



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2024 – 01:46 AM EST

PDB ID : 3W9T
Title : pore-forming CEL-III
Authors : Unno, H.; Goda, S.; Hatakeyama, T.
Deposited on : 2013-04-16
Resolution : 2.90 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

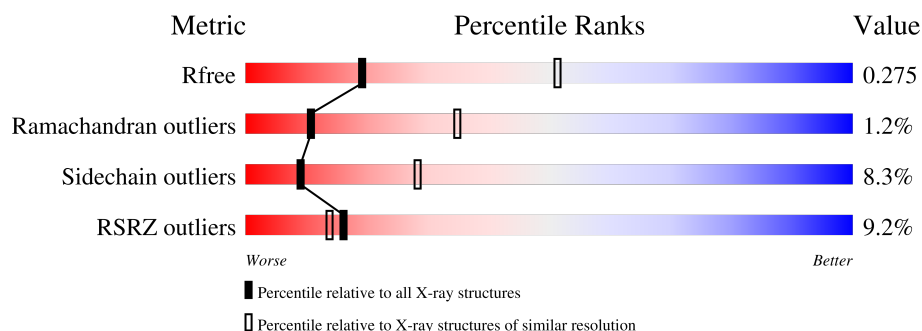
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	164625	2335 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	432	<div> <div>9%</div> <div>92%</div> <div>7%</div> </div>
1	B	432	<div> <div>6%</div> <div>90%</div> <div>9%</div> </div>
1	C	432	<div> <div>7%</div> <div>91%</div> <div>7%</div> </div>
1	D	432	<div> <div>8%</div> <div>91%</div> <div>9%</div> </div>
1	E	432	<div> <div>7%</div> <div>91%</div> <div>8%</div> </div>
1	F	432	<div> <div>13%</div> <div>91%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	432	
2	H	2	
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	
2	Q	2	
2	R	2	
2	S	2	
2	T	2	
2	U	2	
2	V	2	
2	W	2	
2	X	2	
2	Y	2	
2	Z	2	
2	a	2	
2	b	2	
2	c	2	
2	d	2	
2	e	2	

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Mol	Chain	Length	Quality of chain
2	f	2	 50% 50%
2	g	2	 100%
2	h	2	 50% 50%
2	i	2	 50% 50%
2	j	2	 100%
2	k	2	 50% 50%
2	l	2	 50% 50%
2	m	2	 50% 50%
2	n	2	 50% 50%
2	o	2	 100%
2	p	2	 100%
2	q	2	 50% 50%
2	r	2	 50% 50%

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
3	CA	C	1014	-	-	X	-

2 Entry composition [i](#)

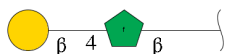
There are 5 unique types of molecules in this entry. The entry contains 24175 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hemolytic lectin CEL-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	C	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	G	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	B	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	F	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	E	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			
1	D	432	Total	C	N	O	S	0	0	0
			3313	2033	562	688	30			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-fructofuranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	M	2	Total	C	O	0	0	0
			23	12	11			
2	N	2	Total	C	O	0	0	0
			23	12	11			
2	O	2	Total	C	O	0	0	0
			23	12	11			
2	P	2	Total	C	O	0	0	0
			23	12	11			
2	Q	2	Total	C	O	0	0	0
			23	12	11			
2	R	2	Total	C	O	0	0	0
			23	12	11			
2	S	2	Total	C	O	0	0	0
			23	12	11			
2	T	2	Total	C	O	0	0	0
			23	12	11			
2	U	2	Total	C	O	0	0	0
			23	12	11			
2	V	2	Total	C	O	0	0	0
			23	12	11			
2	W	2	Total	C	O	0	0	0
			23	12	11			
2	X	2	Total	C	O	0	0	0
			23	12	11			
2	Y	2	Total	C	O	0	0	0
			23	12	11			
2	Z	2	Total	C	O	0	0	0
			23	12	11			
2	a	2	Total	C	O	0	0	0
			23	12	11			
2	b	2	Total	C	O	0	0	0
			23	12	11			
2	c	2	Total	C	O	0	0	0
			23	12	11			
2	d	2	Total	C	O	0	0	0
			23	12	11			
2	e	2	Total	C	O	0	0	0
			23	12	11			
2	f	2	Total	C	O	0	0	0
			23	12	11			
2	g	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	h	2	Total	C	O	0	0	0
			23	12	11			
2	i	2	Total	C	O	0	0	0
			23	12	11			
2	j	2	Total	C	O	0	0	0
			23	12	11			
2	k	2	Total	C	O	0	0	0
			23	12	11			
2	l	2	Total	C	O	0	0	0
			23	12	11			
2	m	2	Total	C	O	0	0	0
			23	12	11			
2	n	2	Total	C	O	0	0	0
			23	12	11			
2	o	2	Total	C	O	0	0	0
			23	12	11			
2	p	2	Total	C	O	0	0	0
			23	12	11			
2	q	2	Total	C	O	0	0	0
			23	12	11			
2	r	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	Ca	0	0
			6	6		
3	C	7	Total	Ca	0	0
			7	7		
3	G	6	Total	Ca	0	0
			6	6		
3	B	6	Total	Ca	0	0
			6	6		
3	F	6	Total	Ca	0	0
			6	6		
3	E	7	Total	Ca	0	0
			7	7		
3	D	6	Total	Ca	0	0
			6	6		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0
4	G	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0

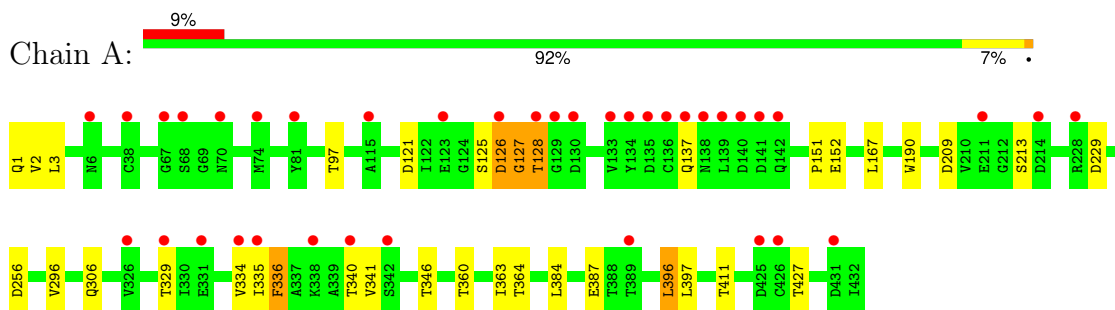
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	C	9	Total O 9 9	0	0
5	G	5	Total O 5 5	0	0
5	B	14	Total O 14 14	0	0
5	F	13	Total O 13 13	0	0
5	E	10	Total O 10 10	0	0
5	D	14	Total O 14 14	0	0

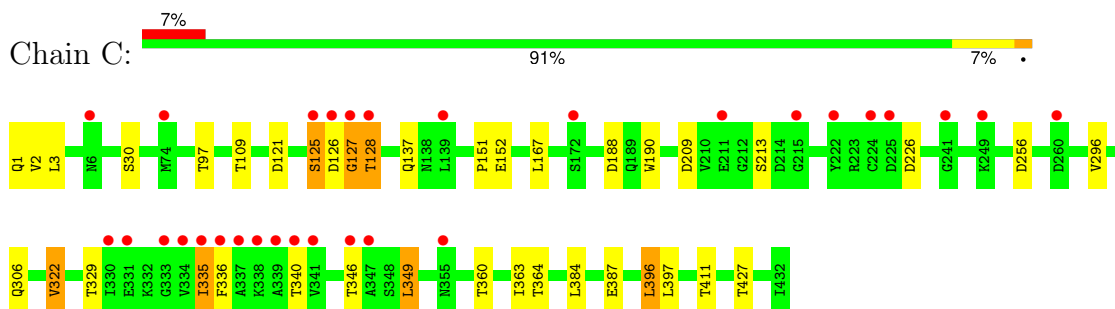
3 Residue-property plots [i](#)

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.

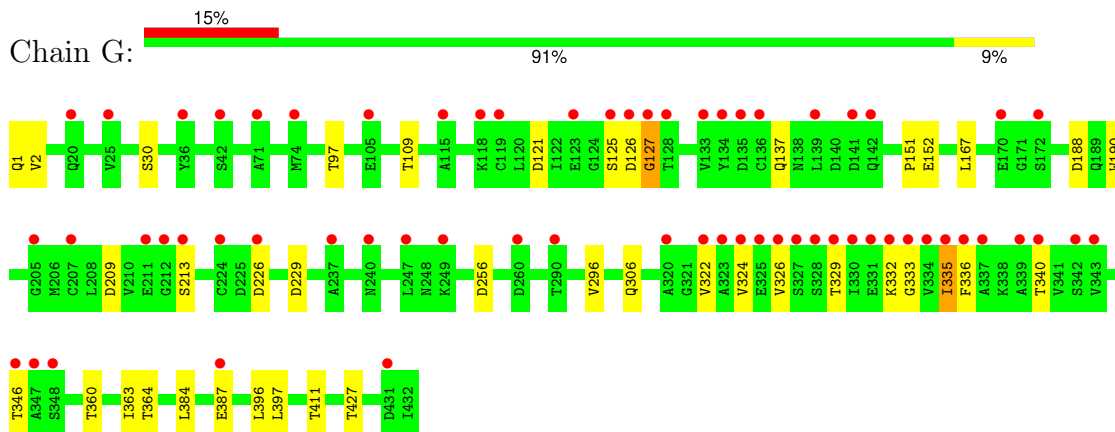
- Molecule 1: Hemolytic lectin CEL-III



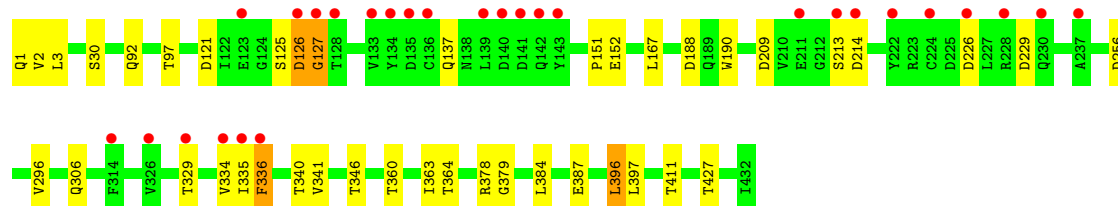
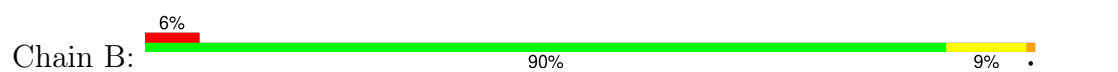
- Molecule 1: Hemolytic lectin CEL-III



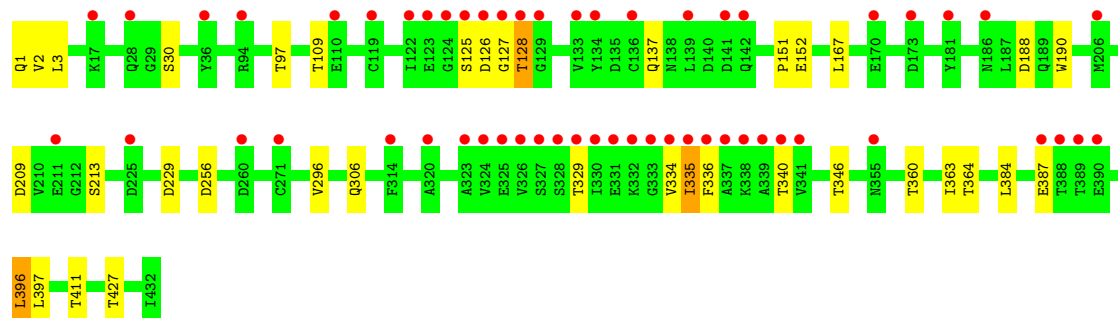
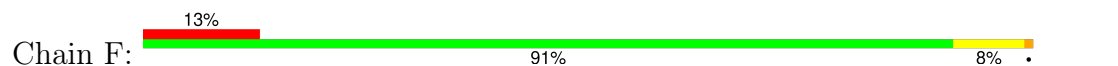
- Molecule 1: Hemolytic lectin CEL-III



