



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:22 PM UTC

PDB ID : 9EY8 / pdb_00009ey8
Title : Crystal structure of human tyrosinase-related protein 1 (TYRP1) in complex with (s)-amino-L-tyrosine
Authors : Ng, Y.M.; Soler-Lopez, M.
Deposited on : 2024-04-09
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

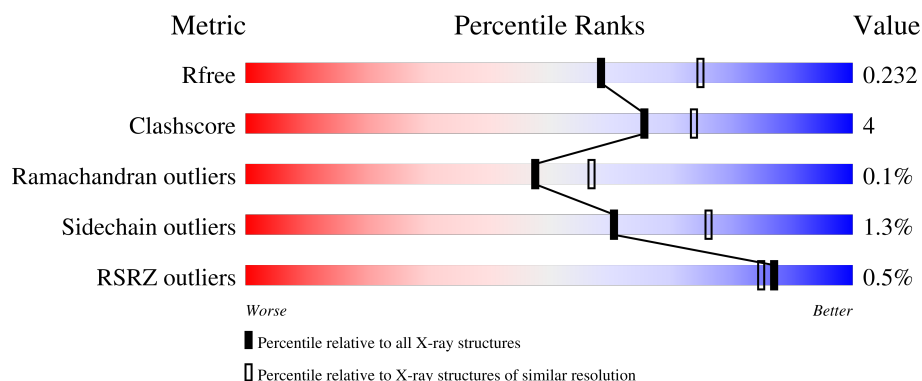
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



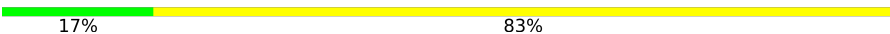
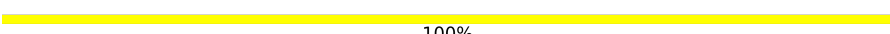
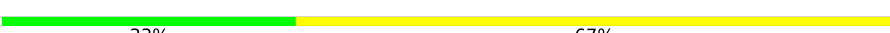
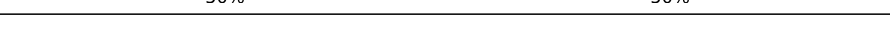
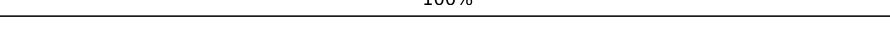
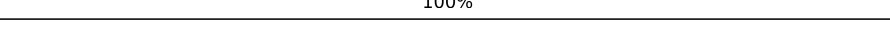
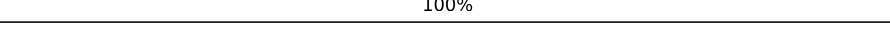
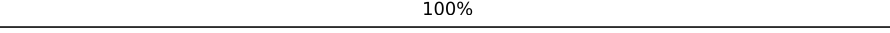
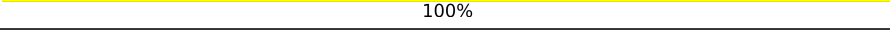
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	AA	450	92% 8% .
1	BA	450	% 90% 10% .
1	CA	450	90% 9% .
1	DA	450	% 90% 10%
2	A	6	17% 50% 33%

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Mol	Chain	Length	Quality of chain
2	C	6	 17% 50% 33%
2	L	6	 17% 83%
2	T	6	 17% 83%
3	B	5	 100%
3	H	5	 100%
4	D	3	 33% 67%
4	W	3	 100%
5	E	4	 100%
5	G	4	 100%
5	S	4	 25% 75%
6	F	2	 100%
6	J	2	 100%
6	K	2	 50% 50%
6	M	2	 50% 50%
6	Q	2	 50% 50%
6	U	2	 100%
6	V	2	 100%
7	I	3	 100%
8	N	7	 86% 14%
9	O	7	 100%
10	P	6	 100%
11	R	2	 50% 50%
11	X	2	 100%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16585 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.

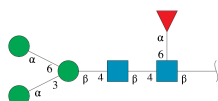
- Molecule 1 is a protein called 5,6-dihydroxyindole-2-carboxylic acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	447	Total	C	N	O	S	0	1	0
			3578	2244	638	673	23			
1	BA	447	Total	C	N	O	S	0	1	0
			3582	2245	640	674	23			
1	CA	447	Total	C	N	O	S	0	0	0
			3571	2239	636	673	23			
1	DA	450	Total	C	N	O	S	0	1	0
			3603	2259	642	679	23			

There are 12 discrepancies between the modelled and reference sequences:

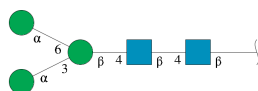
Chain	Residue	Modelled	Actual	Comment	Reference
AA	472	GLU	-	expression tag	UNP P17643
AA	473	ASN	-	expression tag	UNP P17643
AA	474	LEU	-	expression tag	UNP P17643
BA	472	GLU	-	expression tag	UNP P17643
BA	473	ASN	-	expression tag	UNP P17643
BA	474	LEU	-	expression tag	UNP P17643
CA	472	GLU	-	expression tag	UNP P17643
CA	473	ASN	-	expression tag	UNP P17643
CA	474	LEU	-	expression tag	UNP P17643
DA	472	GLU	-	expression tag	UNP P17643
DA	473	ASN	-	expression tag	UNP P17643
DA	474	LEU	-	expression tag	UNP P17643

- Molecule 2 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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



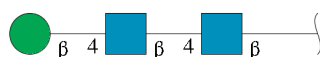
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	6	Total	C	N	O	0	0	0
			71	40	2	29			
2	C	6	Total	C	N	O	0	0	0
			71	40	2	29			
2	L	6	Total	C	N	O	0	0	0
			71	40	2	29			
2	T	6	Total	C	N	O	0	0	0
			71	40	2	29			

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



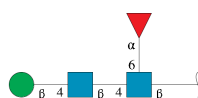
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



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

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



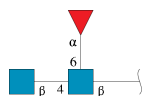
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	G	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	S	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 6 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
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	V	2	Total	C	N	O	0	0	0
			28	16	2	10			

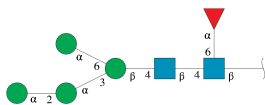
- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	I	3	Total	C	N	O	0	0	0
			38	22	2	14			

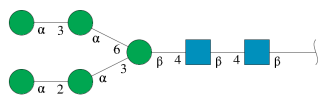
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-

beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



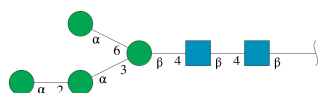
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	N	7	Total	C	N	O	0	0	0
			82	46	2	34			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-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
9	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



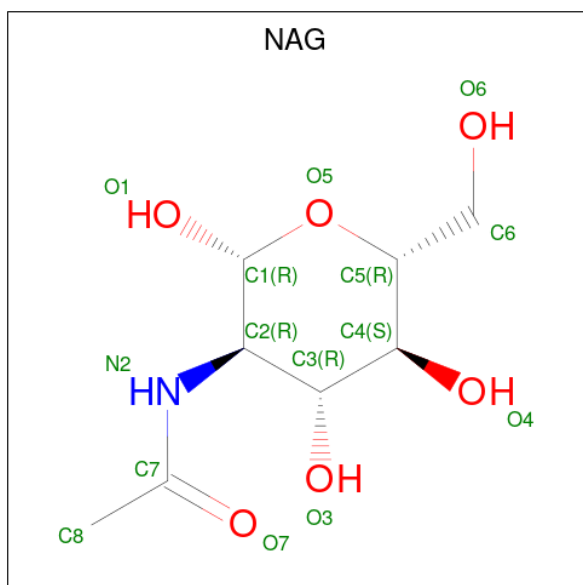
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	P	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	R	2	Total	C	N	O	0	0	0
			24	14	1	9			
11	X	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	AA	1	Total	C	N	O	0	0
			14	8	1	5		
12	CA	1	Total	C	N	O	0	0
			14	8	1	5		
12	DA	1	Total	C	N	O	0	0
			14	8	1	5		
12	DA	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 13 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

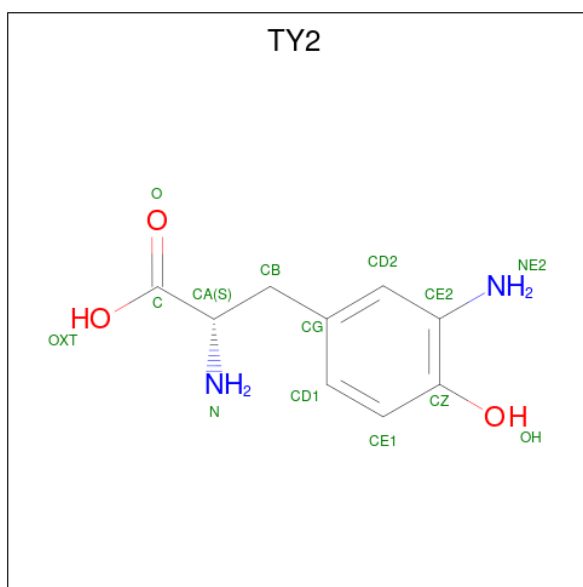


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	AA	1	Total	C	O	0	0
			6	3	3		
13	BA	1	Total	C	O	0	0
			6	3	3		
13	CA	1	Total	C	O	0	0
			6	3	3		
13	DA	1	Total	C	O	0	0
			6	3	3		

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	AA	2	Total	Zn	0	0
			2	2		
14	BA	2	Total	Zn	0	0
			2	2		
14	CA	2	Total	Zn	0	0
			2	2		
14	DA	2	Total	Zn	0	0
			2	2		

- Molecule 15 is 3-AMINO-L-TYROSINE (CCD ID: TY2) (formula: C₉H₁₂N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	CA	1	Total	C	N	O	0	0
			14	9	2	3		

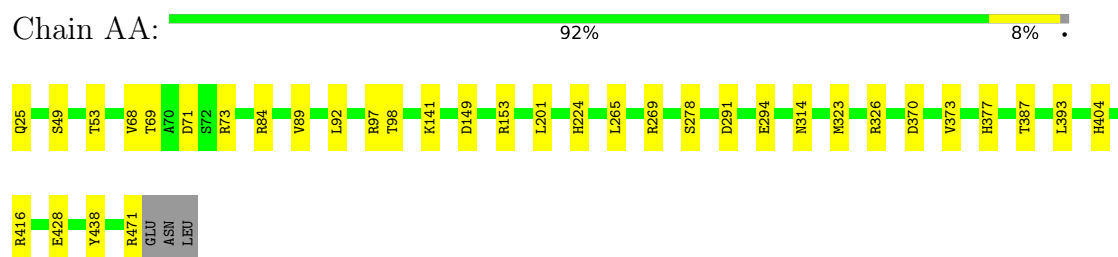
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	AA	313	Total	O	0	0
			313	313		
16	BA	261	Total	O	0	0
			261	261		
16	CA	229	Total	O	0	0
			229	229		
16	DA	196	Total	O	0	0
			196	196		

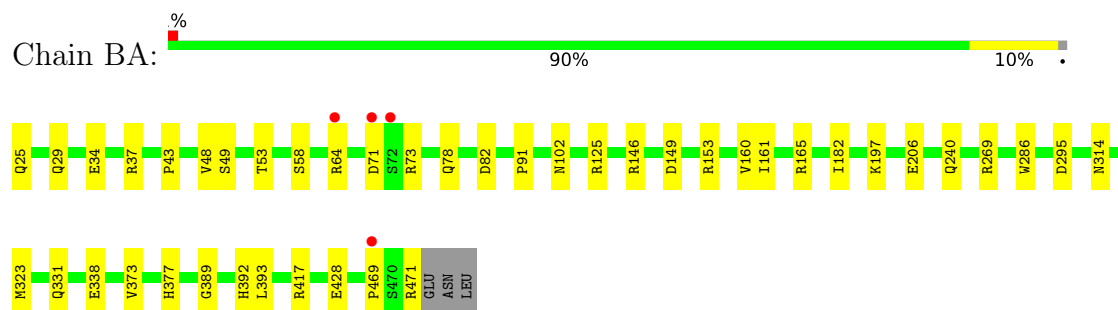
3 Residue-property plots

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

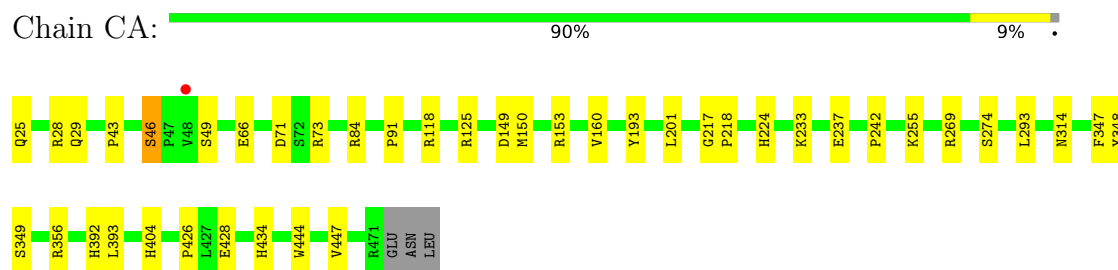
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



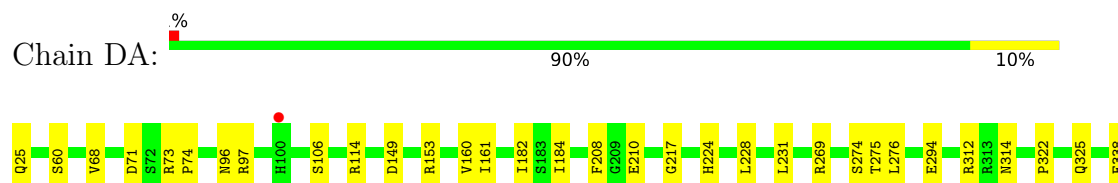
- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase



- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

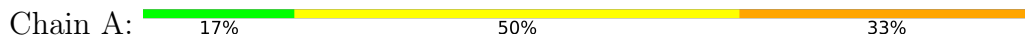


- Molecule 1: 5,6-dihydroxyindole-2-carboxylic acid oxidase

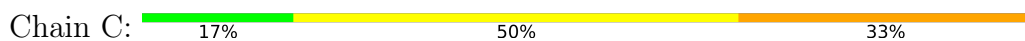




- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



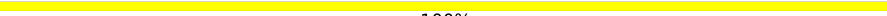
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain H:  100%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain D:  33% 67%

MAG1
MAG2
BMA3

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

Chain W:  100%

MAG1
MAG2
BMA3

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

Chain E:  100%

MAG1
MAG2
BMA3
FUC4

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

Chain G:  100%

MAG1
MAG2
BMA3
FUC4

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

Chain S:  25% 75%

MAG1
MAG2
BMA3
FUC4

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

Chain F:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  50% 50%

MAG1
MAG2

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

Chain M:  50% 50%

MAG1
MAG2

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

Chain Q:  50% 50%

MAG1
MAG2

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

Chain U:  100%

MAG1
MAG2

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

Chain V:  100%

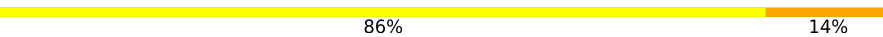
MAG1
MAG2

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

Chain I:  100%

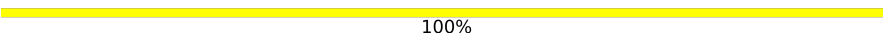
MAG1
MAG2
FUC3

- Molecule 8: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose

Chain N:  86% 14%

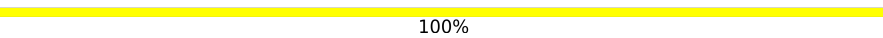
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
FUC7

- Molecule 9: α -D-mannopyranose-(1-2)- α -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-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain O:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

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

Chain P:  100%

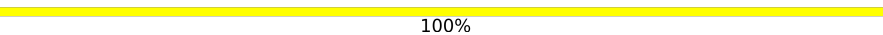
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 11: α -L-fucopyranose-(1-6)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain R:  50% 50%

MAG1
FUC2

- Molecule 11: α -L-fucopyranose-(1-6)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain X:  100%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.97Å 126.97Å 212.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.26 – 2.20 47.26 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.26-2.20) 99.7 (47.26-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.189 , 0.233 0.188 , 0.232	Depositor DCC
R_{free} test set	6092 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16585	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, ZN, FUC, GOL, NAG, MAN, TY2

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	AA	0.37	0/3689	0.53	0/5027
1	BA	0.38	0/3689	0.54	0/5026
1	CA	0.36	0/3678	0.54	2/5012 (0.0%)
1	DA	0.33	0/3714	0.51	0/5061
All	All	0.36	0/14770	0.53	2/20126 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	255	LYS	CA-C-N	5.39	131.25	121.92
1	CA	255	LYS	C-N-CA	5.39	131.25	121.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	3578	0	3343	25	0
1	BA	3582	0	3349	27	0
1	CA	3571	0	3337	27	0
1	DA	3603	0	3366	32	0
2	A	71	0	61	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	71	0	61	1	0
2	L	71	0	61	0	0
2	T	71	0	61	0	0
3	B	61	0	52	0	1
3	H	61	0	52	0	0
4	D	39	0	34	0	0
4	W	39	0	34	0	0
5	E	49	0	43	0	0
5	G	49	0	43	0	0
5	S	49	0	43	0	0
6	F	28	0	25	0	0
6	J	28	0	25	0	0
6	K	28	0	25	1	0
6	M	28	0	25	0	0
6	Q	28	0	25	1	0
6	U	28	0	25	0	0
6	V	28	0	25	0	0
7	I	38	0	34	0	0
8	N	82	0	70	1	0
9	O	83	0	70	0	0
10	P	72	0	61	0	0
11	R	24	0	22	2	0
11	X	24	0	22	0	0
12	AA	14	0	13	0	0
12	CA	14	0	13	0	0
12	DA	28	0	26	0	0
13	AA	6	0	8	0	0
13	BA	6	0	8	1	0
13	CA	6	0	8	1	0
13	DA	6	0	8	0	0
14	AA	2	0	0	0	0
14	BA	2	0	0	0	0
14	CA	2	0	0	0	0
14	DA	2	0	0	0	0
15	CA	14	0	11	0	0
16	AA	313	0	0	9	0
16	BA	261	0	0	10	0
16	CA	229	0	0	4	1
16	DA	196	0	0	9	0
All	All	16585	0	14489	113	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:74:PRO:O	16:DA:601:HOH:O	1.92	0.87
1:BA:125:ARG:NH1	16:BA:603:HOH:O	2.08	0.86
1:BA:25:GLN:N	1:BA:25:GLN:OE1	2.10	0.84
1:BA:269:ARG:NH1	1:BA:314:ASN:OD1	2.11	0.84
1:CA:149:ASP:OD2	1:CA:153:ARG:NH1	2.11	0.83
1:DA:471:ARG:NH1	16:DA:604:HOH:O	2.13	0.80
1:DA:25:GLN:N	1:DA:25:GLN:OE1	2.15	0.79
1:BA:78:GLN:OE1	16:BA:601:HOH:O	2.00	0.79
1:AA:25:GLN:N	1:AA:25:GLN:OE1	2.16	0.78
1:CA:25:GLN:OE1	1:CA:25:GLN:N	2.18	0.76
1:AA:97:ARG:NH1	16:AA:601:HOH:O	2.19	0.75
1:CA:218:PRO:HD2	1:CA:434:HIS:HB3	1.70	0.74
1:AA:25:GLN:NE2	16:AA:602:HOH:O	2.22	0.73
1:CA:29:GLN:HG3	1:CA:43:PRO:HB3	1.74	0.69
1:DA:413:GLU:OE2	16:DA:603:HOH:O	2.11	0.67
1:BA:165:ARG:NH1	16:BA:602:HOH:O	2.01	0.67
1:CA:444:TRP:O	16:CA:601:HOH:O	2.13	0.66
1:DA:345:PRO:HG3	8:N:1:NAG:H83	1.76	0.66
1:DA:184:ILE:O	16:DA:605:HOH:O	2.14	0.65
16:AA:903:HOH:O	2:A:6:FUC:O2	2.14	0.65
1:BA:34:GLU:OE2	1:BA:37:ARG:NH1	2.31	0.64
1:BA:146:ARG:NH1	16:BA:606:HOH:O	2.26	0.64
1:DA:269:ARG:NH1	1:DA:314:ASN:OD1	2.31	0.63
1:CA:46:SER:O	1:CA:46:SER:OG	2.16	0.62
1:DA:417:ARG:NH1	16:DA:602:HOH:O	2.10	0.62
1:CA:71:ASP:HB3	16:CA:754:HOH:O	1.99	0.61
1:CA:73:ARG:NH1	1:CA:428:GLU:OE1	2.35	0.60
1:CA:150:MET:HE3	16:CA:781:HOH:O	2.02	0.59
2:C:2:NAG:O4	2:C:5:MAN:H2	2.04	0.58
1:DA:149:ASP:OD2	1:DA:153:ARG:NH1	2.38	0.57
1:BA:71:ASP:O	16:BA:604:HOH:O	2.17	0.57
1:DA:106:SER:HB2	1:DA:114:ARG:HG2	1.89	0.55
1:AA:471:ARG:NH1	16:AA:611:HOH:O	2.40	0.54
1:CA:293:LEU:HD13	1:CA:392:HIS:CD2	2.42	0.54
13:CA:502:GOL:H11	16:CA:763:HOH:O	2.07	0.54
1:BA:29:GLN:HG3	1:BA:43:PRO:HB3	1.90	0.54
1:BA:64[A]:ARG:NH1	1:BA:102:ASN:OD1	2.41	0.54
1:AA:141:LYS:HD3	1:AA:265:LEU:HD21	1.89	0.53
1:DA:25:GLN:N	1:DA:160:VAL:O	2.41	0.53
1:CA:217:GLY:O	1:CA:356:ARG:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:49:SER:HB2	1:AA:53:THR:HG21	1.90	0.53
1:AA:291:ASP:HB2	1:AA:393:LEU:HD21	1.91	0.52
1:DA:269:ARG:HD3	1:DA:274:SER:HB2	1.92	0.52
1:BA:149:ASP:OD2	1:BA:153:ARG:NH1	2.44	0.51
1:DA:97:ARG:NH2	16:DA:608:HOH:O	2.26	0.50
1:AA:89:VAL:HG23	1:AA:92:LEU:HB2	1.93	0.50
1:BA:25:GLN:N	1:BA:160:VAL:O	2.45	0.50
1:CA:392:HIS:CD2	1:CA:393:LEU:HG	2.47	0.50
1:AA:25:GLN:N	1:AA:25:GLN:CD	2.70	0.50
1:AA:224:HIS:CD2	1:AA:404:HIS:CE1	3.00	0.50
1:AA:323:MET:HE2	16:AA:819:HOH:O	2.11	0.49
1:DA:322:PRO:HA	1:DA:325:GLN:HG3	1.93	0.49
1:CA:118:ARG:HD2	1:CA:242:PRO:HB3	1.94	0.49
1:DA:231:LEU:HA	16:DA:728:HOH:O	2.11	0.49
1:AA:71:ASP:HB3	16:AA:619:HOH:O	2.12	0.48
1:CA:28:ARG:NH1	11:R:1:NAG:H82	2.28	0.48
1:BA:71:ASP:HA	16:BA:810:HOH:O	2.13	0.48
1:AA:416:ARG:HH11	1:AA:416:ARG:HG2	1.79	0.48
1:AA:269:ARG:NH1	1:AA:314:ASN:OD1	2.46	0.47
1:CA:224:HIS:CD2	1:CA:404:HIS:CE1	3.02	0.47
1:DA:224:HIS:CD2	1:DA:404:HIS:CE1	3.02	0.47
1:DA:68:VAL:HG23	1:DA:96:ASN:C	2.40	0.47
1:CA:66:GLU:CD	1:DA:436:ARG:HH12	2.22	0.47
1:AA:149:ASP:O	1:AA:153:ARG:HG3	2.15	0.46
1:BA:73:ARG:NH1	1:BA:428:GLU:OE1	2.48	0.46
1:BA:295:ASP:OD2	6:K:2:NAG:H5	2.15	0.46
1:CA:25:GLN:N	1:CA:160:VAL:O	2.48	0.46
1:CA:28:ARG:HH12	11:R:1:NAG:H82	1.80	0.45
1:DA:208:PHE:CZ	1:DA:210:GLU:HB2	2.51	0.45
1:BA:240:GLN:HG2	16:BA:795:HOH:O	2.16	0.45
1:DA:217:GLY:O	1:DA:356:ARG:HD3	2.16	0.45
1:DA:338:GLU:OE2	1:DA:417:ARG:NH2	2.48	0.45
1:BA:331:GLN:OE1	1:BA:471:ARG:HA	2.17	0.45
1:AA:153:ARG:HD3	16:AA:808:HOH:O	2.16	0.44
1:CA:269:ARG:NH1	1:CA:314:ASN:OD1	2.49	0.44
1:BA:82:ASP:OD2	16:BA:605:HOH:O	2.21	0.44
1:DA:161:ILE:HD13	1:DA:182:ILE:HD12	2.00	0.44
1:BA:286:TRP:HA	13:BA:501:GOL:H31	1.99	0.44
1:AA:294:GLU:HG3	16:AA:815:HOH:O	2.17	0.44
1:CA:233:LYS:O	1:CA:237:GLU:HG2	2.18	0.44
1:BA:58:SER:HB3	1:BA:64[B]:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:392:HIS:NE2	1:CA:393:LEU:HG	2.33	0.44
1:DA:473:ASN:HB2	16:DA:604:HOH:O	2.18	0.43
1:DA:350:ASN:HA	1:DA:369:TYR:CE1	2.53	0.43
1:AA:69:THR:HA	16:AA:668:HOH:O	2.19	0.43
1:DA:275:THR:OG1	1:DA:312:ARG:NH1	2.50	0.43
1:AA:73:ARG:HD2	1:AA:428:GLU:HB3	2.01	0.43
1:AA:370:ASP:O	1:AA:373:VAL:HG12	2.19	0.43
1:DA:294:GLU:H	1:DA:294:GLU:CD	2.27	0.43
1:DA:71:ASP:OD1	1:DA:73:ARG:HG3	2.17	0.43
1:BA:389:GLY:HA3	16:BA:641:HOH:O	2.19	0.42
1:CA:233:LYS:HE3	1:CA:237:GLU:OE1	2.18	0.42
1:AA:68:VAL:CG2	1:AA:98:THR:HG23	2.48	0.42
1:AA:84:ARG:NH2	1:AA:201:LEU:O	2.52	0.42
1:AA:387:THR:HG23	1:AA:393:LEU:HD13	2.02	0.42
1:AA:326:ARG:HB2	1:AA:326:ARG:HH11	1.85	0.42
1:BA:338:GLU:HG2	1:BA:417:ARG:HH22	1.85	0.42
1:BA:165:ARG:HD3	16:BA:602:HOH:O	2.19	0.41
1:BA:392:HIS:CD2	1:BA:393:LEU:HG	2.54	0.41
1:CA:84:ARG:NH2	1:CA:201:LEU:O	2.53	0.41
1:DA:228:LEU:HD11	1:DA:404:HIS:HB3	2.03	0.41
1:CA:118:ARG:CZ	2:A:2:NAG:H62	2.49	0.41
1:DA:393:LEU:HD22	1:DA:396:ASN:HD22	1.85	0.41
1:BA:392:HIS:NE2	1:BA:393:LEU:HG	2.35	0.41
1:CA:125:ARG:HH22	6:Q:1:NAG:H61	1.84	0.41
1:CA:348:TYR:CG	1:CA:349:SER:N	2.89	0.41
1:BA:49:SER:HB2	1:BA:53:THR:HG21	2.03	0.41
1:DA:276:LEU:HD21	1:DA:312:ARG:CZ	2.50	0.41
1:BA:323:MET:HE1	1:BA:373:VAL:HA	2.03	0.41
1:DA:393:LEU:HD22	1:DA:396:ASN:ND2	2.36	0.41
1:DA:71:ASP:HB3	16:DA:700:HOH:O	2.21	0.41
1:AA:201:LEU:HD23	1:AA:201:LEU:HA	1.82	0.41
1:CA:347:PHE:CG	1:CA:426:PRO:HG3	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:5:MAN:O2	16:CA:665:HOH:O[1_655]	2.04	0.16

