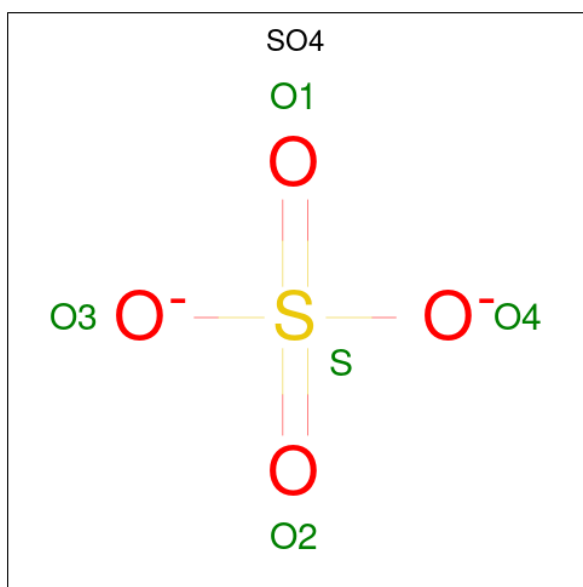
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			6	3	3		
12	A	1	Total	C	O	0	0
			6	3	3		
12	B	1	Total	C	O	0	0
			6	3	3		
12	B	1	Total	C	O	0	0
			6	3	3		
12	C	1	Total	C	O	0	0
			6	3	3		
12	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 13 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			5	2	1	2		
13	C	1	Total	C	N	O	0	0
			5	2	1	2		
13	D	1	Total	C	N	O	0	0
			5	2	1	2		
13	D	1	Total	C	N	O	0	0
			5	2	1	2		
13	E	1	Total	C	N	O	0	0
			5	2	1	2		
13	E	1	Total	C	N	O	0	0
			5	2	1	2		
13	F	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 14 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	D	1	Total	O	S	0	0
			5	4	1		
14	F	1	Total	O	S	0	0
			5	4	1		

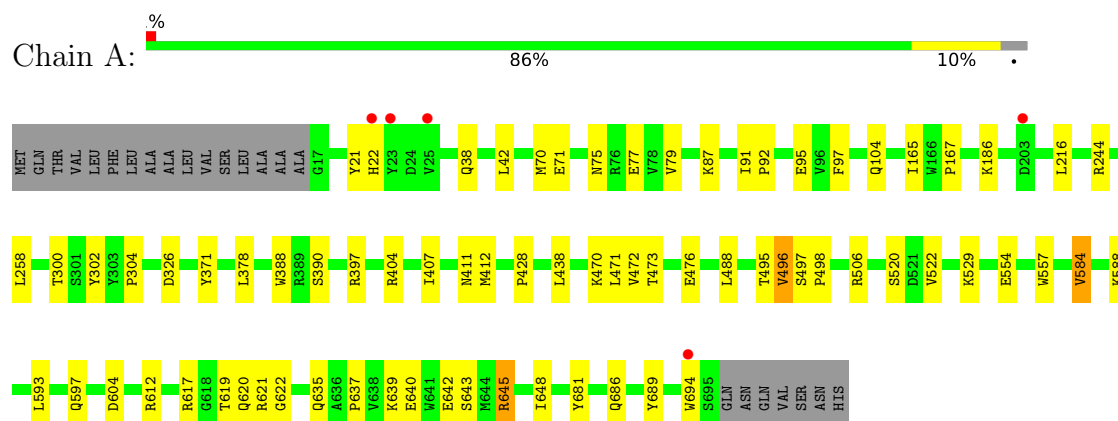
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	286	Total	O	0	0
			286	286		
15	B	339	Total	O	0	0
			339	339		
15	C	210	Total	O	0	0
			210	210		
15	D	227	Total	O	0	0
			227	227		
15	E	267	Total	O	0	0
			267	267		
15	F	260	Total	O	0	0
			260	260		

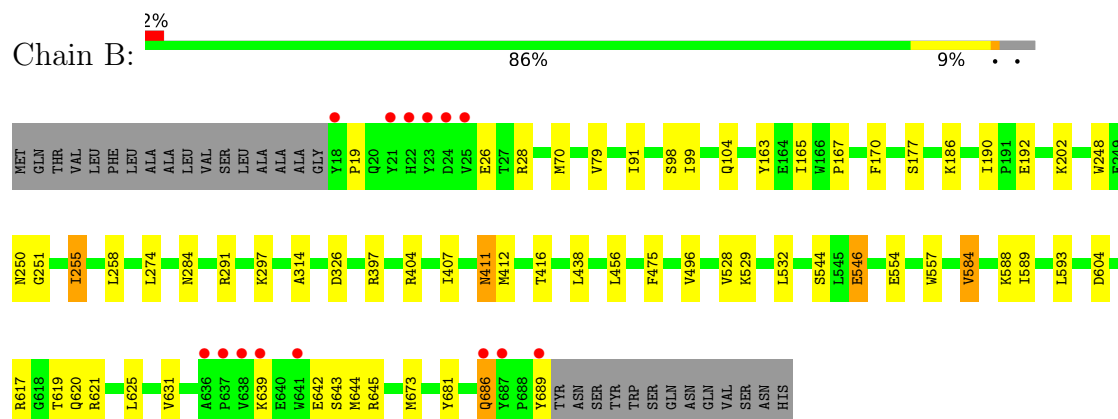
3 Residue-property plots

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.

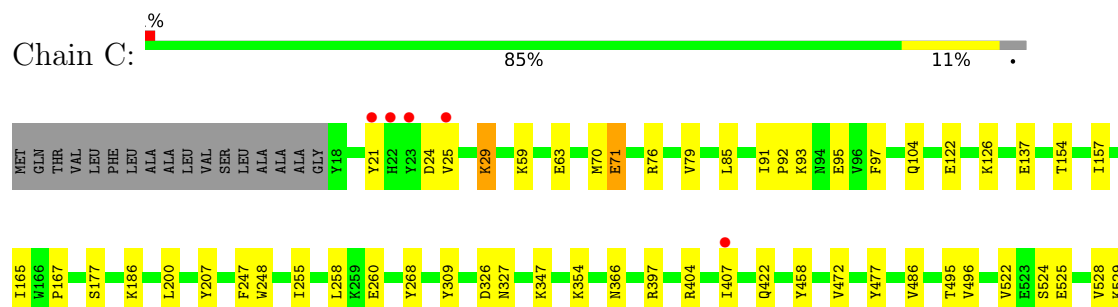
• Molecule 1: Arylphorin



• Molecule 1: Arylphorin

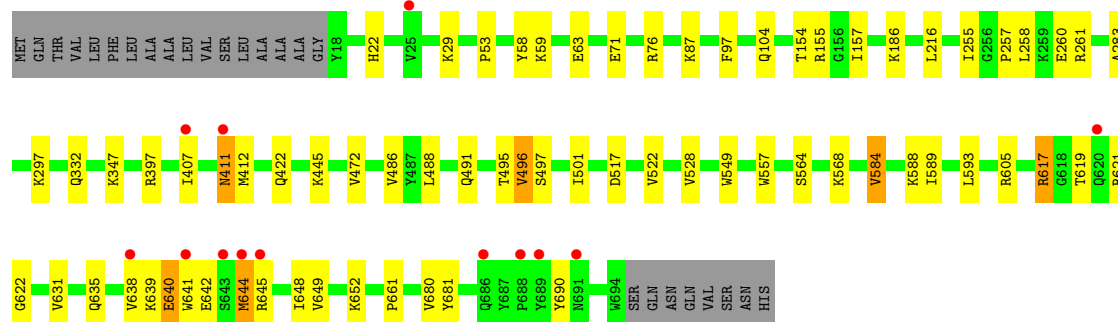
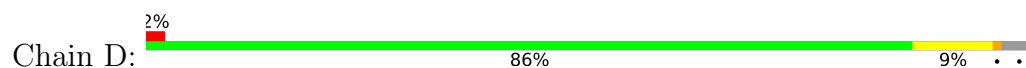


• Molecule 1: Arylphorin

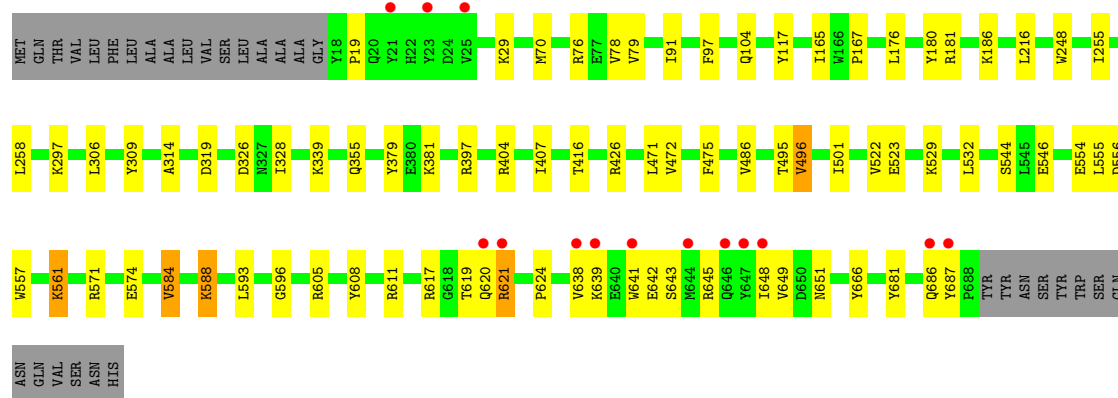
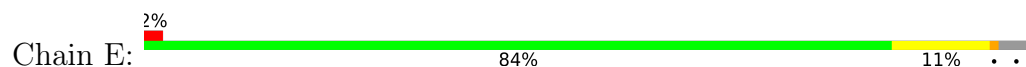




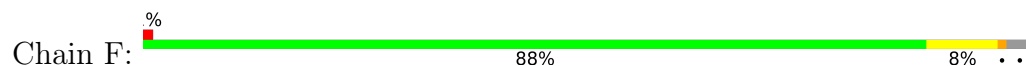
• Molecule 1: Arylphorin



• Molecule 1: Arylphorin



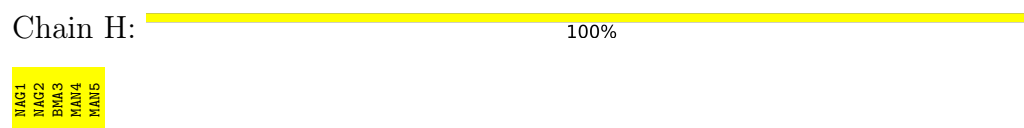
• Molecule 1: Arylphorin



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



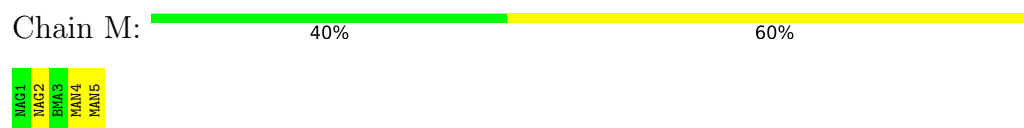
- Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



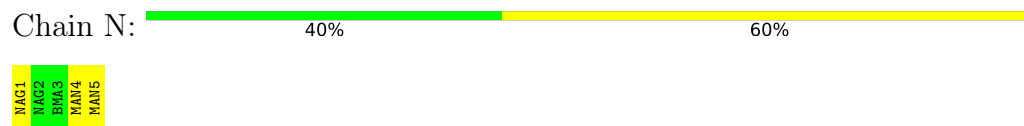
- Molecule 3: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose



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



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



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





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

Chain P: 20% 60% 20%



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

Chain R: 20% 40% 40%



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

Chain I: 67% 33%



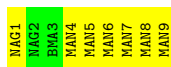
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 100%



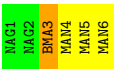
- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 22% 78%



- Molecule 6: 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 Q: 33% 50% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.75Å 196.58Å 224.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.26 – 2.20 49.26 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.26-2.20) 99.9 (49.26-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20_4459, PHENIX 1.20_4459	Depositor
R, R_{free}	0.171 , 0.218 0.171 , 0.218	Depositor DCC
R_{free} test set	10623 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37172	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MPD, CL, MG, MAN, SO4, MES, CU, GOL, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/5989	0.56	2/8153 (0.0%)
1	B	0.42	0/5923	0.55	0/8062
1	C	0.34	0/5974	0.52	1/8132 (0.0%)
1	D	0.37	0/5963	0.55	0/8117
1	E	0.38	0/5894	0.53	1/8021 (0.0%)
1	F	0.36	0/5985	0.53	1/8148 (0.0%)
All	All	0.38	0/35728	0.54	5/48633 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	621	ARG	CG-CD-NE	-6.83	96.98	112.00
1	A	622	GLY	N-CA-C	-6.27	98.33	113.18
1	A	617	ARG	CG-CD-NE	-5.79	99.25	112.00
1	F	622	GLY	N-CA-C	-5.63	99.83	113.18
1	C	622	GLY	N-CA-C	-5.18	100.91	113.18

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	5796	0	5536	50	0
1	B	5734	0	5489	46	0
1	C	5783	0	5525	55	1
1	D	5775	0	5518	50	0
1	E	5711	0	5470	57	0
1	F	5792	0	5533	41	1
2	G	72	0	61	3	0
3	H	61	0	52	0	0
3	K	61	0	52	0	0
3	M	61	0	52	2	0
3	N	61	0	52	1	0
3	O	61	0	52	0	0
3	P	61	0	52	1	0
3	R	61	0	52	1	0
4	I	39	0	34	0	0
4	L	39	0	34	0	0
5	J	105	0	88	0	0
6	Q	72	0	61	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	A	1	0	0	0	0
9	B	4	0	0	0	0
9	C	5	0	0	0	0
9	D	7	0	0	0	0
9	E	3	0	0	0	0
9	F	2	0	0	0	0
10	A	12	0	13	1	0
10	B	12	0	12	0	0
10	E	12	0	12	1	0
11	A	32	0	56	1	0
11	B	16	0	28	0	0
11	C	8	0	14	0	0
11	D	16	0	28	1	0
11	E	8	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	8	0	14	1	0
12	A	12	0	16	2	0
12	B	12	0	16	3	0
12	C	6	0	8	1	0
12	E	6	0	7	0	0
13	C	10	0	4	1	0
13	D	10	0	4	2	0
13	E	10	0	4	1	0
13	F	5	0	2	1	0
14	D	5	0	0	0	0
14	F	5	0	0	0	0
15	A	286	0	0	0	0
15	B	339	0	0	3	0
15	C	210	0	0	4	0
15	D	227	0	0	1	0
15	E	267	0	0	1	0
15	F	260	0	0	1	0
All	All	37172	0	33965	269	1

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 4.

