



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

PDB ID : 7EY2 / pdb_00007ey2
Title : Bifunctional xylosidase/glucosidase LXYL D300N mutant with intermediate substrate xylose
Authors : Gong, W.M.; Yang, L.Y.
Deposited on : 2021-05-29
Resolution : 2.43 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
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

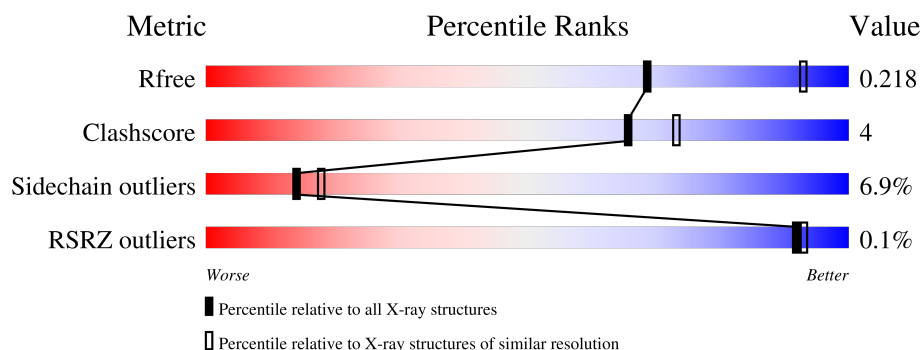
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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

Mol	Chain	Length	Quality of chain
1	A	805	 83% 9% • 6%
1	B	805	 84% 9% • 6%
1	C	805	 82% 10% • 6%
1	D	805	 82% 10% • 6%
1	E	805	 82% 10% • 6%
1	F	805	 83% 9% • 6%

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Mol	Chain	Length	Quality of chain
2	G	3	100%
2	J	3	33% 67%
2	M	3	33% 67%
2	P	3	33% 67%
2	S	3	33% 67%
2	V	3	33% 67%
3	H	7	71% 29%
3	N	7	71% 29%
3	T	7	71% 29%
3	W	7	71% 29%
4	I	5	100%
4	R	5	100%
5	K	8	50% 50%
6	L	6	100%
6	O	6	100%
6	U	6	100%
6	X	6	100%
7	Q	6	83% 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	XYL	C	907	-	X	-	-
11	XYL	D	907	-	X	-	-
5	MAN	K	6	-	-	X	-
5	MAN	K	8	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 37142 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-D-xylosidase/beta-D-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	0	1	0
			5724	3624	958	1125	17			
1	B	758	Total	C	N	O	S	0	1	0
			5736	3632	963	1124	17			
1	C	756	Total	C	N	O	S	0	1	0
			5712	3618	956	1121	17			
1	D	756	Total	C	N	O	S	0	1	0
			5712	3618	956	1121	17			
1	E	757	Total	C	N	O	S	0	1	0
			5726	3626	960	1123	17			
1	F	757	Total	C	N	O	S	0	1	0
			5726	3626	960	1123	17			

There are 18 discrepancies between the modelled and reference sequences:

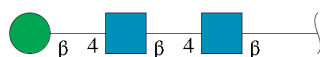
Chain	Residue	Modelled	Actual	Comment	Reference
A	300	ASN	ASP	engineered mutation	UNP G8GLP2
A	804	HIS	-	expression tag	UNP G8GLP2
A	805	HIS	-	expression tag	UNP G8GLP2
B	300	ASN	ASP	engineered mutation	UNP G8GLP2
B	804	HIS	-	expression tag	UNP G8GLP2
B	805	HIS	-	expression tag	UNP G8GLP2
C	300	ASN	ASP	engineered mutation	UNP G8GLP2
C	804	HIS	-	expression tag	UNP G8GLP2
C	805	HIS	-	expression tag	UNP G8GLP2
D	300	ASN	ASP	engineered mutation	UNP G8GLP2
D	804	HIS	-	expression tag	UNP G8GLP2
D	805	HIS	-	expression tag	UNP G8GLP2
E	300	ASN	ASP	engineered mutation	UNP G8GLP2
E	804	HIS	-	expression tag	UNP G8GLP2
E	805	HIS	-	expression tag	UNP G8GLP2
F	300	ASN	ASP	engineered mutation	UNP G8GLP2
F	804	HIS	-	expression tag	UNP G8GLP2

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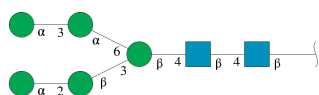
Chain	Residue	Modelled	Actual	Comment	Reference
F	805	HIS	-	expression tag	UNP G8GLP2

- Molecule 2 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.



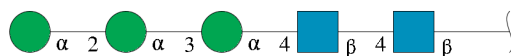
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	S	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	V	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



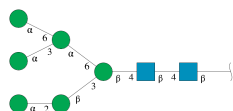
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	7	Total	C	N	O	0	0	0
			83	46	2	35			
3	N	7	Total	C	N	O	0	0	0
			83	46	2	35			
3	T	7	Total	C	N	O	0	0	0
			83	46	2	35			
3	W	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 4 is an oligosaccharide called 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.



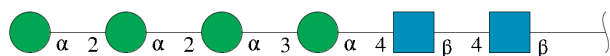
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



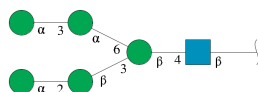
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	K	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



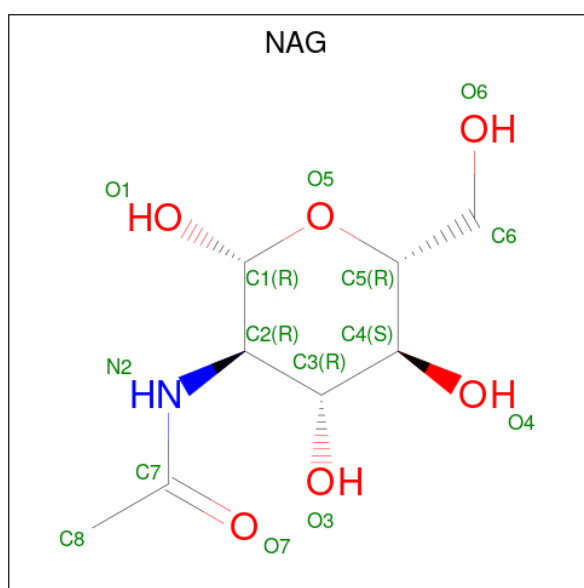
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	6	Total	C	N	O	0	0	0
			72	40	2	30			
6	O	6	Total	C	N	O	0	0	0
			72	40	2	30			
6	U	6	Total	C	N	O	0	0	0
			72	40	2	30			
6	X	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	Q	6	Total	C	N	O	0	0	0
			70	38	1	31			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



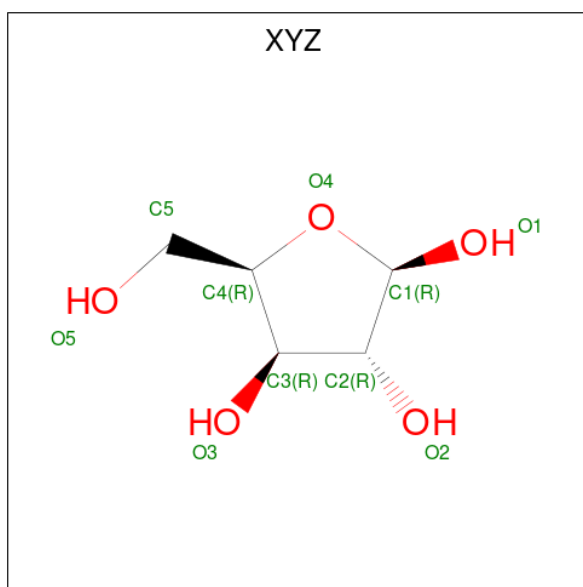
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			13	8	1	4		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

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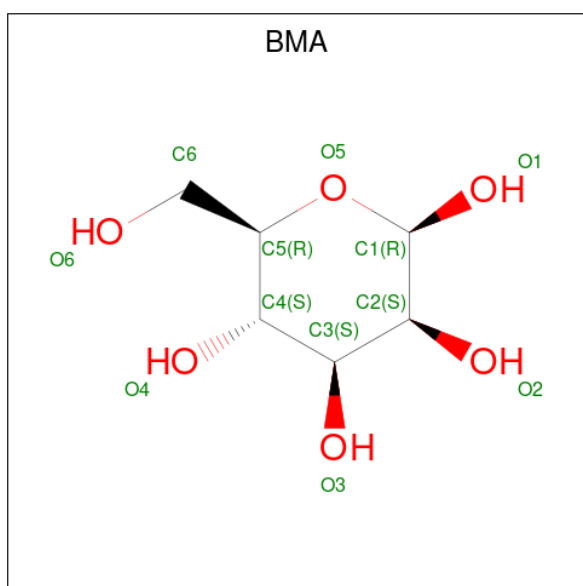
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			13	8	1	4		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			13	8	1	4		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			13	8	1	4		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	D	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		
8	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is beta-D-xylofuranose (CCD ID: XYZ) (formula: C₅H₁₀O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	5	5		
9	B	1	Total	C	O	0	0
			10	5	5		

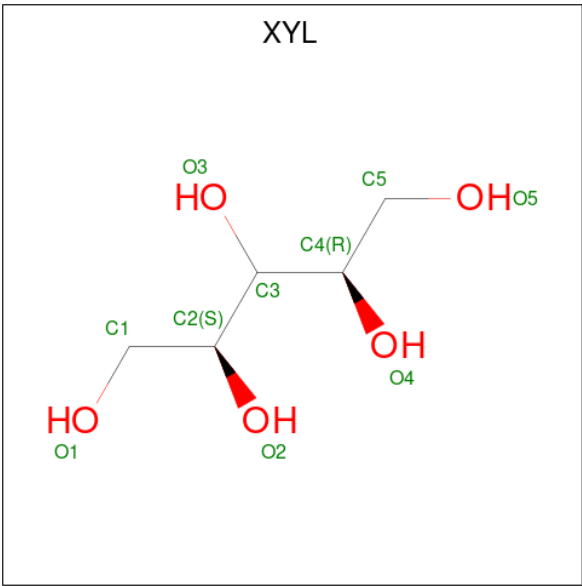
- Molecule 10 is beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 11 is Xylitol (CCD ID: XYL) (formula: $C_5H_{12}O_5$) (labeled as "Ligand of Interest")

by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			10	5	5		
11	D	1	Total	C	O	0	0
			10	5	5		
11	E	1	Total	C	O	0	0
			10	5	5		

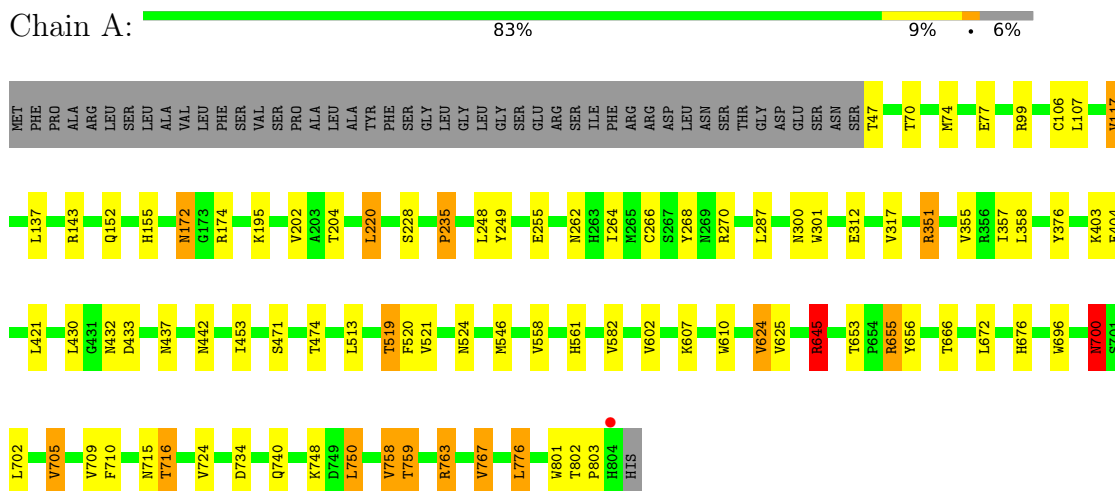
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	239	Total	O	0	0
			239	239		
12	B	304	Total	O	0	0
			304	304		
12	C	177	Total	O	0	0
			177	177		
12	D	177	Total	O	0	0
			177	177		
12	E	204	Total	O	0	0
			204	204		
12	F	200	Total	O	0	0
			200	200		

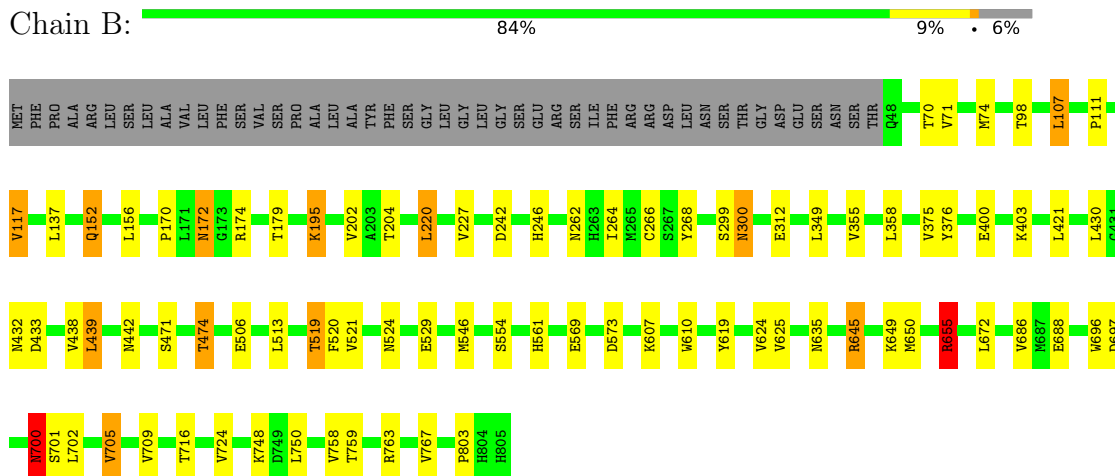
3 Residue-property plots [i](#)

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

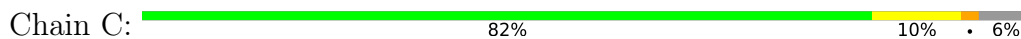
- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

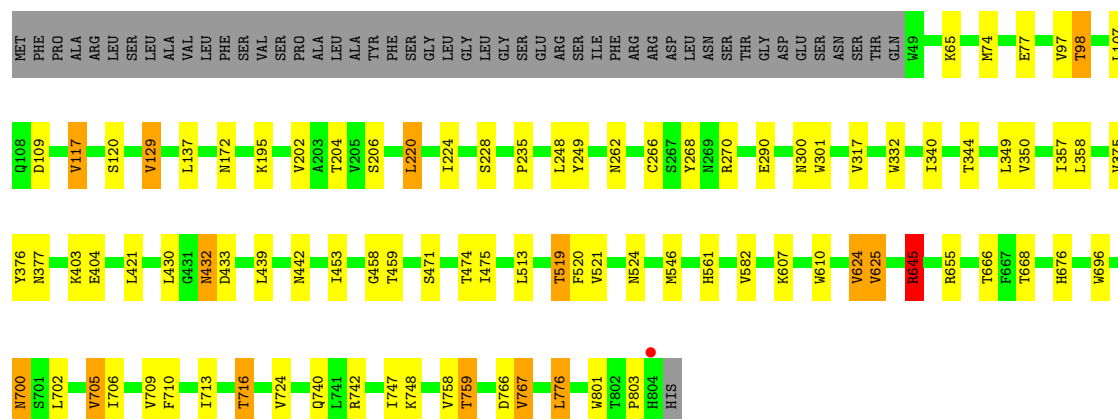


- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase



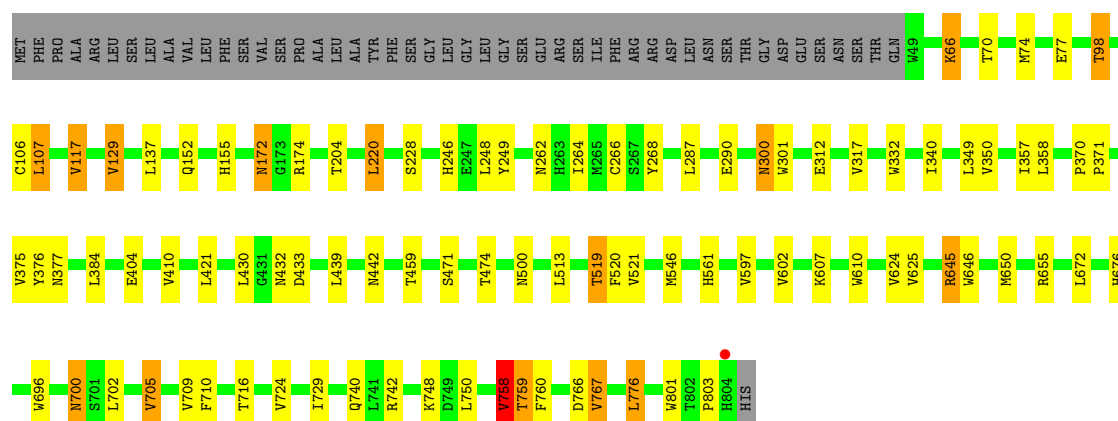
- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase





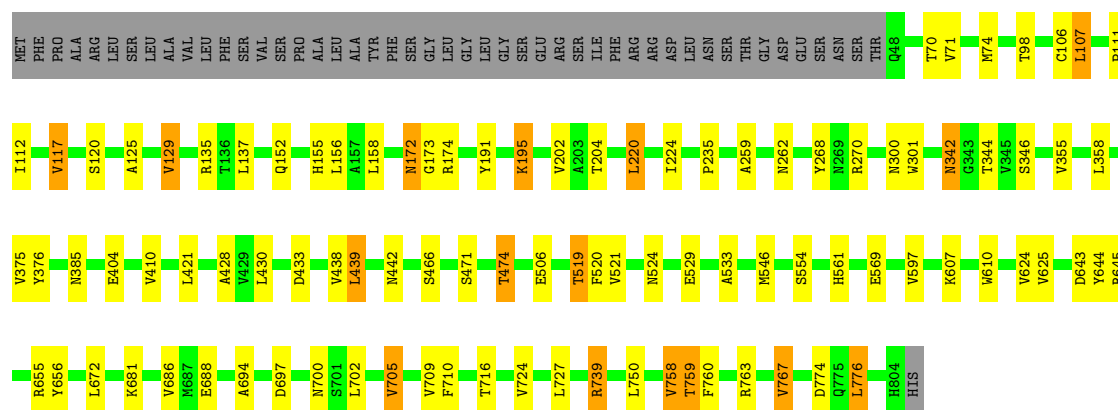
- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain D:  82% 10% • 6%

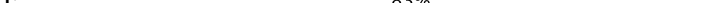


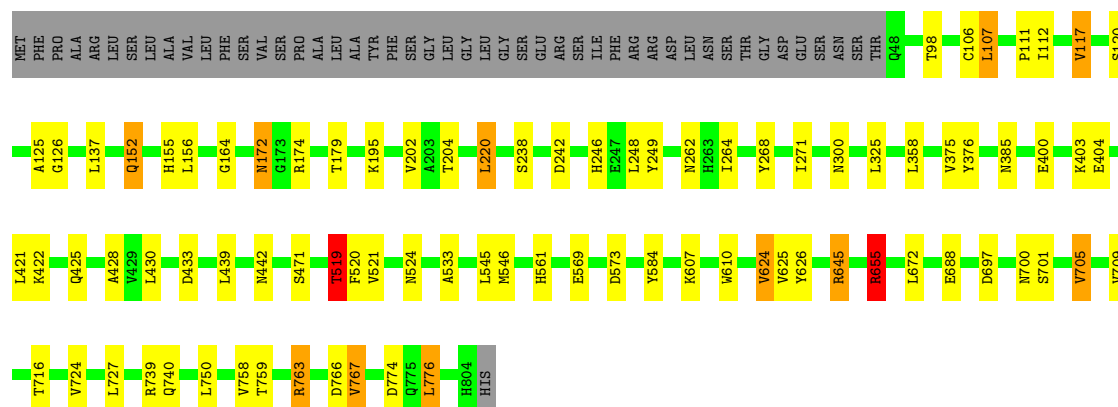
- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain E: 82% 10% • 6%



- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain F:  83% 9% • 6%



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

Chain G: 100%



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

Chain J: 33% 67%



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

Chain M: 33% 67%



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

Chain P: 33% 67%



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

Chain S: 33% 67%



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

Chain V:  33% 67%

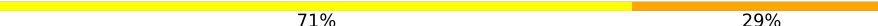
MAG1
MAG2
BMA3

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

Chain H:  71% 29%

MAG1
MAG2
BMA3
BMA4
MAN5
MAN6
MAN7

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

Chain N:  71% 29%

MAG1
MAG2
BMA3
BMA4
MAN5
MAN6
MAN7

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

Chain T:  71% 29%

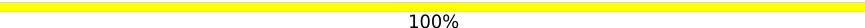
MAG1
MAG2
BMA3
BMA4
MAN5
MAN6
MAN7

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

Chain W:  71% 29%

MAG1
MAG2
BMA3
BMA4
MAN5
MAN6
MAN7

- Molecule 4: 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

Chain I:  100%

MAG1
MAG2
MAN3
MAN4
MAN5

- Molecule 4: 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

Chain R:  100%

MAG1
MAG2
MAN3
MAN4
MAN5

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

Chain K:  50% 50%

MAG1
MAG2
BMA3
BMA4
BMA5
BMA6
BMA7
BMA8

- Molecule 6: alpha-D-mannopyranose-(1-2)-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

Chain L:  100%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

- Molecule 6: alpha-D-mannopyranose-(1-2)-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

Chain O:  100%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

- Molecule 6: alpha-D-mannopyranose-(1-2)-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

Chain U:  100%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

- Molecule 6: alpha-D-mannopyranose-(1-2)-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

Chain X:  100%

MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

● Molecule 7: α -D-mannopyranose-(1-2)- β -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain Q:  83%  17%

MAG1
BMA2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	149.15Å 258.23Å 320.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	160.12 – 2.43 160.12 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.9 (160.12-2.43) 98.9 (160.12-2.43)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.04 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.175 , 0.226 (Not available) , 0.218	Depositor DCC
R_{free} test set	11385 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 3.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.456 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.440 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37142	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	1/5868 (0.0%)	1.10	12/8030 (0.1%)
1	B	1.13	3/5882 (0.1%)	1.08	8/8047 (0.1%)
1	C	1.12	5/5856 (0.1%)	1.09	12/8012 (0.1%)
1	D	1.13	1/5856 (0.0%)	1.11	16/8012 (0.2%)
1	E	1.16	3/5871 (0.1%)	1.11	14/8032 (0.2%)
1	F	1.16	7/5871 (0.1%)	1.11	9/8032 (0.1%)
All	All	1.14	20/35204 (0.1%)	1.10	71/48165 (0.1%)

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	643	ASP	C-O	-7.35	1.17	1.24
1	F	584	TYR	C-O	-6.83	1.17	1.24
1	E	760	PHE	C-O	-6.02	1.18	1.24
1	A	235	PRO	C-O	-5.97	1.17	1.23
1	F	701	SER	C-O	-5.86	1.16	1.23

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	129	VAL	CB-CA-C	-8.33	100.89	112.14
1	C	767	VAL	N-CA-CB	-8.18	101.53	112.16
1	E	129	VAL	N-CA-CB	8.04	121.47	110.54
1	D	767	VAL	N-CA-CB	-7.61	102.27	112.16
1	D	129	VAL	CB-CA-C	-7.59	101.75	112.22

There are no chirality outliers.

There are no planarity outliers.