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	446/450 (99%)	428 (96%)	18 (4%)	0	100	100
1	BA	446/450 (99%)	425 (95%)	20 (4%)	1 (0%)	43	51
1	CA	445/450 (99%)	429 (96%)	16 (4%)	0	100	100
1	DA	449/450 (100%)	423 (94%)	26 (6%)	0	100	100
All	All	1786/1800 (99%)	1705 (96%)	80 (4%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BA	469	PRO

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	AA	397/399 (100%)	394 (99%)	3 (1%)	73	85
1	BA	397/399 (100%)	390 (98%)	7 (2%)	51	68
1	CA	396/399 (99%)	390 (98%)	6 (2%)	57	73
1	DA	400/399 (100%)	396 (99%)	4 (1%)	68	81
All	All	1590/1596 (100%)	1570 (99%)	20 (1%)	61	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	278	SER
1	AA	377	HIS
1	AA	438	TYR
1	BA	48	VAL
1	BA	91	PRO
1	BA	161	ILE
1	BA	182	ILE
1	BA	197	LYS
1	BA	206	GLU
1	BA	377	HIS
1	CA	46	SER
1	CA	49	SER
1	CA	91	PRO
1	CA	193	TYR
1	CA	274	SER
1	CA	447	VAL
1	DA	60	SER
1	DA	363	SER
1	DA	438	TYR
1	DA	474	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	25	GLN
1	AA	81	HIS
1	AA	124	GLN
1	AA	143	HIS
1	AA	250	ASN
1	BA	25	GLN
1	BA	240	GLN
1	BA	390	GLN
1	CA	250	ASN
1	DA	25	GLN

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 ⓘ

93 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	A	1	1,2	14,14,15	0.73	0	17,19,21	1.01	0
2	NAG	A	2	2	14,14,15	0.79	0	17,19,21	1.34	3 (17%)
2	BMA	A	3	2	11,11,12	0.92	0	15,15,17	2.24	2 (13%)
2	MAN	A	4	2	11,11,12	0.68	0	15,15,17	1.31	1 (6%)
2	MAN	A	5	2	11,11,12	0.65	0	15,15,17	1.37	2 (13%)
2	FUC	A	6	2	10,10,11	0.97	0	14,14,16	1.82	5 (35%)
3	NAG	B	1	3,1	14,14,15	0.93	1 (7%)	17,19,21	1.06	2 (11%)
3	NAG	B	2	3	14,14,15	0.72	0	17,19,21	1.25	3 (17%)
3	BMA	B	3	3	11,11,12	1.02	1 (9%)	15,15,17	1.53	3 (20%)
3	MAN	B	4	3	11,11,12	0.67	0	15,15,17	1.75	2 (13%)
3	MAN	B	5	3	11,11,12	0.79	0	15,15,17	0.97	0
2	NAG	C	1	1,2	14,14,15	0.63	0	17,19,21	1.00	0
2	NAG	C	2	2	14,14,15	0.72	0	17,19,21	1.72	3 (17%)
2	BMA	C	3	2	11,11,12	0.94	1 (9%)	15,15,17	3.79	7 (46%)
2	MAN	C	4	2	11,11,12	0.73	0	15,15,17	1.45	1 (6%)
2	MAN	C	5	2	11,11,12	0.58	0	15,15,17	2.61	4 (26%)
2	FUC	C	6	2	10,10,11	0.74	0	14,14,16	1.12	2 (14%)
4	NAG	D	1	4,1	14,14,15	0.69	0	17,19,21	1.02	0
4	NAG	D	2	4	14,14,15	0.78	0	17,19,21	0.83	1 (5%)
4	BMA	D	3	4	11,11,12	1.03	1 (9%)	15,15,17	2.59	4 (26%)
5	NAG	E	1	1,5	14,14,15	0.92	1 (7%)	17,19,21	1.11	1 (5%)
5	NAG	E	2	5	14,14,15	0.79	0	17,19,21	1.48	2 (11%)
5	BMA	E	3	5	11,11,12	0.91	1 (9%)	15,15,17	2.80	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUC	E	4	5	10,10,11	0.67	0	14,14,16	1.24	1 (7%)
6	NAG	F	1	6,1	14,14,15	0.80	0	17,19,21	2.41	3 (17%)
6	NAG	F	2	6	14,14,15	0.66	0	17,19,21	1.14	1 (5%)
5	NAG	G	1	1,5	14,14,15	0.80	0	17,19,21	1.19	2 (11%)
5	NAG	G	2	5	14,14,15	0.83	0	17,19,21	1.21	1 (5%)
5	BMA	G	3	5	11,11,12	0.94	1 (9%)	15,15,17	2.95	4 (26%)
5	FUC	G	4	5	10,10,11	0.79	0	14,14,16	1.16	1 (7%)
3	NAG	H	1	3,1	14,14,15	0.71	0	17,19,21	1.01	1 (5%)
3	NAG	H	2	3	14,14,15	0.77	0	17,19,21	1.53	2 (11%)
3	BMA	H	3	3	11,11,12	0.88	0	15,15,17	1.56	4 (26%)
3	MAN	H	4	3	11,11,12	0.56	0	15,15,17	1.60	1 (6%)
3	MAN	H	5	3	11,11,12	0.70	0	15,15,17	2.64	5 (33%)
7	NAG	I	1	7,1	14,14,15	0.81	0	17,19,21	2.34	3 (17%)
7	NAG	I	2	7	14,14,15	0.69	0	17,19,21	1.03	1 (5%)
7	FUC	I	3	7	10,10,11	0.92	1 (10%)	14,14,16	1.05	0
6	NAG	J	1	6,1	14,14,15	0.70	0	17,19,21	1.05	1 (5%)
6	NAG	J	2	6	14,14,15	0.70	0	17,19,21	1.14	2 (11%)
6	NAG	K	1	6,1	14,14,15	0.79	0	17,19,21	1.08	2 (11%)
6	NAG	K	2	6	14,14,15	0.62	0	17,19,21	1.05	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.74	0	17,19,21	1.11	1 (5%)
2	NAG	L	2	2	14,14,15	0.73	0	17,19,21	1.30	3 (17%)
2	BMA	L	3	2	11,11,12	0.95	0	15,15,17	1.86	2 (13%)
2	MAN	L	4	2	11,11,12	0.56	0	15,15,17	1.18	1 (6%)
2	MAN	L	5	2	11,11,12	0.62	0	15,15,17	1.12	1 (6%)
2	FUC	L	6	2	10,10,11	0.76	0	14,14,16	1.02	0
6	NAG	M	1	6,1	14,14,15	0.76	0	17,19,21	1.23	2 (11%)
6	NAG	M	2	6	14,14,15	0.73	0	17,19,21	0.89	0
8	NAG	N	1	1,8	14,14,15	0.86	0	17,19,21	1.10	1 (5%)
8	NAG	N	2	8	14,14,15	0.77	0	17,19,21	1.24	2 (11%)
8	BMA	N	3	8	11,11,12	0.75	0	15,15,17	2.89	6 (40%)
8	MAN	N	4	8	11,11,12	0.80	0	15,15,17	1.62	2 (13%)
8	MAN	N	5	8	11,11,12	0.62	0	15,15,17	2.20	2 (13%)
8	MAN	N	6	8	11,11,12	0.67	0	15,15,17	1.51	1 (6%)
8	FUC	N	7	8	10,10,11	0.75	0	14,14,16	1.15	1 (7%)
9	NAG	O	1	1,9	14,14,15	0.81	0	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	O	2	9	14,14,15	0.69	0	17,19,21	1.11	1 (5%)
9	BMA	O	3	9	11,11,12	0.78	0	15,15,17	2.81	6 (40%)
9	MAN	O	4	9	11,11,12	0.67	0	15,15,17	1.33	2 (13%)
9	MAN	O	5	9	11,11,12	0.58	0	15,15,17	1.51	1 (6%)
9	MAN	O	6	9	11,11,12	0.70	0	15,15,17	1.18	1 (6%)
9	MAN	O	7	9	11,11,12	0.66	0	15,15,17	1.63	2 (13%)
10	NAG	P	1	1,10	14,14,15	0.72	0	17,19,21	1.30	2 (11%)
10	NAG	P	2	10	14,14,15	0.79	0	17,19,21	1.35	2 (11%)
10	BMA	P	3	10	11,11,12	0.92	0	15,15,17	2.67	5 (33%)
10	MAN	P	4	10	11,11,12	0.61	0	15,15,17	2.01	1 (6%)
10	MAN	P	5	10	11,11,12	0.68	0	15,15,17	1.02	1 (6%)
10	MAN	P	6	10	11,11,12	0.75	0	15,15,17	1.71	2 (13%)
6	NAG	Q	1	6,1	14,14,15	0.63	0	17,19,21	1.23	3 (17%)
6	NAG	Q	2	6	14,14,15	0.68	0	17,19,21	1.21	2 (11%)
11	NAG	R	1	11,1	14,14,15	0.88	1 (7%)	17,19,21	2.50	4 (23%)
11	FUC	R	2	11	10,10,11	0.69	0	14,14,16	1.51	3 (21%)
5	NAG	S	1	1,5	14,14,15	0.96	1 (7%)	17,19,21	1.44	2 (11%)
5	NAG	S	2	5	14,14,15	0.79	0	17,19,21	1.06	1 (5%)
5	BMA	S	3	5	11,11,12	0.93	1 (9%)	15,15,17	2.44	5 (33%)
5	FUC	S	4	5	10,10,11	0.74	0	14,14,16	1.12	0
2	NAG	T	1	1,2	14,14,15	0.81	0	17,19,21	1.03	1 (5%)
2	NAG	T	2	2	14,14,15	0.79	0	17,19,21	0.98	1 (5%)
2	BMA	T	3	2	11,11,12	1.02	1 (9%)	15,15,17	2.04	4 (26%)
2	MAN	T	4	2	11,11,12	0.68	0	15,15,17	1.88	3 (20%)
2	MAN	T	5	2	11,11,12	0.58	0	15,15,17	1.70	2 (13%)
2	FUC	T	6	2	10,10,11	0.81	0	14,14,16	0.94	0
6	NAG	U	1	6,1	14,14,15	0.76	0	17,19,21	1.04	1 (5%)
6	NAG	U	2	6	14,14,15	0.75	1 (7%)	17,19,21	1.22	2 (11%)
6	NAG	V	1	6,1	14,14,15	0.67	0	17,19,21	1.41	3 (17%)
6	NAG	V	2	6	14,14,15	0.70	0	17,19,21	1.22	2 (11%)
4	NAG	W	1	4,1	14,14,15	0.73	0	17,19,21	1.06	2 (11%)
4	NAG	W	2	4	14,14,15	0.72	0	17,19,21	1.33	1 (5%)
4	BMA	W	3	4	11,11,12	1.01	1 (9%)	15,15,17	2.50	5 (33%)
11	NAG	X	1	11,1	14,14,15	0.77	0	17,19,21	2.82	5 (29%)
11	FUC	X	2	11	10,10,11	0.79	1 (10%)	14,14,16	2.04	4 (28%)

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	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	BMA	A	3	2	-	0/2/19/22	0/1/1/1
2	MAN	A	4	2	-	2/2/19/22	0/1/1/1
2	MAN	A	5	2	-	0/2/19/22	0/1/1/1
2	FUC	A	6	2	-	-	0/1/1/1
3	NAG	B	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3	3	-	0/2/19/22	0/1/1/1
3	MAN	B	4	3	-	0/2/19/22	0/1/1/1
3	MAN	B	5	3	-	2/2/19/22	0/1/1/1
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	FUC	C	6	2	-	-	0/1/1/1
4	NAG	D	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	FUC	E	4	5	-	-	0/1/1/1
6	NAG	F	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	FUC	G	4	5	-	-	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	MAN	H	4	3	-	2/2/19/22	0/1/1/1
3	MAN	H	5	3	-	2/2/19/22	1/1/1/1
7	NAG	I	1	7,1	-	3/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	S	2	5	-	1/6/23/26	0/1/1/1
5	BMA	S	3	5	-	0/2/19/22	0/1/1/1
5	FUC	S	4	5	-	-	0/1/1/1
2	NAG	T	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	0/6/23/26	0/1/1/1
2	BMA	T	3	2	-	0/2/19/22	0/1/1/1
2	MAN	T	4	2	-	0/2/19/22	0/1/1/1
2	MAN	T	5	2	-	2/2/19/22	0/1/1/1
2	FUC	T	6	2	-	-	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	NAG	V	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	0/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	BMA	W	3	4	-	0/2/19/22	0/1/1/1
11	NAG	X	1	11,1	-	2/6/23/26	0/1/1/1
11	FUC	X	2	11	-	-	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3	BMA	C2-C3	2.60	1.56	1.52
2	T	3	BMA	C2-C3	2.51	1.56	1.52
5	S	1	NAG	C1-C2	2.48	1.55	1.52
3	B	3	BMA	C2-C3	2.45	1.56	1.52
4	W	3	BMA	C2-C3	2.41	1.56	1.52
5	E	1	NAG	C1-C2	2.26	1.55	1.52
5	G	3	BMA	C2-C3	2.26	1.56	1.52
11	R	1	NAG	C1-C2	2.20	1.55	1.52
5	S	3	BMA	C2-C3	2.17	1.55	1.52
2	C	3	BMA	C2-C3	2.16	1.55	1.52
7	I	3	FUC	O5-C1	-2.15	1.40	1.43
6	U	2	NAG	C1-C2	2.14	1.55	1.52
11	X	2	FUC	C1-C2	2.11	1.57	1.52
3	B	1	NAG	O5-C1	-2.10	1.40	1.43
5	E	3	BMA	C2-C3	2.10	1.55	1.52

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	C1-O5-C5	11.29	127.32	112.19
5	G	3	BMA	C1-O5-C5	9.01	124.26	112.19
5	E	3	BMA	C1-O5-C5	8.90	124.12	112.19
9	O	3	BMA	C1-O5-C5	8.83	124.02	112.19
2	C	5	MAN	C1-O5-C5	8.47	123.53	112.19
10	P	3	BMA	C1-O5-C5	8.33	123.35	112.19
6	F	1	NAG	C2-N2-C7	8.24	133.95	122.90
8	N	3	BMA	C1-O5-C5	8.24	123.23	112.19
7	I	1	NAG	C2-N2-C7	8.05	133.69	122.90
11	R	1	NAG	C2-N2-C7	8.04	133.67	122.90
4	D	3	BMA	C1-O5-C5	7.44	122.16	112.19
11	X	1	NAG	C2-N2-C7	7.20	132.55	122.90
8	N	5	MAN	C1-O5-C5	7.19	121.82	112.19
2	A	3	BMA	C1-O5-C5	7.17	121.79	112.19
5	S	3	BMA	C1-O5-C5	7.04	121.63	112.19
10	P	4	MAN	C1-O5-C5	7.00	121.56	112.19
4	W	3	BMA	C1-O5-C5	6.98	121.54	112.19
11	X	1	NAG	C1-C2-N2	6.31	120.37	110.43
2	L	3	BMA	C1-O5-C5	6.04	120.28	112.19
3	H	5	MAN	C3-C4-C5	-5.98	99.39	110.23
3	B	4	MAN	C1-O5-C5	5.18	119.13	112.19
9	O	5	MAN	C1-O5-C5	5.07	118.97	112.19
2	C	3	BMA	C1-C2-C3	5.06	117.02	109.64
3	H	4	MAN	C1-O5-C5	4.93	118.79	112.19
8	N	6	MAN	C1-O5-C5	4.87	118.72	112.19
2	T	4	MAN	C1-O5-C5	4.85	118.68	112.19
3	H	5	MAN	C2-C3-C4	-4.83	102.36	110.86
9	O	7	MAN	C1-O5-C5	4.83	118.66	112.19
11	X	2	FUC	C1-C2-C3	4.73	116.54	109.64
10	P	6	MAN	C1-O5-C5	4.67	118.45	112.19
2	T	3	BMA	C1-O5-C5	4.63	118.39	112.19
2	T	5	MAN	C1-O5-C5	4.57	118.31	112.19
5	E	2	NAG	C2-N2-C7	4.47	128.89	122.90
3	H	5	MAN	O3-C3-C4	4.47	120.90	110.38
3	H	2	NAG	C1-O5-C5	4.40	118.08	112.19
2	C	3	BMA	C2-C3-C4	4.32	118.45	110.86
2	C	4	MAN	C1-O5-C5	4.25	117.88	112.19
2	A	6	FUC	C1-C2-C3	-4.11	103.67	109.64
2	C	2	NAG	C4-C3-C2	-4.09	105.02	111.02
8	N	3	BMA	O3-C3-C2	-4.06	101.77	110.05
4	W	2	NAG	C2-N2-C7	4.03	128.30	122.90
8	N	4	MAN	C1-O5-C5	3.99	117.53	112.19
11	X	1	NAG	O5-C1-C2	-3.98	105.13	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	C3-C4-C5	3.89	117.28	110.23
11	X	2	FUC	C1-O5-C5	3.88	122.12	112.97
5	S	3	BMA	C3-C4-C5	3.81	117.14	110.23
2	C	5	MAN	C1-C2-C3	3.81	115.19	109.64
2	A	4	MAN	C1-O5-C5	3.73	117.19	112.19
4	W	3	BMA	C3-C4-C5	3.70	116.94	110.23
2	L	4	MAN	C1-O5-C5	3.70	117.14	112.19
4	D	3	BMA	C3-C4-C5	3.68	116.91	110.23
2	C	2	NAG	C1-O5-C5	3.65	117.08	112.19
2	A	5	MAN	C1-O5-C5	3.62	117.03	112.19
5	S	1	NAG	O4-C4-C3	-3.59	101.92	110.38
8	N	4	MAN	O2-C2-C3	3.55	117.50	110.15
2	C	2	NAG	C3-C4-C5	-3.54	103.81	110.23
4	D	3	BMA	C2-C3-C4	3.52	117.05	110.86
9	O	4	MAN	C1-O5-C5	3.51	116.89	112.19
6	V	2	NAG	O5-C1-C2	-3.49	105.90	111.29
5	E	3	BMA	C3-C4-C5	3.46	116.51	110.23
10	P	3	BMA	C3-C4-C5	3.46	116.51	110.23
8	N	3	BMA	C2-C3-C4	3.46	116.94	110.86
2	C	3	BMA	C3-C4-C5	3.45	116.50	110.23
6	F	2	NAG	C1-O5-C5	3.42	116.77	112.19
3	B	3	BMA	C1-O5-C5	3.41	116.76	112.19
2	T	3	BMA	C2-C3-C4	3.36	116.78	110.86
6	V	1	NAG	C3-C4-C5	-3.34	104.17	110.23
3	H	3	BMA	O6-C6-C5	-3.31	100.05	111.33
2	T	4	MAN	C3-C4-C5	-3.25	104.34	110.23
8	N	5	MAN	C1-C2-C3	3.25	114.37	109.64
9	O	6	MAN	C1-O5-C5	3.22	116.50	112.19
3	H	2	NAG	O4-C4-C3	-3.22	102.80	110.38
5	G	1	NAG	C1-O5-C5	3.21	116.49	112.19
3	H	5	MAN	O4-C4-C5	3.19	117.18	109.32
8	N	1	NAG	O3-C3-C2	-3.19	102.78	109.40
11	R	1	NAG	O5-C5-C6	3.17	113.83	107.66
11	R	2	FUC	C1-O5-C5	3.15	120.41	112.97
11	X	1	NAG	O7-C7-N2	3.10	127.46	121.98
9	O	3	BMA	C3-C4-C5	3.08	115.82	110.23
6	F	1	NAG	C8-C7-N2	3.07	121.21	116.12
11	R	1	NAG	C8-C7-N2	3.02	121.13	116.12
2	L	5	MAN	C1-O5-C5	2.97	116.16	112.19
2	T	5	MAN	C3-C4-C5	-2.94	104.90	110.23
5	G	3	BMA	O5-C5-C4	2.94	117.98	110.83
8	N	3	BMA	C3-C4-C5	2.93	115.54	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	C2-C3-C4	2.93	116.01	110.86
2	C	3	BMA	O5-C1-C2	2.87	117.65	110.79
9	O	7	MAN	C1-C2-C3	2.87	113.82	109.64
2	T	3	BMA	C1-C2-C3	2.85	113.80	109.64
5	E	4	FUC	C3-C4-C5	-2.83	105.51	109.81
2	C	3	BMA	O3-C3-C2	-2.82	104.29	110.05
11	X	1	NAG	C8-C7-N2	-2.81	111.46	116.12
6	V	1	NAG	C1-O5-C5	2.79	115.93	112.19
8	N	2	NAG	C1-O5-C5	2.79	115.93	112.19
2	L	2	NAG	C1-C2-N2	2.78	114.81	110.43
2	C	3	BMA	O5-C5-C4	2.76	117.55	110.83
6	Q	1	NAG	O4-C4-C3	-2.73	103.95	110.38
2	A	6	FUC	O5-C5-C4	2.73	114.46	109.55
11	R	2	FUC	C1-C2-C3	2.72	113.60	109.64
7	I	1	NAG	C8-C7-N2	2.71	120.62	116.12
11	X	2	FUC	C3-C4-C5	-2.71	105.70	109.81
10	P	6	MAN	C3-C4-C5	2.70	115.14	110.23
2	A	2	NAG	O4-C4-C3	-2.70	104.02	110.38
5	G	2	NAG	C4-C3-C2	2.69	114.96	111.02
2	T	4	MAN	C1-C2-C3	2.69	113.56	109.64
10	P	3	BMA	C2-C3-C4	2.68	115.57	110.86
7	I	1	NAG	C3-C4-C5	-2.67	105.39	110.23
6	U	1	NAG	O5-C1-C2	-2.66	107.17	111.29
6	Q	1	NAG	C2-N2-C7	2.65	126.45	122.90
6	U	2	NAG	C2-N2-C7	2.65	126.45	122.90
4	W	3	BMA	O4-C4-C3	-2.65	104.14	110.38
5	S	3	BMA	C2-C3-C4	2.64	115.50	110.86
9	O	3	BMA	O5-C5-C4	2.64	117.24	110.83
11	R	1	NAG	O7-C7-C8	-2.63	117.37	122.05
10	P	1	NAG	O5-C1-C2	-2.62	107.24	111.29
3	H	3	BMA	O3-C3-C4	2.60	116.51	110.38
8	N	3	BMA	O4-C4-C3	-2.59	104.27	110.38
2	T	2	NAG	O5-C1-C2	-2.56	107.34	111.29
6	K	1	NAG	C1-O5-C5	2.56	115.61	112.19
3	H	1	NAG	C2-N2-C7	-2.55	119.48	122.90
4	W	3	BMA	O5-C5-C4	2.53	116.99	110.83
5	S	1	NAG	C1-C2-N2	2.53	114.41	110.43
10	P	2	NAG	O5-C1-C2	-2.50	107.43	111.29
5	G	4	FUC	C1-O5-C5	2.49	118.85	112.97
11	R	2	FUC	O5-C5-C4	2.47	114.00	109.55
6	Q	2	NAG	C1-O5-C5	2.46	115.49	112.19
5	S	3	BMA	O5-C5-C4	2.45	116.80	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	O5-C1-C2	-2.44	107.51	111.29
6	J	1	NAG	O4-C4-C3	-2.44	104.62	110.38
2	L	2	NAG	C1-O5-C5	2.44	115.46	112.19
10	P	5	MAN	C1-O5-C5	2.44	115.46	112.19
2	A	6	FUC	O3-C3-C4	2.44	116.13	110.38
10	P	3	BMA	O4-C4-C3	-2.44	104.62	110.38
3	H	3	BMA	C1-O5-C5	2.44	115.45	112.19
8	N	2	NAG	O4-C4-C3	-2.44	104.63	110.38
5	E	3	BMA	O5-C5-C4	2.43	116.75	110.83
3	B	4	MAN	C1-C2-C3	2.41	113.16	109.64
3	B	2	NAG	O5-C1-C2	-2.40	107.58	111.29
9	O	1	NAG	O4-C4-C3	-2.40	104.72	110.38
9	O	3	BMA	C2-C3-C4	2.40	115.08	110.86
5	E	2	NAG	O5-C1-C2	-2.39	107.60	111.29
5	E	3	BMA	C2-C3-C4	2.37	115.03	110.86
6	V	2	NAG	C1-O5-C5	2.37	115.36	112.19
9	O	3	BMA	O4-C4-C3	-2.37	104.80	110.38
6	Q	2	NAG	C2-N2-C7	2.36	126.07	122.90
2	L	1	NAG	C1-O5-C5	2.35	115.33	112.19
5	E	3	BMA	O4-C4-C3	-2.34	104.85	110.38
6	K	1	NAG	O4-C4-C3	-2.34	104.85	110.38
2	L	3	BMA	O3-C3-C4	2.34	115.90	110.38
4	W	3	BMA	C2-C3-C4	2.34	114.98	110.86
2	A	6	FUC	O4-C4-C5	2.34	114.89	109.74
10	P	1	NAG	C1-O5-C5	2.29	115.26	112.19
6	M	1	NAG	C1-O5-C5	2.28	115.25	112.19
9	O	2	NAG	C1-O5-C5	2.28	115.24	112.19
3	B	1	NAG	O5-C1-C2	-2.28	107.77	111.29
6	J	2	NAG	C3-C4-C5	-2.27	106.12	110.23
4	D	3	BMA	O5-C5-C4	2.26	116.33	110.83
3	B	1	NAG	C1-O5-C5	2.26	115.22	112.19
7	I	2	NAG	C1-O5-C5	2.25	115.20	112.19
6	K	2	NAG	C1-O5-C5	2.21	115.15	112.19
9	O	4	MAN	O2-C2-C3	2.21	114.73	110.15
2	T	1	NAG	O4-C4-C5	2.20	114.75	109.32
2	L	2	NAG	O5-C1-C2	-2.20	107.89	111.29
2	C	5	MAN	C3-C4-C5	-2.20	106.25	110.23
2	T	3	BMA	O4-C4-C3	-2.19	105.21	110.38
3	B	3	BMA	O3-C3-C4	2.19	115.53	110.38
9	O	3	BMA	O3-C3-C2	-2.19	105.59	110.05
2	A	2	NAG	O3-C3-C2	-2.18	104.86	109.40
8	N	3	BMA	O3-C3-C4	2.18	115.52	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	O5-C1-C2	-2.18	107.92	111.29
5	S	3	BMA	O4-C4-C3	-2.18	105.24	110.38
3	B	3	BMA	O5-C5-C6	2.16	111.87	107.66
2	C	6	FUC	O3-C3-C2	-2.16	105.65	110.05
6	U	2	NAG	C1-O5-C5	2.15	115.06	112.19
6	F	1	NAG	O4-C4-C3	-2.13	105.36	110.38
2	A	6	FUC	O5-C1-C2	-2.12	105.73	110.79
3	B	2	NAG	C2-N2-C7	2.11	125.73	122.90
2	A	5	MAN	O2-C2-C1	-2.11	104.39	109.22
6	Q	1	NAG	C4-C3-C2	2.11	114.11	111.02
10	P	2	NAG	C3-C4-C5	-2.11	106.40	110.23
2	A	3	BMA	O4-C4-C3	-2.10	105.42	110.38
3	H	3	BMA	O5-C5-C4	2.10	115.93	110.83
11	X	2	FUC	O4-C4-C5	2.09	114.35	109.74
10	P	3	BMA	O5-C5-C4	2.09	115.91	110.83
6	V	1	NAG	O4-C4-C5	2.08	114.45	109.32
4	D	2	NAG	O5-C1-C2	-2.08	108.07	111.29
4	W	1	NAG	O4-C4-C3	-2.08	105.47	110.38
5	S	2	NAG	C2-N2-C7	2.07	125.68	122.90
8	N	7	FUC	O3-C3-C2	-2.06	105.84	110.05
2	C	6	FUC	C1-C2-C3	2.06	112.65	109.64
5	G	1	NAG	O4-C4-C3	-2.06	105.53	110.38
6	J	2	NAG	O4-C4-C5	2.05	114.38	109.32
3	H	5	MAN	O2-C2-C3	-2.05	105.91	110.15
3	B	2	NAG	O4-C4-C3	-2.04	105.57	110.38
2	C	5	MAN	O5-C1-C2	2.04	115.65	110.79
6	M	1	NAG	O5-C1-C2	-2.04	108.14	111.29
4	W	1	NAG	C2-N2-C7	2.03	125.62	122.90

