



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 07:18 PM UTC

PDB ID : 4UOJ / pdb_00004uoj
Title : Structure of Fungal beta-mannosidase (GH2) from Trichoderma harzianum
Authors : Muniz, J.R.C.; Aparicio, R.; Santos, J.C.; Nascimento, A.S.; Golubev, A.M.; Polikarpov, I.
Deposited on : 2014-06-04
Resolution : 2.50 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

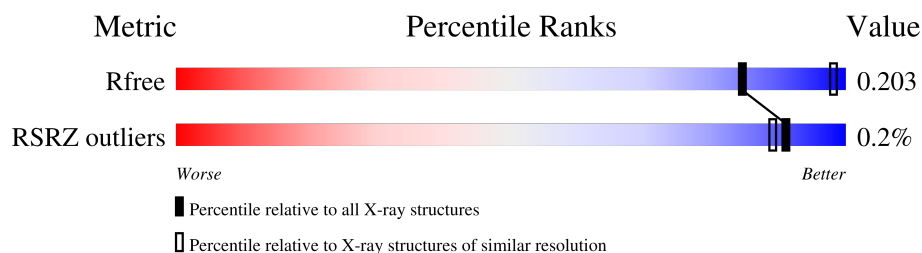
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 16996 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.

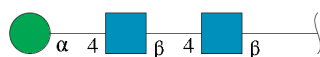
- Molecule 1 is a protein called BETA-MANNOSIDASE GH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	917	Total	C	N	O	S	0	2	0
			7259	4654	1213	1376	16			
1	B	917	Total	C	N	O	S	0	1	0
			7234	4634	1210	1374	16			

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

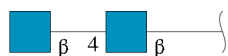
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	J	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 3 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.



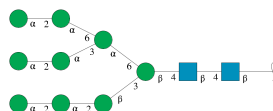
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



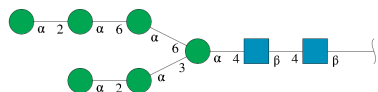
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	11	Total	C	N	O	0	0	0
			127	70	2	55			
5	K	11	Total	C	N	O	0	0	0
			127	70	2	55			

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

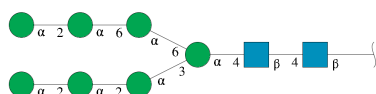


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(3-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

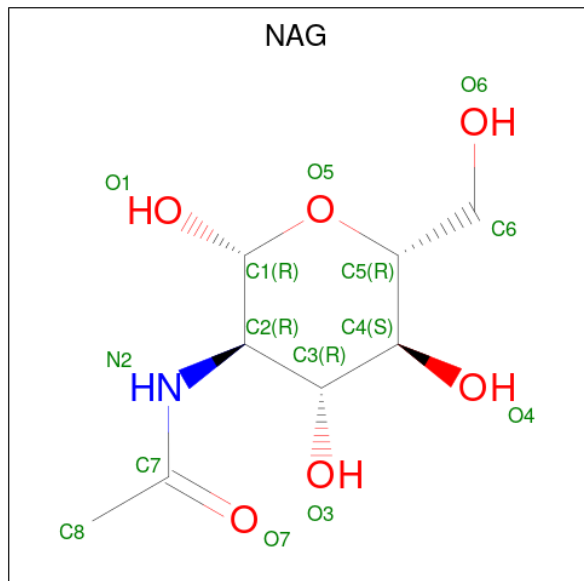
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]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
8	I	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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

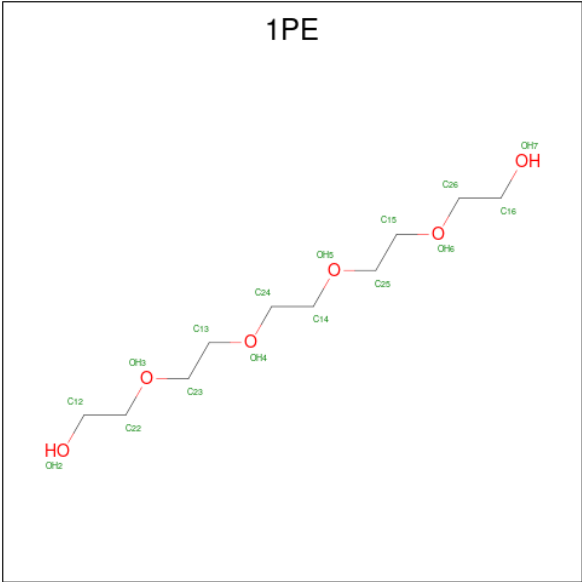
- Molecule 10 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	16	Total	Cd	0	0
			16	16		
10	B	12	Total	Cd	0	0
			12	12		

- Molecule 11 is SODIUM ION (CCD ID: NA) (formula: Na).

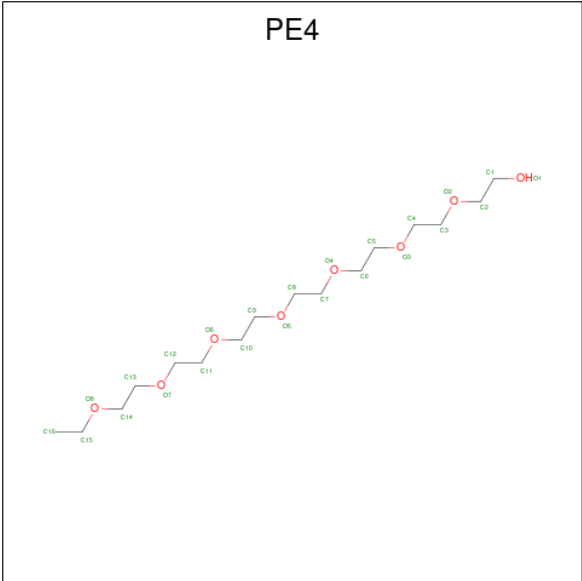
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Na	0	0
			2	2		
11	B	1	Total	Na	0	0
			1	1		

- Molecule 12 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 13 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 14 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	1	Total	Cl	0	0
			1	1		

- Molecule 15 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	1	Total	Ca	0	0
			1	1		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	731	Total	O	0	0
			731	731		
16	B	769	Total	O	0	0
			769	769		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	165.16Å 165.63Å 123.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.23 – 2.50 116.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (117.23-2.50) 99.1 (116.95-2.50)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.179 , 0.201 0.180 , 0.203	Depositor DCC
R_{free} test set	5871 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.350 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16996	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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](#)

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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](#)

65 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	1,2	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	C	2	2	14,14,15	0.37	0	17,19,21	0.76	0
2	BMA	C	3	2	11,11,12	0.52	0	15,15,17	0.66	0
2	MAN	C	4	2	11,11,12	0.44	0	15,15,17	0.94	1 (6%)
2	MAN	C	5	2	11,11,12	0.51	0	15,15,17	0.58	0
2	MAN	C	6	2	11,11,12	0.59	0	13,15,17	1.10	1 (7%)
3	NAG	D	1	3,1	14,14,15	0.40	0	17,19,21	2.61	4 (23%)
3	NAG	D	2	3	14,14,15	0.72	0	17,19,21	0.90	1 (5%)
3	MAN	D	3	3	11,11,12	0.57	0	15,15,17	1.14	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.57	0	17,19,21	0.85	0
4	NAG	E	2	4	14,14,15	0.61	0	17,19,21	0.71	0
5	NAG	F	1	1,5	14,14,15	0.43	0	17,19,21	0.84	1 (5%)
5	MAN	F	10	5	11,11,12	0.30	0	15,15,17	0.90	1 (6%)
5	MAN	F	11	5	11,11,12	0.55	0	15,15,17	0.81	1 (6%)
5	NAG	F	2	5	14,14,15	0.96	1 (7%)	17,19,21	1.66	2 (11%)
5	BMA	F	3	5	11,11,12	0.40	0	15,15,17	1.42	1 (6%)
5	BMA	F	4	5	11,11,12	0.35	0	15,15,17	1.55	3 (20%)
5	MAN	F	5	5	11,11,12	0.24	0	15,15,17	1.06	1 (6%)
5	MAN	F	6	5	11,11,12	0.50	0	15,15,17	0.70	1 (6%)
5	MAN	F	7	5	11,11,12	0.82	0	15,15,17	2.39	1 (6%)
5	MAN	F	8	5	11,11,12	0.73	0	15,15,17	1.50	2 (13%)
5	MAN	F	9	5	11,11,12	0.41	0	15,15,17	0.71	0
6	NAG	G	1	1,6	14,14,15	0.67	1 (7%)	17,19,21	0.72	0
6	NAG	G	2	6	14,14,15	0.92	0	17,19,21	1.30	3 (17%)
6	MAN	G	3	6	11,11,12	0.48	0	15,15,17	1.42	1 (6%)
6	MAN	G	4	6	11,11,12	0.88	0	15,15,17	0.93	1 (6%)
6	MAN	G	5	6	11,11,12	0.61	0	15,15,17	0.77	1 (6%)
6	MAN	G	6	6	11,11,12	0.49	0	15,15,17	0.92	1 (6%)
6	MAN	G	7	6	11,11,12	0.40	0	15,15,17	1.20	1 (6%)
6	MAN	G	8	6	11,11,12	0.41	0	15,15,17	1.05	1 (6%)
7	NAG	H	1	1,7	14,14,15	0.51	0	17,19,21	0.76	0
7	NAG	H	2	7	14,14,15	1.01	1 (7%)	19,19,21	2.48	3 (15%)
8	NAG	I	1	8,1	14,14,15	0.62	0	17,19,21	0.55	0
8	NAG	I	2	8	14,14,15	0.42	0	17,19,21	0.66	0
8	MAN	I	3	8	11,11,12	0.69	0	15,15,17	1.26	1 (6%)
8	MAN	I	4	8	11,11,12	0.40	0	15,15,17	0.84	1 (6%)
8	MAN	I	5	8	11,11,12	0.46	0	15,15,17	1.26	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	I	6	8	11,11,12	0.60	0	15,15,17	1.39	2 (13%)
8	MAN	I	7	8	11,11,12	0.79	0	15,15,17	1.02	1 (6%)
8	MAN	I	8	8	11,11,12	0.60	0	15,15,17	0.85	1 (6%)
8	MAN	I	9	8	11,11,12	0.65	0	15,15,17	0.82	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.27	0	17,19,21	0.66	0
2	NAG	J	2	2	14,14,15	0.49	0	17,19,21	0.99	0
2	BMA	J	3	2	11,11,12	0.40	0	15,15,17	0.67	0
2	MAN	J	4	2	11,11,12	0.23	0	15,15,17	1.03	1 (6%)
2	MAN	J	5	2	11,11,12	0.40	0	15,15,17	0.61	0
2	MAN	J	6	2	10,10,12	1.15	1 (10%)	13,13,17	2.12	3 (23%)
5	NAG	K	1	1,5	14,14,15	0.47	0	17,19,21	0.86	1 (5%)
5	MAN	K	10	5	11,11,12	0.35	0	15,15,17	0.68	0
5	MAN	K	11	5	11,11,12	0.47	0	15,15,17	0.76	1 (6%)
5	NAG	K	2	5	14,14,15	0.29	0	17,19,21	0.62	0
5	BMA	K	3	5	11,11,12	0.52	0	15,15,17	1.63	1 (6%)
5	BMA	K	4	5	11,11,12	0.54	0	15,15,17	1.53	2 (13%)
5	MAN	K	5	5	11,11,12	0.22	0	15,15,17	0.90	1 (6%)
5	MAN	K	6	5	11,11,12	0.39	0	15,15,17	0.81	1 (6%)
5	MAN	K	7	5	11,11,12	0.56	0	15,15,17	1.60	2 (13%)
5	MAN	K	8	5	11,11,12	0.68	0	15,15,17	0.51	0
5	MAN	K	9	5	11,11,12	0.38	0	15,15,17	0.89	1 (6%)
7	NAG	L	1	1,7	14,14,15	0.60	0	17,19,21	0.79	0
7	NAG	L	2	7	14,14,15	0.91	1 (7%)	19,19,21	2.39	3 (15%)
3	NAG	M	1	3,1	14,14,15	0.27	0	17,19,21	0.98	1 (5%)
3	NAG	M	2	3	14,14,15	0.72	0	17,19,21	0.73	0
3	MAN	M	3	3	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
4	NAG	N	1	1,4	14,14,15	0.96	0	17,19,21	1.71	4 (23%)
4	NAG	N	2	4	14,14,15	0.70	0	17,19,21	0.66	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/18/22	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	MAN	D	3	3	-	2/2/19/22	1/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	F	10	5	-	0/2/19/22	0/1/1/1
5	MAN	F	11	5	-	0/2/19/22	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	BMA	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
6	NAG	G	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	1/6/23/26	0/1/1/1
6	MAN	G	3	6	-	2/2/19/22	1/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	1/2/19/22	0/1/1/1
6	MAN	G	6	6	-	0/2/19/22	0/1/1/1
6	MAN	G	7	6	-	0/2/19/22	0/1/1/1
6	MAN	G	8	6	-	0/2/19/22	0/1/1/1
7	NAG	H	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/22/26	0/1/1/1
8	NAG	I	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	MAN	I	3	8	-	0/2/19/22	1/1/1/1
8	MAN	I	4	8	-	0/2/19/22	0/1/1/1
8	MAN	I	5	8	-	0/2/19/22	0/1/1/1
8	MAN	I	6	8	-	2/2/19/22	0/1/1/1
8	MAN	I	7	8	-	0/2/19/22	0/1/1/1
8	MAN	I	8	8	-	0/2/19/22	0/1/1/1
8	MAN	I	9	8	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	J	4	2	-	0/2/19/22	0/1/1/1
2	MAN	J	5	2	-	0/2/19/22	0/1/1/1
2	MAN	J	6	2	-	0/2/16/22	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	K	10	5	-	0/2/19/22	0/1/1/1
5	MAN	K	11	5	-	0/2/19/22	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	BMA	K	4	5	-	0/2/19/22	0/1/1/1
5	MAN	K	5	5	-	0/2/19/22	0/1/1/1
5	MAN	K	6	5	-	0/2/19/22	0/1/1/1
5	MAN	K	7	5	-	0/2/19/22	0/1/1/1
5	MAN	K	8	5	-	0/2/19/22	0/1/1/1
5	MAN	K	9	5	-	0/2/19/22	0/1/1/1
7	NAG	L	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/22/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	MAN	M	3	3	-	1/2/19/22	1/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	2	NAG	C1-C2	3.25	1.56	1.52
7	L	2	NAG	C1-C2	2.90	1.56	1.52
2	J	6	MAN	O5-C1	2.26	1.49	1.44
5	F	2	NAG	O5-C1	-2.23	1.40	1.43
6	G	1	NAG	C1-C2	2.02	1.55	1.52