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	A	5724	0	5509	40	0
1	B	5736	0	5525	34	0
1	C	5712	0	5505	41	0
1	D	5712	0	5505	38	0
1	E	5726	0	5519	36	0
1	F	5726	0	5518	32	0
2	G	39	0	34	4	0
2	J	39	0	34	2	0
2	M	39	0	34	4	0
2	P	39	0	34	5	0
2	S	39	0	34	2	0
2	V	39	0	34	2	0
3	H	83	0	70	3	0
3	N	83	0	70	4	0
3	T	83	0	70	4	0
3	W	83	0	70	3	0
4	I	61	0	52	0	0
4	R	61	0	52	0	0
5	K	94	0	77	12	0
6	L	72	0	61	0	0
6	O	72	0	61	0	0
6	U	72	0	61	0	0
6	X	72	0	61	0	0
7	Q	70	0	60	3	0
8	A	55	0	50	0	0
8	B	42	0	38	2	0
8	C	55	0	50	0	0
8	D	68	0	61	3	0
8	E	42	0	39	2	0
8	F	42	0	38	0	0
9	A	10	0	7	1	0
9	B	10	0	7	1	0
10	A	11	0	10	0	0
11	C	10	0	12	2	0
11	D	10	0	12	0	0
11	E	10	0	12	1	0
12	A	239	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	B	304	0	0	3	0
12	C	177	0	0	3	0
12	D	177	0	0	2	0
12	E	204	0	0	5	0
12	F	200	0	0	3	0
All	All	37142	0	34386	269	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 4.

The worst 5 of 269 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:8:MAN:O6	5:K:8:MAN:C6	1.66	1.40
5:K:6:MAN:C5	5:K:8:MAN:O6	1.68	1.36
3:W:1:NAG:O4	3:W:1:NAG:C4	1.73	1.36
2:M:1:NAG:C4	2:M:1:NAG:O4	1.73	1.36
5:K:1:NAG:O4	5:K:1:NAG:C4	1.77	1.33

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	610/650 (94%)	567 (93%)	43 (7%)	14	17
1	B	612/650 (94%)	569 (93%)	43 (7%)	14	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	609/650 (94%)	567 (93%)	42 (7%)	14	18
1	D	609/650 (94%)	569 (93%)	40 (7%)	15	19
1	E	611/650 (94%)	566 (93%)	45 (7%)	13	15
1	F	611/650 (94%)	572 (94%)	39 (6%)	16	21
All	All	3662/3900 (94%)	3410 (93%)	252 (7%)	14	18

5 of 252 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	624	VAL
1	F	202	VAL
1	D	358	LEU
1	F	172	ASN
1	F	625	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	369	ASN
1	F	262	ASN
1	E	442	ASN
1	F	147	GLN
1	F	561	HIS

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 ⓘ

94 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	G	1	2,1	14,14,15	3.65	1 (7%)	17,19,21	1.42	2 (11%)
2	NAG	G	2	2	14,14,15	1.09	0	17,19,21	1.97	6 (35%)
2	BMA	G	3	2	11,11,12	1.07	1 (9%)	15,15,17	1.32	3 (20%)
3	NAG	H	1	3,1	14,14,15	3.99	2 (14%)	17,19,21	1.89	4 (23%)
3	NAG	H	2	3	14,14,15	0.58	0	17,19,21	1.08	1 (5%)
3	BMA	H	3	3	11,11,12	0.67	0	15,15,17	2.00	3 (20%)
3	BMA	H	4	3	11,11,12	1.26	1 (9%)	15,15,17	2.67	7 (46%)
3	MAN	H	5	3	11,11,12	1.12	1 (9%)	15,15,17	1.30	2 (13%)
3	MAN	H	6	3	11,11,12	1.00	0	15,15,17	3.77	6 (40%)
3	MAN	H	7	3	11,11,12	0.61	0	15,15,17	1.47	5 (33%)
4	NAG	I	1	4,1	14,14,15	0.91	1 (7%)	17,19,21	1.55	4 (23%)
4	NAG	I	2	4	14,14,15	0.73	0	17,19,21	2.47	7 (41%)
4	MAN	I	3	4	11,11,12	1.39	1 (9%)	15,15,17	1.84	6 (40%)
4	MAN	I	4	4	11,11,12	1.29	1 (9%)	15,15,17	2.70	5 (33%)
4	MAN	I	5	4	11,11,12	0.66	0	15,15,17	2.51	5 (33%)
2	NAG	J	1	2,1	14,14,15	3.87	1 (7%)	17,19,21	1.58	3 (17%)
2	NAG	J	2	2	14,14,15	0.47	0	17,19,21	1.26	2 (11%)
2	BMA	J	3	2	11,11,12	0.90	0	15,15,17	1.44	2 (13%)
5	NAG	K	1	5,1	14,14,15	3.79	1 (7%)	17,19,21	2.46	5 (29%)
5	NAG	K	2	5	14,14,15	0.69	0	17,19,21	1.19	2 (11%)
5	BMA	K	3	5	11,11,12	0.51	0	15,15,17	2.40	6 (40%)
5	BMA	K	4	5	11,11,12	1.40	2 (18%)	15,15,17	2.57	7 (46%)
5	MAN	K	5	5	11,11,12	1.23	2 (18%)	15,15,17	1.81	6 (40%)
5	MAN	K	6	5	11,11,12	1.85	1 (9%)	15,15,17	2.70	7 (46%)
5	MAN	K	7	5	11,11,12	0.68	0	15,15,17	1.25	2 (13%)
5	MAN	K	8	5	11,11,12	2.22	2 (18%)	15,15,17	3.97	8 (53%)
6	NAG	L	1	6,1	14,14,15	0.49	0	17,19,21	1.37	2 (11%)
6	NAG	L	2	6	14,14,15	0.84	0	17,19,21	1.99	5 (29%)
6	MAN	L	3	6	11,11,12	1.37	1 (9%)	15,15,17	2.00	6 (40%)
6	MAN	L	4	6	11,11,12	0.95	0	15,15,17	2.32	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	L	5	6	11,11,12	0.67	0	15,15,17	2.66	5 (33%)
6	MAN	L	6	6	11,11,12	0.74	0	15,15,17	1.81	2 (13%)
2	NAG	M	1	2,1	14,14,15	3.37	1 (7%)	17,19,21	1.45	2 (11%)
2	NAG	M	2	2	14,14,15	1.08	0	17,19,21	1.92	6 (35%)
2	BMA	M	3	2	11,11,12	1.36	1 (9%)	15,15,17	1.24	1 (6%)
3	NAG	N	1	3,1	14,14,15	4.35	2 (14%)	17,19,21	2.27	6 (35%)
3	NAG	N	2	3	14,14,15	0.70	0	17,19,21	1.01	1 (5%)
3	BMA	N	3	3	11,11,12	0.89	0	15,15,17	2.45	4 (26%)
3	BMA	N	4	3	11,11,12	1.25	1 (9%)	15,15,17	2.67	8 (53%)
3	MAN	N	5	3	11,11,12	1.19	1 (9%)	15,15,17	1.49	4 (26%)
3	MAN	N	6	3	11,11,12	0.93	0	15,15,17	3.76	6 (40%)
3	MAN	N	7	3	11,11,12	0.67	0	15,15,17	1.41	1 (6%)
6	NAG	O	1	6,1	14,14,15	0.80	0	17,19,21	1.47	3 (17%)
6	NAG	O	2	6	14,14,15	0.93	1 (7%)	17,19,21	1.69	6 (35%)
6	MAN	O	3	6	11,11,12	1.25	0	15,15,17	2.22	6 (40%)
6	MAN	O	4	6	11,11,12	1.41	1 (9%)	15,15,17	2.63	5 (33%)
6	MAN	O	5	6	11,11,12	0.76	0	15,15,17	2.17	5 (33%)
6	MAN	O	6	6	11,11,12	0.82	0	15,15,17	1.63	4 (26%)
2	NAG	P	1	2,1	14,14,15	3.74	1 (7%)	17,19,21	1.49	3 (17%)
2	NAG	P	2	2	14,14,15	1.04	0	17,19,21	2.00	5 (29%)
2	BMA	P	3	2	11,11,12	1.15	1 (9%)	15,15,17	1.43	2 (13%)
7	NAG	Q	1	7	15,15,15	0.68	0	21,21,21	1.57	4 (19%)
7	BMA	Q	2	7	11,11,12	0.64	0	15,15,17	2.60	5 (33%)
7	BMA	Q	3	7	11,11,12	1.32	2 (18%)	15,15,17	2.43	6 (40%)
7	MAN	Q	4	7	11,11,12	1.20	0	15,15,17	1.45	3 (20%)
7	MAN	Q	5	7	11,11,12	1.24	1 (9%)	15,15,17	3.88	6 (40%)
7	MAN	Q	6	7	11,11,12	0.50	0	15,15,17	1.09	1 (6%)
4	NAG	R	1	4,1	14,14,15	0.85	0	17,19,21	1.27	1 (5%)
4	NAG	R	2	4	14,14,15	0.78	0	17,19,21	1.78	6 (35%)
4	MAN	R	3	4	11,11,12	1.22	1 (9%)	15,15,17	1.99	4 (26%)
4	MAN	R	4	4	11,11,12	1.27	1 (9%)	15,15,17	2.69	6 (40%)
4	MAN	R	5	4	11,11,12	1.40	2 (18%)	15,15,17	2.35	6 (40%)
2	NAG	S	1	2,1	14,14,15	4.05	1 (7%)	17,19,21	1.72	6 (35%)
2	NAG	S	2	2	14,14,15	0.59	0	17,19,21	1.12	1 (5%)
2	BMA	S	3	2	11,11,12	1.05	0	15,15,17	1.38	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	T	1	3,1	14,14,15	3.86	1 (7%)	17,19,21	2.36	4 (23%)
3	NAG	T	2	3	14,14,15	0.78	0	17,19,21	1.08	1 (5%)
3	BMA	T	3	3	11,11,12	0.67	0	15,15,17	2.30	5 (33%)
3	BMA	T	4	3	11,11,12	1.17	1 (9%)	15,15,17	2.39	7 (46%)
3	MAN	T	5	3	11,11,12	0.97	1 (9%)	15,15,17	2.33	6 (40%)
3	MAN	T	6	3	11,11,12	1.19	2 (18%)	15,15,17	3.80	7 (46%)
3	MAN	T	7	3	11,11,12	0.84	0	15,15,17	1.76	6 (40%)
6	NAG	U	1	6,1	14,14,15	0.62	0	17,19,21	1.17	2 (11%)
6	NAG	U	2	6	14,14,15	0.88	0	17,19,21	1.63	3 (17%)
6	MAN	U	3	6	11,11,12	1.46	3 (27%)	15,15,17	2.17	6 (40%)
6	MAN	U	4	6	11,11,12	1.09	0	15,15,17	2.81	6 (40%)
6	MAN	U	5	6	11,11,12	0.66	0	15,15,17	2.71	5 (33%)
6	MAN	U	6	6	11,11,12	1.09	1 (9%)	15,15,17	1.76	4 (26%)
2	NAG	V	1	2,1	14,14,15	4.04	1 (7%)	17,19,21	1.38	3 (17%)
2	NAG	V	2	2	14,14,15	0.59	0	17,19,21	1.44	1 (5%)
2	BMA	V	3	2	11,11,12	1.16	1 (9%)	15,15,17	1.62	2 (13%)
3	NAG	W	1	3,1	14,14,15	3.42	1 (7%)	17,19,21	2.24	4 (23%)
3	NAG	W	2	3	14,14,15	0.75	0	17,19,21	1.20	1 (5%)
3	BMA	W	3	3	11,11,12	0.56	0	15,15,17	2.36	5 (33%)
3	BMA	W	4	3	11,11,12	1.24	2 (18%)	15,15,17	2.49	6 (40%)
3	MAN	W	5	3	11,11,12	1.37	2 (18%)	15,15,17	2.78	6 (40%)
3	MAN	W	6	3	11,11,12	1.16	1 (9%)	15,15,17	3.90	5 (33%)
3	MAN	W	7	3	11,11,12	0.85	0	15,15,17	1.55	3 (20%)
6	NAG	X	1	6,1	14,14,15	0.78	1 (7%)	17,19,21	1.58	3 (17%)
6	NAG	X	2	6	14,14,15	0.95	0	17,19,21	1.58	2 (11%)
6	MAN	X	3	6	11,11,12	1.55	2 (18%)	15,15,17	2.15	5 (33%)
6	MAN	X	4	6	11,11,12	1.09	1 (9%)	15,15,17	2.72	6 (40%)
6	MAN	X	5	6	11,11,12	0.57	0	15,15,17	1.87	4 (26%)
6	MAN	X	6	6	11,11,12	0.94	0	15,15,17	1.38	2 (13%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	N	7	3	-	0/2/19/22	0/1/1/1
6	NAG	O	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1
6	MAN	O	3	6	-	1/2/19/22	0/1/1/1
6	MAN	O	4	6	-	2/2/19/22	0/1/1/1
6	MAN	O	5	6	-	2/2/19/22	0/1/1/1
6	MAN	O	6	6	-	2/2/19/22	0/1/1/1
2	NAG	P	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	P	2	2	-	0/6/23/26	0/1/1/1
2	BMA	P	3	2	-	1/2/19/22	0/1/1/1
7	NAG	Q	1	7	-	0/6/26/26	0/1/1/1
7	BMA	Q	2	7	-	0/2/19/22	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	6	7	-	0/2/19/22	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	MAN	R	3	4	-	1/2/19/22	0/1/1/1
4	MAN	R	4	4	-	1/2/19/22	0/1/1/1
4	MAN	R	5	4	-	1/2/19/22	0/1/1/1
2	NAG	S	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	BMA	S	3	2	-	2/2/19/22	0/1/1/1
3	NAG	T	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	BMA	T	4	3	-	0/2/19/22	0/1/1/1
3	MAN	T	5	3	-	0/2/19/22	0/1/1/1
3	MAN	T	6	3	-	2/2/19/22	0/1/1/1
3	MAN	T	7	3	-	0/2/19/22	0/1/1/1
6	NAG	U	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	MAN	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	2/2/19/22	0/1/1/1
6	MAN	U	5	6	-	0/2/19/22	0/1/1/1
6	MAN	U	6	6	-	0/2/19/22	0/1/1/1
2	NAG	V	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	V	2	2	-	0/6/23/26	0/1/1/1
2	BMA	V	3	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	W	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	BMA	W	3	3	-	0/2/19/22	0/1/1/1
3	BMA	W	4	3	-	0/2/19/22	0/1/1/1
3	MAN	W	5	3	-	1/2/19/22	0/1/1/1
3	MAN	W	6	3	-	2/2/19/22	0/1/1/1
3	MAN	W	7	3	-	0/2/19/22	0/1/1/1
6	NAG	X	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	MAN	X	3	6	-	2/2/19/22	0/1/1/1
6	MAN	X	4	6	-	2/2/19/22	0/1/1/1
6	MAN	X	5	6	-	0/2/19/22	0/1/1/1
6	MAN	X	6	6	-	2/2/19/22	0/1/1/1

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	NAG	O4-C4	15.85	1.82	1.43
2	S	1	NAG	O4-C4	14.97	1.80	1.43
2	V	1	NAG	O4-C4	14.91	1.79	1.43
3	H	1	NAG	O4-C4	14.46	1.78	1.43
2	J	1	NAG	O4-C4	14.16	1.78	1.43

The worst 5 of 395 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	5	MAN	C1-O5-C5	12.71	129.22	112.19
3	N	6	MAN	C1-O5-C5	12.17	128.50	112.19
3	H	6	MAN	C1-O5-C5	12.04	128.32	112.19
3	W	6	MAN	C1-O5-C5	11.56	127.68	112.19
3	T	6	MAN	C1-O5-C5	11.04	126.98	112.19

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	S	3	BMA	O5-C5-C6-O6
2	J	3	BMA	O5-C5-C6-O6
3	H	6	MAN	O5-C5-C6-O6
6	X	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	S	3	BMA	C4-C5-C6-O6

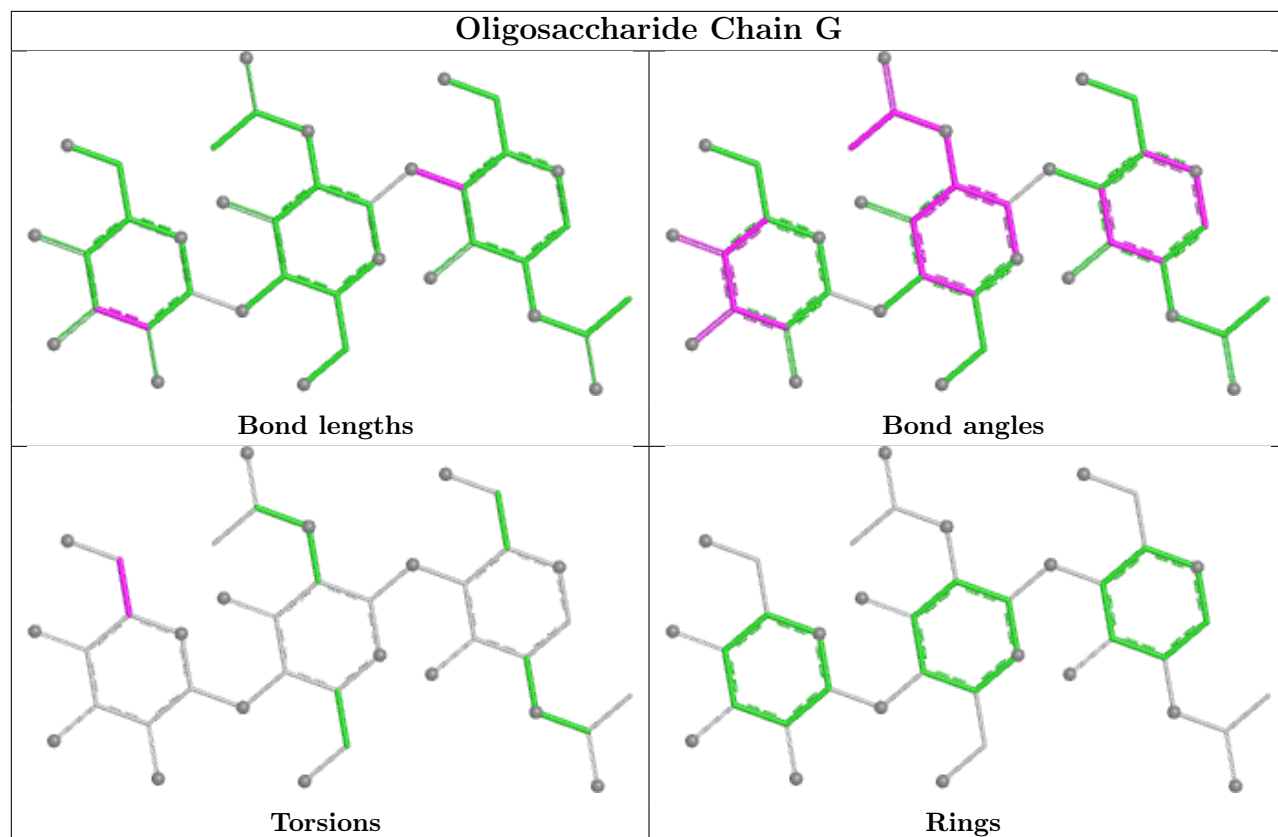
There are no ring outliers.

26 monomers are involved in 48 short contacts:

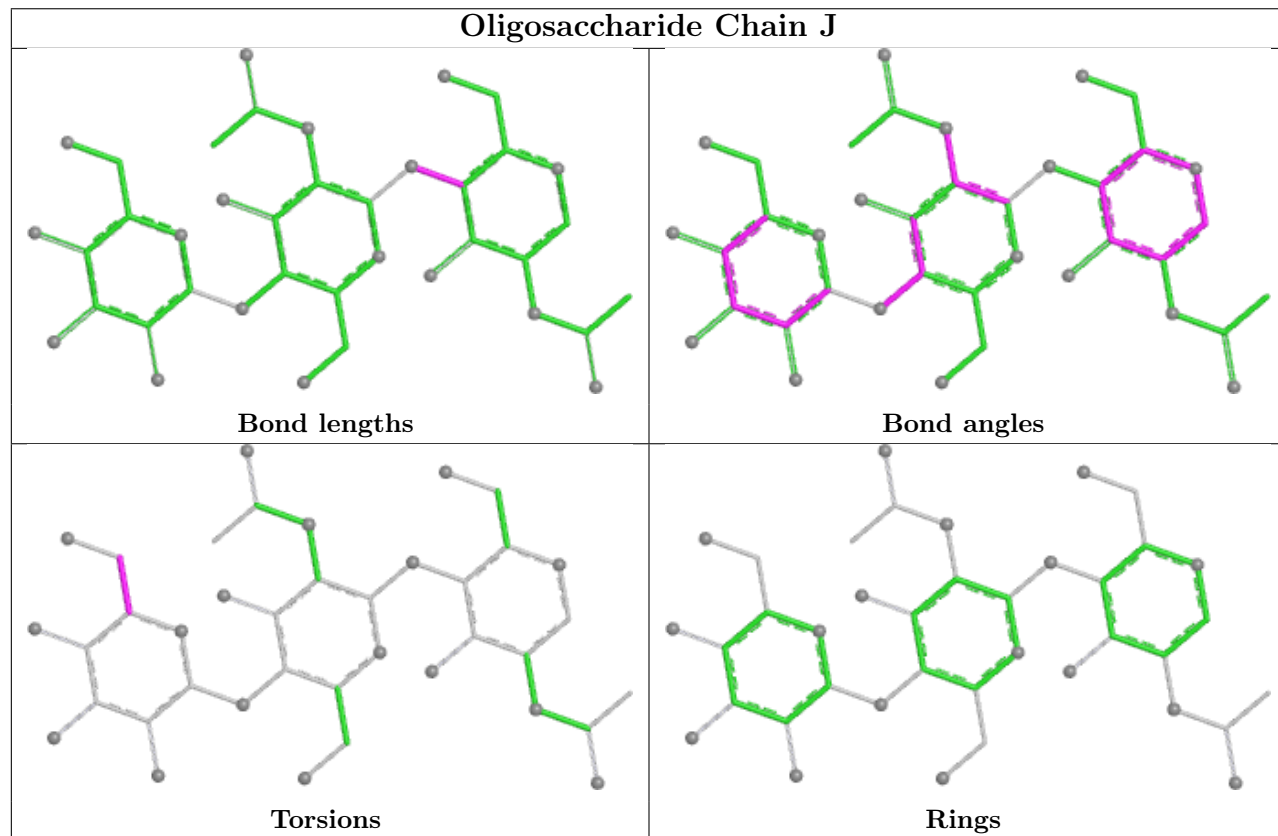
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	2	NAG	1	0
2	M	1	NAG	4	0
5	K	1	NAG	4	0
3	N	1	NAG	4	0
7	Q	1	NAG	3	0
2	P	2	NAG	1	0
2	V	1	NAG	2	0
2	S	1	NAG	2	0
3	W	2	NAG	1	0
5	K	8	MAN	8	0
2	M	2	NAG	1	0
2	P	1	NAG	5	0
3	H	2	NAG	1	0
2	J	1	NAG	2	0
2	G	3	BMA	2	0
5	K	6	MAN	6	0
3	N	2	NAG	1	0
2	V	2	NAG	1	0
5	K	2	NAG	1	0
2	G	1	NAG	2	0
2	S	2	NAG	1	0
3	H	1	NAG	3	0
2	G	2	NAG	1	0
2	J	2	NAG	1	0
3	T	1	NAG	4	0
3	W	1	NAG	3	0