The worst 5 of 269 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:620:GLN:HE22	1:E:624:PRO:HD3	1.42	0.85
1:F:634:TYR:OH	1:F:645:ARG:NH2	2.11	0.82
1:B:284:ASN:OD1	1:B:617:ARG:NH2	2.15	0.80
1:F:116:TYR:OH	1:F:253:GLN:NE2	2.15	0.80
1:B:28:ARG:NH1	1:B:604:ASP:OD2	2.10	0.79

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ASP:OD2	1:F:59:LYS:NZ[4_455]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	678/702 (97%)	665 (98%)	12 (2%)	1 (0%)	48	57
1	B	671/702 (96%)	662 (99%)	9 (1%)	0	100	100
1	C	677/702 (96%)	665 (98%)	12 (2%)	0	100	100
1	D	675/702 (96%)	665 (98%)	10 (2%)	0	100	100
1	E	669/702 (95%)	661 (99%)	8 (1%)	0	100	100
1	F	677/702 (96%)	666 (98%)	11 (2%)	0	100	100
All	All	4047/4212 (96%)	3984 (98%)	62 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	640	GLU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	620/637 (97%)	609 (98%)	11 (2%)	51	68
1	B	614/637 (96%)	604 (98%)	10 (2%)	55	71
1	C	619/637 (97%)	608 (98%)	11 (2%)	51	68
1	D	618/637 (97%)	602 (97%)	16 (3%)	40	55
1	E	612/637 (96%)	601 (98%)	11 (2%)	51	68
1	F	620/637 (97%)	607 (98%)	13 (2%)	47	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3703/3822 (97%)	3631 (98%)	72 (2%)	50 66

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	638	VAL
1	F	686	GLN
1	F	22	HIS
1	F	438	LEU
1	C	486	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	243	ASN
1	F	253	GLN
1	F	626	GLN
1	C	566	GLN
1	C	69	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

62 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	G	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	0.49	0
2	NAG	G	2	2	14,14,15	0.56	1 (7%)	17,19,21	0.60	0
2	BMA	G	3	2	11,11,12	0.95	0	15,15,17	0.93	1 (6%)
2	MAN	G	4	2	11,11,12	0.95	0	15,15,17	1.06	1 (6%)
2	MAN	G	5	2	11,11,12	0.94	1 (9%)	15,15,17	1.21	2 (13%)
2	MAN	G	6	2	11,11,12	1.42	3 (27%)	15,15,17	1.25	2 (13%)
3	NAG	H	1	3,1	14,14,15	0.54	0	17,19,21	0.89	1 (5%)
3	NAG	H	2	3	14,14,15	0.35	0	17,19,21	0.71	1 (5%)
3	BMA	H	3	3	11,11,12	0.61	0	15,15,17	0.99	1 (6%)
3	MAN	H	4	3	11,11,12	1.20	1 (9%)	15,15,17	1.41	5 (33%)
3	MAN	H	5	3	11,11,12	1.09	1 (9%)	15,15,17	1.14	1 (6%)
4	NAG	I	1	4,1	14,14,15	0.29	0	17,19,21	0.72	1 (5%)
4	NAG	I	2	4	14,14,15	0.34	0	17,19,21	0.62	0
4	BMA	I	3	4	11,11,12	0.94	0	15,15,17	1.01	0
5	NAG	J	1	1,5	14,14,15	0.69	1 (7%)	17,19,21	0.93	0
5	NAG	J	2	5	14,14,15	0.21	0	17,19,21	0.45	0
5	BMA	J	3	5	11,11,12	0.90	0	15,15,17	0.71	0
5	MAN	J	4	5	11,11,12	0.89	1 (9%)	15,15,17	1.32	1 (6%)
5	MAN	J	5	5	11,11,12	0.99	1 (9%)	15,15,17	1.63	4 (26%)
5	MAN	J	6	5	11,11,12	0.83	1 (9%)	15,15,17	1.05	2 (13%)
5	MAN	J	7	5	11,11,12	0.91	0	15,15,17	0.99	2 (13%)
5	MAN	J	8	5	11,11,12	1.06	1 (9%)	15,15,17	0.94	1 (6%)
5	MAN	J	9	5	11,11,12	0.73	0	15,15,17	1.08	1 (6%)
3	NAG	K	1	3,1	14,14,15	0.32	0	17,19,21	0.44	0
3	NAG	K	2	3	14,14,15	0.58	1 (7%)	17,19,21	0.64	1 (5%)
3	BMA	K	3	3	11,11,12	0.84	0	15,15,17	1.19	1 (6%)
3	MAN	K	4	3	11,11,12	0.98	1 (9%)	15,15,17	1.05	2 (13%)
3	MAN	K	5	3	11,11,12	1.13	1 (9%)	15,15,17	0.93	0
4	NAG	L	1	4,1	14,14,15	0.49	0	17,19,21	0.64	0
4	NAG	L	2	4	14,14,15	0.27	0	17,19,21	0.55	0
4	BMA	L	3	4	11,11,12	0.79	0	15,15,17	0.86	0
3	NAG	M	1	3,1	14,14,15	0.23	0	17,19,21	0.55	0
3	NAG	M	2	3	14,14,15	0.52	0	17,19,21	0.55	0
3	BMA	M	3	3	11,11,12	0.84	0	15,15,17	0.70	0
3	MAN	M	4	3	11,11,12	0.87	0	15,15,17	1.06	1 (6%)
3	MAN	M	5	3	11,11,12	1.06	1 (9%)	15,15,17	1.21	2 (13%)
3	NAG	N	1	3,1	14,14,15	0.64	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	N	2	3	14,14,15	0.37	0	17,19,21	0.57	0
3	BMA	N	3	3	11,11,12	0.81	0	15,15,17	0.80	0
3	MAN	N	4	3	11,11,12	1.08	0	15,15,17	0.86	1 (6%)
3	MAN	N	5	3	11,11,12	0.78	0	15,15,17	1.29	2 (13%)
3	NAG	O	1	3,1	14,14,15	0.73	1 (7%)	17,19,21	0.74	0
3	NAG	O	2	3	14,14,15	0.51	0	17,19,21	0.54	0
3	BMA	O	3	3	11,11,12	0.88	0	15,15,17	0.79	0
3	MAN	O	4	3	11,11,12	1.10	0	15,15,17	0.99	1 (6%)
3	MAN	O	5	3	11,11,12	1.03	1 (9%)	15,15,17	1.24	1 (6%)
3	NAG	P	1	3,1	14,14,15	0.79	1 (7%)	17,19,21	0.59	0
3	NAG	P	2	3	14,14,15	0.35	0	17,19,21	0.38	0
3	BMA	P	3	3	11,11,12	0.91	0	15,15,17	1.02	1 (6%)
3	MAN	P	4	3	11,11,12	0.69	0	15,15,17	1.08	1 (6%)
3	MAN	P	5	3	11,11,12	1.22	2 (18%)	15,15,17	0.79	0
6	NAG	Q	1	6,1	14,14,15	0.31	0	17,19,21	0.64	0
6	NAG	Q	2	6	14,14,15	0.49	0	17,19,21	0.59	0
6	BMA	Q	3	6	11,11,12	0.71	0	15,15,17	1.13	2 (13%)
6	MAN	Q	4	6	11,11,12	0.85	0	15,15,17	1.14	2 (13%)
6	MAN	Q	5	6	11,11,12	0.94	1 (9%)	15,15,17	0.81	1 (6%)
6	MAN	Q	6	6	11,11,12	1.07	1 (9%)	15,15,17	0.91	1 (6%)
3	NAG	R	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	0.68	0
3	NAG	R	2	3	14,14,15	0.51	0	17,19,21	0.43	0
3	BMA	R	3	3	11,11,12	0.44	0	15,15,17	1.48	1 (6%)
3	MAN	R	4	3	11,11,12	0.92	0	15,15,17	1.03	1 (6%)
3	MAN	R	5	3	11,11,12	1.09	1 (9%)	15,15,17	1.02	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
2	MAN	G	4	2	-	2/2/19/22	0/1/1/1
2	MAN	G	5	2	-	0/2/19/22	0/1/1/1
2	MAN	G	6	2	-	0/2/19/22	0/1/1/1

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

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

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	4	MAN	C1-C2	2.69	1.58	1.52
3	O	1	NAG	O5-C1	-2.66	1.39	1.43
2	G	6	MAN	O5-C1	-2.53	1.39	1.43
2	G	1	NAG	O5-C1	-2.47	1.39	1.43
3	R	1	NAG	C1-C2	2.43	1.55	1.52

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	3	BMA	C1-O5-C5	4.85	118.69	112.19
5	J	4	MAN	C1-O5-C5	4.20	117.82	112.19
5	J	5	MAN	C1-O5-C5	3.75	117.22	112.19
3	N	5	MAN	C1-O5-C5	3.72	117.18	112.19
5	J	5	MAN	O2-C2-C3	-3.65	102.60	110.15

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6

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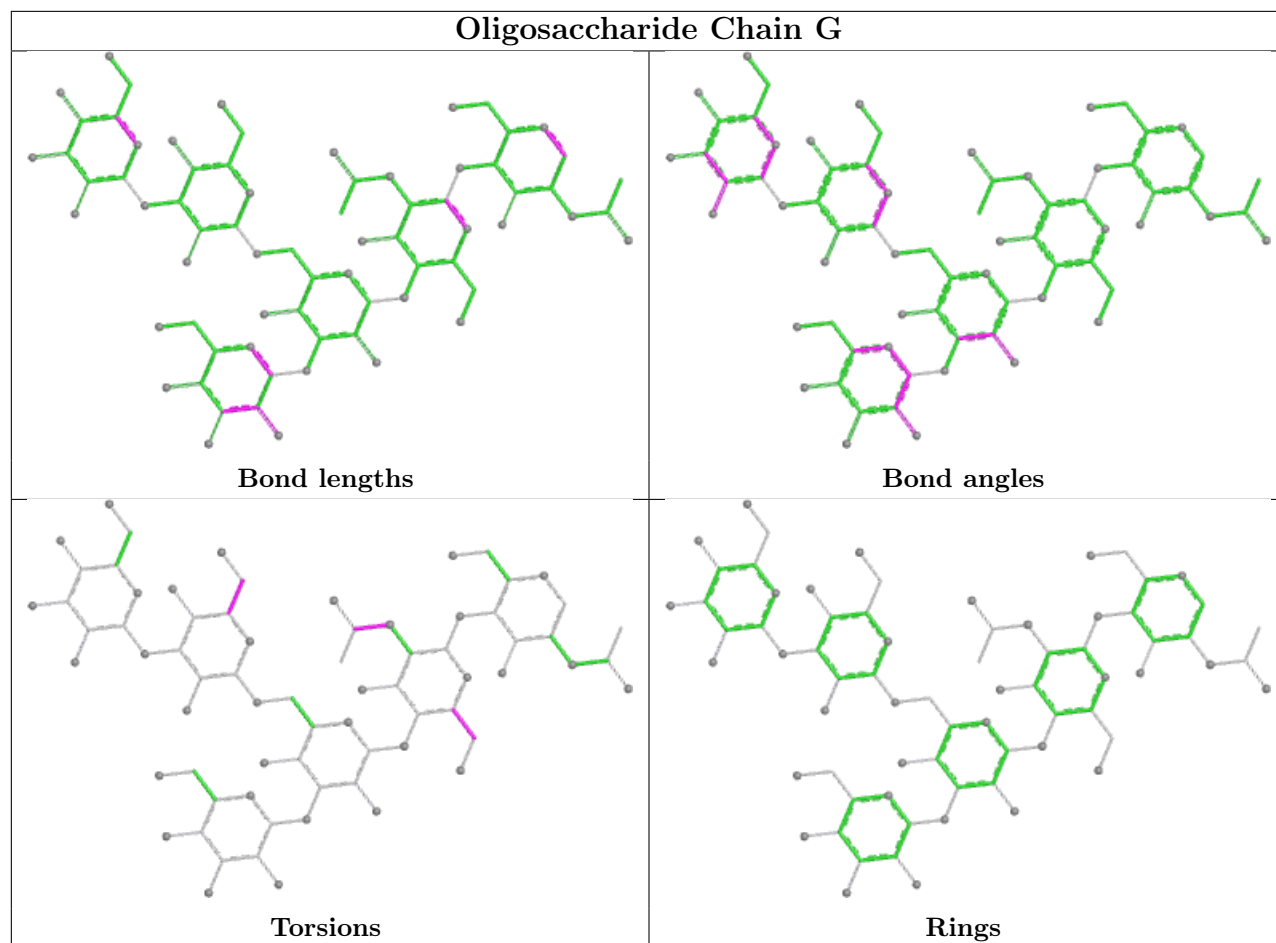
Mol	Chain	Res	Type	Atoms
5	J	7	MAN	O5-C5-C6-O6
2	G	4	MAN	O5-C5-C6-O6
3	O	4	MAN	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6