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	7	MAN	O3-C3-C4	-8.78	89.69	110.38
7	H	2	NAG	C1-C2-N2	-8.74	100.60	110.73
7	L	2	NAG	C1-C2-N2	-8.50	100.88	110.73
3	D	1	NAG	C1-O5-C5	8.18	123.15	112.19
2	J	6	MAN	C1-C2-C3	-5.96	100.94	110.61

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
8	I	6	MAN	O5-C5-C6-O6
3	D	3	MAN	C4-C5-C6-O6
4	N	1	NAG	C8-C7-N2-C2

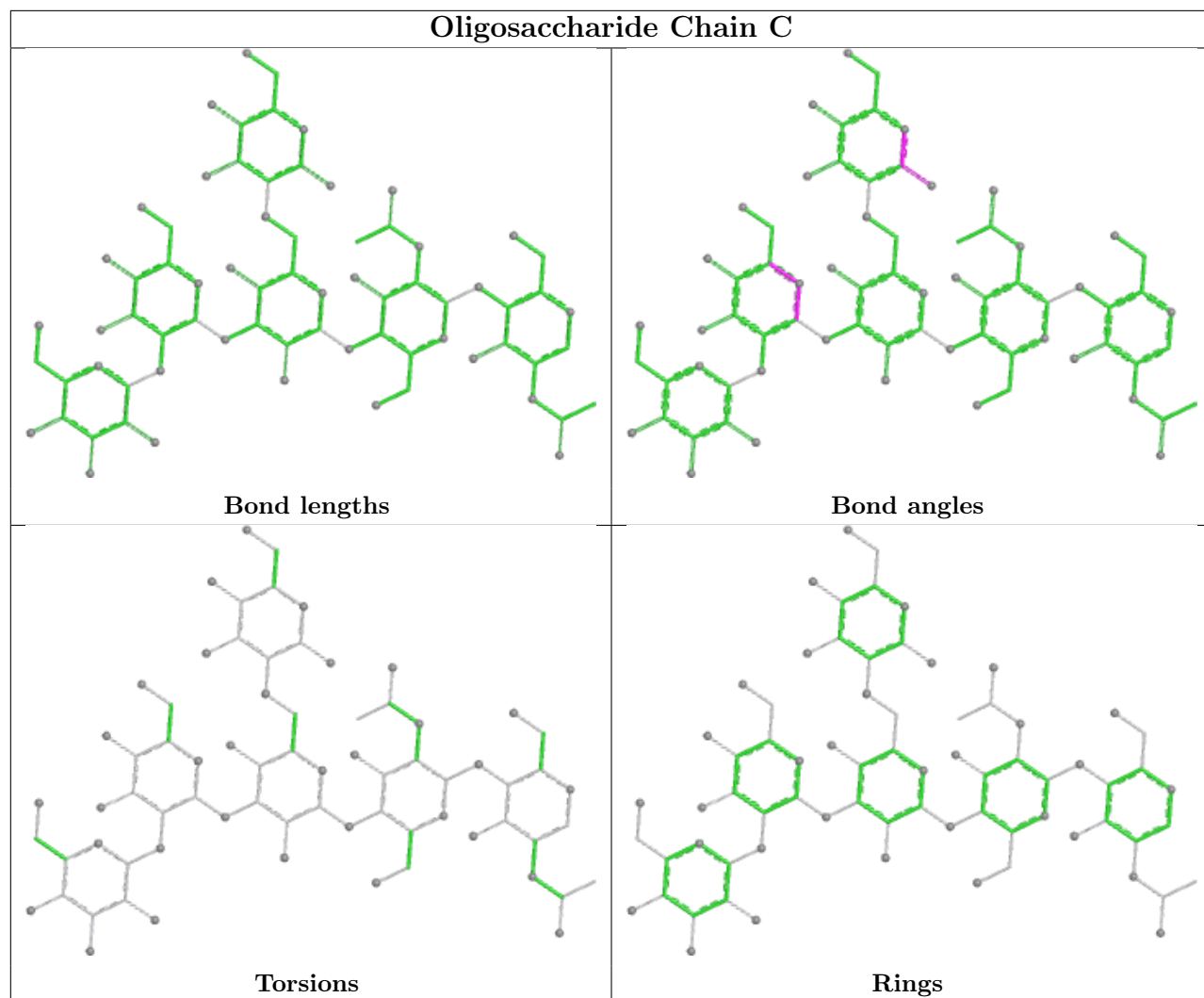
All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	3	MAN	C1-C2-C3-C4-C5-O5
8	I	3	MAN	C1-C2-C3-C4-C5-O5
3	D	3	MAN	C1-C2-C3-C4-C5-O5
6	G	3	MAN	C1-C2-C3-C4-C5-O5

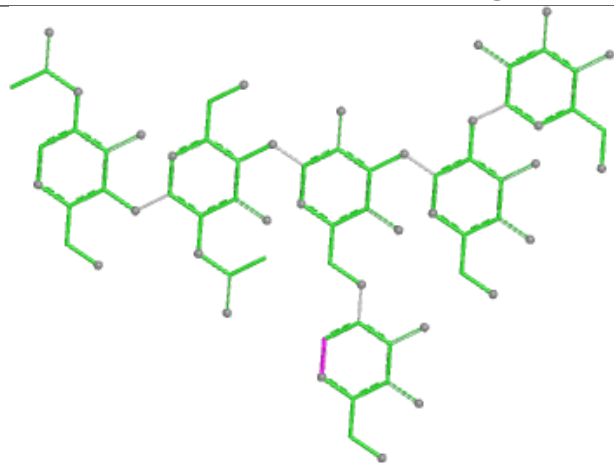
No monomer is involved in short contacts.

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

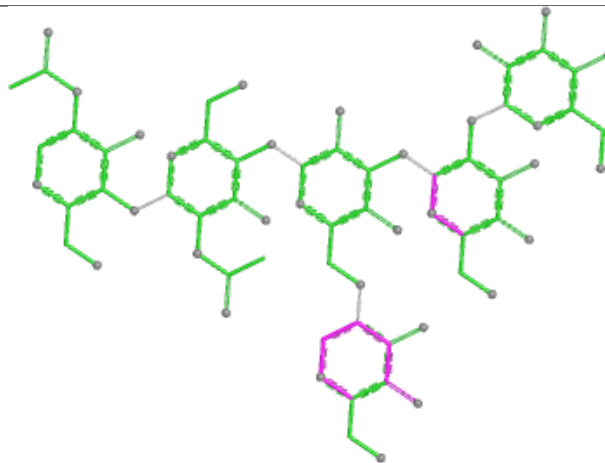
Oligosaccharide Chain C



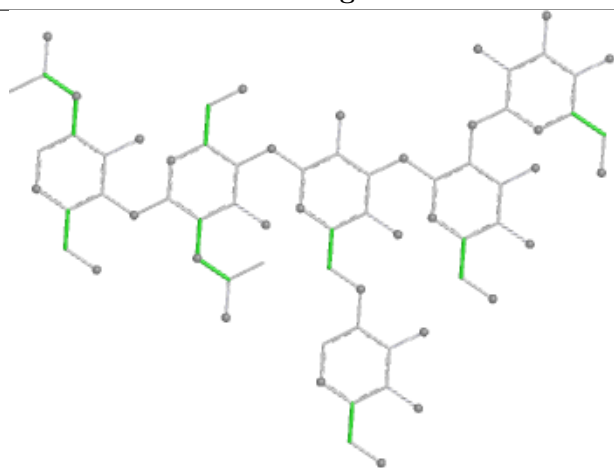
Oligosaccharide Chain J



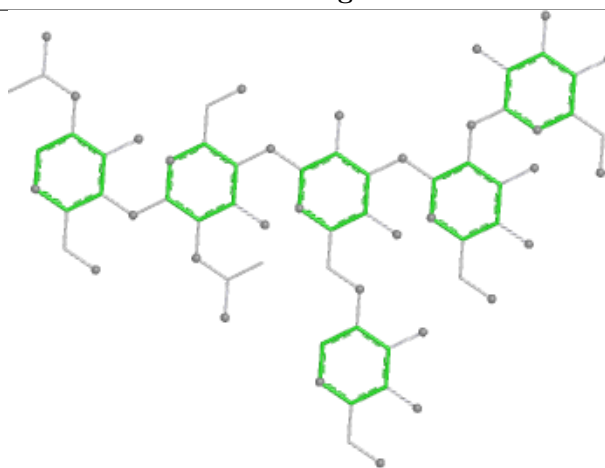
Bond lengths



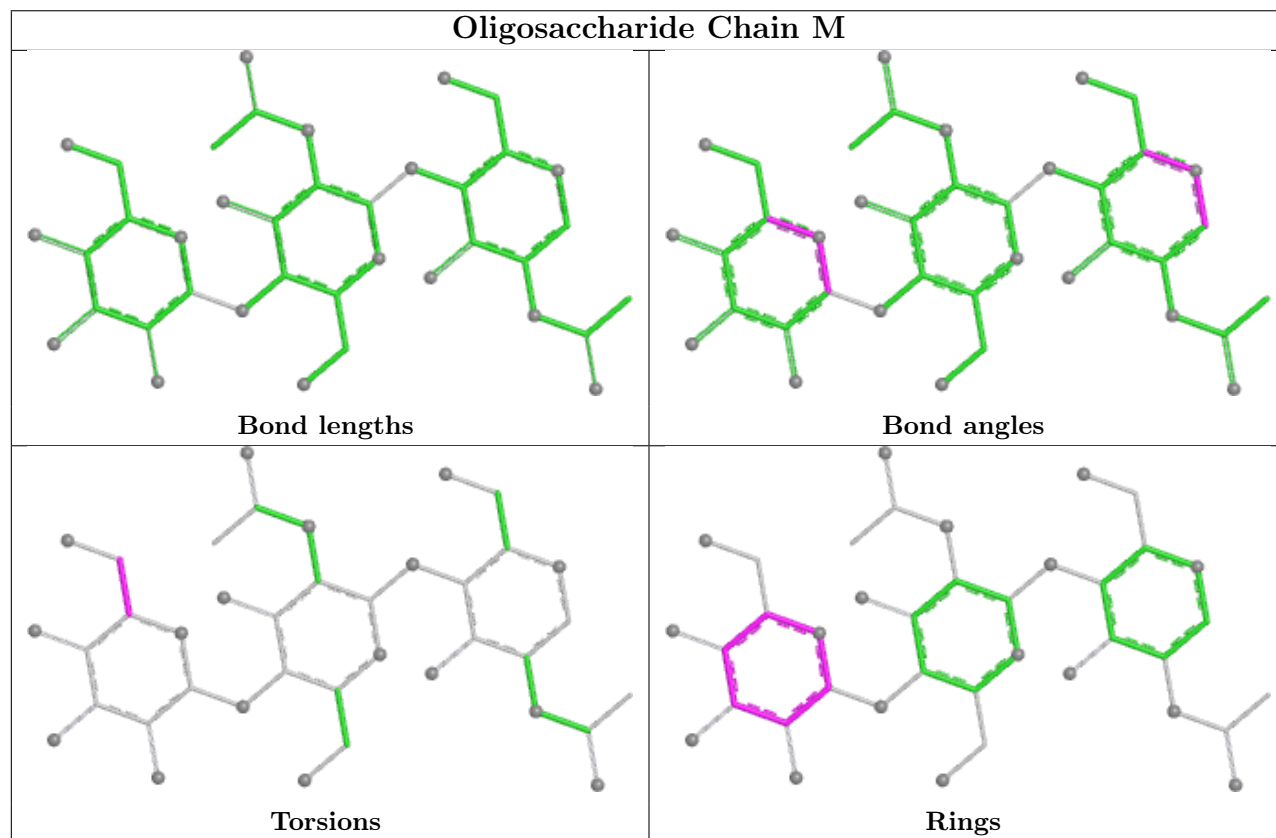
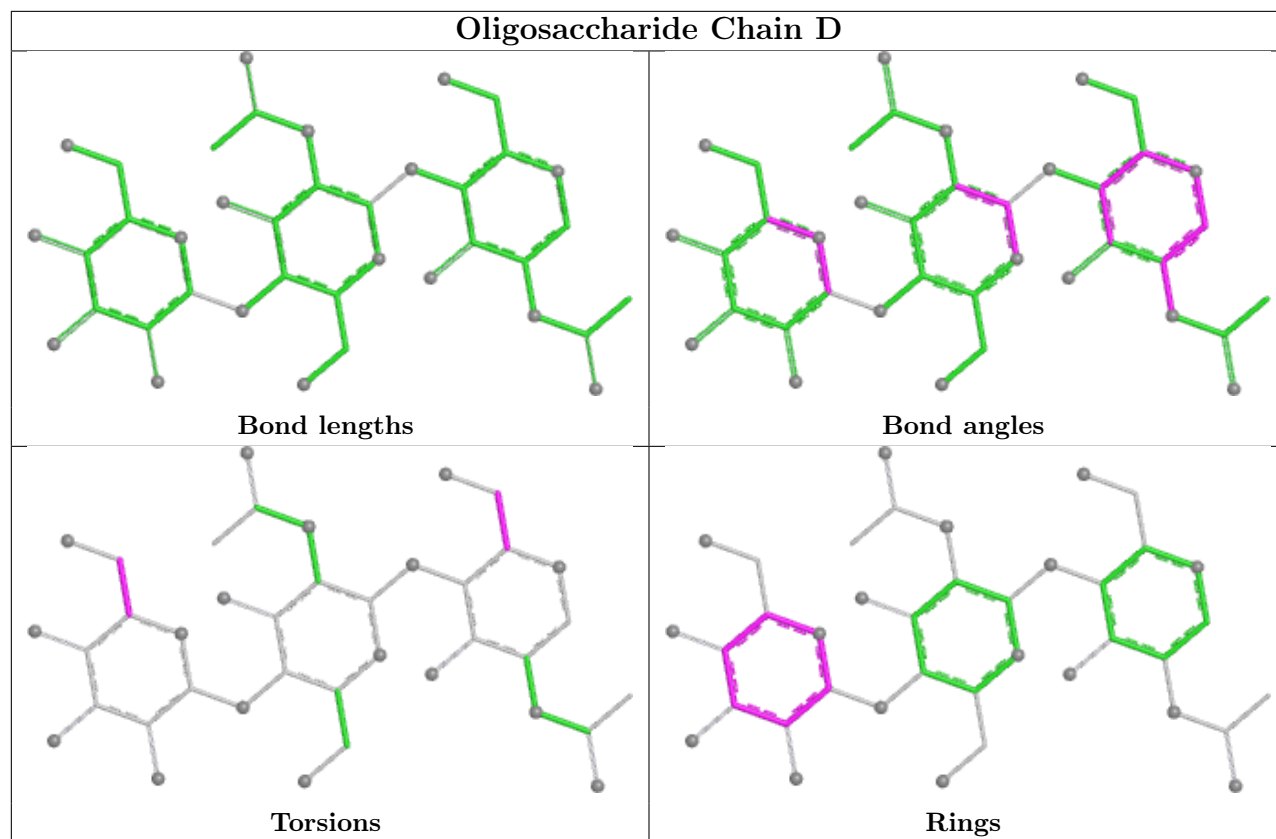
Bond angles

