



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:47 AM UTC

PDB ID : 8UWA / pdb_00008uwa
Title : VH1-18 QxxV class antibody 09-1B12 bound to A/Perth/16/2009 H3N2 hemagglutinin
Authors : Maurer, D.P.
Deposited on : 2023-11-06
Resolution : 4.02 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

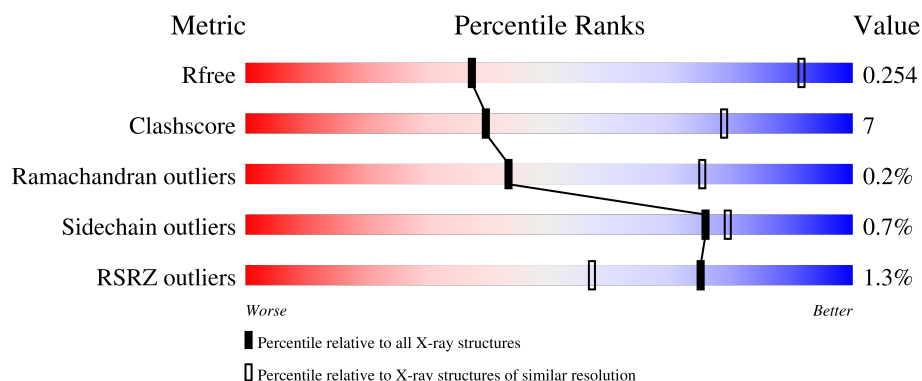
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.02 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.



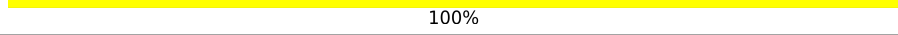
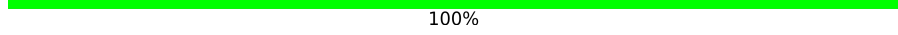
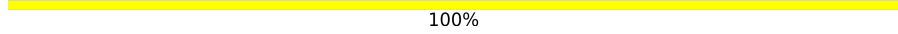
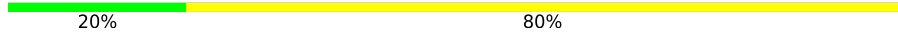
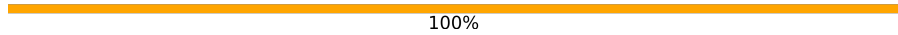
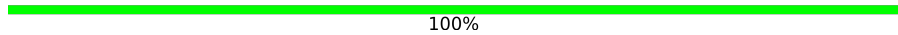
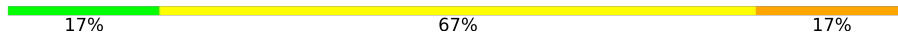
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1095 (4.24-3.80)
Clashscore	190562	1142 (4.24-3.80)
Ramachandran outliers	187476	1074 (4.24-3.80)
Sidechain outliers	187428	1065 (4.24-3.80)
RSRZ outliers	180081	1095 (4.24-3.80)

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	D	216	2% 85% 14% .
1	E	216	82% 17% .
1	G	216	% 85% 15%
2	A	514	2% 80% 14% 5%
2	B	514	% 78% 16% 5%

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Mol	Chain	Length	Quality of chain
2	C	514	
3	F	240	
3	H	240	
3	U	240	
4	I	4	
4	Q	4	
5	J	7	
6	K	3	
6	Z	3	
6	a	3	
7	L	5	
7	M	5	
7	R	5	
7	S	5	
7	T	5	
7	V	5	
8	N	4	
8	P	4	
9	O	2	
9	W	2	
9	b	2	
10	X	6	
10	Y	6	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 22979 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 09-1B12 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	216	Total	C	N	O	S	0	0	0
			1681	1050	291	335	5			
1	E	216	Total	C	N	O	S	0	0	0
			1681	1050	291	335	5			
1	G	216	Total	C	N	O	S	0	0	0
			1681	1050	291	335	5			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	489	Total	C	N	O	S	15	0	0
			3866	2410	690	748	18			
2	B	486	Total	C	N	O	S	7	0	0
			3837	2391	685	743	18			
2	C	490	Total	C	N	O	S	19	0	0
			3873	2414	691	750	18			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	ALA	-	expression tag	UNP C6KNH7
A	506	GLY	-	expression tag	UNP C6KNH7
A	507	SER	-	expression tag	UNP C6KNH7
A	508	SER	-	expression tag	UNP C6KNH7
A	509	LEU	-	expression tag	UNP C6KNH7
A	510	GLU	-	expression tag	UNP C6KNH7
A	511	VAL	-	expression tag	UNP C6KNH7
A	512	LEU	-	expression tag	UNP C6KNH7
A	513	PHE	-	expression tag	UNP C6KNH7
A	514	GLN	-	expression tag	UNP C6KNH7
B	505	ALA	-	expression tag	UNP C6KNH7
B	506	GLY	-	expression tag	UNP C6KNH7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	507	SER	-	expression tag	UNP C6KNH7
B	508	SER	-	expression tag	UNP C6KNH7
B	509	LEU	-	expression tag	UNP C6KNH7
B	510	GLU	-	expression tag	UNP C6KNH7
B	511	VAL	-	expression tag	UNP C6KNH7
B	512	LEU	-	expression tag	UNP C6KNH7
B	513	PHE	-	expression tag	UNP C6KNH7
B	514	GLN	-	expression tag	UNP C6KNH7
C	505	ALA	-	expression tag	UNP C6KNH7
C	506	GLY	-	expression tag	UNP C6KNH7
C	507	SER	-	expression tag	UNP C6KNH7
C	508	SER	-	expression tag	UNP C6KNH7
C	509	LEU	-	expression tag	UNP C6KNH7
C	510	GLU	-	expression tag	UNP C6KNH7
C	511	VAL	-	expression tag	UNP C6KNH7
C	512	LEU	-	expression tag	UNP C6KNH7
C	513	PHE	-	expression tag	UNP C6KNH7
C	514	GLN	-	expression tag	UNP C6KNH7

- Molecule 3 is a protein called 09-1B12 heavy chain.

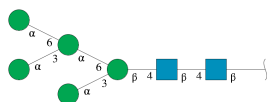
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	230	Total	C	N	O	S	0	0	0
			1725	1089	293	336	7			
3	H	239	Total	C	N	O	S	0	0	0
			1790	1129	303	351	7			
3	U	230	Total	C	N	O	S	0	0	0
			1725	1089	293	336	7			

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



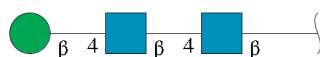
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



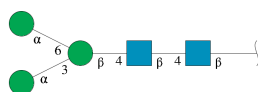
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



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

- Molecule 7 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
7	L	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	M	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

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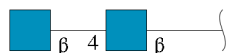
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	S	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	T	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	V	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is an oligosaccharide called 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.



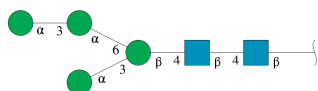
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	N	4	Total	C	N	O	0	0	0
			50	28	2	20			
8	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



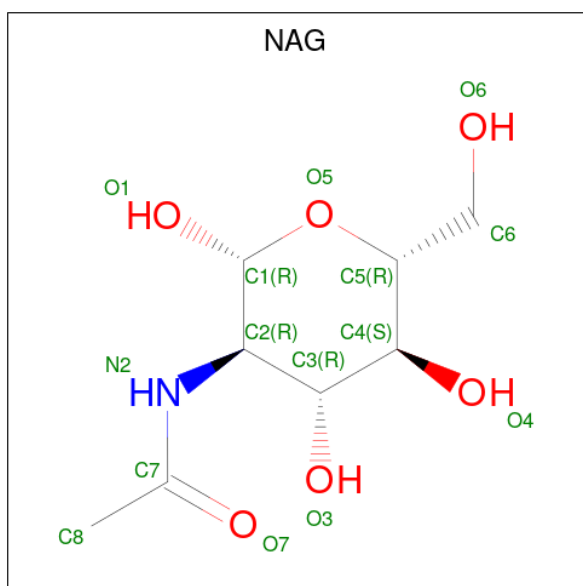
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	b	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 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
10	X	6	Total	C	N	O	0	0	0
			72	40	2	30			
10	Y	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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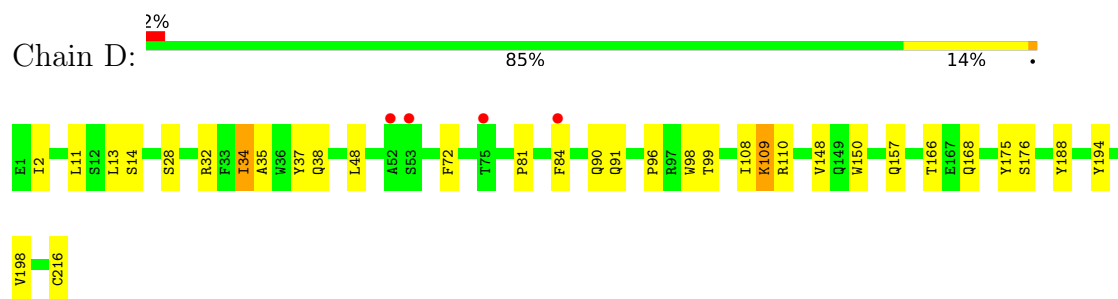
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			14	8	1	5		
11	C	1	Total	C	N	O	0	0
			14	8	1	5		

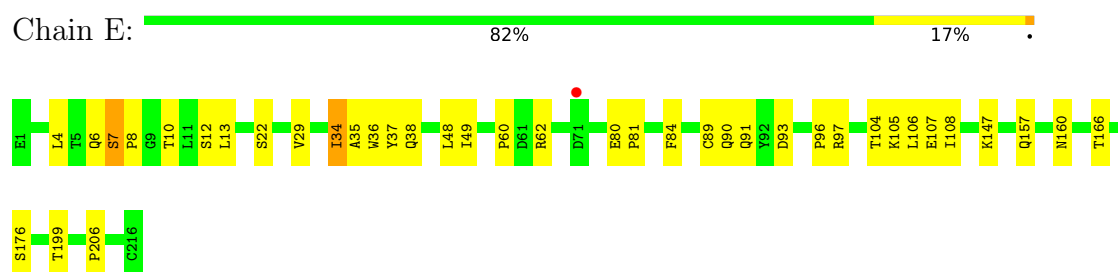
3 Residue-property plots [i](#)

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

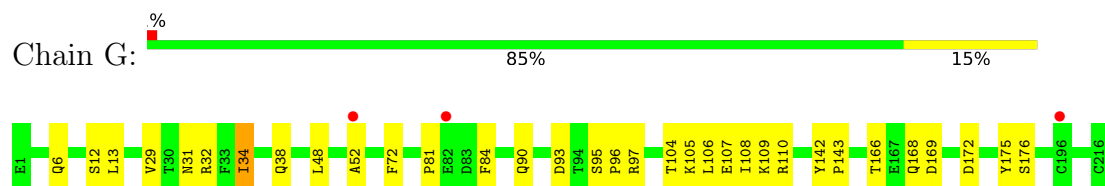
- Molecule 1: 09-1B12 light chain



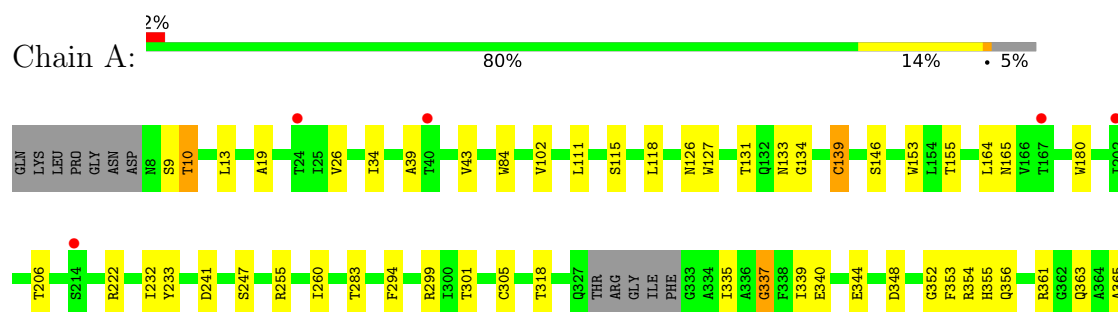
- Molecule 1: 09-1B12 light chain



- Molecule 1: 09-1B12 light chain

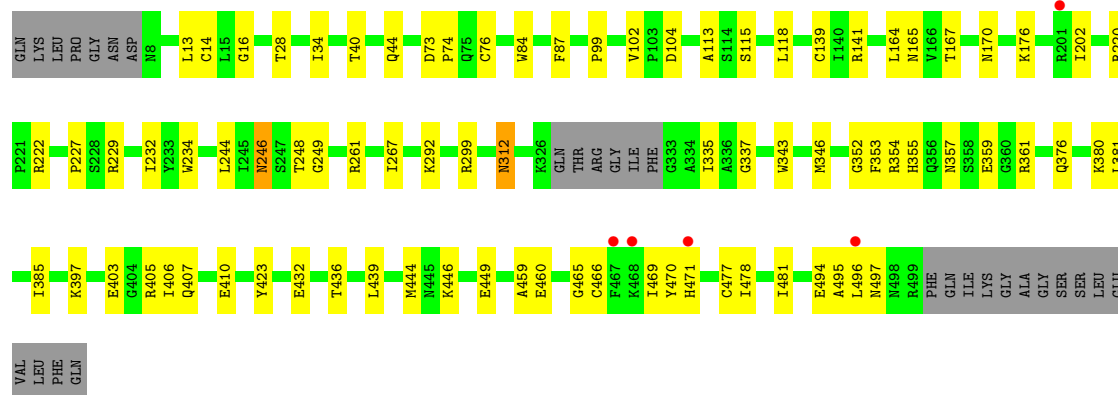
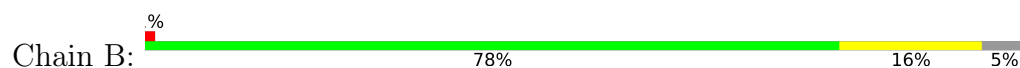


- Molecule 2: Hemagglutinin

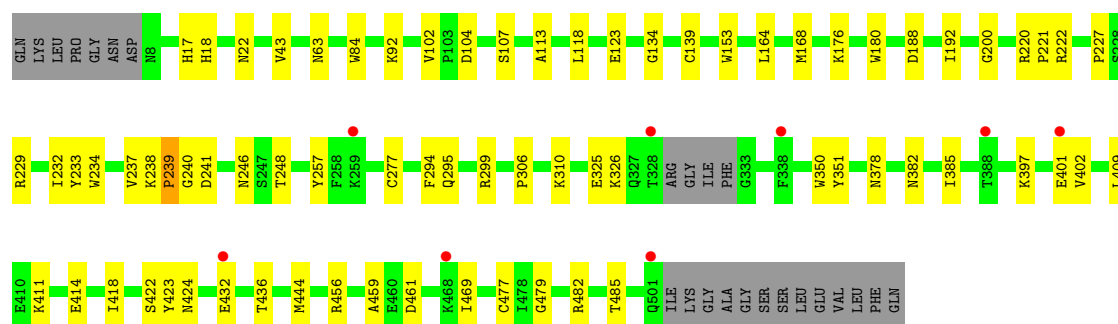
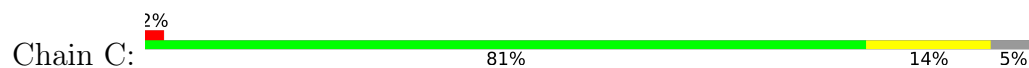




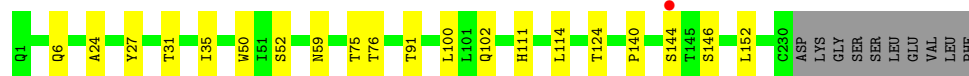
• Molecule 2: Hemagglutinin



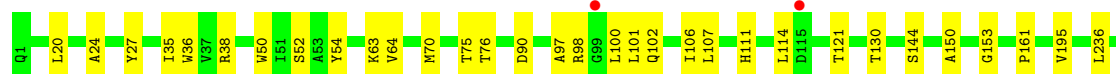
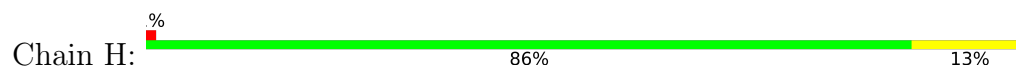
• Molecule 2: Hemagglutinin



• Molecule 3: 09-1B12 heavy chain



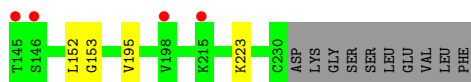
• Molecule 3: 09-1B12 heavy chain





- Molecule 3: 09-1B12 heavy chain

Chain U: 2% 80% 15% .