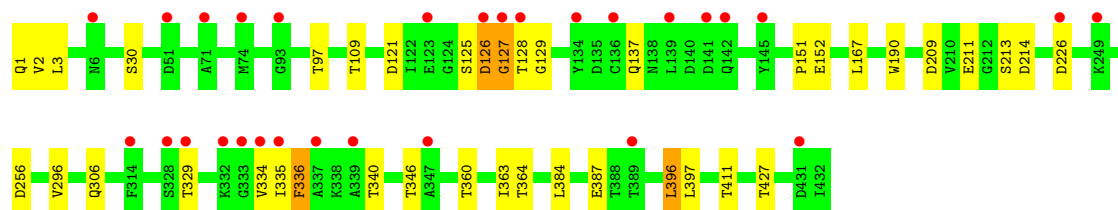
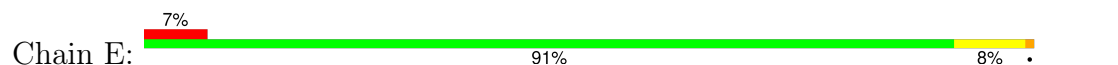
- Molecule 1: Hemolytic lectin CEL-III



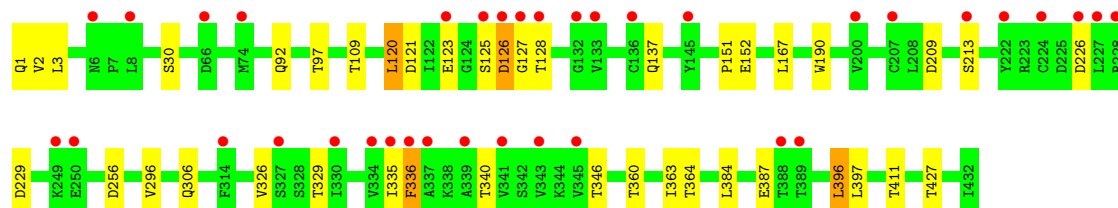
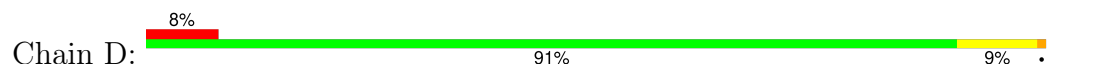
- Molecule 1: Hemolytic lectin CEL-III



- Molecule 1: Hemolytic lectin CEL-III



- Molecule 1: Hemolytic lectin CEL-III



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose





- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain I:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain J:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain K:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain L:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain M:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain N:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain O:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain P:  50% 50%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain Q:  50% 50%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain R:  100%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain S:  50% 50%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain T:  50% 50%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain U:  100%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain V:  50% 50%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain W:  50% 50%



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain X: 



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain Y: 



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain Z: 

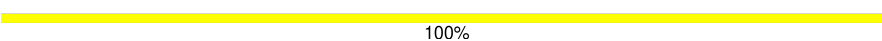


- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain a: 



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain b: 



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain c: 



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain d: 



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain e:  100%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain f:  50% 50%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain g:  100%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain h:  50% 50%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain i:  50% 50%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain j:  100%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain k:  50% 50%

FRU1
GAL2

- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain l:  50% 50%



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain m:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain n:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain o:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain p:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain q:



- Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-fructofuranose

Chain r:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.80Å 228.65Å 133.02Å 90.00° 127.13° 90.00°	Depositor
Resolution (Å)	48.20 – 2.90 48.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.20-2.90) 98.4 (48.20-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.239 , 0.273 0.239 , 0.275	Depositor DCC
R_{free} test set	5793 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24175	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, CA, MG, PCA, FRU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.47	1/3366 (0.0%)	0.70	3/4566 (0.1%)
1	B	0.47	1/3366 (0.0%)	0.72	4/4566 (0.1%)
1	C	0.46	0/3366	0.71	5/4566 (0.1%)
1	D	0.45	0/3366	0.68	2/4566 (0.0%)
1	E	0.47	0/3366	0.69	2/4566 (0.0%)
1	F	0.49	0/3366	0.70	2/4566 (0.0%)
1	G	0.45	0/3366	0.71	1/4566 (0.0%)
All	All	0.47	2/23562 (0.0%)	0.70	19/31962 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	3
1	G	0	4
All	All	0	25

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	ASP	CG-OD2	-7.12	1.08	1.25
1	B	379	GLY	N-CA	-5.95	1.37	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASP	CB-CG-OD1	13.30	130.27	118.30
1	C	128	THR	N-CA-C	-10.58	82.44	111.00
1	B	378	ARG	C-N-CA	9.70	142.68	122.30
1	A	126	ASP	OD1-CG-OD2	-8.37	107.39	123.30
1	B	378	ARG	CA-C-N	7.94	132.07	116.20
1	C	349	LEU	CA-CB-CG	6.93	131.23	115.30
1	E	129	GLY	N-CA-C	6.81	130.11	113.10
1	B	378	ARG	O-C-N	-6.64	111.91	123.20
1	C	349	LEU	CB-CG-CD1	6.01	121.23	111.00
1	D	120	LEU	CB-CG-CD2	5.99	121.17	111.00
1	E	396	LEU	CA-CB-CG	5.77	128.56	115.30
1	B	396	LEU	CA-CB-CG	5.74	128.50	115.30
1	D	396	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	396	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	396	LEU	CA-CB-CG	5.26	127.40	115.30
1	G	2	VAL	CG1-CB-CG2	5.20	119.23	110.90
1	F	2	VAL	CG1-CB-CG2	5.18	119.19	110.90
1	F	396	LEU	CA-CB-CG	5.08	127.00	115.30
1	C	322	VAL	CG1-CB-CG2	5.02	118.94	110.90

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	PRO	Peptide
1	A	335	ILE	Peptide
1	B	126	ASP	Peptide
1	B	127	GLY	Peptide
1	B	151	PRO	Peptide
1	B	335	ILE	Peptide
1	C	125	SER	Peptide
1	C	127	GLY	Peptide
1	C	151	PRO	Peptide
1	C	335	ILE	Peptide
1	D	126	ASP	Peptide
1	D	127	GLY	Peptide
1	D	151	PRO	Peptide
1	D	335	ILE	Peptide
1	E	126	ASP	Peptide
1	E	127	GLY	Peptide
1	E	151	PRO	Peptide
1	E	335	ILE	Peptide
1	F	127	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	F	151	PRO	Peptide
1	F	335	ILE	Peptide
1	G	127	GLY	Peptide
1	G	151	PRO	Peptide
1	G	332	LYS	Peptide
1	G	335	ILE	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/432 (100%)	407 (95%)	18 (4%)	5 (1%)	11	35
1	B	430/432 (100%)	410 (95%)	16 (4%)	4 (1%)	14	43
1	C	430/432 (100%)	410 (95%)	13 (3%)	7 (2%)	8	28
1	D	430/432 (100%)	411 (96%)	15 (4%)	4 (1%)	14	43
1	E	430/432 (100%)	408 (95%)	17 (4%)	5 (1%)	11	35
1	F	430/432 (100%)	410 (95%)	15 (4%)	5 (1%)	11	35
1	G	430/432 (100%)	411 (96%)	12 (3%)	7 (2%)	8	28
All	All	3010/3024 (100%)	2867 (95%)	106 (4%)	37 (1%)	11	35

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	126	ASP
1	C	128	THR
1	C	336	PHE
1	G	126	ASP

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Mol	Chain	Res	Type
1	G	336	PHE
1	B	126	ASP
1	F	126	ASP
1	F	128	THR
1	F	336	PHE
1	E	126	ASP
1	E	127	GLY
1	D	126	ASP
1	A	127	GLY
1	A	336	PHE
1	C	127	GLY
1	G	127	GLY
1	B	336	PHE
1	E	336	PHE
1	D	336	PHE
1	C	152	GLU
1	B	226	ASP
1	E	152	GLU
1	D	152	GLU
1	D	226	ASP
1	A	126	ASP
1	A	128	THR
1	C	226	ASP
1	G	152	GLU
1	G	226	ASP
1	G	333	GLY
1	B	152	GLU
1	F	152	GLU
1	A	152	GLU
1	G	335	ILE
1	E	226	ASP
1	C	335	ILE
1	F	335	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	340 (92%)	30 (8%)	9	29
1	B	370/370 (100%)	337 (91%)	33 (9%)	8	26
1	C	370/370 (100%)	340 (92%)	30 (8%)	9	29
1	D	370/370 (100%)	337 (91%)	33 (9%)	8	26
1	E	370/370 (100%)	339 (92%)	31 (8%)	9	28
1	F	370/370 (100%)	341 (92%)	29 (8%)	10	31
1	G	370/370 (100%)	340 (92%)	30 (8%)	9	29
All	All	2590/2590 (100%)	2374 (92%)	216 (8%)	9	28

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	3	LEU
1	A	97	THR
1	A	121	ASP
1	A	125	SER
1	A	128	THR
1	A	137	GLN
1	A	167	LEU
1	A	190	TRP
1	A	209	ASP
1	A	213	SER
1	A	229	ASP
1	A	256	ASP
1	A	296	VAL
1	A	306	GLN
1	A	329	THR
1	A	334	VAL
1	A	336	PHE
1	A	340	THR
1	A	341	VAL
1	A	346	THR
1	A	360	THR
1	A	363	ILE
1	A	364	THR
1	A	384	LEU
1	A	387	GLU
1	A	396	LEU
1	A	397	LEU
1	A	411	THR

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Mol	Chain	Res	Type
1	A	427	THR
1	C	2	VAL
1	C	3	LEU
1	C	30	SER
1	C	97	THR
1	C	109	THR
1	C	121	ASP
1	C	125	SER
1	C	137	GLN
1	C	167	LEU
1	C	188	ASP
1	C	190	TRP
1	C	209	ASP
1	C	213	SER
1	C	256	ASP
1	C	296	VAL
1	C	306	GLN
1	C	322	VAL
1	C	329	THR
1	C	340	THR
1	C	346	THR
1	C	349	LEU
1	C	360	THR
1	C	363	ILE
1	C	364	THR
1	C	384	LEU
1	C	387	GLU
1	C	396	LEU
1	C	397	LEU
1	C	411	THR
1	C	427	THR
1	G	30	SER
1	G	97	THR
1	G	109	THR
1	G	121	ASP
1	G	125	SER
1	G	137	GLN
1	G	167	LEU
1	G	188	ASP
1	G	190	TRP
1	G	209	ASP
1	G	213	SER

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Mol	Chain	Res	Type
1	G	229	ASP
1	G	256	ASP
1	G	296	VAL
1	G	306	GLN
1	G	322	VAL
1	G	324	VAL
1	G	326	VAL
1	G	329	THR
1	G	340	THR
1	G	346	THR
1	G	360	THR
1	G	363	ILE
1	G	364	THR
1	G	384	LEU
1	G	387	GLU
1	G	396	LEU
1	G	397	LEU
1	G	411	THR
1	G	427	THR
1	B	2	VAL
1	B	3	LEU
1	B	30	SER
1	B	92	GLN
1	B	97	THR
1	B	121	ASP
1	B	125	SER
1	B	137	GLN
1	B	167	LEU
1	B	188	ASP
1	B	190	TRP
1	B	209	ASP
1	B	213	SER
1	B	214	ASP
1	B	229	ASP
1	B	256	ASP
1	B	296	VAL
1	B	306	GLN
1	B	329	THR
1	B	334	VAL
1	B	336	PHE
1	B	340	THR
1	B	341	VAL

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Mol	Chain	Res	Type
1	B	346	THR
1	B	360	THR
1	B	363	ILE
1	B	364	THR
1	B	384	LEU
1	B	387	GLU
1	B	396	LEU
1	B	397	LEU
1	B	411	THR
1	B	427	THR
1	F	3	LEU
1	F	30	SER
1	F	97	THR
1	F	109	THR
1	F	125	SER
1	F	128	THR
1	F	137	GLN
1	F	167	LEU
1	F	188	ASP
1	F	190	TRP
1	F	209	ASP
1	F	213	SER
1	F	229	ASP
1	F	256	ASP
1	F	296	VAL
1	F	306	GLN
1	F	329	THR
1	F	334	VAL
1	F	340	THR
1	F	346	THR
1	F	360	THR
1	F	363	ILE
1	F	364	THR
1	F	384	LEU
1	F	387	GLU
1	F	396	LEU
1	F	397	LEU
1	F	411	THR
1	F	427	THR
1	E	2	VAL
1	E	3	LEU
1	E	30	SER