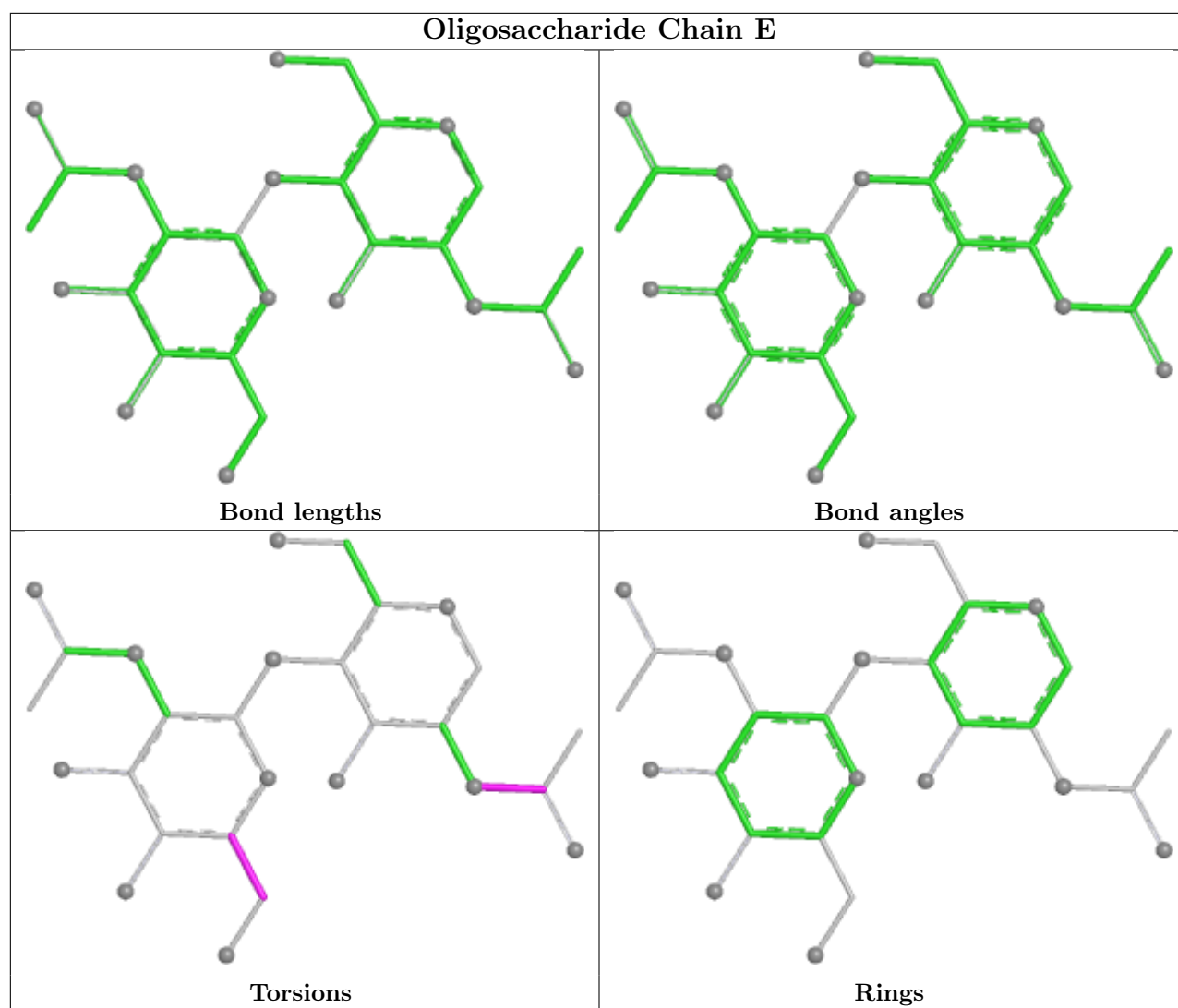


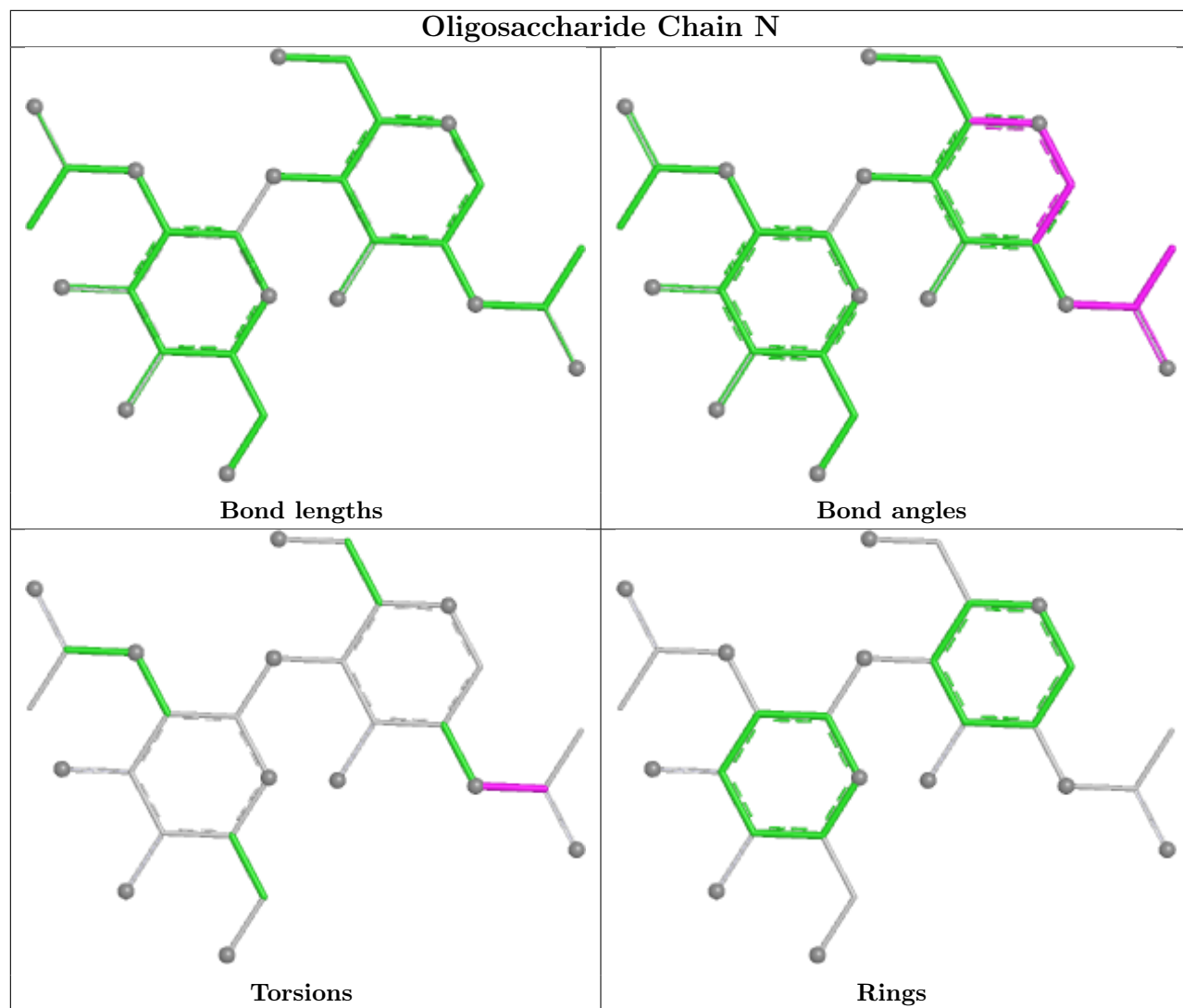
Torsions

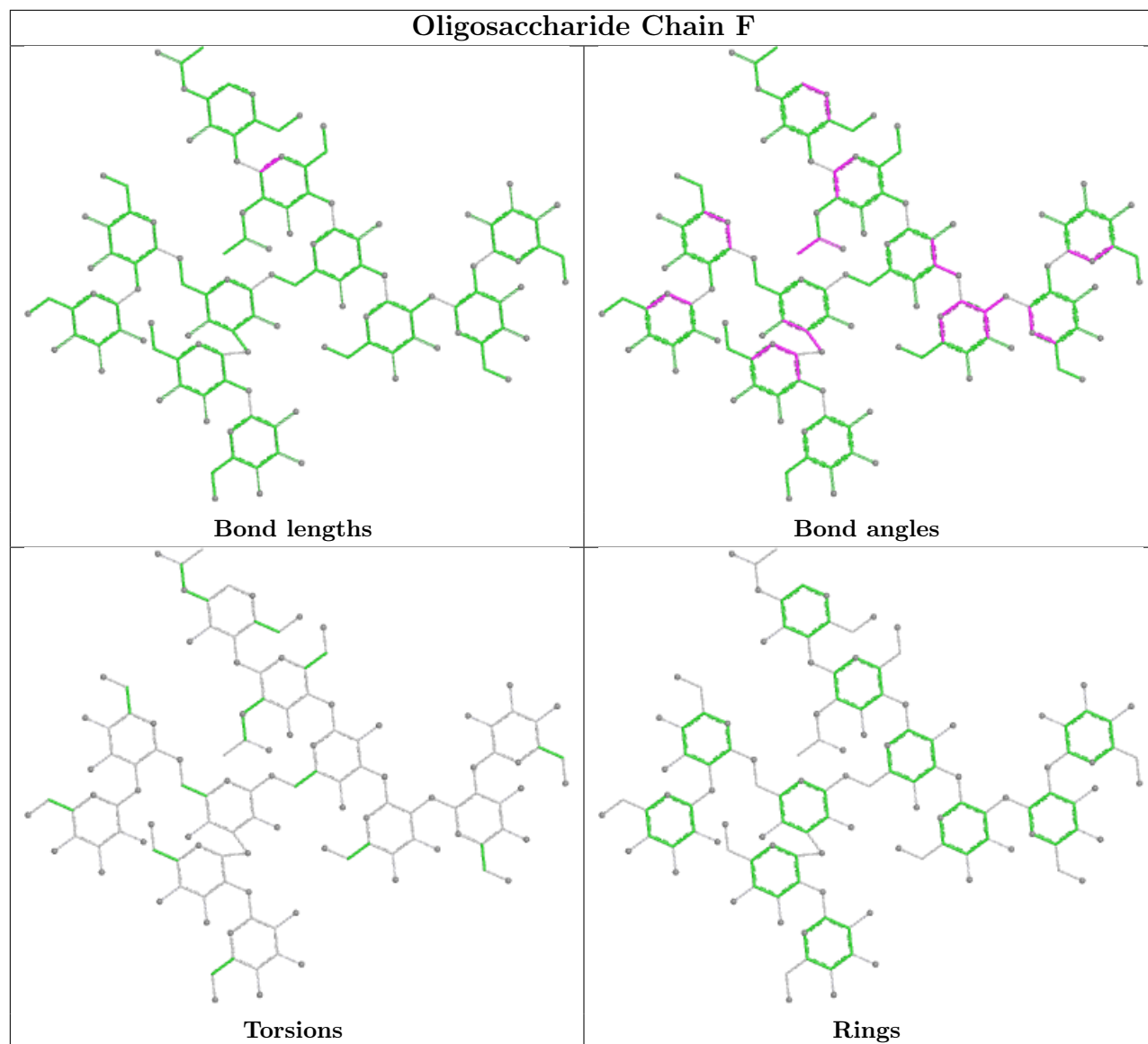


Rings

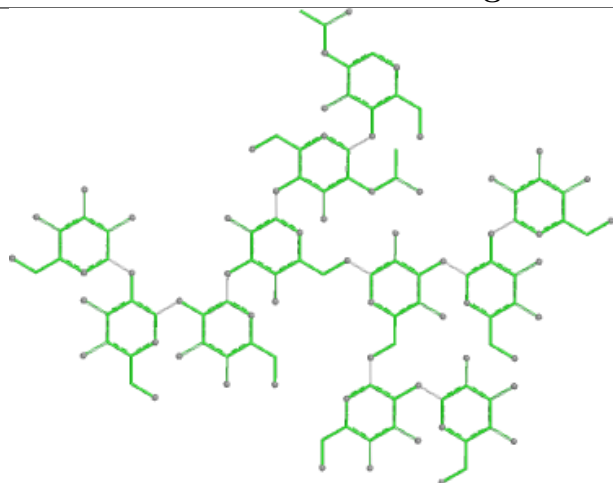




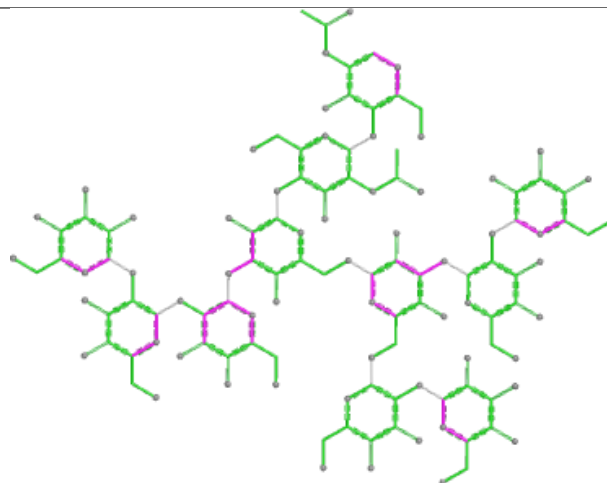




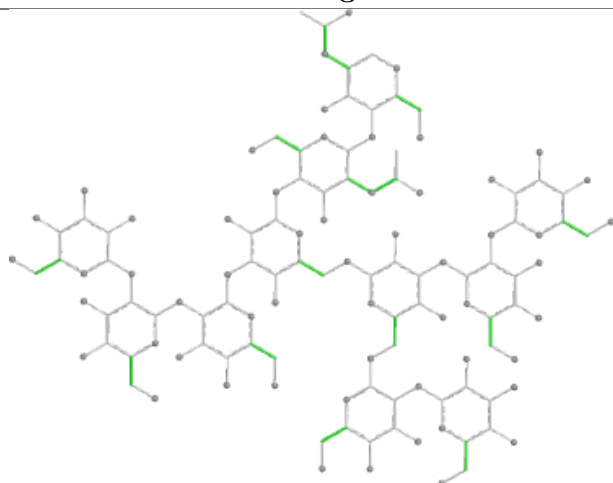
Oligosaccharide Chain K



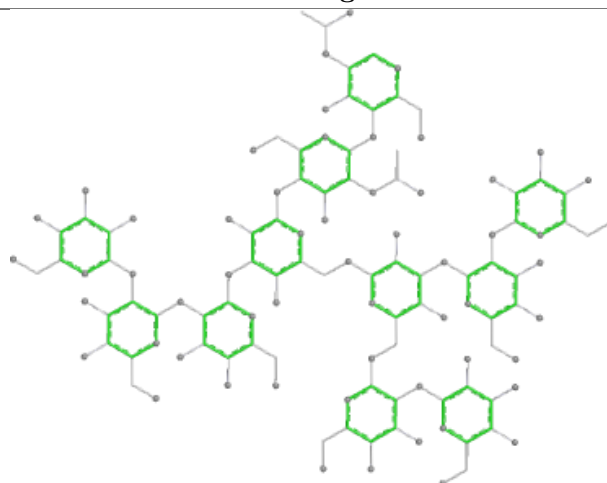
Bond lengths



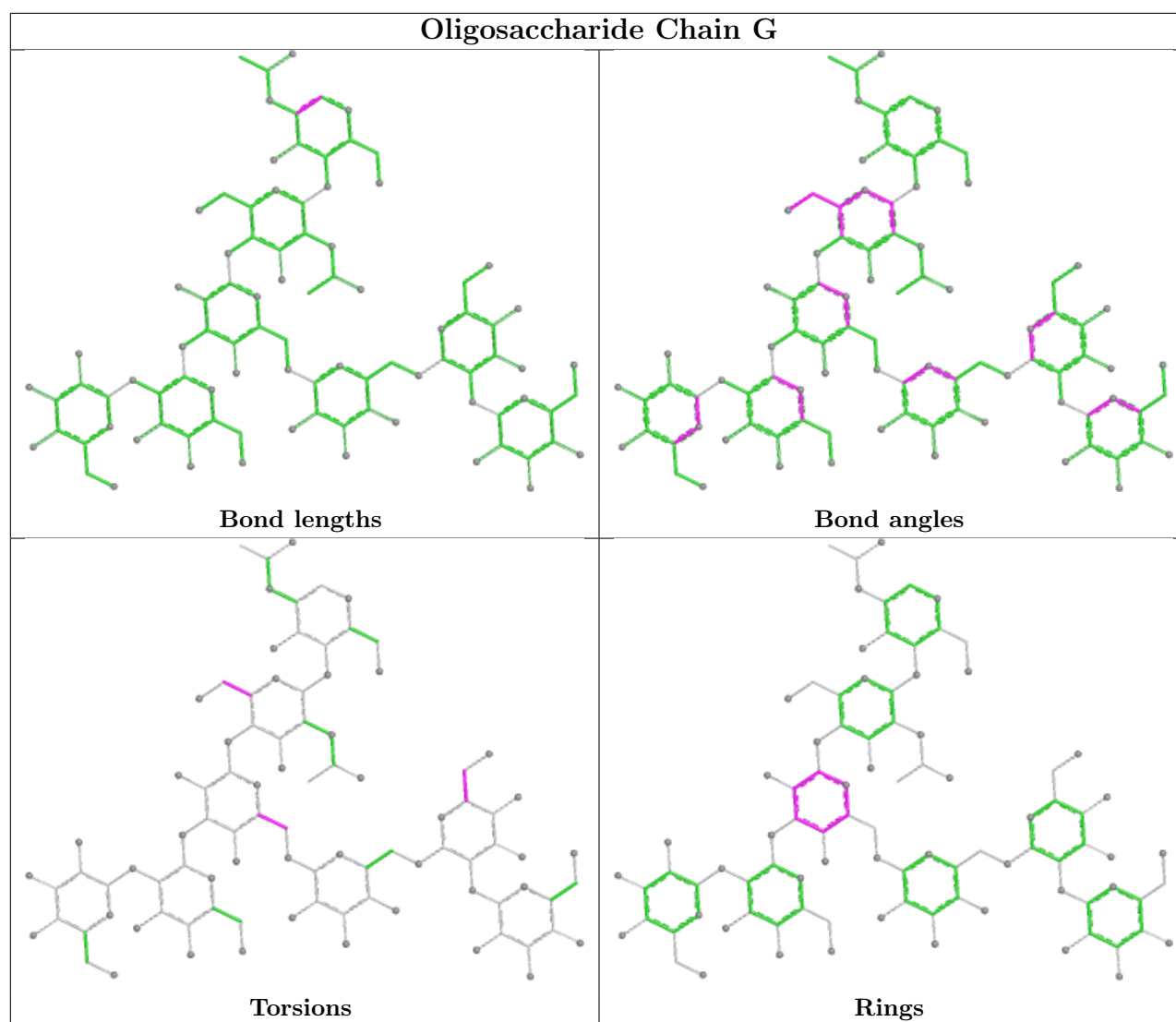
Bond angles

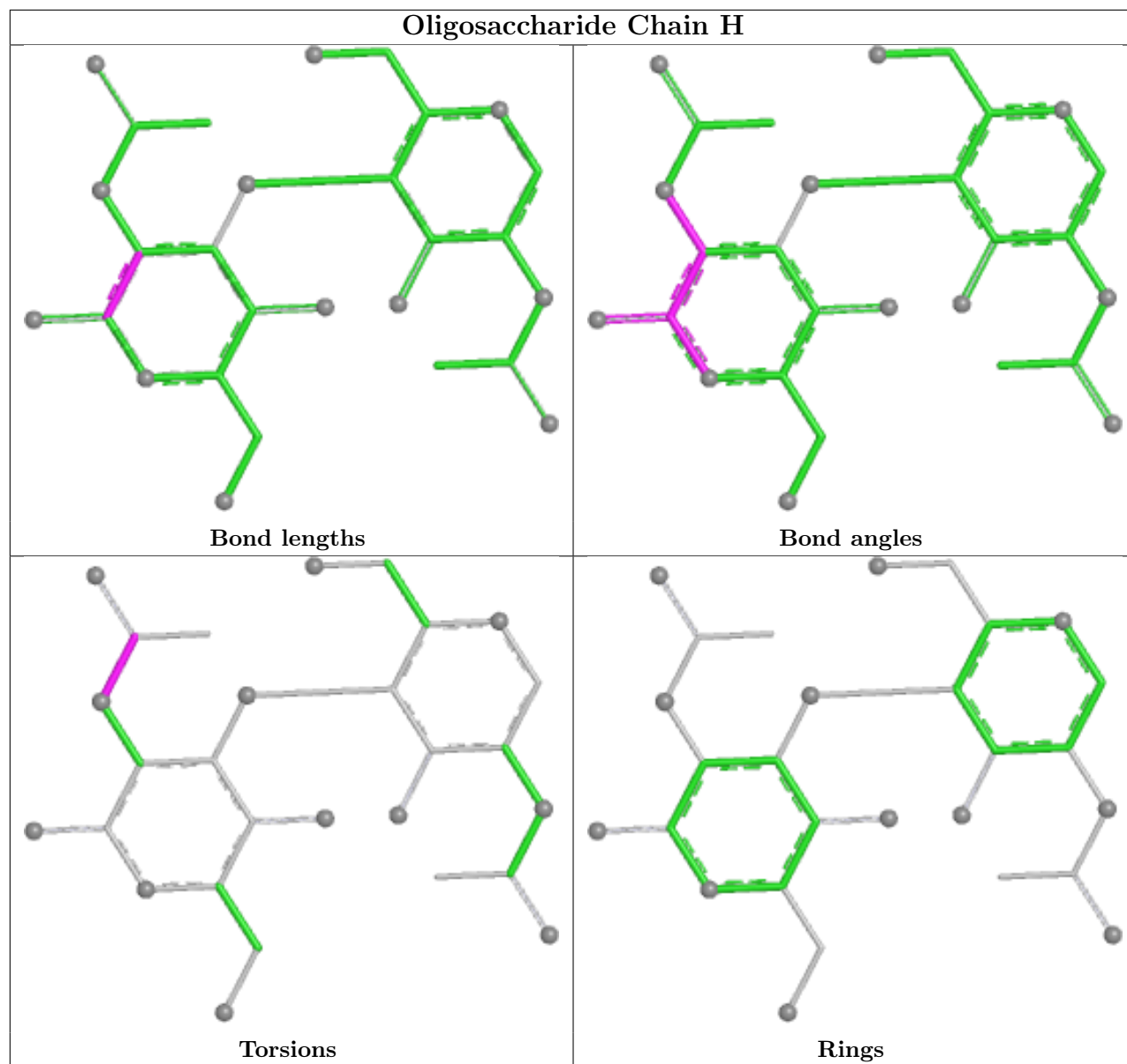


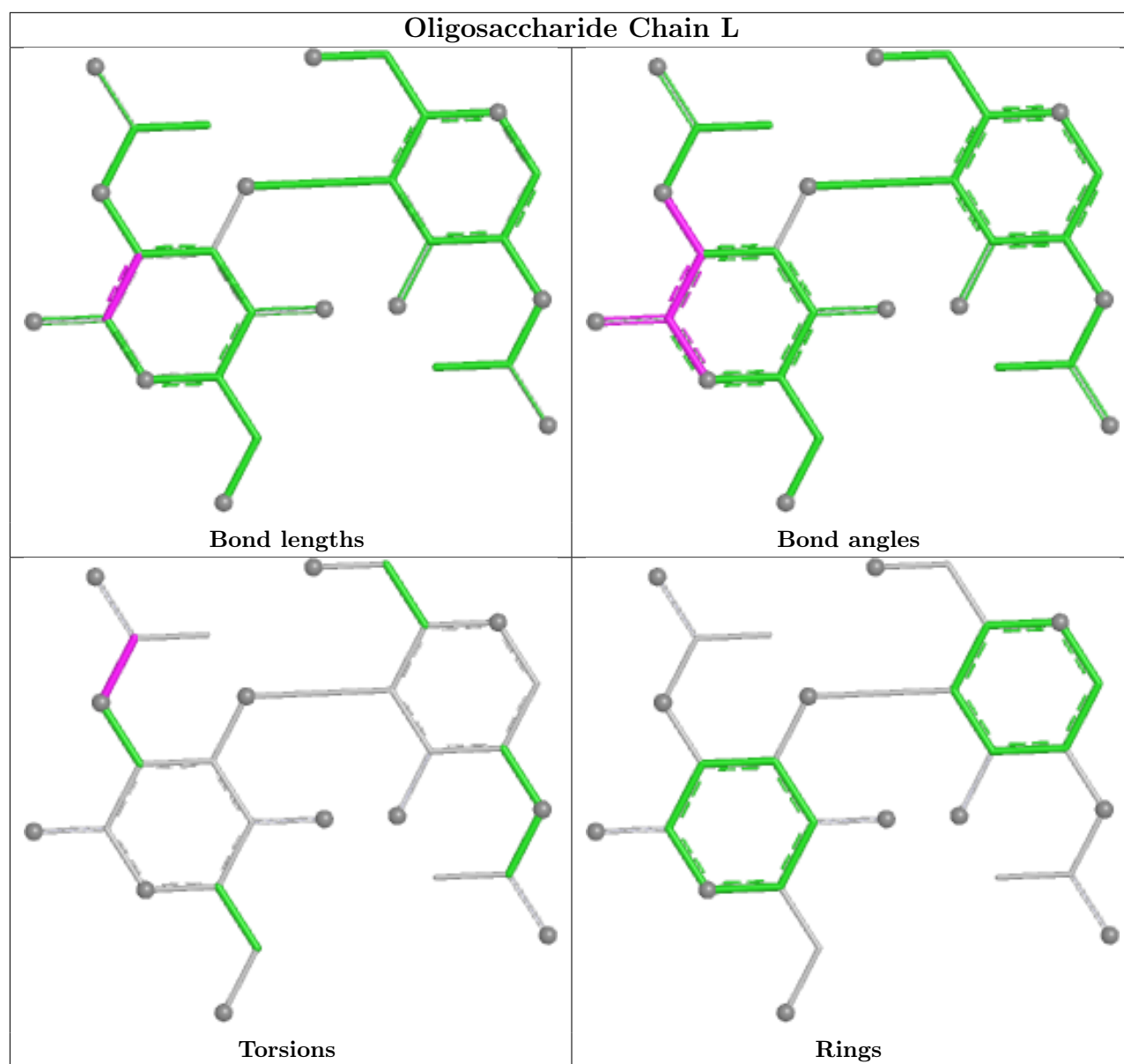
Torsions

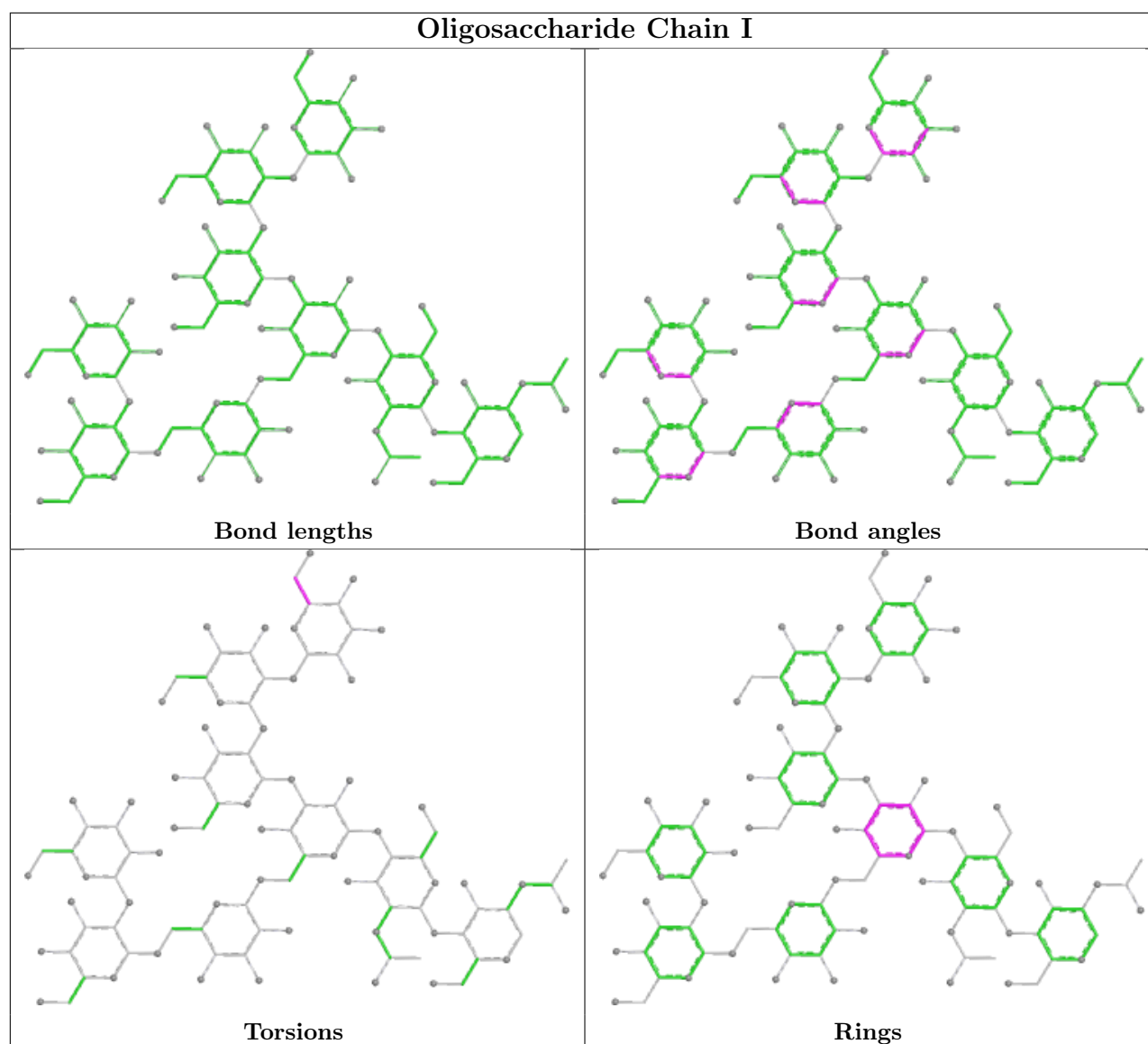


Rings









4.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 33 are monoatomic - leaving 14 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	$\# Z > 2$
9	NAG	B	1002	1	14,14,15	0.60	0	17,19,21	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	A	1005	1	14,14,15	0.37	0	17,19,21	0.82	1 (5%)
9	NAG	B	1001	1	14,14,15	0.45	0	17,19,21	0.76	0
12	1PE	A	1023	-	8,8,15	0.36	0	7,7,14	0.73	0
9	NAG	A	1002	1	14,14,15	0.44	0	17,19,21	0.78	1 (5%)