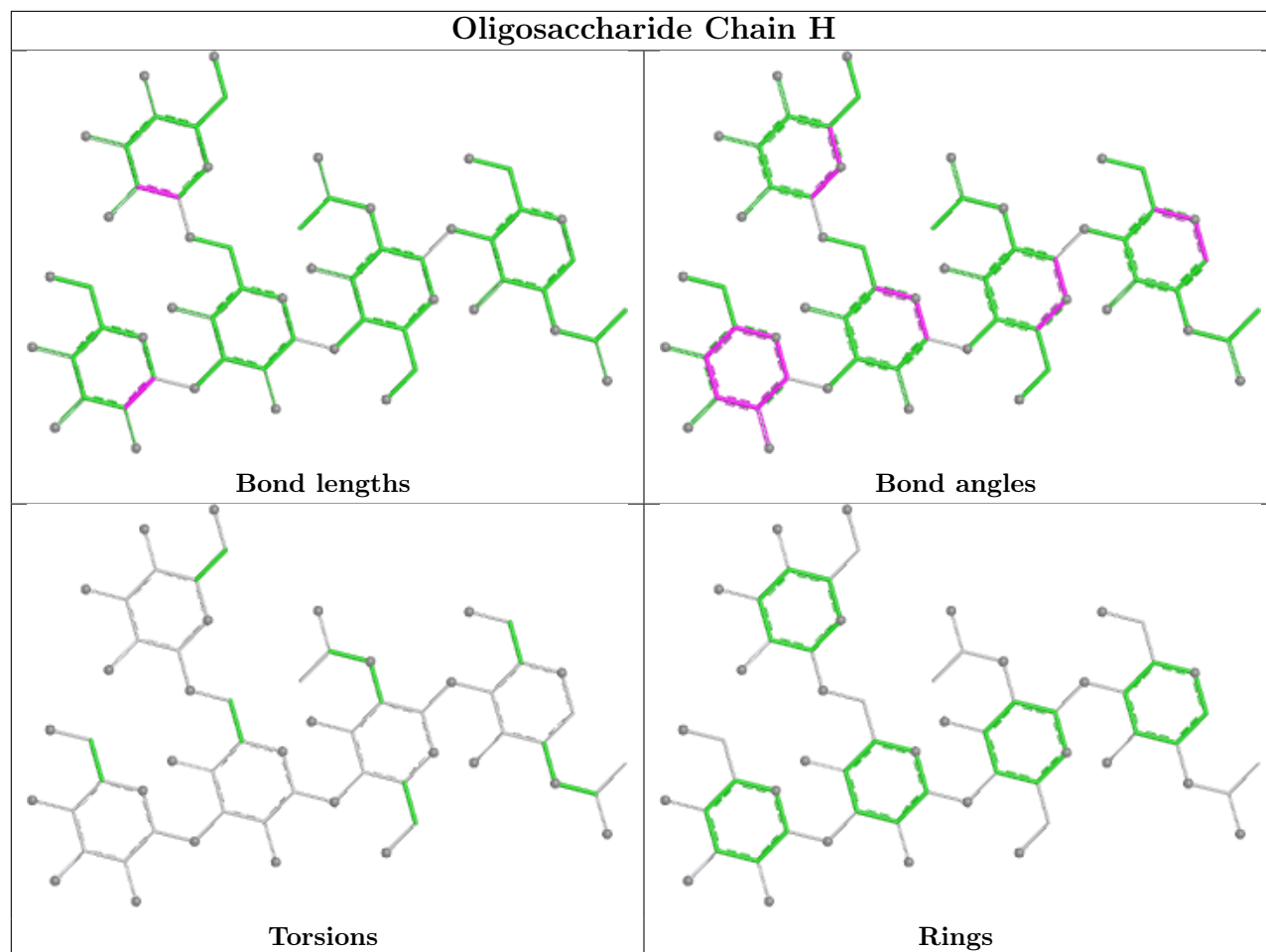
There are no ring outliers.

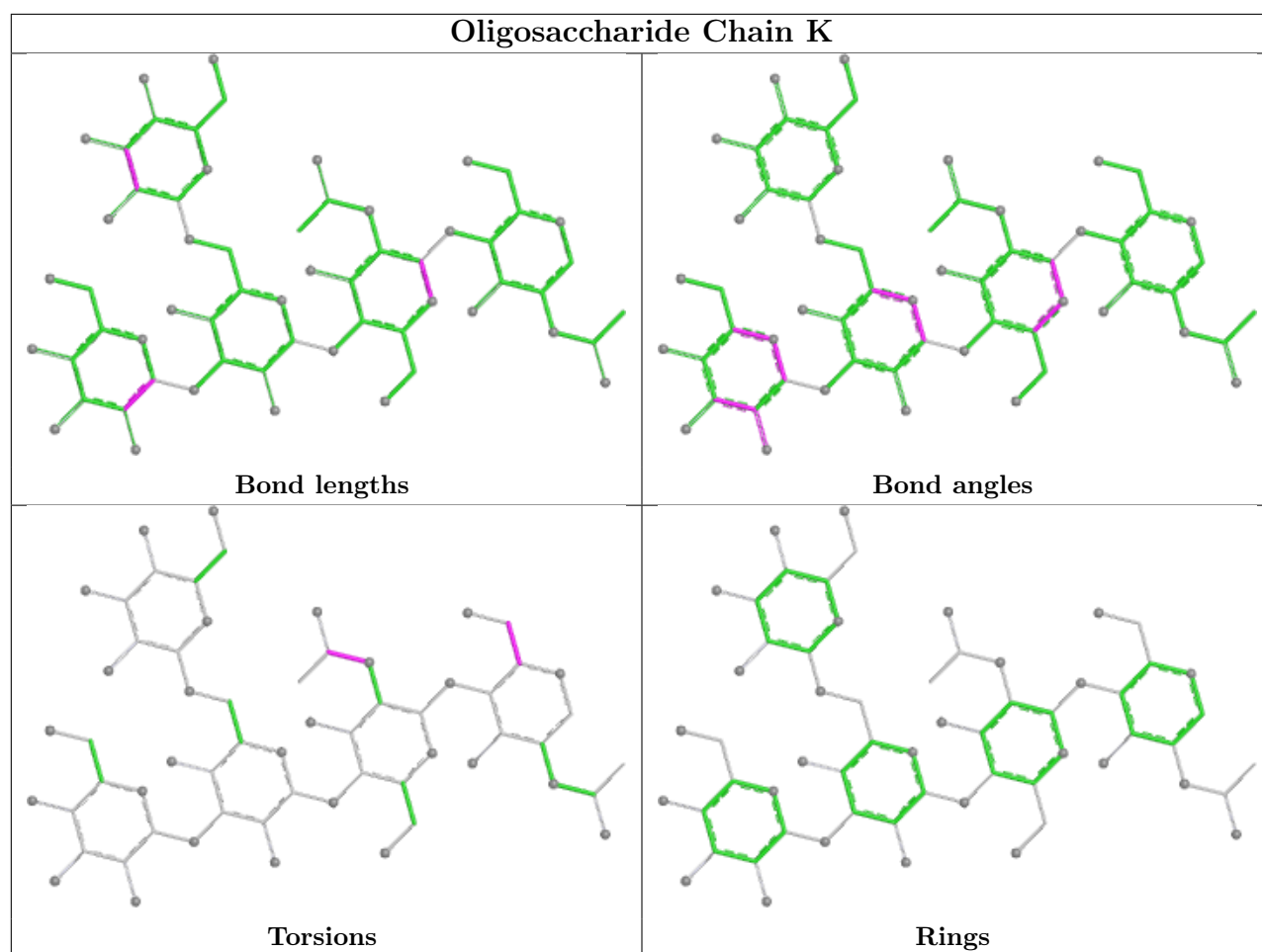
9 monomers are involved in 9 short contacts:

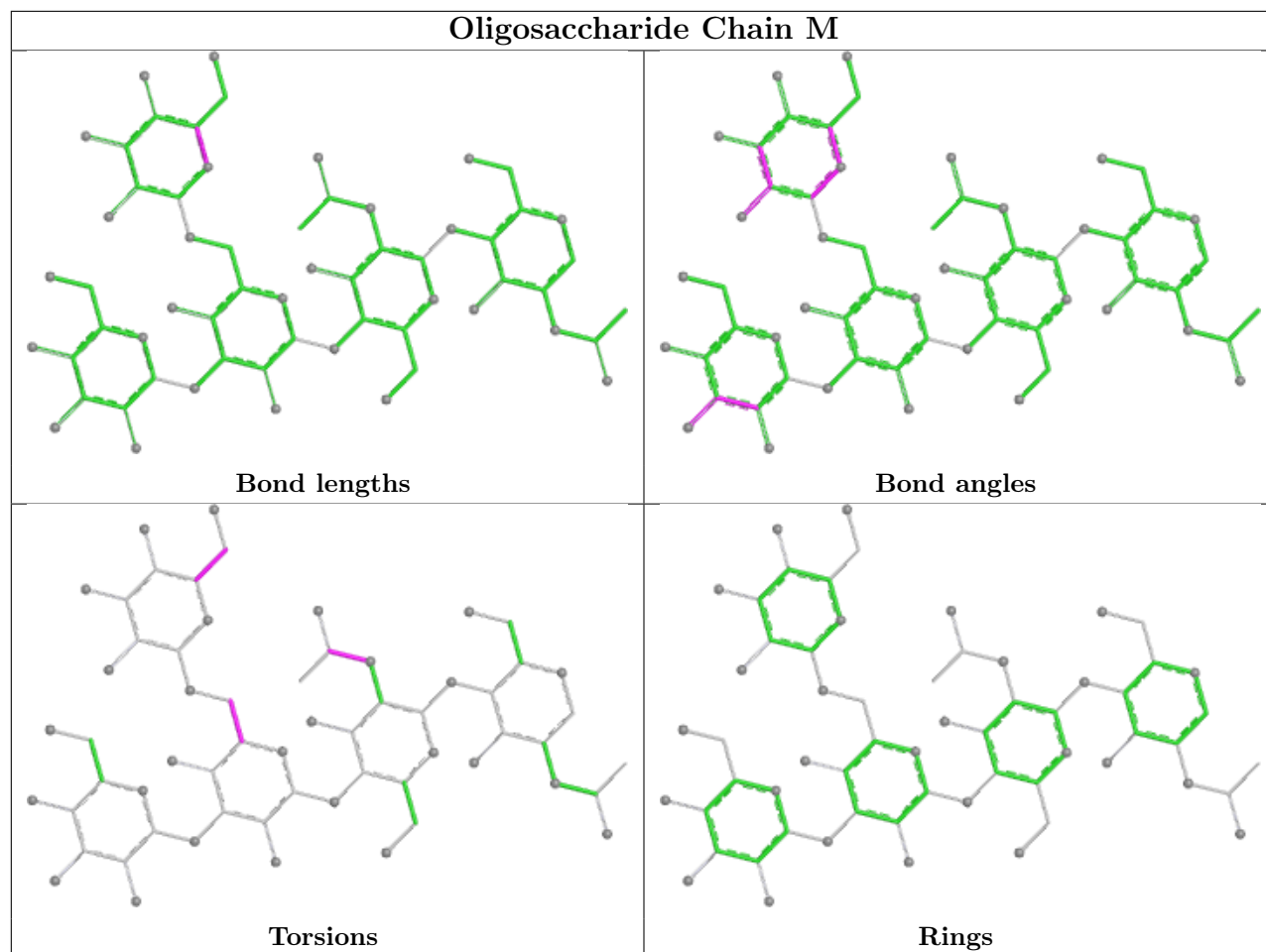
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	5	MAN	1	0
3	P	1	NAG	1	0
3	M	2	NAG	2	0
2	G	1	NAG	1	0
6	Q	3	BMA	1	0
3	N	1	NAG	1	0
2	G	5	MAN	1	0
2	G	3	BMA	1	0
3	R	3	BMA	1	0