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	X	1	NAG	C1-C2-N2-C7
2	C	3	BMA	O5-C5-C6-O6
3	B	5	MAN	O5-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
10	P	6	MAN	O5-C5-C6-O6
11	R	1	NAG	O5-C5-C6-O6
10	P	4	MAN	O5-C5-C6-O6
2	C	5	MAN	C4-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	H	3	BMA	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
8	N	5	MAN	O5-C5-C6-O6
7	I	2	NAG	C4-C5-C6-O6
2	T	5	MAN	C4-C5-C6-O6
3	H	5	MAN	C4-C5-C6-O6
2	T	5	MAN	O5-C5-C6-O6
2	A	4	MAN	C4-C5-C6-O6
3	H	5	MAN	O5-C5-C6-O6
9	O	4	MAN	O5-C5-C6-O6
3	B	5	MAN	C4-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
9	O	4	MAN	C4-C5-C6-O6
11	R	1	NAG	C4-C5-C6-O6
10	P	4	MAN	C4-C5-C6-O6
2	A	4	MAN	O5-C5-C6-O6
4	W	1	NAG	C8-C7-N2-C2
4	W	1	NAG	O7-C7-N2-C2
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
11	R	1	NAG	C8-C7-N2-C2
11	R	1	NAG	O7-C7-N2-C2
2	L	4	MAN	O5-C5-C6-O6
9	O	6	MAN	C4-C5-C6-O6
10	P	6	MAN	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
9	O	6	MAN	O5-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
3	H	4	MAN	C4-C5-C6-O6
10	P	5	MAN	C4-C5-C6-O6
9	O	7	MAN	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
2	L	4	MAN	C4-C5-C6-O6
8	N	5	MAN	C4-C5-C6-O6
6	F	1	NAG	C1-C2-N2-C7
10	P	5	MAN	O5-C5-C6-O6
10	P	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C3-C2-N2-C7
7	I	1	NAG	C3-C2-N2-C7
11	R	1	NAG	C3-C2-N2-C7
9	O	7	MAN	O5-C5-C6-O6
9	O	2	NAG	C4-C5-C6-O6
10	P	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
4	D	1	NAG	C1-C2-N2-C7
5	E	2	NAG	C1-C2-N2-C7
5	G	2	NAG	C1-C2-N2-C7
5	S	2	NAG	C1-C2-N2-C7
6	Q	1	NAG	C1-C2-N2-C7
11	R	1	NAG	C1-C2-N2-C7
11	X	1	NAG	C3-C2-N2-C7
3	H	4	MAN	O5-C5-C6-O6

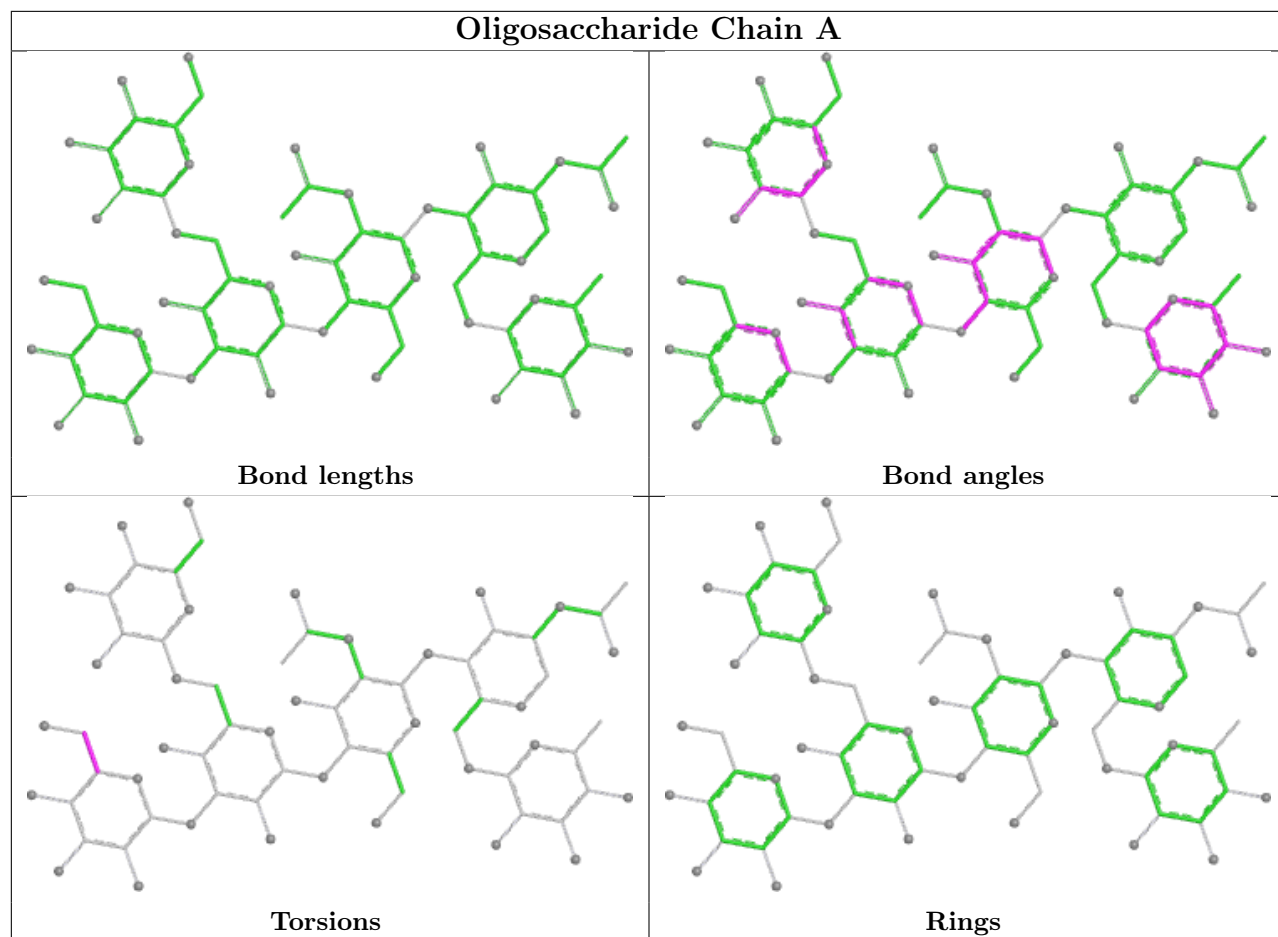
All (2) ring outliers are listed below:

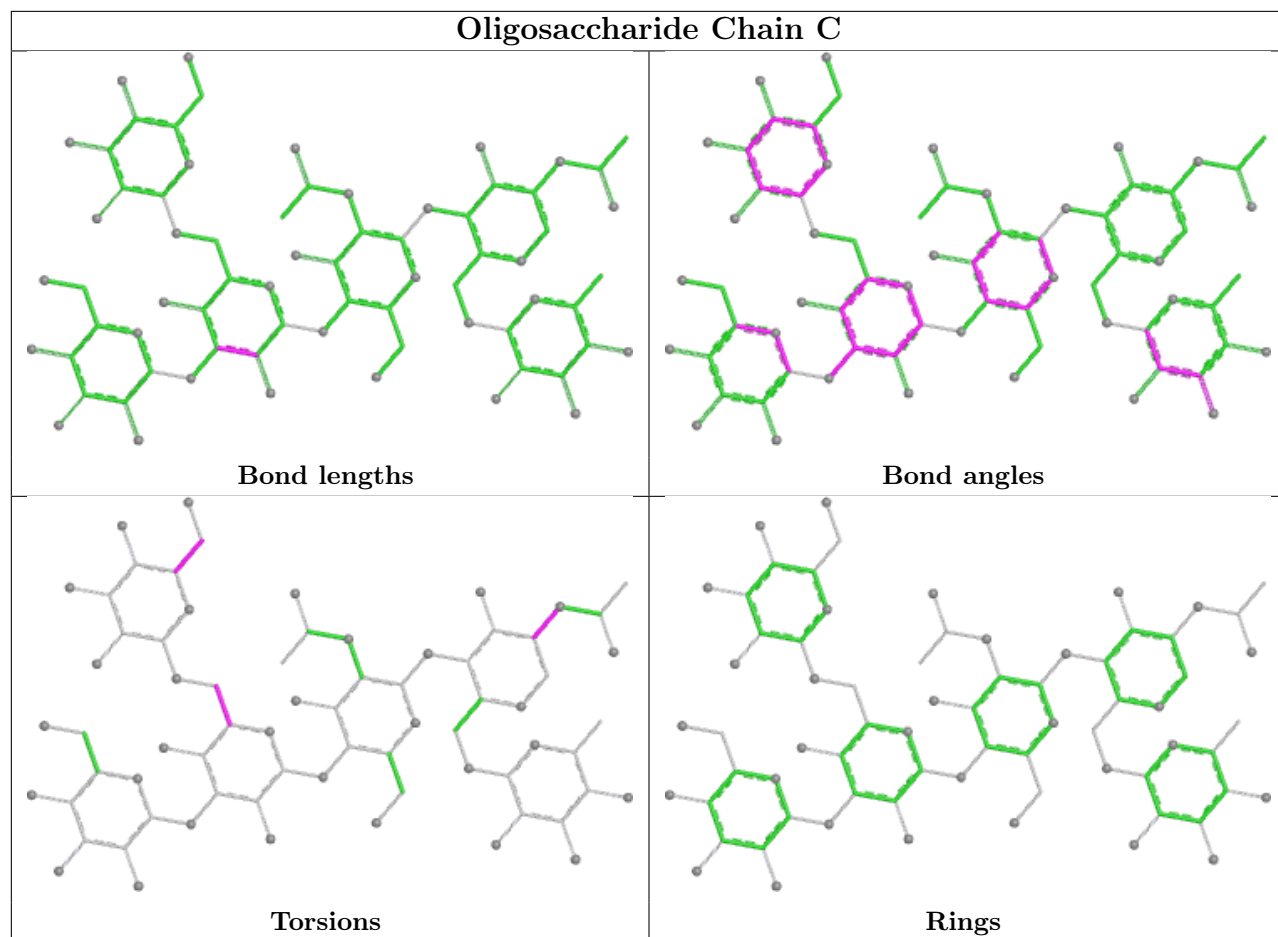
Mol	Chain	Res	Type	Atoms
8	N	5	MAN	C1-C2-C3-C4-C5-O5
3	H	5	MAN	C1-C2-C3-C4-C5-O5

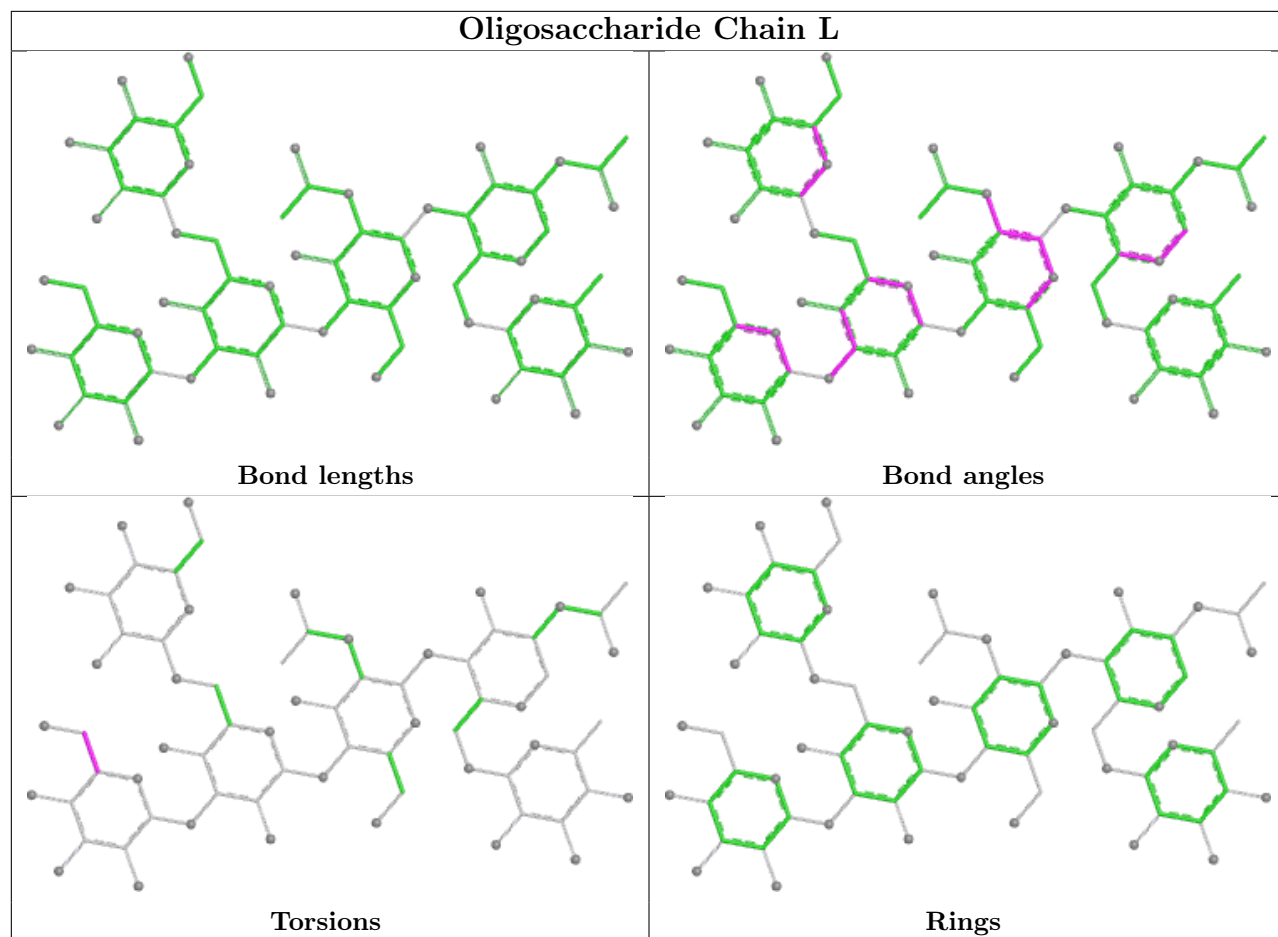
9 monomers are involved in 9 short contacts:

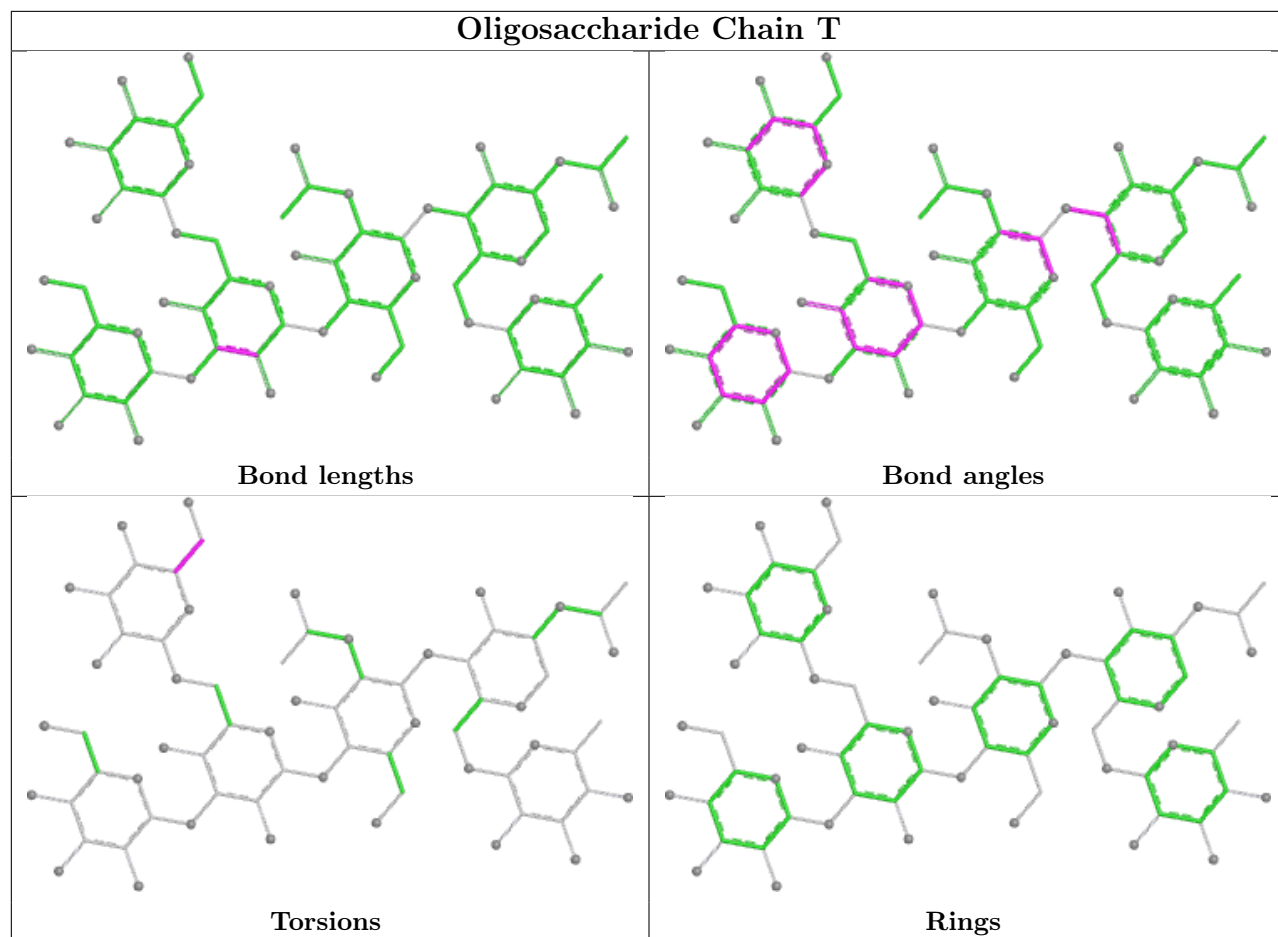
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6	FUC	1	0
2	C	2	NAG	1	0
2	C	5	MAN	1	0
6	K	2	NAG	1	0
11	R	1	NAG	2	0
3	B	5	MAN	0	1
6	Q	1	NAG	1	0
8	N	1	NAG	1	0
2	A	2	NAG	1	0

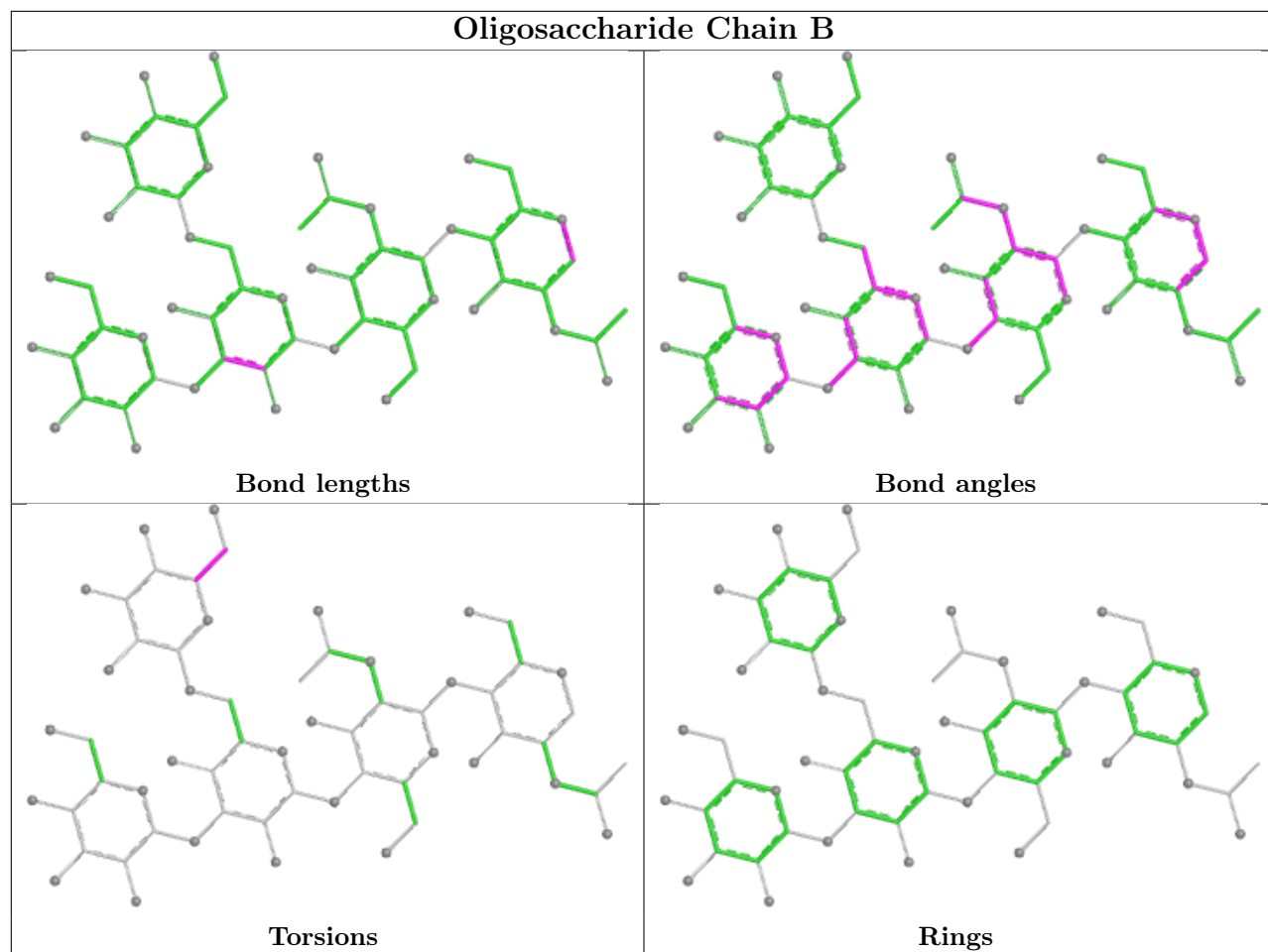
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