9	NAG	A	1004	1	14,14,15	0.57	0	17,19,21	0.57	0
9	NAG	A	1001	1	14,14,15	0.55	0	17,19,21	0.86	1 (5%)
9	NAG	B	1003	1	14,14,15	0.63	0	17,19,21	0.46	0
9	NAG	B	1004	1	14,14,15	0.68	1 (7%)	17,19,21	0.89	1 (5%)
13	PE4	B	1020	-	15,15,23	0.50	0	14,14,22	0.32	0
9	NAG	B	1005	1	14,14,15	0.49	0	17,19,21	1.17	1 (5%)
13	PE4	A	1024	-	9,9,23	0.50	0	8,8,22	0.52	0
12	1PE	B	1018	-	8,8,15	0.37	0	7,7,14	0.84	0
9	NAG	A	1003	1	14,14,15	0.64	0	17,19,21	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
12	1PE	A	1023	-	-	6/6/6/13	-
9	NAG	A	1002	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1001	1	-	1/6/23/26	0/1/1/1
9	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
13	PE4	B	1020	-	-	9/13/13/21	-
9	NAG	B	1005	1	-	0/6/23/26	0/1/1/1
13	PE4	A	1024	-	-	5/7/7/21	-
12	1PE	B	1018	-	-	6/6/6/13	-
9	NAG	A	1003	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1004	NAG	C1-C2	2.25	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1004	NAG	C1-O5-C5	3.19	116.47	112.19
9	B	1005	NAG	C2-N2-C7	-2.88	119.04	122.90
9	A	1001	NAG	C1-O5-C5	2.80	115.94	112.19