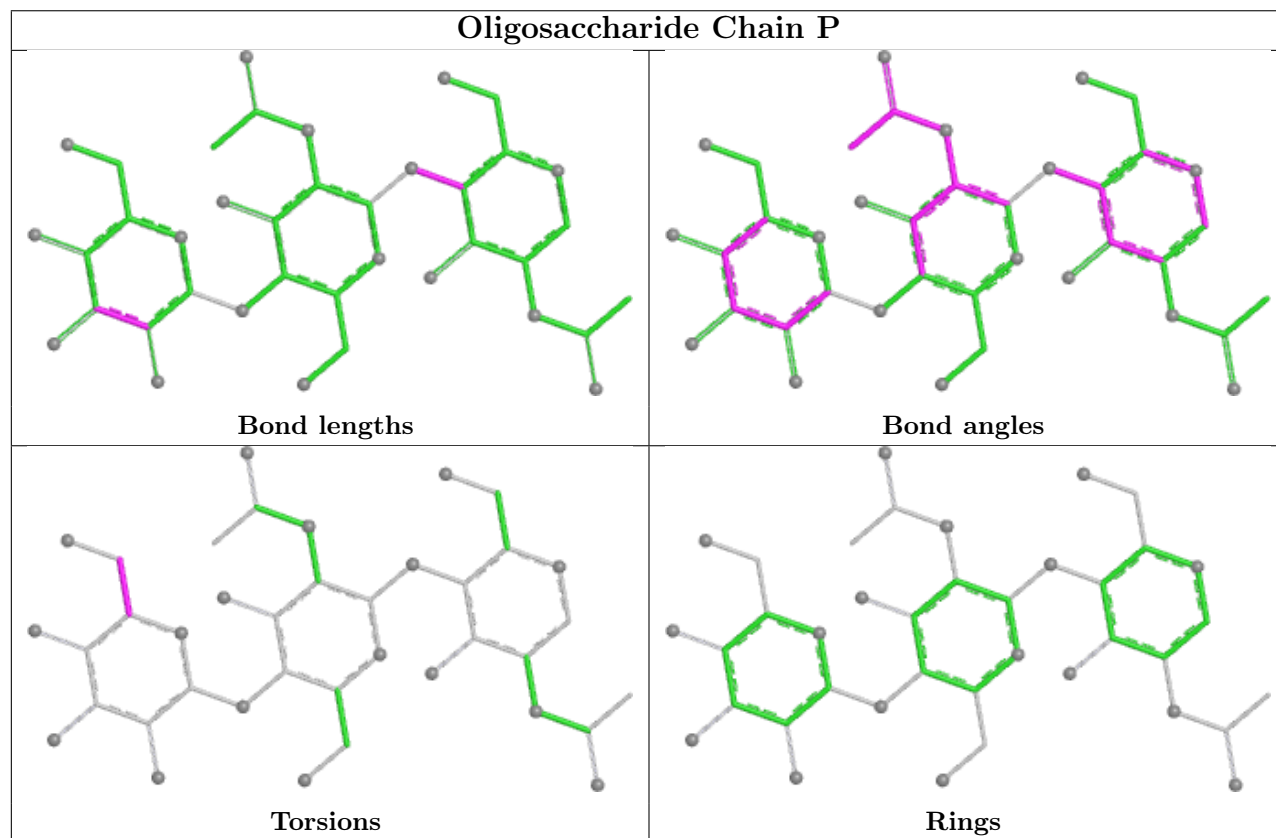
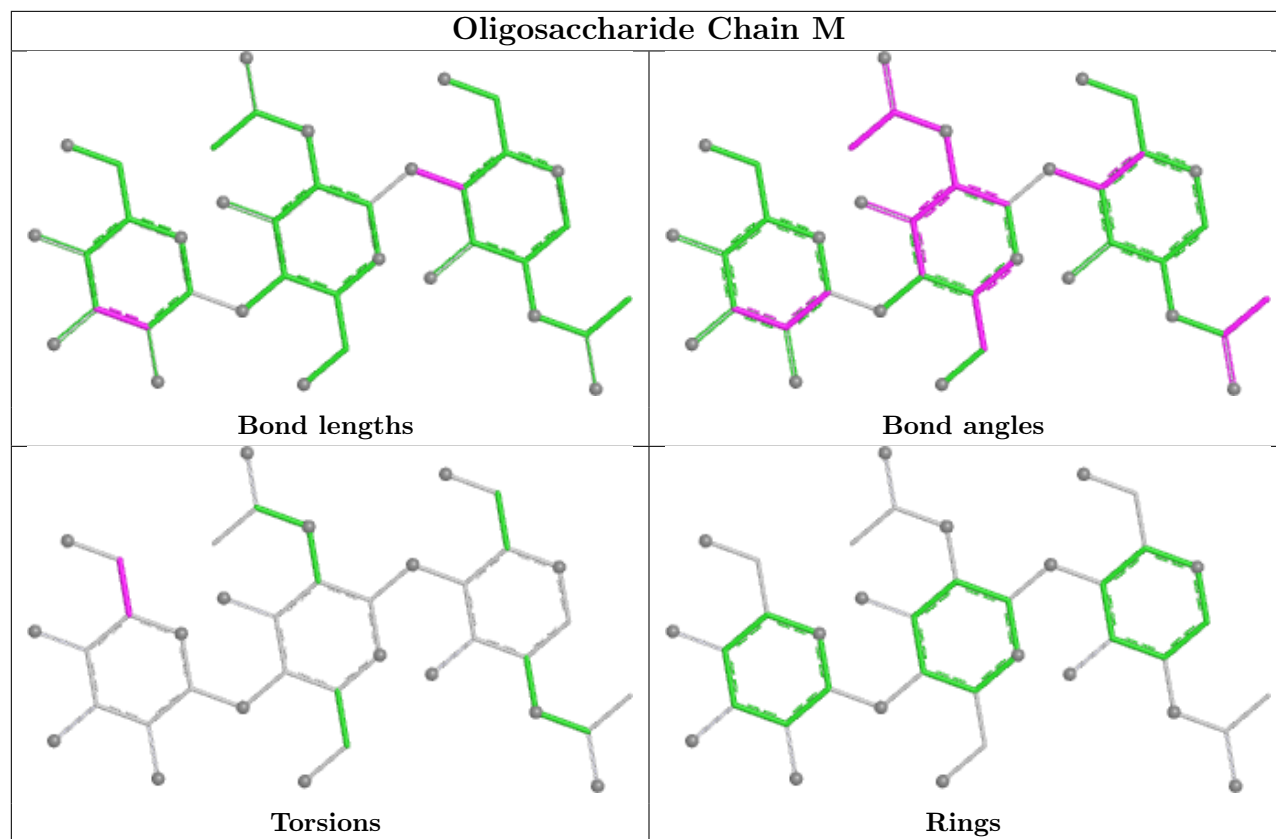
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

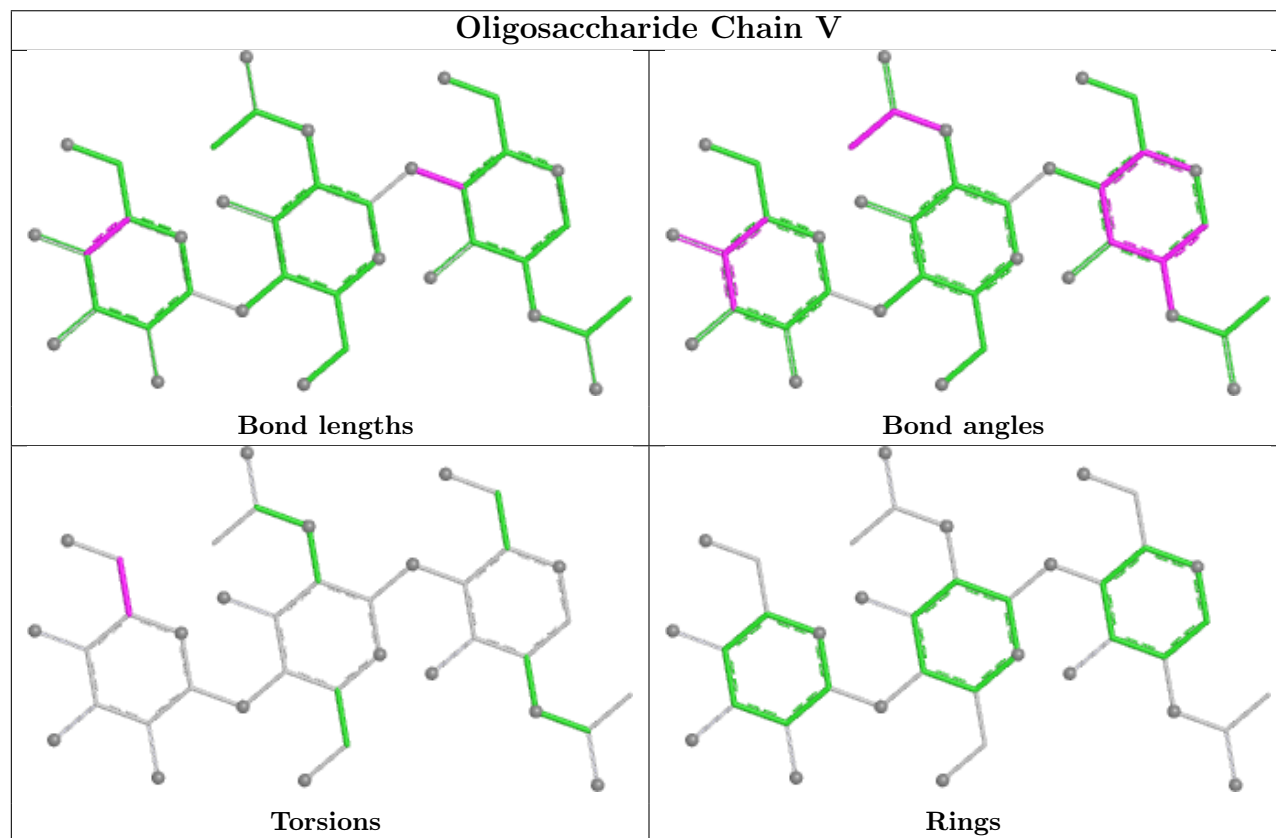
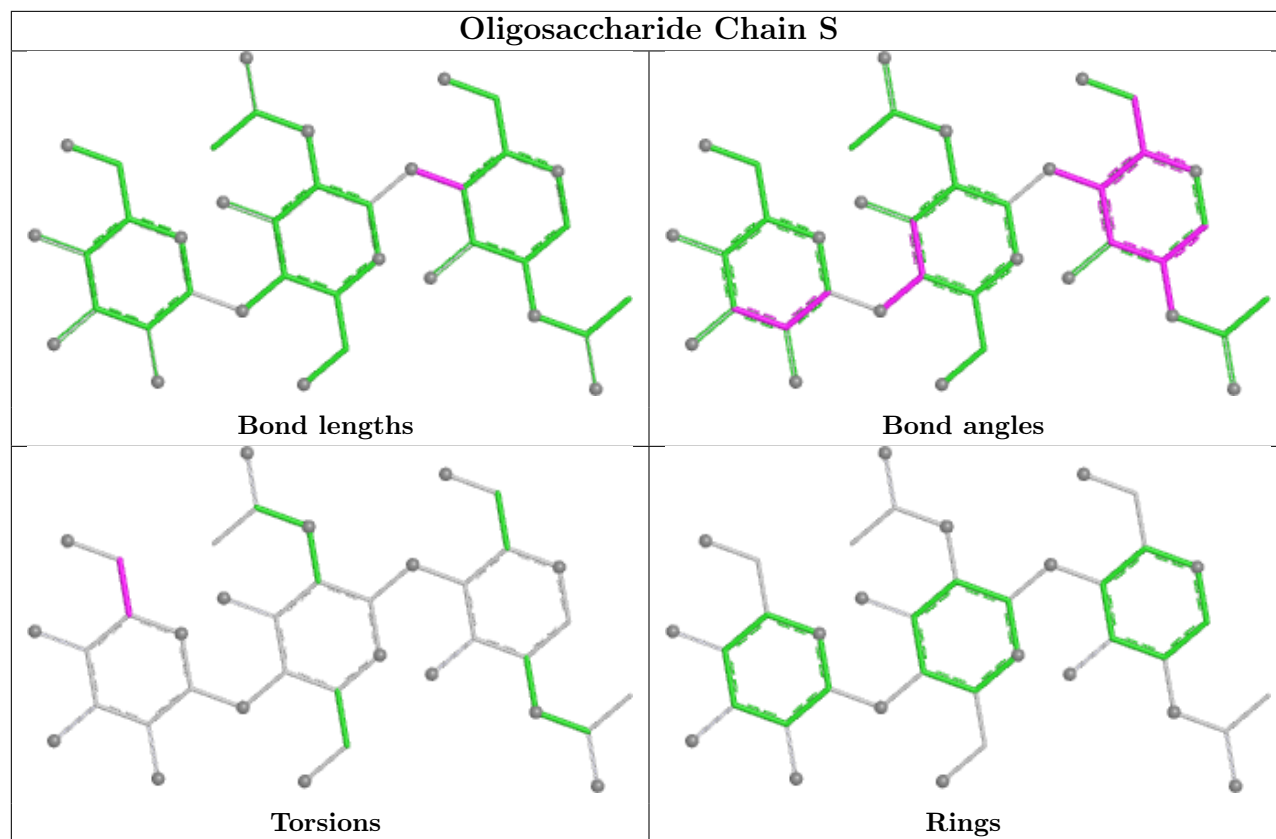
Oligosaccharide Chain G