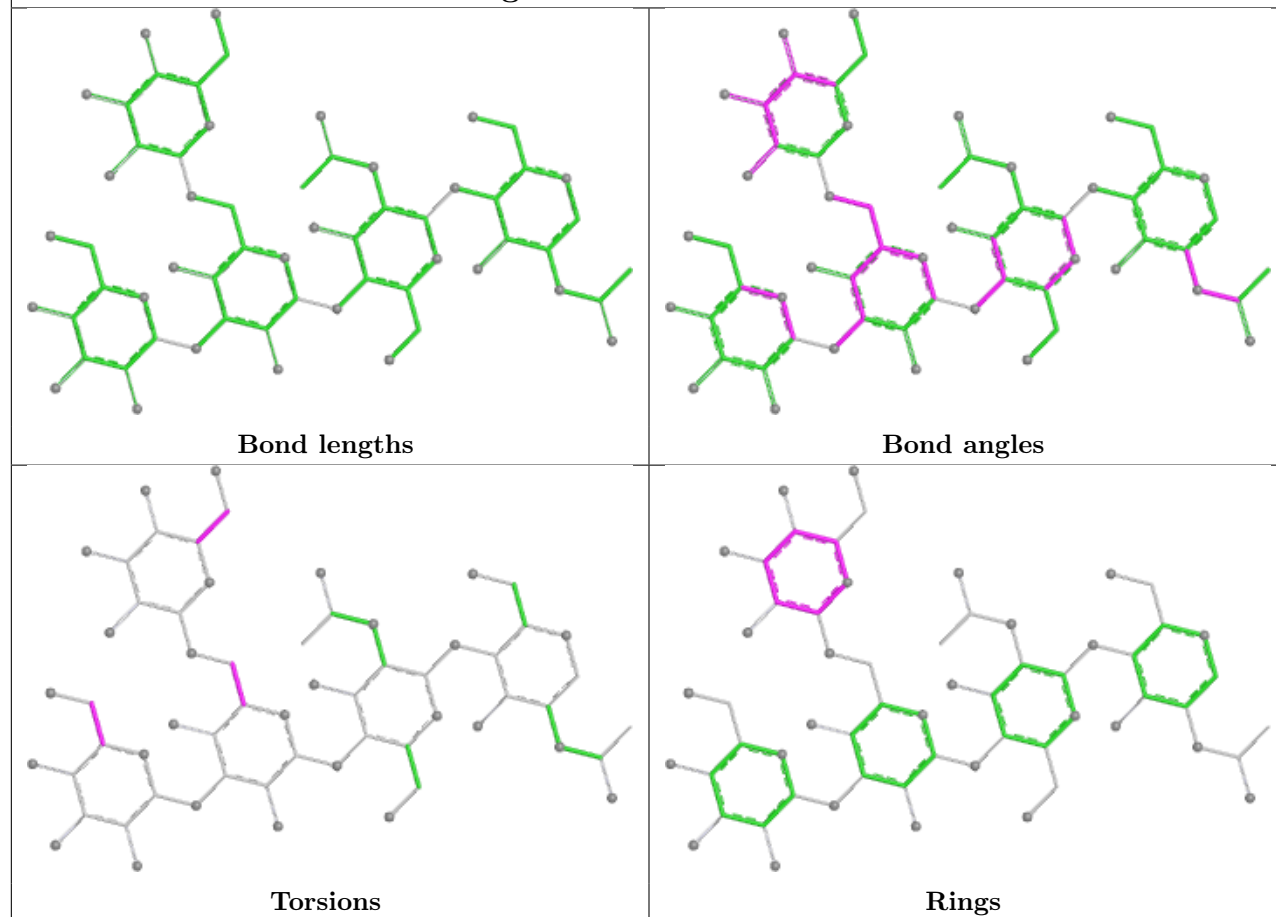




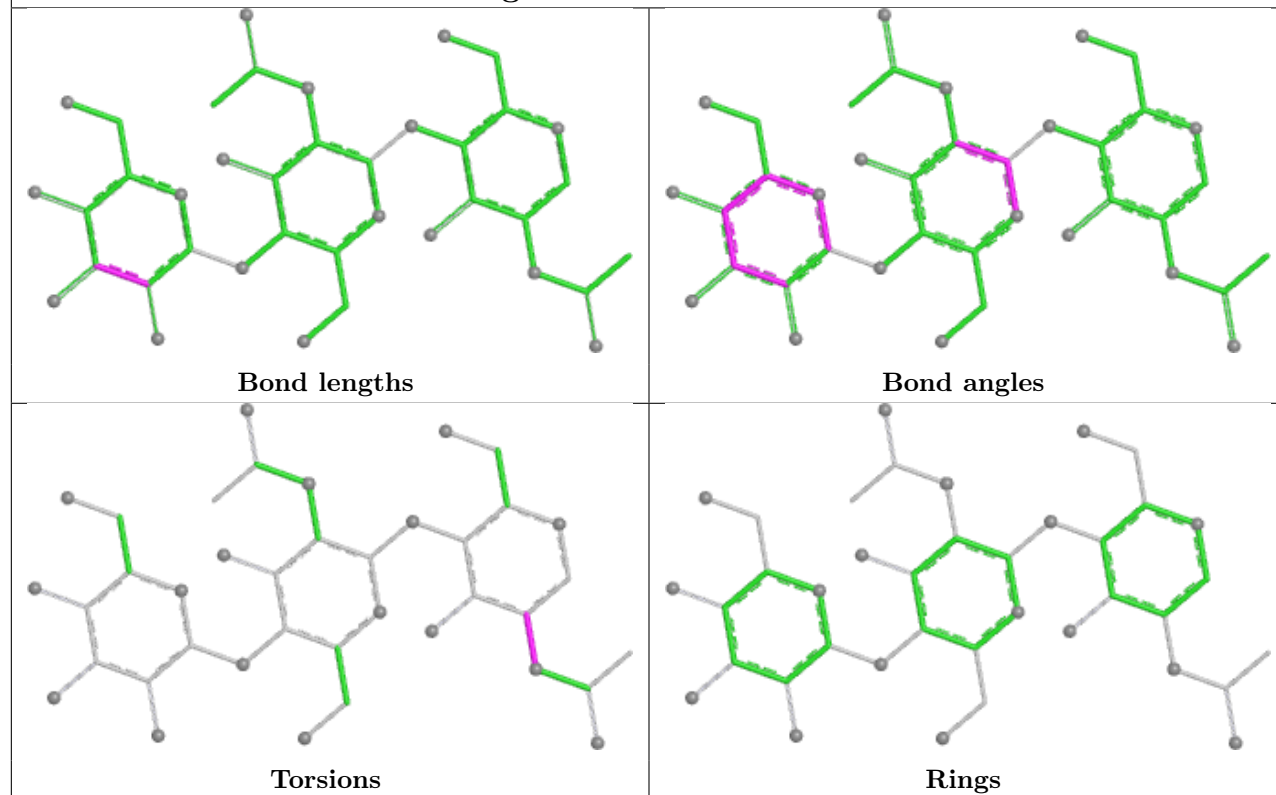


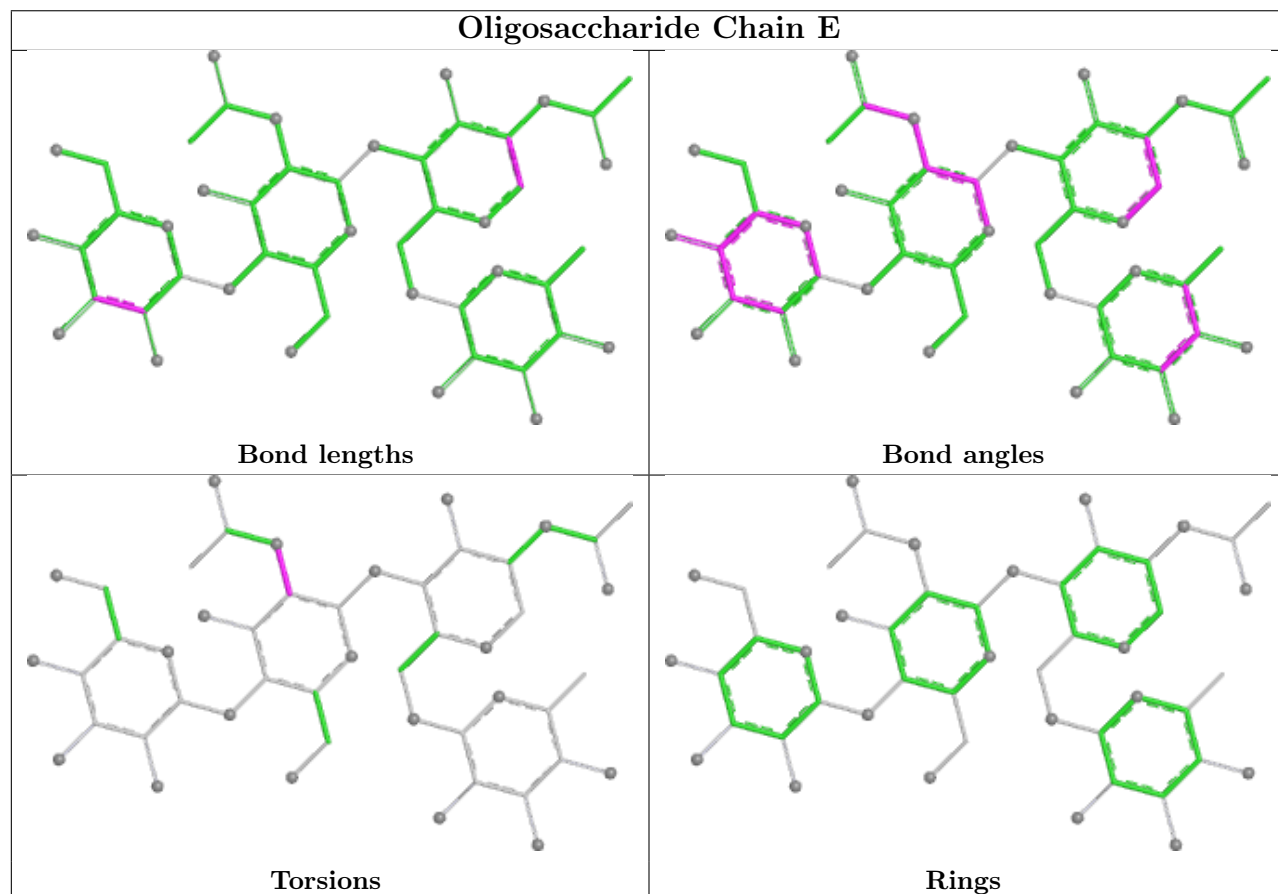
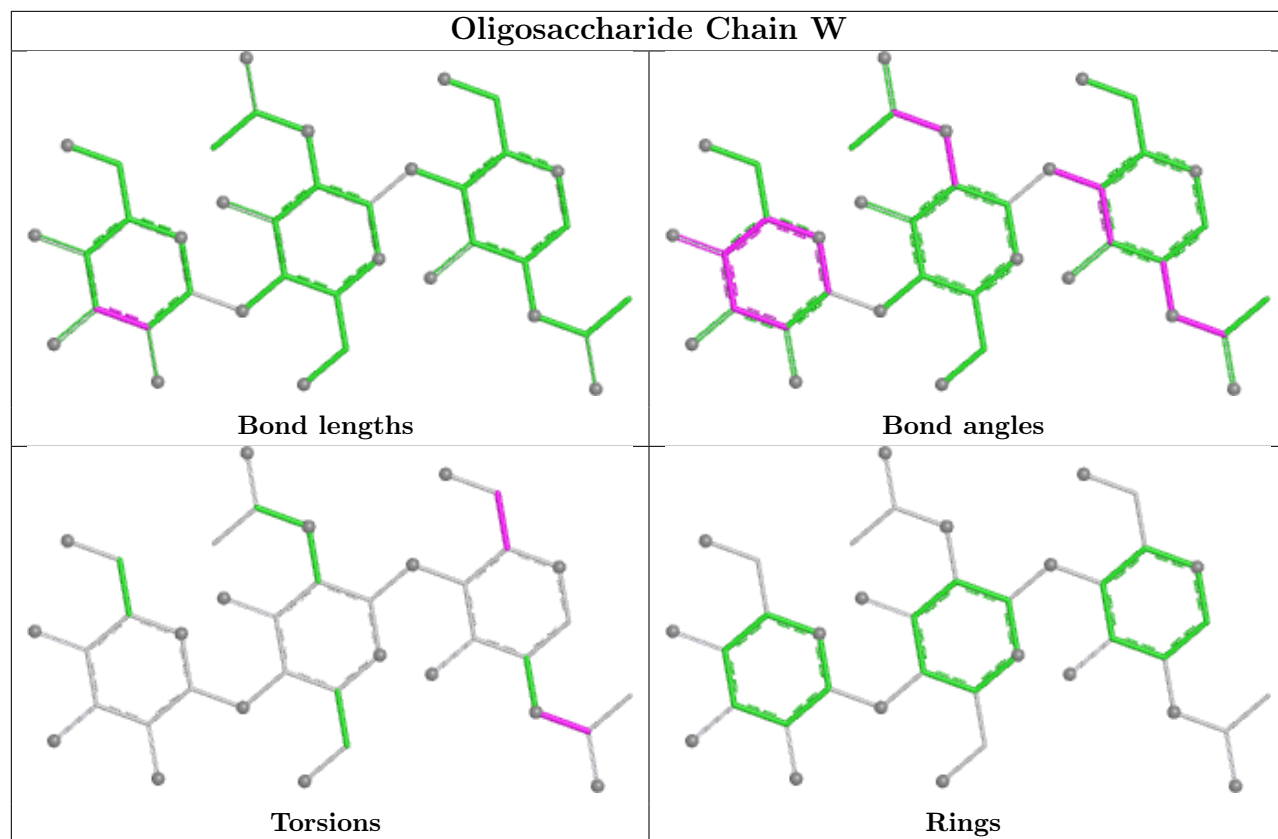


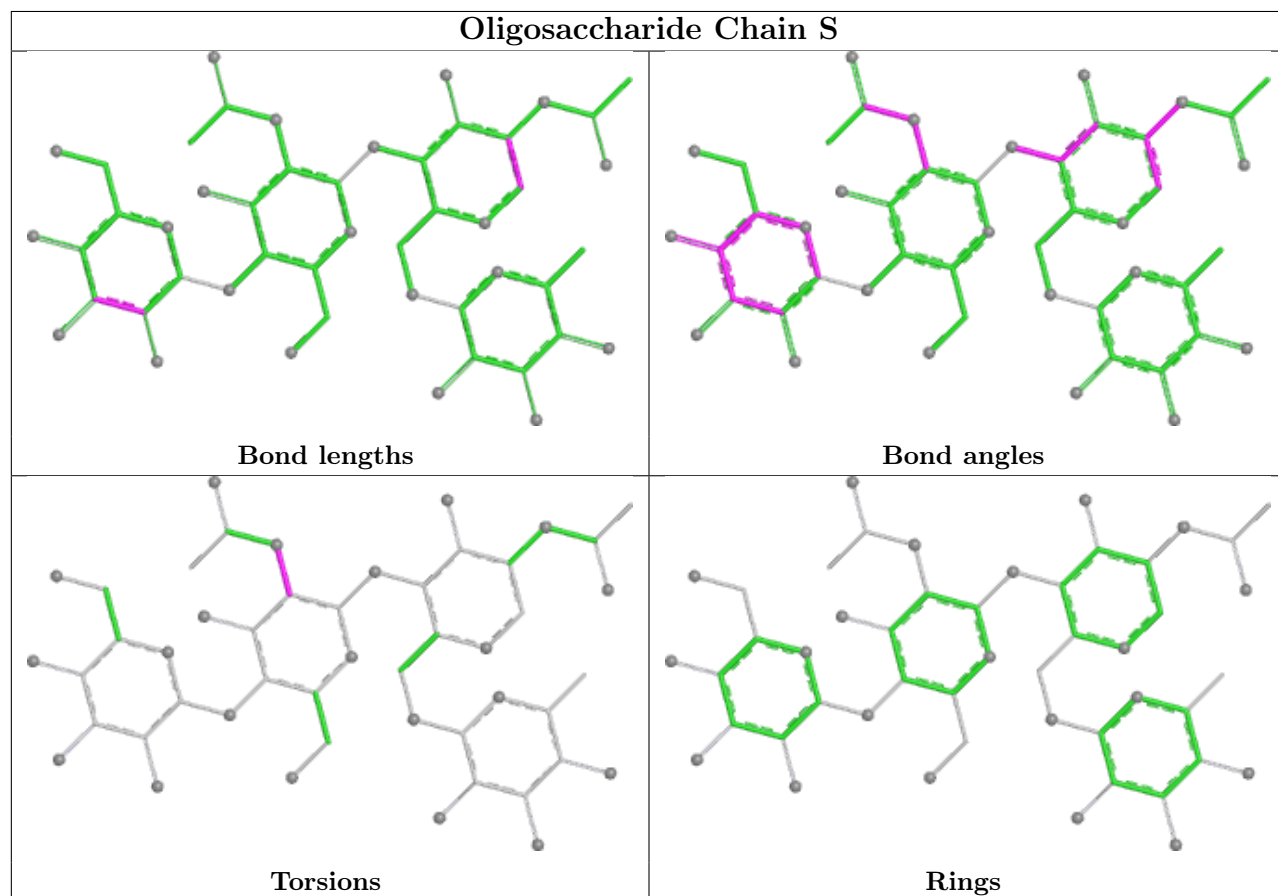
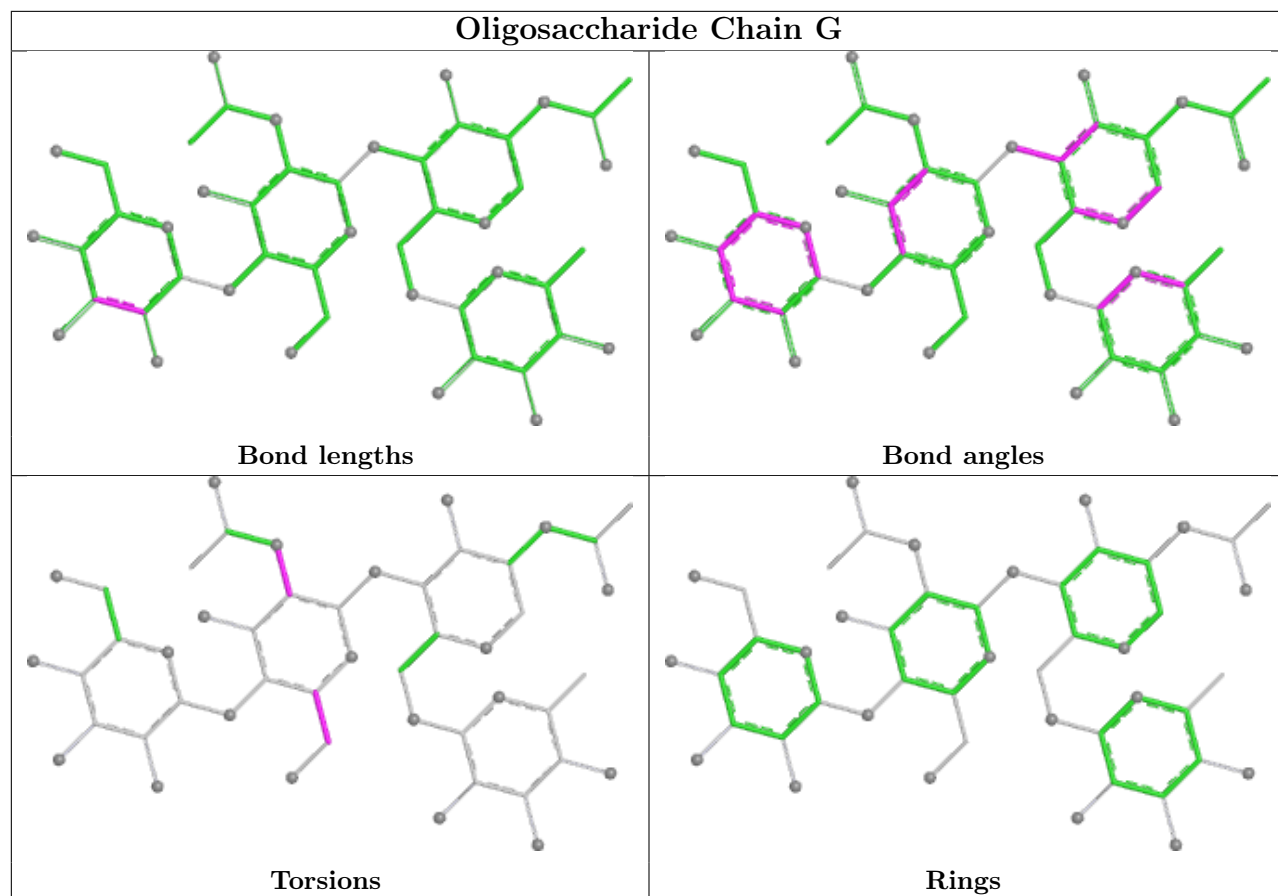
Oligosaccharide Chain H