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

Chain I: 50% 50%



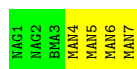
- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 75% 25%



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

Chain J: 43% 57%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 100%



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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

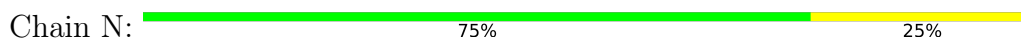




- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

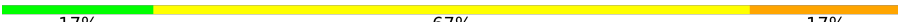


- Molecule 10: α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain X:  17% 83%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 10: 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

Chain Y:  17% 67% 17%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.04Å 158.04Å 417.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.21 – 4.02 50.21 – 4.02	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.21-4.02) 99.7 (50.21-4.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.230 , 0.254 0.231 , 0.254	Depositor DCC
R_{free} test set	2004 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	106.8	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	22979	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	D	0.16	0/1719	0.40	0/2332
1	E	0.17	0/1719	0.43	0/2332
1	G	0.16	0/1719	0.37	0/2332
2	A	0.18	0/3945	0.42	1/5338 (0.0%)
2	B	0.17	0/3915	0.38	0/5298
2	C	0.20	0/3952	0.39	1/5348 (0.0%)
3	F	0.15	0/1766	0.37	0/2412
3	H	0.14	0/1831	0.36	0/2499
3	U	0.17	0/1766	0.41	0/2412
All	All	0.17	0/22332	0.39	2/30303 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	337	GLY	N-CA-C	7.41	121.50	111.20
2	C	239	PRO	CA-N-CD	-5.89	103.76	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	7	SER	Peptide

5.2 Too-close contacts

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	D	1681	0	1632	26	0
1	E	1681	0	1633	31	0
1	G	1681	0	1632	25	0
2	A	3866	0	3743	52	0
2	B	3837	0	3716	57	0
2	C	3873	0	3750	52	0
3	F	1725	0	1701	14	0
3	H	1790	0	1767	21	0
3	U	1725	0	1700	30	0
4	I	50	0	43	0	0
4	Q	50	0	43	0	0
5	J	83	0	70	0	0
6	K	39	0	34	0	0
6	Z	39	0	34	0	0
6	a	39	0	34	2	0
7	L	61	0	52	6	0
7	M	61	0	52	0	0
7	R	61	0	52	1	0
7	S	61	0	52	2	0
7	T	61	0	52	1	0
7	V	61	0	52	3	0
8	N	50	0	43	0	0
8	P	50	0	43	2	0
9	O	28	0	25	2	0
9	W	28	0	25	0	0
9	b	28	0	25	1	0
10	X	72	0	61	3	0
10	Y	72	0	61	1	0
11	A	28	0	26	0	0
11	B	42	0	39	1	0
11	C	56	0	52	0	0
All	All	22979	0	22244	303	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 303 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)
3:U:35:ILE:HD11	3:U:114:LEU:HD21	1.51	0.89
1:E:7:SER:HB3	1:E:22:SER:HB3	1.57	0.86
1:D:34:ILE:HA	1:D:90:GLN:O	1.76	0.85
1:E:34:ILE:HA	1:E:90:GLN:O	1.81	0.81
2:A:115:SER:HB2	2:A:260:ILE:HD12	1.63	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	214/216 (99%)	201 (94%)	11 (5%)	2 (1%)	14	48
1	E	214/216 (99%)	202 (94%)	10 (5%)	2 (1%)	14	48
1	G	214/216 (99%)	204 (95%)	9 (4%)	1 (0%)	24	60
2	A	485/514 (94%)	457 (94%)	27 (6%)	1 (0%)	43	75
2	B	482/514 (94%)	462 (96%)	20 (4%)	0	100	100
2	C	486/514 (95%)	467 (96%)	19 (4%)	0	100	100
3	F	228/240 (95%)	219 (96%)	9 (4%)	0	100	100
3	H	237/240 (99%)	229 (97%)	8 (3%)	0	100	100
3	U	228/240 (95%)	220 (96%)	8 (4%)	0	100	100
All	All	2788/2910 (96%)	2661 (95%)	121 (4%)	6 (0%)	43	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	8	PRO
1	D	34	ILE
1	G	34	ILE
2	A	10	THR
1	D	109	LYS

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	D	189/189 (100%)	188 (100%)	1 (0%)	81	82
1	E	189/189 (100%)	188 (100%)	1 (0%)	81	82
1	G	189/189 (100%)	189 (100%)	0	100	100
2	A	427/447 (96%)	422 (99%)	5 (1%)	63	73
2	B	424/447 (95%)	419 (99%)	5 (1%)	63	73
2	C	428/447 (96%)	424 (99%)	4 (1%)	70	77
3	F	191/200 (96%)	191 (100%)	0	100	100
3	H	199/200 (100%)	199 (100%)	0	100	100
3	U	191/200 (96%)	191 (100%)	0	100	100
All	All	2427/2508 (97%)	2411 (99%)	16 (1%)	76	79

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	277	CYS
2	C	139	CYS
2	B	139	CYS
2	C	63	ASN
2	B	76	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	216	ASN
2	C	298	ASN
3	U	39	GLN
2	C	296	ASN
2	C	378	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 ⓘ

80 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	$\# Z > 2$
4	NAG	I	1	4,2	14,14,15	1.13	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	I	2	4	14,14,15	0.29	0	17,19,21	0.56	0
4	BMA	I	3	4	11,11,12	0.68	0	15,15,17	0.76	0
4	MAN	I	4	4	11,11,12	0.84	1 (9%)	15,15,17	1.14	2 (13%)
5	NAG	J	1	5,2	14,14,15	0.45	0	17,19,21	0.66	0
5	NAG	J	2	5	14,14,15	0.39	0	17,19,21	0.54	0
5	BMA	J	3	5	11,11,12	0.88	0	15,15,17	1.00	0
5	MAN	J	4	5	11,11,12	0.77	0	15,15,17	0.89	1 (6%)
5	MAN	J	5	5	11,11,12	0.92	0	15,15,17	1.19	2 (13%)
5	MAN	J	6	5	11,11,12	0.60	0	15,15,17	1.00	2 (13%)
5	MAN	J	7	5	11,11,12	0.92	0	15,15,17	0.98	2 (13%)
6	NAG	K	1	2,6	14,14,15	0.69	0	17,19,21	0.86	1 (5%)
6	NAG	K	2	6	14,14,15	0.63	0	17,19,21	1.01	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BMA	K	3	6	11,11,12	1.22	2 (18%)	15,15,17	1.11	1 (6%)
7	NAG	L	1	7,2	14,14,15	0.35	0	17,19,21	0.83	1 (5%)
7	NAG	L	2	7	14,14,15	0.33	0	17,19,21	1.07	1 (5%)
7	BMA	L	3	7	11,11,12	1.03	0	15,15,17	0.77	0
7	MAN	L	4	7	11,11,12	1.20	2 (18%)	15,15,17	1.16	2 (13%)
7	MAN	L	5	7	11,11,12	1.33	2 (18%)	15,15,17	1.24	2 (13%)
7	NAG	M	1	7,2	14,14,15	0.99	1 (7%)	17,19,21	1.00	1 (5%)
7	NAG	M	2	7	14,14,15	0.95	1 (7%)	17,19,21	1.02	2 (11%)
7	BMA	M	3	7	11,11,12	1.85	3 (27%)	15,15,17	2.19	4 (26%)
7	MAN	M	4	7	11,11,12	1.32	2 (18%)	15,15,17	1.55	2 (13%)
7	MAN	M	5	7	11,11,12	0.94	1 (9%)	15,15,17	1.08	2 (13%)
8	NAG	N	1	2,8	14,14,15	0.34	0	17,19,21	0.61	0
8	NAG	N	2	8	14,14,15	0.22	0	17,19,21	0.63	0
8	BMA	N	3	8	11,11,12	0.92	0	15,15,17	0.73	0
8	MAN	N	4	8	11,11,12	0.84	1 (9%)	15,15,17	1.12	2 (13%)
9	NAG	O	1	2,9	14,14,15	0.33	0	17,19,21	1.17	2 (11%)
9	NAG	O	2	9	14,14,15	0.23	0	17,19,21	0.96	1 (5%)
8	NAG	P	1	2,8	14,14,15	0.53	0	17,19,21	1.88	5 (29%)
8	NAG	P	2	8	14,14,15	0.55	0	17,19,21	0.47	0
8	BMA	P	3	8	11,11,12	1.02	1 (9%)	15,15,17	0.97	2 (13%)
8	MAN	P	4	8	11,11,12	1.29	2 (18%)	15,15,17	1.13	2 (13%)
4	NAG	Q	1	4,2	14,14,15	0.21	0	17,19,21	0.60	0
4	NAG	Q	2	4	14,14,15	0.38	0	17,19,21	0.67	0
4	BMA	Q	3	4	11,11,12	0.79	0	15,15,17	0.70	0
4	MAN	Q	4	4	11,11,12	0.90	1 (9%)	15,15,17	1.10	2 (13%)
7	NAG	R	1	7,2	14,14,15	1.32	1 (7%)	17,19,21	1.40	2 (11%)
7	NAG	R	2	7	14,14,15	0.76	1 (7%)	17,19,21	1.06	2 (11%)
7	BMA	R	3	7	11,11,12	1.88	3 (27%)	15,15,17	1.98	3 (20%)
7	MAN	R	4	7	11,11,12	1.46	2 (18%)	15,15,17	1.55	2 (13%)
7	MAN	R	5	7	11,11,12	1.31	2 (18%)	15,15,17	1.31	2 (13%)
7	NAG	S	1	7,2	14,14,15	0.63	1 (7%)	17,19,21	0.81	1 (5%)
7	NAG	S	2	7	14,14,15	0.54	0	17,19,21	1.60	2 (11%)
7	BMA	S	3	7	11,11,12	1.00	1 (9%)	15,15,17	0.88	1 (6%)
7	MAN	S	4	7	11,11,12	1.37	2 (18%)	15,15,17	1.25	1 (6%)
7	MAN	S	5	7	11,11,12	0.75	0	15,15,17	1.12	2 (13%)
7	NAG	T	1	7,2	14,14,15	0.27	0	17,19,21	0.72	0
7	NAG	T	2	7	14,14,15	0.42	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	T	3	7	11,11,12	0.75	0	15,15,17	0.74	0
7	MAN	T	4	7	11,11,12	0.79	0	15,15,17	0.98	2 (13%)
7	MAN	T	5	7	11,11,12	0.90	0	15,15,17	0.99	2 (13%)
7	NAG	V	1	7,2	14,14,15	0.58	0	17,19,21	0.66	0
7	NAG	V	2	7	14,14,15	0.62	0	17,19,21	1.10	1 (5%)
7	BMA	V	3	7	11,11,12	1.11	1 (9%)	15,15,17	1.49	2 (13%)
7	MAN	V	4	7	11,11,12	0.87	0	15,15,17	1.11	1 (6%)
7	MAN	V	5	7	11,11,12	1.09	1 (9%)	15,15,17	1.00	2 (13%)
9	NAG	W	1	2,9	14,14,15	0.38	0	17,19,21	0.64	0
9	NAG	W	2	9	14,14,15	0.40	0	17,19,21	0.47	0
10	NAG	X	1	10,2	14,14,15	0.66	1 (7%)	17,19,21	0.89	0
10	NAG	X	2	10	14,14,15	1.06	1 (7%)	17,19,21	1.35	1 (5%)
10	BMA	X	3	10	11,11,12	1.20	1 (9%)	15,15,17	1.37	1 (6%)
10	MAN	X	4	10	11,11,12	0.92	0	15,15,17	0.98	1 (6%)
10	MAN	X	5	10	11,11,12	0.98	1 (9%)	15,15,17	1.03	1 (6%)
10	MAN	X	6	10	11,11,12	0.84	1 (9%)	15,15,17	1.04	1 (6%)
10	NAG	Y	1	10,2	14,14,15	0.42	0	17,19,21	0.66	0
10	NAG	Y	2	10	14,14,15	0.36	0	17,19,21	0.78	1 (5%)
10	BMA	Y	3	10	11,11,12	0.75	0	15,15,17	1.13	1 (6%)
10	MAN	Y	4	10	11,11,12	1.35	2 (18%)	15,15,17	1.62	2 (13%)
10	MAN	Y	5	10	11,11,12	0.88	0	15,15,17	0.85	1 (6%)
10	MAN	Y	6	10	11,11,12	0.83	0	15,15,17	1.00	2 (13%)
6	NAG	Z	1	2,6	14,14,15	0.23	0	17,19,21	0.48	0
6	NAG	Z	2	6	14,14,15	0.20	0	17,19,21	0.60	0
6	BMA	Z	3	6	11,11,12	0.66	0	15,15,17	0.70	0
6	NAG	a	1	2,6	14,14,15	0.32	0	17,19,21	0.45	0
6	NAG	a	2	6	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
6	BMA	a	3	6	11,11,12	1.80	4 (36%)	15,15,17	1.96	4 (26%)
9	NAG	b	1	2,9	14,14,15	0.99	1 (7%)	17,19,21	1.31	2 (11%)
9	NAG	b	2	9	14,14,15	0.30	0	17,19,21	0.72	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
4	NAG	I	1	4,2	-	0/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	R	3	7	-	2/2/19/22	0/1/1/1
7	MAN	R	4	7	-	1/2/19/22	1/1/1/1
7	MAN	R	5	7	-	2/2/19/22	1/1/1/1
7	NAG	S	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	BMA	S	3	7	-	2/2/19/22	0/1/1/1
7	MAN	S	4	7	-	1/2/19/22	1/1/1/1
7	MAN	S	5	7	-	0/2/19/22	0/1/1/1
7	NAG	T	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	BMA	T	3	7	-	0/2/19/22	0/1/1/1
7	MAN	T	4	7	-	1/2/19/22	0/1/1/1
7	MAN	T	5	7	-	0/2/19/22	0/1/1/1
7	NAG	V	1	7,2	-	4/6/23/26	0/1/1/1
7	NAG	V	2	7	-	2/6/23/26	0/1/1/1
7	BMA	V	3	7	-	1/2/19/22	0/1/1/1
7	MAN	V	4	7	-	1/2/19/22	0/1/1/1
7	MAN	V	5	7	-	0/2/19/22	0/1/1/1
9	NAG	W	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	W	2	9	-	1/6/23/26	0/1/1/1
10	NAG	X	1	10,2	-	3/6/23/26	0/1/1/1
10	NAG	X	2	10	-	2/6/23/26	0/1/1/1
10	BMA	X	3	10	-	1/2/19/22	0/1/1/1
10	MAN	X	4	10	-	1/2/19/22	0/1/1/1
10	MAN	X	5	10	-	0/2/19/22	0/1/1/1
10	MAN	X	6	10	-	1/2/19/22	0/1/1/1
10	NAG	Y	1	10,2	-	4/6/23/26	0/1/1/1
10	NAG	Y	2	10	-	2/6/23/26	0/1/1/1
10	BMA	Y	3	10	-	2/2/19/22	0/1/1/1
10	MAN	Y	4	10	-	0/2/19/22	0/1/1/1
10	MAN	Y	5	10	-	1/2/19/22	0/1/1/1
10	MAN	Y	6	10	-	0/2/19/22	0/1/1/1
6	NAG	Z	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	0/2/19/22	0/1/1/1
6	NAG	a	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	4/6/23/26	0/1/1/1
6	BMA	a	3	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	b	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	b	2	9	-	0/6/23/26	0/1/1/1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	1	NAG	O5-C1	-4.51	1.36	1.43
7	M	3	BMA	C4-C5	3.95	1.61	1.53
4	I	1	NAG	O5-C1	-3.76	1.37	1.43
7	R	3	BMA	C4-C5	3.70	1.60	1.53
6	a	3	BMA	C4-C5	3.66	1.60	1.53

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	1	NAG	C1-O5-C5	5.56	119.64	112.19
7	S	2	NAG	C3-C4-C5	5.08	119.44	110.23
7	M	3	BMA	C1-C2-C3	-5.04	102.30	109.64
10	X	2	NAG	C1-O5-C5	5.03	118.92	112.19
7	M	3	BMA	C1-O5-C5	-4.51	106.14	112.19

There are no chirality outliers.

5 of 95 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	P	1	NAG	C1-C2-N2-C7
9	O	2	NAG	C1-C2-N2-C7
9	b	1	NAG	C1-C2-N2-C7
10	X	1	NAG	C1-C2-N2-C7
7	M	3	BMA	C4-C5-C6-O6

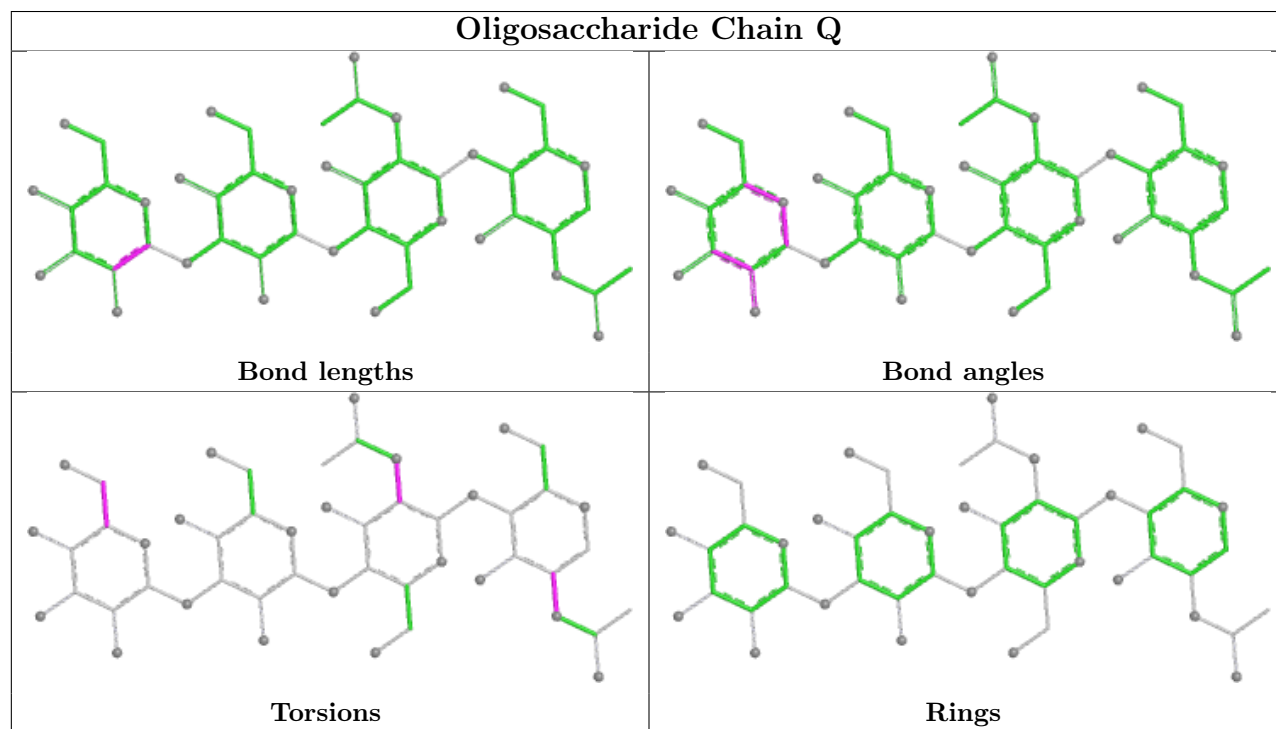
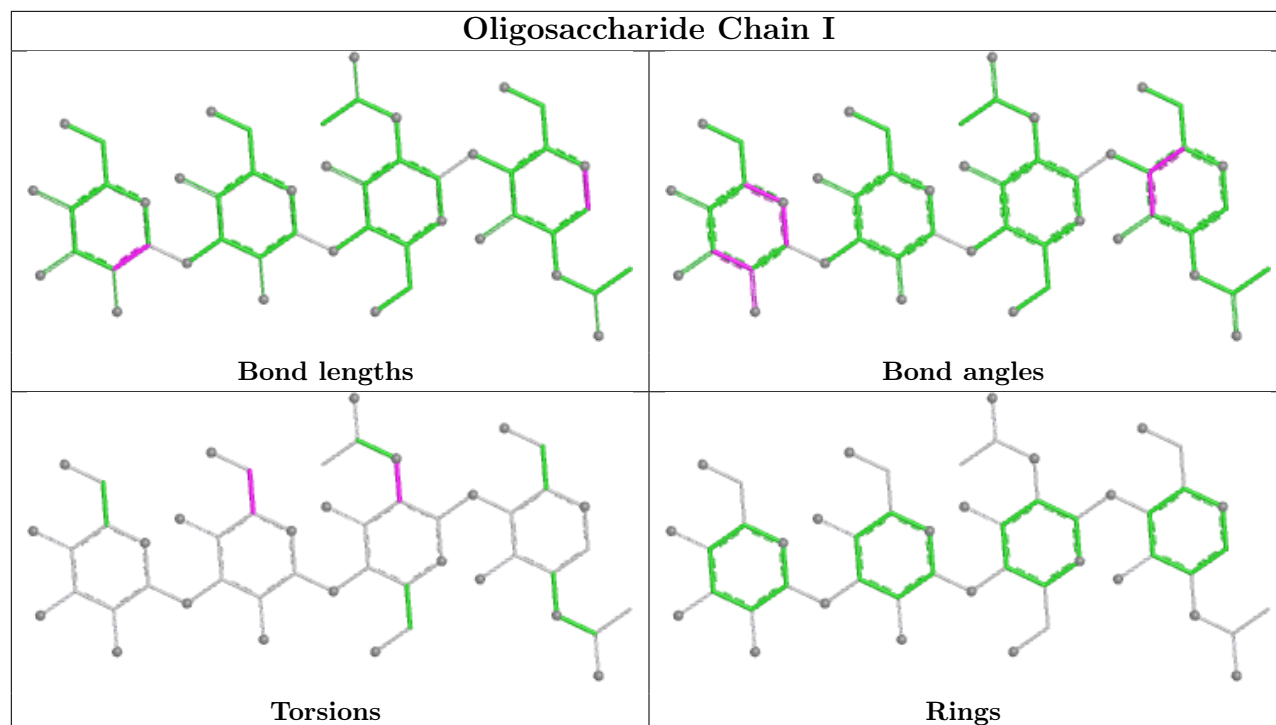
5 of 7 ring outliers are listed below:

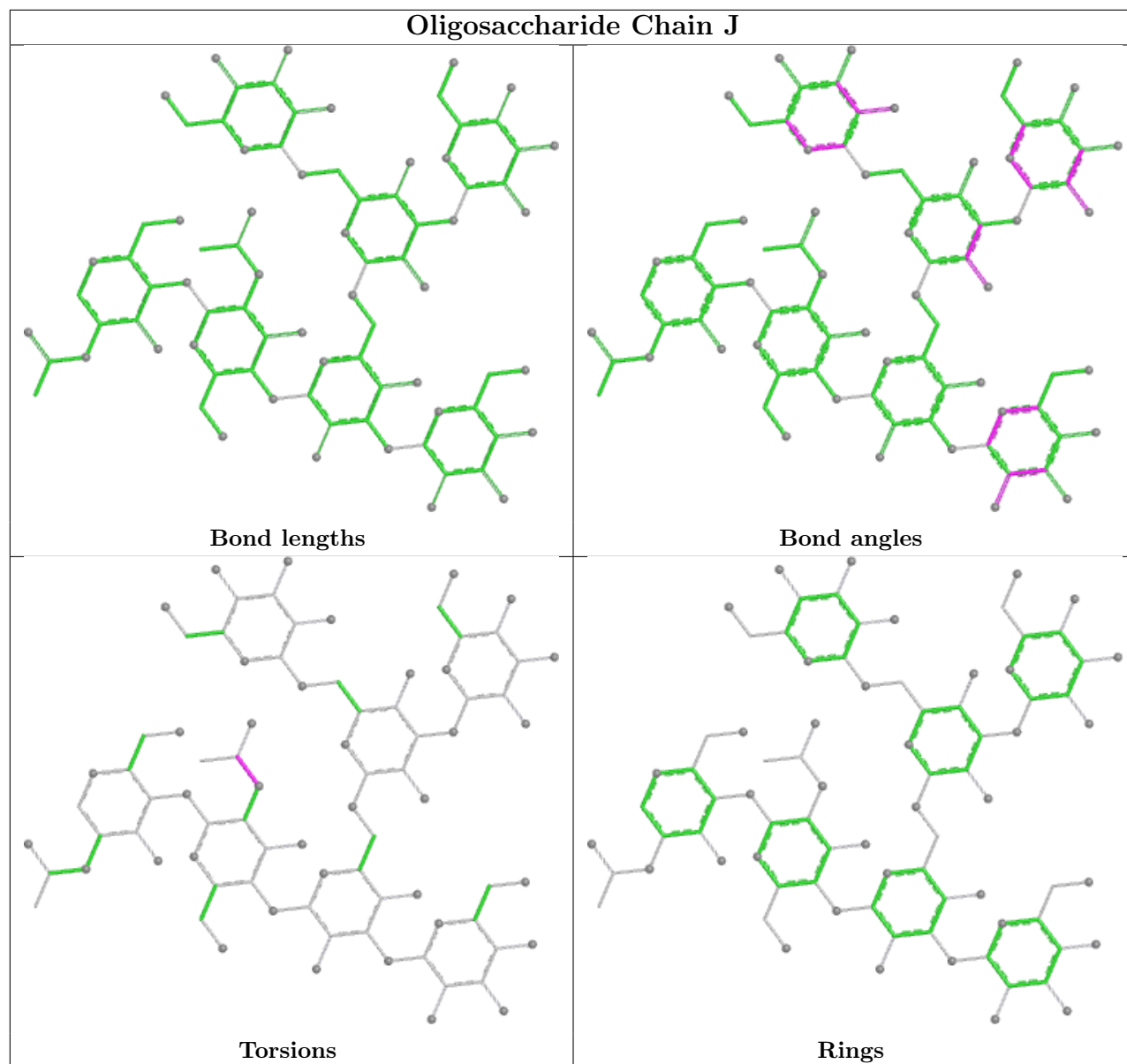
Mol	Chain	Res	Type	Atoms
7	R	4	MAN	C1-C2-C3-C4-C5-O5
7	R	5	MAN	C1-C2-C3-C4-C5-O5
7	S	4	MAN	C1-C2-C3-C4-C5-O5
7	M	5	MAN	C1-C2-C3-C4-C5-O5
7	L	4	MAN	C1-C2-C3-C4-C5-O5

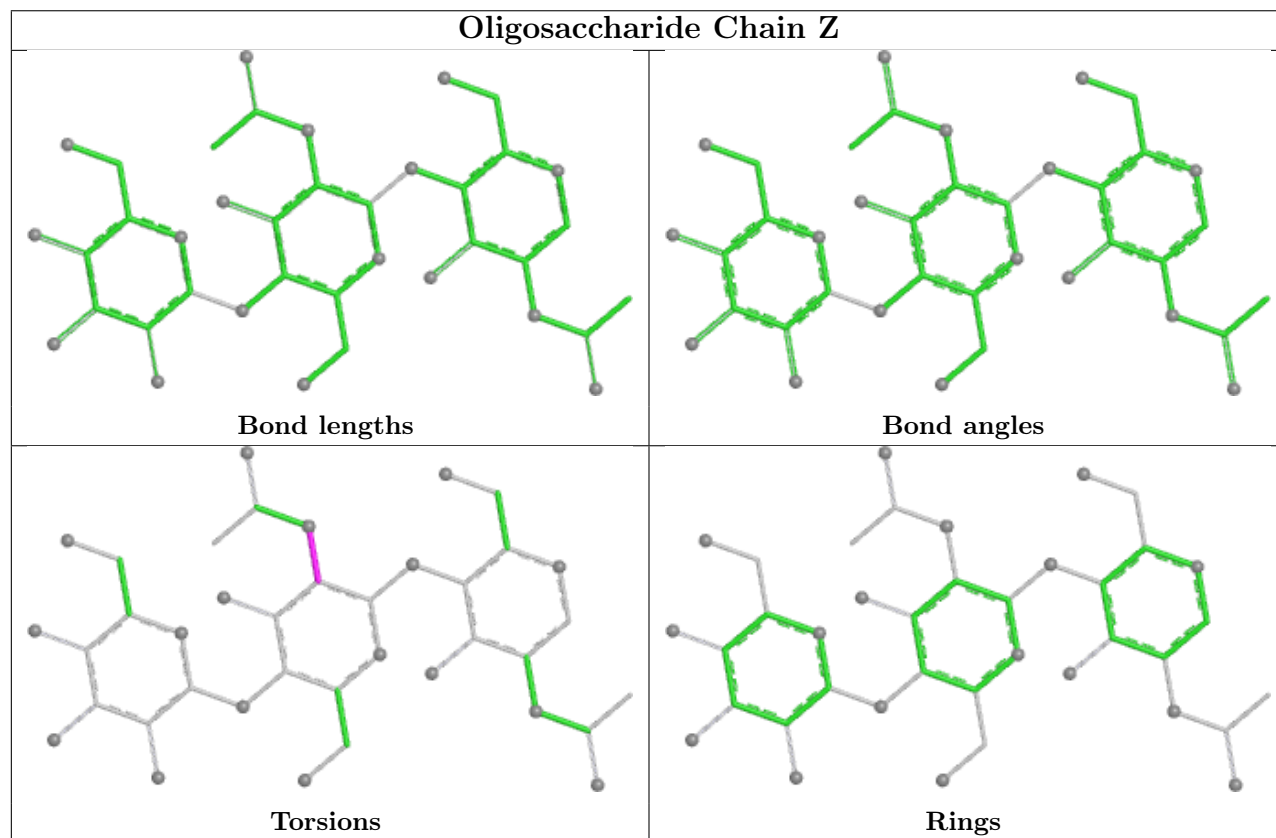
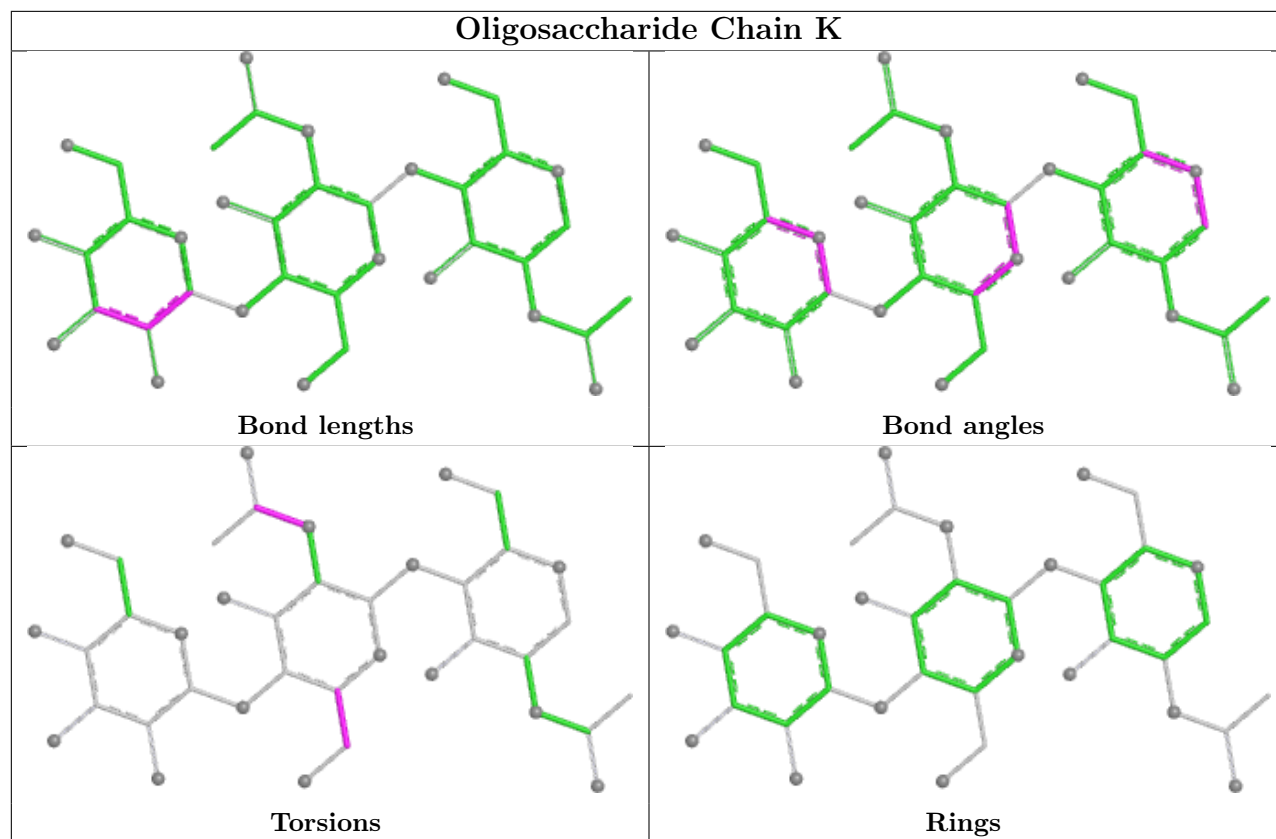
29 monomers are involved in 24 short contacts:

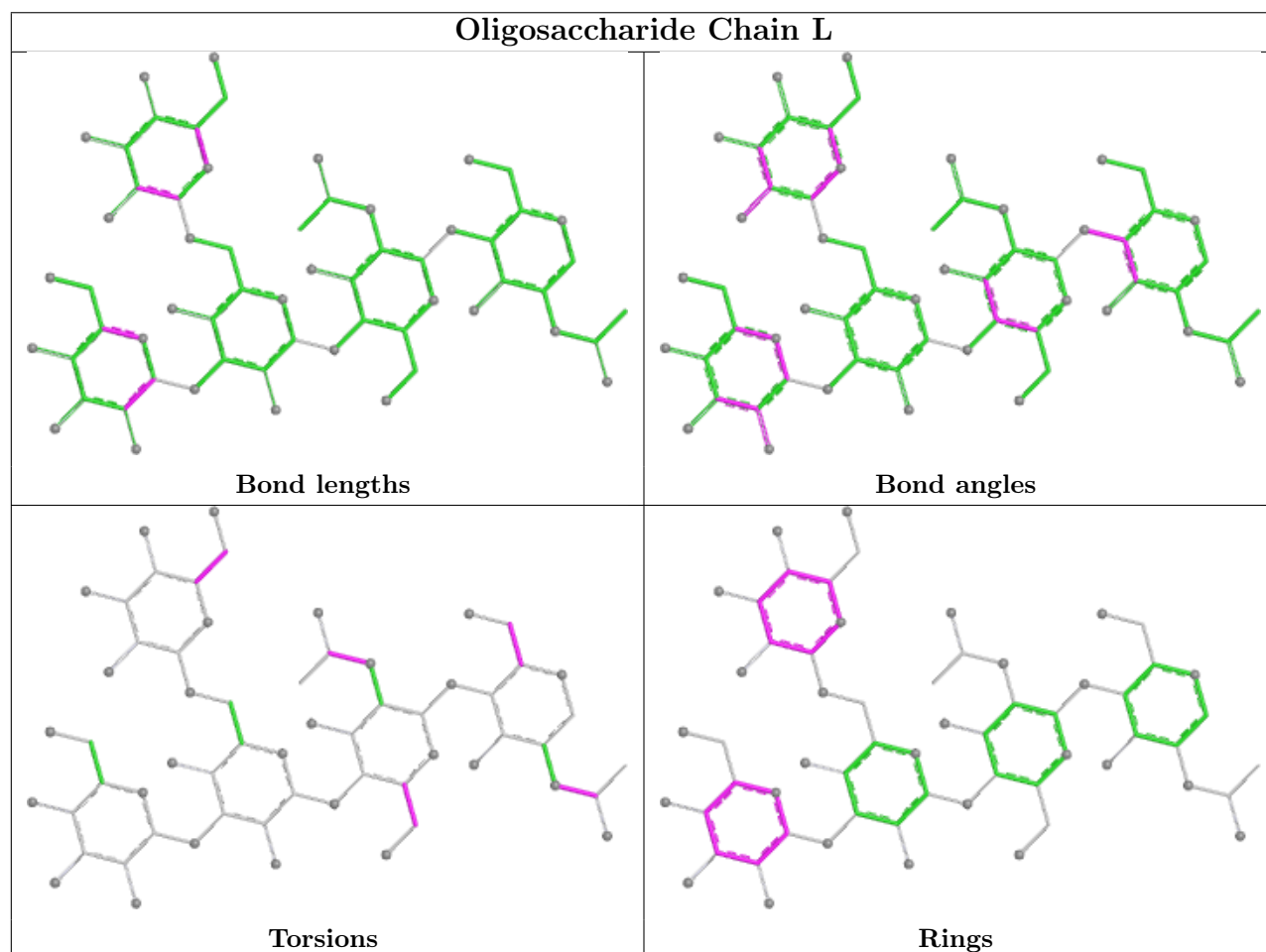
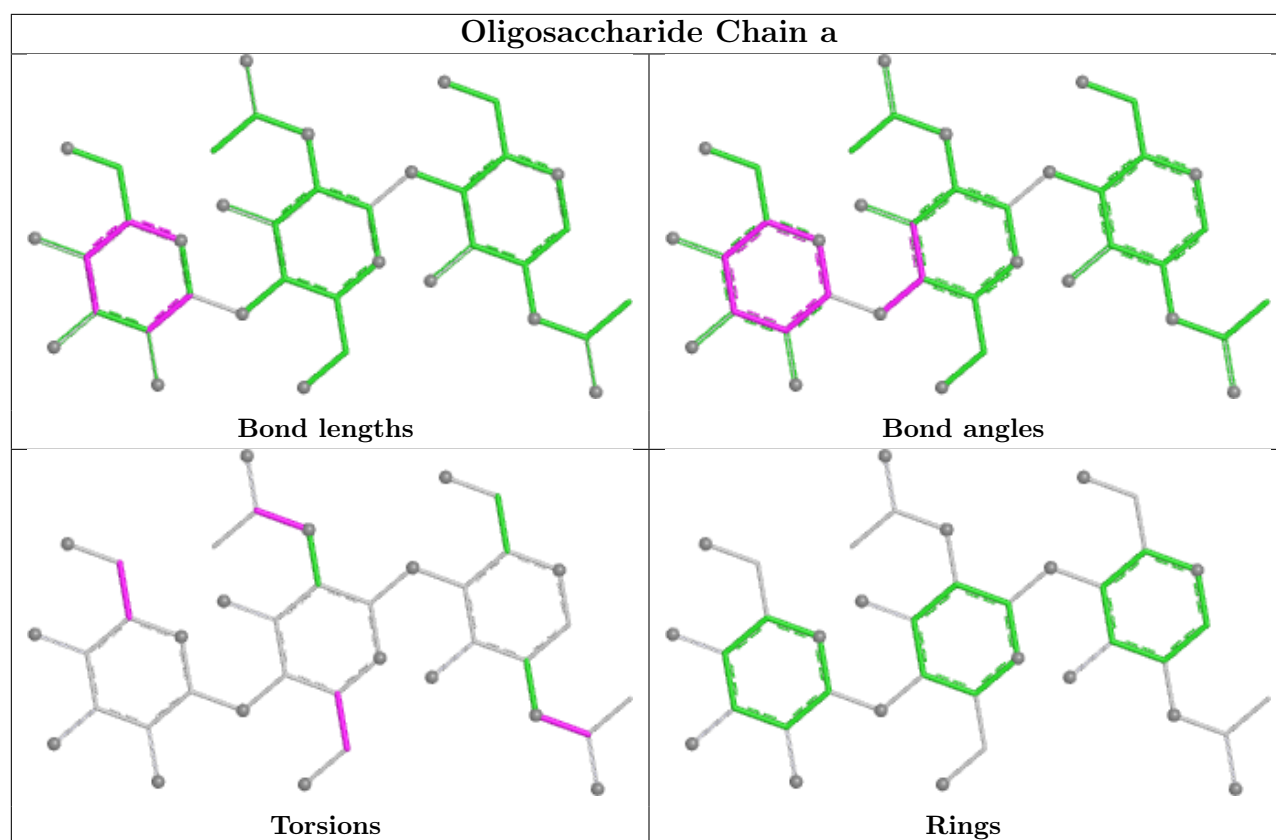
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	V	3	BMA	1	0
8	P	3	BMA	1	0
7	L	2	NAG	4	0
7	S	4	MAN	1	0
10	Y	2	NAG	1	0
10	X	2	NAG	1	0
8	P	4	MAN	1	0
9	O	1	NAG	2	0
9	b	1	NAG	1	0
7	V	2	NAG	1	0
7	L	4	MAN	1	0
7	V	5	MAN	1	0
10	X	5	MAN	1	0
7	R	5	MAN	1	0
10	X	4	MAN	1	0
6	a	1	NAG	2	0
7	R	3	BMA	1	0
7	V	1	NAG	1	0
10	X	6	MAN	1	0
8	P	1	NAG	1	0
9	O	2	NAG	1	0
7	L	3	BMA	2	0
7	T	1	NAG	1	0
10	X	3	BMA	1	0
6	a	2	NAG	1	0
7	S	1	NAG	1	0
7	L	5	MAN	1	0
7	S	3	BMA	1	0
7	T	2	NAG	1	0