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Mol	Chain	Res	Type
1	E	97	THR
1	E	109	THR
1	E	121	ASP
1	E	125	SER
1	E	128	THR
1	E	137	GLN
1	E	167	LEU
1	E	190	TRP
1	E	209	ASP
1	E	213	SER
1	E	214	ASP
1	E	256	ASP
1	E	296	VAL
1	E	306	GLN
1	E	329	THR
1	E	334	VAL
1	E	336	PHE
1	E	340	THR
1	E	346	THR
1	E	360	THR
1	E	363	ILE
1	E	364	THR
1	E	384	LEU
1	E	387	GLU
1	E	396	LEU
1	E	397	LEU
1	E	411	THR
1	E	427	THR
1	D	2	VAL
1	D	3	LEU
1	D	30	SER
1	D	92	GLN
1	D	97	THR
1	D	109	THR
1	D	120	LEU
1	D	121	ASP
1	D	125	SER
1	D	128	THR
1	D	137	GLN
1	D	167	LEU
1	D	190	TRP
1	D	209	ASP

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Mol	Chain	Res	Type
1	D	213	SER
1	D	229	ASP
1	D	256	ASP
1	D	296	VAL
1	D	306	GLN
1	D	326	VAL
1	D	329	THR
1	D	336	PHE
1	D	340	THR
1	D	346	THR
1	D	360	THR
1	D	363	ILE
1	D	364	THR
1	D	384	LEU
1	D	387	GLU
1	D	396	LEU
1	D	397	LEU
1	D	411	THR
1	D	427	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	270	GLN
1	A	301	ASN
1	A	306	GLN
1	C	32	ASN
1	C	270	GLN
1	C	301	ASN
1	C	306	GLN
1	G	32	ASN
1	G	301	ASN
1	G	306	GLN
1	B	32	ASN
1	B	301	ASN
1	B	306	GLN
1	F	32	ASN
1	F	138	ASN
1	F	270	GLN
1	F	301	ASN
1	F	306	GLN

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Mol	Chain	Res	Type
1	E	32	ASN
1	E	138	ASN
1	E	270	GLN
1	E	301	ASN
1	E	306	GLN
1	D	32	ASN
1	D	270	GLN
1	D	301	ASN
1	D	306	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PCA	F	1	1	7,8,9	0.53	0	9,10,12	2.25	4 (44%)
1	PCA	B	1	1	7,8,9	0.51	0	9,10,12	2.14	2 (22%)
1	PCA	E	1	1	7,8,9	0.48	0	9,10,12	2.37	3 (33%)
1	PCA	A	1	1	7,8,9	0.58	0	9,10,12	2.31	3 (33%)
1	PCA	D	1	1	7,8,9	0.65	0	9,10,12	2.24	2 (22%)
1	PCA	G	1	1	7,8,9	0.65	0	9,10,12	2.19	3 (33%)
1	PCA	C	1	1	7,8,9	0.52	0	9,10,12	2.30	4 (44%)

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
1	PCA	F	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	E	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	G	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	PCA	CB-CA-C	5.05	119.59	112.66
1	E	1	PCA	CB-CA-C	4.95	119.45	112.66
1	C	1	PCA	CB-CA-C	4.53	118.87	112.66
1	A	1	PCA	CB-CA-C	4.41	118.70	112.66
1	F	1	PCA	CA-N-CD	-4.32	98.79	113.58
1	B	1	PCA	CB-CA-C	4.30	118.55	112.66
1	G	1	PCA	CB-CA-C	4.18	118.38	112.66
1	A	1	PCA	CA-N-CD	-3.93	100.12	113.58
1	C	1	PCA	CA-N-CD	-3.73	100.80	113.58
1	E	1	PCA	CA-N-CD	-3.73	100.81	113.58
1	B	1	PCA	CA-N-CD	-3.66	101.05	113.58
1	G	1	PCA	CA-N-CD	-3.62	101.19	113.58
1	D	1	PCA	CA-N-CD	-3.48	101.65	113.58
1	F	1	PCA	CB-CA-C	3.43	117.36	112.66
1	F	1	PCA	CB-CG-CD	-2.38	100.73	104.41
1	F	1	PCA	OE-CD-CG	-2.37	122.48	126.72
1	A	1	PCA	OE-CD-CG	-2.25	122.71	126.72
1	G	1	PCA	OE-CD-CG	-2.18	122.83	126.72
1	E	1	PCA	OE-CD-CG	-2.13	122.92	126.72
1	C	1	PCA	CB-CG-CD	-2.12	101.13	104.41
1	C	1	PCA	OE-CD-CG	-2.03	123.09	126.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

74 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	FRU	H	1	2	11,12,12	0.64	0	10,18,18	0.88	0
2	GAL	H	2	2,3	11,11,12	0.32	0	15,15,17	1.28	1 (6%)
2	FRU	I	1	2	11,12,12	0.64	0	10,18,18	0.86	0
2	GAL	I	2	2,3	11,11,12	0.73	0	15,15,17	2.01	2 (13%)
2	FRU	J	1	2	11,12,12	0.70	1 (9%)	10,18,18	1.02	0
2	GAL	J	2	2,3	11,11,12	0.39	0	15,15,17	0.87	0
2	FRU	K	1	2	11,12,12	0.59	0	10,18,18	0.71	0
2	GAL	K	2	2,3	11,11,12	0.28	0	15,15,17	0.93	1 (6%)
2	FRU	L	1	2	11,12,12	0.55	0	10,18,18	0.83	0
2	GAL	L	2	2,3	11,11,12	0.33	0	15,15,17	0.79	0
2	FRU	M	1	2	11,12,12	0.72	0	10,18,18	1.04	0
2	GAL	M	2	2,3	11,11,12	0.75	0	15,15,17	1.82	3 (20%)
2	FRU	N	1	2	11,12,12	0.67	0	10,18,18	0.70	0
2	GAL	N	2	2,3	11,11,12	0.49	0	15,15,17	1.92	3 (20%)
2	FRU	O	1	2	11,12,12	0.62	0	10,18,18	0.81	0
2	GAL	O	2	2,3	11,11,12	0.34	0	15,15,17	1.52	4 (26%)
2	FRU	P	1	2	11,12,12	0.69	0	10,18,18	0.62	0
2	GAL	P	2	2,3	11,11,12	0.55	0	15,15,17	1.25	1 (6%)
2	FRU	Q	1	2	11,12,12	0.70	0	10,18,18	1.07	1 (10%)
2	GAL	Q	2	2,3	11,11,12	0.37	0	15,15,17	0.97	0
2	FRU	R	1	2	11,12,12	0.61	0	10,18,18	0.97	0
2	GAL	R	2	2,3	11,11,12	0.36	0	15,15,17	0.46	0
2	FRU	S	1	2	11,12,12	0.67	0	10,18,18	0.66	0
2	GAL	S	2	2,3	11,11,12	0.31	0	15,15,17	1.07	1 (6%)
2	FRU	T	1	2	11,12,12	0.65	0	10,18,18	0.88	0
2	GAL	T	2	2,3	11,11,12	0.40	0	15,15,17	2.09	2 (13%)
2	FRU	U	1	2	11,12,12	0.59	0	10,18,18	0.84	0
2	GAL	U	2	2,3	11,11,12	0.33	0	15,15,17	0.87	0
2	FRU	V	1	2	11,12,12	0.62	0	10,18,18	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	V	2	2,3	11,11,12	0.44	0	15,15,17	1.91	2 (13%)
2	FRU	W	1	2	11,12,12	0.72	0	10,18,18	1.45	1 (10%)
2	GAL	W	2	2,3	11,11,12	0.33	0	15,15,17	0.81	0
2	FRU	X	1	2	11,12,12	0.72	0	10,18,18	0.91	0
2	GAL	X	2	2,3	11,11,12	0.72	0	15,15,17	2.03	4 (26%)
2	FRU	Y	1	2	11,12,12	0.64	0	10,18,18	0.74	0
2	GAL	Y	2	2,3	11,11,12	0.28	0	15,15,17	0.74	0
2	FRU	Z	1	2	11,12,12	0.69	0	10,18,18	0.81	0
2	GAL	Z	2	2,3	11,11,12	0.36	0	15,15,17	2.57	4 (26%)
2	FRU	a	1	2	11,12,12	0.56	0	10,18,18	1.08	0
2	GAL	a	2	2,3	11,11,12	0.44	0	15,15,17	1.82	1 (6%)
2	FRU	b	1	2	11,12,12	0.98	1 (9%)	10,18,18	1.19	0
2	GAL	b	2	2	11,11,12	0.56	0	15,15,17	2.99	5 (33%)
2	FRU	c	1	2	11,12,12	0.77	0	10,18,18	1.05	1 (10%)
2	GAL	c	2	2,3	11,11,12	0.38	0	15,15,17	0.77	0
2	FRU	d	1	2	11,12,12	0.73	0	10,18,18	0.54	0
2	GAL	d	2	2,3	11,11,12	0.30	0	15,15,17	0.78	0
2	FRU	e	1	2	11,12,12	0.88	1 (9%)	10,18,18	0.93	0
2	GAL	e	2	2,3	11,11,12	0.70	0	15,15,17	1.94	2 (13%)
2	FRU	f	1	2	11,12,12	0.60	0	10,18,18	0.58	0
2	GAL	f	2	2,3	11,11,12	0.42	0	15,15,17	1.11	1 (6%)
2	FRU	g	1	2	11,12,12	1.03	1 (9%)	10,18,18	1.13	1 (10%)
2	GAL	g	2	2	11,11,12	0.68	0	15,15,17	2.04	7 (46%)
2	FRU	h	1	2	11,12,12	0.59	0	10,18,18	0.95	0
2	GAL	h	2	2,3	11,11,12	0.58	0	15,15,17	1.29	1 (6%)
2	FRU	i	1	2	11,12,12	0.60	0	10,18,18	0.86	0
2	GAL	i	2	2,3	11,11,12	0.40	0	15,15,17	1.21	1 (6%)
2	FRU	j	1	2	11,12,12	0.74	1 (9%)	10,18,18	0.84	0
2	GAL	j	2	2,3	11,11,12	0.51	0	15,15,17	1.14	2 (13%)
2	FRU	k	1	2	11,12,12	0.65	0	10,18,18	0.84	0
2	GAL	k	2	2,3	11,11,12	0.53	0	15,15,17	1.11	1 (6%)
2	FRU	l	1	2	11,12,12	0.61	0	10,18,18	0.81	0
2	GAL	l	2	2,3	11,11,12	0.65	0	15,15,17	1.78	2 (13%)
2	FRU	m	1	2	11,12,12	0.78	0	10,18,18	1.07	0
2	GAL	m	2	2	11,11,12	0.46	0	15,15,17	2.00	4 (26%)
2	FRU	n	1	2	11,12,12	0.70	1 (9%)	10,18,18	1.11	0
2	GAL	n	2	2,3	11,11,12	0.41	0	15,15,17	0.75	0
2	FRU	o	1	2	11,12,12	0.64	0	10,18,18	0.96	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	o	2	2,3	11,11,12	0.46	0	15,15,17	1.57	1 (6%)
2	FRU	p	1	2	11,12,12	0.67	0	10,18,18	0.78	0
2	GAL	p	2	2,3	11,11,12	0.58	0	15,15,17	1.11	0
2	FRU	q	1	2	11,12,12	0.64	0	10,18,18	0.84	0
2	GAL	q	2	2,3	11,11,12	0.40	0	15,15,17	2.18	1 (6%)
2	FRU	r	1	2	11,12,12	0.51	0	10,18,18	0.95	0
2	GAL	r	2	2,3	11,11,12	0.33	0	15,15,17	1.58	4 (26%)