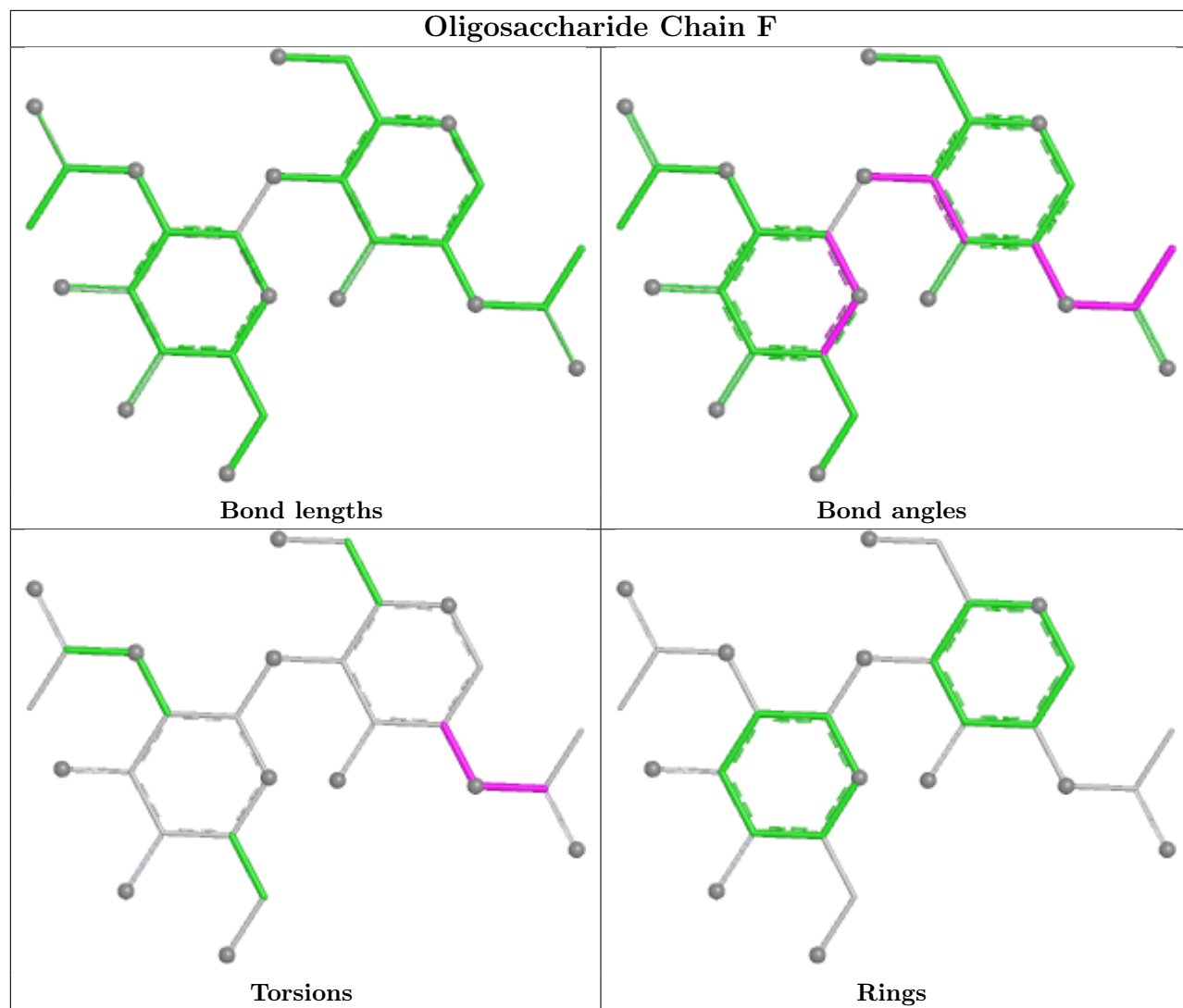


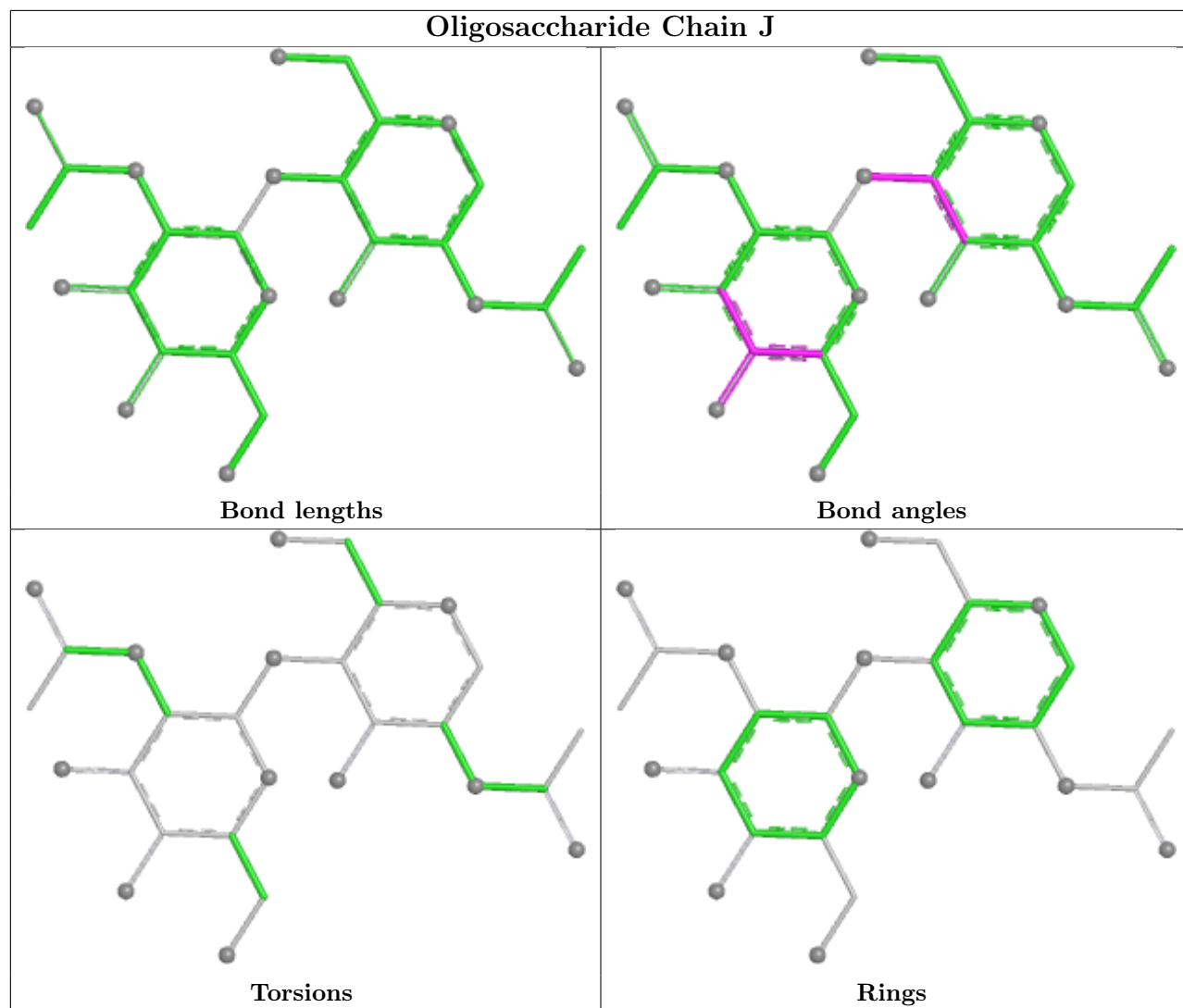
Oligosaccharide Chain D

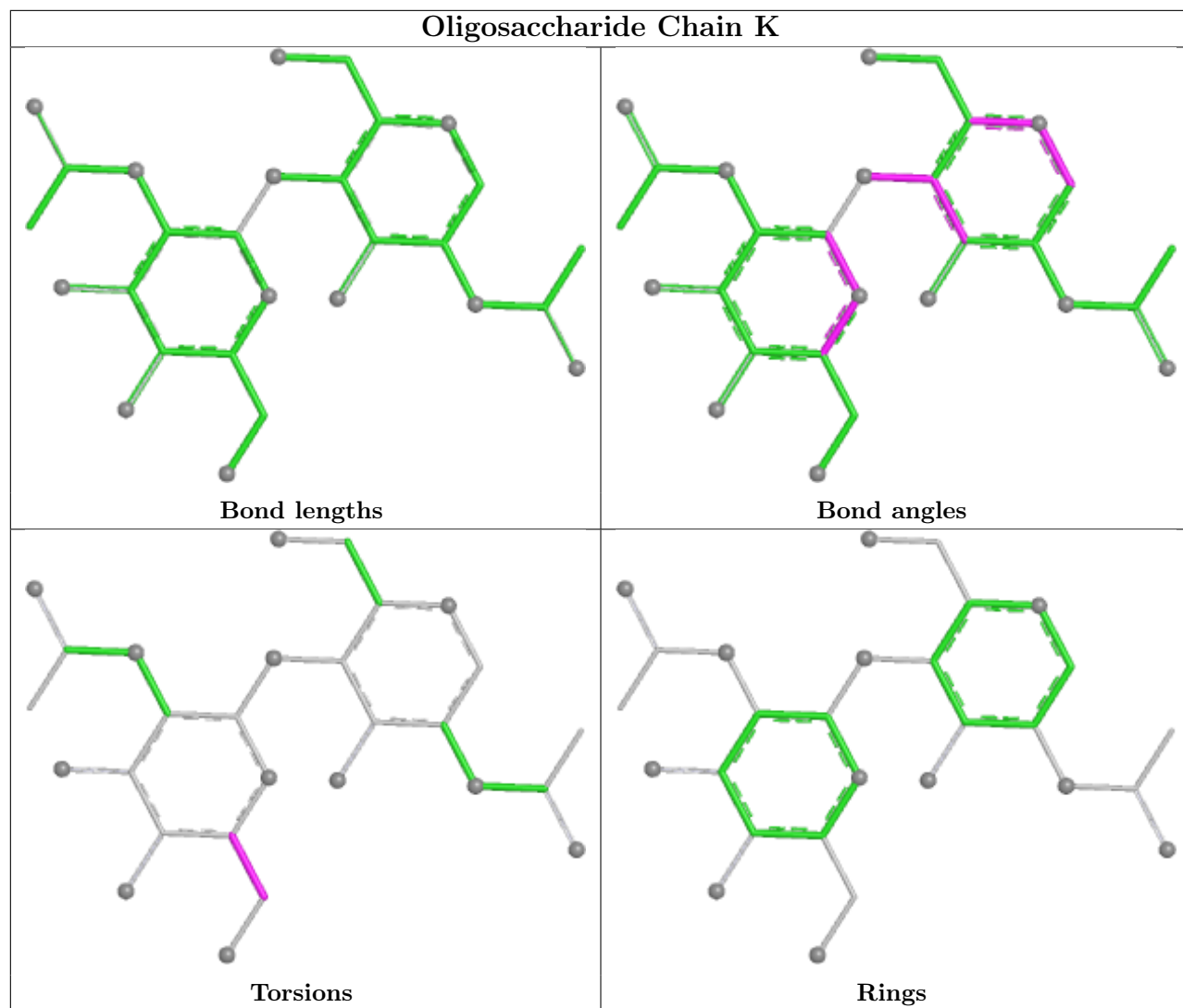


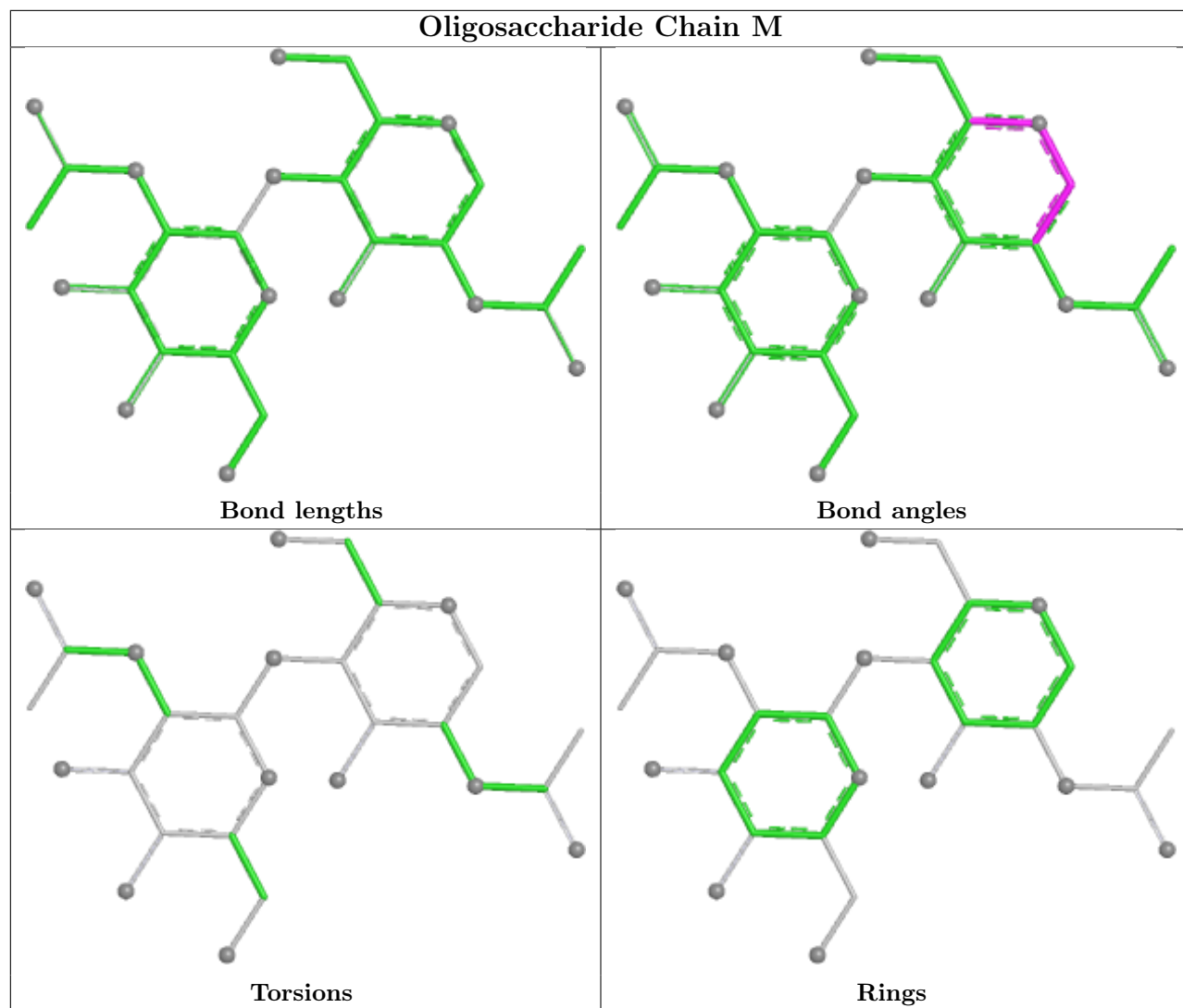


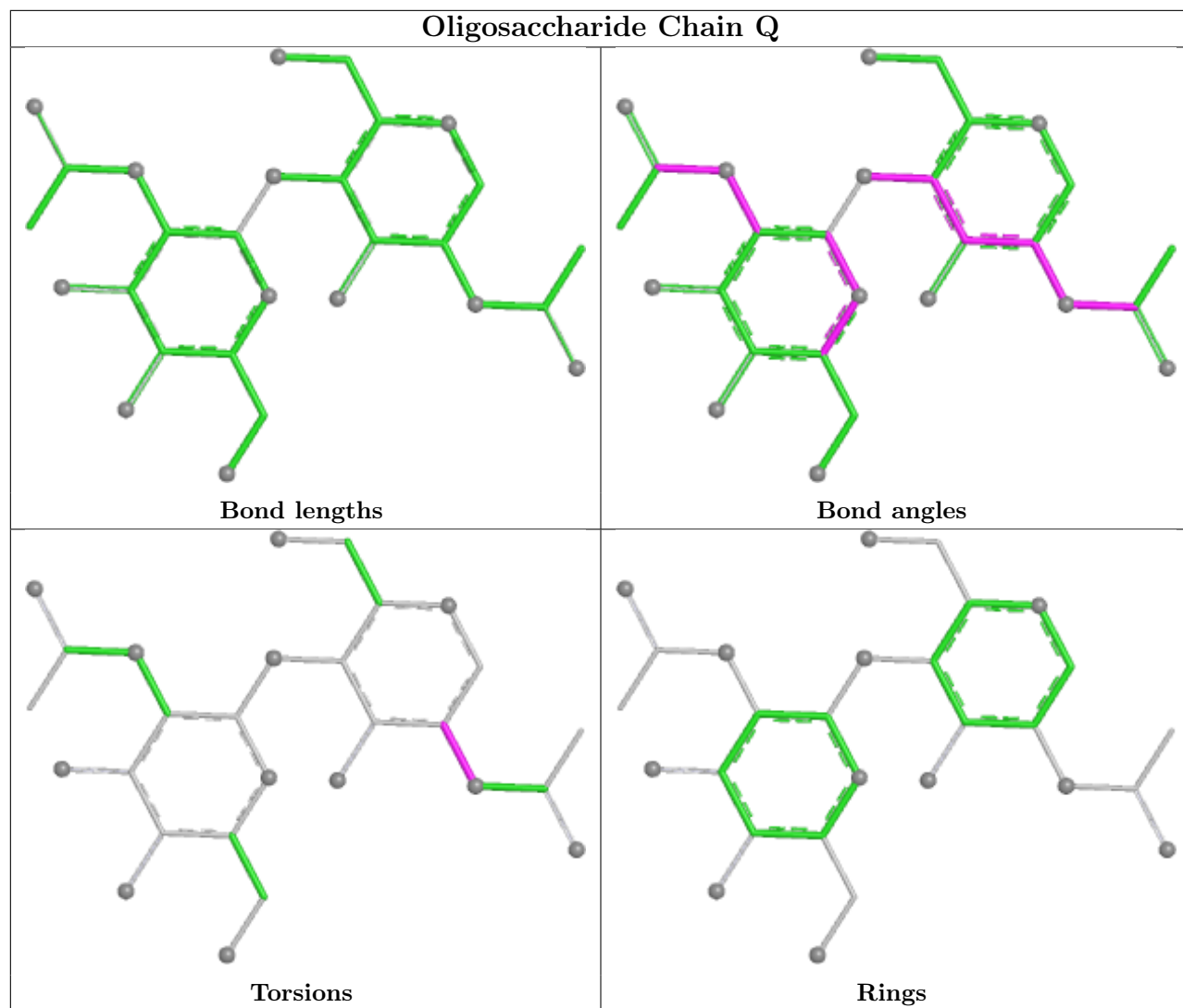


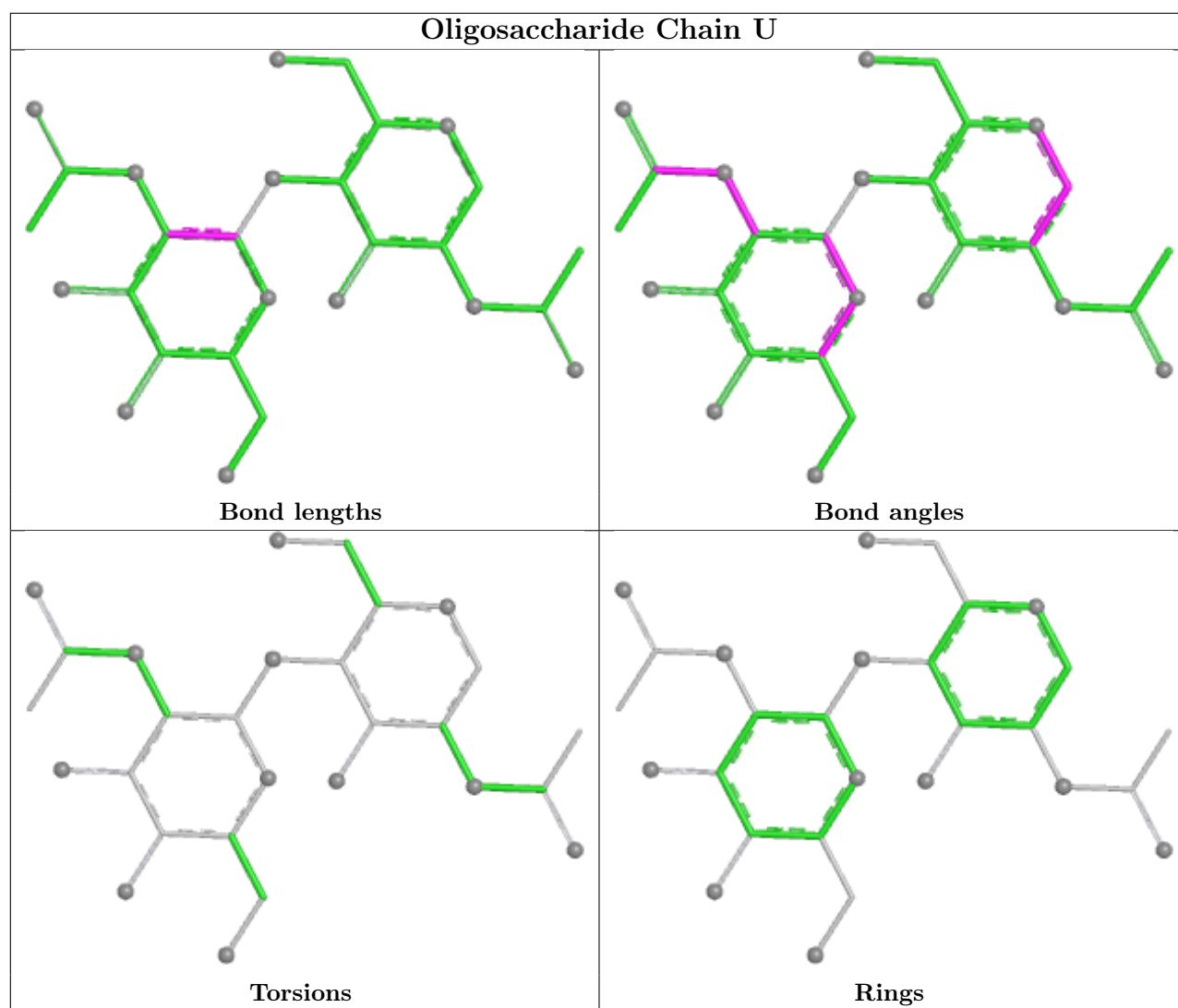


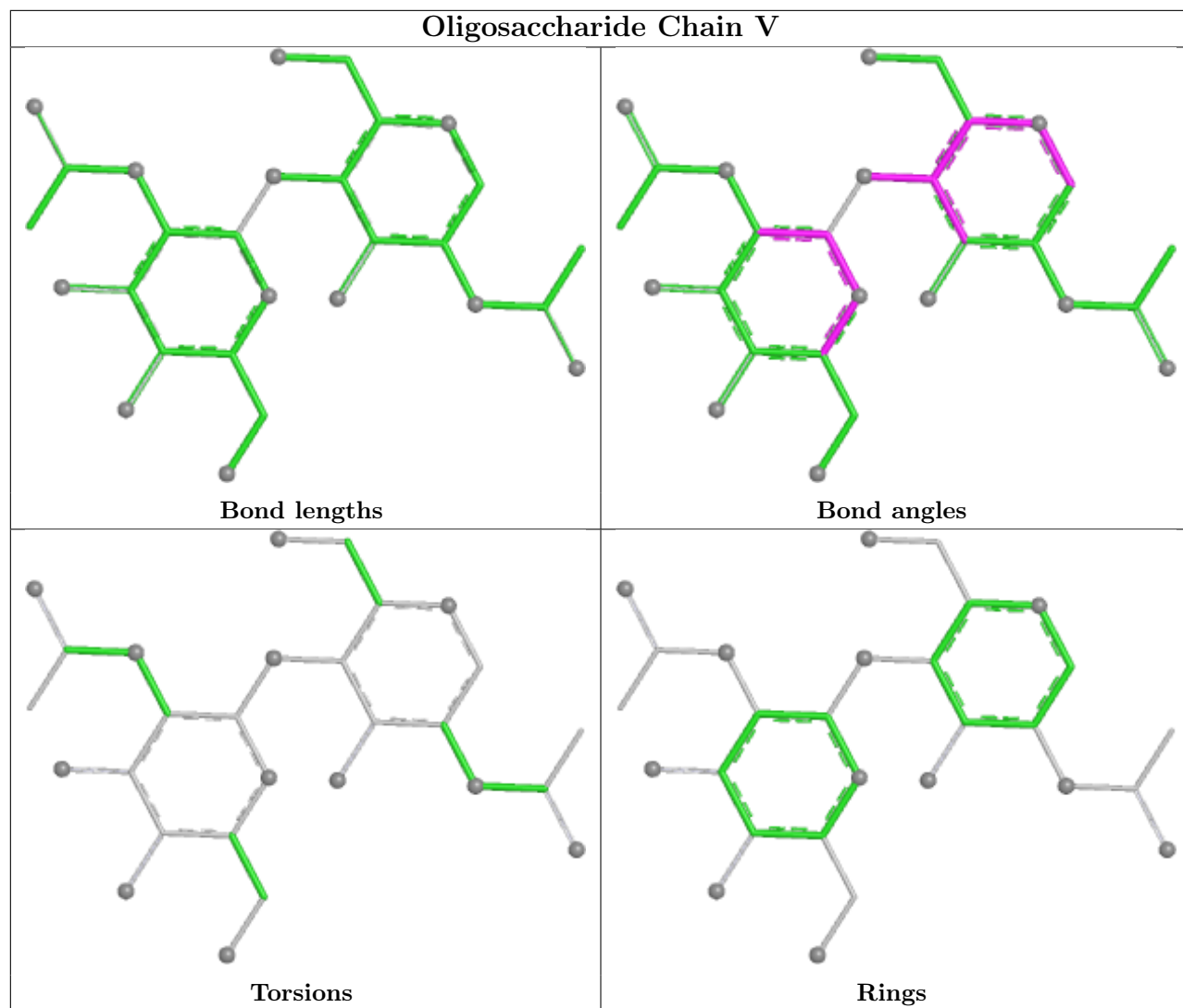


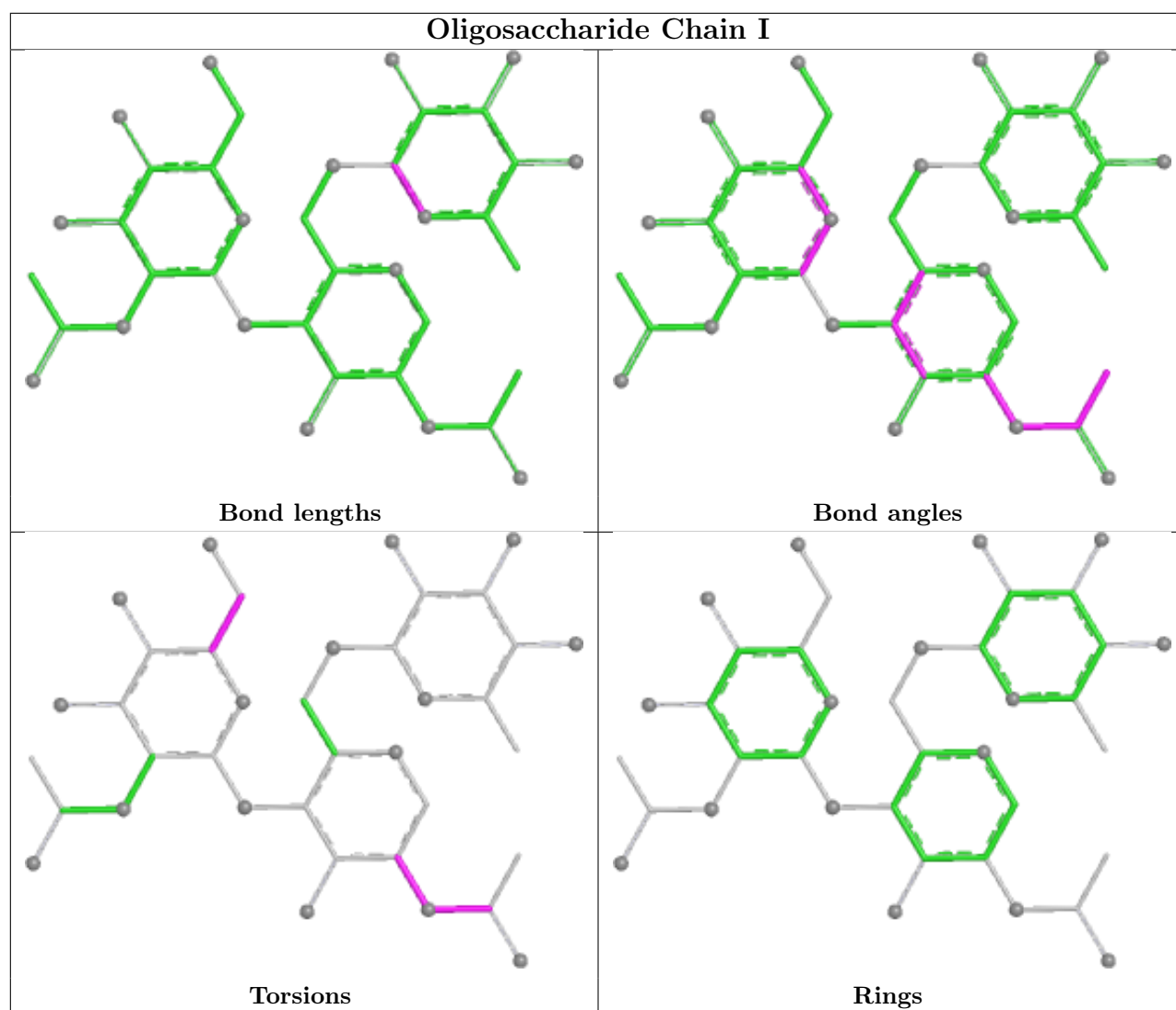


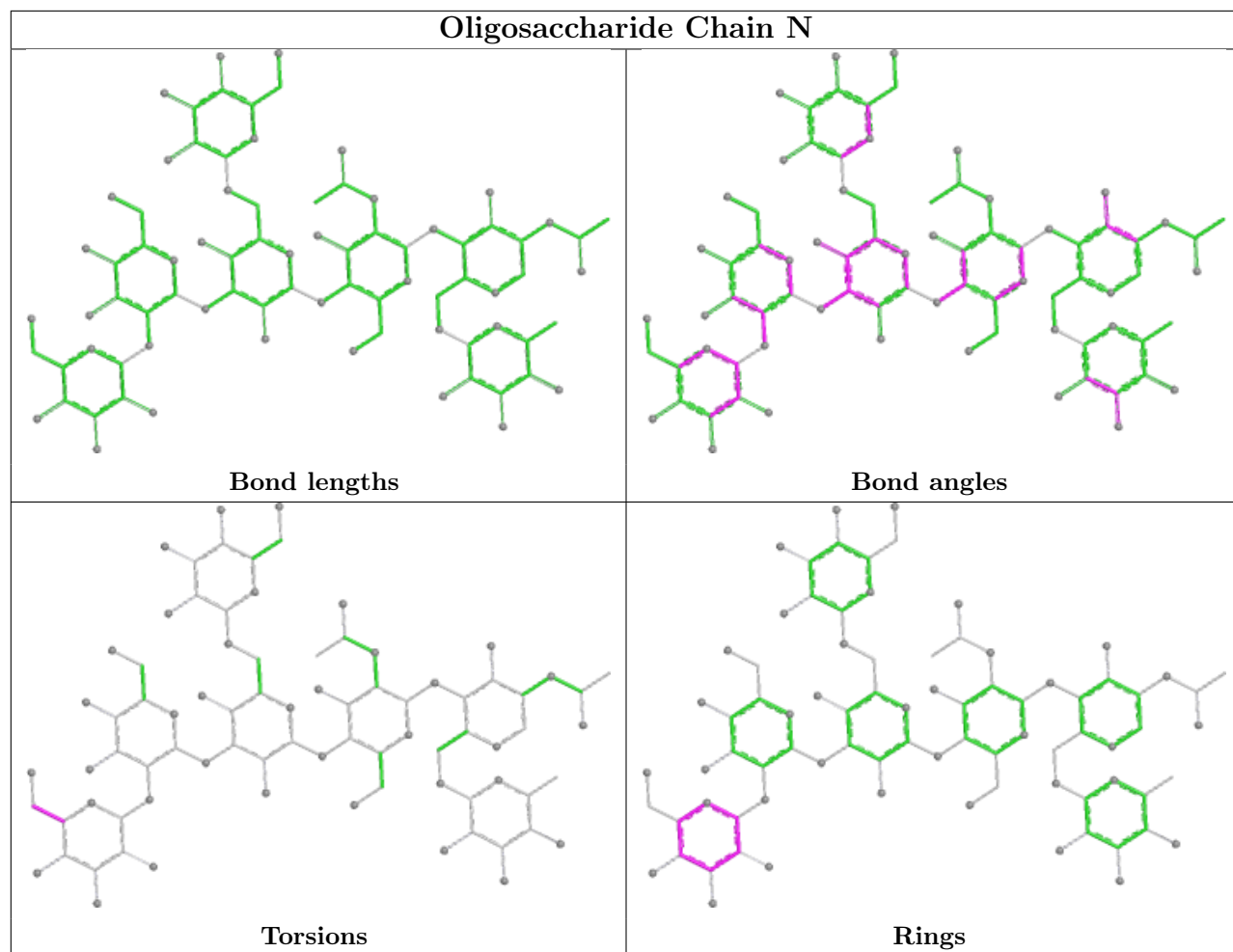


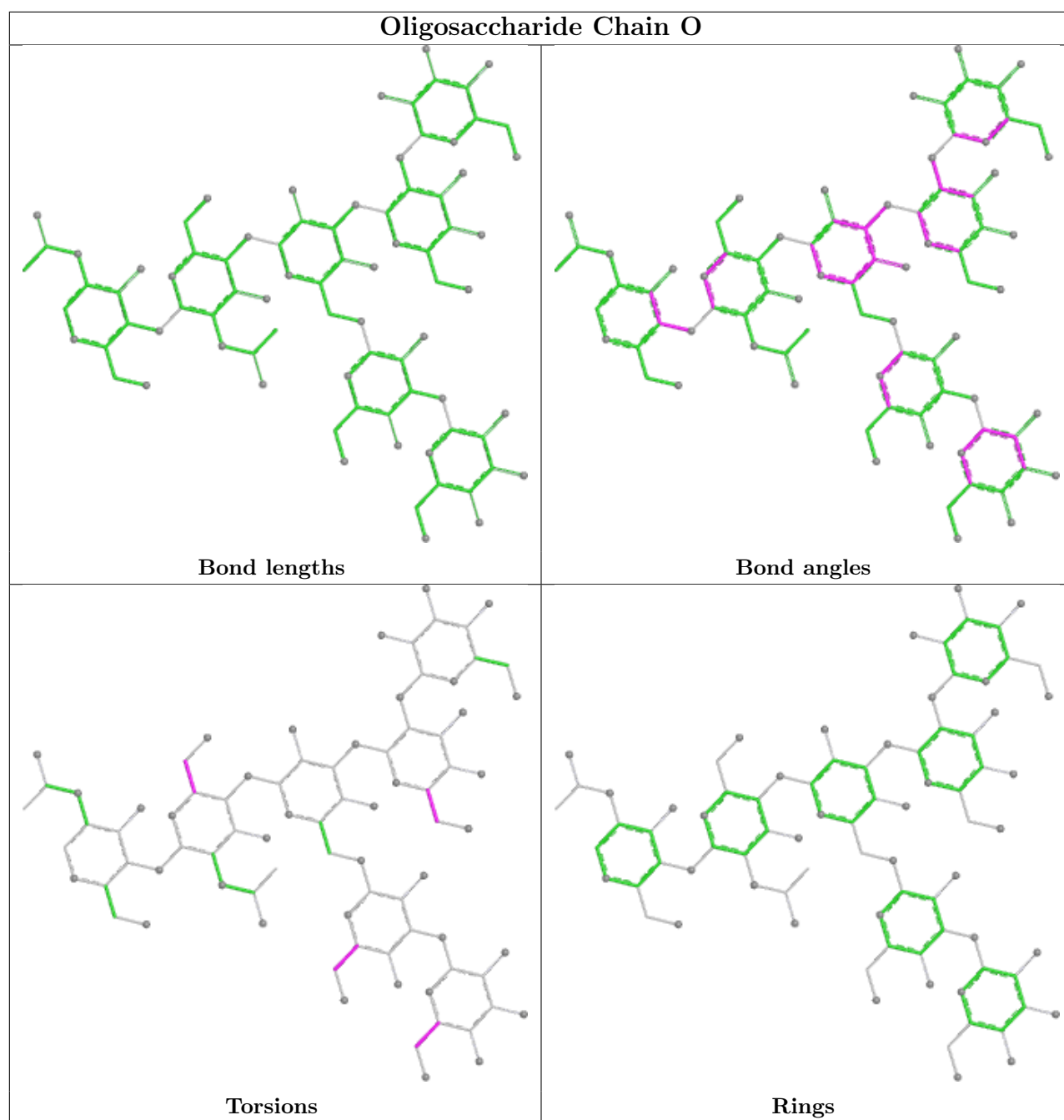


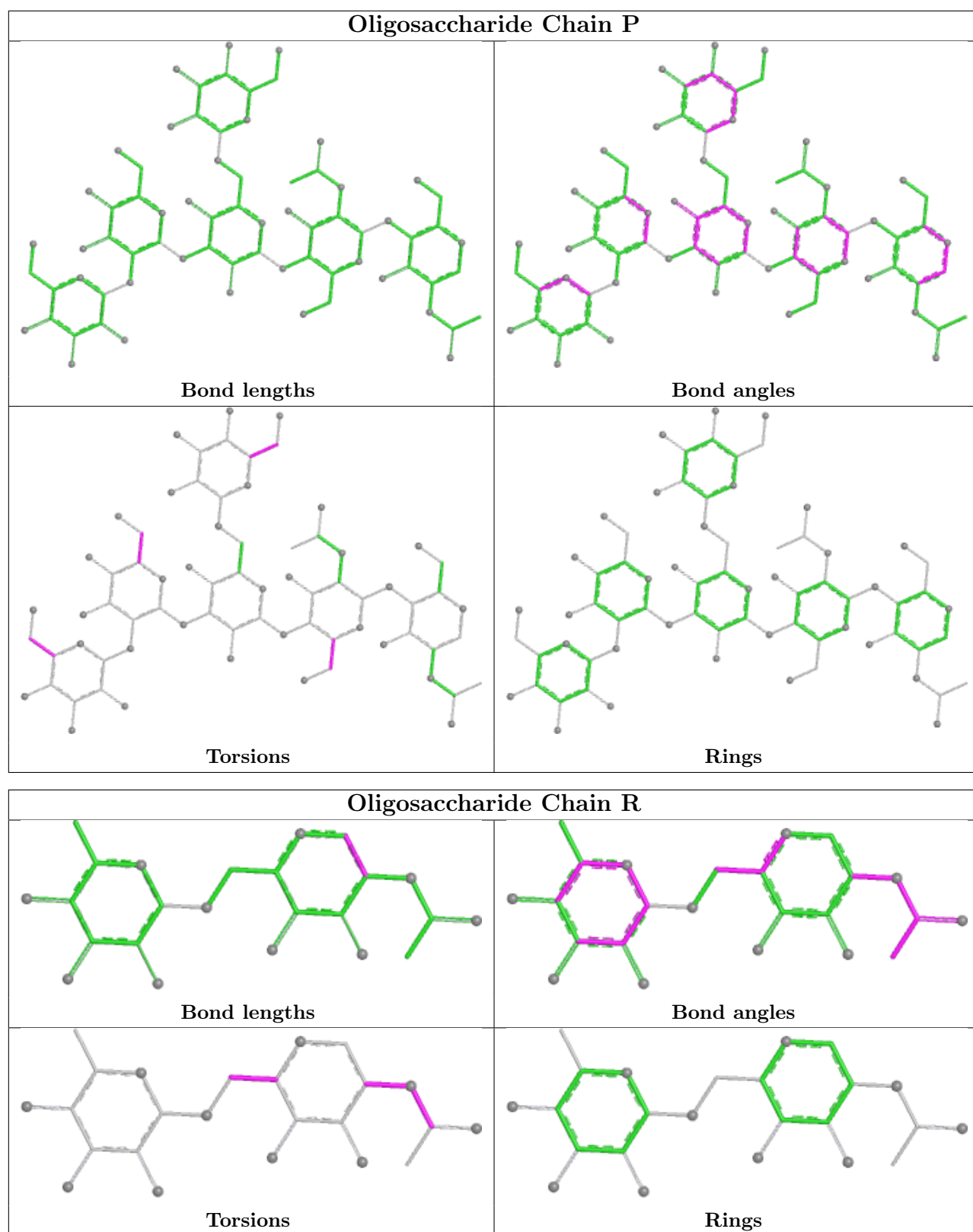


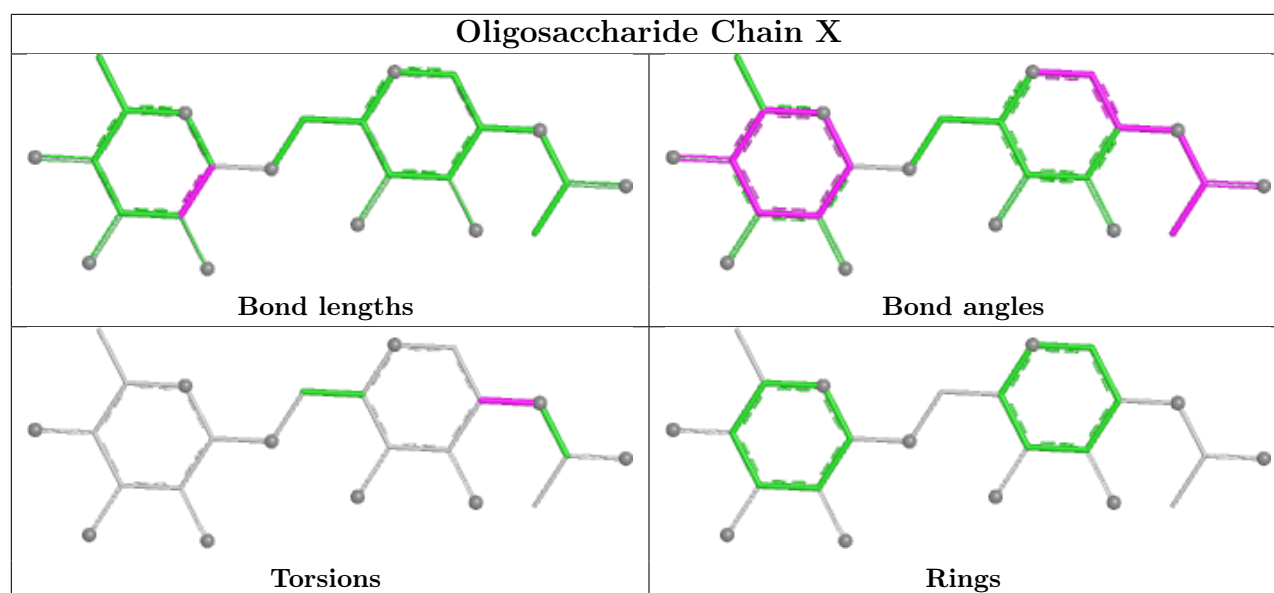












5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	DA	502	1	14,14,15	0.81	0	17,19,21	1.18	1 (5%)
12	NAG	CA	501	1	14,14,15	0.93	1 (7%)	17,19,21	1.58	2 (11%)
12	NAG	DA	501	1	14,14,15	0.88	1 (7%)	17,19,21	2.09	3 (17%)
13	GOL	AA	502	-	5,5,5	0.22	0	5,5,5	0.55	0
12	NAG	AA	501	1	14,14,15	0.94	0	17,19,21	2.36	5 (29%)
15	TY2	CA	503	-	13,14,14	1.21	2 (15%)	15,19,19	2.05	3 (20%)
13	GOL	DA	503	-	5,5,5	0.36	0	5,5,5	0.48	0
13	GOL	CA	502	-	5,5,5	0.32	0	5,5,5	0.57	0
13	GOL	BA	501	-	5,5,5	0.27	0	5,5,5	0.32	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	DA	502	1	-	2/6/23/26	0/1/1/1
12	NAG	CA	501	1	-	2/6/23/26	0/1/1/1
12	NAG	DA	501	1	-	0/6/23/26	0/1/1/1
13	GOL	AA	502	-	-	4/4/4/4	-
12	NAG	AA	501	1	-	3/6/23/26	0/1/1/1
15	TY2	CA	503	-	-	2/8/8/8	0/1/1/1
13	GOL	DA	503	-	-	4/4/4/4	-
13	GOL	CA	502	-	-	2/4/4/4	-
13	GOL	BA	501	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	CA	501	NAG	C1-C2	2.73	1.56	1.52
15	CA	503	TY2	CE2-CZ	-2.16	1.38	1.40
15	CA	503	TY2	CE2-NE2	2.15	1.45	1.38
12	DA	501	NAG	O5-C1	-2.04	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AA	501	NAG	C2-N2-C7	7.55	133.02	122.90
12	DA	501	NAG	C1-O5-C5	-6.85	103.00	112.19
15	CA	503	TY2	CE2-CD2-CG	-6.37	118.85	122.10
12	CA	501	NAG	C1-O5-C5	4.55	118.29	112.19
12	DA	501	NAG	C1-C2-N2	3.67	116.22	110.43
12	CA	501	NAG	C2-N2-C7	3.25	127.25	122.90
12	AA	501	NAG	O7-C7-N2	3.22	127.67	121.98
12	DA	502	NAG	C1-O5-C5	2.94	116.13	112.19
12	DA	501	NAG	O5-C1-C2	-2.50	107.43	111.29
15	CA	503	TY2	CG-CB-CA	-2.25	109.53	114.13
15	CA	503	TY2	OXT-C-O	-2.22	119.05	124.08
12	AA	501	NAG	O5-C5-C4	-2.18	105.51	110.83
12	AA	501	NAG	C4-C3-C2	2.17	114.19	111.02
12	AA	501	NAG	C1-O5-C5	-2.15	109.31	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

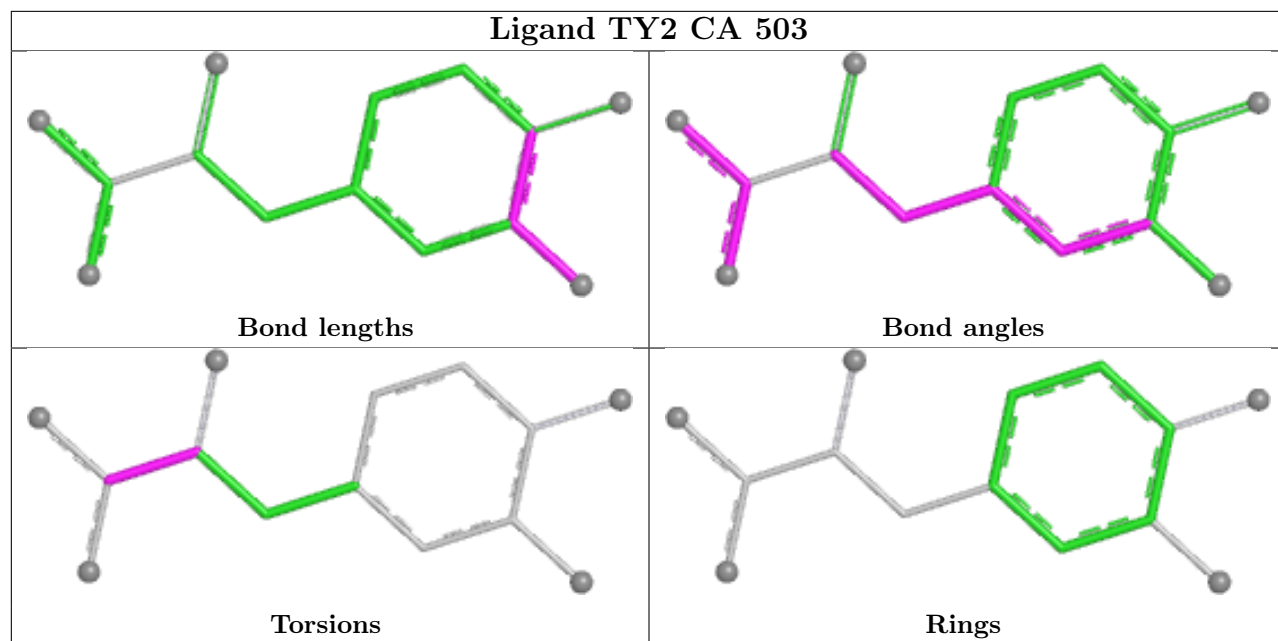
Mol	Chain	Res	Type	Atoms
12	AA	501	NAG	C3-C2-N2-C7
13	AA	502	GOL	O1-C1-C2-O2
13	AA	502	GOL	O1-C1-C2-C3
13	AA	502	GOL	C1-C2-C3-O3
13	AA	502	GOL	O2-C2-C3-O3
13	BA	501	GOL	C1-C2-C3-O3
13	BA	501	GOL	O2-C2-C3-O3
13	CA	502	GOL	C1-C2-C3-O3
13	DA	503	GOL	O1-C1-C2-C3
13	DA	503	GOL	C1-C2-C3-O3
12	CA	501	NAG	C8-C7-N2-C2
12	CA	501	NAG	O7-C7-N2-C2
15	CA	503	TY2	OXT-C-CA-N
13	CA	502	GOL	O2-C2-C3-O3
13	DA	503	GOL	O1-C1-C2-O2
13	DA	503	GOL	O2-C2-C3-O3
12	AA	501	NAG	O5-C5-C6-O6
12	DA	502	NAG	C4-C5-C6-O6
12	DA	502	NAG	O5-C5-C6-O6
15	CA	503	TY2	O-C-CA-N
12	AA	501	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	CA	502	GOL	1	0
13	BA	501	GOL	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	AA	447/450 (99%)	-0.40	0	100 100	20, 37, 53, 73	2 (0%)
1	BA	447/450 (99%)	-0.33	4 (0%)	81 79	18, 38, 52, 80	1 (0%)
1	CA	447/450 (99%)	-0.19	1 (0%)	91 90	28, 40, 58, 75	0
1	DA	450/450 (100%)	-0.10	4 (0%)	81 79	31, 45, 61, 82	1 (0%)
All	All	1791/1800 (99%)	-0.25	9 (0%)	87 85	18, 40, 57, 82	4 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DA	474	LEU	5.5
1	BA	64[A]	ARG	3.4
1	DA	473	ASN	3.3
1	BA	469	PRO	3.2
1	CA	48	VAL	2.9
1	BA	72	SER	2.7
1	DA	472	GLU	2.3