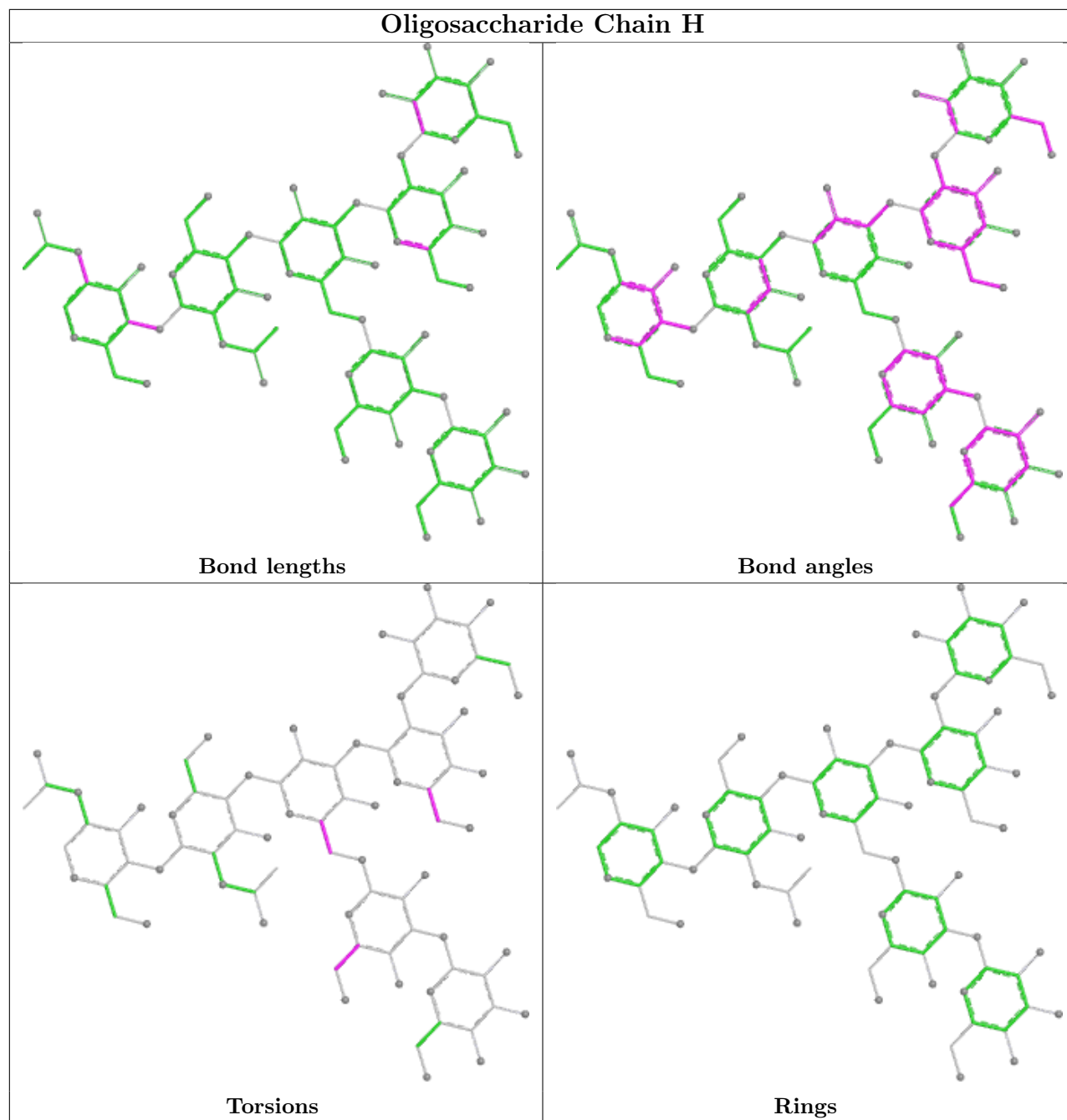


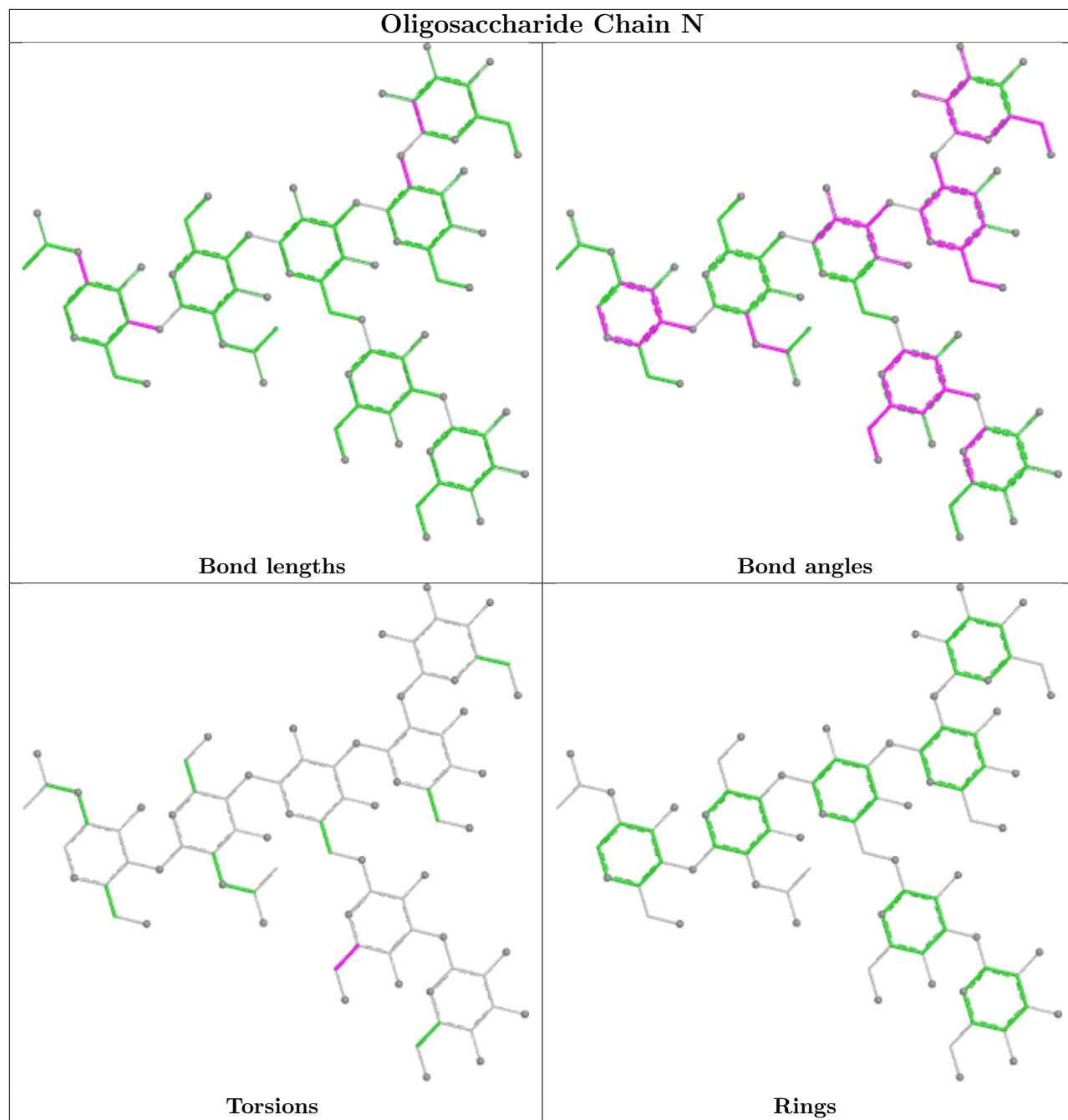
Oligosaccharide Chain J

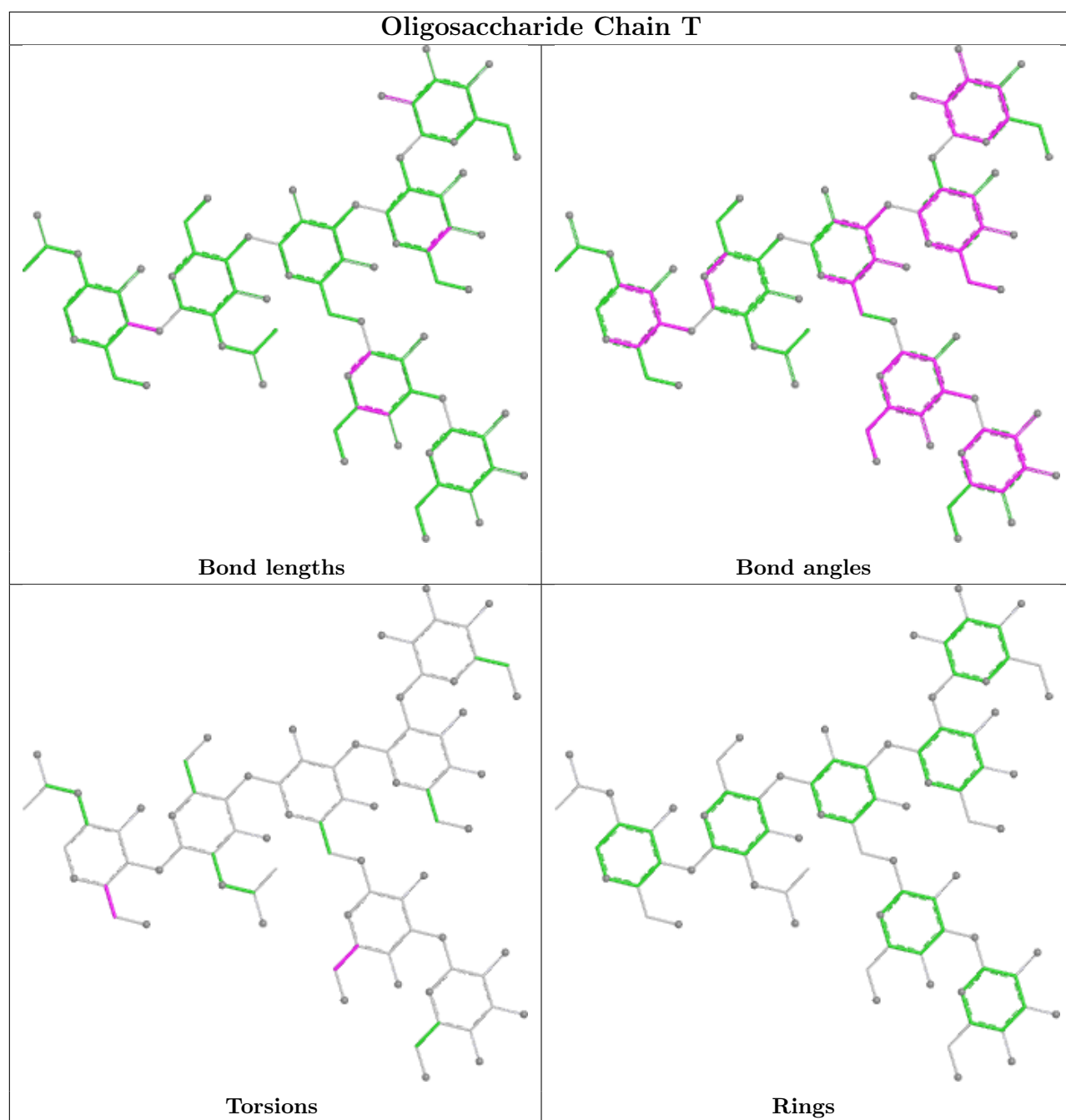


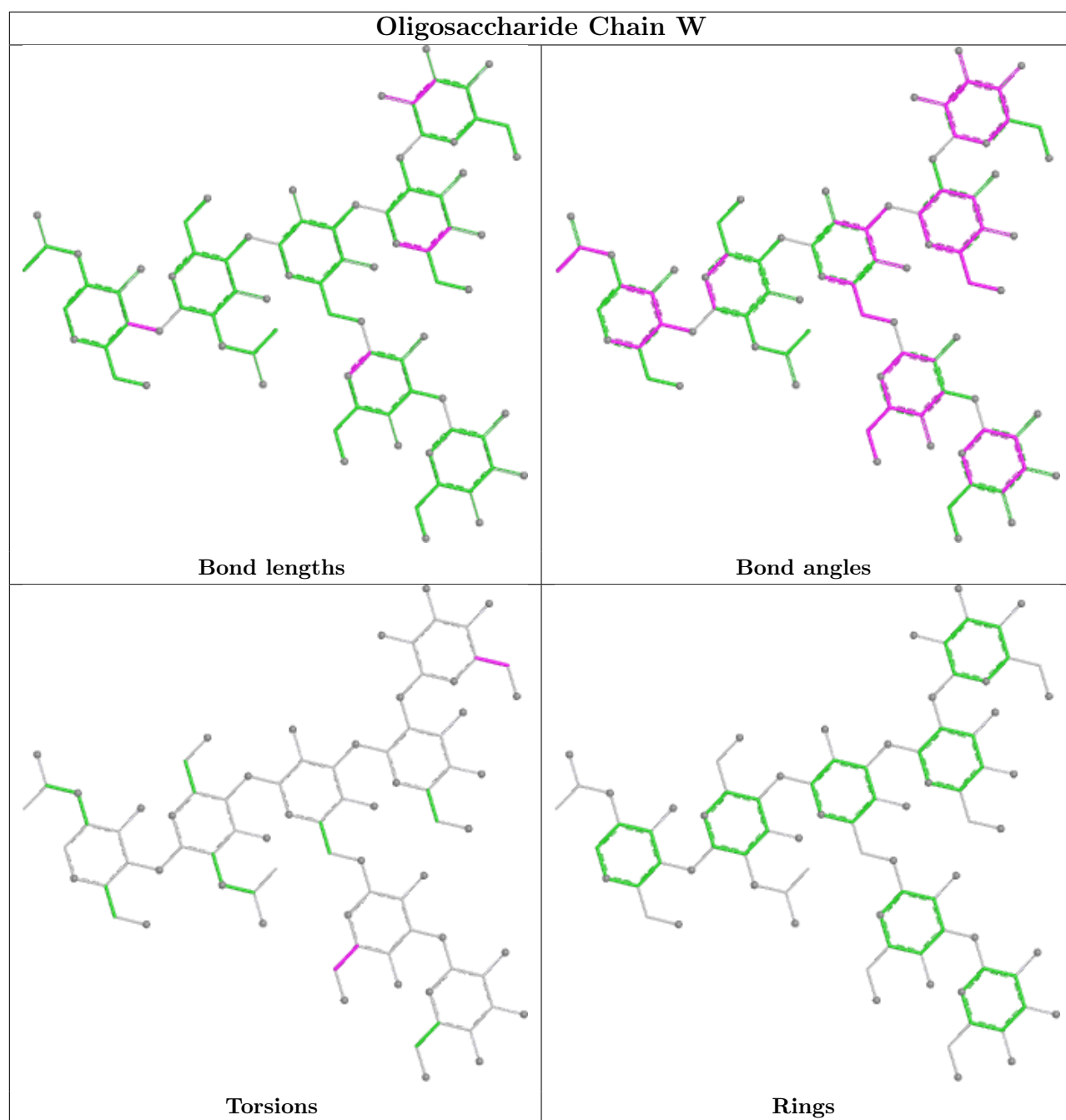


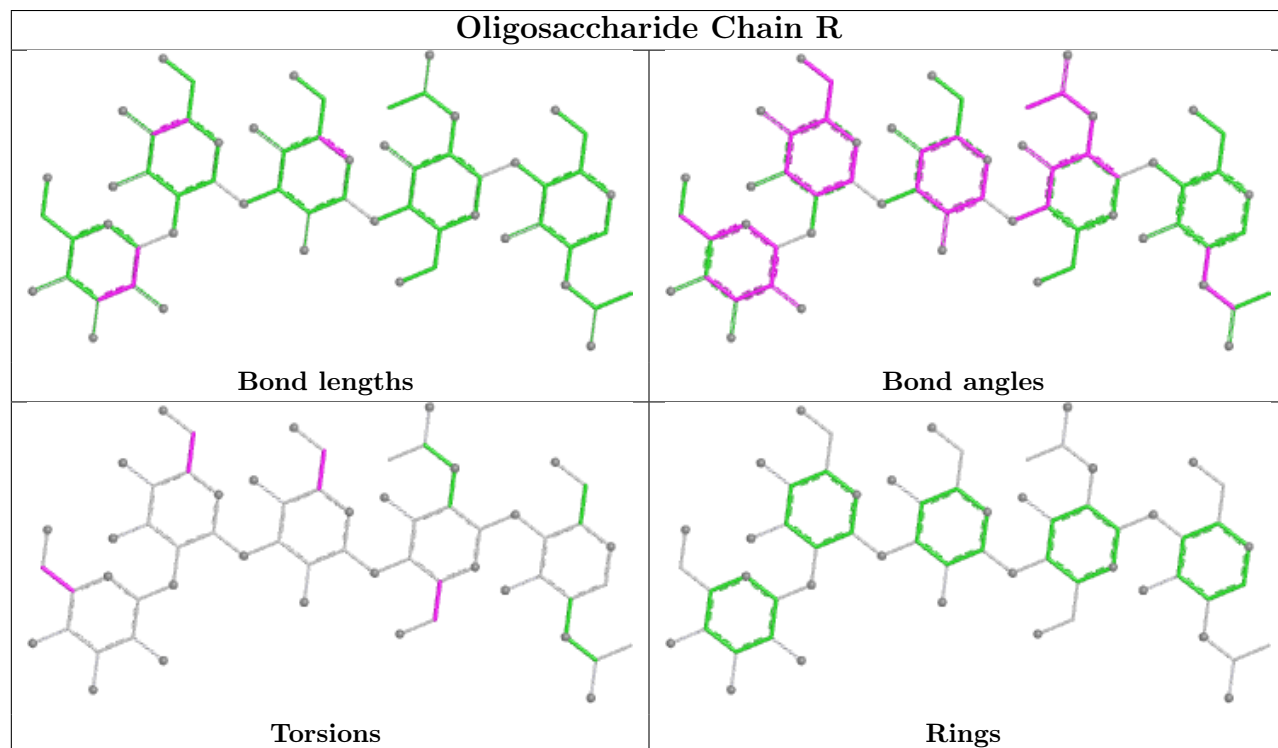
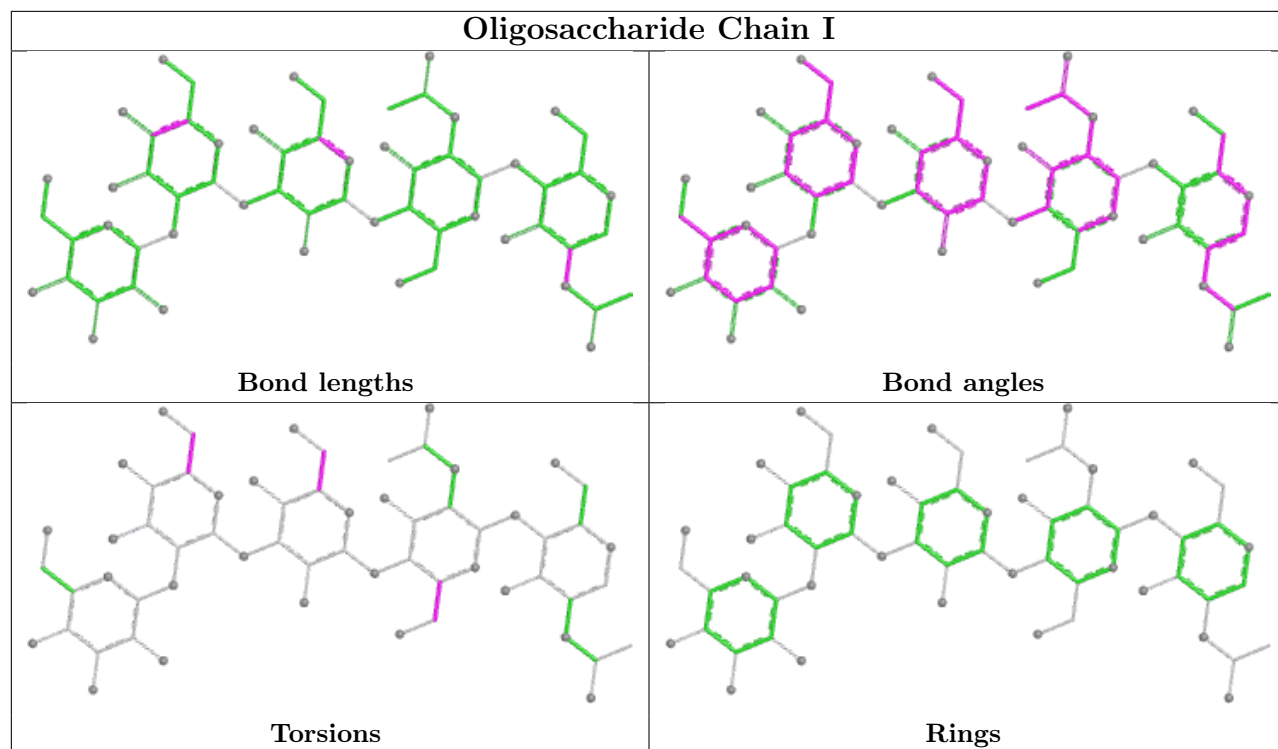