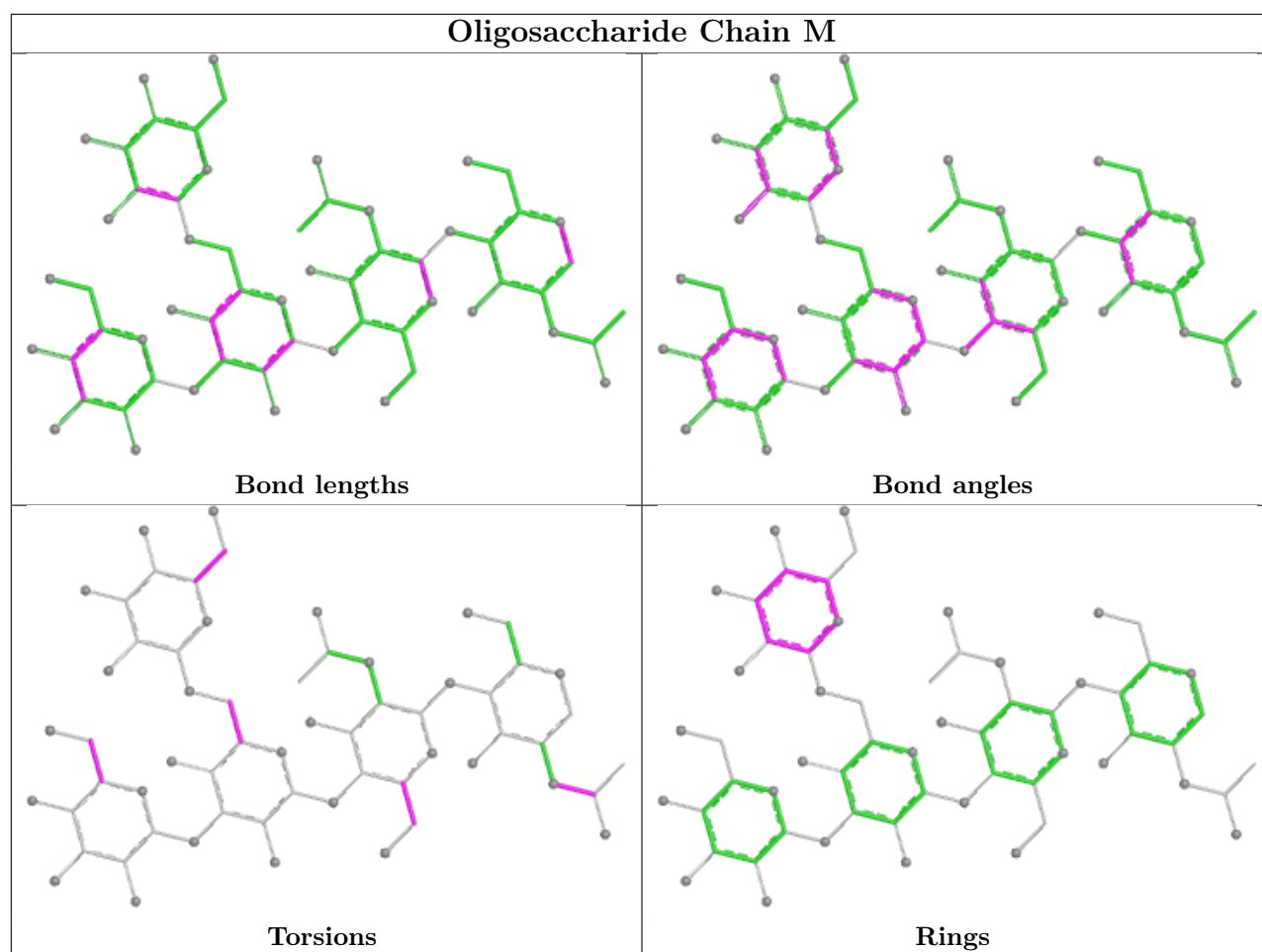
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