9	A	1002	NAG	C1-O5-C5	2.40	115.41	112.19
9	A	1005	NAG	C2-N2-C7	-2.25	119.88	122.90

There are no chirality outliers.

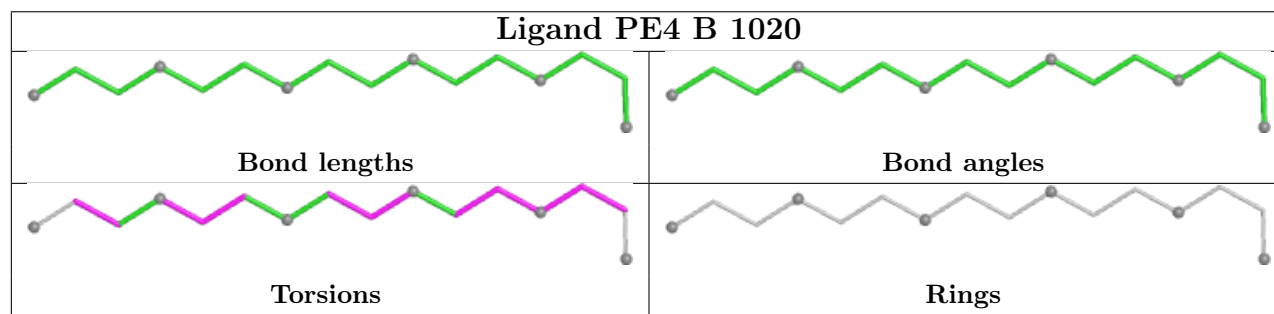
5 of 30 torsion outliers are listed below:

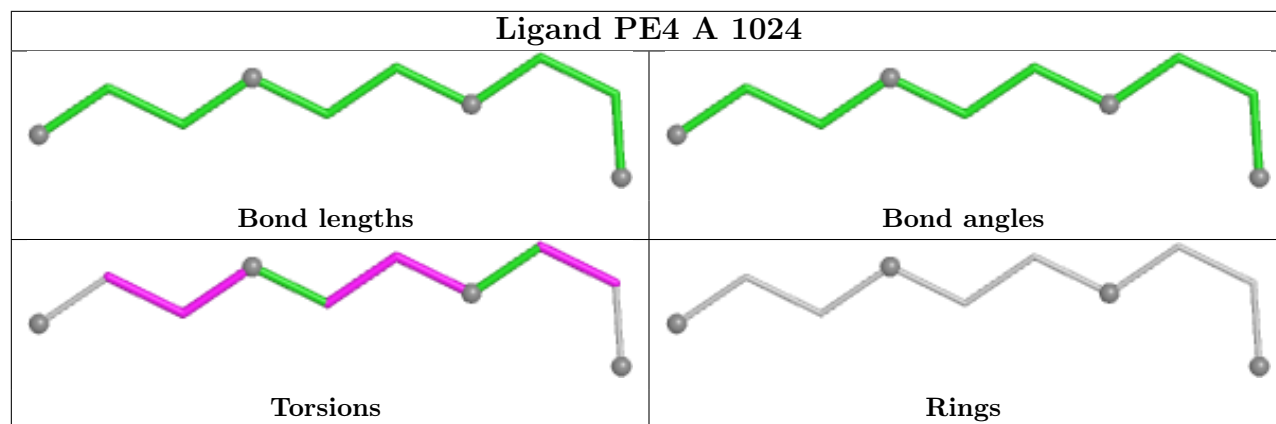
Mol	Chain	Res	Type	Atoms
13	B	1020	PE4	O2-C3-C4-O3
13	B	1020	PE4	O4-C7-C8-O5
13	A	1024	PE4	O2-C3-C4-O3
12	A	1023	1PE	OH5-C14-C24-OH4
13	A	1024	PE4	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	917/942 (97%)	-1.36	2 (0%) 91 89	25, 51, 85, 114	2 (0%)
1	B	917/942 (97%)	-1.43	1 (0%) 92 90	31, 48, 76, 113	1 (0%)
All	All	1834/1884 (97%)	-1.40	3 (0%) 91 89	25, 49, 81, 114	3 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	838	SER	2.7
1	A	838	SER	2.2
1	A	147	LYS	2.0

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
8	MAN	I	6	11/12	0.90	0.25	71,74,77,77	11
2	MAN	J	6	10/12	0.96	0.05	24,26,26,27	0
7	NAG	H	2	14/15	0.97	0.07	58,67,69,73	0
7	NAG	L	2	14/15	0.97	0.07	59,66,70,71	0
6	MAN	G	8	11/12	0.97	0.07	55,61,68,71	0
2	MAN	C	6	11/12	0.98	0.06	65,67,70,71	0