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	FRU	H	1	2	-	5/5/24/24	0/1/1/1
2	GAL	H	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	I	1	2	-	2/5/24/24	0/1/1/1
2	GAL	I	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	J	1	2	-	4/5/24/24	0/1/1/1
2	GAL	J	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	K	1	2	-	2/5/24/24	0/1/1/1
2	GAL	K	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	L	1	2	-	3/5/24/24	0/1/1/1
2	GAL	L	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	M	1	2	-	0/5/24/24	0/1/1/1
2	GAL	M	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	N	1	2	-	3/5/24/24	0/1/1/1
2	GAL	N	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	O	1	2	-	3/5/24/24	0/1/1/1
2	GAL	O	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	P	1	2	-	3/5/24/24	0/1/1/1
2	GAL	P	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	Q	1	2	-	3/5/24/24	0/1/1/1
2	GAL	Q	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	R	1	2	-	3/5/24/24	0/1/1/1
2	GAL	R	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	S	1	2	-	0/5/24/24	0/1/1/1
2	GAL	S	2	2,3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	T	1	2	-	4/5/24/24	0/1/1/1
2	GAL	T	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	U	1	2	-	3/5/24/24	0/1/1/1
2	GAL	U	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	V	1	2	-	4/5/24/24	0/1/1/1
2	GAL	V	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	W	1	2	-	3/5/24/24	0/1/1/1
2	GAL	W	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	X	1	2	-	5/5/24/24	0/1/1/1
2	GAL	X	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	Y	1	2	-	2/5/24/24	0/1/1/1
2	GAL	Y	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	Z	1	2	-	2/5/24/24	0/1/1/1
2	GAL	Z	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	a	1	2	-	2/5/24/24	0/1/1/1
2	GAL	a	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	b	1	2	-	3/5/24/24	0/1/1/1
2	GAL	b	2	2	-	2/2/19/22	0/1/1/1
2	FRU	c	1	2	-	0/5/24/24	0/1/1/1
2	GAL	c	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	d	1	2	-	1/5/24/24	0/1/1/1
2	GAL	d	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	e	1	2	-	2/5/24/24	0/1/1/1
2	GAL	e	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	f	1	2	-	3/5/24/24	0/1/1/1
2	GAL	f	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	g	1	2	-	3/5/24/24	0/1/1/1
2	GAL	g	2	2	-	0/2/19/22	0/1/1/1
2	FRU	h	1	2	-	2/5/24/24	0/1/1/1
2	GAL	h	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	i	1	2	-	3/5/24/24	0/1/1/1
2	GAL	i	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	j	1	2	-	3/5/24/24	0/1/1/1
2	GAL	j	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	k	1	2	-	2/5/24/24	0/1/1/1
2	GAL	k	2	2,3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	l	1	2	-	3/5/24/24	0/1/1/1
2	GAL	l	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	m	1	2	-	2/5/24/24	0/1/1/1
2	GAL	m	2	2	-	0/2/19/22	0/1/1/1
2	FRU	n	1	2	-	2/5/24/24	0/1/1/1
2	GAL	n	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	o	1	2	-	5/5/24/24	0/1/1/1
2	GAL	o	2	2,3	-	0/2/19/22	0/1/1/1
2	FRU	p	1	2	-	3/5/24/24	0/1/1/1
2	GAL	p	2	2,3	-	2/2/19/22	0/1/1/1
2	FRU	q	1	2	-	5/5/24/24	0/1/1/1
2	GAL	q	2	2,3	-	1/2/19/22	0/1/1/1
2	FRU	r	1	2	-	4/5/24/24	0/1/1/1
2	GAL	r	2	2,3	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	1	FRU	O2-C2	2.12	1.44	1.40
2	j	1	FRU	O2-C2	2.11	1.44	1.40
2	J	1	FRU	O2-C2	2.09	1.44	1.40
2	g	1	FRU	O5-C2	-2.08	1.40	1.43
2	b	1	FRU	O2-C2	2.08	1.44	1.40
2	n	1	FRU	O2-C2	2.07	1.44	1.40

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	2	GAL	C1-O5-C5	-9.71	99.17	112.19
2	q	2	GAL	C1-O5-C5	7.69	122.50	112.19
2	T	2	GAL	C1-O5-C5	6.62	121.06	112.19
2	I	2	GAL	C1-O5-C5	6.46	120.85	112.19
2	a	2	GAL	C1-O5-C5	6.15	120.43	112.19
2	Z	2	GAL	C1-O5-C5	6.09	120.34	112.19
2	V	2	GAL	C1-O5-C5	5.96	120.17	112.19
2	N	2	GAL	C1-O5-C5	5.51	119.57	112.19
2	l	2	GAL	C1-O5-C5	5.39	119.41	112.19
2	o	2	GAL	C1-O5-C5	5.26	119.23	112.19
2	X	2	GAL	C1-O5-C5	5.15	119.09	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	2	GAL	C1-C2-C3	4.71	116.50	109.64
2	M	2	GAL	C3-C4-C5	4.61	118.60	110.23
2	e	2	GAL	C1-O5-C5	4.50	118.22	112.19
2	m	2	GAL	O3-C3-C2	-4.42	101.03	110.05
2	Z	2	GAL	C2-C3-C4	4.35	118.51	110.86
2	M	2	GAL	C1-O5-C5	4.29	117.93	112.19
2	Z	2	GAL	C1-C2-C3	3.98	115.44	109.64
2	m	2	GAL	C1-C2-C3	-3.87	104.02	109.64
2	Z	2	GAL	C3-C4-C5	3.86	117.23	110.23
2	P	2	GAL	C1-O5-C5	3.84	117.33	112.19
2	g	2	GAL	C1-C2-C3	-3.43	104.65	109.64
2	g	2	GAL	O3-C3-C2	-3.25	103.42	110.05
2	b	2	GAL	O5-C5-C6	3.25	113.98	107.66
2	N	2	GAL	O5-C5-C4	3.20	118.61	110.83
2	r	2	GAL	C1-O5-C5	3.15	116.41	112.19
2	l	2	GAL	O5-C5-C6	3.10	113.69	107.66
2	g	2	GAL	O5-C5-C4	-3.10	103.29	110.83
2	X	2	GAL	O4-C4-C5	3.08	116.90	109.32
2	h	2	GAL	C1-O5-C5	3.05	116.27	112.19
2	N	2	GAL	C3-C4-C5	3.01	115.69	110.23
2	W	1	FRU	O4-C4-C3	-3.00	103.16	112.16
2	g	2	GAL	C1-O5-C5	-2.87	108.34	112.19
2	r	2	GAL	C1-C2-C3	2.87	113.82	109.64
2	H	2	GAL	O5-C5-C6	2.86	113.23	107.66
2	m	2	GAL	O5-C5-C6	2.79	113.10	107.66
2	m	2	GAL	O5-C5-C4	-2.77	104.08	110.83
2	b	2	GAL	O5-C5-C4	-2.73	104.17	110.83
2	X	2	GAL	C1-C2-C3	2.73	113.61	109.64
2	g	1	FRU	C6-C5-C4	-2.72	108.67	115.10
2	k	2	GAL	O5-C5-C6	2.69	112.90	107.66
2	V	2	GAL	C1-C2-C3	2.68	113.55	109.64
2	O	2	GAL	C1-C2-C3	2.60	113.43	109.64
2	I	2	GAL	C1-C2-C3	2.60	113.42	109.64
2	r	2	GAL	C3-C4-C5	-2.54	105.63	110.23
2	j	2	GAL	O3-C3-C4	-2.48	104.53	110.38
2	g	2	GAL	O5-C5-C6	2.43	112.39	107.66
2	i	2	GAL	C1-C2-C3	2.42	113.17	109.64
2	Q	1	FRU	C6-C5-C4	-2.42	109.39	115.10
2	O	2	GAL	O4-C4-C5	2.38	115.19	109.32
2	O	2	GAL	C3-C4-C5	-2.38	105.92	110.23
2	K	2	GAL	C1-O5-C5	2.34	115.32	112.19
2	b	2	GAL	C1-C2-C3	-2.32	106.27	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	2	GAL	C1-O5-C5	2.29	115.26	112.19
2	f	2	GAL	C3-C4-C5	2.27	114.34	110.23
2	M	2	GAL	O5-C5-C4	2.26	116.33	110.83
2	r	2	GAL	O5-C5-C6	2.25	112.04	107.66
2	b	2	GAL	O3-C3-C4	-2.24	105.10	110.38
2	g	2	GAL	O2-C2-C3	2.24	114.78	110.15
2	j	2	GAL	O5-C5-C6	2.12	111.80	107.66
2	c	1	FRU	C6-C5-C4	-2.08	110.18	115.10
2	S	2	GAL	C1-C2-C3	2.05	112.63	109.64
2	o	1	FRU	O4-C4-C3	-2.05	106.01	112.16
2	X	2	GAL	O5-C5-C4	2.04	115.80	110.83
2	T	2	GAL	O5-C5-C4	2.03	115.76	110.83
2	g	2	GAL	O4-C4-C3	-2.02	105.63	110.38

There are no chirality outliers.

All (148) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FRU	O1-C1-C2-C3
2	H	1	FRU	O1-C1-C2-O2
2	H	1	FRU	O1-C1-C2-O5
2	I	1	FRU	O1-C1-C2-O2
2	J	1	FRU	O1-C1-C2-C3
2	J	1	FRU	O1-C1-C2-O2
2	J	1	FRU	O1-C1-C2-O5
2	N	1	FRU	O1-C1-C2-C3
2	N	1	FRU	O1-C1-C2-O2
2	N	1	FRU	O1-C1-C2-O5
2	O	1	FRU	O1-C1-C2-C3
2	O	1	FRU	O1-C1-C2-O2
2	O	1	FRU	O1-C1-C2-O5
2	U	1	FRU	O1-C1-C2-C3
2	U	1	FRU	O1-C1-C2-O2
2	U	1	FRU	O1-C1-C2-O5
2	X	1	FRU	O1-C1-C2-C3
2	X	1	FRU	O1-C1-C2-O2
2	a	1	FRU	O5-C5-C6-O6
2	b	1	FRU	O1-C1-C2-C3
2	b	1	FRU	O1-C1-C2-O2
2	b	1	FRU	O1-C1-C2-O5
2	g	1	FRU	O1-C1-C2-C3
2	g	1	FRU	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	h	1	FRU	O1-C1-C2-O2
2	i	1	FRU	O1-C1-C2-C3
2	i	1	FRU	O1-C1-C2-O2
2	l	1	FRU	O1-C1-C2-C3
2	l	1	FRU	O1-C1-C2-O2
2	l	1	FRU	O1-C1-C2-O5
2	n	1	FRU	O5-C5-C6-O6
2	o	1	FRU	O1-C1-C2-O2
2	p	1	FRU	O1-C1-C2-O2
2	q	1	FRU	O1-C1-C2-O2
2	r	1	FRU	O1-C1-C2-O2
2	H	1	FRU	O5-C5-C6-O6
2	P	1	FRU	O5-C5-C6-O6
2	R	1	FRU	O5-C5-C6-O6
2	r	1	FRU	O5-C5-C6-O6
2	H	1	FRU	C4-C5-C6-O6
2	a	1	FRU	C4-C5-C6-O6
2	K	1	FRU	O5-C5-C6-O6
2	Z	1	FRU	O5-C5-C6-O6
2	p	1	FRU	O5-C5-C6-O6
2	P	1	FRU	C4-C5-C6-O6
2	n	1	FRU	C4-C5-C6-O6
2	r	1	FRU	C4-C5-C6-O6
2	J	2	GAL	O5-C5-C6-O6
2	b	2	GAL	O5-C5-C6-O6
2	L	1	FRU	O5-C5-C6-O6
2	Q	1	FRU	O5-C5-C6-O6
2	V	1	FRU	O5-C5-C6-O6
2	Y	1	FRU	O5-C5-C6-O6
2	q	1	FRU	O5-C5-C6-O6
2	V	2	GAL	O5-C5-C6-O6
2	L	1	FRU	C4-C5-C6-O6
2	Q	1	FRU	C4-C5-C6-O6
2	R	1	FRU	C4-C5-C6-O6
2	V	1	FRU	C4-C5-C6-O6
2	Y	1	FRU	C4-C5-C6-O6
2	o	1	FRU	C4-C5-C6-O6
2	p	1	FRU	C4-C5-C6-O6
2	l	2	GAL	O5-C5-C6-O6
2	r	2	GAL	O5-C5-C6-O6
2	H	2	GAL	O5-C5-C6-O6
2	f	2	GAL	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	j	2	GAL	O5-C5-C6-O6
2	b	2	GAL	C4-C5-C6-O6
2	l	2	GAL	C4-C5-C6-O6
2	J	2	GAL	C4-C5-C6-O6
2	Z	1	FRU	C4-C5-C6-O6
2	V	2	GAL	C4-C5-C6-O6
2	U	2	GAL	O5-C5-C6-O6
2	p	2	GAL	O5-C5-C6-O6
2	c	2	GAL	O5-C5-C6-O6
2	c	2	GAL	C4-C5-C6-O6
2	j	2	GAL	C4-C5-C6-O6
2	n	2	GAL	C4-C5-C6-O6
2	r	2	GAL	C4-C5-C6-O6
2	k	2	GAL	O5-C5-C6-O6
2	k	2	GAL	C4-C5-C6-O6
2	N	2	GAL	O5-C5-C6-O6
2	H	2	GAL	C4-C5-C6-O6
2	U	2	GAL	C4-C5-C6-O6
2	n	2	GAL	O5-C5-C6-O6
2	f	2	GAL	C4-C5-C6-O6
2	o	1	FRU	O5-C5-C6-O6
2	N	2	GAL	C4-C5-C6-O6
2	P	2	GAL	O5-C5-C6-O6
2	W	2	GAL	C4-C5-C6-O6
2	Y	2	GAL	O5-C5-C6-O6
2	R	2	GAL	C4-C5-C6-O6
2	X	1	FRU	O1-C1-C2-O5
2	g	1	FRU	O1-C1-C2-O5
2	i	1	FRU	O1-C1-C2-O5
2	K	1	FRU	C4-C5-C6-O6
2	q	1	FRU	C4-C5-C6-O6
2	X	1	FRU	O5-C5-C6-O6
2	q	2	GAL	C4-C5-C6-O6
2	k	1	FRU	C4-C5-C6-O6
2	R	2	GAL	O5-C5-C6-O6
2	X	2	GAL	C4-C5-C6-O6
2	p	2	GAL	C4-C5-C6-O6
2	e	1	FRU	O5-C5-C6-O6
2	q	1	FRU	O1-C1-C2-O5
2	Z	2	GAL	O5-C5-C6-O6
2	W	1	FRU	O5-C5-C6-O6
2	O	2	GAL	C4-C5-C6-O6