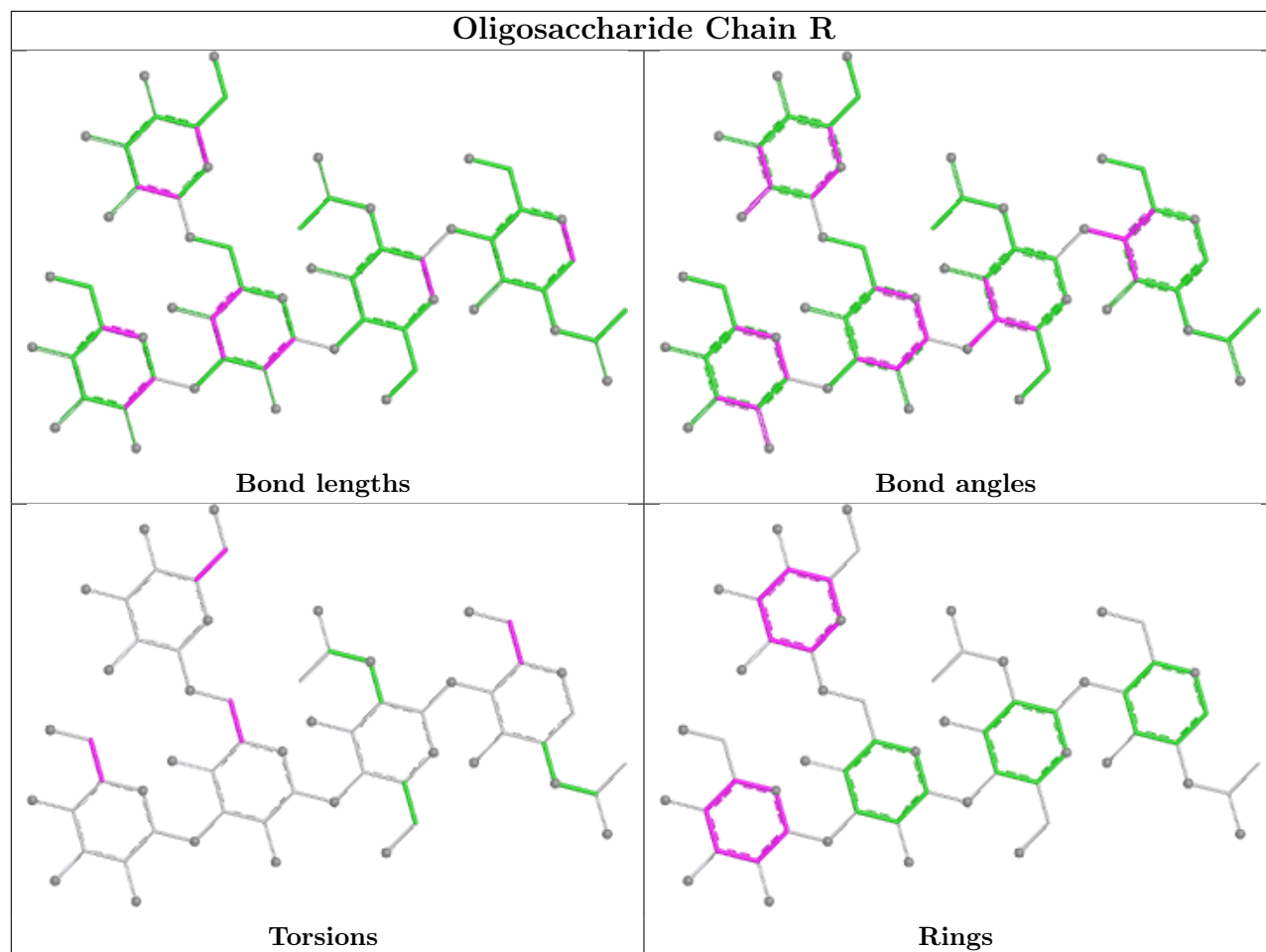


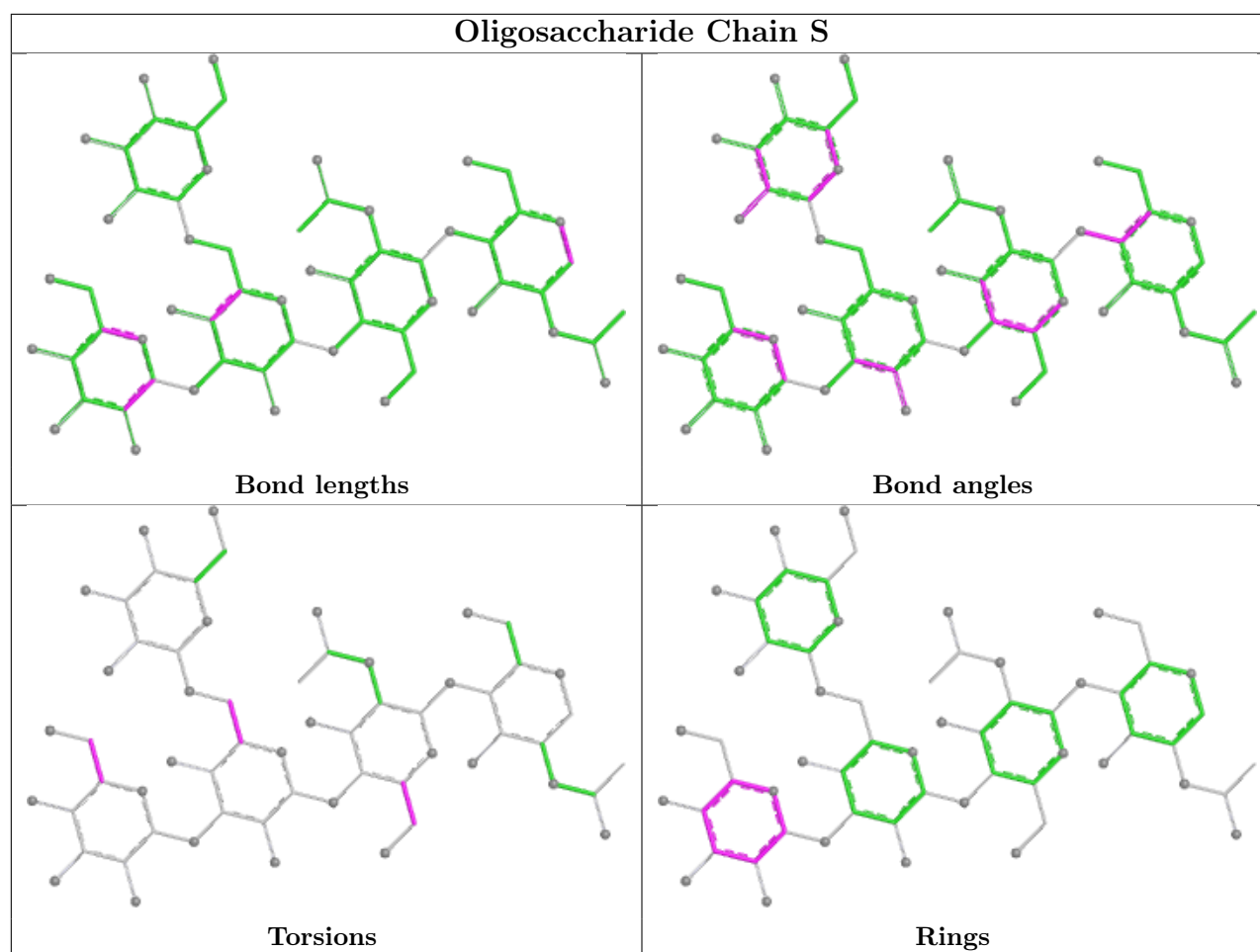


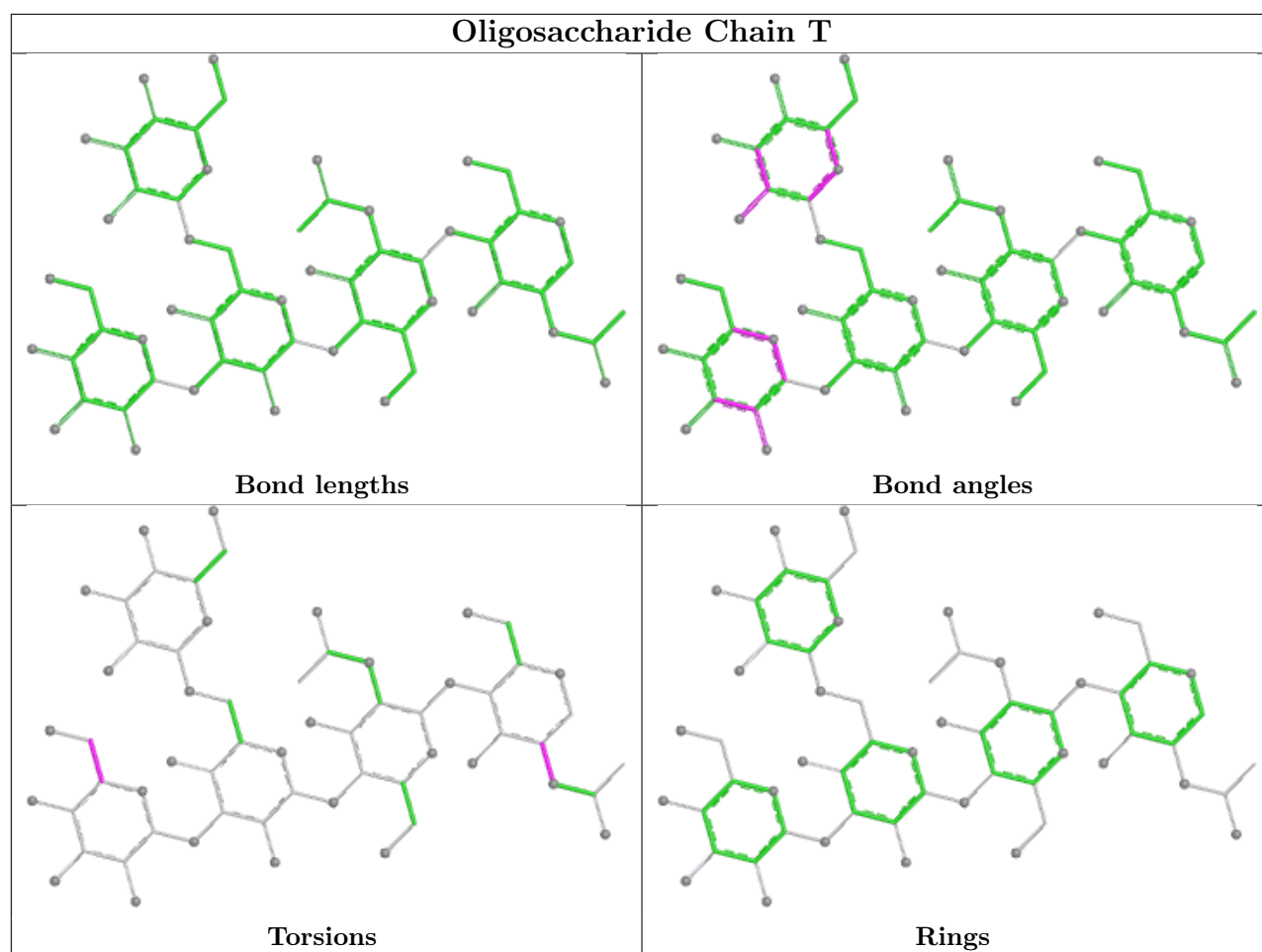


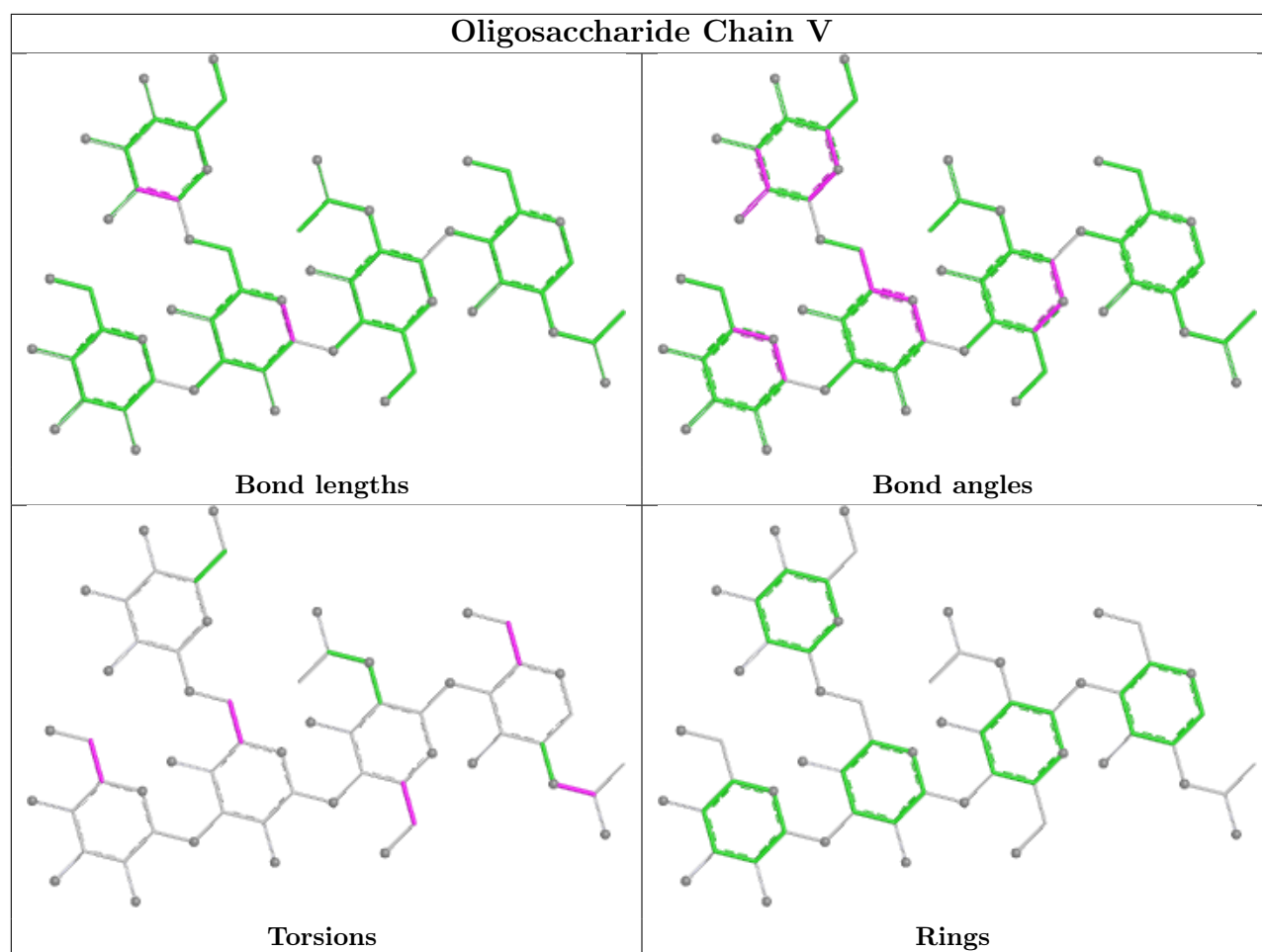


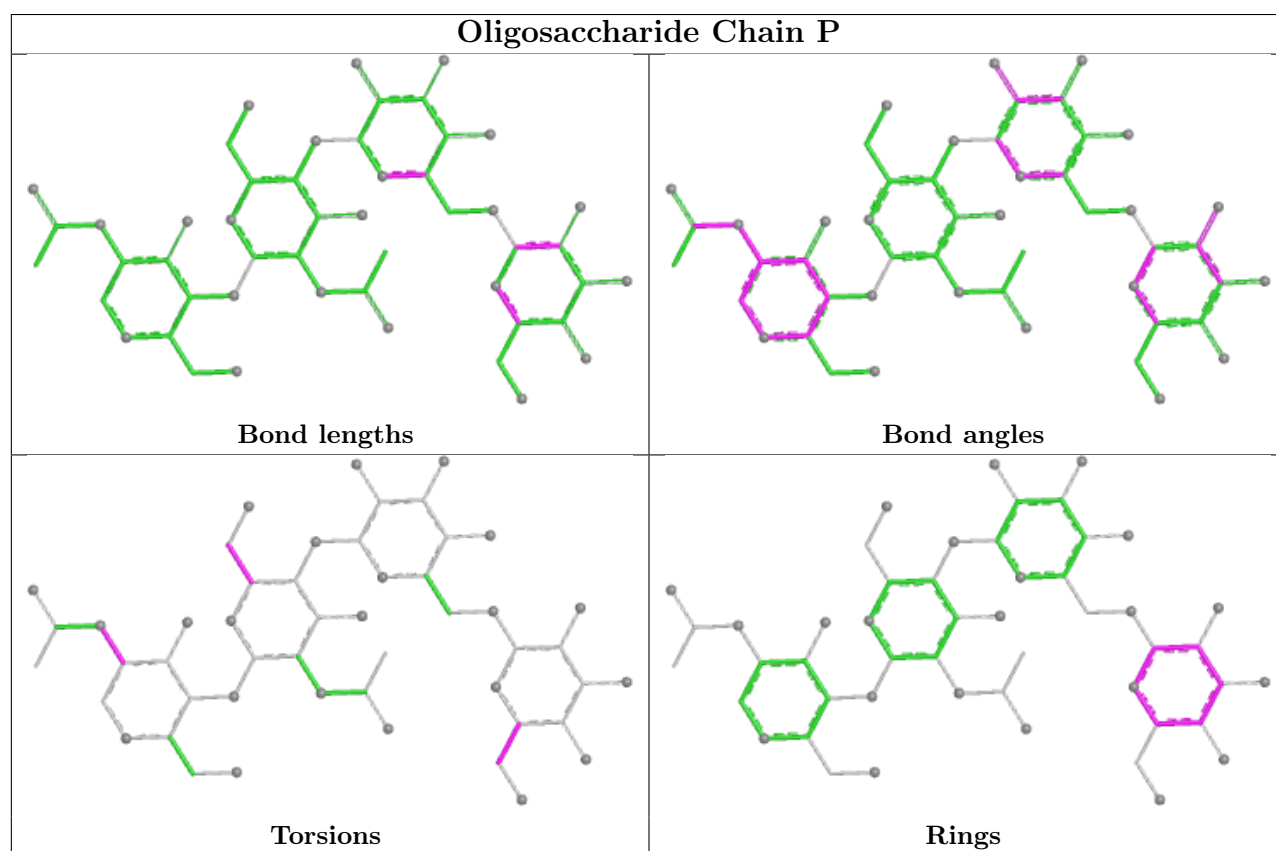
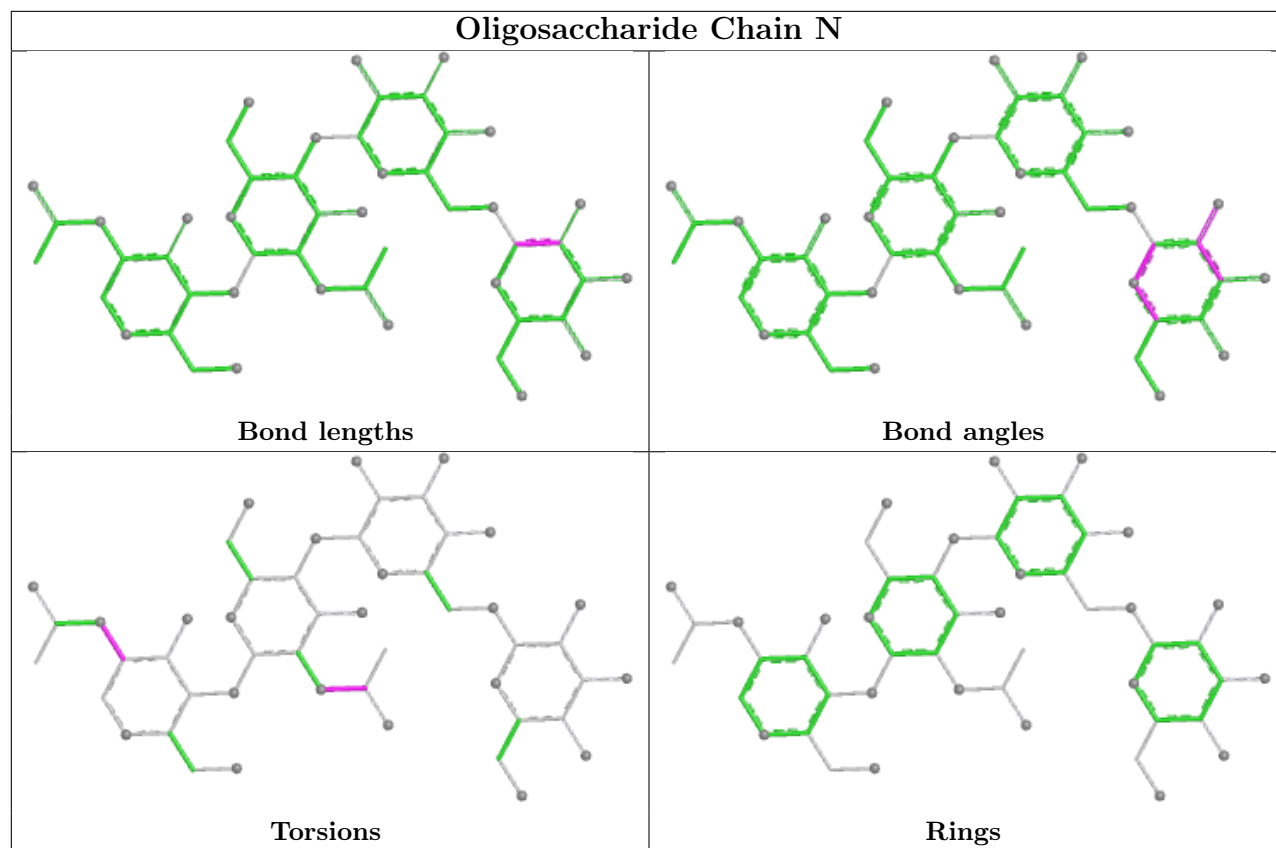