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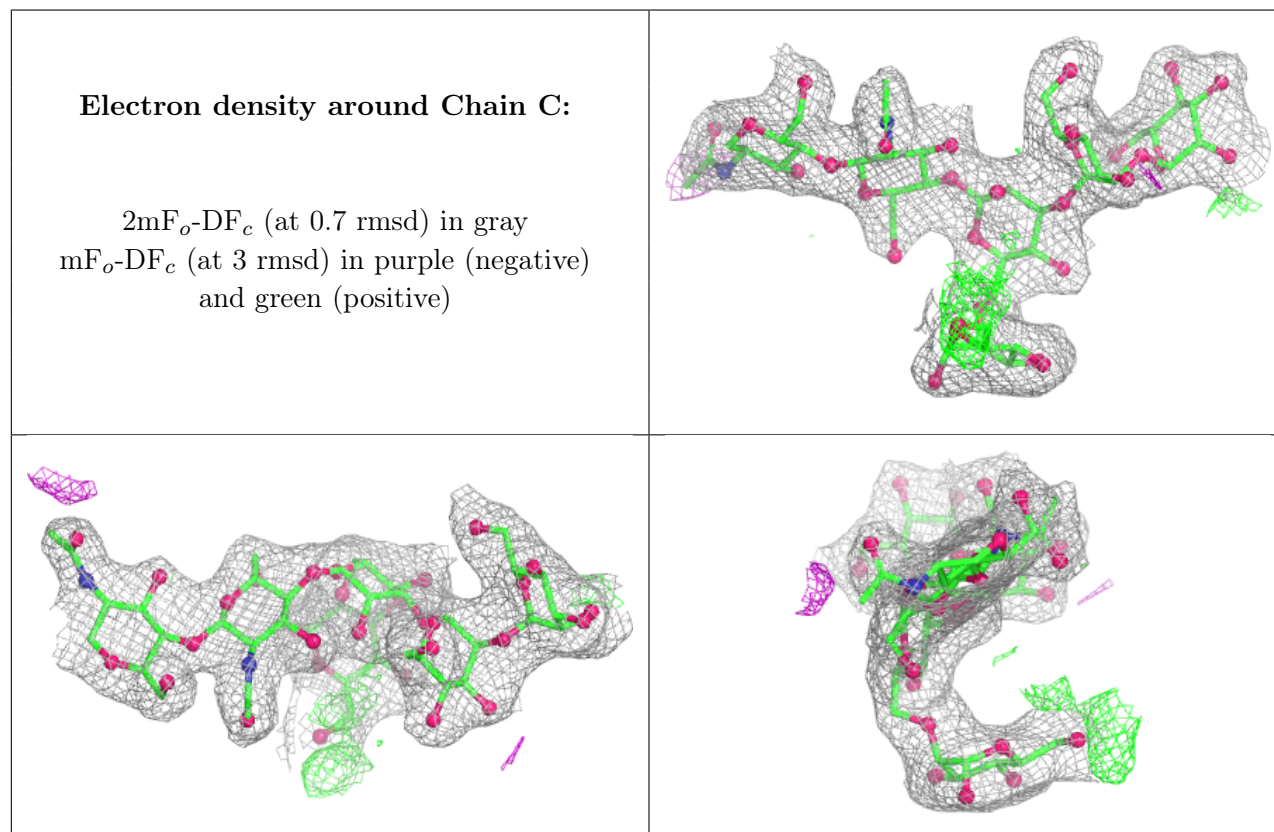
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	D	3	11/12	0.98	0.05	52,56,62,63	0
3	MAN	M	3	11/12	0.98	0.05	51,56,61,62	0
8	MAN	I	5	11/12	0.98	0.07	55,61,69,73	0
6	MAN	G	4	11/12	0.98	0.05	61,65,67,67	0
8	MAN	I	7	11/12	0.98	0.07	63,67,68,68	0
8	MAN	I	9	11/12	0.98	0.09	59,66,69,71	0
4	NAG	E	2	14/15	0.99	0.04	53,58,68,72	0
4	NAG	N	1	14/15	0.99	0.03	37,44,52,59	0
4	NAG	N	2	14/15	0.99	0.03	49,55,63,63	0
5	BMA	F	3	11/12	0.99	0.03	47,47,50,51	0
5	BMA	F	4	11/12	0.99	0.04	44,45,51,51	0
5	MAN	F	5	11/12	0.99	0.03	47,50,51,54	0
5	MAN	F	6	11/12	0.99	0.03	57,62,63,64	0
5	MAN	F	7	11/12	0.99	0.03	50,52,55,59	0
5	MAN	F	8	11/12	0.99	0.04	53,55,60,61	0
5	MAN	F	9	11/12	0.99	0.03	56,57,59,59	0
5	MAN	F	11	11/12	0.99	0.03	46,50,51,52	0
5	BMA	K	3	11/12	0.99	0.03	44,46,50,50	0
5	BMA	K	4	11/12	0.99	0.03	40,46,51,52	0
5	MAN	K	5	11/12	0.99	0.02	44,49,52,53	0
5	MAN	K	6	11/12	0.99	0.03	55,60,64,64	0
5	MAN	K	8	11/12	0.99	0.03	48,50,55,56	0
5	MAN	K	9	11/12	0.99	0.03	49,52,54,54	0
5	MAN	K	11	11/12	0.99	0.03	48,51,54,55	0
6	NAG	G	2	14/15	0.99	0.03	52,56,60,65	0
6	MAN	G	3	11/12	0.99	0.03	61,62,64,67	0
2	NAG	J	1	14/15	0.99	0.04	41,44,46,46	0
6	MAN	G	5	11/12	0.99	0.04	57,58,62,64	0
6	MAN	G	6	11/12	0.99	0.06	60,63,66,68	0
6	MAN	G	7	11/12	0.99	0.03	62,64,66,67	0
2	BMA	J	3	11/12	0.99	0.03	43,47,50,50	0
2	MAN	J	5	11/12	0.99	0.04	40,45,48,49	0
7	NAG	L	1	14/15	0.99	0.03	46,50,53,55	0
2	NAG	C	2	14/15	0.99	0.04	43,45,49,53	0
8	NAG	I	1	14/15	0.99	0.04	39,47,52,52	0
8	MAN	I	4	11/12	0.99	0.04	61,63,67,67	0
2	MAN	C	5	11/12	0.99	0.03	40,50,52,55	0
3	NAG	M	1	14/15	0.99	0.03	37,39,42,43	0
2	NAG	C	1	14/15	0.99	0.06	42,44,50,51	0
8	MAN	I	8	11/12	0.99	0.07	58,62,66,67	0
4	NAG	E	1	14/15	0.99	0.03	39,43,51,54	0
5	NAG	F	1	14/15	1.00	0.03	44,47,48,49	0

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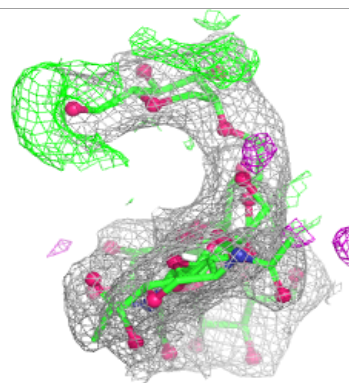
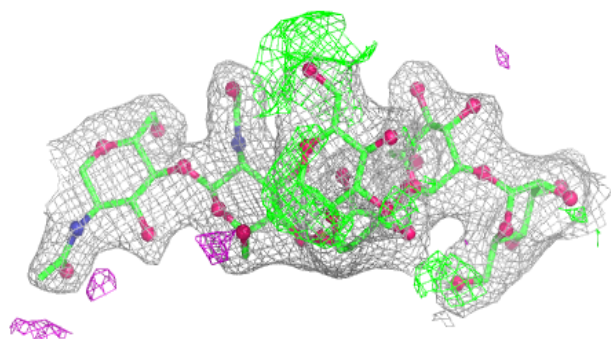
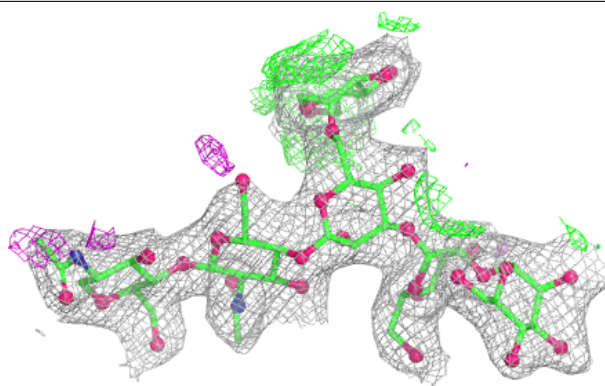
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	K	1	14/15	1.00	0.03	42,44,46,47	0
5	NAG	K	2	14/15	1.00	0.02	40,42,46,46	0
5	NAG	F	2	14/15	1.00	0.02	44,47,58,59	0
2	MAN	J	4	11/12	1.00	0.02	41,44,48,48	0
7	NAG	H	1	14/15	1.00	0.03	46,50,54,56	0
3	NAG	M	2	14/15	1.00	0.03	39,44,50,50	0
2	BMA	C	3	11/12	1.00	0.02	46,50,57,61	0
5	MAN	K	7	11/12	1.00	0.02	45,47,49,51	0
2	NAG	J	2	14/15	1.00	0.03	38,43,48,53	0
8	NAG	I	2	14/15	1.00	0.03	47,55,58,63	0
8	MAN	I	3	11/12	1.00	0.02	57,61,64,68	0
3	NAG	D	1	14/15	1.00	0.02	40,42,49,50	0
5	MAN	K	10	11/12	1.00	0.03	43,44,49,52	0
3	NAG	D	2	14/15	1.00	0.02	38,46,51,53	0
6	NAG	G	1	14/15	1.00	0.03	43,53,59,61	0
2	MAN	C	4	11/12	1.00	0.02	38,47,49,50	0
5	MAN	F	10	11/12	1.00	0.02	47,49,51,52	0

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

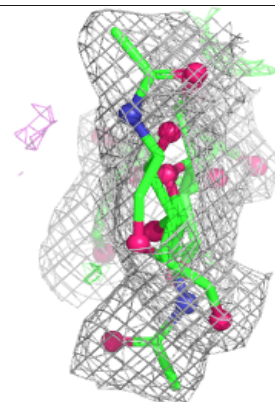
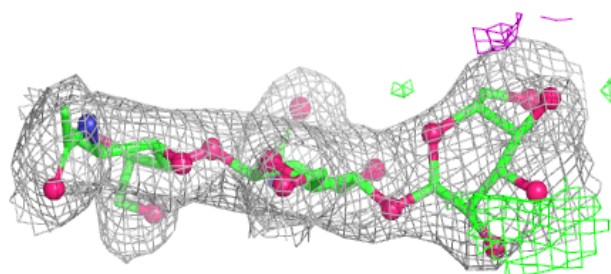
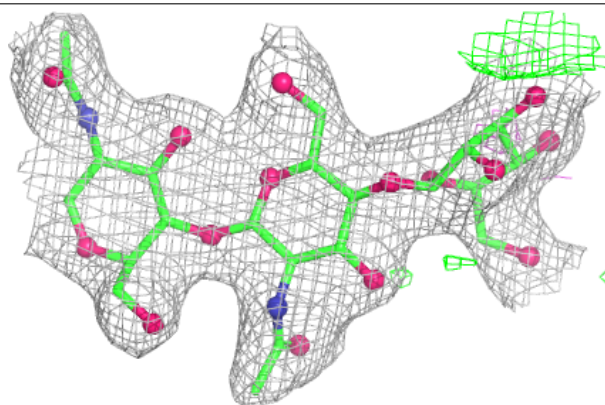


Electron density around Chain J:

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

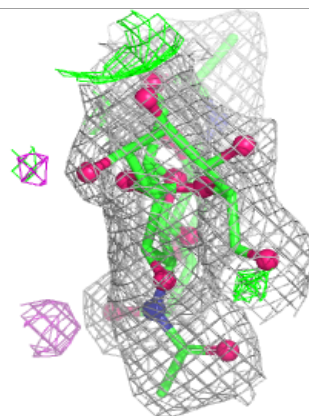
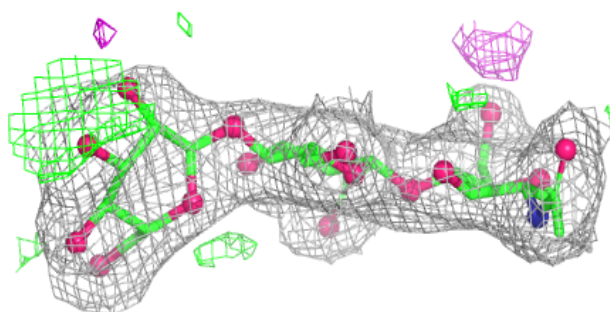
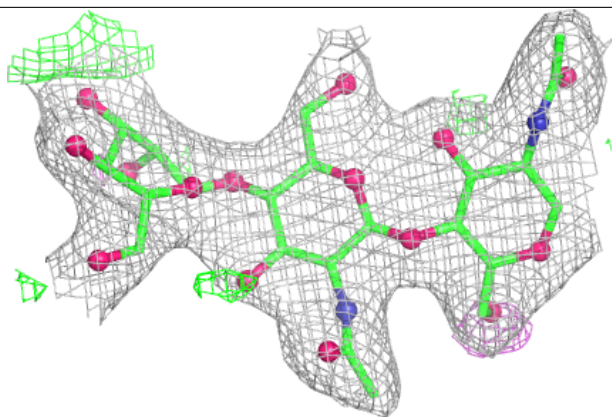
**Electron density around Chain D:**

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

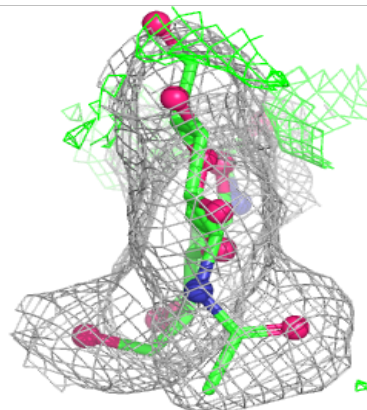
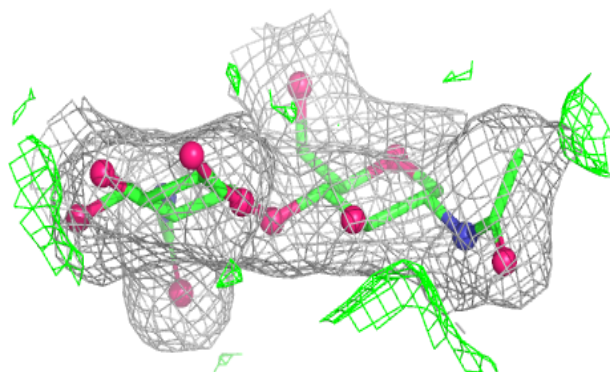
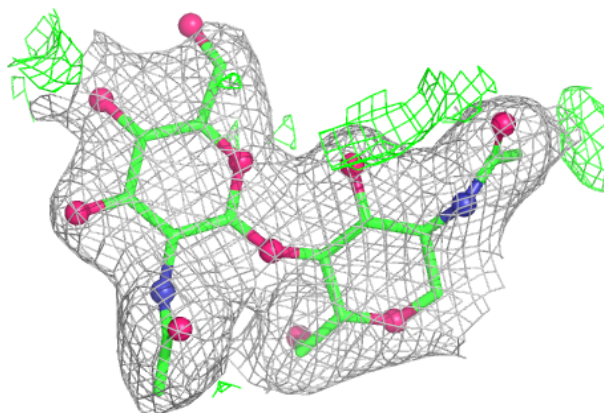