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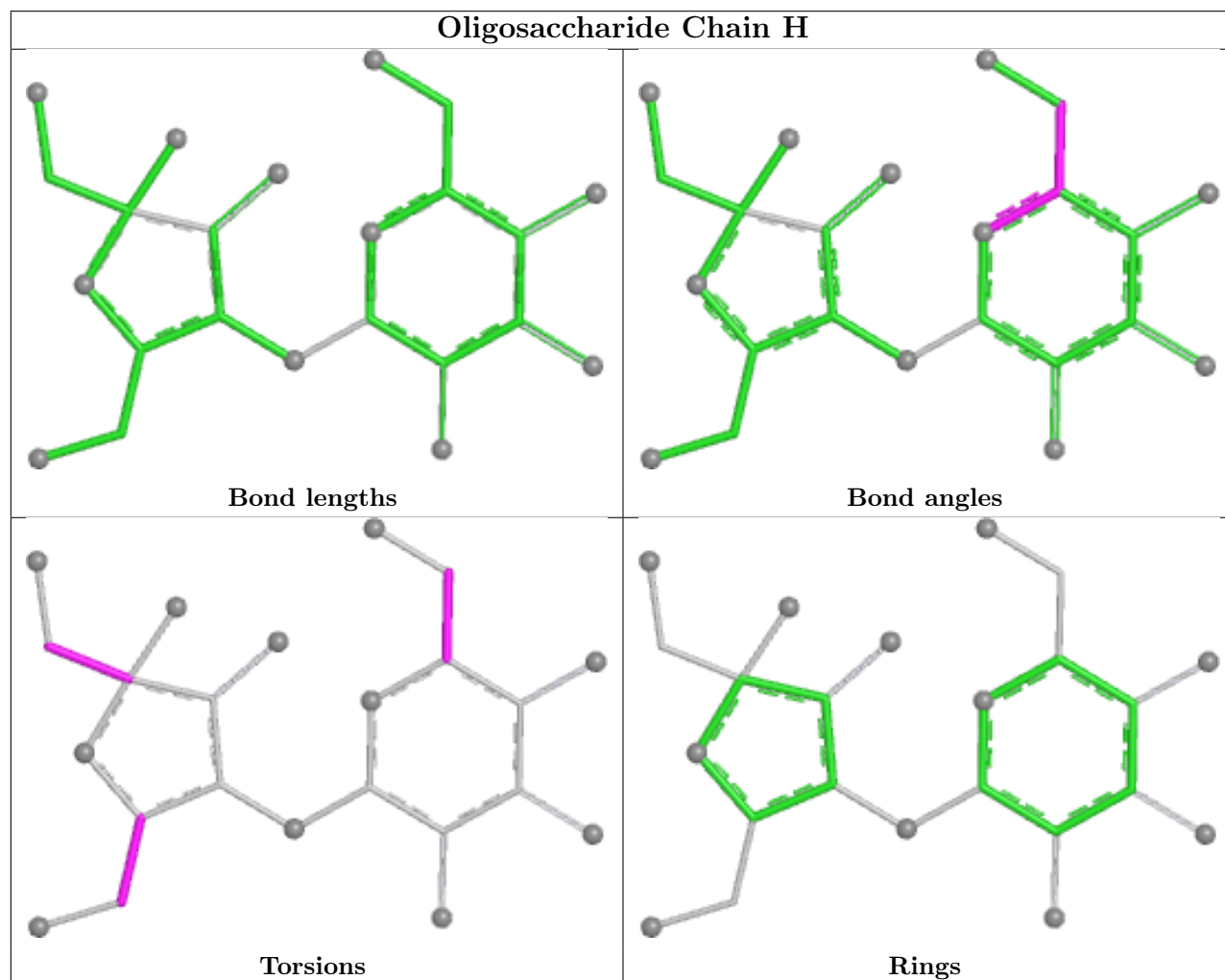
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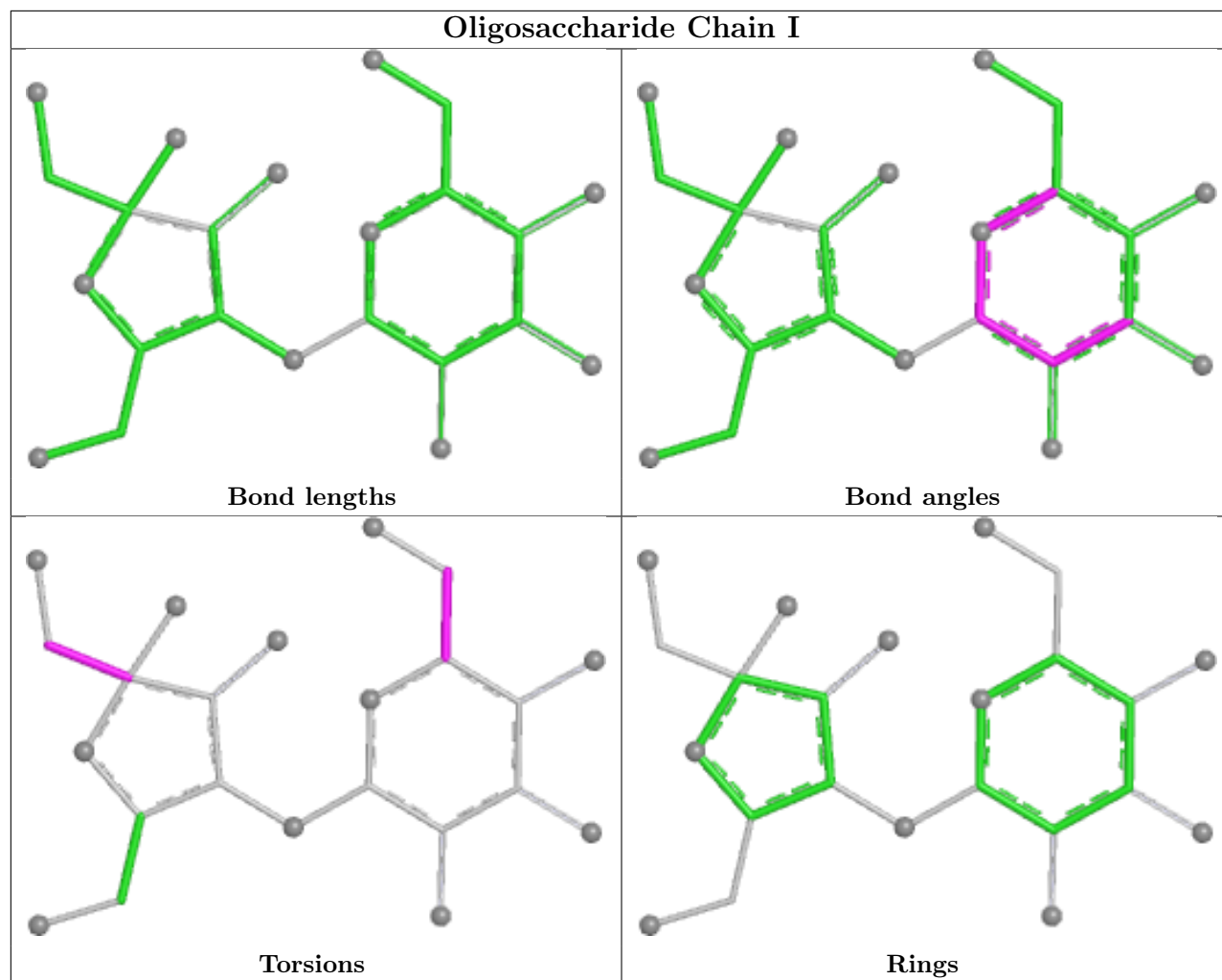
Mol	Chain	Res	Type	Atoms
2	M	2	GAL	O5-C5-C6-O6
2	T	2	GAL	C4-C5-C6-O6
2	e	2	GAL	O5-C5-C6-O6
2	T	1	FRU	O1-C1-C2-O5
2	d	1	FRU	O5-C5-C6-O6
2	P	2	GAL	C4-C5-C6-O6
2	W	2	GAL	O5-C5-C6-O6
2	V	1	FRU	O1-C1-C2-C3
2	o	1	FRU	O1-C1-C2-C3
2	V	1	FRU	O1-C1-C2-O5
2	j	1	FRU	O1-C1-C2-O5
2	X	1	FRU	C4-C5-C6-O6
2	Y	2	GAL	C4-C5-C6-O6
2	k	1	FRU	O5-C5-C6-O6
2	O	2	GAL	O5-C5-C6-O6
2	h	1	FRU	O1-C1-C2-O5
2	T	1	FRU	O1-C1-C2-O2
2	f	1	FRU	O1-C1-C2-O2
2	j	1	FRU	O1-C1-C2-O2
2	T	1	FRU	O1-C1-C2-C3
2	f	1	FRU	O1-C1-C2-C3
2	q	1	FRU	O1-C1-C2-C3
2	m	1	FRU	O5-C5-C6-O6
2	I	1	FRU	O1-C1-C2-O5
2	e	1	FRU	C4-C5-C6-O6
2	Q	1	FRU	O1-C1-C2-O5
2	f	1	FRU	O1-C1-C2-O5
2	m	1	FRU	O1-C1-C2-O5
2	o	1	FRU	O1-C1-C2-O5
2	J	1	FRU	O5-C5-C6-O6
2	L	1	FRU	O1-C1-C2-C3
2	P	1	FRU	O1-C1-C2-C3
2	R	1	FRU	O1-C1-C2-C3
2	j	1	FRU	O1-C1-C2-C3
2	r	1	FRU	O1-C1-C2-O5
2	M	2	GAL	C4-C5-C6-O6
2	W	1	FRU	C4-C5-C6-O6
2	I	2	GAL	C4-C5-C6-O6
2	T	1	FRU	C4-C5-C6-O6
2	W	1	FRU	O1-C1-C2-C3