1	DA	100[A]	HIS	2.0
1	BA	71	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	1	14/15	-	-	34,40,49,51	0
2	NAG	A	2	14/15	-	-	35,43,47,47	0
2	BMA	A	3	11/12	-	-	39,40,47,54	0
2	MAN	A	4	11/12	-	-	45,49,56,58	0
2	MAN	A	5	11/12	-	-	54,58,66,68	0
2	FUC	A	6	10/11	-	-	55,62,69,69	0
2	NAG	C	1	14/15	-	-	43,51,59,60	0
2	NAG	C	2	14/15	-	-	57,68,87,93	0
2	BMA	C	3	11/12	-	-	96,101,106,106	0
2	MAN	C	4	11/12	-	-	74,101,105,106	0
2	MAN	C	5	11/12	-	-	95,102,104,105	0
2	FUC	C	6	10/11	-	-	42,48,54,55	0
3	BMA	H	3	11/12	0.32	0.15	51,60,69,76	0
5	BMA	S	3	11/12	0.38	0.12	87,92,95,97	0
4	BMA	W	3	11/12	0.39	0.17	68,90,95,96	0
8	NAG	N	2	14/15	0.44	0.15	50,63,77,83	0
6	NAG	U	2	14/15	0.49	0.15	66,80,86,89	0
2	FUC	L	6	10/11	-	-	65,71,73,74	0
6	NAG	V	1	14/15	0.55	0.17	43,60,66,68	0
5	BMA	G	3	11/12	0.60	0.14	77,86,88,91	0
6	NAG	U	1	14/15	0.63	0.14	50,57,69,70	0
2	MAN	L	4	11/12	0.63	0.13	51,56,64,70	0
6	NAG	J	1	14/15	0.66	0.13	59,72,81,88	0
2	FUC	T	6	10/11	-	-	51,57,61,66	0
3	NAG	B	1	14/15	-	-	36,41,44,45	0
3	NAG	B	2	14/15	-	-	39,48,59,62	0
3	BMA	B	3	11/12	-	-	65,73,83,85	0
3	MAN	B	4	11/12	-	-	78,87,93,94	0
3	MAN	B	5	11/12	-	-	79,83,88,89	0
8	NAG	N	1	14/15	0.67	0.12	40,47,50,51	0
7	NAG	I	2	14/15	0.67	0.14	79,82,85,87	0
9	NAG	O	2	14/15	0.67	0.14	73,83,92,94	0
3	MAN	H	4	11/12	-	-	77,80,85,87	0
3	MAN	H	5	11/12	-	-	37,54,61,70	0
4	NAG	D	1	14/15	-	-	41,47,56,56	0
4	NAG	D	2	14/15	-	-	61,68,82,87	0
4	BMA	D	3	11/12	-	-	89,95,98,99	0
6	NAG	J	2	14/15	0.69	0.12	82,91,97,104	0
6	NAG	M	2	14/15	0.73	0.10	61,72,79,81	0
2	BMA	T	3	11/12	0.73	0.12	89,92,94,95	0
6	NAG	M	1	14/15	0.75	0.11	47,54,65,67	0
6	NAG	Q	2	14/15	0.77	0.11	75,91,102,102	0
2	NAG	T	2	14/15	0.77	0.12	66,74,79,83	0

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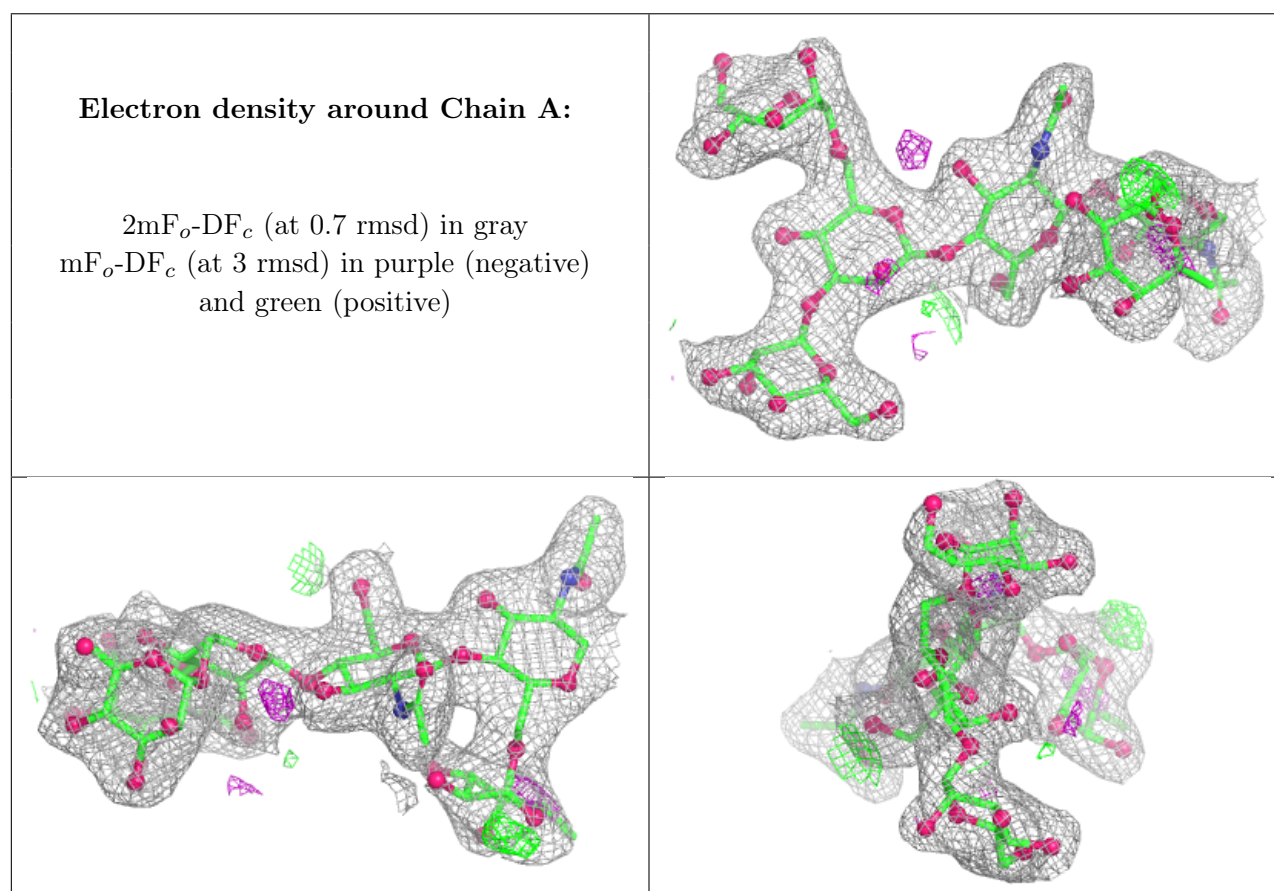
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FUC	E	4	10/11	-	-	58,71,81,85	0
2	MAN	L	5	11/12	0.78	0.13	67,69,72,78	0
2	MAN	T	4	11/12	0.78	0.16	96,99,101,102	0
10	MAN	P	5	11/12	0.78	0.12	53,60,66,67	0
5	FUC	G	4	10/11	-	-	43,50,56,58	0
6	NAG	K	2	14/15	0.81	0.10	65,70,77,83	0
5	NAG	S	2	14/15	0.81	0.11	68,73,81,85	0
10	MAN	P	4	11/12	0.82	0.11	68,73,78,79	0
5	FUC	S	4	10/11	-	-	65,71,75,79	0
3	NAG	H	2	14/15	0.82	0.10	48,52,56,60	0
4	NAG	W	2	14/15	0.83	0.12	75,86,90,90	0
5	NAG	G	2	14/15	0.83	0.11	62,74,84,88	0
11	NAG	X	1	14/15	0.85	0.11	60,75,88,90	0
7	NAG	I	1	14/15	0.87	0.09	56,67,76,83	0
2	BMA	L	3	11/12	0.88	0.09	44,51,55,68	0
2	NAG	L	1	14/15	0.88	0.09	39,47,51,60	0
5	NAG	G	1	14/15	0.88	0.10	47,54,60,62	0
6	NAG	K	1	14/15	0.89	0.09	42,48,56,56	0
4	NAG	W	1	14/15	0.90	0.10	66,75,79,83	0
9	NAG	O	1	14/15	0.91	0.08	42,48,61,64	0
6	NAG	Q	1	14/15	0.91	0.08	50,71,79,89	0
10	NAG	P	2	14/15	0.91	0.09	64,69,79,79	0
6	NAG	V	2	14/15	-	-	68,74,81,85	0
2	NAG	L	2	14/15	0.92	0.08	48,52,58,60	0
2	MAN	T	5	11/12	0.92	0.09	74,88,93,94	11
7	FUC	I	3	10/11	-	-	57,72,74,76	0
11	NAG	R	1	14/15	0.92	0.09	54,69,88,93	0
6	NAG	F	2	14/15	0.92	0.09	80,87,92,93	0
8	BMA	N	3	11/12	-	-	90,94,96,100	0
8	MAN	N	4	11/12	-	-	95,102,110,112	0
8	MAN	N	5	11/12	-	-	106,112,121,123	0
8	MAN	N	6	11/12	-	-	91,94,100,100	0
8	FUC	N	7	10/11	-	-	37,46,50,53	0
2	NAG	T	1	14/15	0.93	0.07	57,62,68,68	0
10	BMA	P	3	11/12	0.93	0.07	76,79,90,96	0
9	BMA	O	3	11/12	-	-	101,109,116,125	0
9	MAN	O	4	11/12	-	-	95,107,109,109	0
9	MAN	O	5	11/12	-	-	83,97,101,103	0
9	MAN	O	6	11/12	-	-	125,129,132,136	0
9	MAN	O	7	11/12	-	-	126,140,143,145	0
6	NAG	F	1	14/15	0.93	0.09	52,63,78,85	0
5	NAG	S	1	14/15	0.94	0.07	56,63,66,66	0