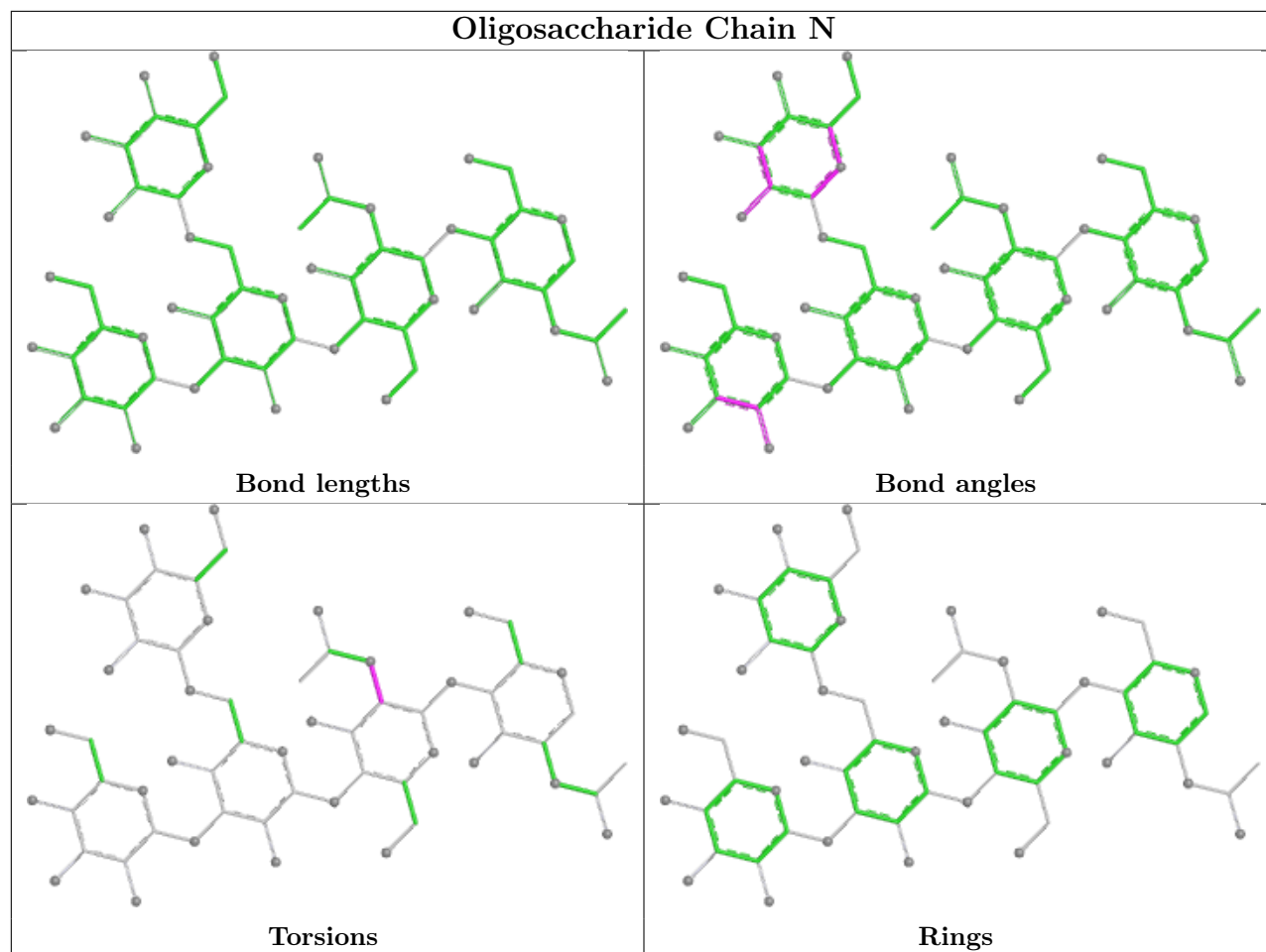
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

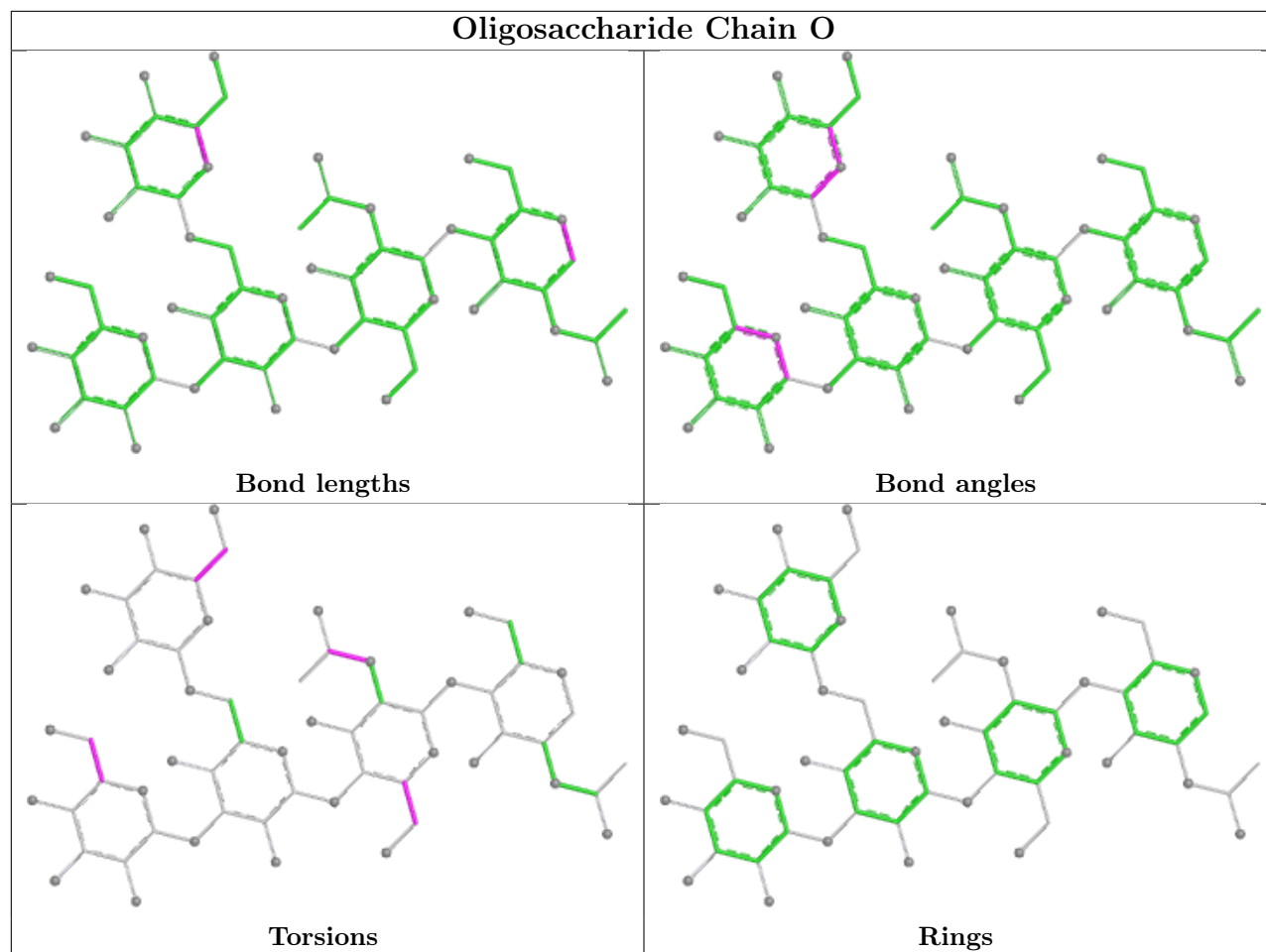


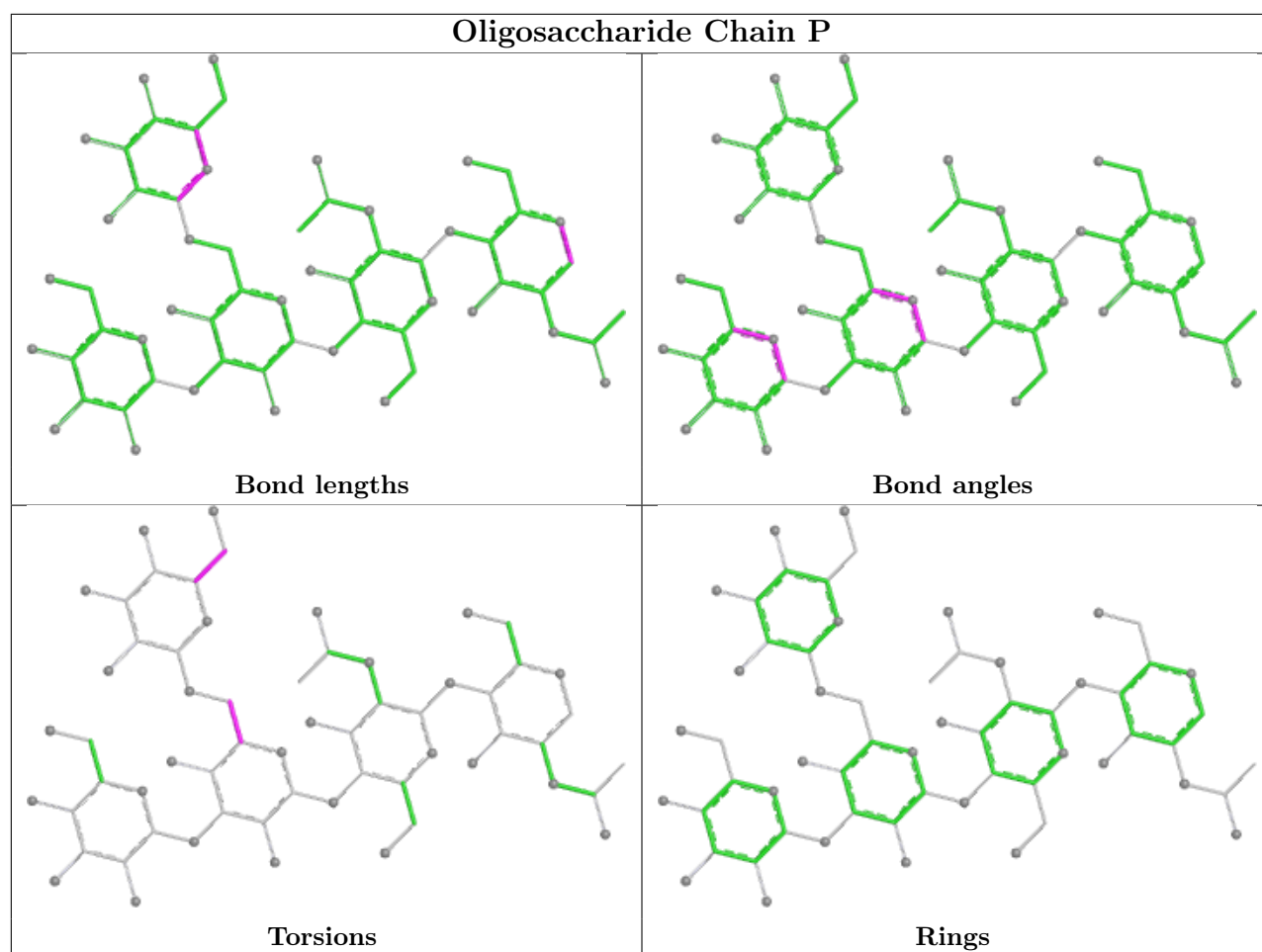


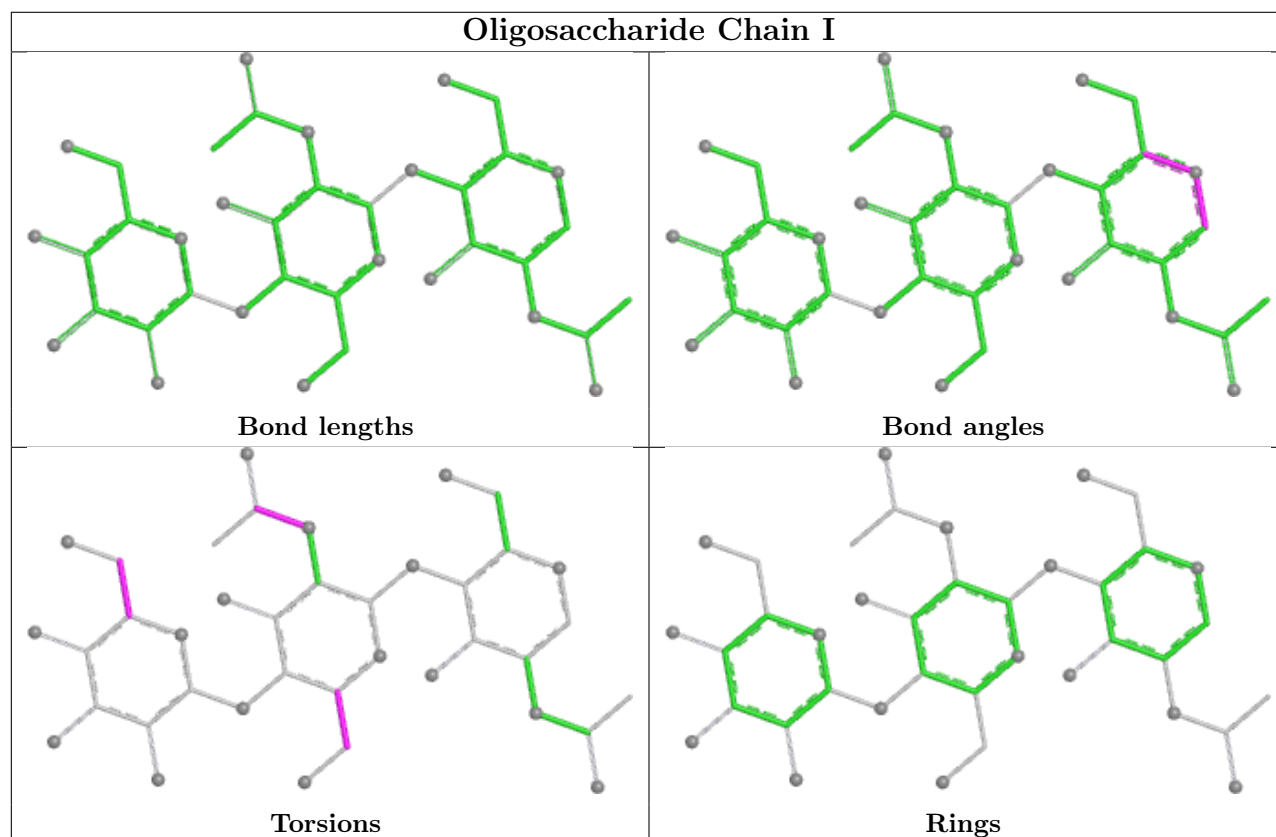
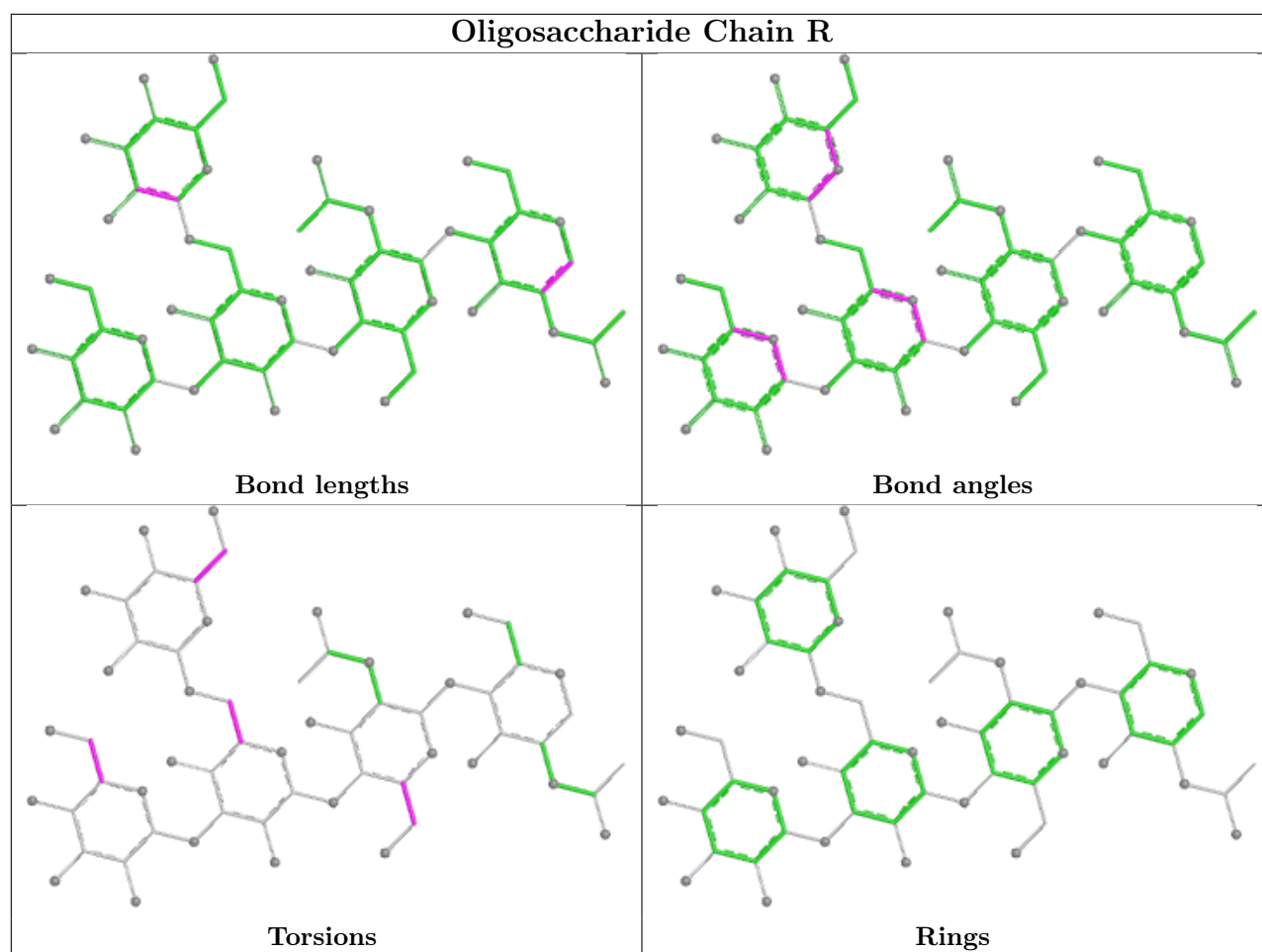