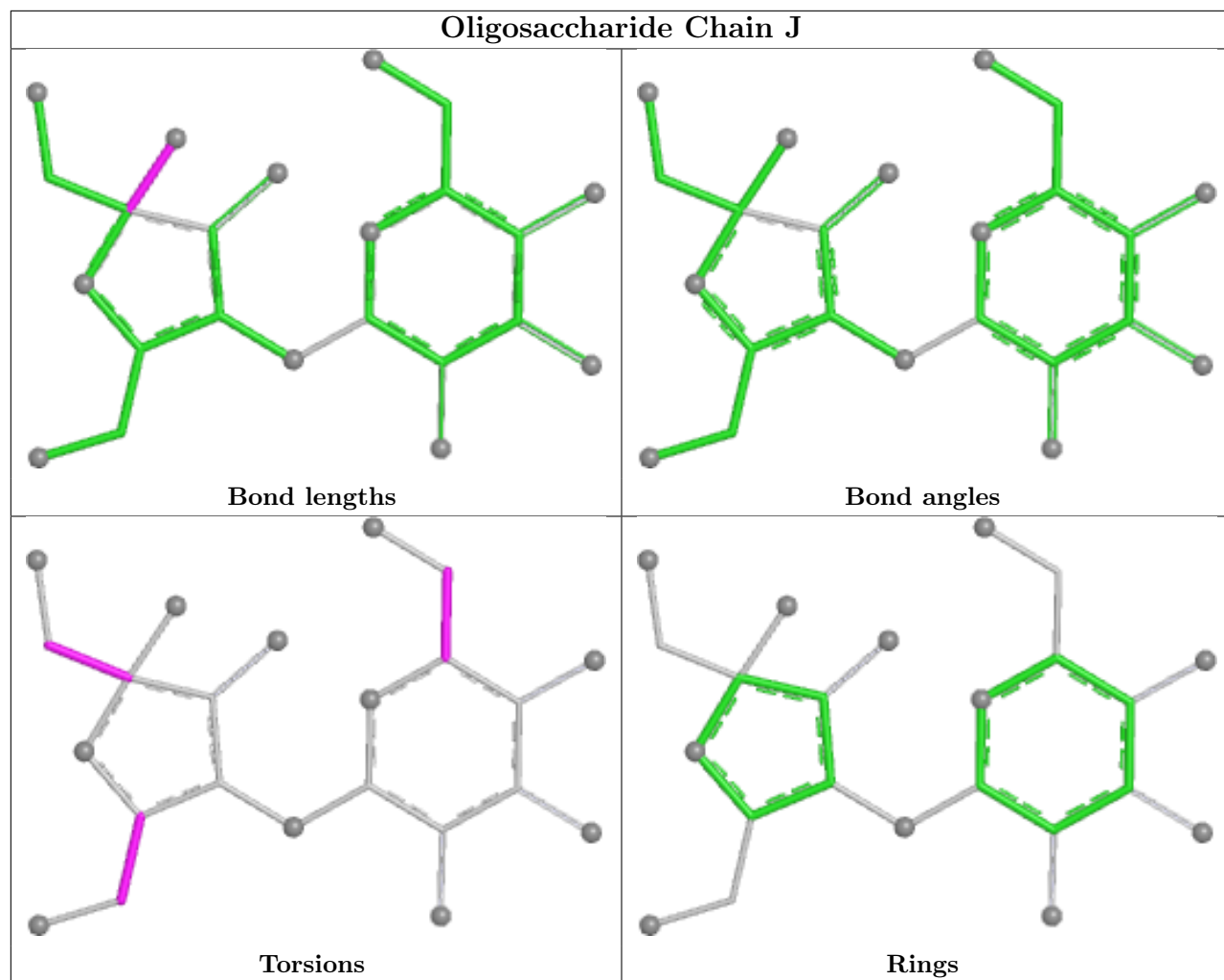
There are no ring outliers.

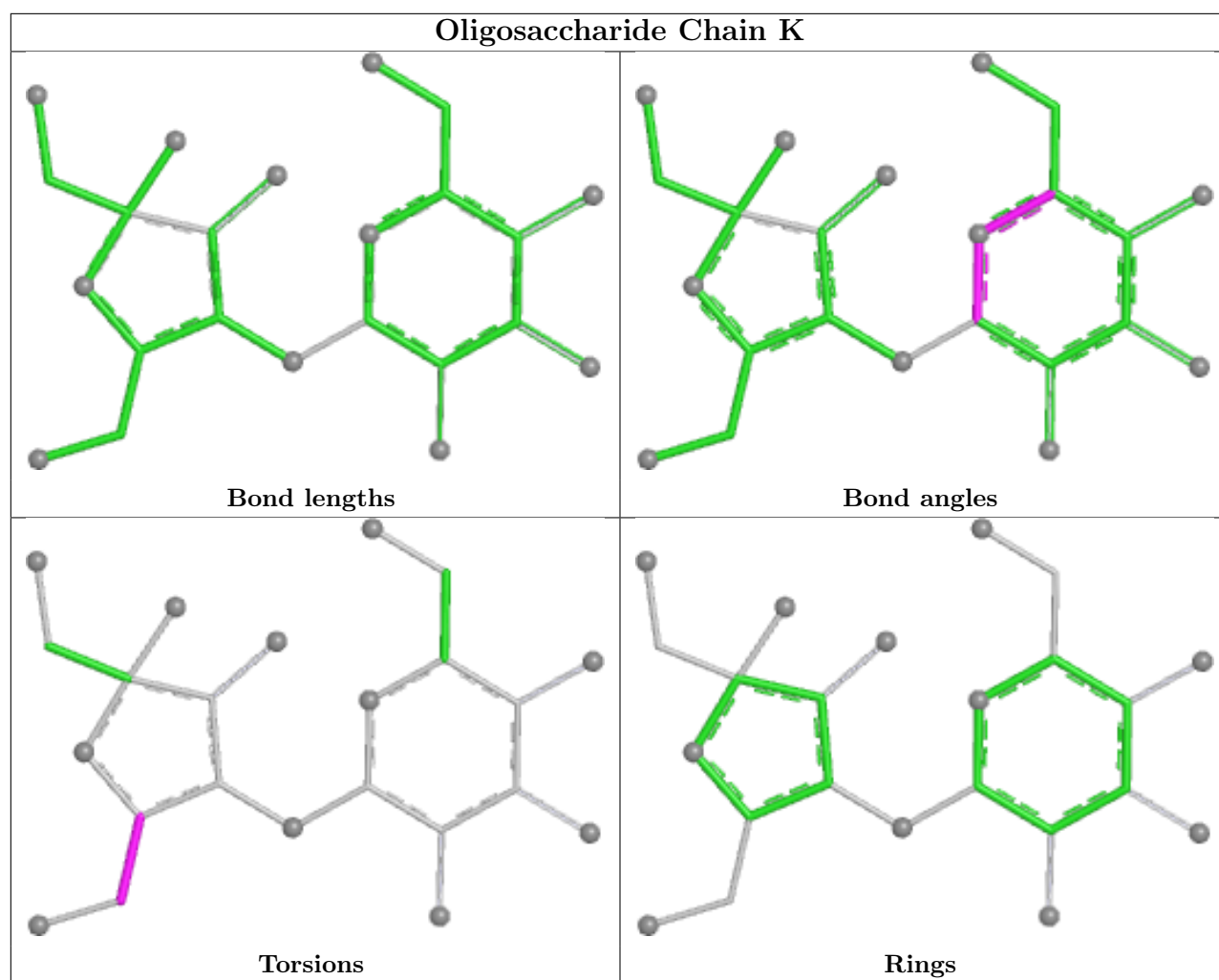
No monomer is involved in short contacts.

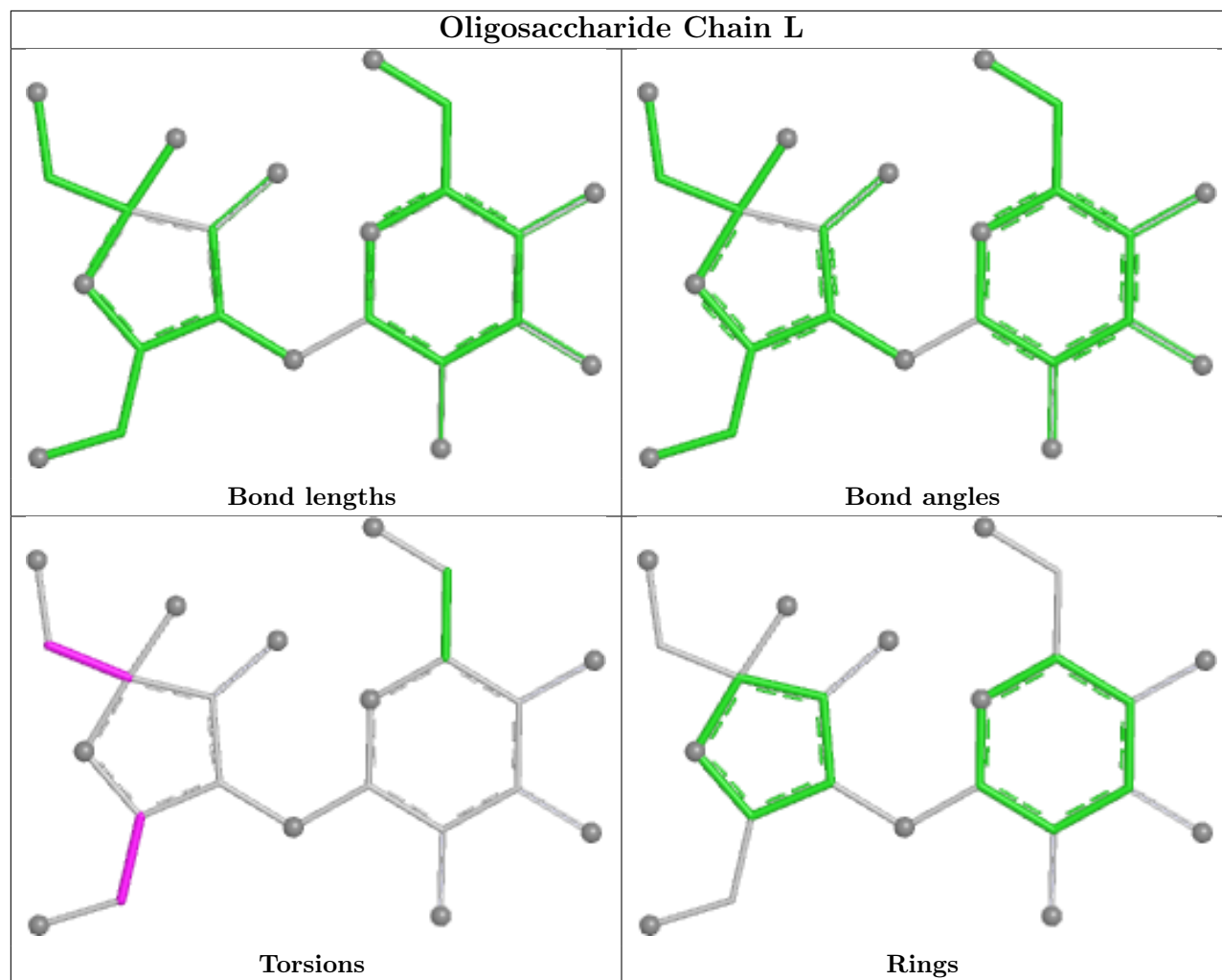
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