Electron density around Chain M:

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

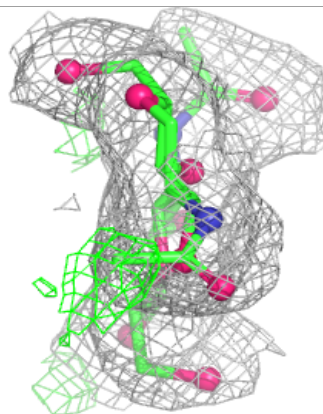
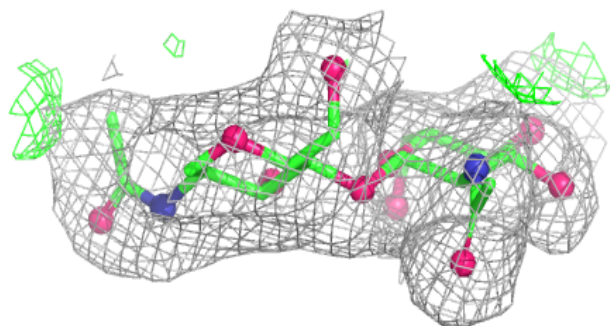
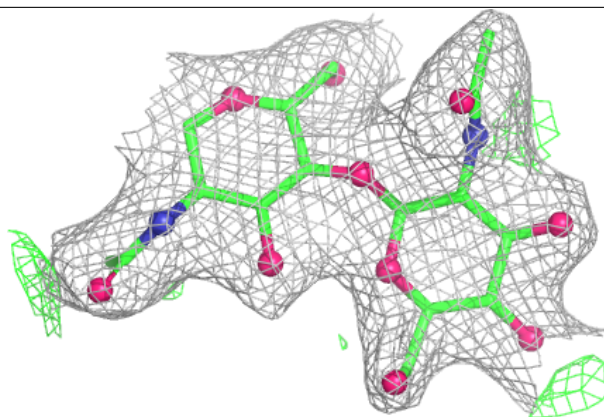
**Electron density around Chain E:**

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



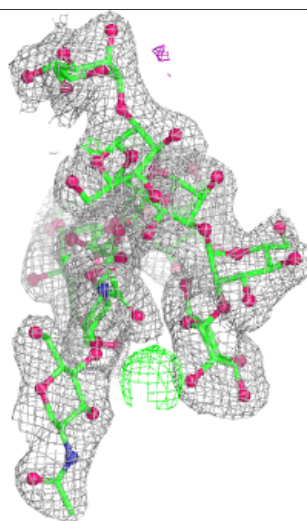
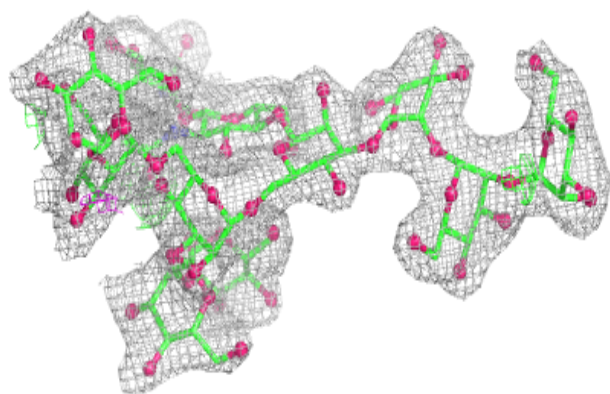
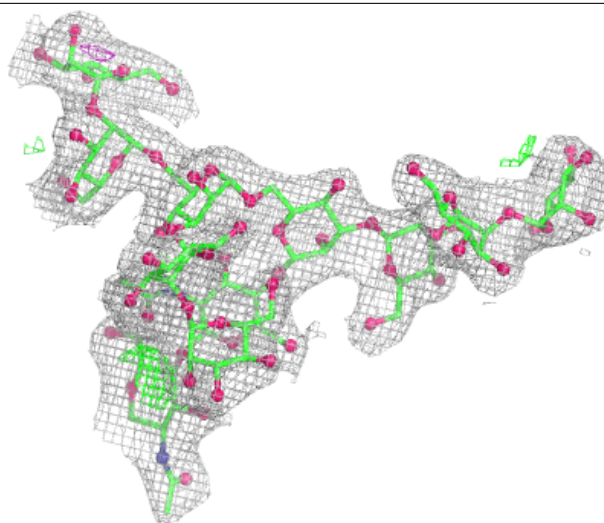
Electron density around Chain N:

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



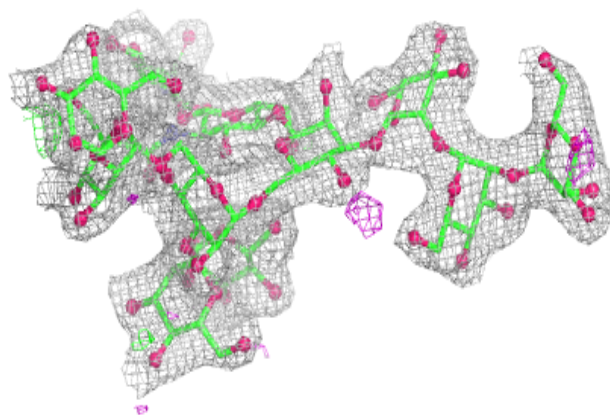
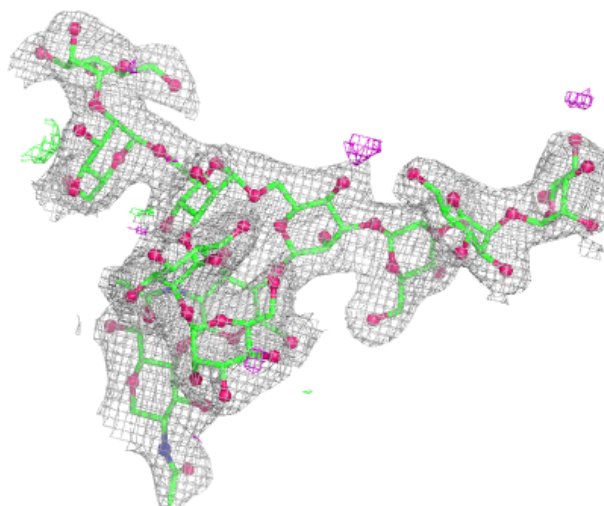
Electron density around Chain F:

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



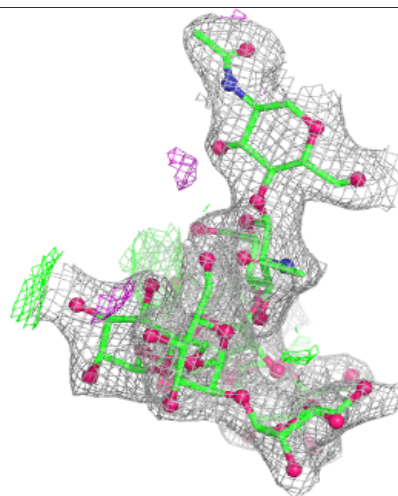
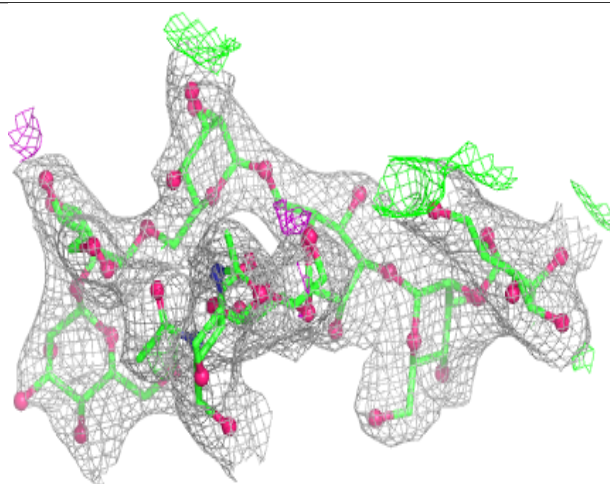
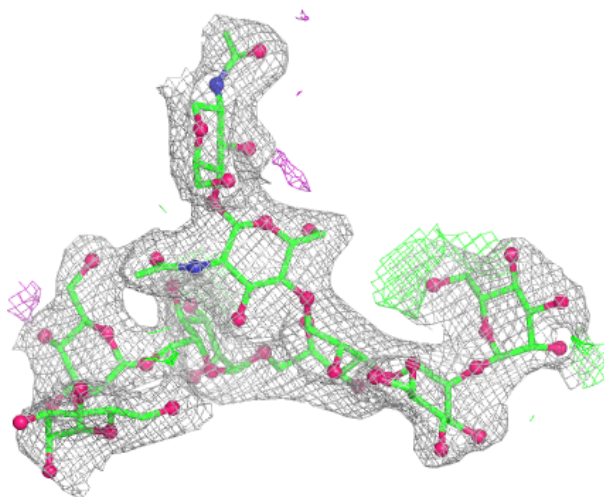
Electron density around Chain K:

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



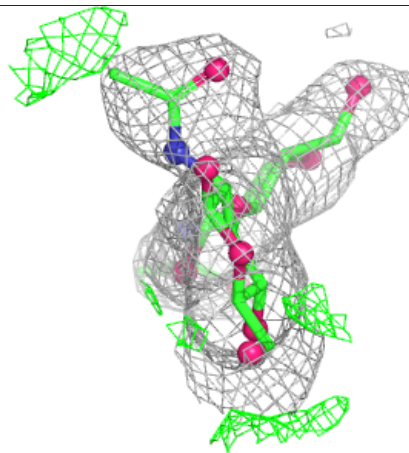
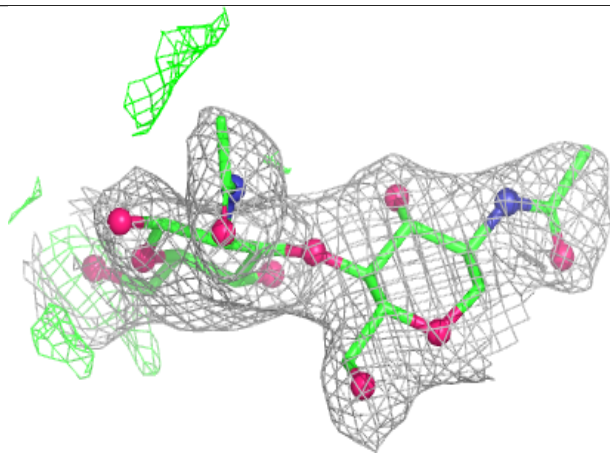
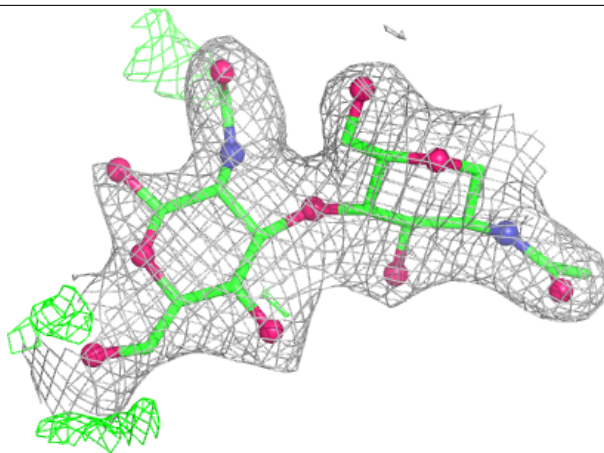
Electron density around Chain G:

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



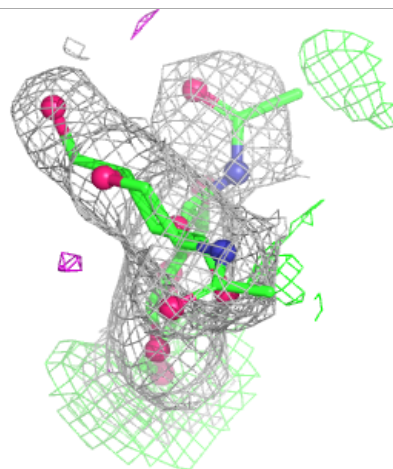
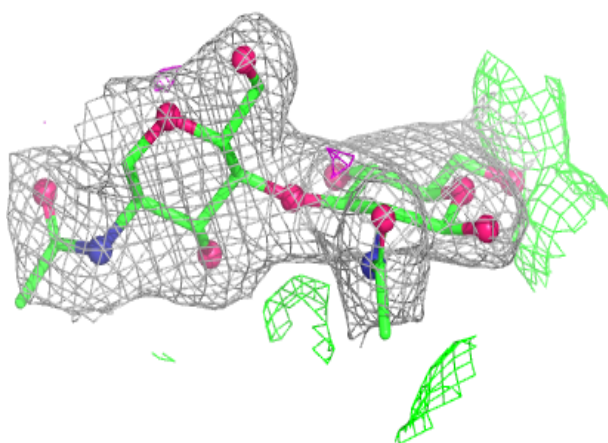
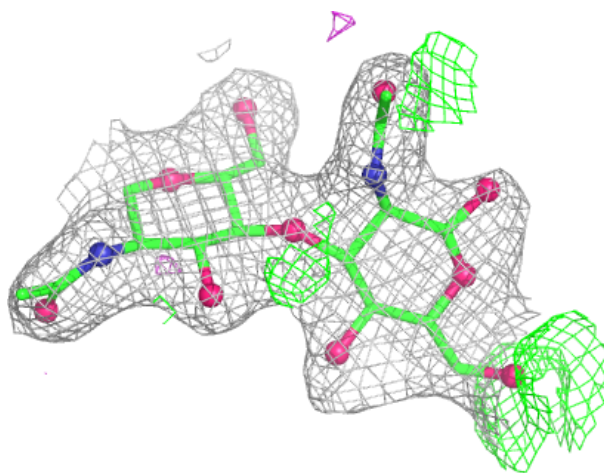
Electron density around Chain H:

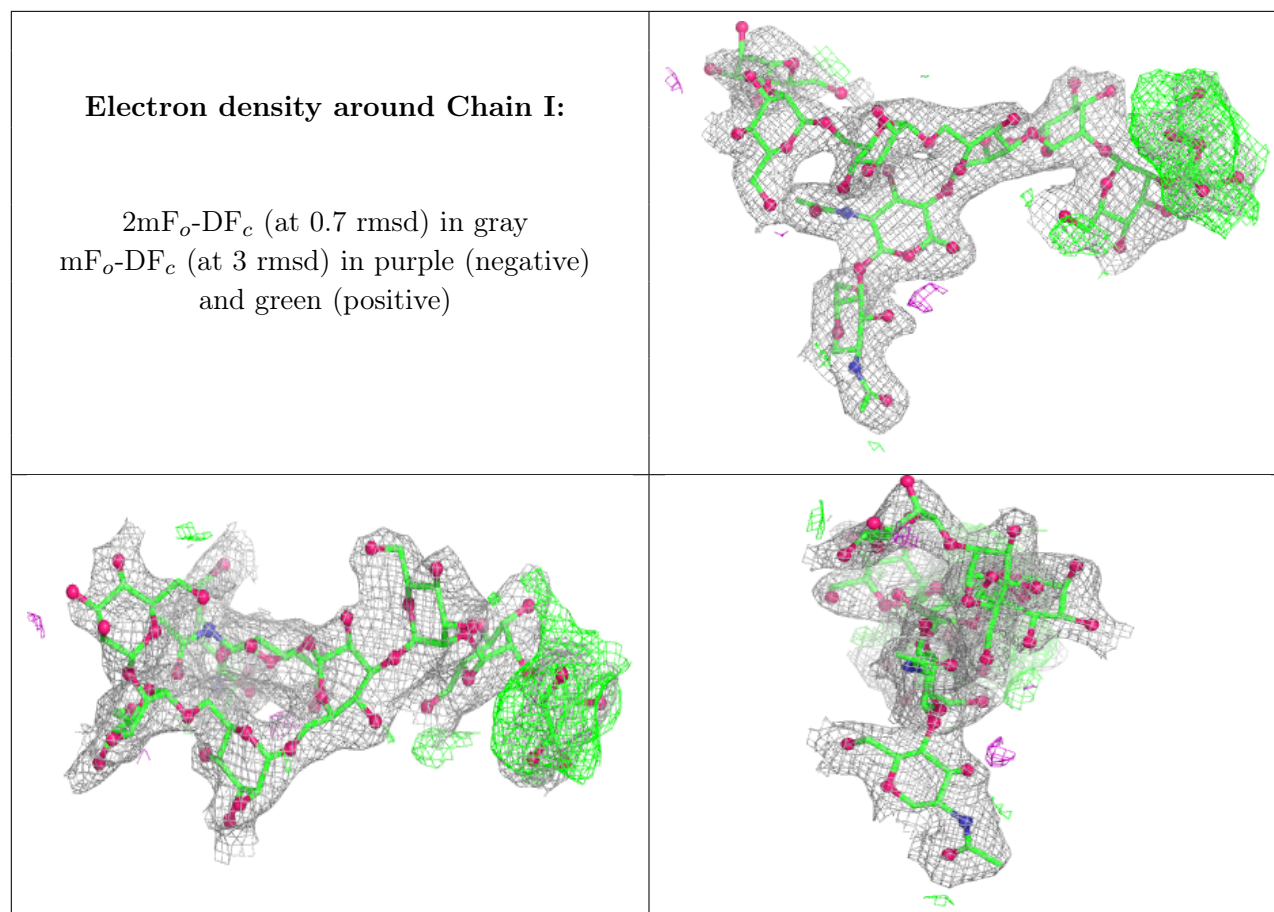
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
9	NAG	A	1005	14/15	0.97	0.06	24,25,26,27	14
9	NAG	A	1004	14/15	0.98	0.04	51,60,63,65	0
9	NAG	A	1002	14/15	0.98	0.05	62,65,68,70	0
9	NAG	B	1002	14/15	0.98	0.05	54,57,65,65	0
9	NAG	B	1005	14/15	0.98	0.06	24,25,26,27	14
11	NA	A	1022	1/1	0.98	0.17	55,55,55,55	0
12	1PE	A	1023	9/16	0.98	0.05	51,52,53,53	0
9	NAG	B	1003	14/15	0.99	0.04	39,44,50,50	0
9	NAG	B	1004	14/15	0.99	0.04	59,62,64,70	0
9	NAG	A	1003	14/15	0.99	0.04	40,46,49,52	0
10	CD	A	1006	1/1	0.99	0.06	54,54,54,54	1
10	CD	A	1007	1/1	0.99	0.03	82,82,82,82	1

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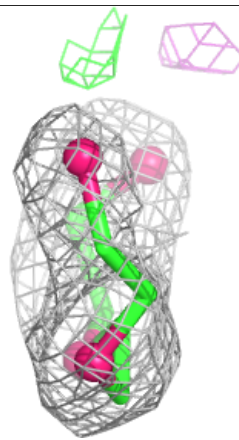
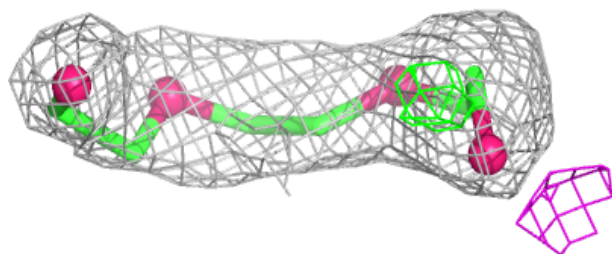
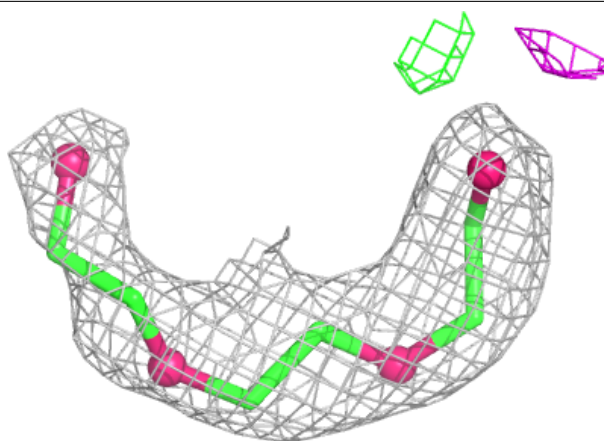
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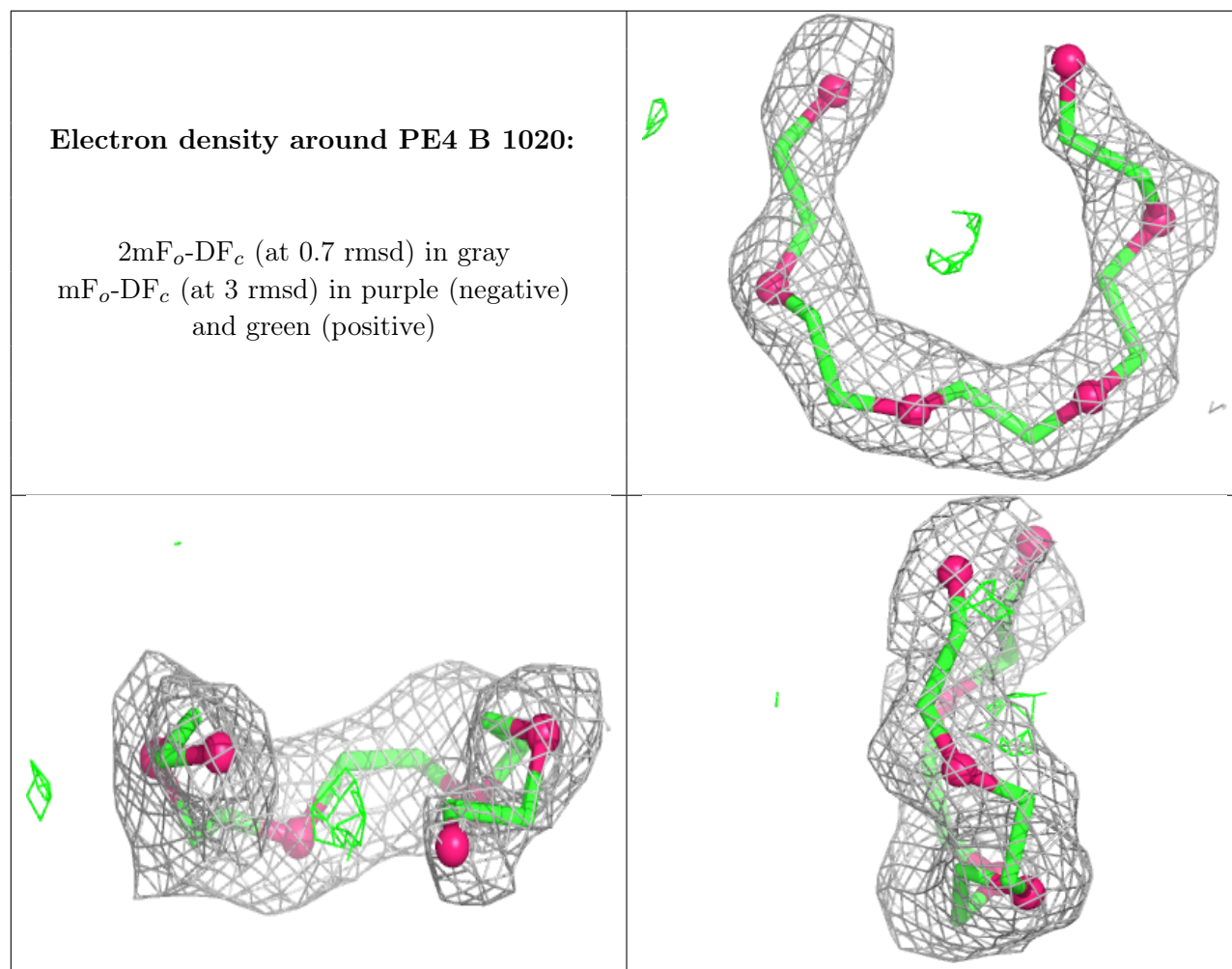
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	CD	A	1008	1/1	0.99	0.04	73,73,73,73	1
10	CD	A	1009	1/1	0.99	0.04	141,141,141,141	0
10	CD	A	1025	1/1	0.99	0.03	120,120,120,120	0
10	CD	B	1011	1/1	0.99	0.03	35,35,35,35	1
10	CD	B	1022	1/1	0.99	0.04	114,114,114,114	0
11	NA	A	1021	1/1	0.99	0.12	48,48,48,48	0
9	NAG	B	1001	14/15	0.99	0.04	63,66,69,70	0
11	NA	B	1017	1/1	0.99	0.18	57,57,57,57	0
9	NAG	A	1001	14/15	0.99	0.04	65,68,71,71	0
12	1PE	B	1018	9/16	0.99	0.05	51,53,54,54	0
13	PE4	A	1024	10/24	0.99	0.05	58,63,65,67	0
13	PE4	B	1020	16/24	0.99	0.06	56,62,69,71	0
10	CD	A	1020	1/1	1.00	0.02	102,102,102,102	0
10	CD	A	1010	1/1	1.00	0.05	94,94,94,94	0
10	CD	B	1006	1/1	1.00	0.05	58,58,58,58	1
10	CD	B	1007	1/1	1.00	0.04	127,127,127,127	0
10	CD	B	1008	1/1	1.00	0.06	94,94,94,94	0
10	CD	B	1009	1/1	1.00	0.01	54,54,54,54	0
10	CD	B	1010	1/1	1.00	0.01	59,59,59,59	0
10	CD	A	1011	1/1	1.00	0.01	41,41,41,41	0
10	CD	B	1012	1/1	1.00	0.01	56,56,56,56	1
10	CD	B	1013	1/1	1.00	0.01	83,83,83,83	1
10	CD	B	1014	1/1	1.00	0.01	95,95,95,95	0
10	CD	B	1015	1/1	1.00	0.01	47,47,47,47	0
10	CD	B	1016	1/1	1.00	0.02	79,79,79,79	0
10	CD	A	1012	1/1	1.00	0.01	40,40,40,40	0
10	CD	A	1013	1/1	1.00	0.01	39,39,39,39	0
10	CD	A	1014	1/1	1.00	0.01	55,55,55,55	0
10	CD	A	1015	1/1	1.00	0.01	47,47,47,47	1
10	CD	A	1016	1/1	1.00	0.02	58,58,58,58	1
10	CD	A	1017	1/1	1.00	0.03	63,63,63,63	1
10	CD	A	1018	1/1	1.00	0.01	47,47,47,47	0
10	CD	A	1019	1/1	1.00	0.01	39,39,39,39	0
14	CL	B	1019	1/1	1.00	0.05	53,53,53,53	0
15	CA	B	1021	1/1	1.00	0.02	54,54,54,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PE4 A 1024:

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





5.5 Other polymers [i](#)

There are no such residues in this entry.