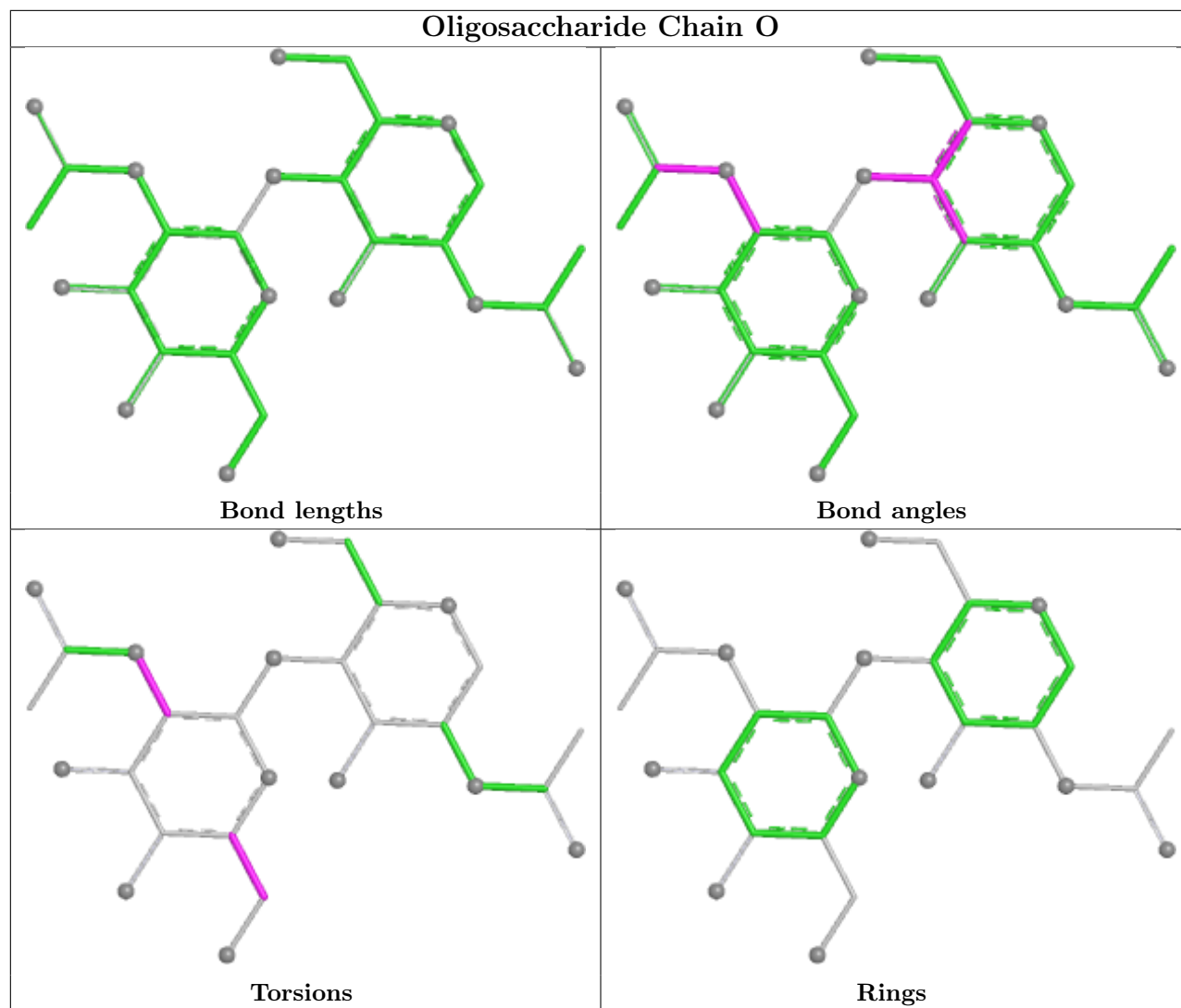


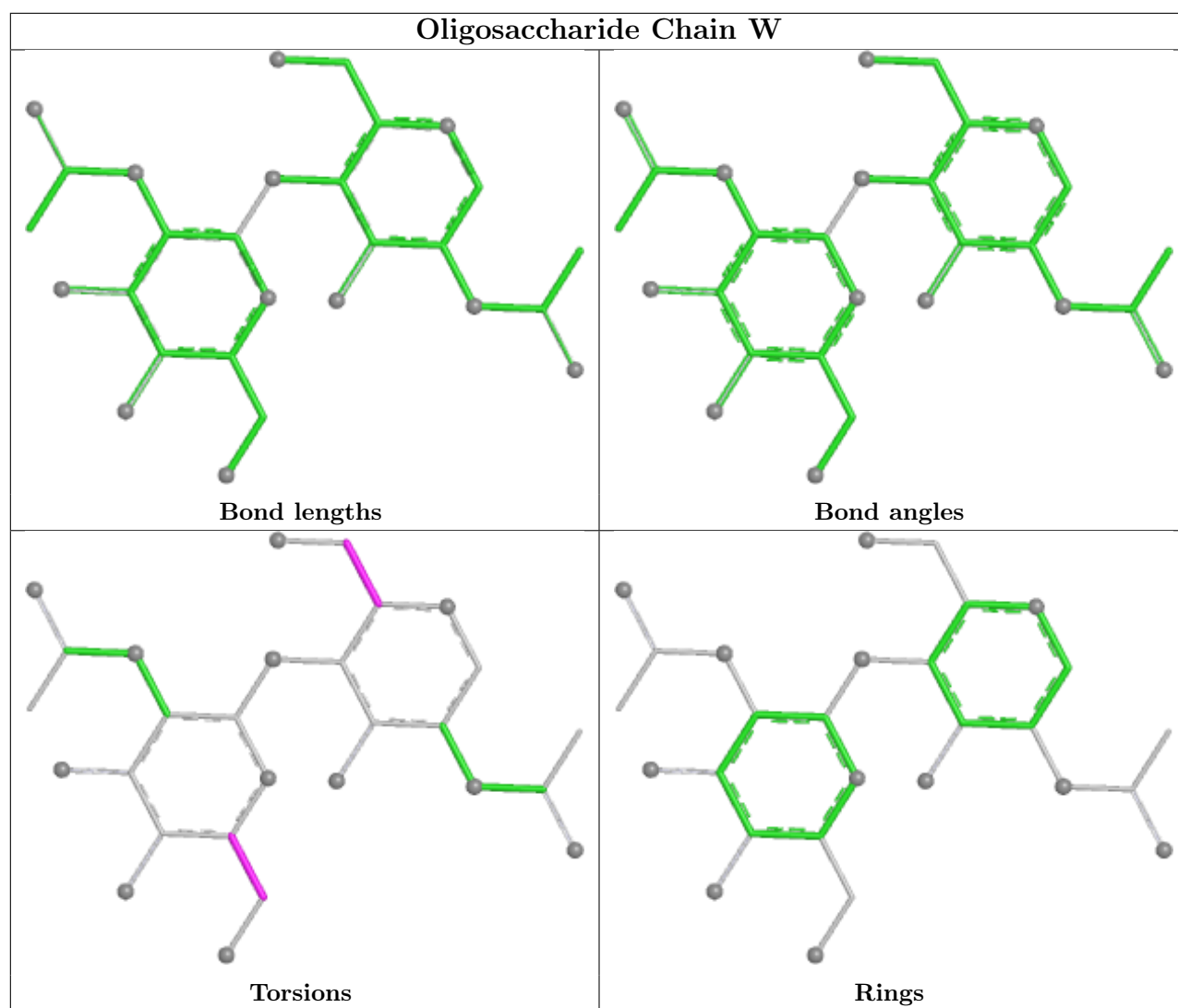


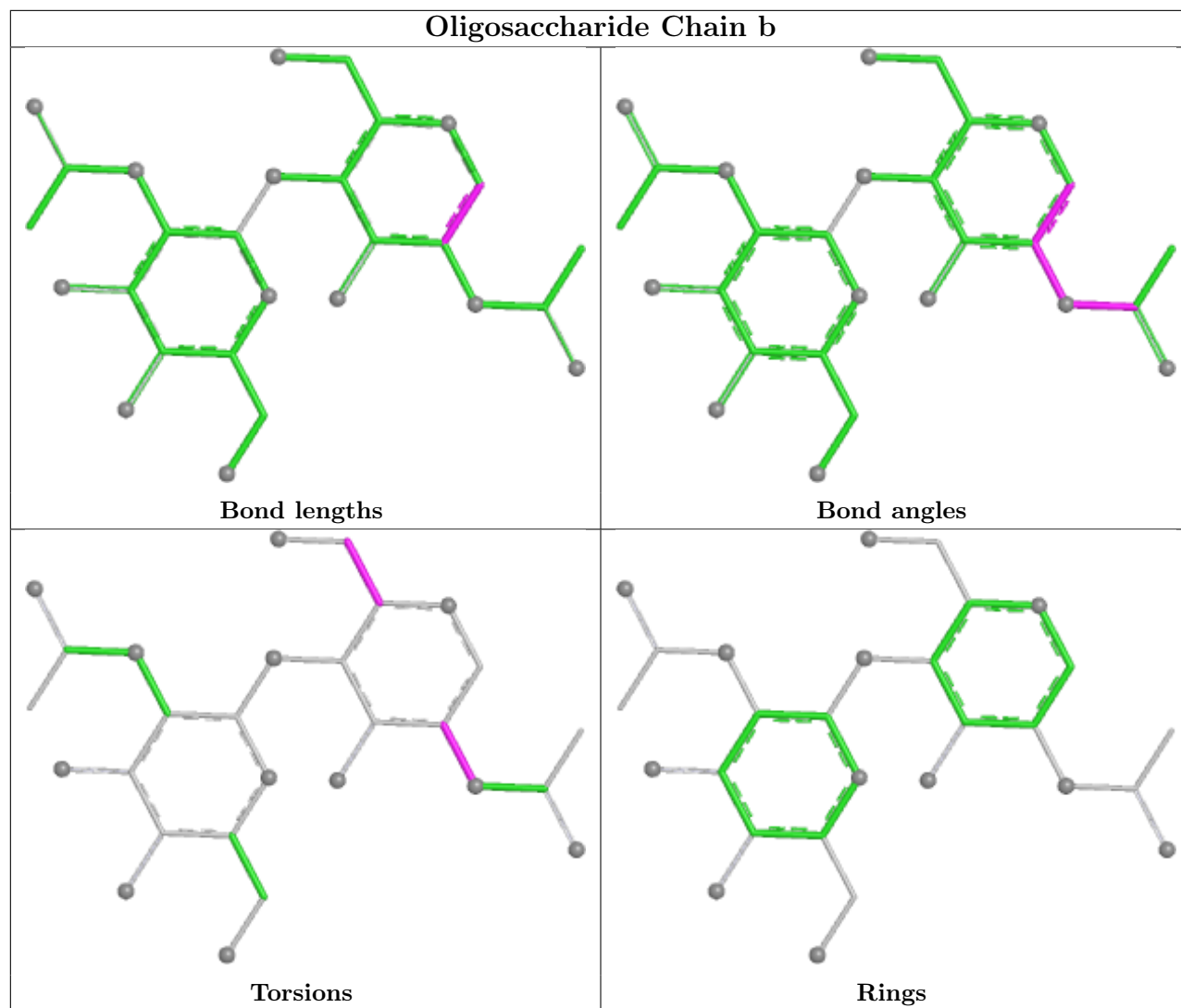


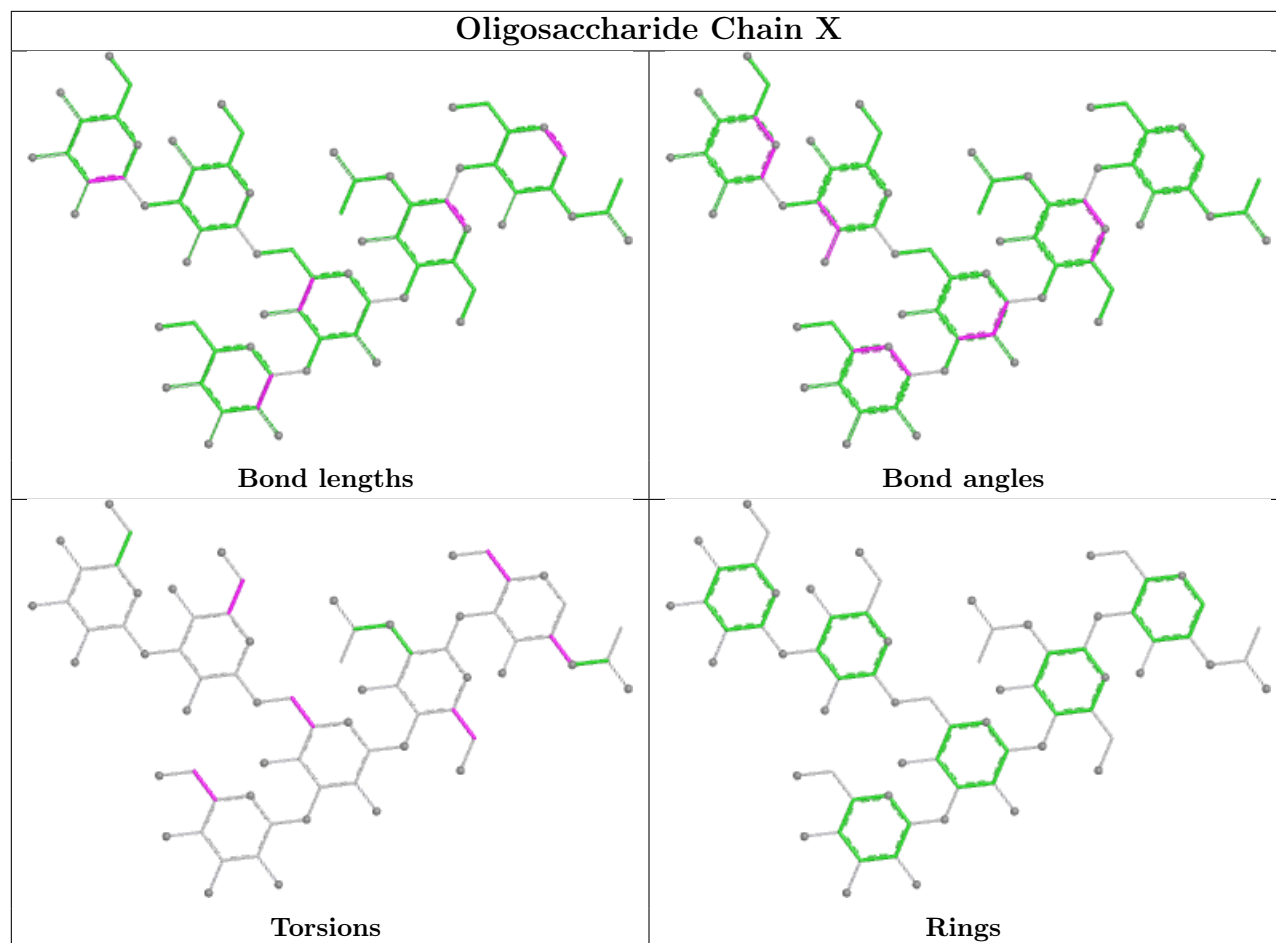


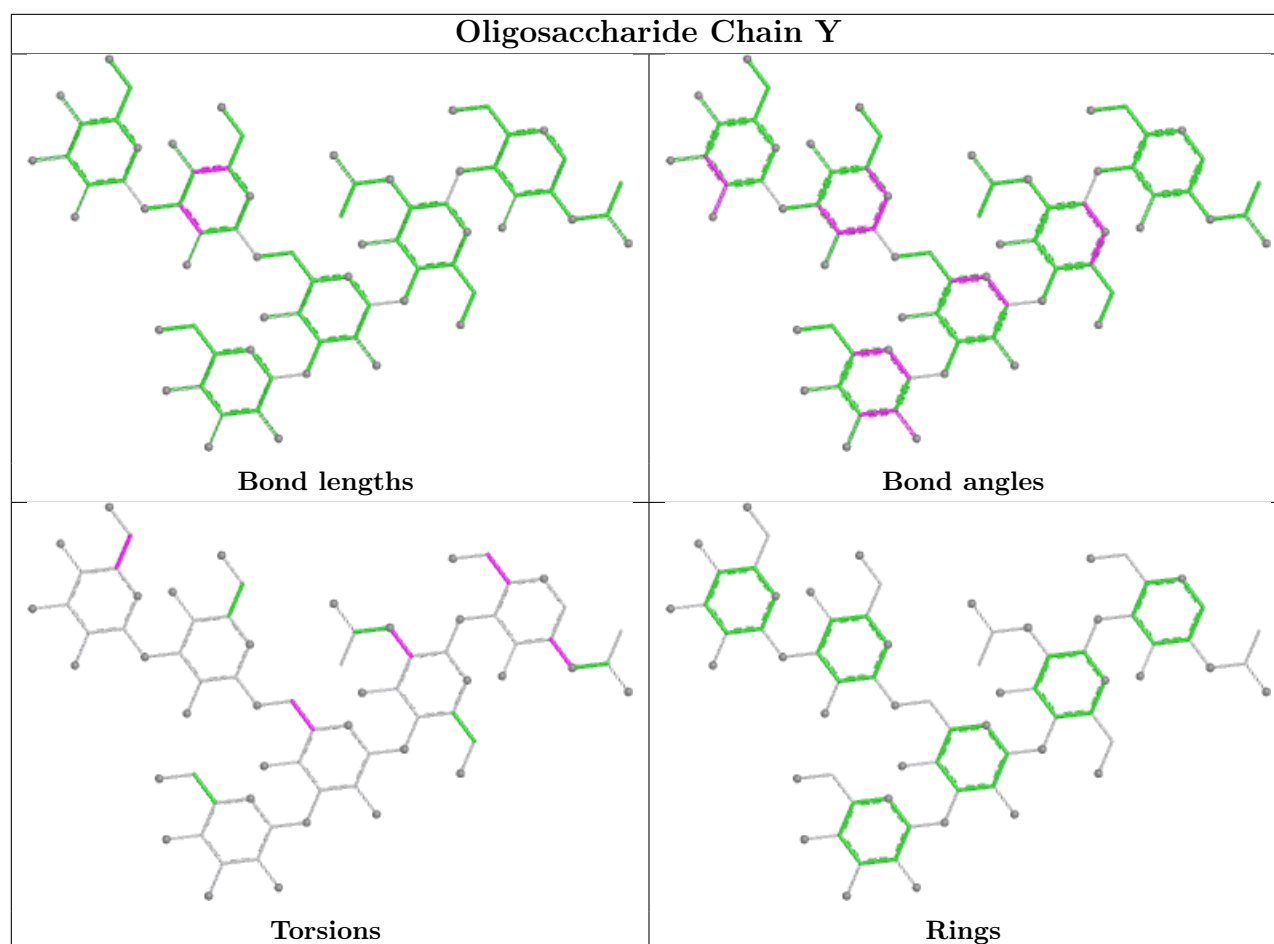












5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	NAG	A	602	2	14,14,15	0.52	0	17,19,21	0.76	1 (5%)
11	NAG	C	602	2	14,14,15	0.39	0	17,19,21	1.19	2 (11%)
11	NAG	B	601	2	14,14,15	0.38	0	17,19,21	0.48	0
11	NAG	C	601	2	14,14,15	0.28	0	17,19,21	0.44	0
11	NAG	A	601	2	14,14,15	0.47	0	17,19,21	1.34	1 (5%)
11	NAG	C	604	2	14,14,15	1.50	1 (7%)	17,19,21	1.73	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	B	602	2	14,14,15	0.49	0	17,19,21	0.42	0
11	NAG	B	603	2	14,14,15	0.91	1 (7%)	17,19,21	0.95	1 (5%)
11	NAG	C	603	2	14,14,15	0.47	0	17,19,21	0.50	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
11	NAG	A	602	2	-	2/6/23/26	0/1/1/1
11	NAG	C	602	2	-	2/6/23/26	0/1/1/1
11	NAG	B	601	2	-	0/6/23/26	0/1/1/1
11	NAG	C	601	2	-	1/6/23/26	0/1/1/1
11	NAG	A	601	2	-	1/6/23/26	0/1/1/1
11	NAG	C	604	2	-	1/6/23/26	0/1/1/1
11	NAG	B	602	2	-	3/6/23/26	0/1/1/1
11	NAG	B	603	2	-	2/6/23/26	0/1/1/1
11	NAG	C	603	2	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	604	NAG	O5-C1	5.20	1.52	1.43
11	B	603	NAG	O5-C1	-3.04	1.38	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	604	NAG	C1-O5-C5	6.62	121.05	112.19
11	A	601	NAG	C1-O5-C5	4.28	117.92	112.19
11	C	602	NAG	C2-N2-C7	3.38	127.43	122.90
11	B	603	NAG	C3-C4-C5	2.28	114.38	110.23
11	A	602	NAG	C1-O5-C5	2.27	115.23	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	602	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
11	B	602	NAG	C8-C7-N2-C2
11	B	602	NAG	O7-C7-N2-C2
11	B	603	NAG	C8-C7-N2-C2
11	B	603	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	603	NAG	1	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	D	216/216 (100%)	0.11	4 (1%) 66 49	76, 103, 131, 162	0
1	E	216/216 (100%)	0.17	1 (0%) 87 73	85, 119, 144, 199	0
1	G	216/216 (100%)	0.21	3 (1%) 73 55	83, 121, 154, 175	0
2	A	489/514 (95%)	0.28	9 (1%) 67 50	24, 106, 137, 169	3 (0%)
2	B	486/514 (94%)	0.10	5 (1%) 79 61	27, 110, 140, 154	1 (0%)
2	C	490/514 (95%)	0.25	8 (1%) 70 52	23, 112, 139, 171	4 (0%)
3	F	230/240 (95%)	0.04	1 (0%) 88 75	82, 102, 152, 192	0
3	H	239/240 (99%)	0.10	2 (0%) 82 65	79, 104, 151, 197	0
3	U	230/240 (95%)	0.03	4 (1%) 69 52	77, 100, 136, 212	0
All	All	2812/2910 (96%)	0.16	37 (1%) 75 57	23, 109, 143, 212	8 (0%)

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	52	ALA	3.5
2	C	468	LYS	3.2
1	E	71	ASP	3.1
2	A	468	LYS	3.0
2	C	501	GLN	2.9

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	I	1	14/15	-	-	126,148,165,170	0
4	NAG	I	2	14/15	-	-	164,179,190,196	0
4	BMA	I	3	11/12	-	-	187,196,202,203	0
4	MAN	I	4	11/12	-	-	149,178,192,196	0
7	BMA	L	3	11/12	0.05	0.16	155,165,173,176	0
10	MAN	Y	6	11/12	0.12	0.15	173,191,197,198	0
7	NAG	S	1	14/15	0.13	0.17	102,131,146,152	0
9	NAG	W	2	14/15	0.15	0.20	144,177,189,194	0
7	MAN	S	5	11/12	0.20	0.18	151,166,173,177	0
10	MAN	Y	5	11/12	0.22	0.15	192,201,209,214	0
10	MAN	Y	4	11/12	0.22	0.17	180,201,209,211	0
7	MAN	M	5	11/12	0.24	0.17	152,181,188,196	0
5	MAN	J	5	11/12	-	-	162,171,182,186	0
5	MAN	J	6	11/12	-	-	111,143,149,157	0
5	MAN	J	7	11/12	-	-	139,160,169,169	0
7	MAN	V	4	11/12	0.24	0.17	120,145,157,159	0
9	NAG	W	1	14/15	0.25	0.19	139,157,179,188	0
7	BMA	M	3	11/12	0.29	0.14	177,182,189,191	0
5	MAN	J	4	11/12	0.29	0.15	142,155,168,175	0
7	NAG	S	2	14/15	0.36	0.18	134,152,159,162	0
4	BMA	Q	3	11/12	0.36	0.15	168,174,185,194	0
6	NAG	a	1	14/15	-	-	157,183,203,206	0
6	NAG	a	2	14/15	-	-	199,204,209,214	0
6	BMA	a	3	11/12	-	-	154,195,205,206	0
4	MAN	Q	4	11/12	0.41	0.16	170,187,192,192	0
7	MAN	S	4	11/12	0.41	0.17	143,180,186,188	0
7	MAN	M	4	11/12	0.41	0.12	162,186,190,192	0
7	MAN	L	4	11/12	-	-	164,174,181,182	0
7	MAN	L	5	11/12	-	-	138,165,171,171	0
5	BMA	J	3	11/12	0.42	0.12	146,151,155,157	0
10	MAN	X	4	11/12	0.43	0.13	166,179,187,189	0
7	MAN	T	4	11/12	0.47	0.18	218,230,236,238	0
7	MAN	R	4	11/12	0.47	0.11	137,161,177,181	0
7	BMA	T	3	11/12	0.48	0.13	211,219,226,228	0
7	MAN	V	5	11/12	0.49	0.15	144,164,175,182	0
6	BMA	Z	3	11/12	0.52	0.11	156,168,174,177	0
8	MAN	N	4	11/12	0.52	0.12	171,191,195,195	0
10	MAN	X	6	11/12	0.54	0.13	166,177,181,182	0
7	MAN	R	5	11/12	-	-	172,186,199,202	0
7	BMA	R	3	11/12	0.55	0.11	157,179,198,200	0
10	BMA	X	3	11/12	0.56	0.12	171,176,181,183	0

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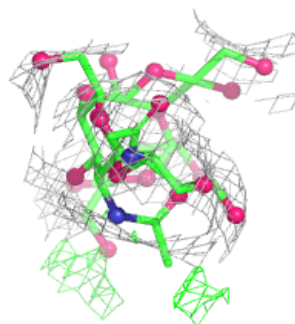
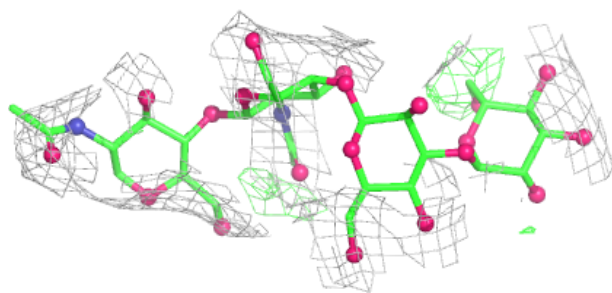
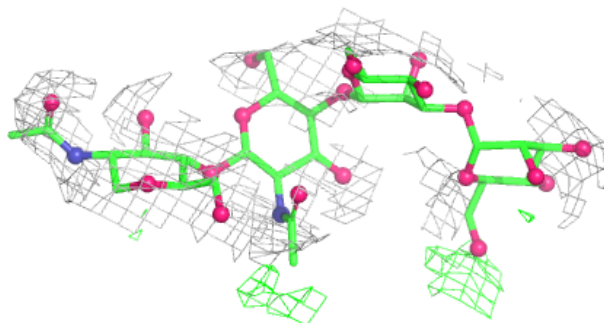
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	P	1	14/15	0.57	0.15	108,133,141,142	0
10	MAN	X	5	11/12	0.57	0.17	143,174,183,184	0
8	NAG	P	2	14/15	0.59	0.13	124,140,155,170	0
7	MAN	T	5	11/12	0.61	0.12	168,200,210,212	0
7	NAG	L	2	14/15	0.67	0.15	140,150,173,178	0
8	BMA	N	3	11/12	0.67	0.10	168,178,187,187	0
7	BMA	V	3	11/12	0.70	0.11	147,158,163,167	0
7	NAG	T	2	14/15	0.70	0.17	170,186,201,211	0
9	NAG	O	2	14/15	0.71	0.14	154,182,192,194	0
7	BMA	S	3	11/12	0.72	0.13	169,181,185,187	0
7	NAG	R	2	14/15	0.72	0.12	183,198,202,202	0
6	NAG	K	1	14/15	0.73	0.16	120,137,160,171	0
4	NAG	Q	1	14/15	0.73	0.24	110,114,122,135	0
7	NAG	V	1	14/15	0.74	0.17	125,143,159,160	0
4	NAG	Q	2	14/15	0.74	0.19	135,154,166,169	0
10	NAG	X	2	14/15	0.75	0.13	119,160,176,177	0
7	NAG	V	2	14/15	0.75	0.18	138,152,160,172	0
5	NAG	J	2	14/15	0.76	0.11	147,156,160,163	0
7	NAG	L	1	14/15	0.76	0.20	107,121,132,149	0
8	BMA	P	3	11/12	-	-	166,176,184,193	0
8	MAN	P	4	11/12	-	-	150,180,191,193	0
10	BMA	Y	3	11/12	0.76	0.08	174,182,191,194	0
7	NAG	T	1	14/15	0.77	0.21	122,162,176,180	0
9	NAG	O	1	14/15	0.80	0.13	149,172,182,192	0
5	NAG	J	1	14/15	0.81	0.14	132,140,158,161	0
9	NAG	b	1	14/15	-	-	177,191,209,214	0
9	NAG	b	2	14/15	-	-	199,213,218,219	0
7	NAG	M	1	14/15	0.81	0.20	131,147,165,179	0
6	NAG	K	2	14/15	0.81	0.12	111,155,163,167	0
6	NAG	Z	2	14/15	0.81	0.09	127,136,155,162	0
8	NAG	N	1	14/15	0.82	0.20	102,117,133,143	0
7	NAG	M	2	14/15	0.82	0.21	152,181,195,200	0
10	NAG	X	1	14/15	0.83	0.15	105,131,155,168	0
8	NAG	N	2	14/15	0.88	0.14	149,164,177,177	0
10	NAG	Y	2	14/15	0.88	0.10	146,158,169,175	0
7	NAG	R	1	14/15	0.89	0.10	161,181,187,194	0
6	NAG	Z	1	14/15	0.90	0.09	93,113,125,132	0
10	NAG	Y	1	14/15	0.93	0.12	114,125,140,159	0
6	BMA	K	3	11/12	0.95	0.07	131,154,164,170	0