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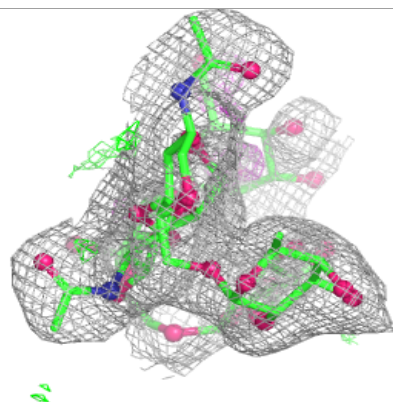
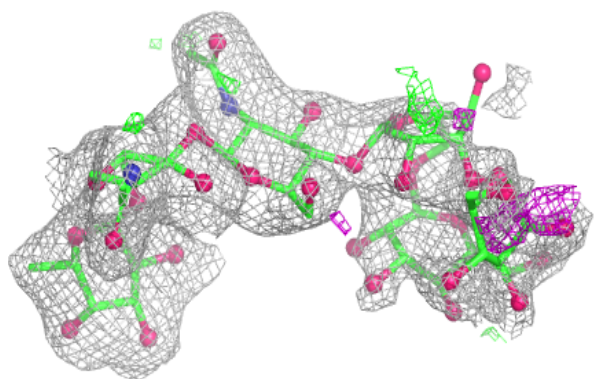
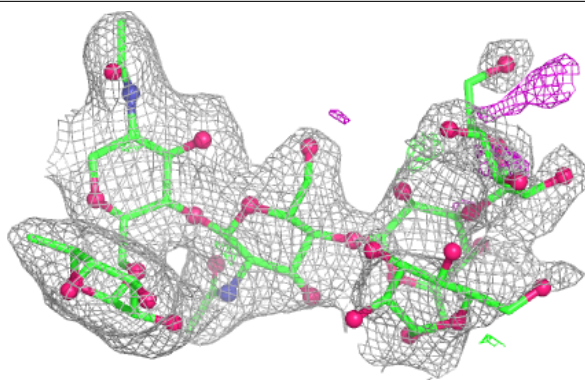
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	E	2	14/15	0.94	0.08	68,74,79,79	0
10	NAG	P	1	14/15	0.94	0.07	45,48,57,63	0
5	BMA	E	3	11/12	0.95	0.06	68,75,81,82	0
10	MAN	P	6	11/12	-	-	89,95,99,102	0
5	NAG	E	1	14/15	0.95	0.08	33,53,70,70	0
11	FUC	R	2	10/11	-	-	79,97,101,103	0
3	NAG	H	1	14/15	0.95	0.06	45,49,52,52	0
11	FUC	X	2	10/11	-	-	79,82,91,92	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.

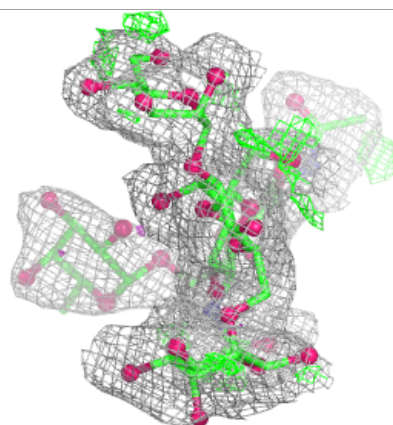
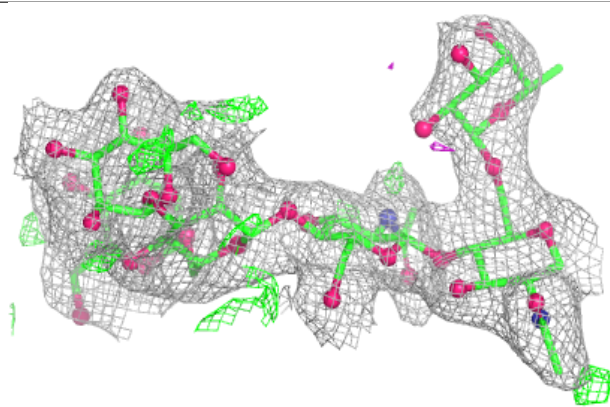
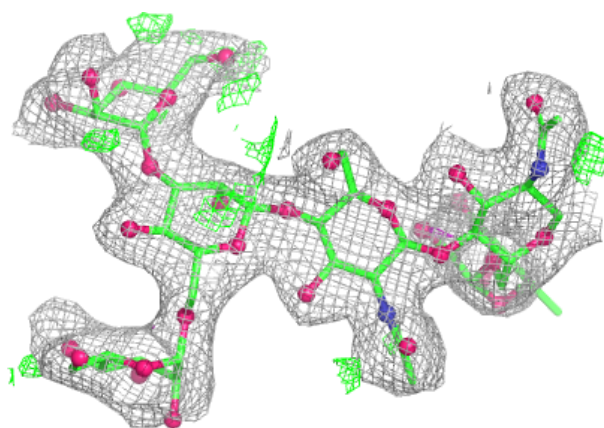


Electron density around Chain C:

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

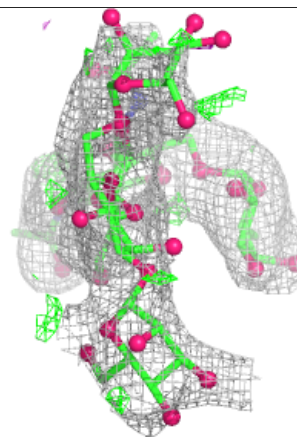
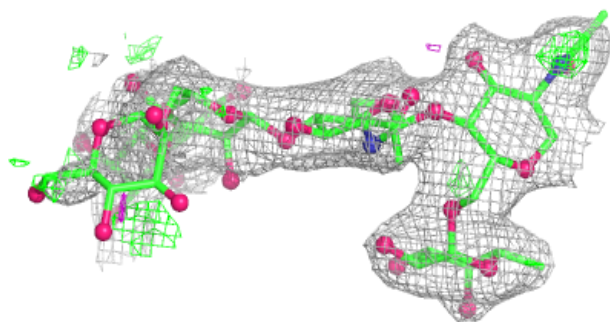
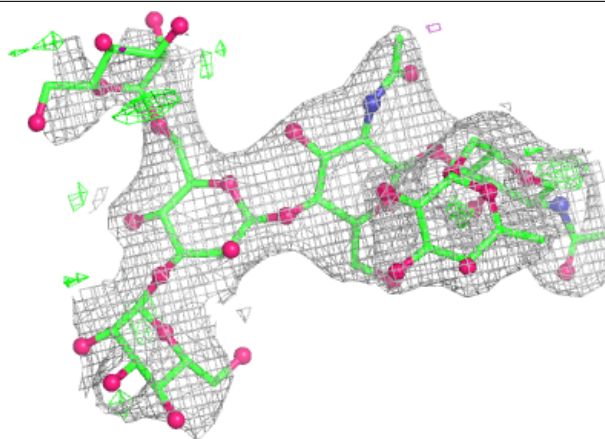
**Electron density around Chain L:**

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



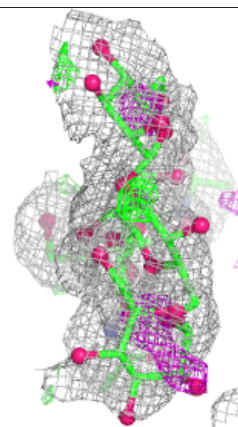
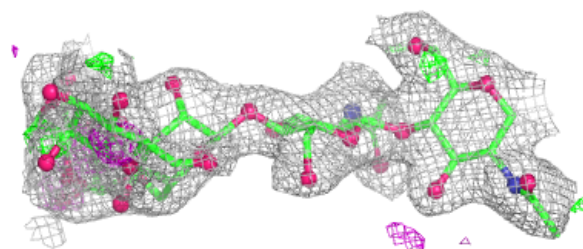
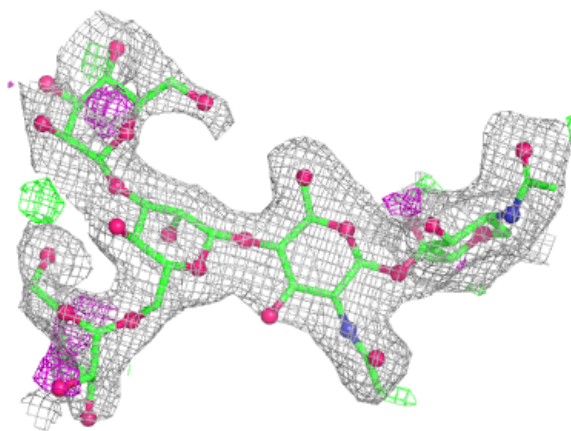
Electron density around Chain T:

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



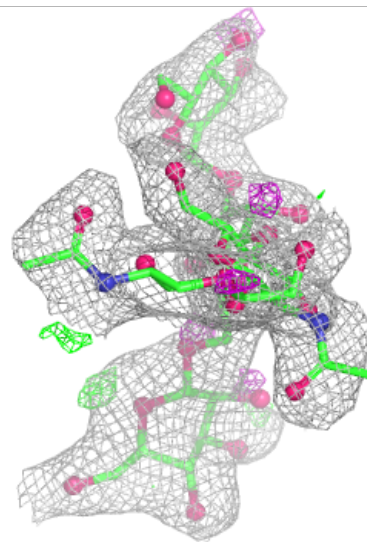
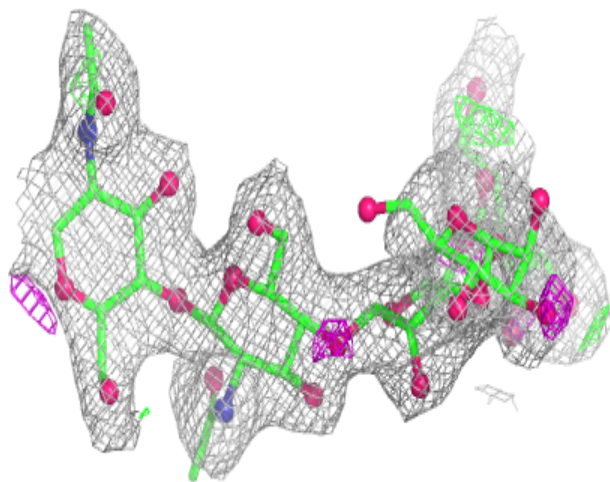
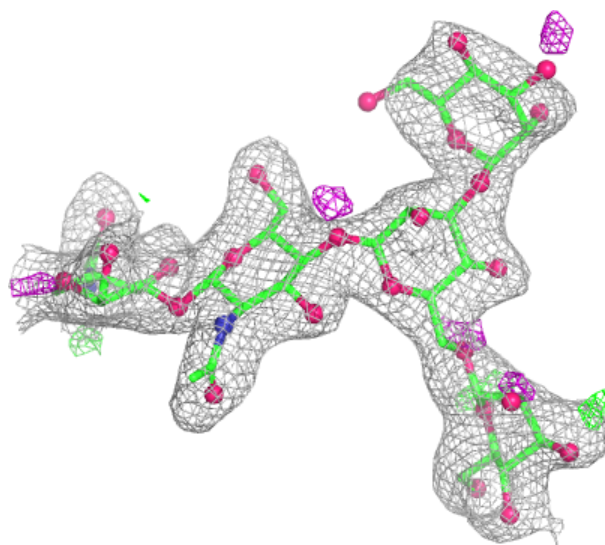
Electron density around Chain B:

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



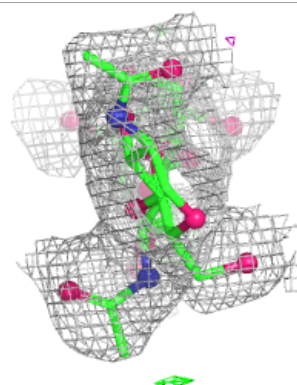
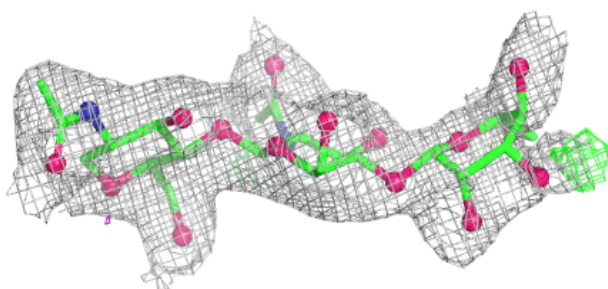
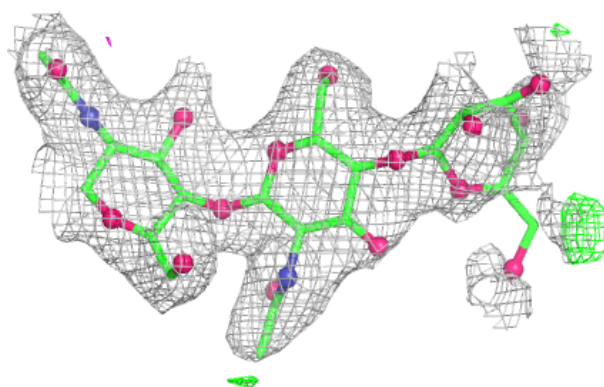
Electron density around Chain H:

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

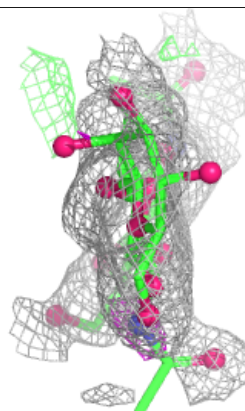
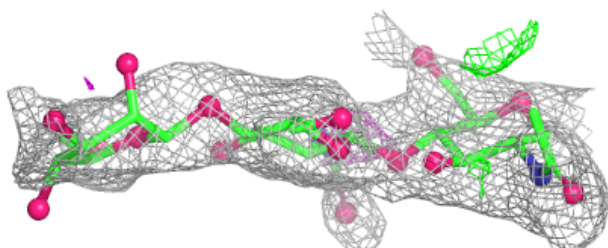
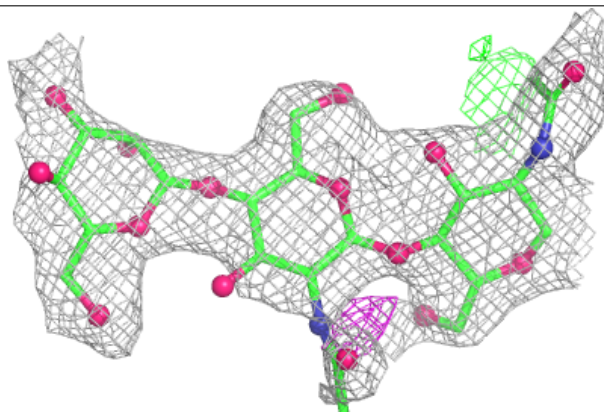


Electron density around Chain D:

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

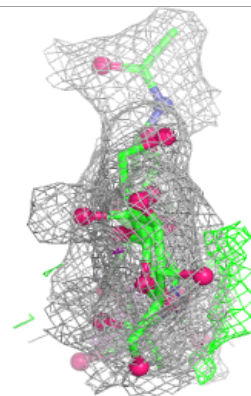
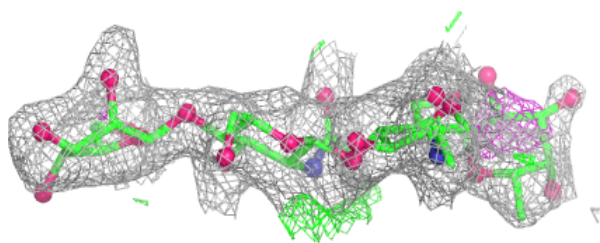
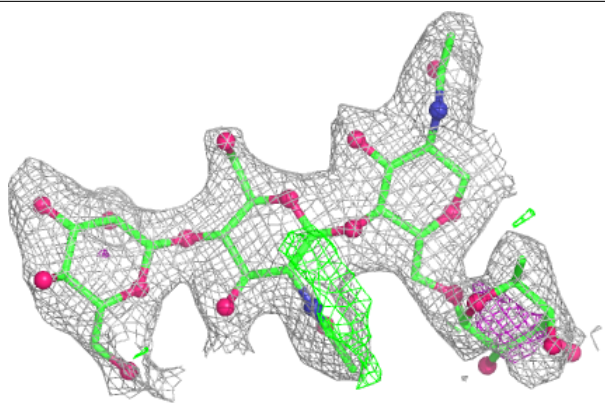
**Electron density around Chain W:**

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

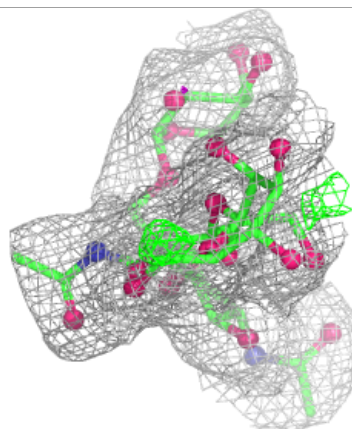
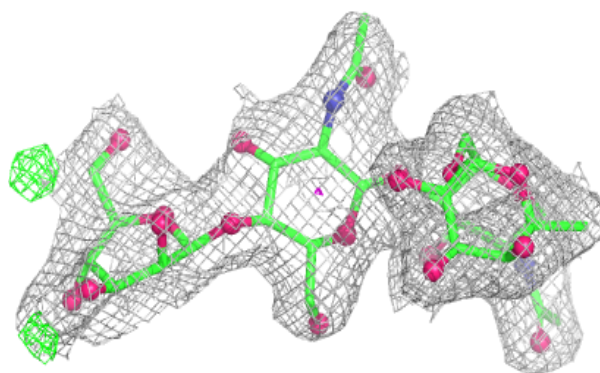
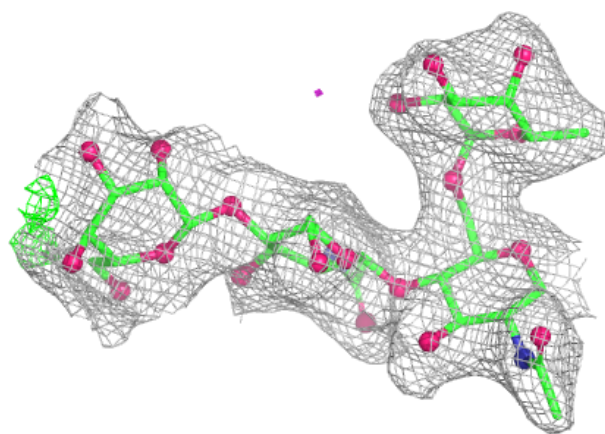


Electron density around Chain E:

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

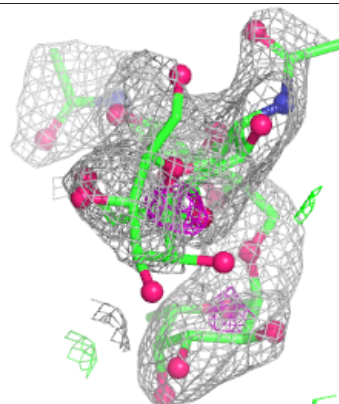
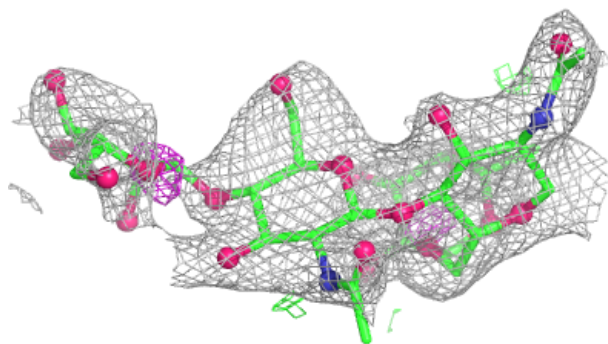
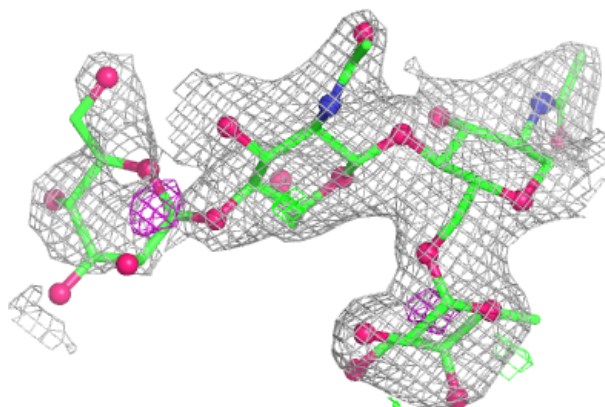
**Electron density around Chain G:**

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



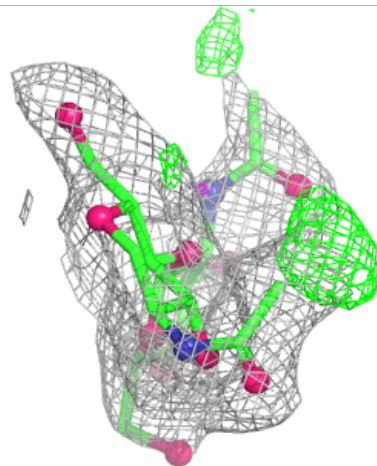
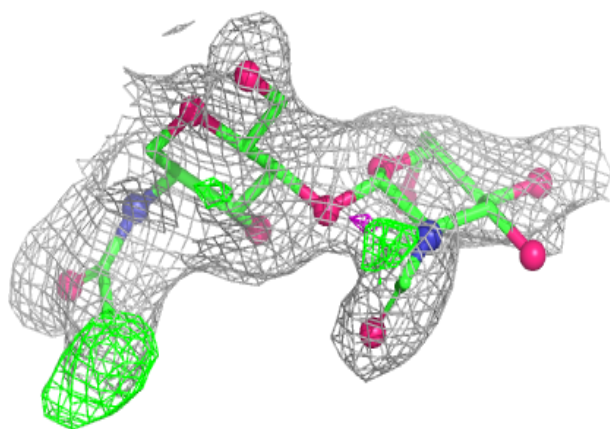
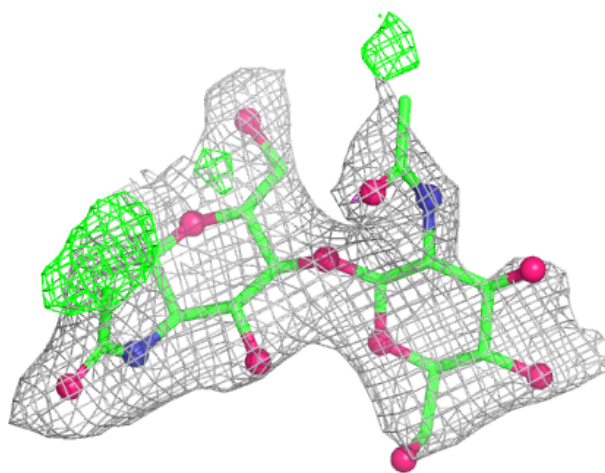
Electron density around Chain S:

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



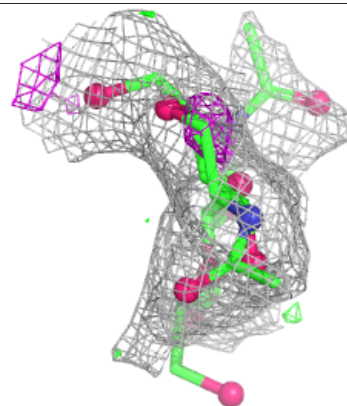
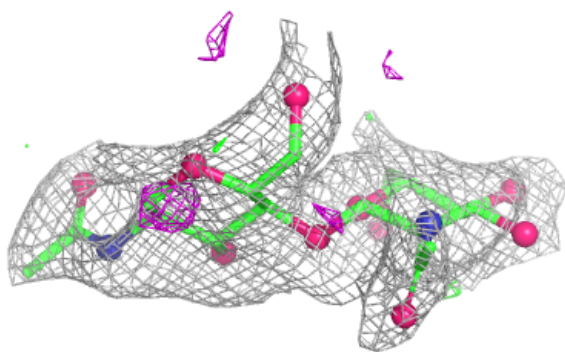
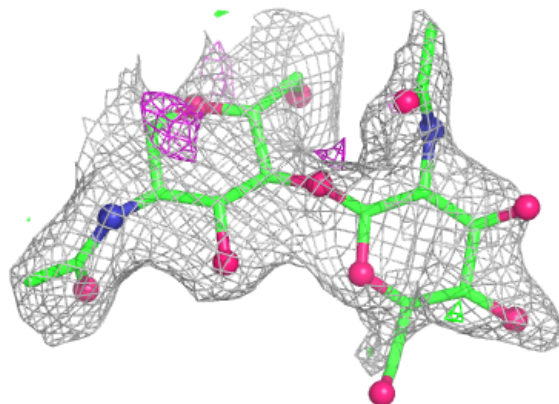
Electron density around Chain F:

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



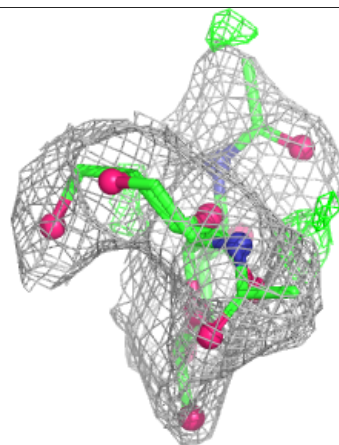
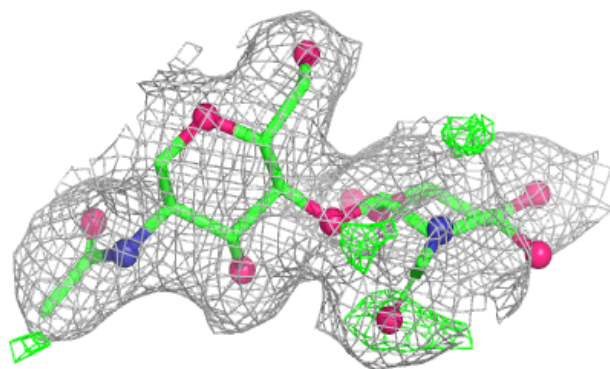
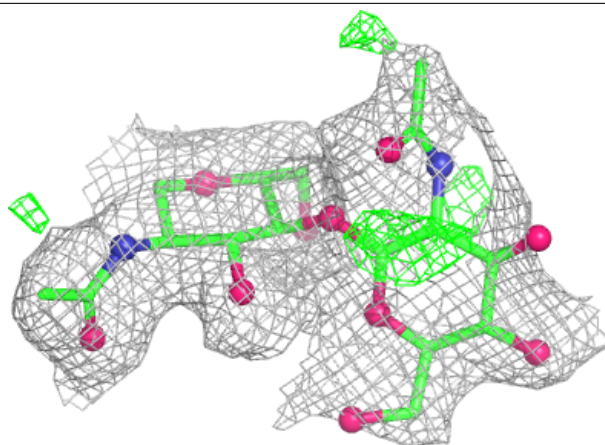
Electron density around Chain J:

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



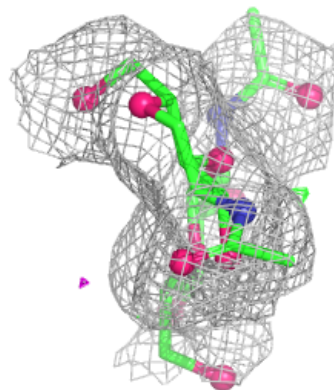
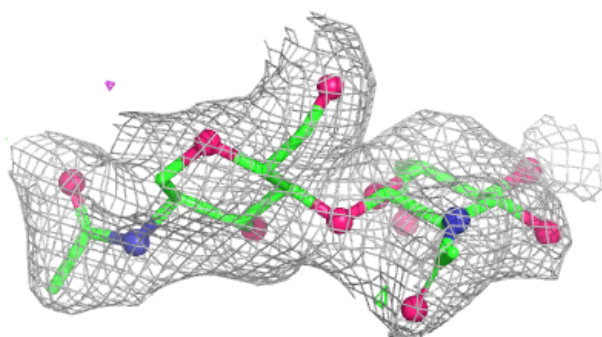
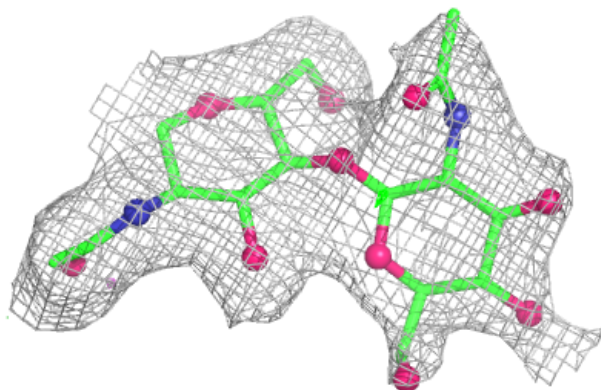
Electron density around Chain K:

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



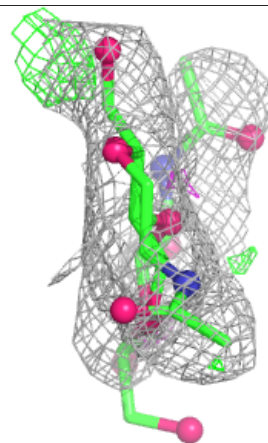
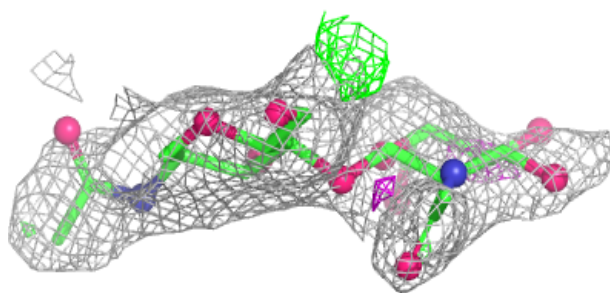
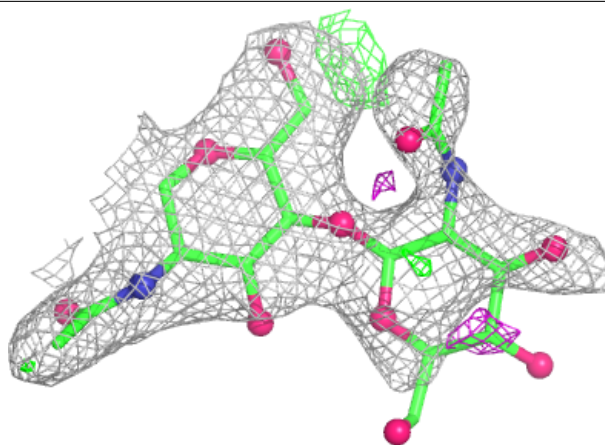
Electron density around Chain M:

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



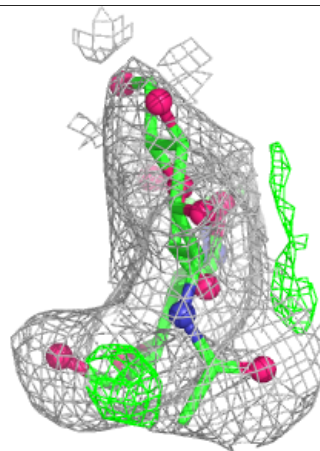
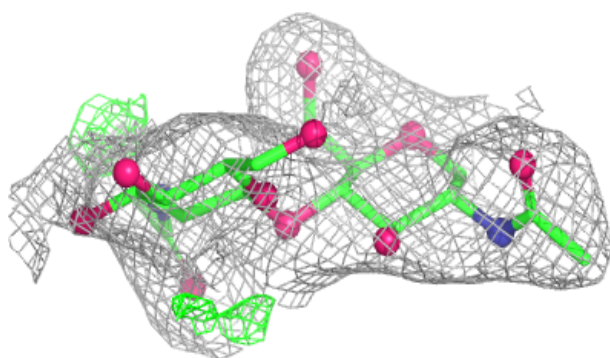
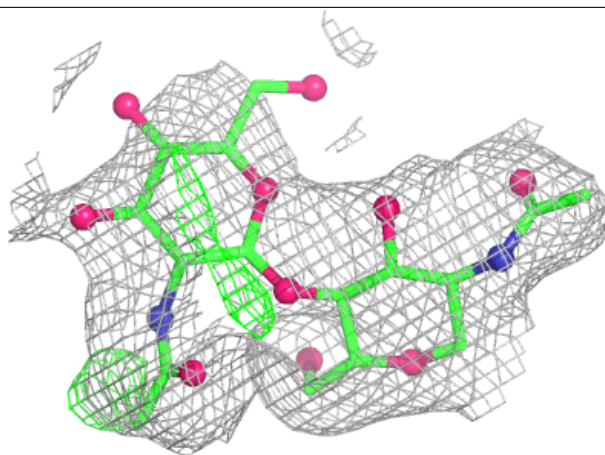
Electron density around Chain Q:

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



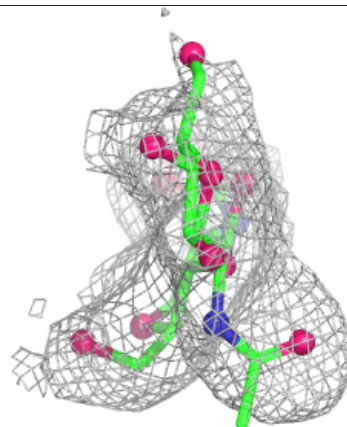
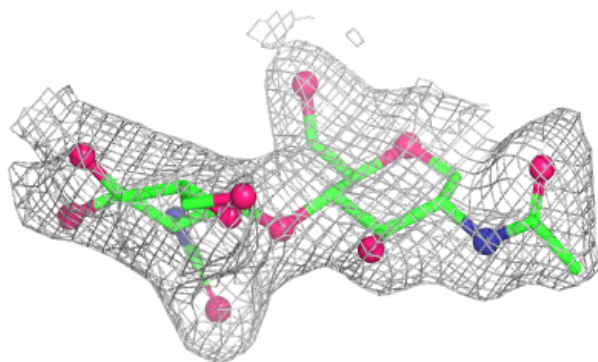
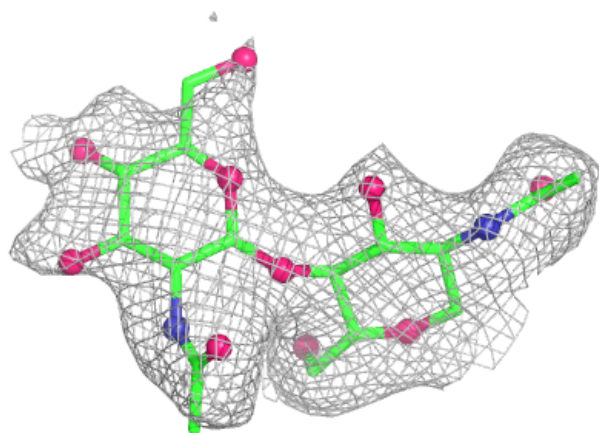
Electron density around Chain U:

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



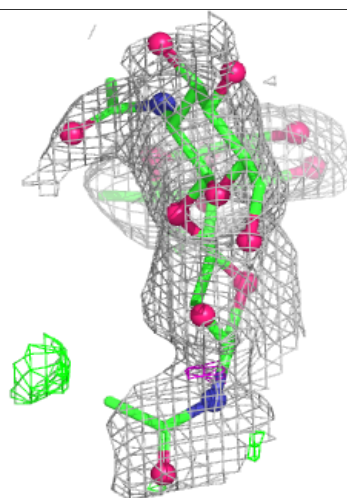
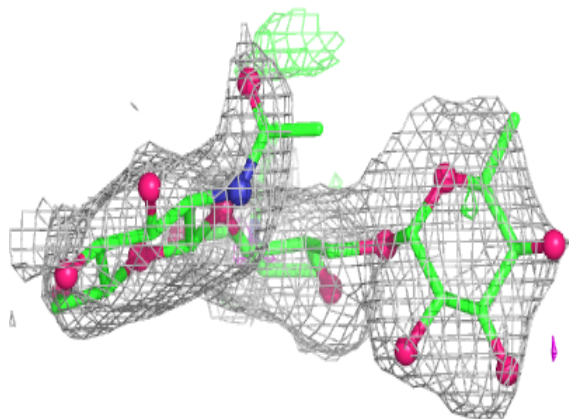
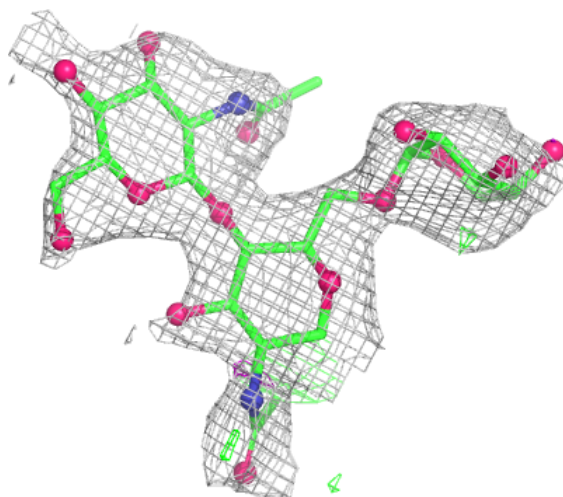
Electron density around Chain V:

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



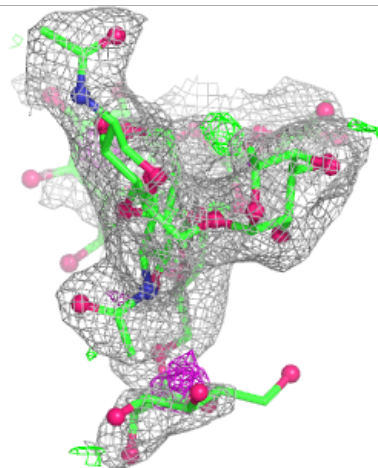
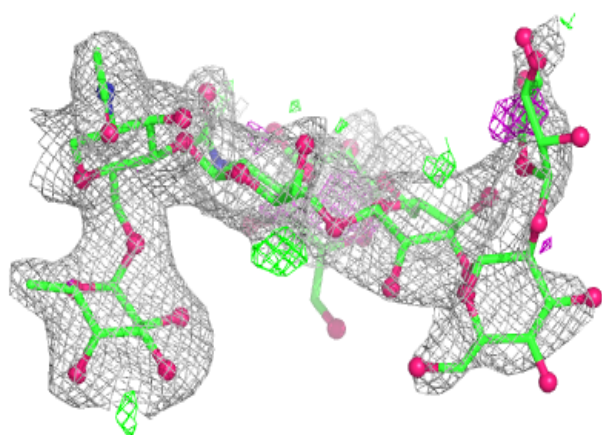
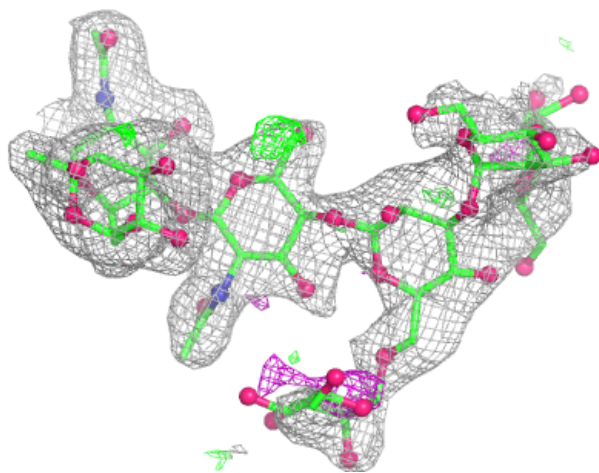
Electron density around Chain I:

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



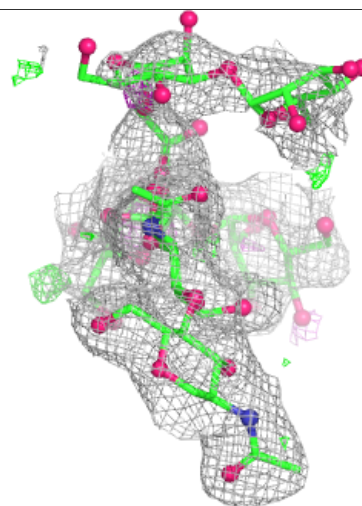
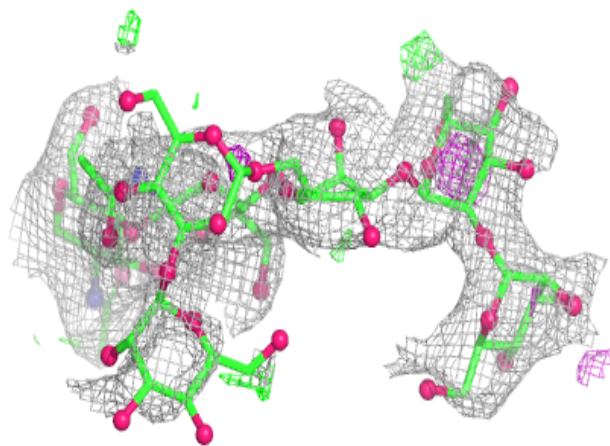
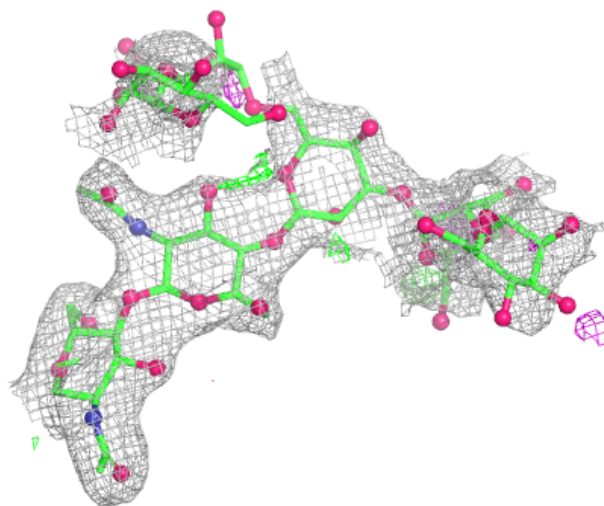
Electron density around Chain N:

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



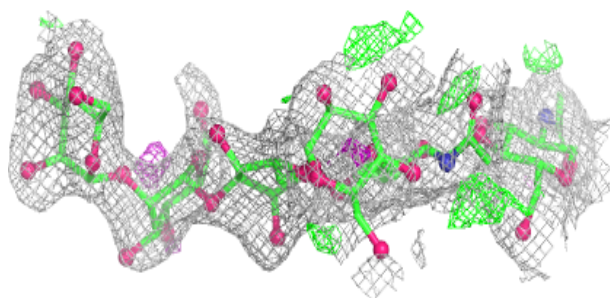
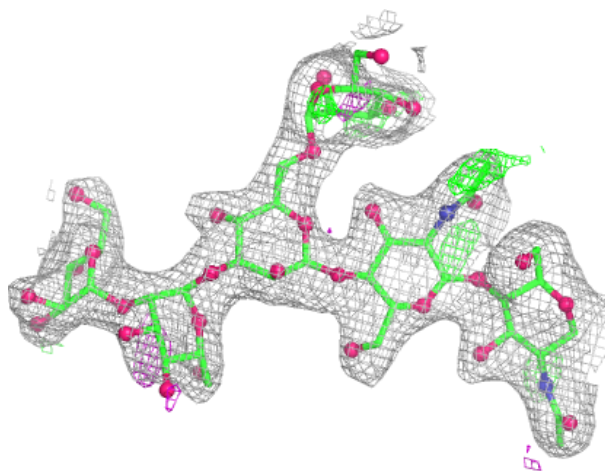
Electron density around Chain O:

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



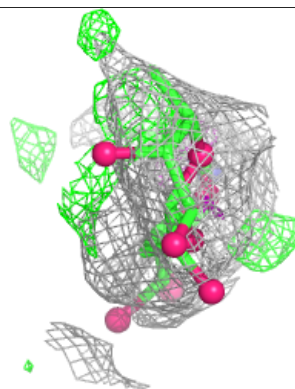
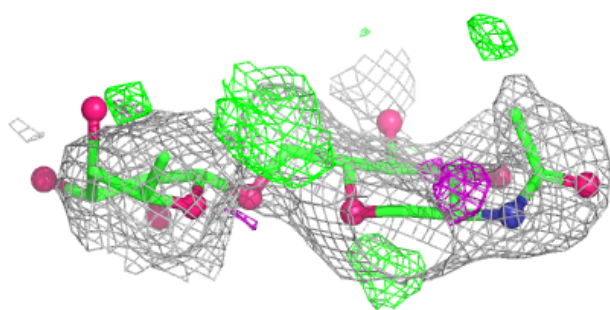
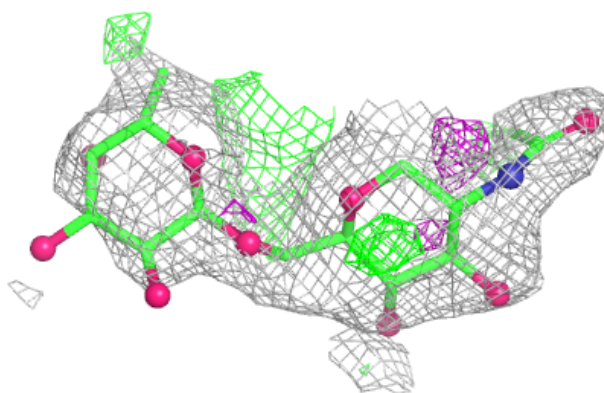
Electron density around Chain P:

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

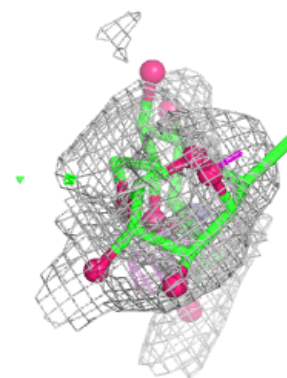
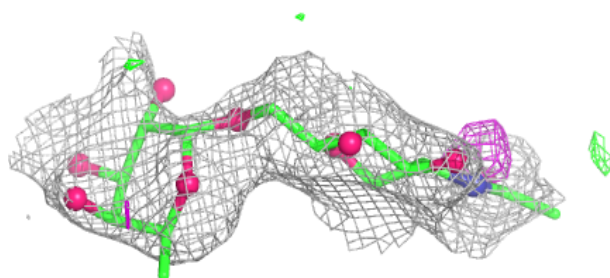
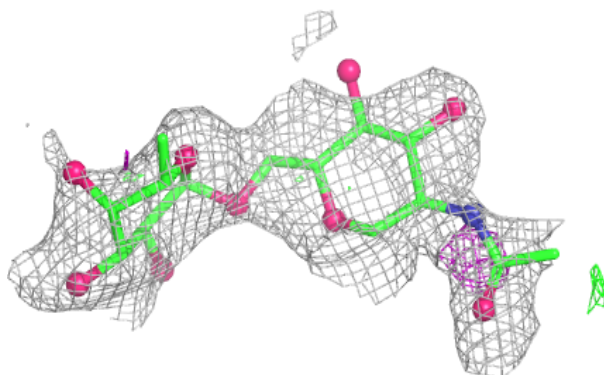


Electron density around Chain R:

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

**Electron density around Chain 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 ⓘ

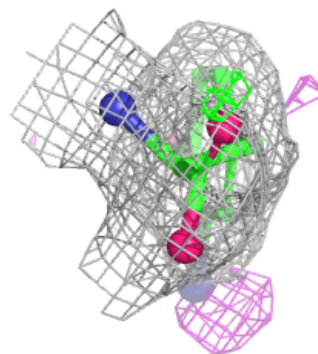
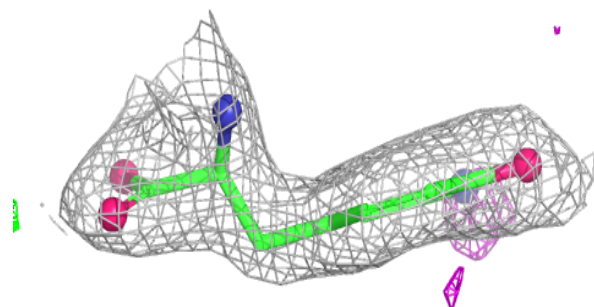
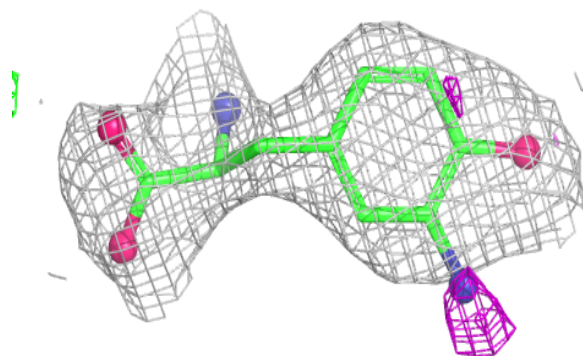
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	NAG	DA	502	14/15	0.29	0.16	80,90,98,98	0
12	NAG	DA	501	14/15	0.56	0.17	68,77,85,90	0
12	NAG	CA	501	14/15	0.62	0.12	69,81,91,94	0
12	NAG	AA	501	14/15	0.66	0.13	70,75,78,87	0
13	GOL	AA	502	6/6	0.81	0.15	38,56,63,65	0
13	GOL	CA	502	6/6	0.82	0.13	40,44,56,60	0
13	GOL	BA	501	6/6	0.86	0.12	42,51,59,61	0
13	GOL	DA	503	6/6	0.87	0.11	47,52,59,61	0
15	TY2	CA	503	14/14	0.91	0.10	34,46,56,59	0
14	ZN	BA	503	1/1	0.99	0.05	31,31,31,31	0
14	ZN	BA	502	1/1	1.00	0.02	30,30,30,30	0
14	ZN	AA	503	1/1	1.00	0.04	28,28,28,28	0
14	ZN	CA	504	1/1	1.00	0.02	30,30,30,30	0
14	ZN	CA	505	1/1	1.00	0.04	33,33,33,33	0
14	ZN	DA	504	1/1	1.00	0.02	33,33,33,33	0
14	ZN	DA	505	1/1	1.00	0.01	32,32,32,32	0
14	ZN	AA	504	1/1	1.00	0.03	28,28,28,28	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 TY2 CA 503:

$2mF_o-DF_c$ (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.