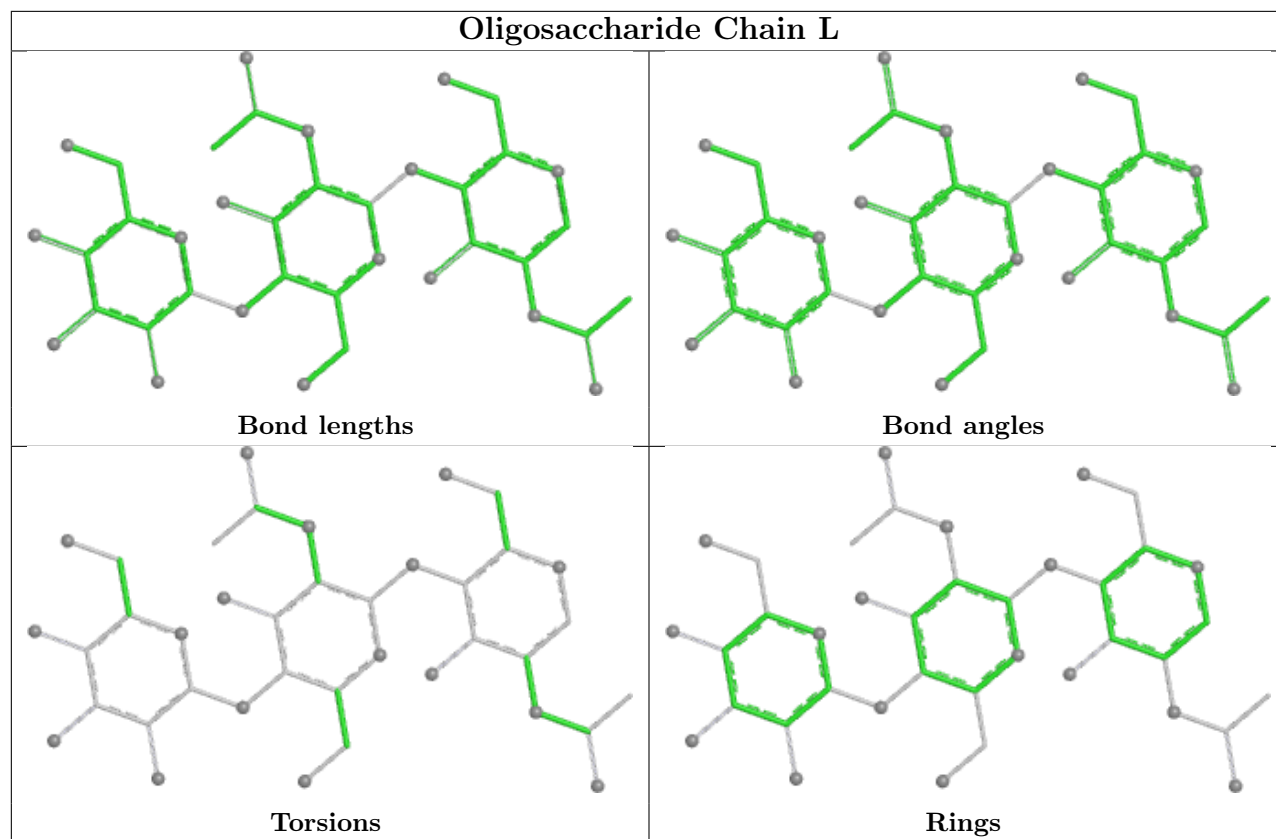




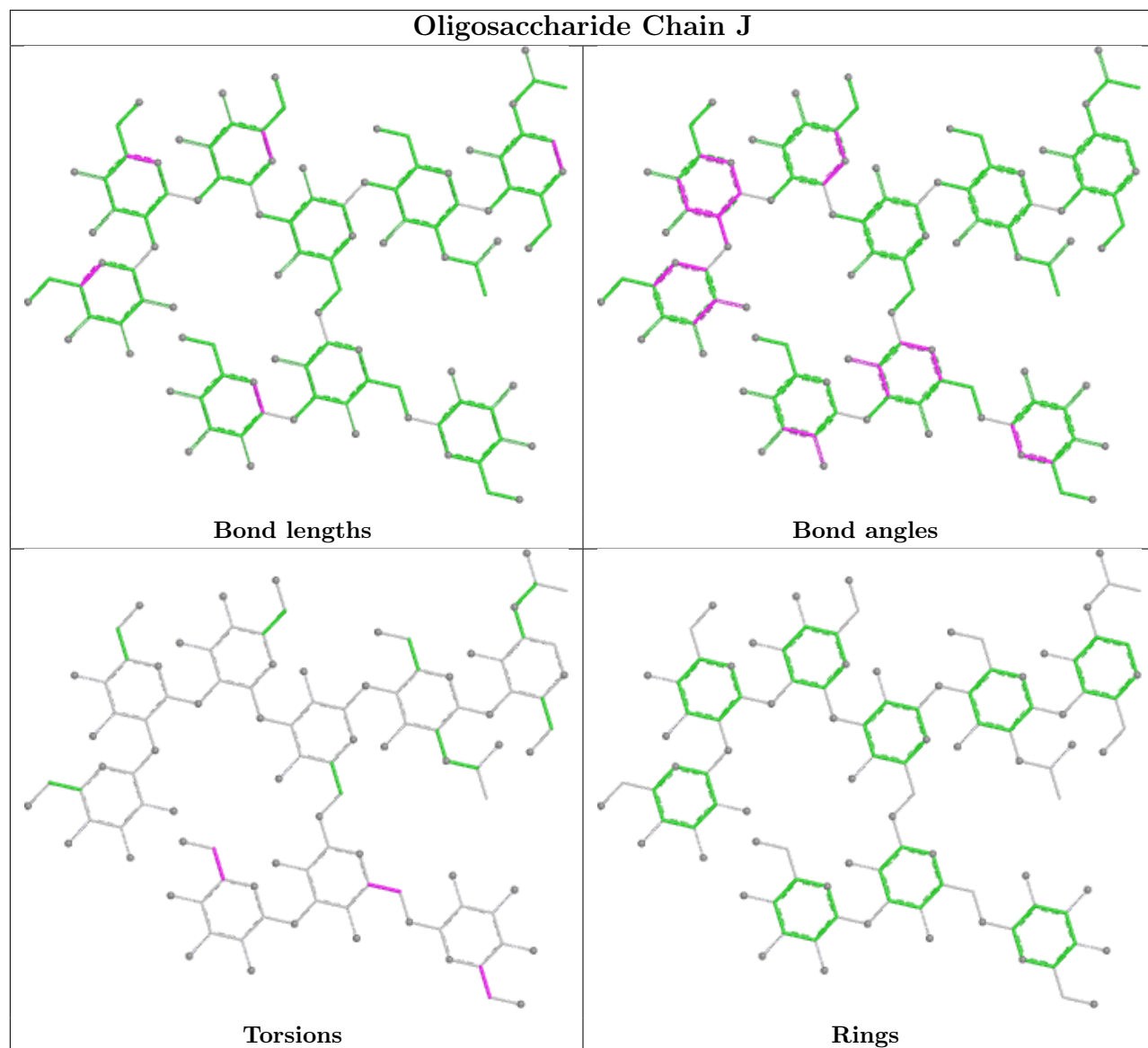


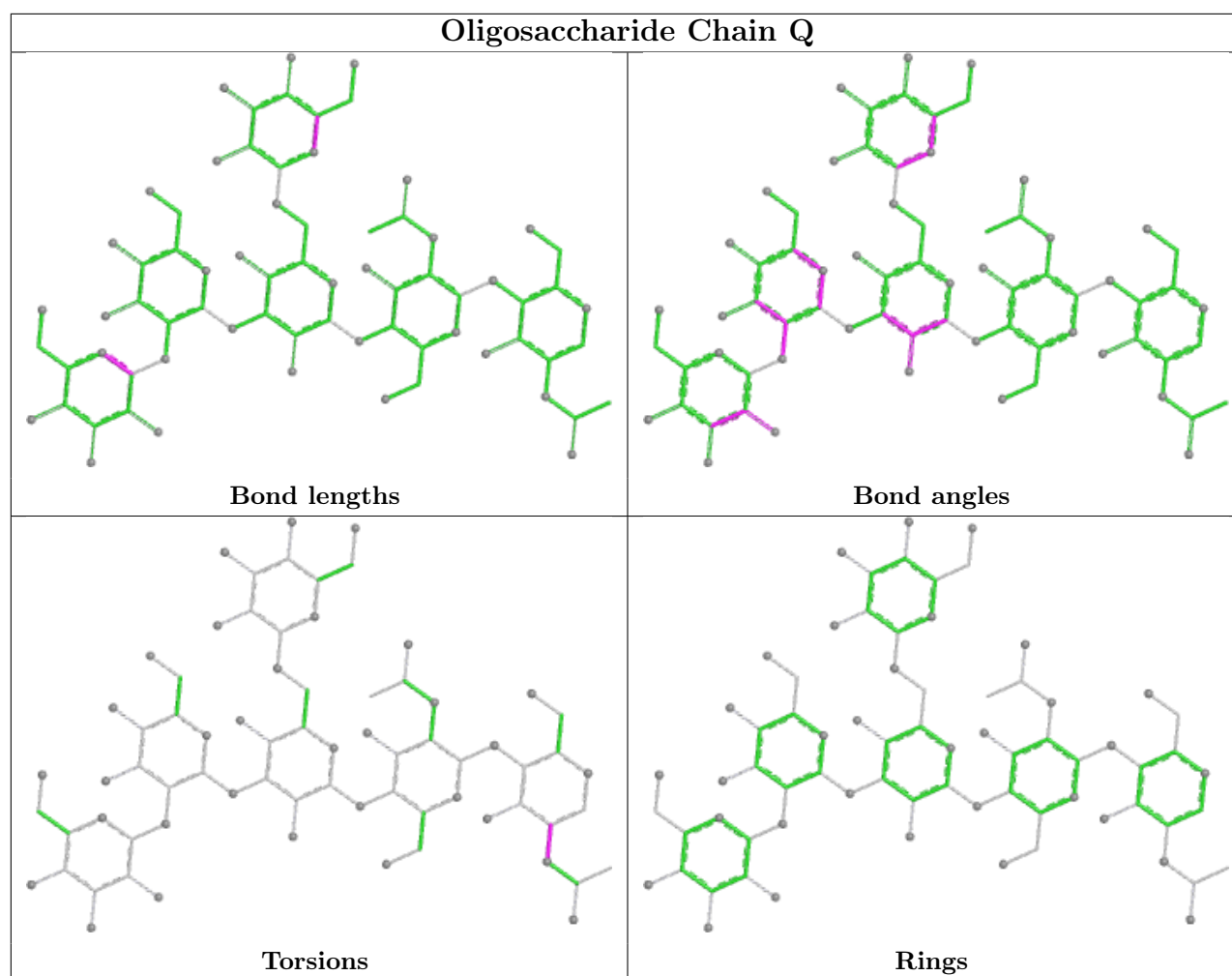






Oligosaccharide Chain J





5.6 Ligand geometry [i](#)

Of 62 ligands modelled in this entry, 33 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	$\# Z > 2$
11	MPD	A	907	-	7,7,7	0.23	0	9,10,10	0.27	0
12	GOL	B	911	-	5,5,5	0.66	0	5,5,5	1.37	0
12	GOL	C	909	-	5,5,5	1.05	0	5,5,5	1.29	0
13	GLY	D	913	-	4,4,4	1.12	0	3,4,4	0.87	0
13	GLY	F	907	-	4,4,4	0.78	0	3,4,4	1.84	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	GLY	C	910	-	4,4,4	1.03	0	3,4,4	1.00	0
13	GLY	E	909	-	4,4,4	1.05	0	3,4,4	1.86	2 (66%)
11	MPD	A	908	-	7,7,7	0.29	0	9,10,10	0.50	0
12	GOL	A	910	-	5,5,5	0.89	0	5,5,5	0.74	0
10	MES	E	906	-	12,12,12	2.28	1 (8%)	15,16,16	2.49	8 (53%)
11	MPD	A	905	-	7,7,7	0.46	0	9,10,10	0.41	0
13	GLY	E	910	-	4,4,4	0.95	0	3,4,4	1.60	1 (33%)
11	MPD	B	909	-	7,7,7	0.49	0	9,10,10	0.67	0
12	GOL	A	909	-	5,5,5	1.03	0	5,5,5	0.98	0
10	MES	B	907	-	12,12,12	2.27	1 (8%)	15,16,16	1.82	3 (20%)
14	SO4	F	905	-	4,4,4	0.48	0	6,6,6	0.41	0
11	MPD	F	906	-	7,7,7	0.30	0	9,10,10	0.31	0
11	MPD	A	906	-	7,7,7	0.34	0	9,10,10	0.38	0
13	GLY	D	912	-	4,4,4	1.09	1 (25%)	3,4,4	1.92	2 (66%)
11	MPD	D	911	-	7,7,7	0.30	0	9,10,10	0.67	0
13	GLY	C	911	-	4,4,4	1.09	0	3,4,4	1.56	0
11	MPD	C	908	-	7,7,7	0.34	0	9,10,10	0.77	0
11	MPD	E	907	-	7,7,7	0.35	0	9,10,10	0.53	0
12	GOL	E	908	-	5,5,5	1.13	1 (20%)	5,5,5	1.86	1 (20%)
14	SO4	D	909	-	4,4,4	0.34	0	6,6,6	0.20	0
11	MPD	B	908	-	7,7,7	0.35	0	9,10,10	0.42	0
11	MPD	D	910	-	7,7,7	0.33	0	9,10,10	0.43	0
10	MES	A	904	-	12,12,12	2.20	1 (8%)	15,16,16	1.94	4 (26%)
12	GOL	B	910	-	5,5,5	1.06	1 (20%)	5,5,5	1.79	1 (20%)

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	MPD	A	907	-	-	3/5/5/5	-
12	GOL	B	911	-	-	0/4/4/4	-
12	GOL	C	909	-	-	2/4/4/4	-
13	GLY	D	913	-	-	0/2/2/2	-
13	GLY	F	907	-	-	0/2/2/2	-
13	GLY	C	910	-	-	0/2/2/2	-
13	GLY	E	909	-	-	2/2/2/2	-
11	MPD	A	908	-	-	4/5/5/5	-
12	GOL	A	910	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MES	E	906	-	-	5/6/14/14	0/1/1/1
11	MPD	A	905	-	-	0/5/5/5	-
13	GLY	E	910	-	-	0/2/2/2	-
11	MPD	B	909	-	-	0/5/5/5	-
12	GOL	A	909	-	-	0/4/4/4	-
10	MES	B	907	-	-	4/6/14/14	0/1/1/1
11	MPD	F	906	-	-	0/5/5/5	-
11	MPD	A	906	-	-	2/5/5/5	-
13	GLY	D	912	-	-	2/2/2/2	-
11	MPD	D	911	-	-	3/5/5/5	-
13	GLY	C	911	-	-	2/2/2/2	-
11	MPD	C	908	-	-	0/5/5/5	-
11	MPD	E	907	-	-	0/5/5/5	-
12	GOL	E	908	-	-	4/4/4/4	-
11	MPD	B	908	-	-	4/5/5/5	-
11	MPD	D	910	-	-	0/5/5/5	-
10	MES	A	904	-	-	5/6/14/14	0/1/1/1
12	GOL	B	910	-	-	0/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	906	MES	C8-S	-7.55	1.67	1.77
10	B	907	MES	C8-S	-7.43	1.67	1.77
10	A	904	MES	C8-S	-7.23	1.67	1.77
12	B	910	GOL	C1-C2	2.22	1.60	1.51
13	D	912	GLY	OXT-C	-2.09	1.23	1.30

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	907	MES	C5-N4-C3	5.21	120.07	108.84
10	E	906	MES	O2S-S-C8	4.57	113.63	106.73
10	E	906	MES	C5-N4-C3	4.07	117.60	108.84
10	A	904	MES	O2S-S-C8	4.07	112.87	106.73
12	E	908	GOL	C3-C2-C1	-3.65	98.43	111.80

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	904	MES	C8-C7-N4-C5
10	A	904	MES	C7-C8-S-O1S
11	A	907	MPD	C1-C2-C3-C4
11	A	907	MPD	O2-C2-C3-C4
11	A	908	MPD	C2-C3-C4-C5

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	909	GOL	1	0
13	D	913	GLY	1	0
13	F	907	GLY	1	0
13	C	910	GLY	1	0
11	A	908	MPD	1	0
10	E	906	MES	1	0
13	E	910	GLY	1	0
12	A	909	GOL	2	0
11	F	906	MPD	1	0
13	D	912	GLY	1	0
11	D	911	MPD	1	0
10	A	904	MES	1	0