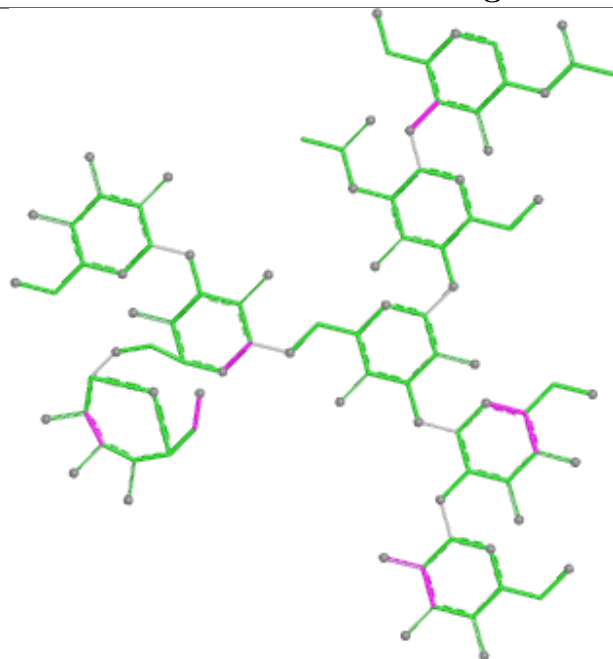




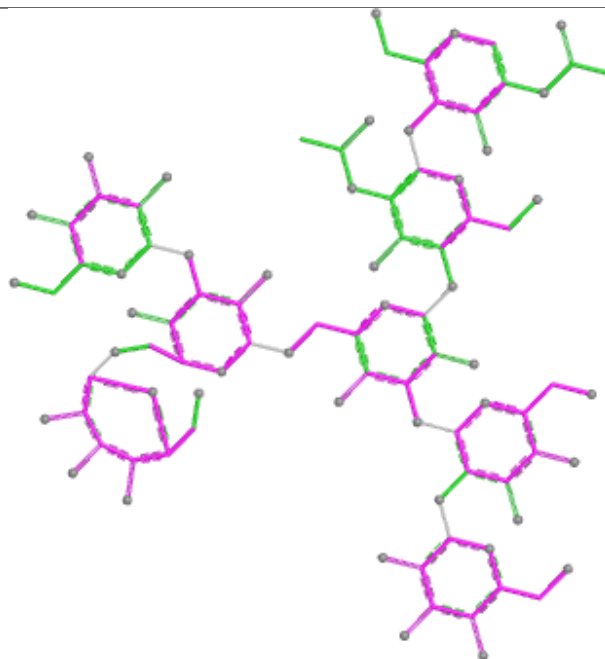




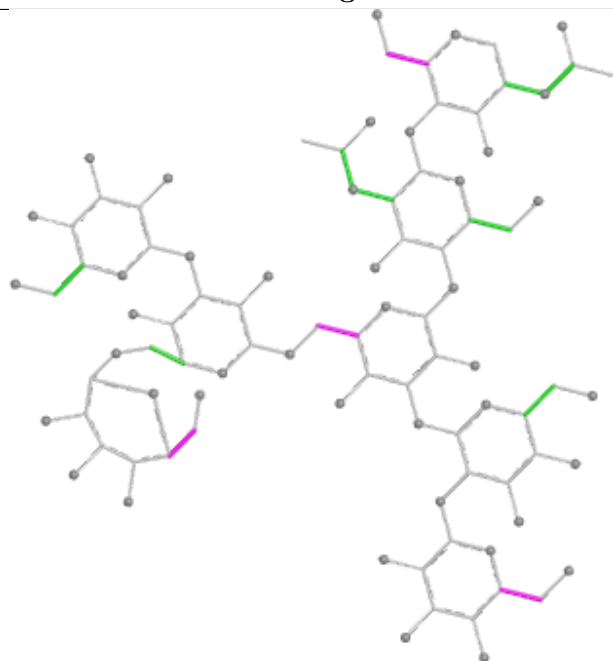
Oligosaccharide Chain K



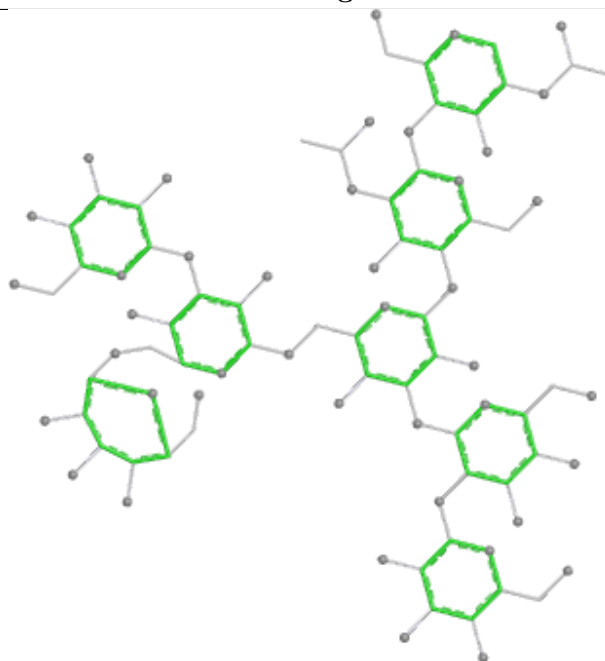
Bond lengths



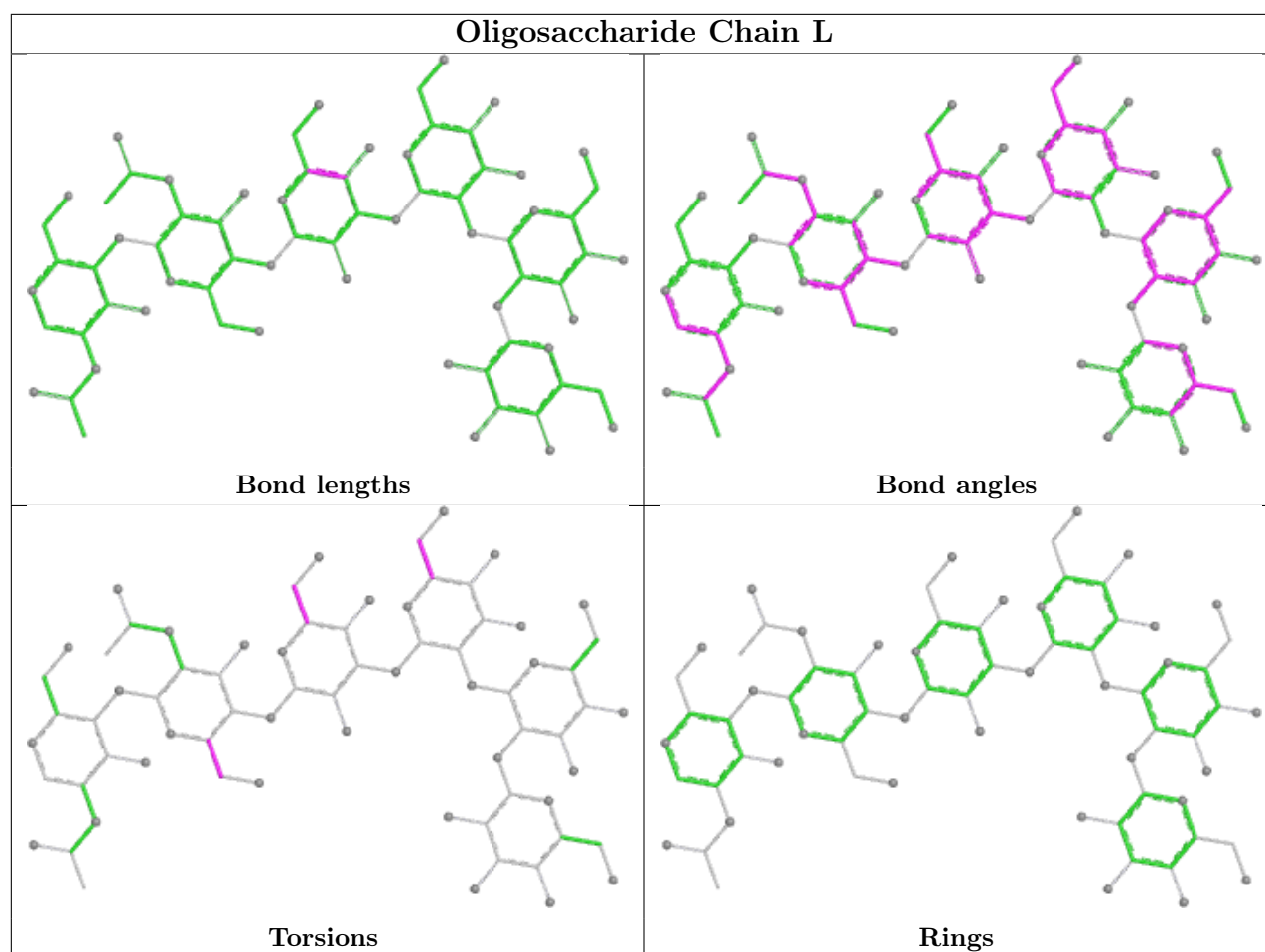
Bond angles

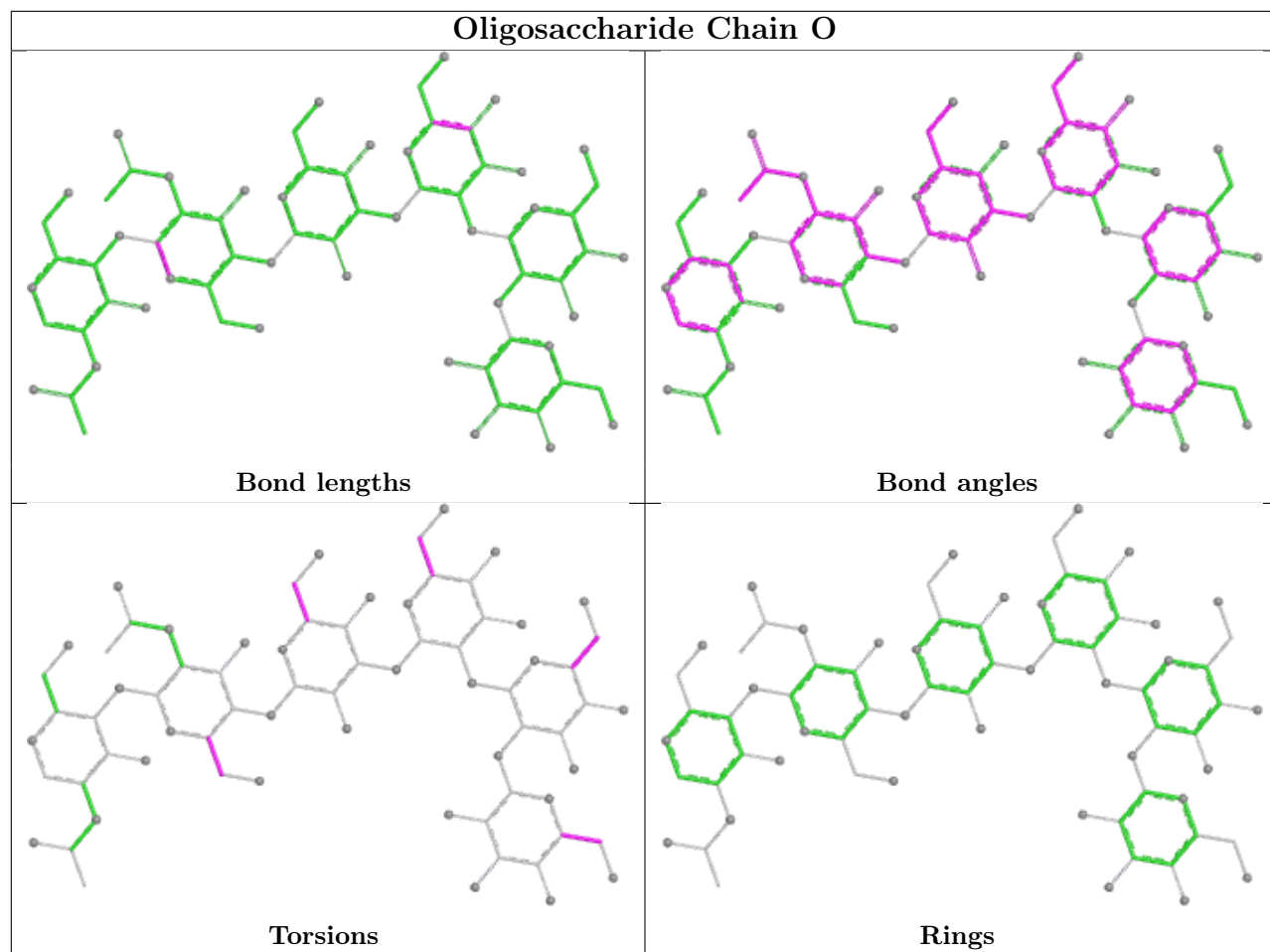


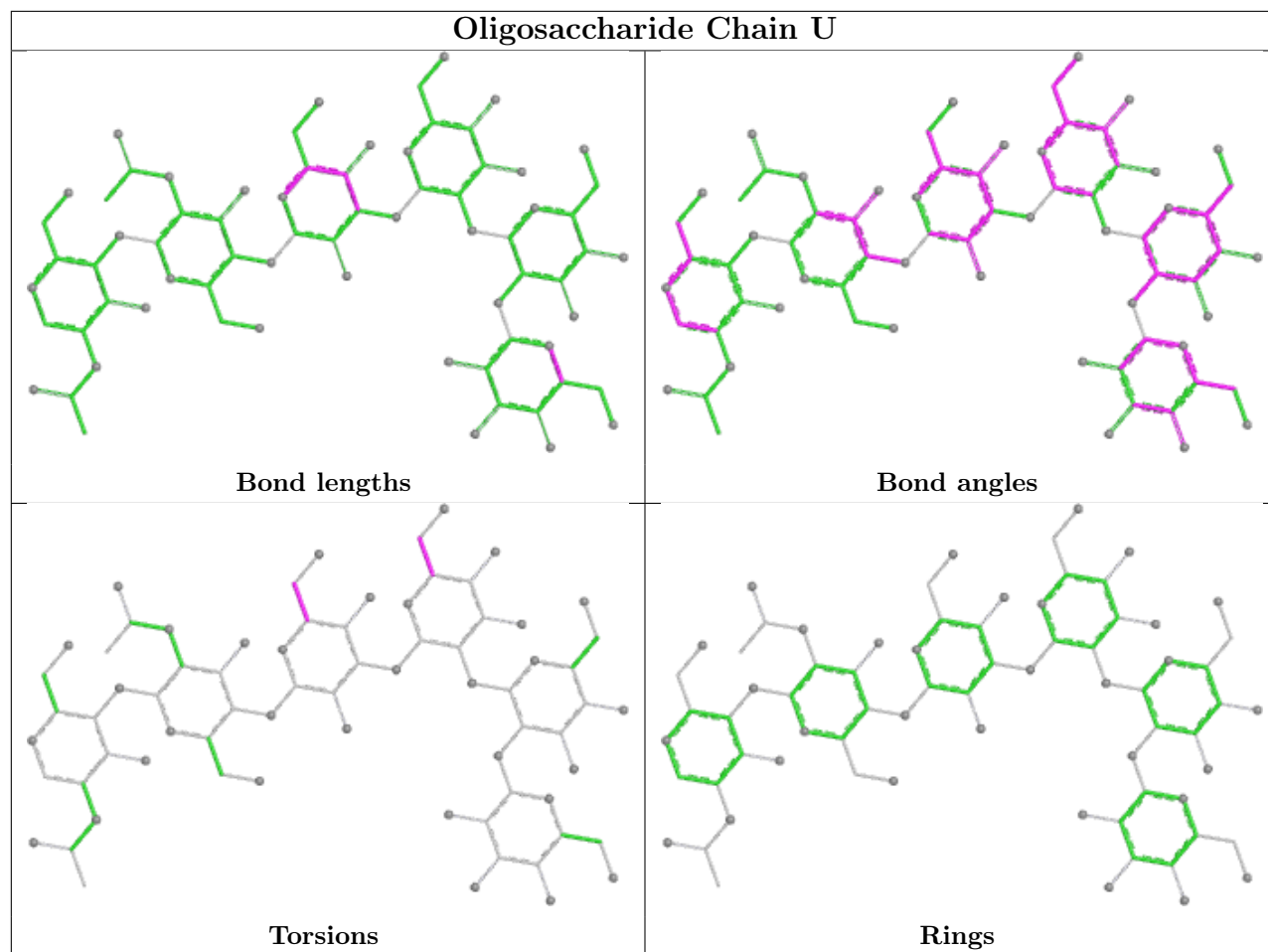
Torsions

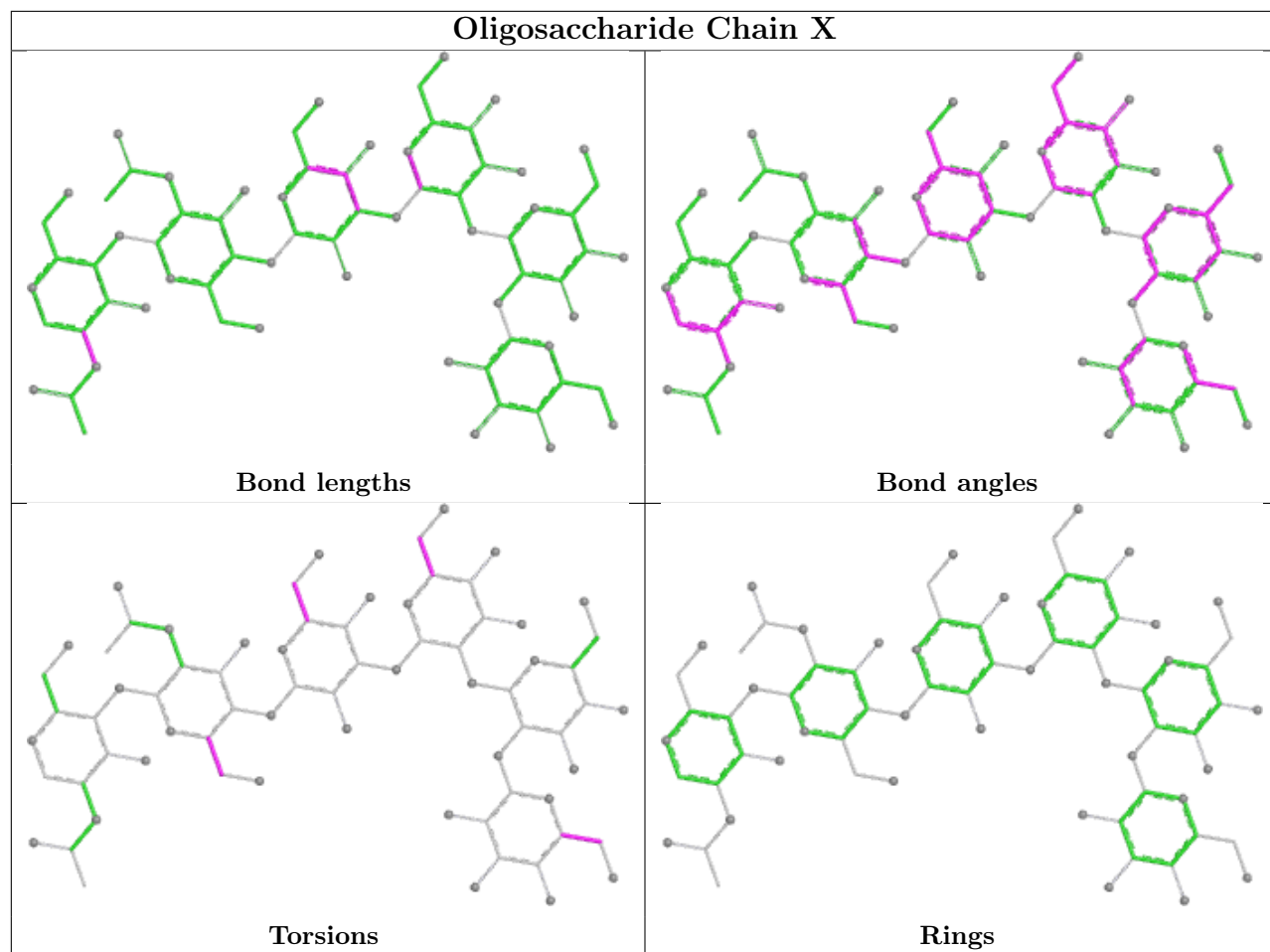


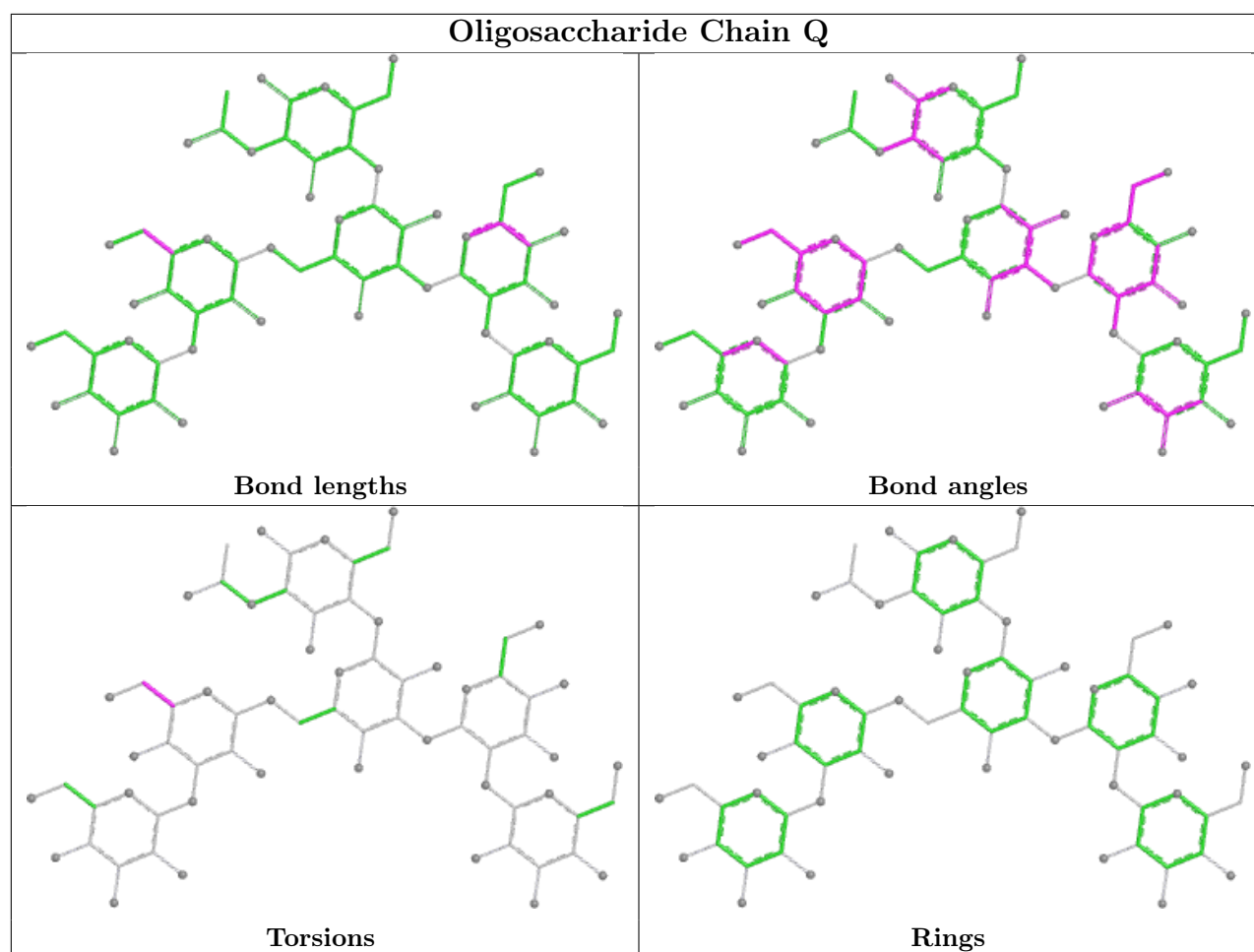
Rings











5.6 Ligand geometry [i](#)

28 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$
8	NAG	A	903	1	14,14,15	0.95	1 (7%)	17,19,21	1.15	0
9	XYZ	A	907	-	10,10,10	1.01	1 (10%)	13,14,14	2.79	6 (46%)
11	XYL	D	907	-	9,9,9	1.17	1 (11%)	11,11,11	2.43	6 (54%)
8	NAG	B	904	1	14,14,15	0.42	0	17,19,21	1.55	5 (29%)
8	NAG	E	904	1	14,14,15	0.34	0	17,19,21	1.71	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	C	905	1	14,14,15	0.76	1 (7%)	17,19,21	1.23	4 (23%)
8	NAG	B	903	1	14,14,15	0.50	0	17,19,21	1.34	1 (5%)
8	NAG	D	905	1	14,14,15	2.02	4 (28%)	17,19,21	3.69	9 (52%)
10	BMA	A	908	-	11,11,12	1.13	2 (18%)	15,15,17	1.95	5 (33%)
8	NAG	D	902	1	13,13,15	1.04	2 (15%)	12,17,21	1.46	2 (16%)
8	NAG	A	906	1	14,14,15	0.66	0	17,19,21	2.34	4 (23%)
8	NAG	B	905	1	14,14,15	1.77	2 (14%)	17,19,21	3.72	10 (58%)
8	NAG	F	903	1	14,14,15	1.15	2 (14%)	17,19,21	2.17	6 (35%)
8	NAG	A	905	1	14,14,15	0.78	1 (7%)	17,19,21	1.05	0
11	XYL	C	907	-	9,9,9	1.30	1 (11%)	11,11,11	2.49	5 (45%)
8	NAG	A	904	1	13,13,15	1.16	1 (7%)	15,17,21	3.14	5 (33%)
8	NAG	E	903	1	14,14,15	1.62	3 (21%)	17,19,21	2.54	5 (29%)
8	NAG	E	905	1	14,14,15	0.82	0	17,19,21	3.71	9 (52%)
8	NAG	C	903	1	14,14,15	1.09	1 (7%)	17,19,21	1.90	4 (23%)
8	NAG	F	905	1	14,14,15	0.54	0	17,19,21	3.39	7 (41%)
9	XYZ	B	906	-	10,10,10	1.26	1 (10%)	13,14,14	2.20	7 (53%)
8	NAG	D	906	1	14,14,15	0.60	0	17,19,21	1.95	3 (17%)
8	NAG	D	903	1	14,14,15	0.90	1 (7%)	17,19,21	1.22	4 (23%)
8	NAG	C	906	1	14,14,15	0.45	0	17,19,21	1.52	2 (11%)
8	NAG	D	904	1	13,13,15	1.23	1 (7%)	15,17,21	2.85	3 (20%)
8	NAG	C	904	1	13,13,15	0.91	1 (7%)	15,17,21	2.26	3 (20%)
8	NAG	F	904	1	14,14,15	0.46	0	17,19,21	1.42	3 (17%)
11	XYL	E	906	-	9,9,9	1.29	1 (11%)	11,11,11	2.24	5 (45%)

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
8	NAG	A	903	1	-	0/6/23/26	0/1/1/1
9	XYZ	A	907	-	-	2/2/18/18	0/1/1/1
11	XYL	D	907	-	-	6/12/12/12	-
8	NAG	B	904	1	-	1/6/23/26	0/1/1/1
8	NAG	E	904	1	-	0/6/23/26	0/1/1/1
8	NAG	C	905	1	-	0/6/23/26	0/1/1/1
8	NAG	B	903	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	905	1	-	1/6/23/26	0/1/1/1
10	BMA	A	908	-	-	2/2/19/22	0/1/1/1
8	NAG	D	902	1	-	0/6/19/26	0/1/1/1
8	NAG	A	906	1	-	2/6/23/26	0/1/1/1
8	NAG	B	905	1	-	1/6/23/26	0/1/1/1
8	NAG	F	903	1	-	2/6/23/26	0/1/1/1
8	NAG	A	905	1	-	0/6/23/26	0/1/1/1
11	XYL	C	907	-	-	8/12/12/12	-
8	NAG	A	904	1	-	1/6/19/26	0/1/1/1
8	NAG	E	903	1	-	0/6/23/26	0/1/1/1
8	NAG	E	905	1	-	2/6/23/26	0/1/1/1
8	NAG	C	903	1	-	2/6/23/26	0/1/1/1
8	NAG	F	905	1	-	3/6/23/26	0/1/1/1
9	XYZ	B	906	-	-	1/2/18/18	0/1/1/1
8	NAG	D	906	1	-	2/6/23/26	0/1/1/1
8	NAG	D	903	1	-	0/6/23/26	0/1/1/1
8	NAG	C	906	1	-	0/6/23/26	0/1/1/1
8	NAG	D	904	1	-	1/6/19/26	0/1/1/1
8	NAG	C	904	1	-	0/6/19/26	0/1/1/1
8	NAG	F	904	1	-	0/6/23/26	0/1/1/1
11	XYL	E	906	-	-	2/12/12/12	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	905	NAG	C1-C2	5.53	1.59	1.52
8	B	905	NAG	C1-C2	-4.91	1.45	1.52
8	E	903	NAG	C1-C2	4.43	1.58	1.52
8	B	905	NAG	C3-C2	3.80	1.60	1.52
8	D	904	NAG	C1-C2	3.61	1.55	1.51

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	905	NAG	O5-C1-C2	-11.52	93.46	111.29
8	E	905	NAG	C1-O5-C5	10.28	125.97	112.19
8	A	904	NAG	C3-C2-C1	10.14	118.83	109.50
8	D	904	NAG	C3-C2-C1	9.19	117.95	109.50
8	B	905	NAG	C1-C2-N2	8.18	123.32	110.43

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

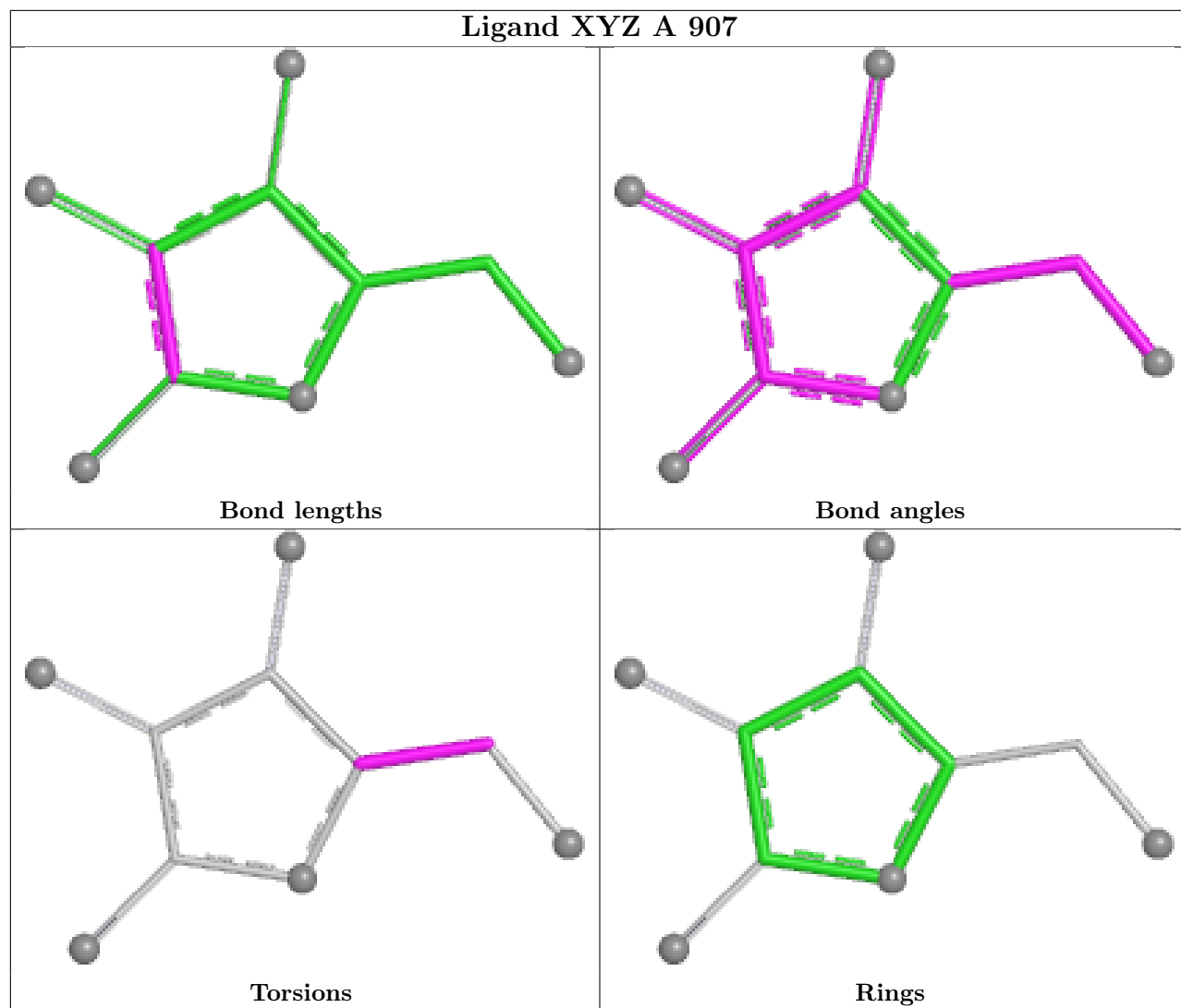
Mol	Chain	Res	Type	Atoms
8	B	905	NAG	C3-C2-N2-C7
8	E	905	NAG	C3-C2-N2-C7
8	F	905	NAG	C3-C2-N2-C7
11	C	907	XYL	O1-C1-C2-C3
11	C	907	XYL	O1-C1-C2-O2

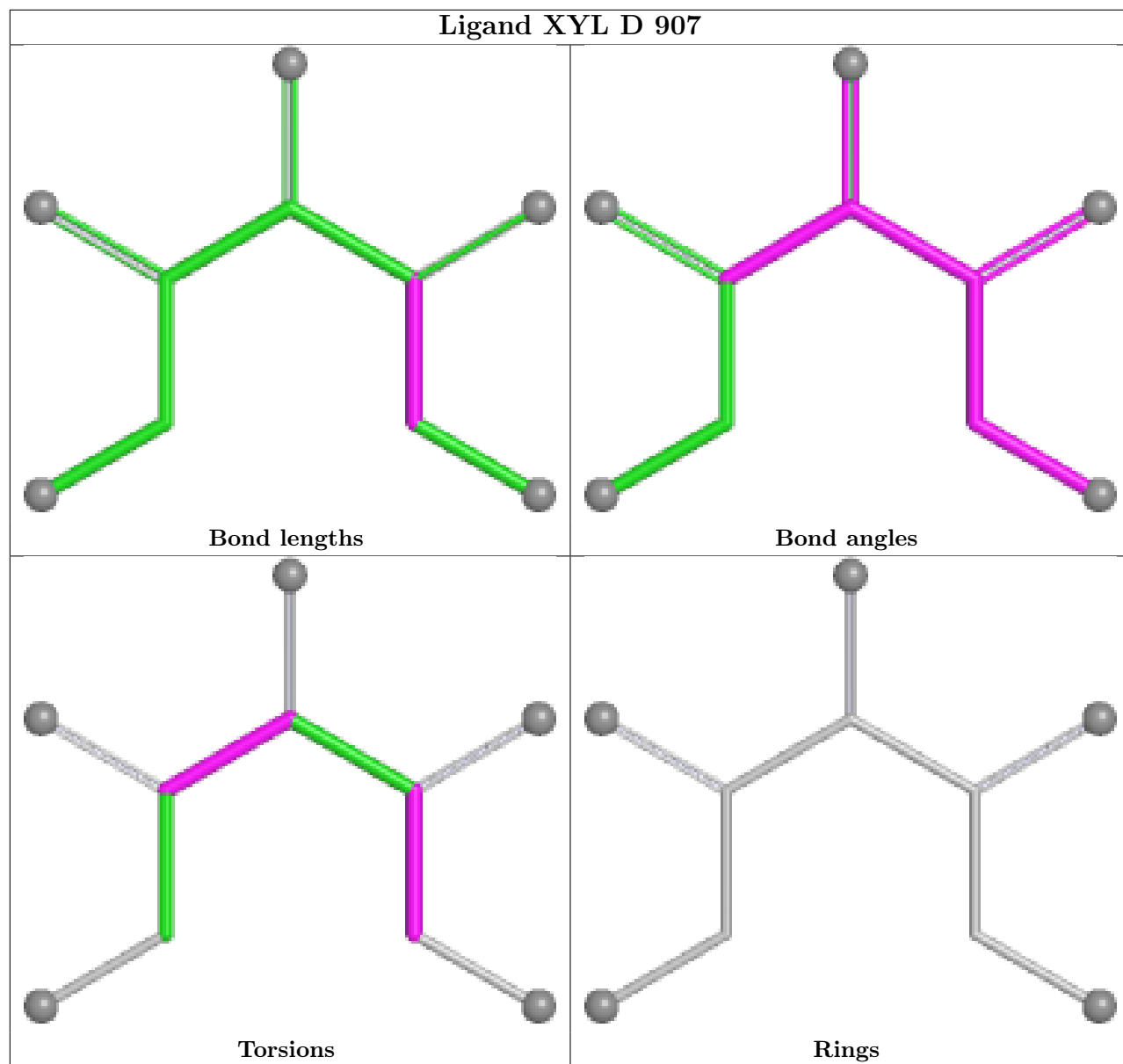
There are no ring outliers.