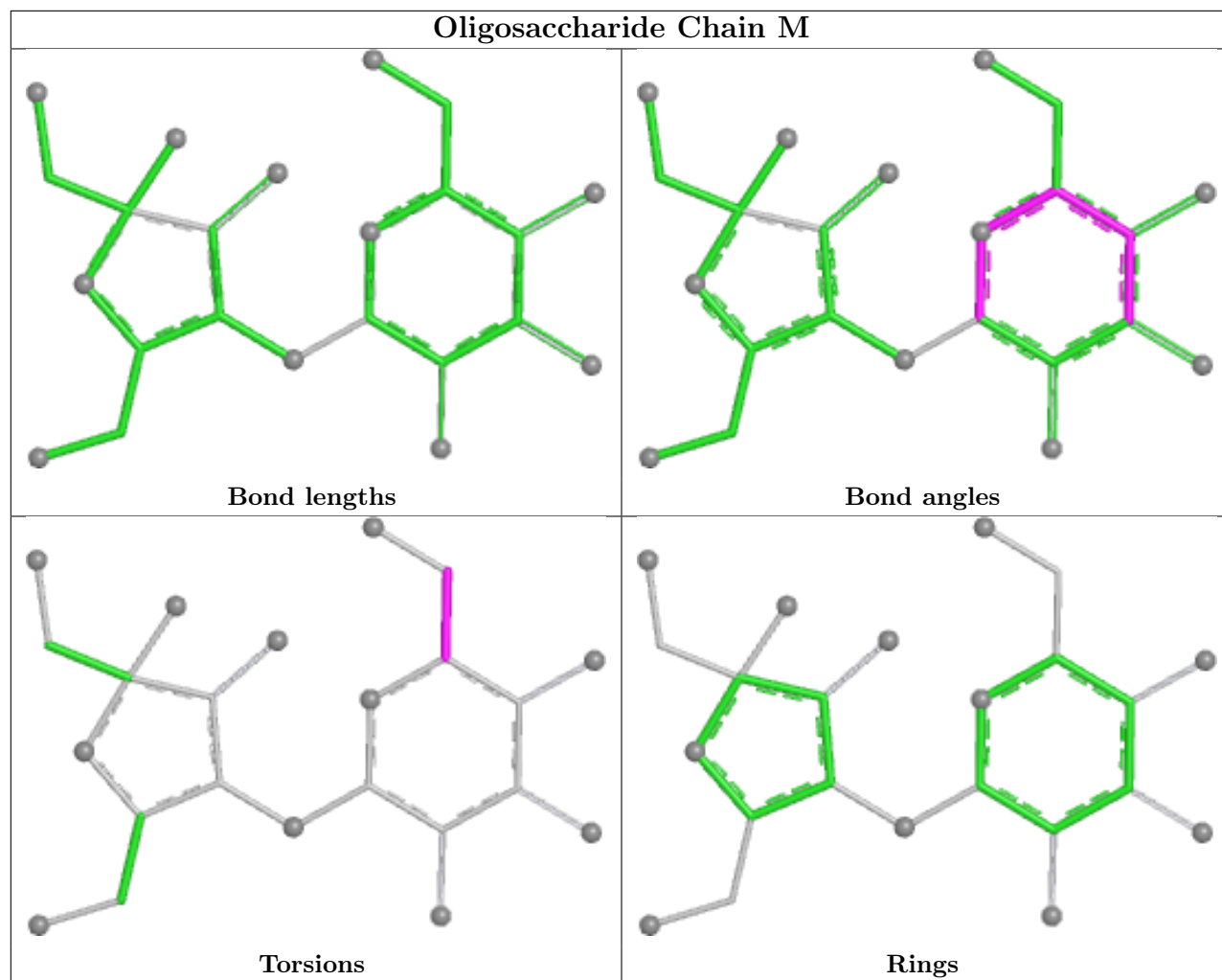


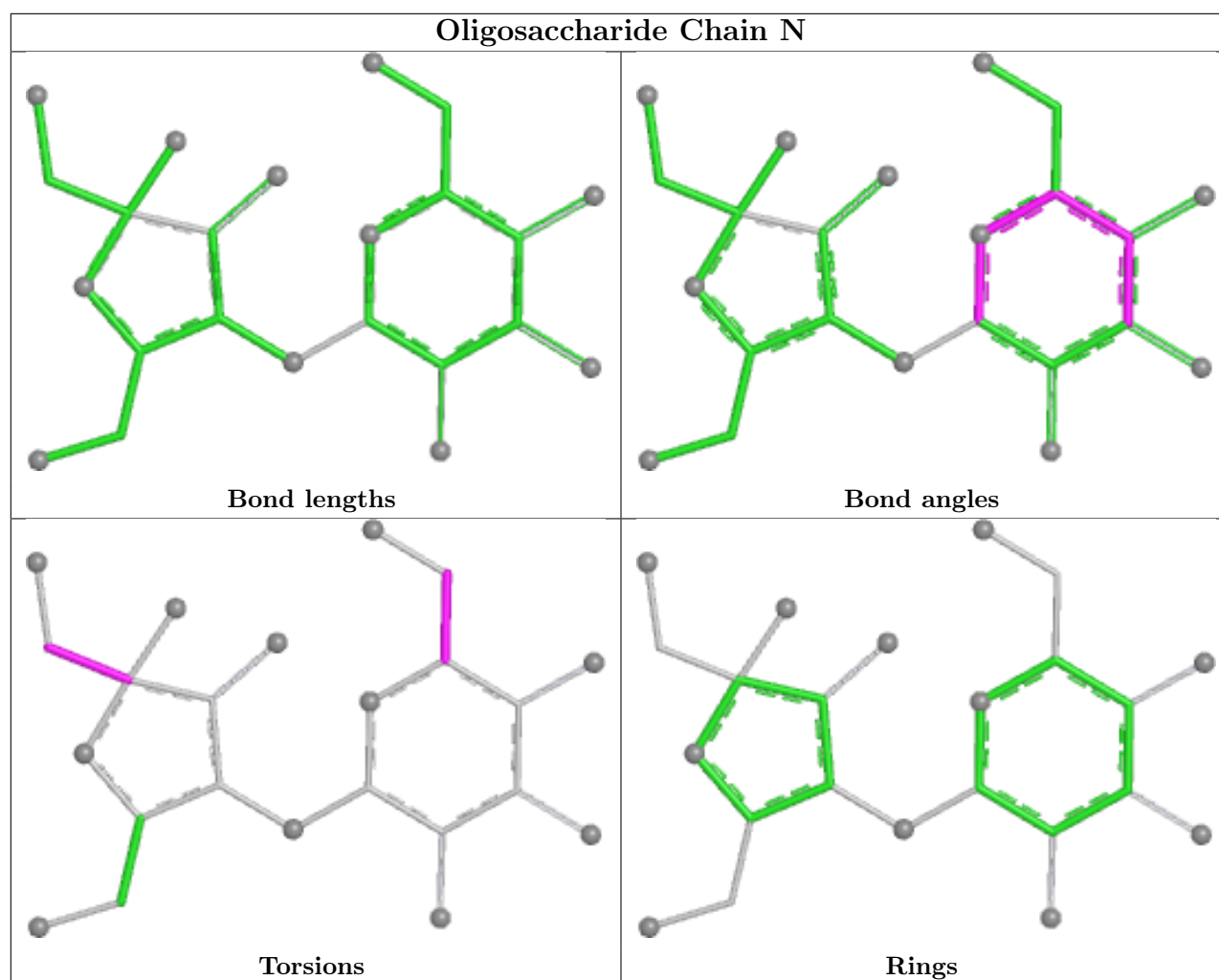


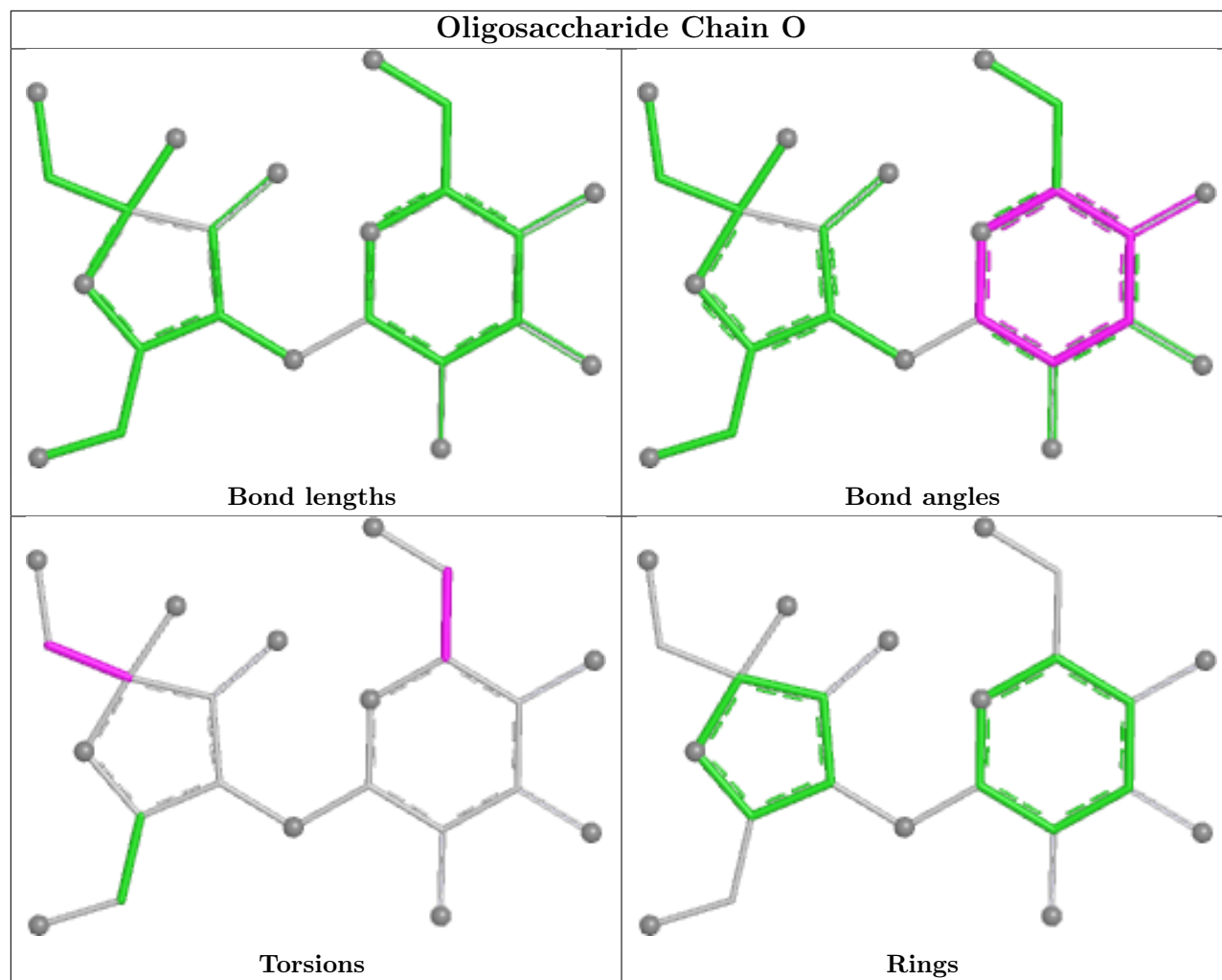