12	B	910	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	679/702 (96%)	-0.42	5 (0%) 84 82	23, 38, 67, 117	1 (0%)
1	B	672/702 (95%)	-0.46	14 (2%) 63 60	22, 36, 63, 132	1 (0%)
1	C	678/702 (96%)	-0.23	7 (1%) 79 77	25, 47, 80, 141	1 (0%)
1	D	677/702 (96%)	-0.26	13 (1%) 66 63	29, 43, 82, 142	0
1	E	671/702 (95%)	-0.33	14 (2%) 63 60	26, 39, 80, 147	0
1	F	678/702 (96%)	-0.28	9 (1%) 75 73	27, 43, 80, 123	1 (0%)
All	All	4055/4212 (96%)	-0.33	62 (1%) 72 69	22, 41, 77, 147	4 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	641	TRP	4.9
1	E	641	TRP	4.3
1	B	636	ALA	3.7
1	B	641	TRP	3.7
1	F	644	MET	3.5

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($\text{\AA}^2$)	Q<0.9
3	MAN	P	4	11/12	0.36	0.13	108,113,119,121	0
3	MAN	R	4	11/12	0.37	0.12	102,108,112,113	0
3	MAN	O	5	11/12	0.39	0.15	100,106,107,111	0
3	BMA	R	3	11/12	0.50	0.13	96,101,106,110	0
3	MAN	M	5	11/12	0.51	0.14	101,105,109,109	0
3	MAN	N	4	11/12	0.51	0.12	98,105,116,120	0
4	BMA	I	3	11/12	0.51	0.14	73,79,86,95	0
3	MAN	R	5	11/12	0.55	0.14	97,101,104,105	0
5	MAN	J	9	11/12	0.56	0.15	82,90,96,103	0
3	MAN	P	5	11/12	0.57	0.14	83,95,96,96	0
6	MAN	Q	6	11/12	0.57	0.13	84,89,96,98	0
3	MAN	K	5	11/12	0.58	0.13	86,88,95,95	0
6	MAN	Q	5	11/12	0.61	0.14	108,112,117,119	0
3	MAN	N	5	11/12	0.61	0.14	100,102,108,111	0
4	NAG	I	2	14/15	0.63	0.13	64,69,74,80	0
4	BMA	L	3	11/12	0.64	0.11	92,97,99,100	0
5	MAN	J	8	11/12	0.66	0.12	82,84,88,90	0
3	MAN	H	4	11/12	0.67	0.13	77,81,84,85	0
2	MAN	G	5	11/12	0.67	0.15	85,99,108,113	0
3	MAN	H	5	11/12	0.68	0.11	77,84,91,92	0
3	MAN	K	4	11/12	0.69	0.13	95,100,105,112	0
3	BMA	P	3	11/12	0.70	0.11	90,96,103,107	0
3	BMA	K	3	11/12	0.72	0.10	81,82,87,91	0
2	MAN	G	4	11/12	0.73	0.12	84,88,93,95	0
3	BMA	N	3	11/12	0.76	0.10	73,82,90,98	0
3	NAG	O	2	14/15	0.77	0.10	50,57,62,64	0
6	MAN	Q	4	11/12	0.79	0.12	76,81,91,95	0
3	MAN	M	4	11/12	0.79	0.13	66,75,79,86	0
2	MAN	G	6	11/12	0.79	0.12	53,59,66,67	0
3	MAN	O	4	11/12	0.80	0.10	64,73,75,75	0
3	BMA	O	3	11/12	0.80	0.09	62,71,81,89	0
5	MAN	J	5	11/12	0.81	0.10	68,71,74,79	0
3	BMA	H	3	11/12	0.82	0.10	71,74,78,79	0
5	MAN	J	4	11/12	0.83	0.10	66,68,71,74	0
4	NAG	L	2	14/15	0.85	0.10	73,78,92,94	0
6	BMA	Q	3	11/12	0.87	0.09	68,79,82,82	0
3	NAG	M	2	14/15	0.87	0.09	58,62,64,69	0
3	NAG	H	1	14/15	0.88	0.09	45,49,53,56	0
5	BMA	J	3	11/12	0.88	0.07	58,61,66,67	0
3	NAG	P	2	14/15	0.89	0.09	54,66,78,83	0
6	NAG	Q	2	14/15	0.89	0.09	50,55,65,66	0
4	NAG	L	1	14/15	0.89	0.09	53,59,68,73	0
4	NAG	I	1	14/15	0.89	0.09	43,57,64,68	0

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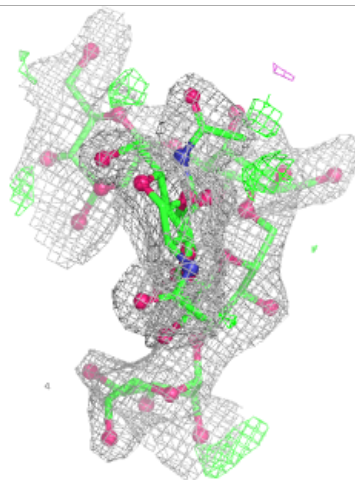
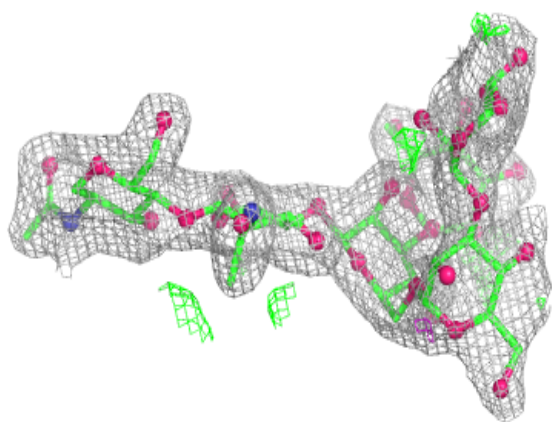
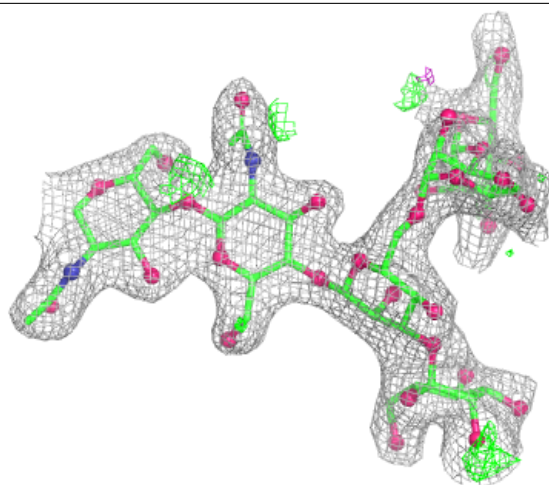
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MAN	J	6	11/12	0.89	0.09	58,68,75,77	0
3	BMA	M	3	11/12	0.89	0.07	73,79,89,91	0
2	NAG	G	2	14/15	0.90	0.07	48,51,58,60	0
3	NAG	N	2	14/15	0.90	0.10	57,64,67,71	0
3	NAG	K	2	14/15	0.90	0.09	59,65,72,72	0
2	BMA	G	3	11/12	0.91	0.07	60,68,73,80	0
3	NAG	R	2	14/15	0.91	0.08	67,73,82,88	0
5	MAN	J	7	11/12	0.92	0.08	64,70,81,81	0
3	NAG	O	1	14/15	0.92	0.08	41,46,50,53	0
6	NAG	Q	1	14/15	0.93	0.07	42,47,51,54	0
3	NAG	K	1	14/15	0.93	0.07	50,54,57,59	0
5	NAG	J	1	14/15	0.93	0.08	33,42,49,49	0
5	NAG	J	2	14/15	0.93	0.07	44,50,57,60	0
3	NAG	N	1	14/15	0.93	0.08	43,48,55,58	0
3	NAG	H	2	14/15	0.93	0.07	55,59,63,68	0
3	NAG	R	1	14/15	0.94	0.07	50,58,64,69	0
3	NAG	M	1	14/15	0.94	0.08	47,56,60,62	0
2	NAG	G	1	14/15	0.95	0.06	40,45,47,49	0
3	NAG	P	1	14/15	0.96	0.06	40,46,54,57	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.