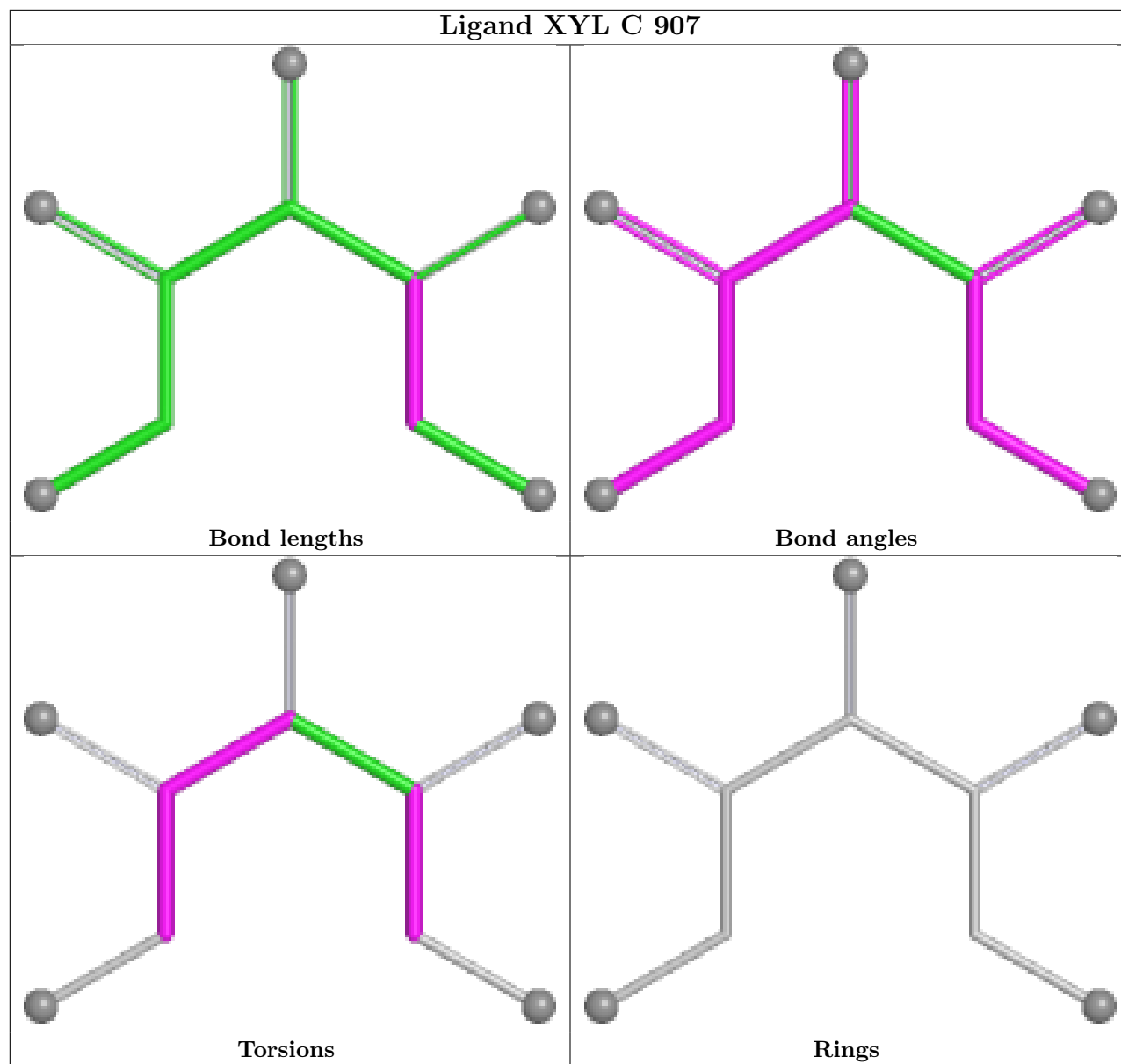
7 monomers are involved in 12 short contacts:

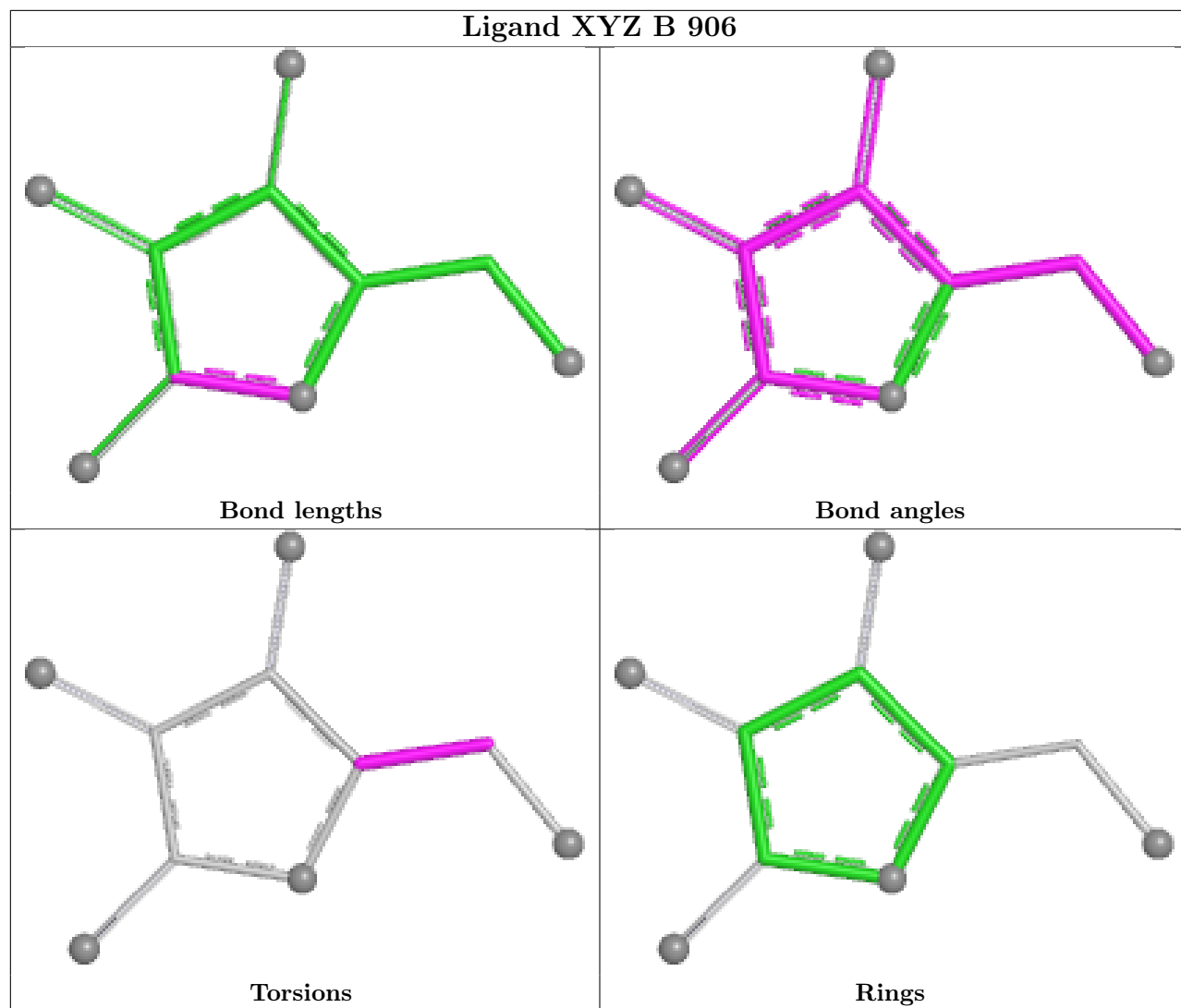
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	907	XYZ	1	0
8	D	902	NAG	3	0
8	B	905	NAG	2	0
11	C	907	XYL	2	0
8	E	905	NAG	2	0
9	B	906	XYZ	1	0
11	E	906	XYL	1	0

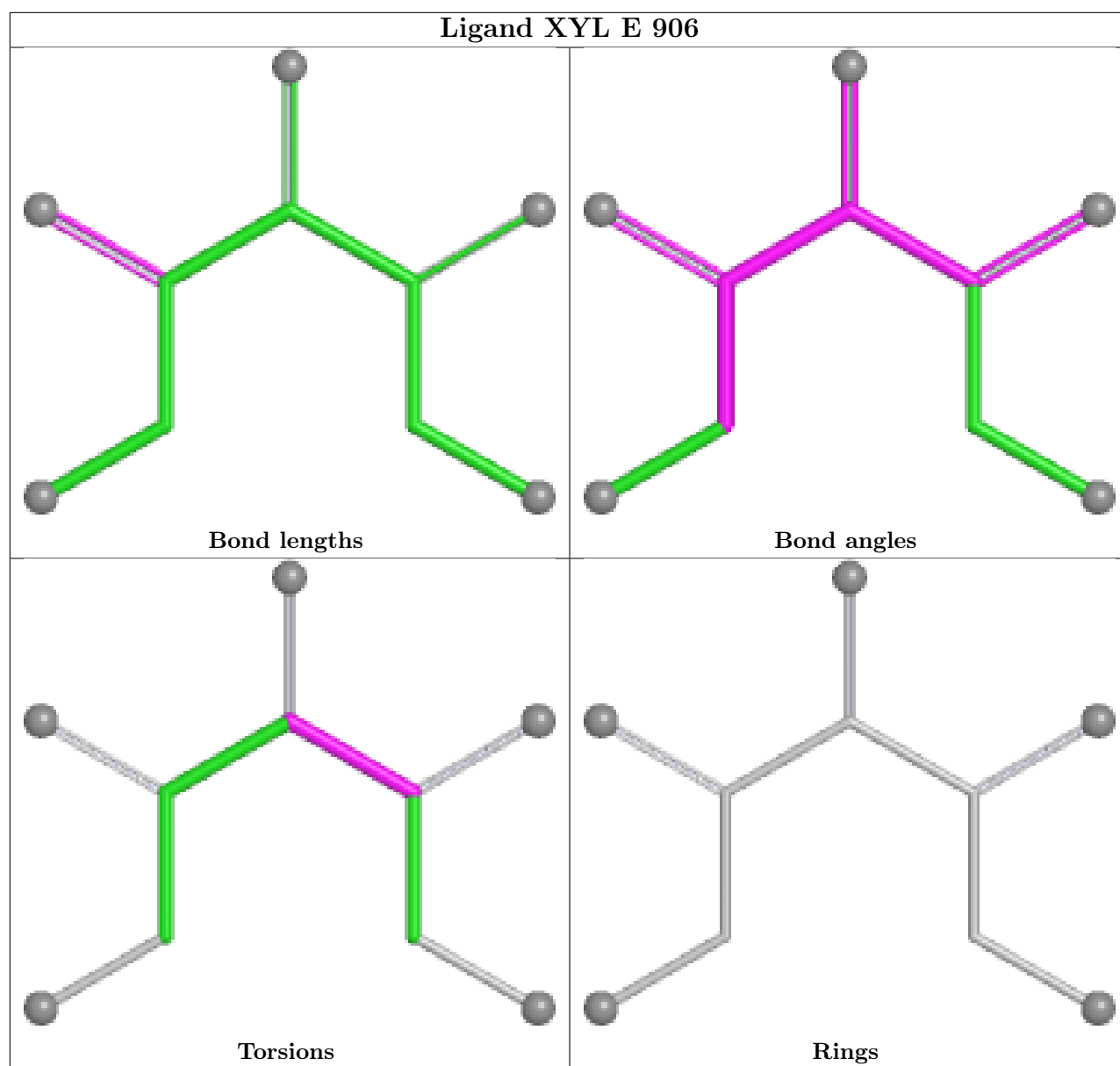
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	758/805 (94%)	-1.38	1 (0%) 92 93	18, 29, 47, 98	1 (0%)
1	B	758/805 (94%)	-1.40	0 100 100	18, 27, 44, 90	1 (0%)
1	C	756/805 (93%)	-1.36	1 (0%) 92 93	19, 29, 46, 92	1 (0%)
1	D	756/805 (93%)	-1.37	1 (0%) 92 93	18, 29, 46, 102	1 (0%)
1	E	757/805 (94%)	-1.38	0 100 100	18, 27, 44, 85	1 (0%)
1	F	757/805 (94%)	-1.40	0 100 100	18, 27, 44, 88	1 (0%)
All	All	4542/4830 (94%)	-1.38	3 (0%) 92 93	18, 28, 45, 102	6 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	804	HIS	2.5
1	C	804	HIS	2.4
1	A	804	HIS	2.2

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	I	5	11/12	0.95	0.08	72,82,90,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	V	3	11/12	0.96	0.07	62,74,82,85	0
3	MAN	T	5	11/12	0.96	0.07	55,58,68,75	0
2	BMA	J	3	11/12	0.96	0.07	56,69,76,85	0
5	MAN	K	5	11/12	0.96	0.07	50,59,71,72	0
6	MAN	L	3	11/12	0.96	0.07	32,50,57,59	0
6	MAN	O	5	11/12	0.96	0.09	77,85,91,100	0
6	MAN	U	3	11/12	0.96	0.07	33,48,56,59	0
6	MAN	X	3	11/12	0.96	0.07	40,47,56,56	0
3	MAN	W	5	11/12	0.97	0.06	52,54,64,64	0
3	MAN	W	6	11/12	0.97	0.06	39,42,44,45	0
4	MAN	I	3	11/12	0.97	0.07	51,56,59,59	0
4	MAN	I	4	11/12	0.97	0.06	52,60,67,70	0
2	BMA	G	3	11/12	0.97	0.08	62,75,79,80	0
3	BMA	N	4	11/12	0.97	0.06	47,52,57,59	0
5	MAN	K	8	11/12	0.97	0.08	57,77,86,86	0
3	MAN	N	5	11/12	0.97	0.08	47,53,59,60	0
6	MAN	L	5	11/12	0.97	0.08	62,68,82,86	0
6	MAN	O	3	11/12	0.97	0.06	46,52,56,56	0
2	BMA	S	3	11/12	0.97	0.06	61,68,76,76	0
6	MAN	O	6	11/12	0.97	0.08	80,93,100,103	0
3	MAN	T	6	11/12	0.97	0.05	40,42,45,46	0
6	MAN	U	5	11/12	0.97	0.07	59,63,71,75	0
3	MAN	T	7	11/12	0.97	0.06	41,46,52,53	0
7	MAN	Q	4	11/12	0.97	0.07	45,48,58,60	0
7	MAN	Q	5	11/12	0.97	0.06	36,44,51,54	0
3	BMA	H	4	11/12	0.98	0.04	44,48,53,53	0
3	MAN	H	5	11/12	0.98	0.06	45,52,58,59	0
3	MAN	H	7	11/12	0.98	0.05	47,52,54,59	0
4	MAN	R	3	11/12	0.98	0.05	51,55,60,63	0
4	MAN	R	4	11/12	0.98	0.06	51,56,61,61	0
4	MAN	R	5	11/12	0.98	0.07	60,69,85,89	0
5	BMA	K	4	11/12	0.98	0.04	41,45,49,52	0
3	BMA	N	3	11/12	0.98	0.04	37,39,44,46	0
2	NAG	M	2	14/15	0.98	0.05	41,45,57,68	0
2	BMA	M	3	11/12	0.98	0.07	58,70,77,78	0
3	MAN	N	6	11/12	0.98	0.05	40,46,49,51	0
6	MAN	L	6	11/12	0.98	0.07	59,66,72,74	0
3	MAN	N	7	11/12	0.98	0.04	44,46,49,50	0
6	MAN	O	4	11/12	0.98	0.06	50,59,66,66	0
3	BMA	T	4	11/12	0.98	0.04	43,45,50,50	0
2	NAG	P	2	14/15	0.98	0.05	44,50,59,70	0
2	BMA	P	3	11/12	0.98	0.06	61,68,76,78	0

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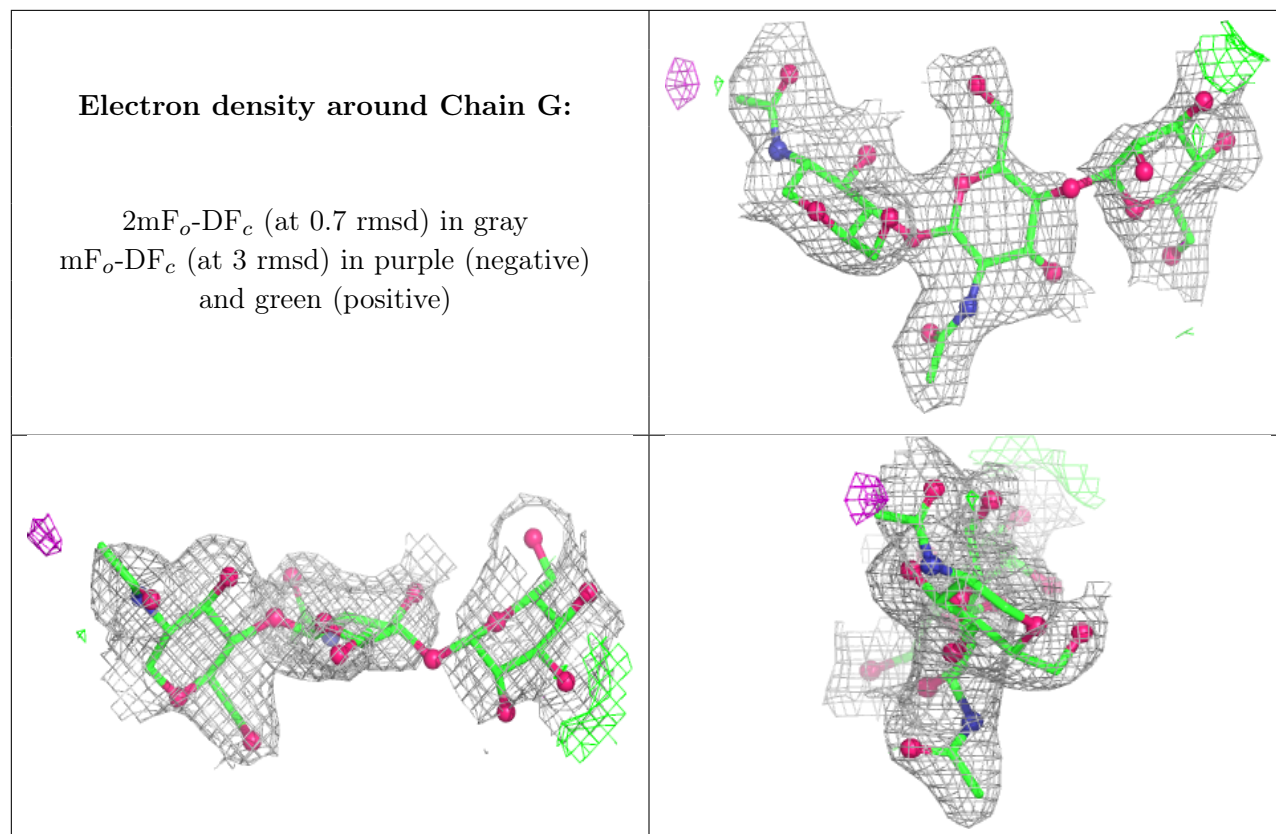
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	U	4	11/12	0.98	0.04	40,43,48,58	0
2	NAG	S	2	14/15	0.98	0.05	36,40,46,54	0
2	NAG	J	2	14/15	0.98	0.04	37,43,50,57	0
6	MAN	X	4	11/12	0.98	0.04	41,42,52,52	0
6	MAN	X	5	11/12	0.98	0.05	57,62,66,71	0
6	MAN	X	6	11/12	0.98	0.08	57,66,72,72	0
7	BMA	Q	3	11/12	0.98	0.05	46,50,54,56	0
2	NAG	G	2	14/15	0.98	0.05	43,52,66,76	0
3	MAN	W	7	11/12	0.98	0.05	38,43,45,47	0
7	MAN	Q	6	11/12	0.98	0.05	45,49,51,51	0
2	NAG	V	2	14/15	0.99	0.05	36,41,48,55	0
2	NAG	M	1	14/15	0.99	0.04	28,33,37,38	0
3	NAG	H	1	14/15	0.99	0.03	25,27,33,36	0
5	NAG	K	1	14/15	0.99	0.04	25,27,31,36	0
5	NAG	K	2	14/15	0.99	0.04	24,26,30,33	0
5	BMA	K	3	11/12	0.99	0.03	29,32,39,46	0
3	NAG	T	1	14/15	0.99	0.03	25,26,31,36	0
3	NAG	T	2	14/15	0.99	0.03	22,25,29,31	0
5	MAN	K	6	11/12	0.99	0.04	41,50,79,88	0
5	MAN	K	7	11/12	0.99	0.04	41,45,48,49	0
3	BMA	T	3	11/12	0.99	0.03	28,31,36,37	0
6	NAG	L	1	14/15	0.99	0.02	20,21,25,26	0
6	NAG	L	2	14/15	0.99	0.04	27,30,36,40	0
3	NAG	H	2	14/15	0.99	0.04	35,37,40,41	0
6	MAN	L	4	11/12	0.99	0.04	40,42,49,60	0
3	BMA	H	3	11/12	0.99	0.03	37,37,44,48	0
2	NAG	G	1	14/15	0.99	0.04	29,32,35,42	0
6	NAG	O	1	14/15	0.99	0.04	23,27,30,32	0
6	NAG	O	2	14/15	0.99	0.06	28,34,44,45	0
2	NAG	S	1	14/15	0.99	0.03	28,36,38,40	0
3	NAG	W	1	14/15	0.99	0.04	23,26,30,34	0
3	NAG	W	2	14/15	0.99	0.03	24,27,30,32	0
3	BMA	W	3	11/12	0.99	0.03	30,33,36,37	0
6	NAG	U	1	14/15	0.99	0.03	20,23,27,27	0
6	NAG	U	2	14/15	0.99	0.03	25,30,34,37	0
3	BMA	W	4	11/12	0.99	0.04	42,47,53,53	0
3	MAN	H	6	11/12	0.99	0.04	37,46,50,51	0
2	NAG	J	1	14/15	0.99	0.04	27,34,36,37	0
6	MAN	U	6	11/12	0.99	0.07	49,60,64,65	0
6	NAG	X	1	14/15	0.99	0.03	20,23,28,32	0
6	NAG	X	2	14/15	0.99	0.03	28,32,38,39	0
3	NAG	N	1	14/15	0.99	0.04	27,28,34,36	0

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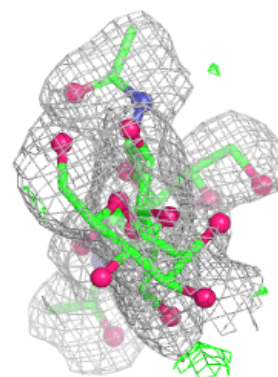
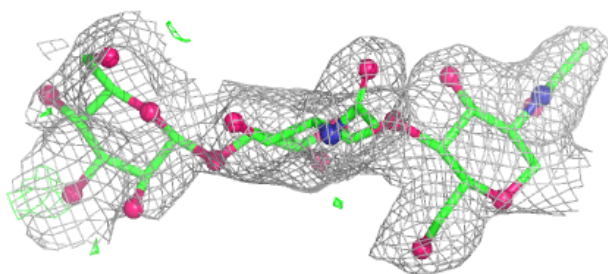
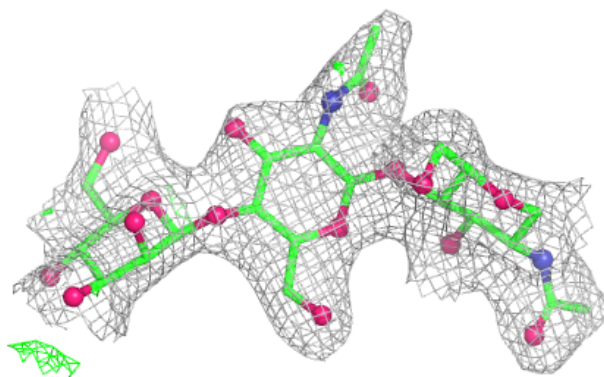
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	I	1	14/15	0.99	0.03	22,26,30,31	0
4	NAG	I	2	14/15	0.99	0.05	27,34,47,48	0
3	NAG	N	2	14/15	0.99	0.06	34,39,42,44	0
7	NAG	Q	1	15/15	0.99	0.04	35,37,41,42	0
7	BMA	Q	2	11/12	0.99	0.04	40,41,44,47	0
2	NAG	P	1	14/15	0.99	0.05	28,33,35,40	0
2	NAG	V	1	14/15	0.99	0.04	31,34,37,38	0
4	NAG	R	1	14/15	0.99	0.05	23,25,29,30	0
4	NAG	R	2	14/15	0.99	0.04	27,32,40,48	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.