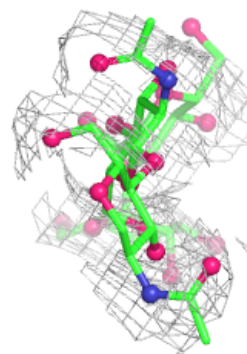
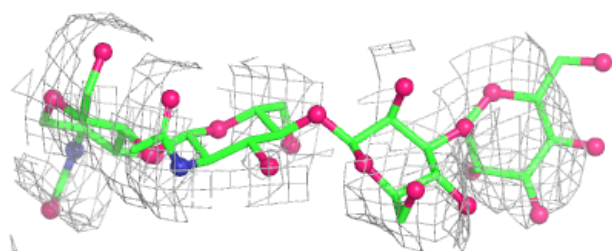
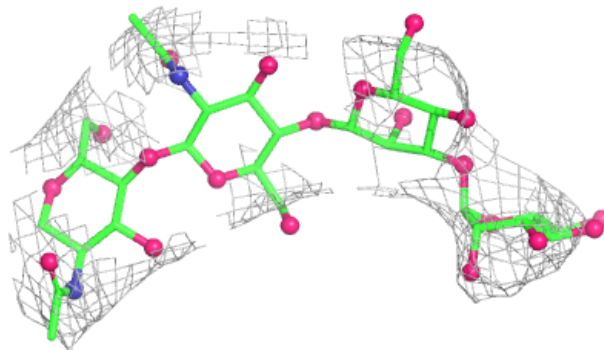
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

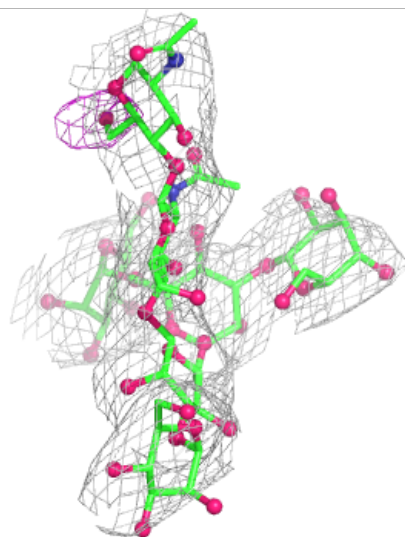
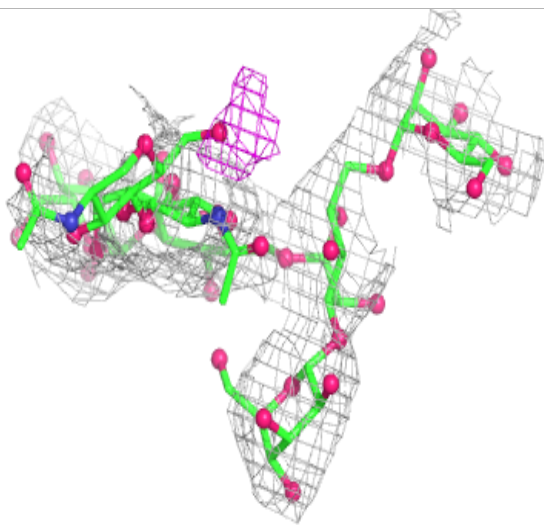
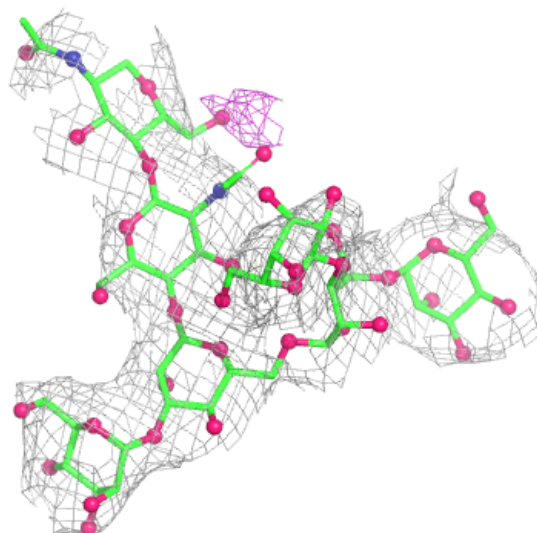
**Electron density around Chain Q:**

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



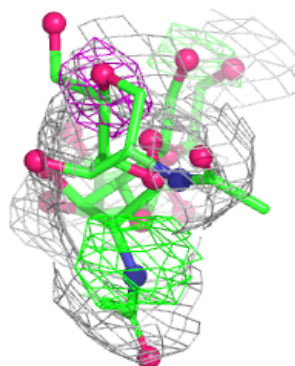
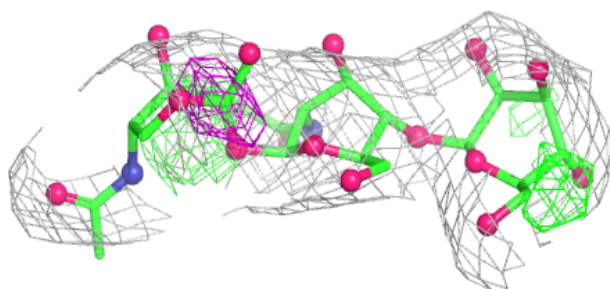
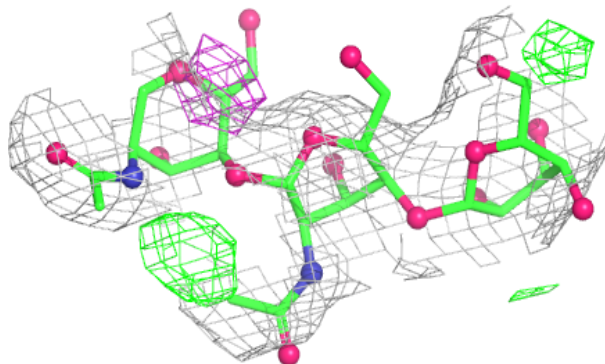
Electron density around Chain J:

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

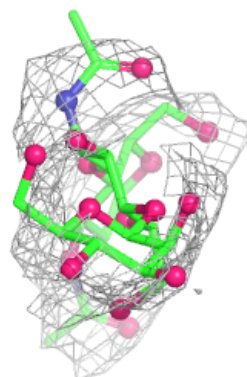
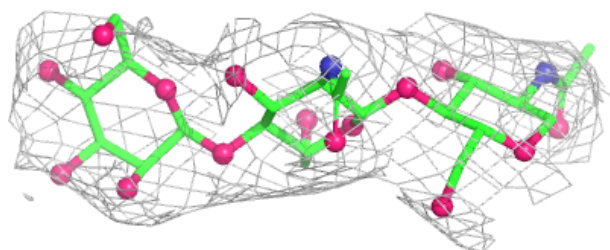
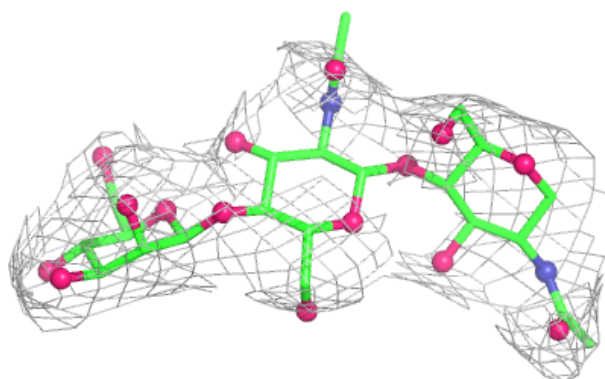


Electron density around Chain K:

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

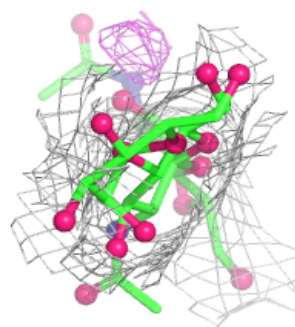
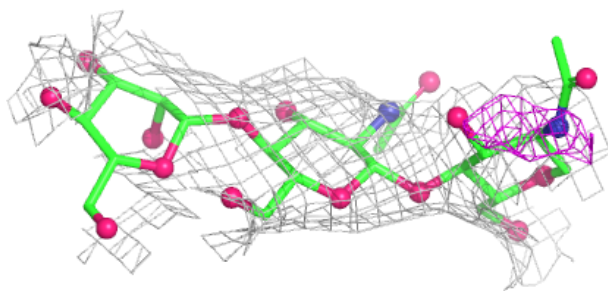
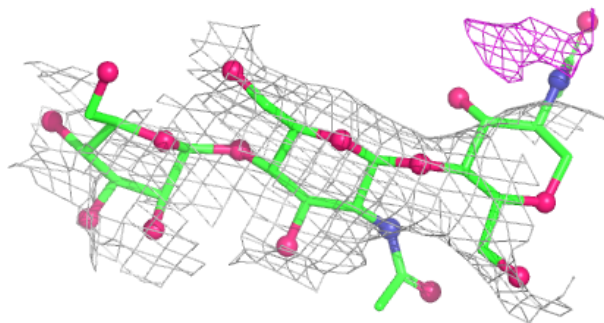
**Electron density around Chain Z:**

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

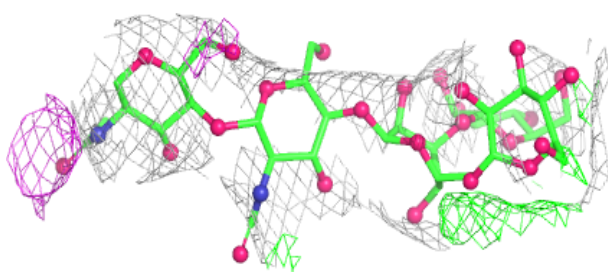
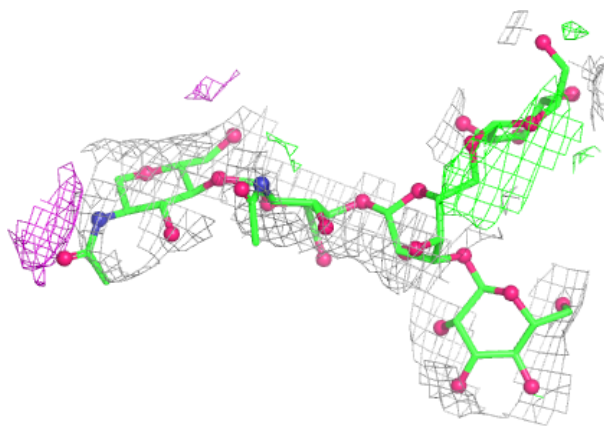


Electron density around Chain a:

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

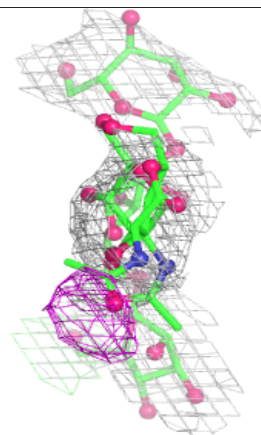
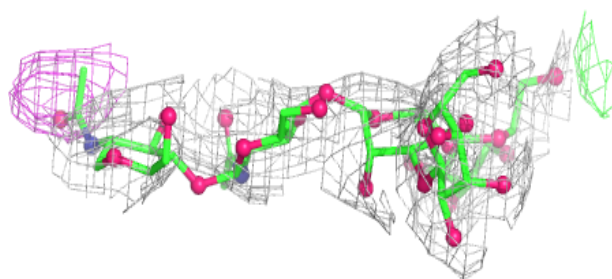
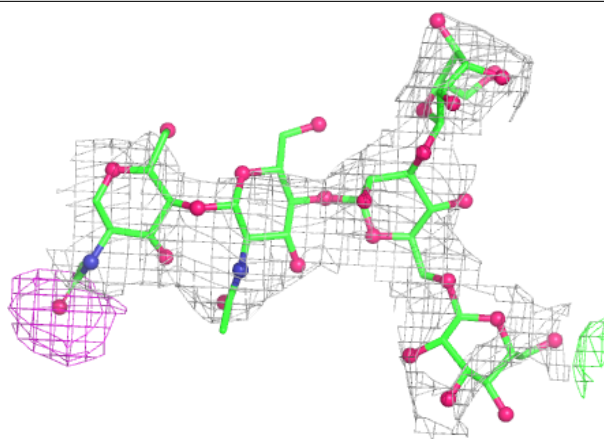
**Electron density around Chain L:**

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



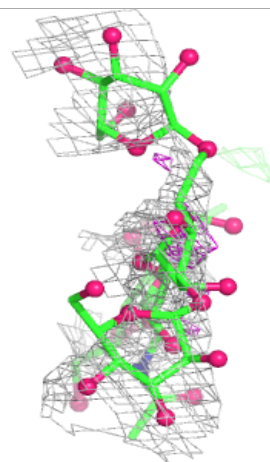
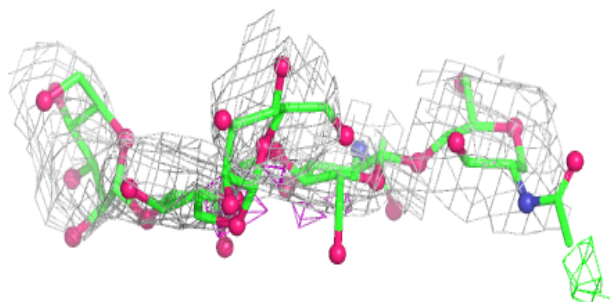
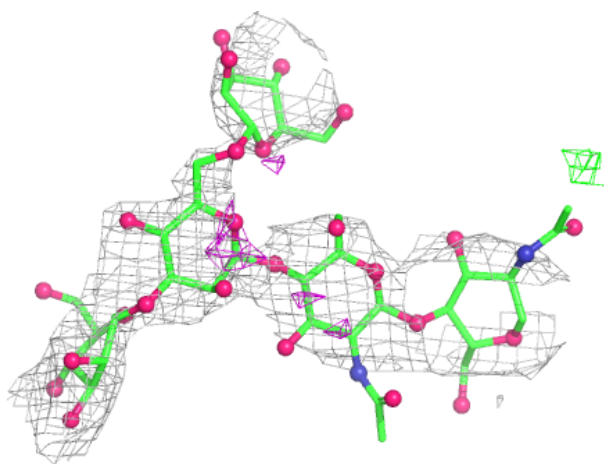
Electron density around Chain M:

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



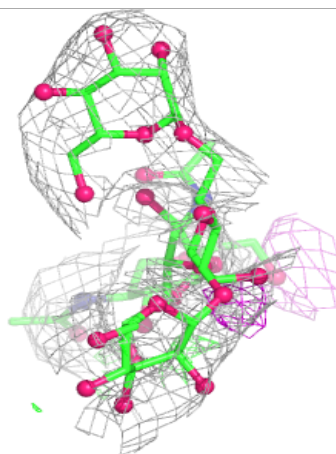
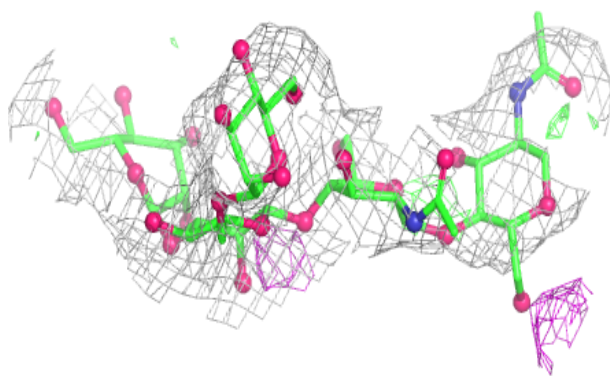
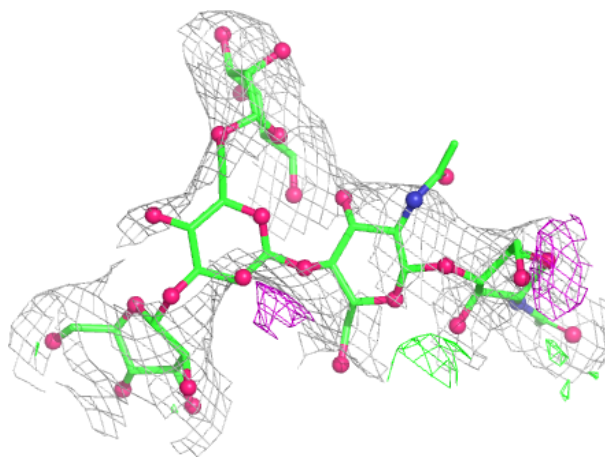
Electron density around Chain R:

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



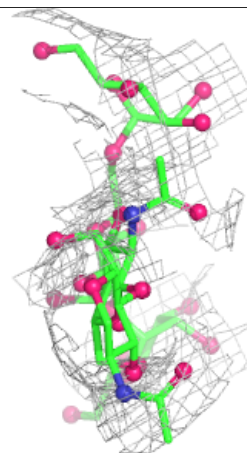
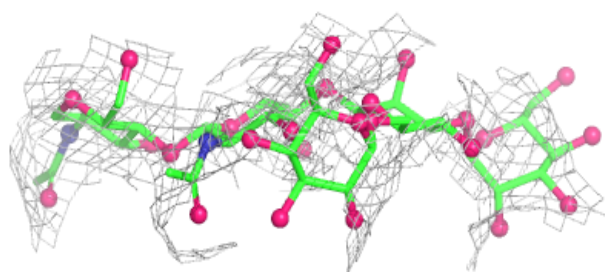
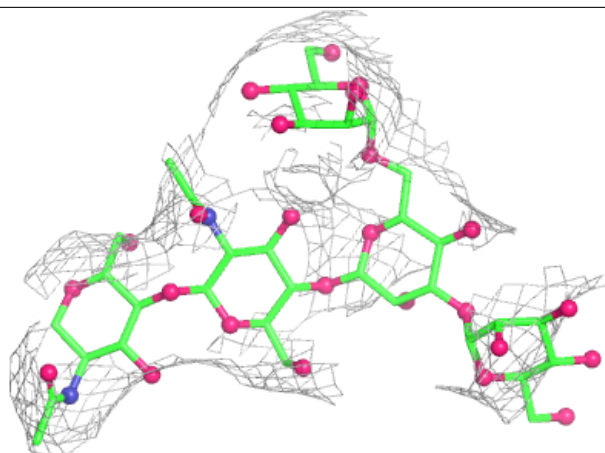
Electron density around Chain S:

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

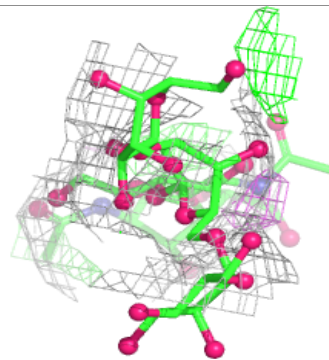
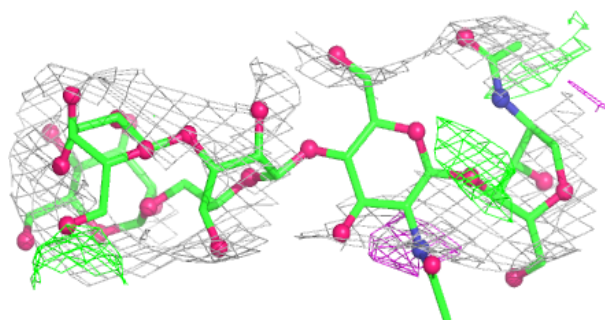
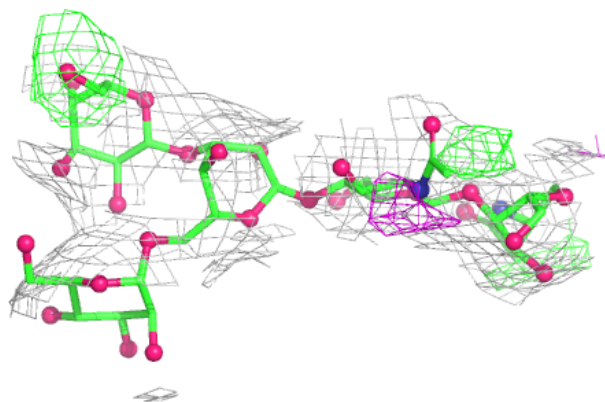


Electron density around Chain T:

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

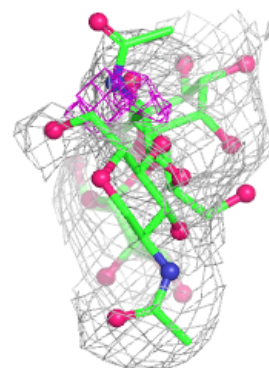
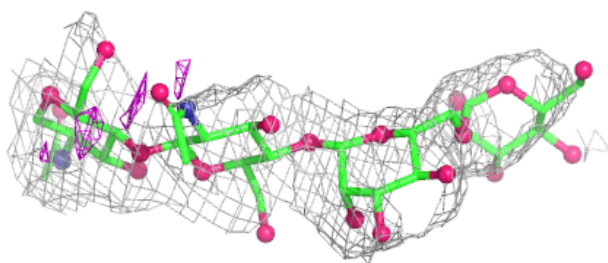
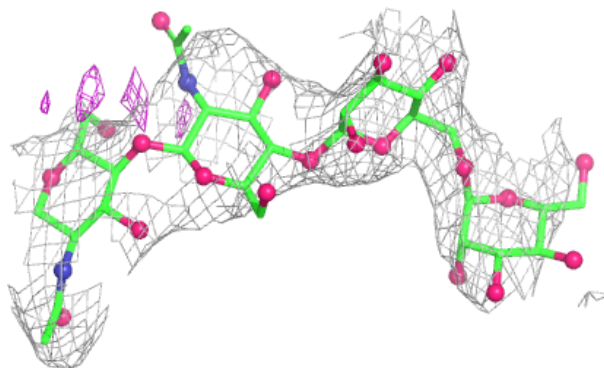
**Electron density around Chain V:**

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

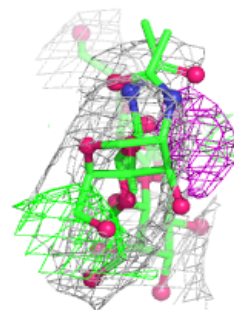
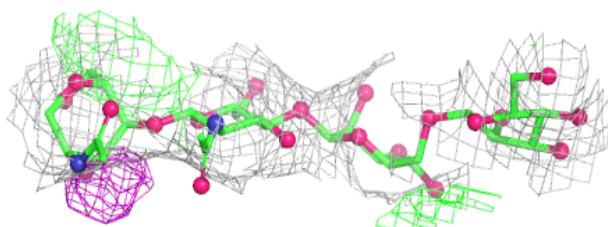
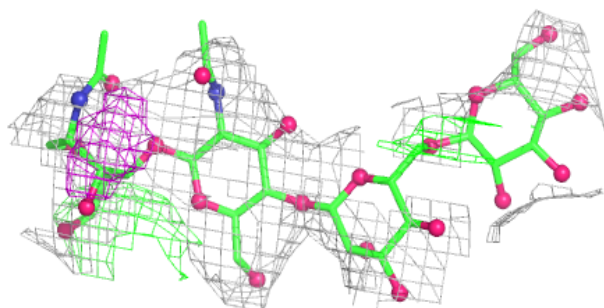


Electron density around Chain N:

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

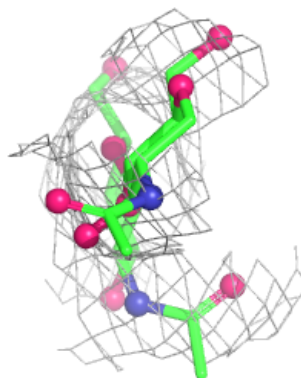
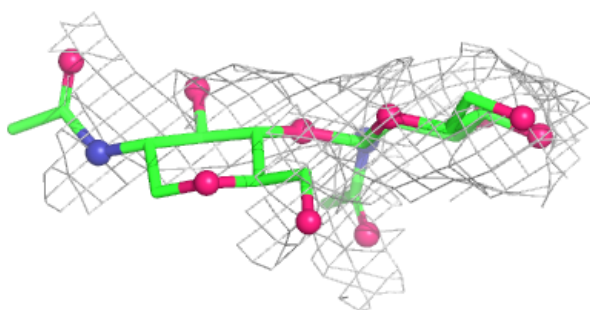
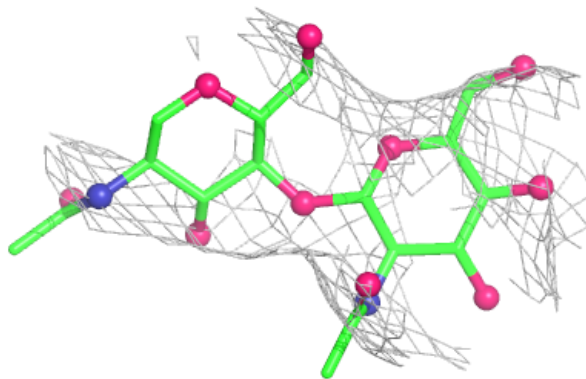
**Electron density around Chain P:**

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



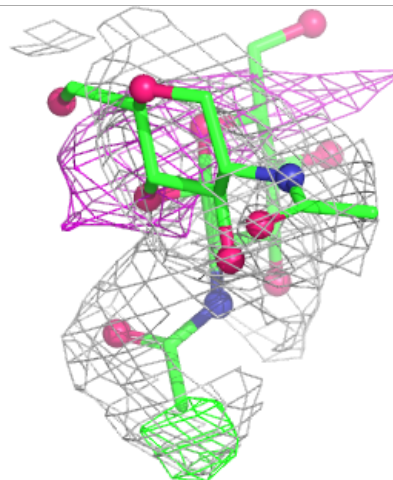
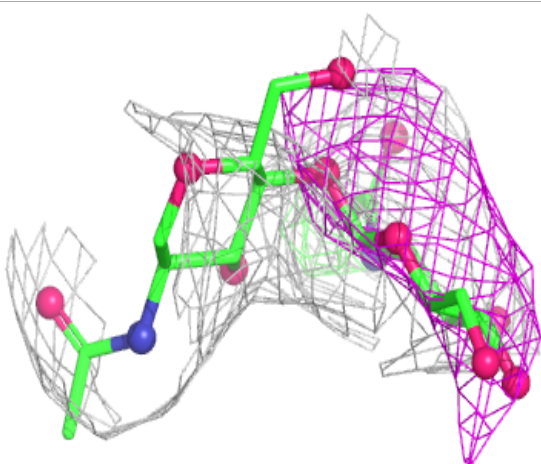
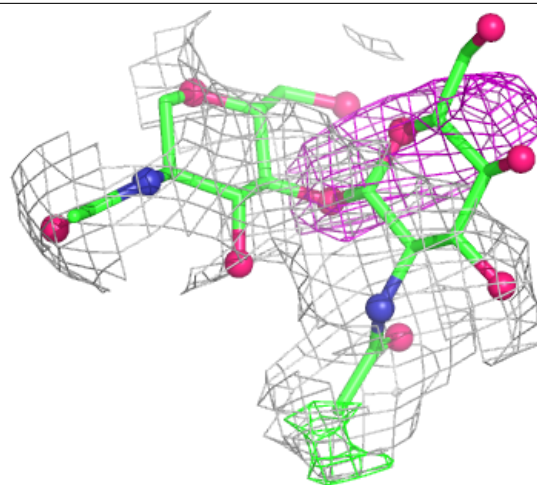
Electron density around Chain O:

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



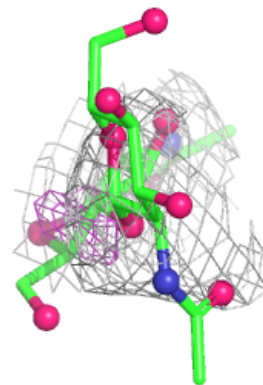
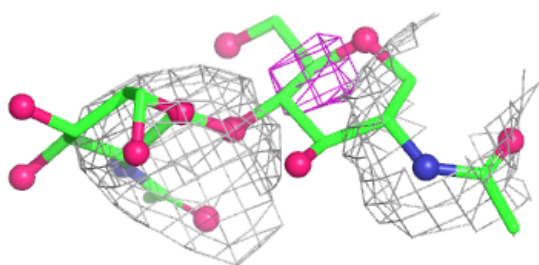
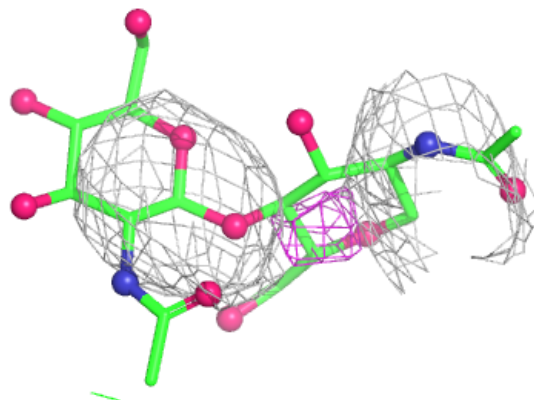
Electron density around Chain W:

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



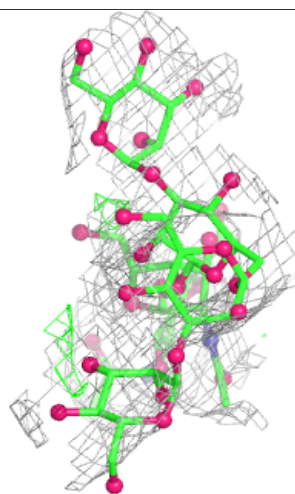
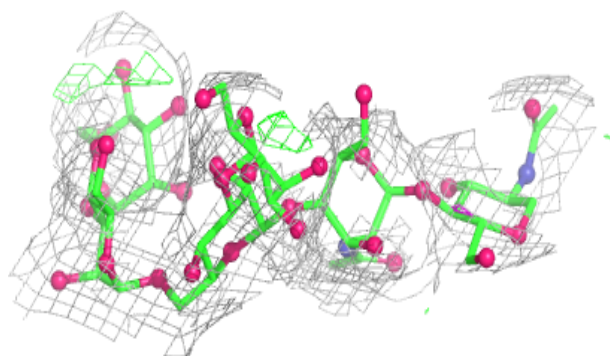
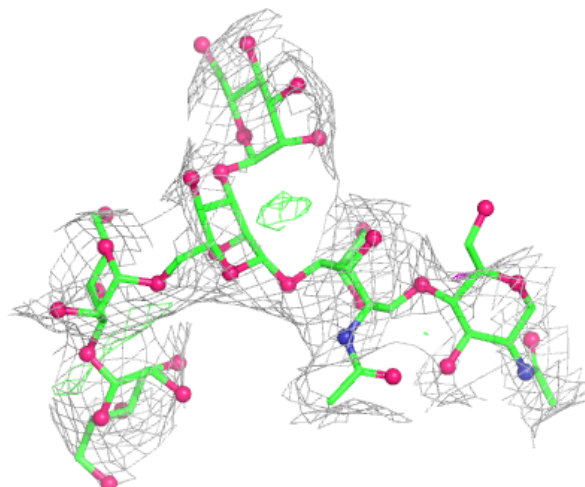
Electron density around Chain b:

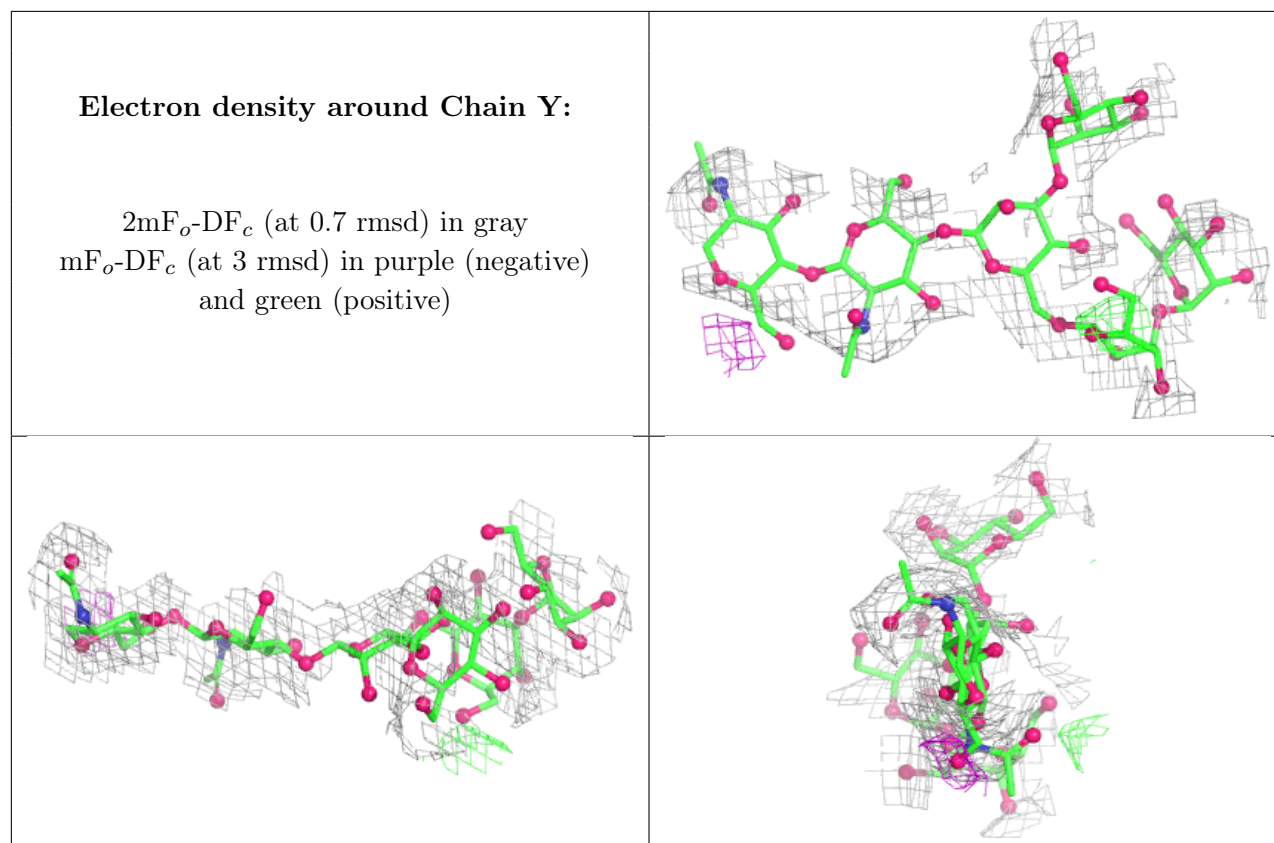
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain X:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	NAG	B	603	14/15	0.29	0.22	139,166,172,175	0
11	NAG	C	604	14/15	0.48	0.17	156,164,179,180	0
11	NAG	A	602	14/15	0.52	0.15	136,165,171,175	0
11	NAG	B	602	14/15	0.53	0.15	127,137,144,149	0
11	NAG	B	601	14/15	0.56	0.15	147,156,165,168	0
11	NAG	C	601	14/15	0.62	0.15	135,153,166,176	0
11	NAG	A	601	14/15	0.63	0.14	122,147,157,165	0
11	NAG	C	602	14/15	0.67	0.22	134,147,165,173	0
11	NAG	C	603	14/15	0.69	0.14	124,149,158,160	0

6.5 Other polymers [i](#)

There are no such residues in this entry.