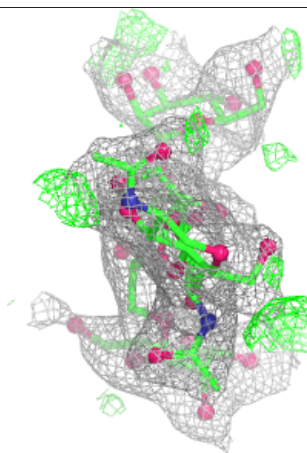
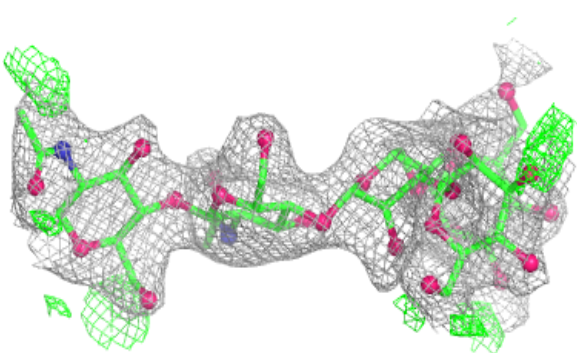
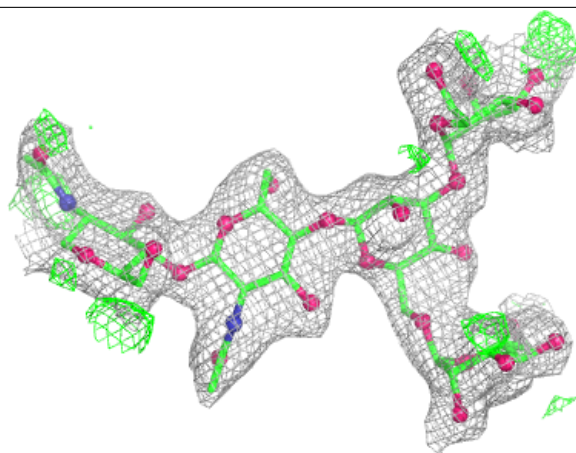
Electron density around Chain G:

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

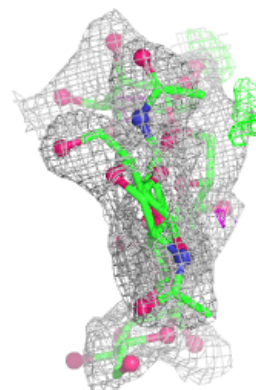
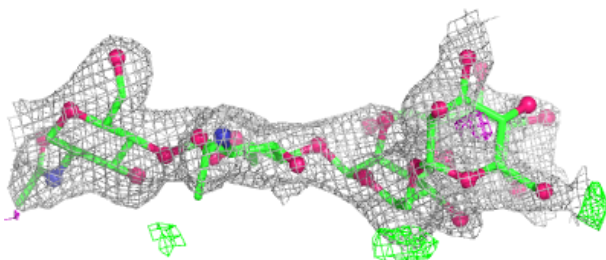
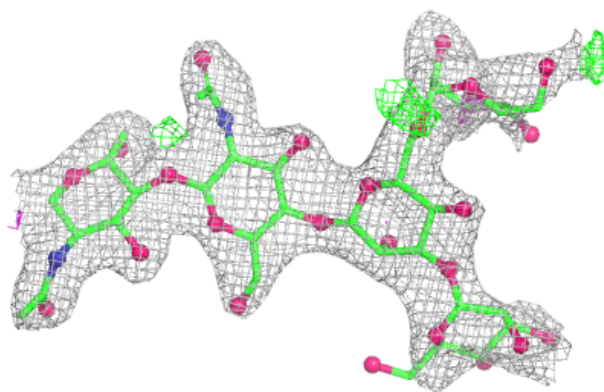


Electron density around Chain H:

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

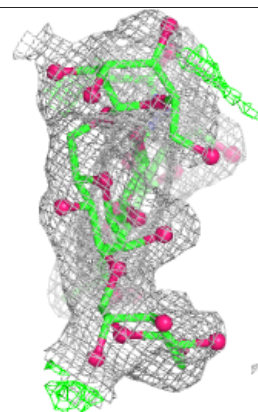
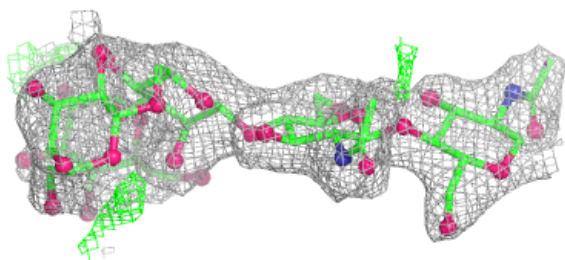
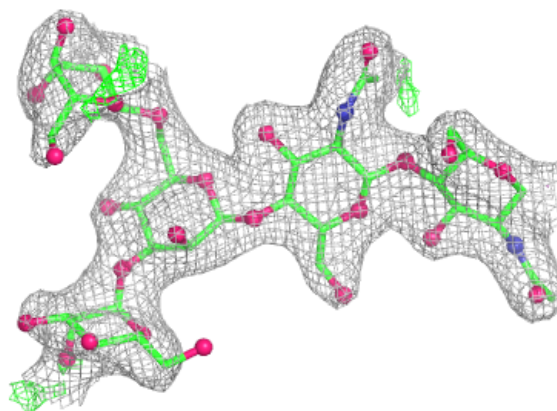
**Electron density around Chain K:**

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



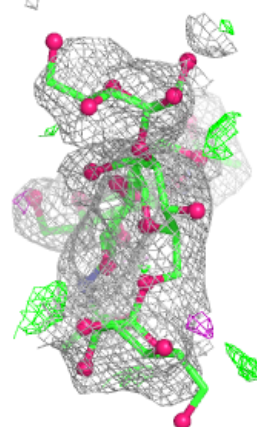
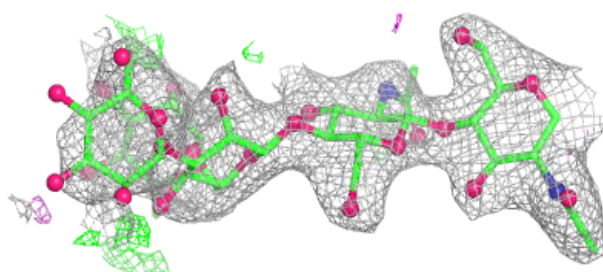
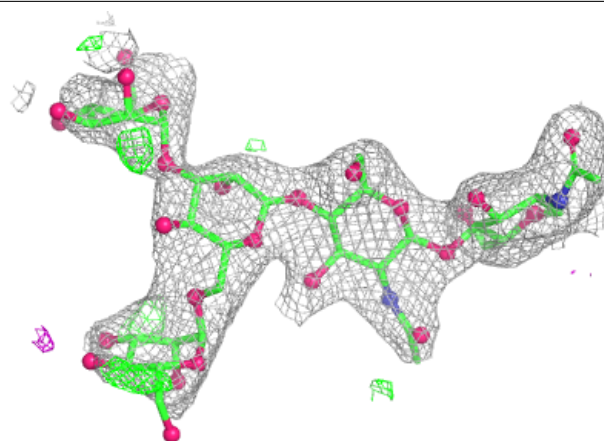
Electron density around Chain M:

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



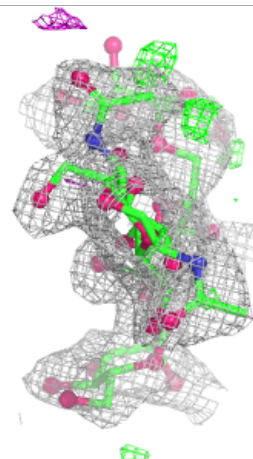
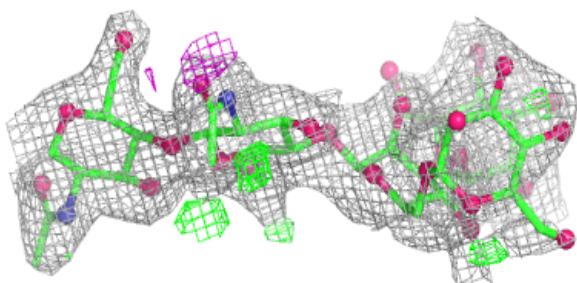
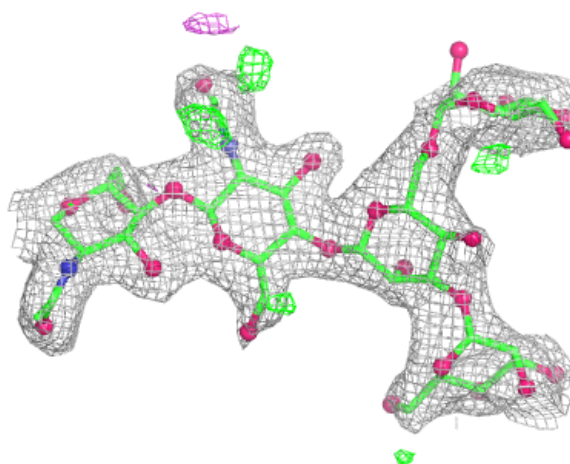
Electron density around Chain N:

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



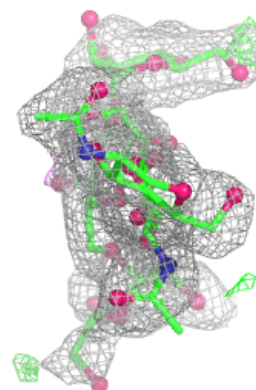
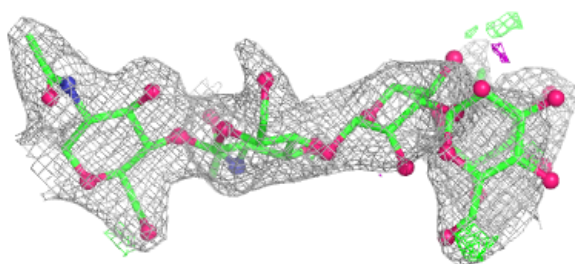
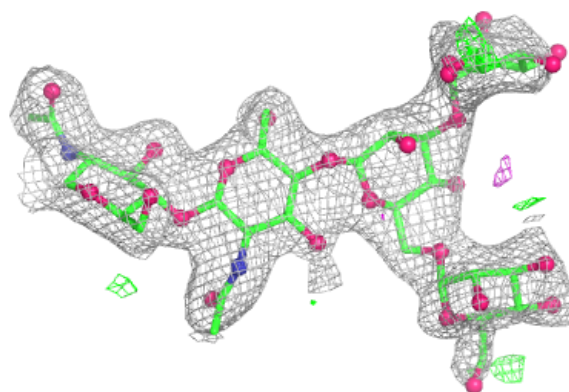
Electron density around Chain O:

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



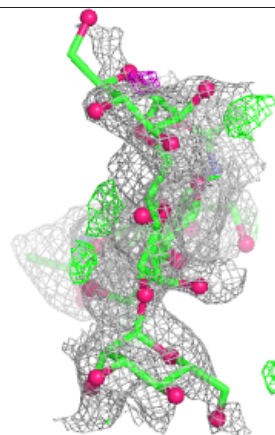
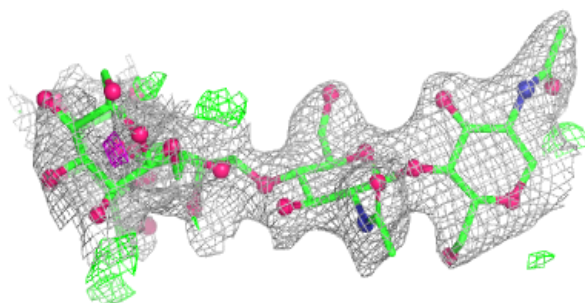
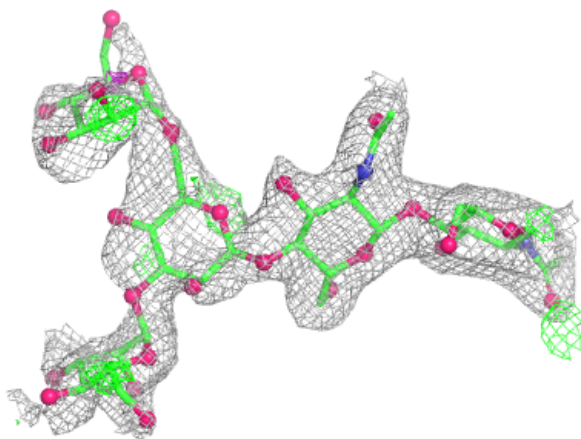
Electron density around Chain P:

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



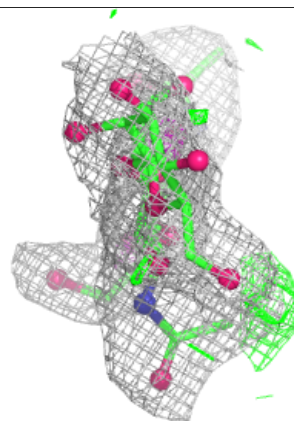
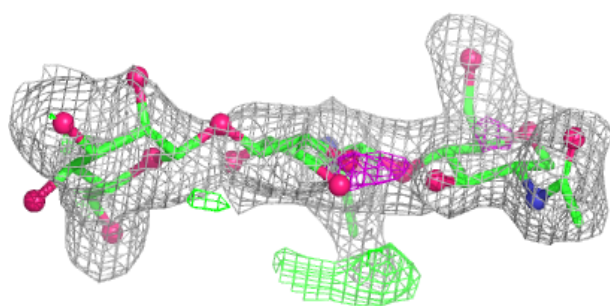
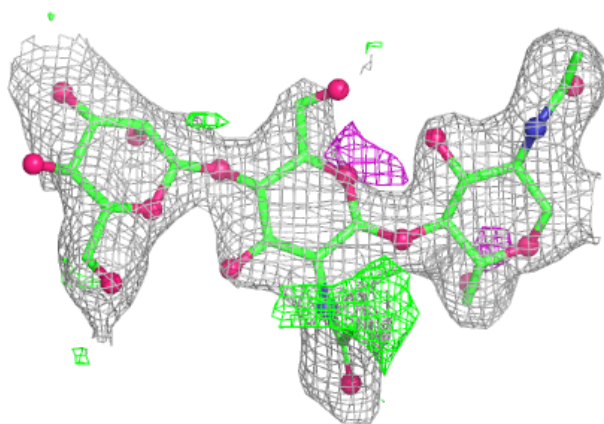
Electron density around Chain R:

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

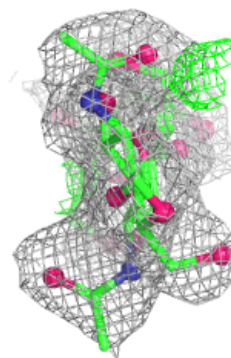
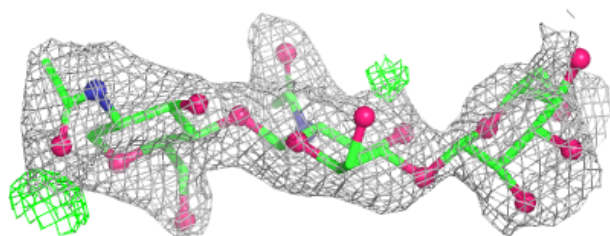
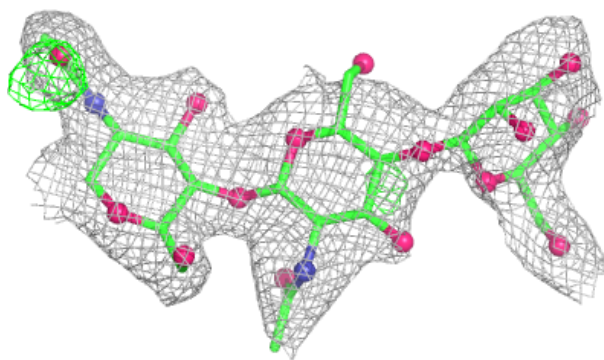


Electron density around Chain I:

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

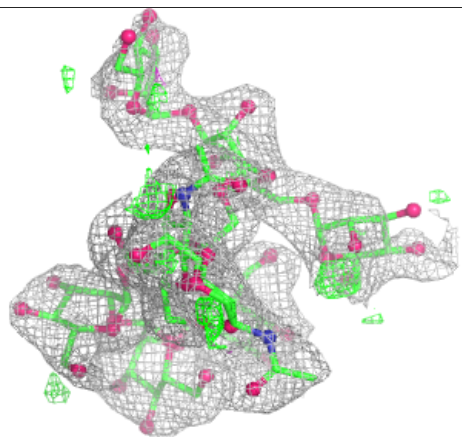
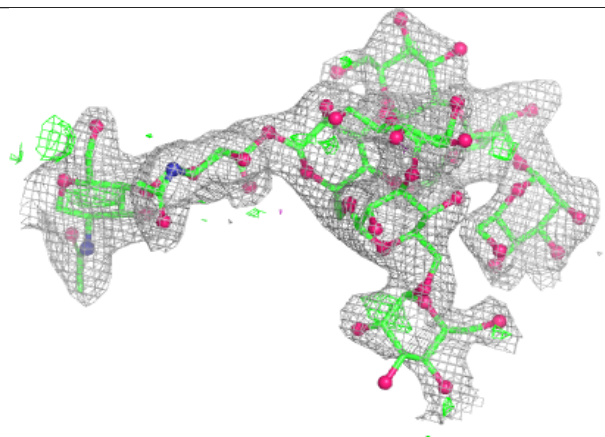
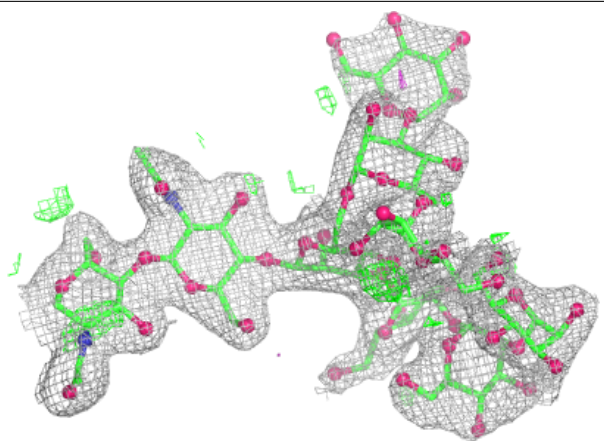
**Electron density around Chain L:**

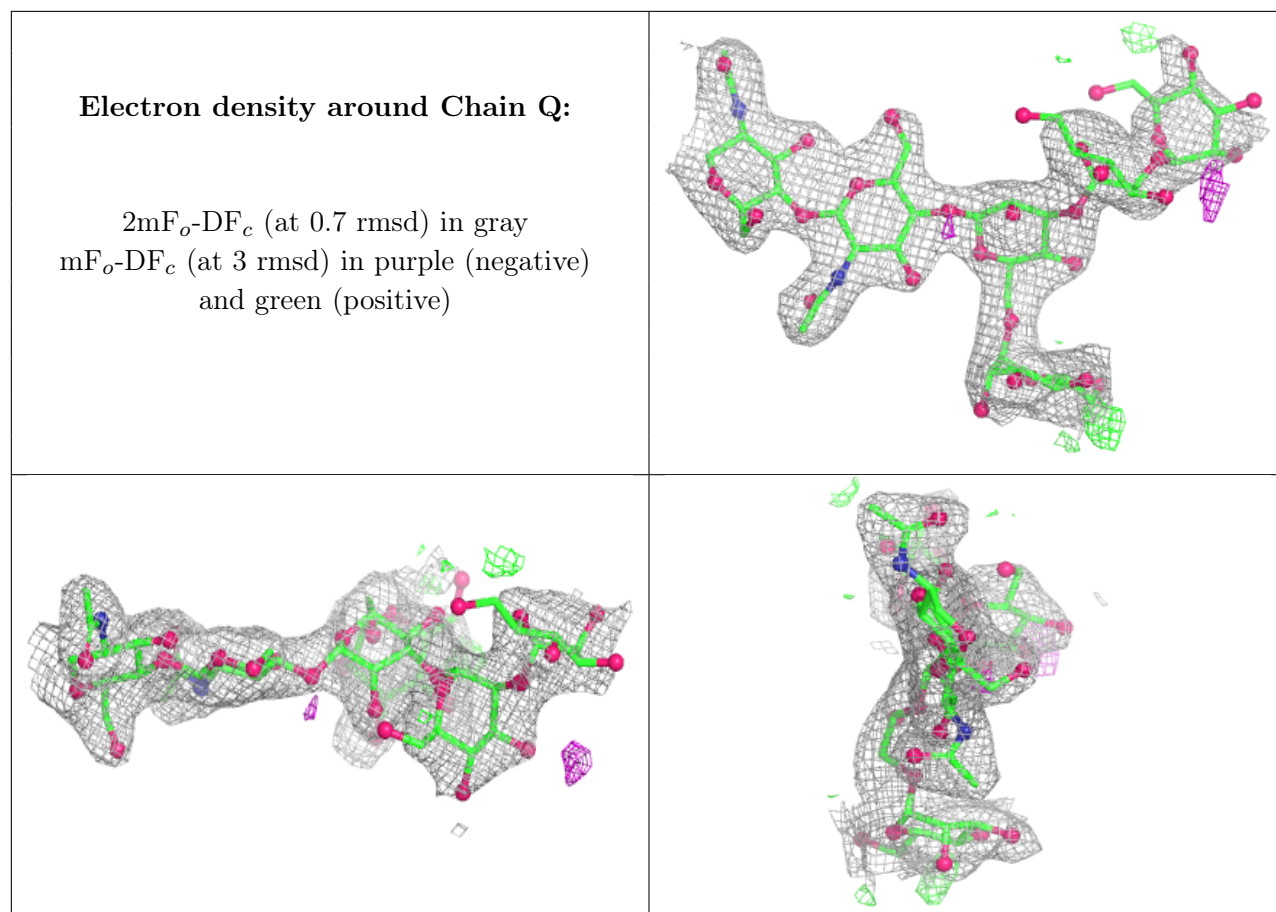
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	GLY	C	911	5/5	0.76	0.12	61,62,70,73	0
14	SO4	D	909	5/5	0.77	0.10	69,75,78,89	0
13	GLY	D	912	5/5	0.81	0.14	46,49,52,53	0
13	GLY	D	913	5/5	0.84	0.12	32,34,38,44	0
10	MES	A	904	12/12	0.84	0.14	46,50,60,60	0
9	CL	B	906	1/1	0.86	0.17	79,79,79,79	0
11	MPD	D	911	8/8	0.86	0.13	44,53,56,62	0
9	CL	D	905	1/1	0.86	0.14	71,71,71,71	0
14	SO4	F	905	5/5	0.86	0.14	49,50,55,77	0
9	CL	E	903	1/1	0.87	0.12	73,73,73,73	0
9	CL	A	903	1/1	0.87	0.16	85,85,85,85	0
11	MPD	A	906	8/8	0.87	0.12	44,52,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CL	C	904	1/1	0.88	0.14	68,68,68,68	0
9	CL	E	904	1/1	0.88	0.15	72,72,72,72	0
9	CL	D	903	1/1	0.88	0.14	76,76,76,76	0
9	CL	B	904	1/1	0.88	0.17	78,78,78,78	0
13	GLY	E	909	5/5	0.88	0.09	46,47,49,51	0
11	MPD	A	907	8/8	0.88	0.13	44,49,58,62	0
11	MPD	B	908	8/8	0.88	0.11	40,46,55,56	0
9	CL	F	904	1/1	0.89	0.13	78,78,78,78	0
9	CL	E	905	1/1	0.89	0.13	68,68,68,68	0
12	GOL	C	909	6/6	0.89	0.11	49,52,53,58	0
12	GOL	A	909	6/6	0.90	0.09	43,48,50,50	0
13	GLY	F	907	5/5	0.90	0.08	34,38,42,45	0
11	MPD	C	908	8/8	0.91	0.10	38,45,47,47	0
10	MES	B	907	12/12	0.91	0.10	38,47,55,57	0
8	MG	C	902	1/1	0.91	0.17	57,57,57,57	0
12	GOL	B	911	6/6	0.91	0.10	38,42,43,53	0
9	CL	C	906	1/1	0.91	0.19	73,73,73,73	0
9	CL	B	903	1/1	0.91	0.09	67,67,67,67	0
9	CL	D	906	1/1	0.92	0.09	65,65,65,65	0
13	GLY	C	910	5/5	0.92	0.08	32,37,39,42	0
13	GLY	E	910	5/5	0.92	0.09	44,44,50,52	0
9	CL	D	908	1/1	0.93	0.09	56,56,56,56	0
10	MES	E	906	12/12	0.93	0.10	42,50,53,60	0
12	GOL	E	908	6/6	0.93	0.07	29,30,32,33	0
8	MG	A	902	1/1	0.93	0.14	54,54,54,54	0
11	MPD	E	907	8/8	0.93	0.08	33,36,41,41	0
9	CL	D	907	1/1	0.93	0.15	72,72,72,72	0
9	CL	F	903	1/1	0.94	0.13	57,57,57,57	0
9	CL	C	905	1/1	0.94	0.12	72,72,72,72	0
11	MPD	F	906	8/8	0.94	0.07	33,37,42,42	0
9	CL	B	905	1/1	0.94	0.20	72,72,72,72	0
11	MPD	B	909	8/8	0.95	0.07	34,38,41,42	0
12	GOL	B	910	6/6	0.95	0.07	25,26,31,33	0
9	CL	D	902	1/1	0.95	0.16	66,66,66,66	0
11	MPD	D	910	8/8	0.95	0.07	40,41,42,45	0
9	CL	C	903	1/1	0.95	0.10	71,71,71,71	0
11	MPD	A	908	8/8	0.95	0.08	38,44,48,48	0
9	CL	D	904	1/1	0.95	0.13	58,58,58,58	0
8	MG	E	902	1/1	0.96	0.15	48,48,48,48	0
8	MG	F	902	1/1	0.96	0.10	55,55,55,55	0
11	MPD	A	905	8/8	0.96	0.05	31,37,39,42	0
9	CL	C	907	1/1	0.97	0.13	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	GOL	A	910	6/6	0.98	0.06	29,30,34,37	0
8	MG	B	902	1/1	0.98	0.10	49,49,49,49	0
7	CU	C	901	1/1	0.99	0.04	35,35,35,35	0
7	CU	D	901	1/1	0.99	0.06	38,38,38,38	0
7	CU	E	901	1/1	0.99	0.04	37,37,37,37	0
7	CU	F	901	1/1	0.99	0.06	39,39,39,39	0
7	CU	A	901	1/1	0.99	0.06	34,34,34,34	0
7	CU	B	901	1/1	0.99	0.04	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.