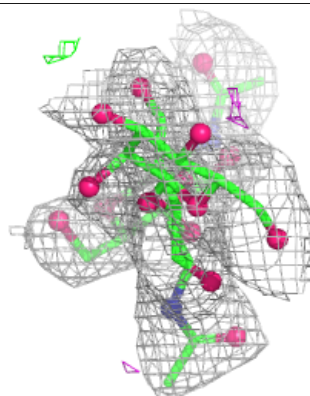
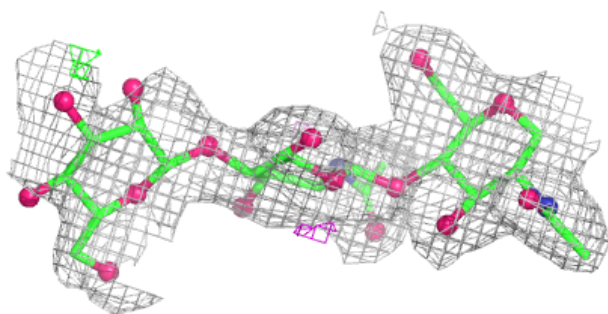
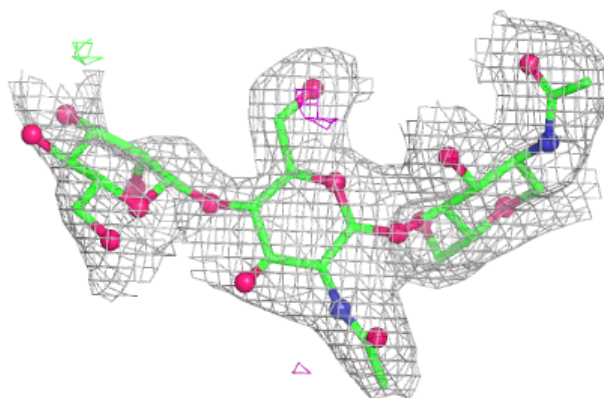


Electron density around Chain J:

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

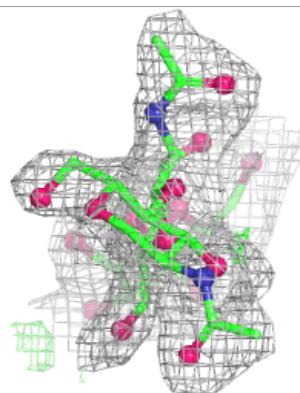
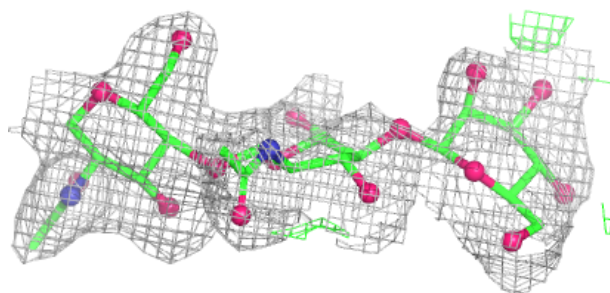
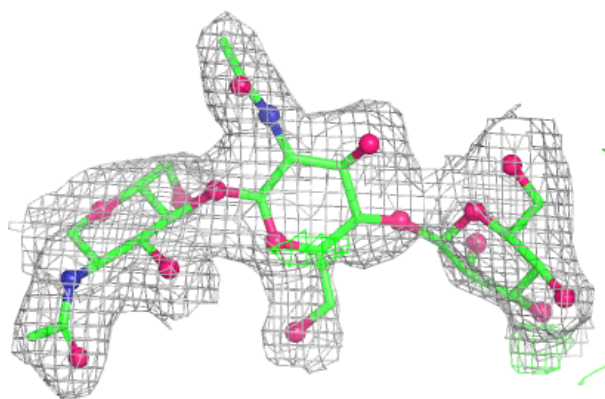
**Electron density around Chain M:**

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

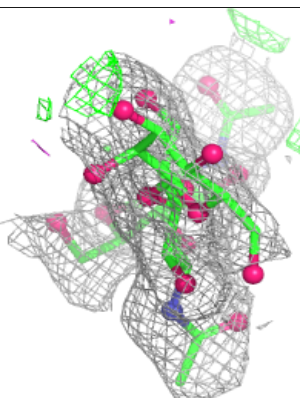
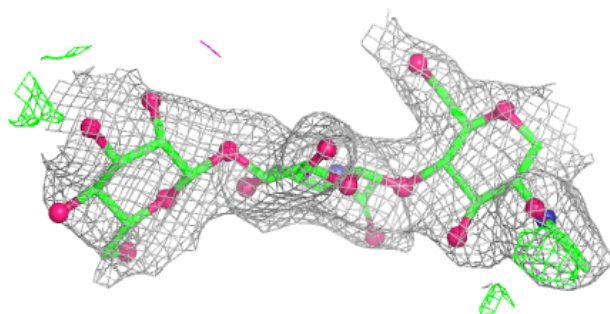
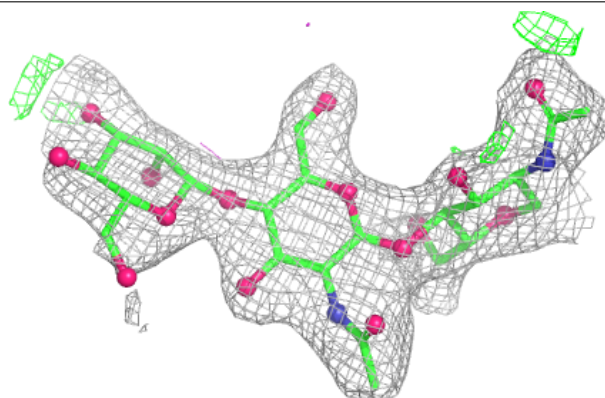


Electron density around Chain P:

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

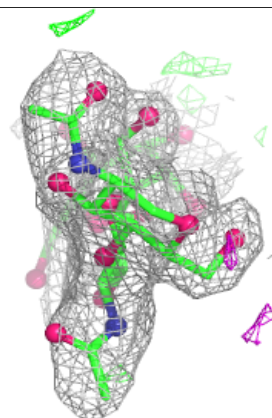
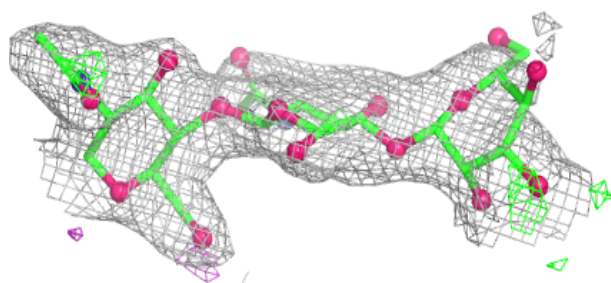
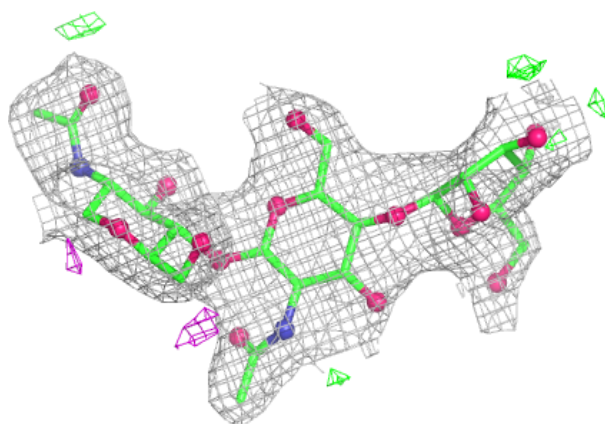
**Electron density around Chain S:**

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



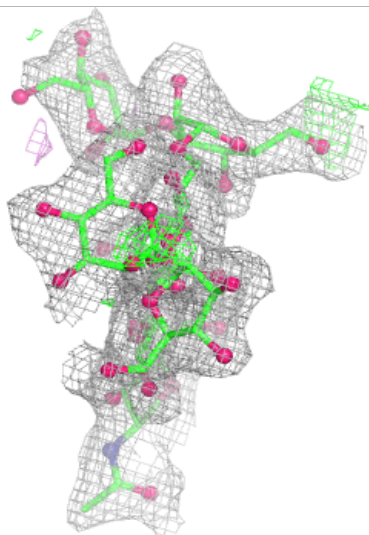
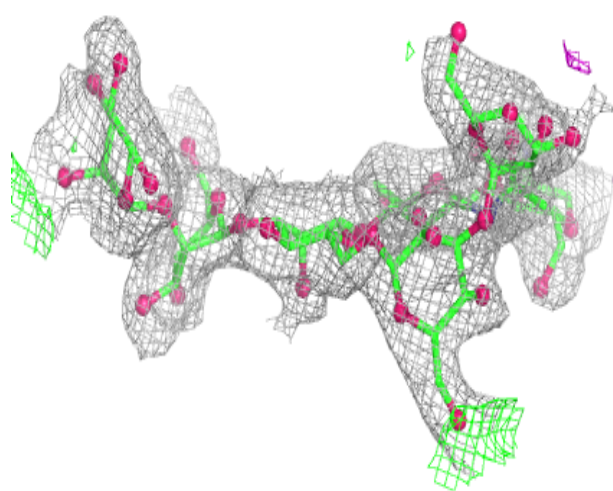
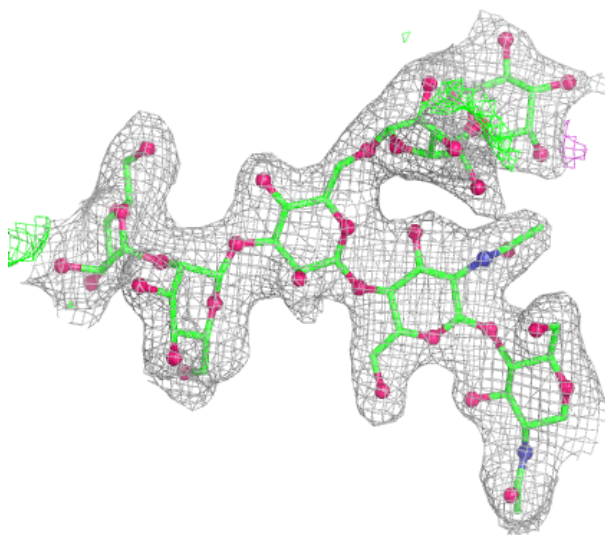
Electron density around Chain V:

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



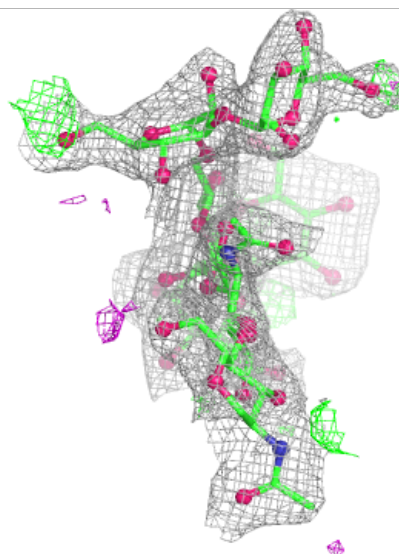
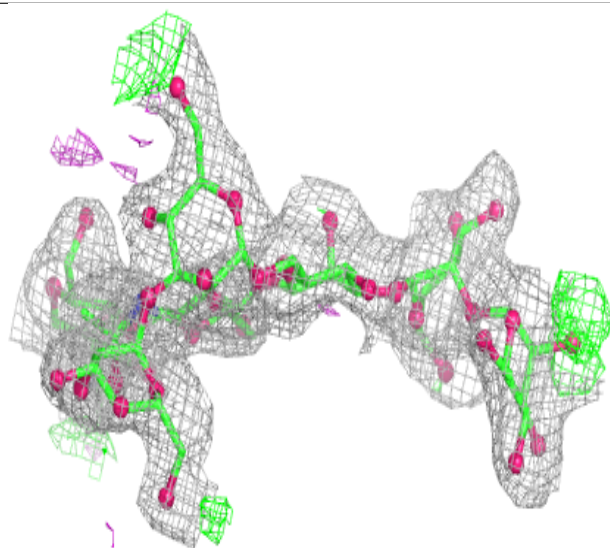
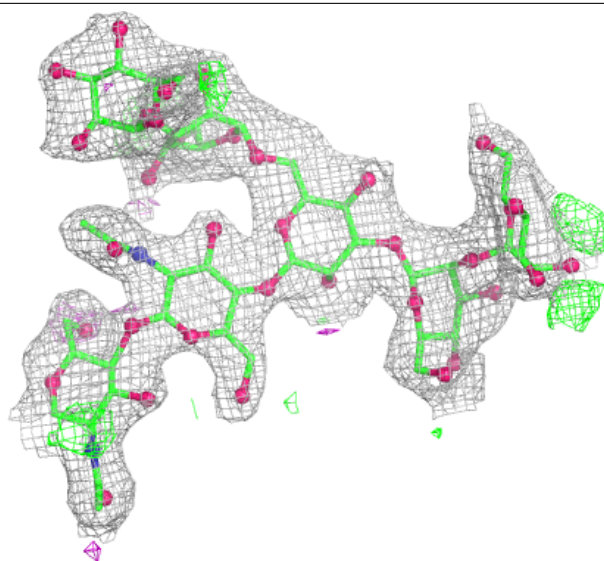
Electron density around Chain H:

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



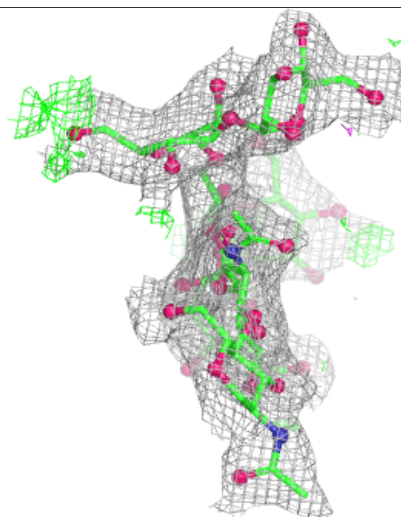
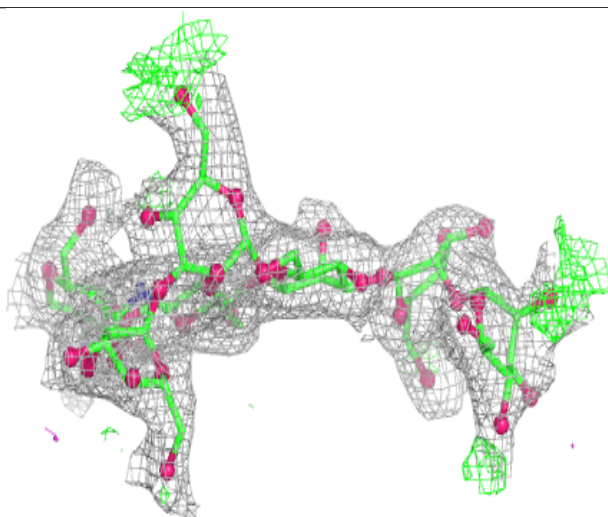
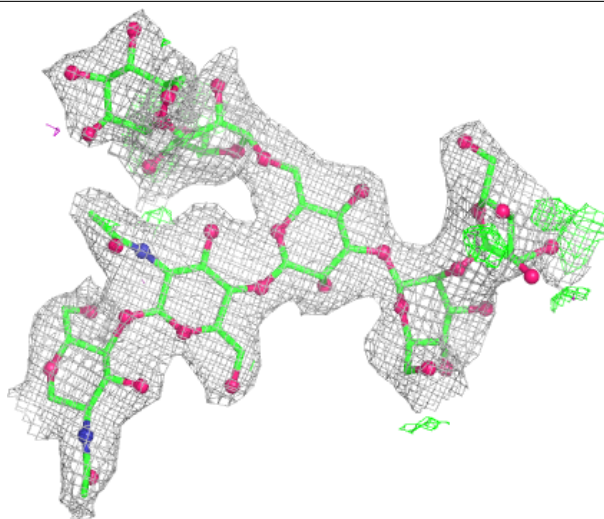
Electron density around Chain N:

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and green (positive)



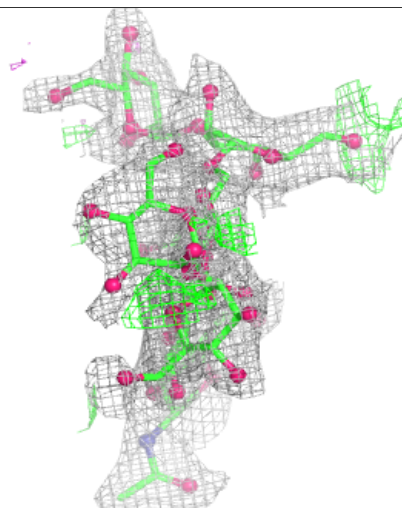
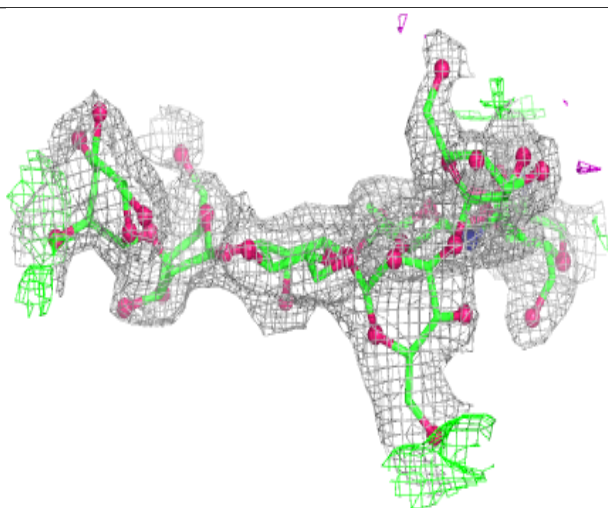
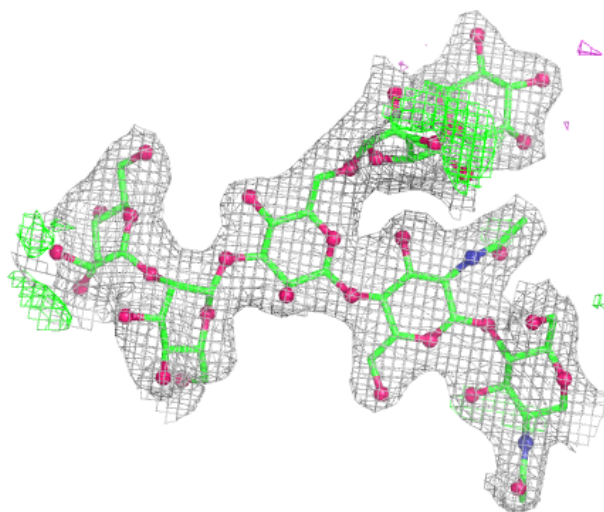
Electron density around Chain T:

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and green (positive)



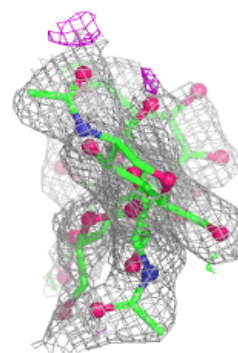
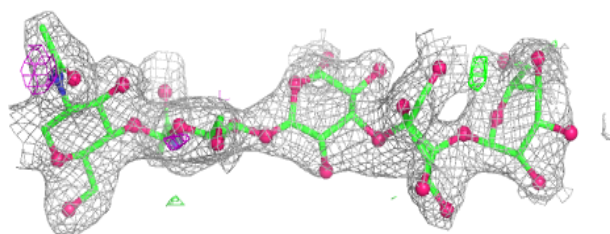
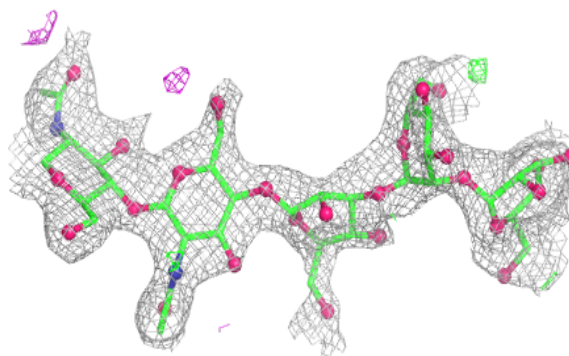
Electron density around Chain W:

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

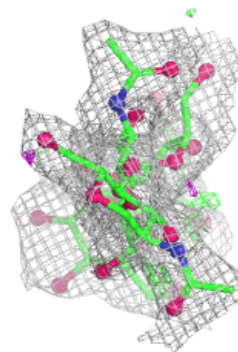
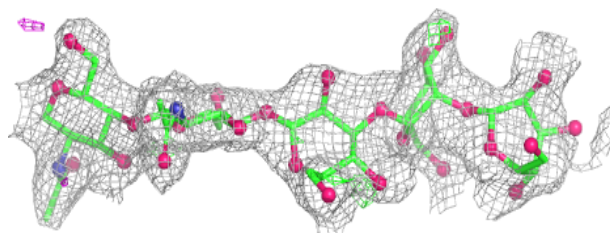
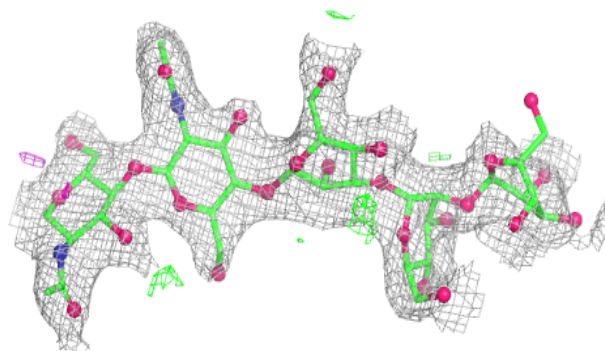


Electron density around Chain I:

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

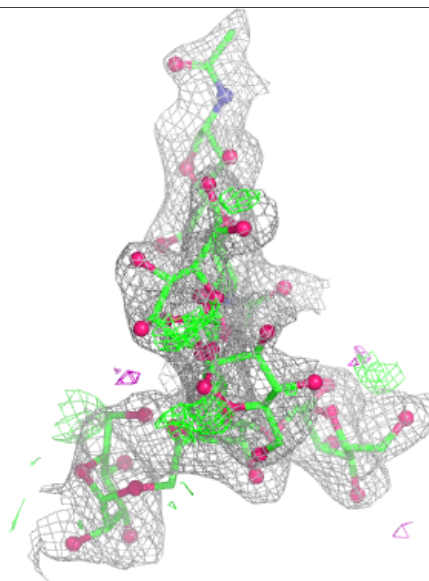
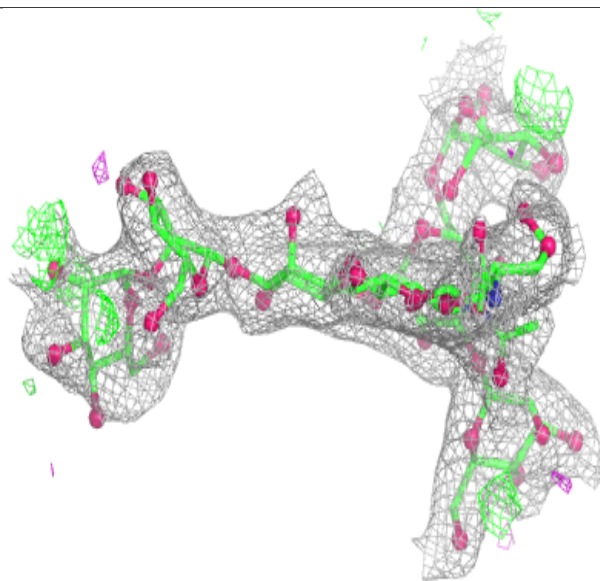
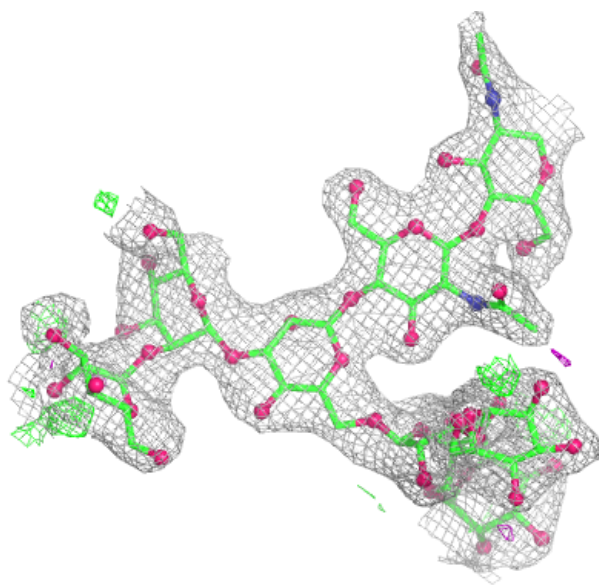
**Electron density around Chain R:**

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



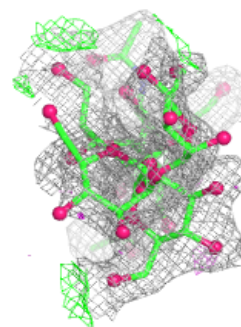
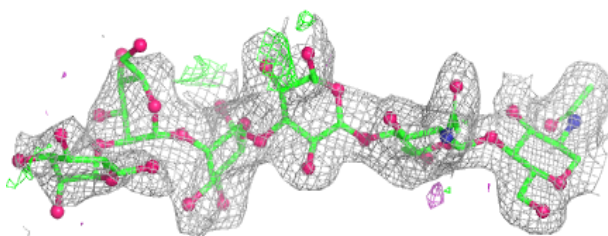
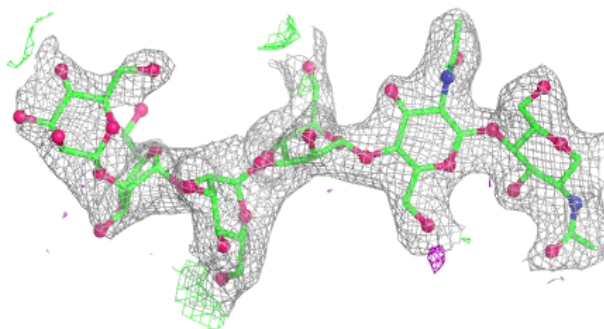
Electron density around Chain K:

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

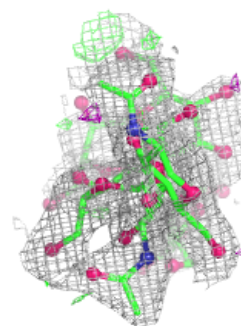
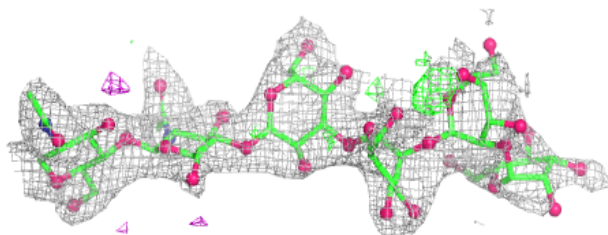
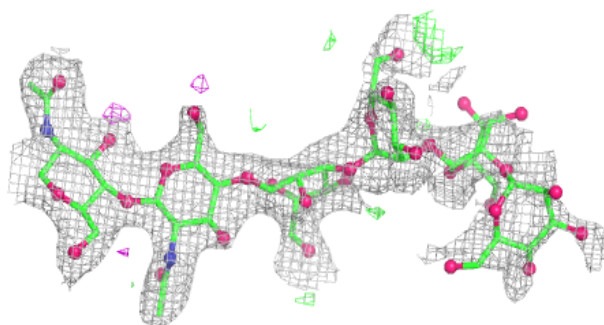


Electron density around Chain L:

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

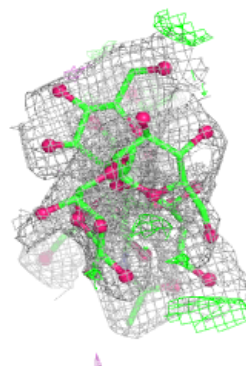
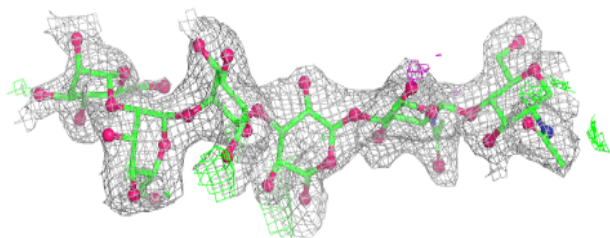
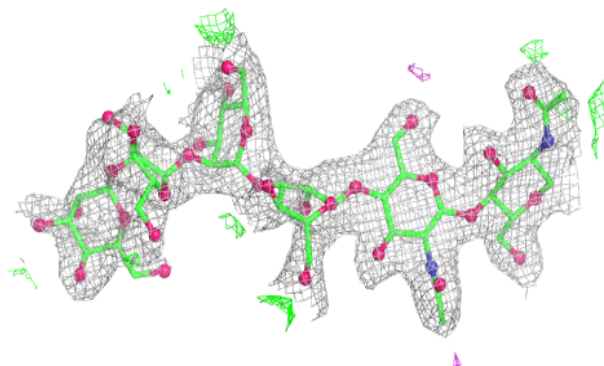
**Electron density around Chain O:**

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

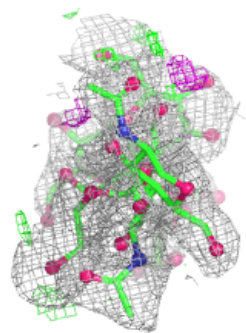
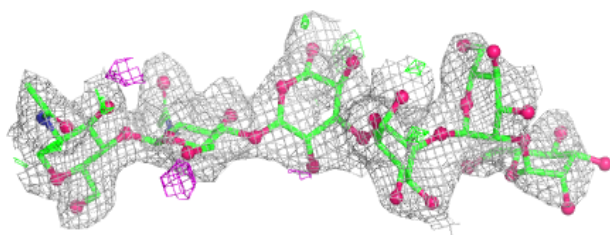
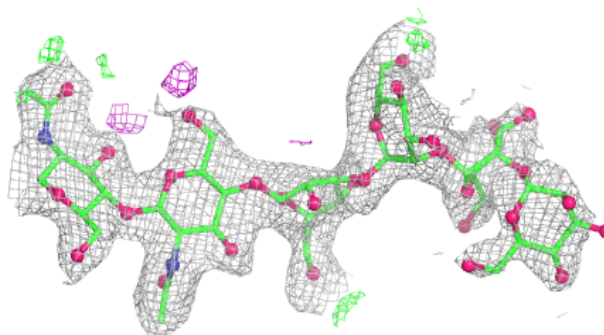


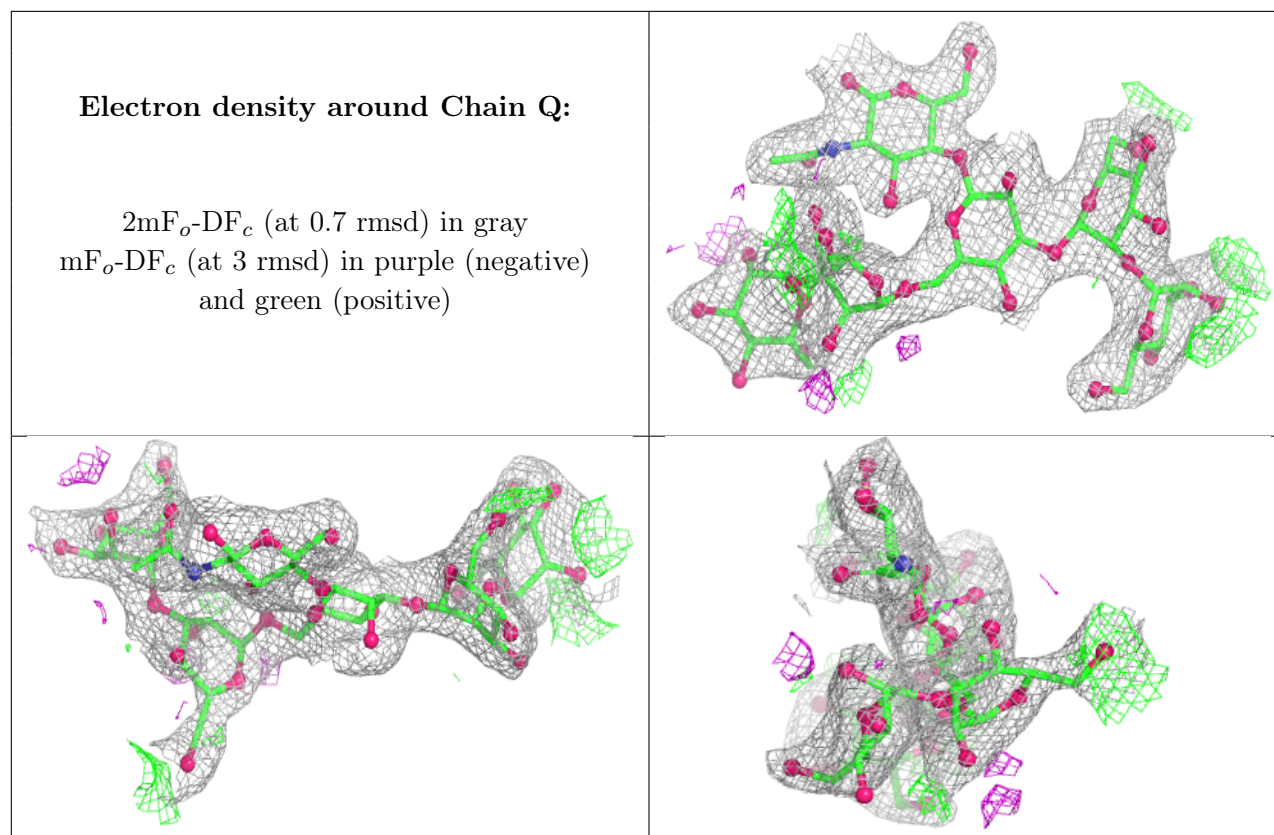
Electron density around Chain U:

$2mF_o-DF_c$ (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
8	NAG	A	903	14/15	0.96	0.06	54,62,74,74	0
8	NAG	A	906	14/15	0.96	0.09	70,75,80,84	0
8	NAG	C	906	14/15	0.96	0.09	36,42,45,46	14
8	NAG	D	906	14/15	0.96	0.07	69,78,84,84	0
10	BMA	A	908	11/12	0.97	0.06	79,88,92,95	0
8	NAG	C	904	13/15	0.98	0.04	54,55,61,61	0
8	NAG	A	904	13/15	0.98	0.05	45,51,56,57	0
8	NAG	D	903	14/15	0.98	0.05	55,63,67,68	0
8	NAG	D	904	13/15	0.98	0.05	51,56,63,63	0
8	NAG	B	905	14/15	0.98	0.05	40,45,49,50	0
8	NAG	E	903	14/15	0.98	0.05	48,56,65,66	0
8	NAG	F	903	14/15	0.98	0.04	54,59,65,70	0
8	NAG	C	903	14/15	0.98	0.05	55,63,75,77	0
8	NAG	B	904	14/15	0.99	0.03	30,35,38,39	0

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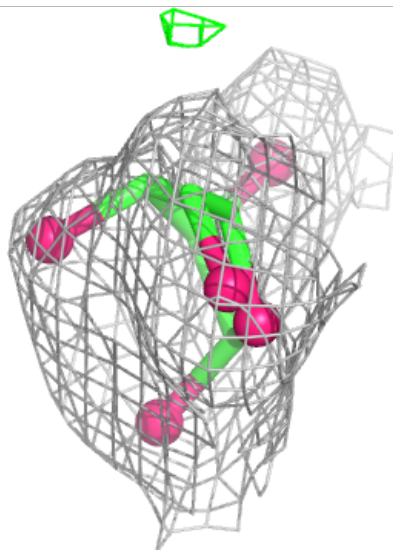
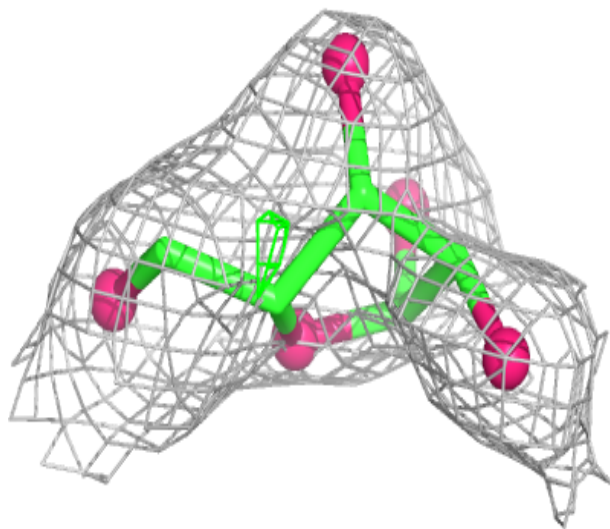
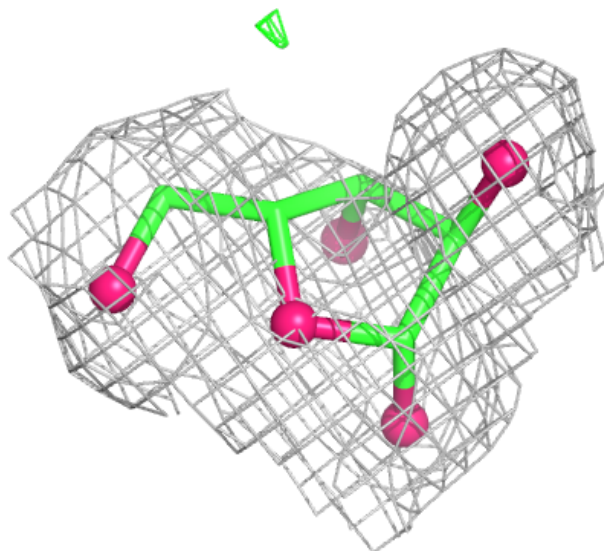
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	D	905	14/15	0.99	0.03	22,28,32,35	0
8	NAG	C	905	14/15	0.99	0.03	24,29,33,34	0
8	NAG	A	905	14/15	0.99	0.04	23,28,30,31	0
8	NAG	E	904	14/15	0.99	0.04	30,34,38,41	0
8	NAG	E	905	14/15	0.99	0.04	37,46,51,52	0
8	NAG	D	902	13/15	0.99	0.03	24,27,35,35	0
8	NAG	F	904	14/15	0.99	0.03	28,32,36,39	0
8	NAG	F	905	14/15	0.99	0.05	35,44,53,53	0
9	XYZ	A	907	10/10	0.99	0.04	37,47,54,54	0
9	XYZ	B	906	10/10	0.99	0.04	40,53,58,65	0
8	NAG	B	903	14/15	0.99	0.04	52,56,66,66	0
11	XYL	C	907	10/10	0.99	0.06	37,45,50,67	0
11	XYL	D	907	10/10	0.99	0.05	39,42,48,63	0
11	XYL	E	906	10/10	0.99	0.04	32,43,49,53	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.

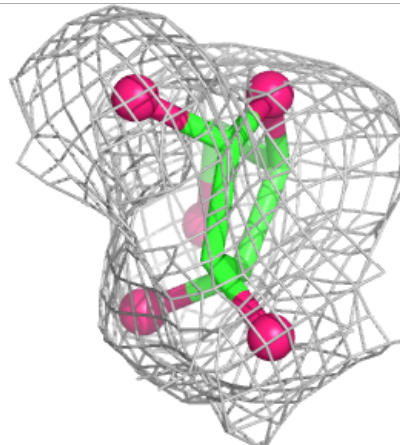
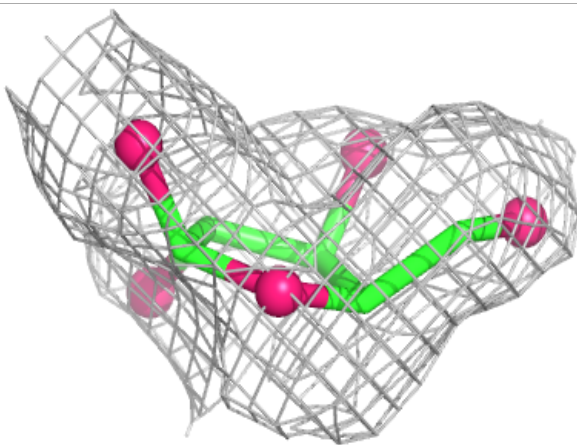
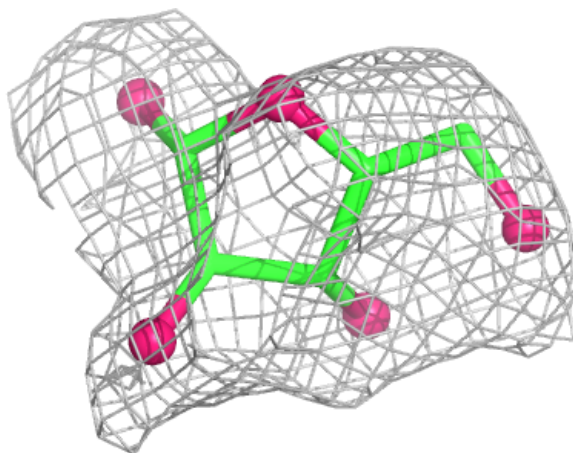
Electron density around XYZ A 907:

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



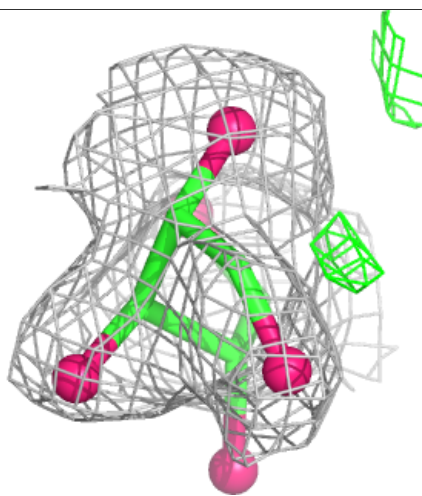
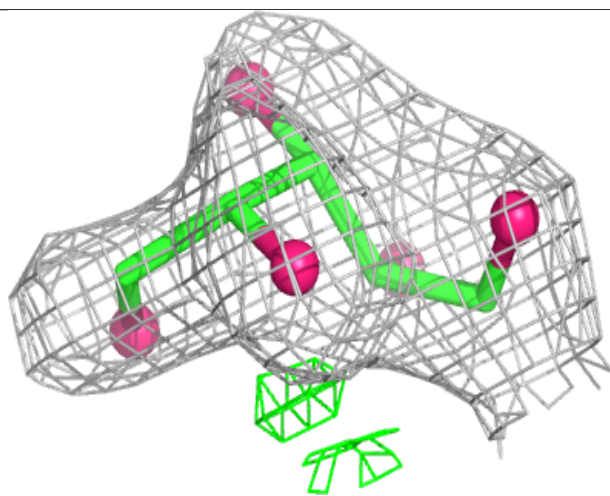
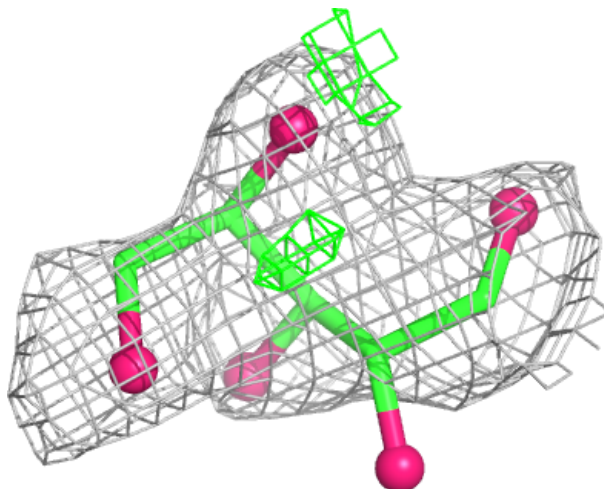
Electron density around XYZ B 906:

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



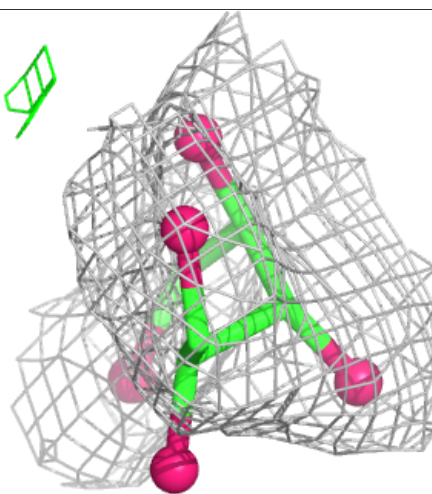
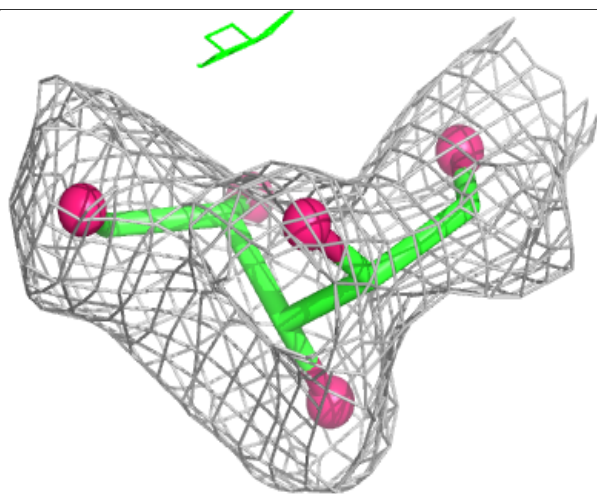
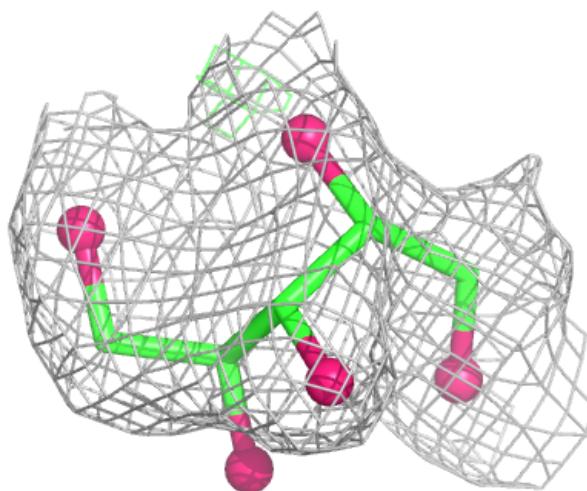
Electron density around XYL C 907:

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



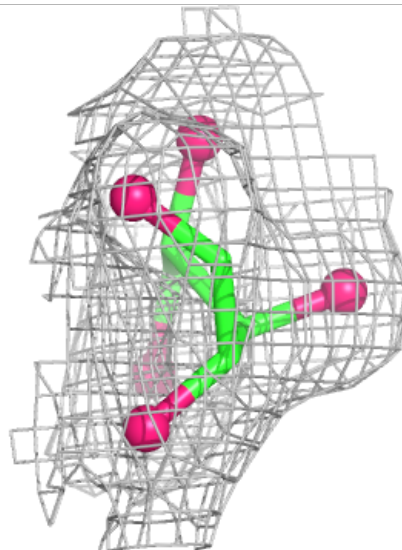
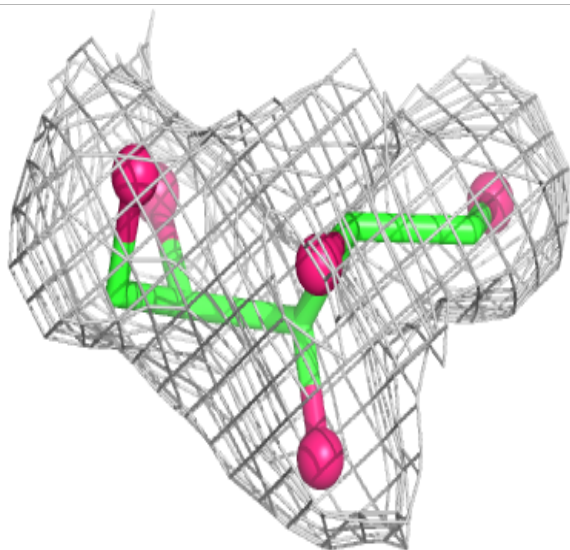
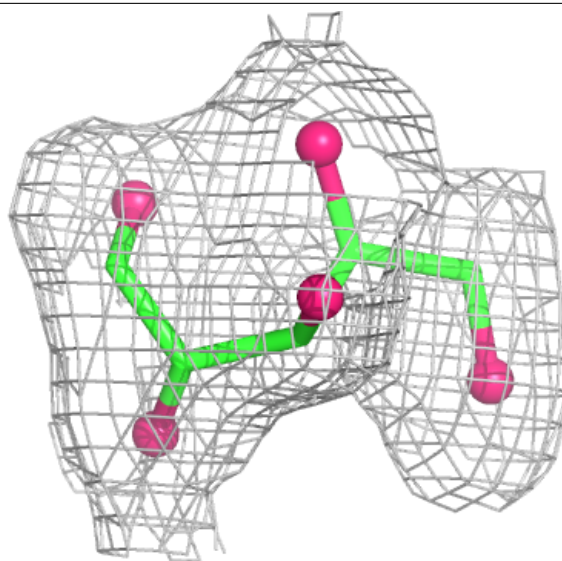
Electron density around XYL D 907:

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



Electron density around XYL E 906:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.