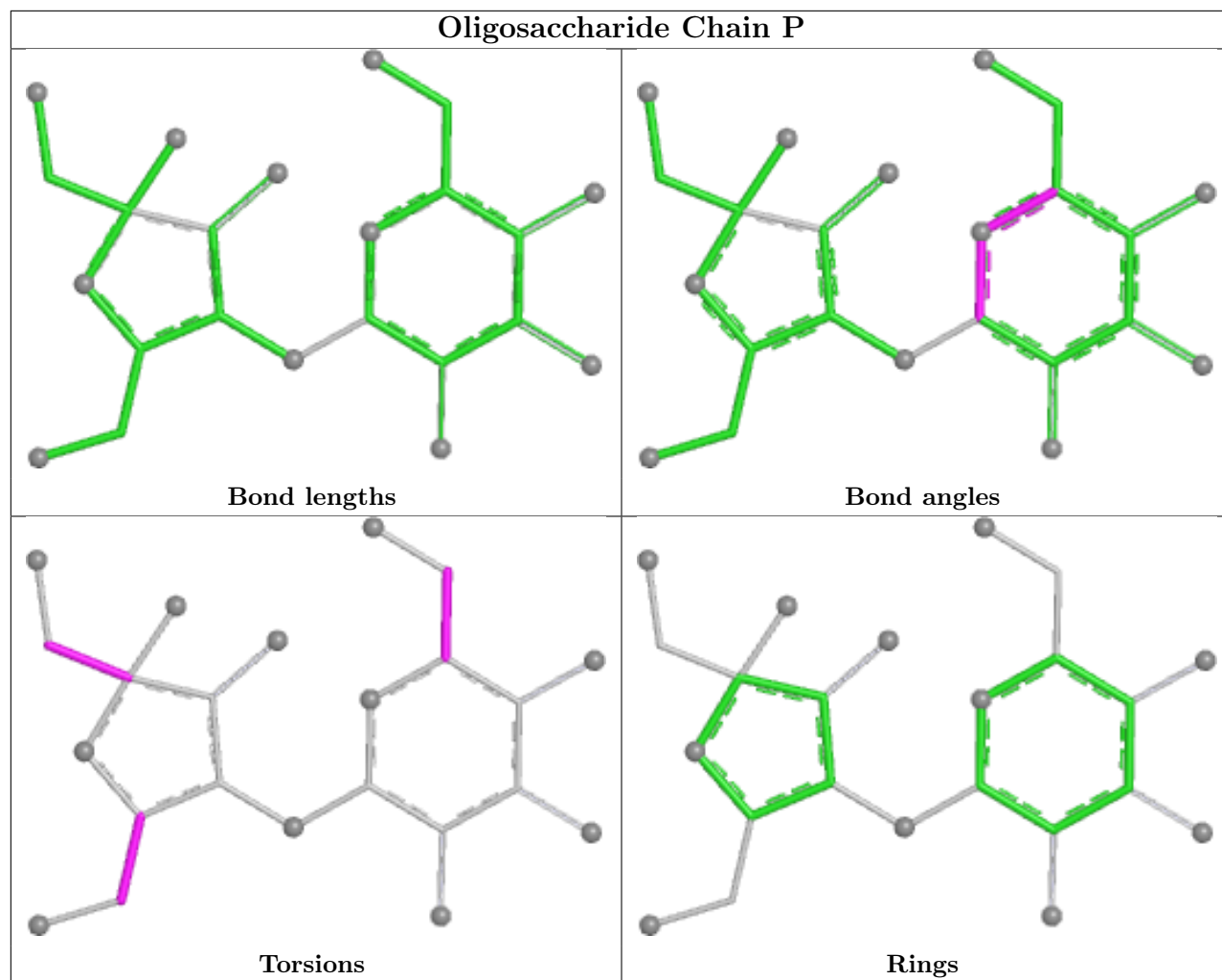


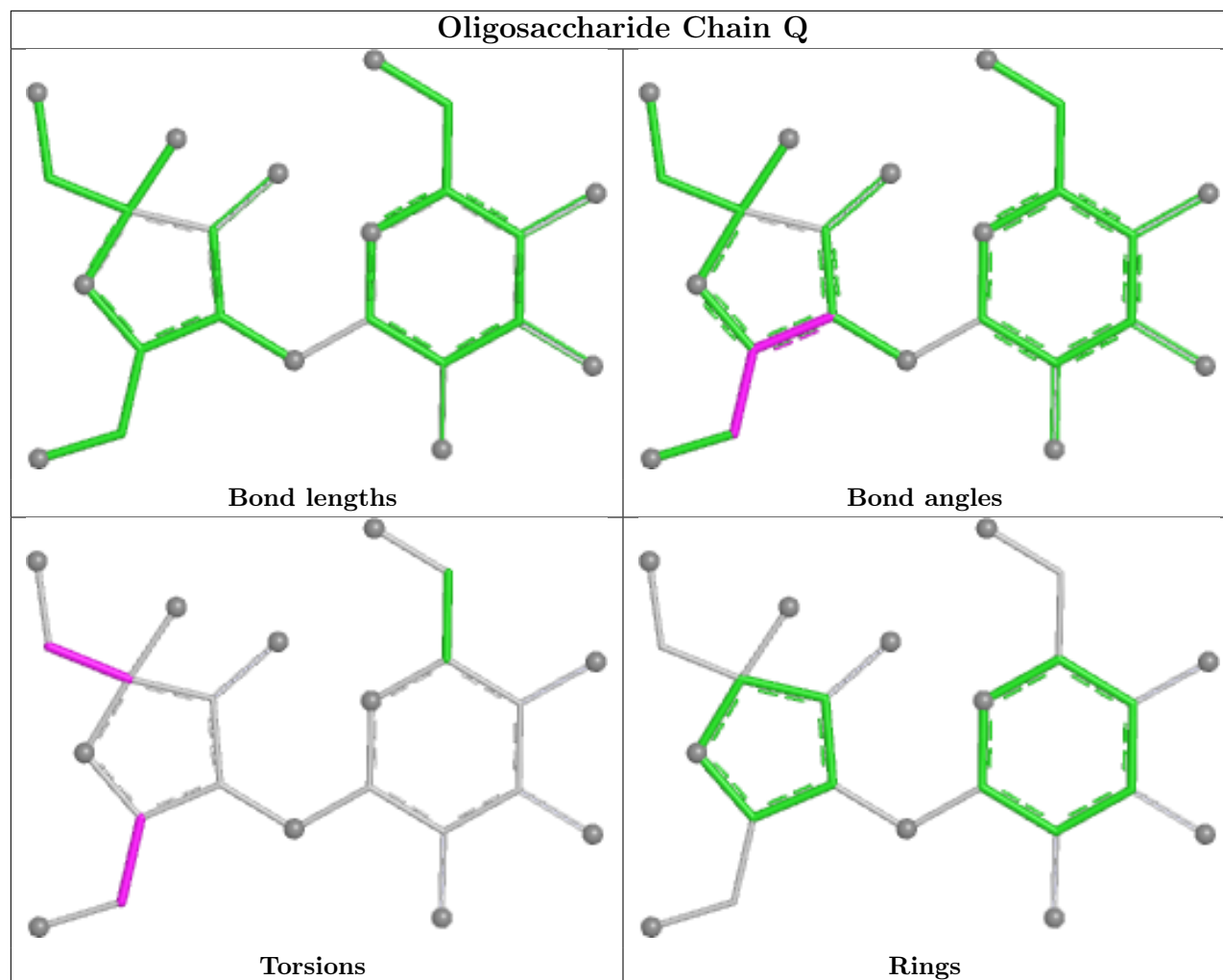


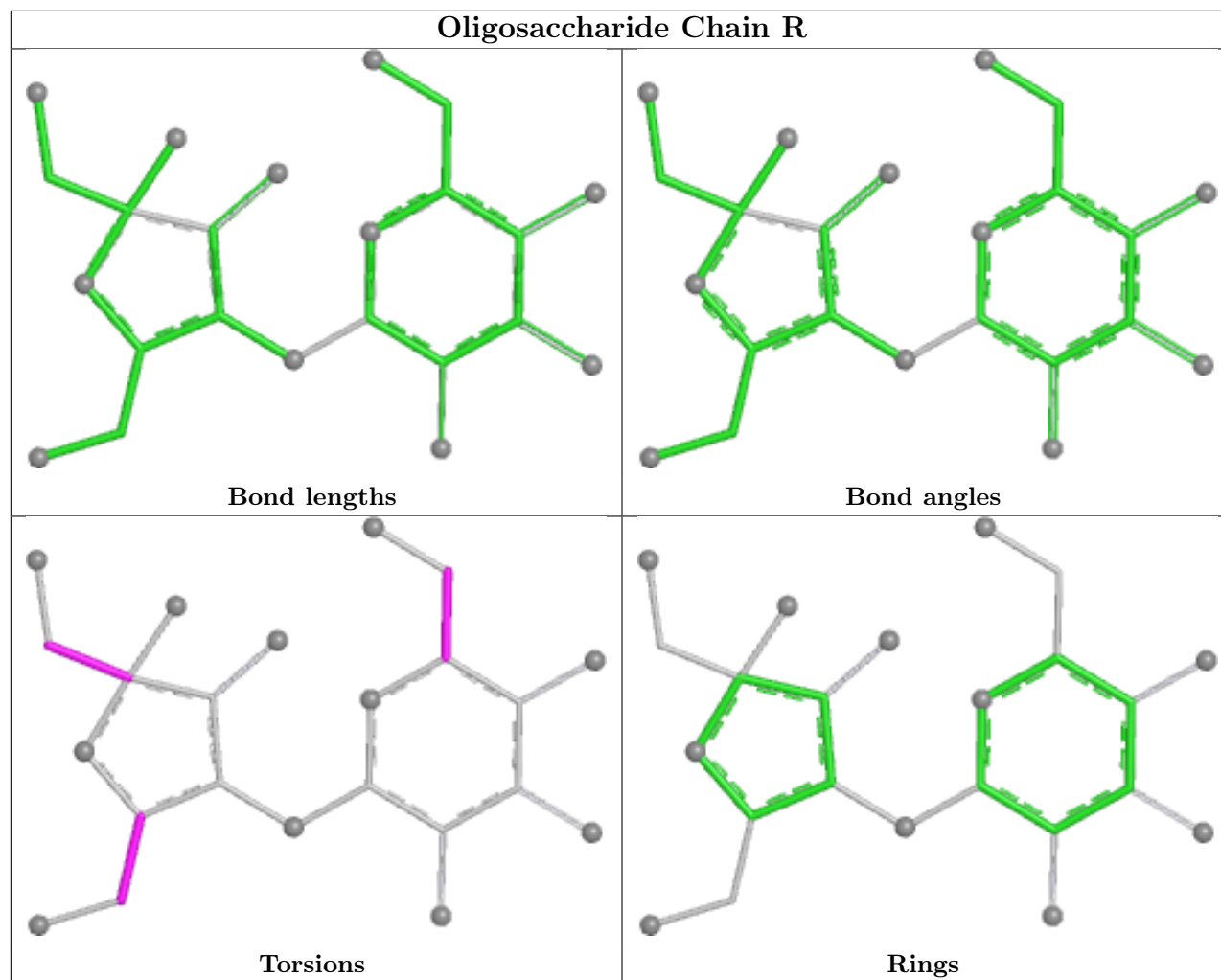


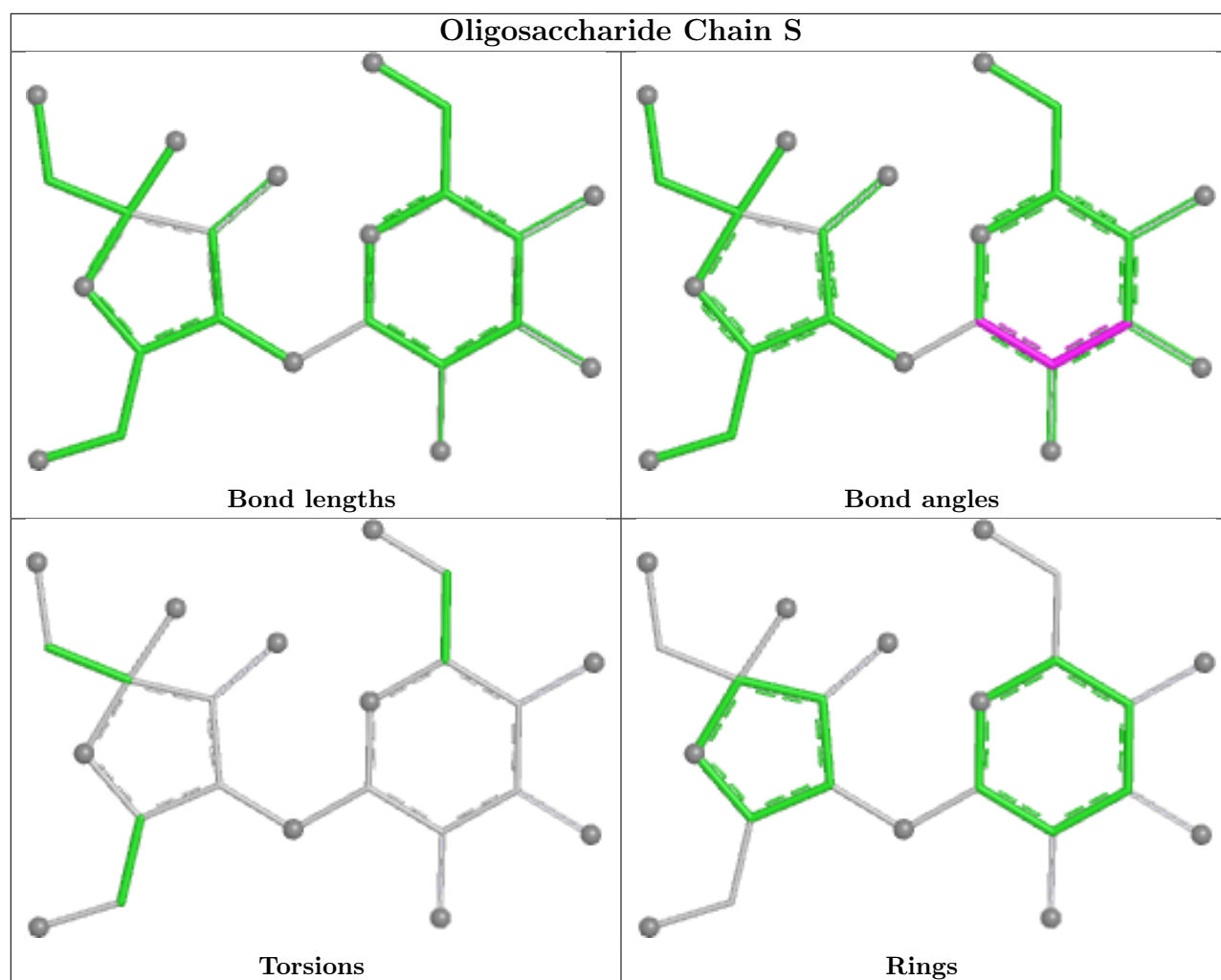


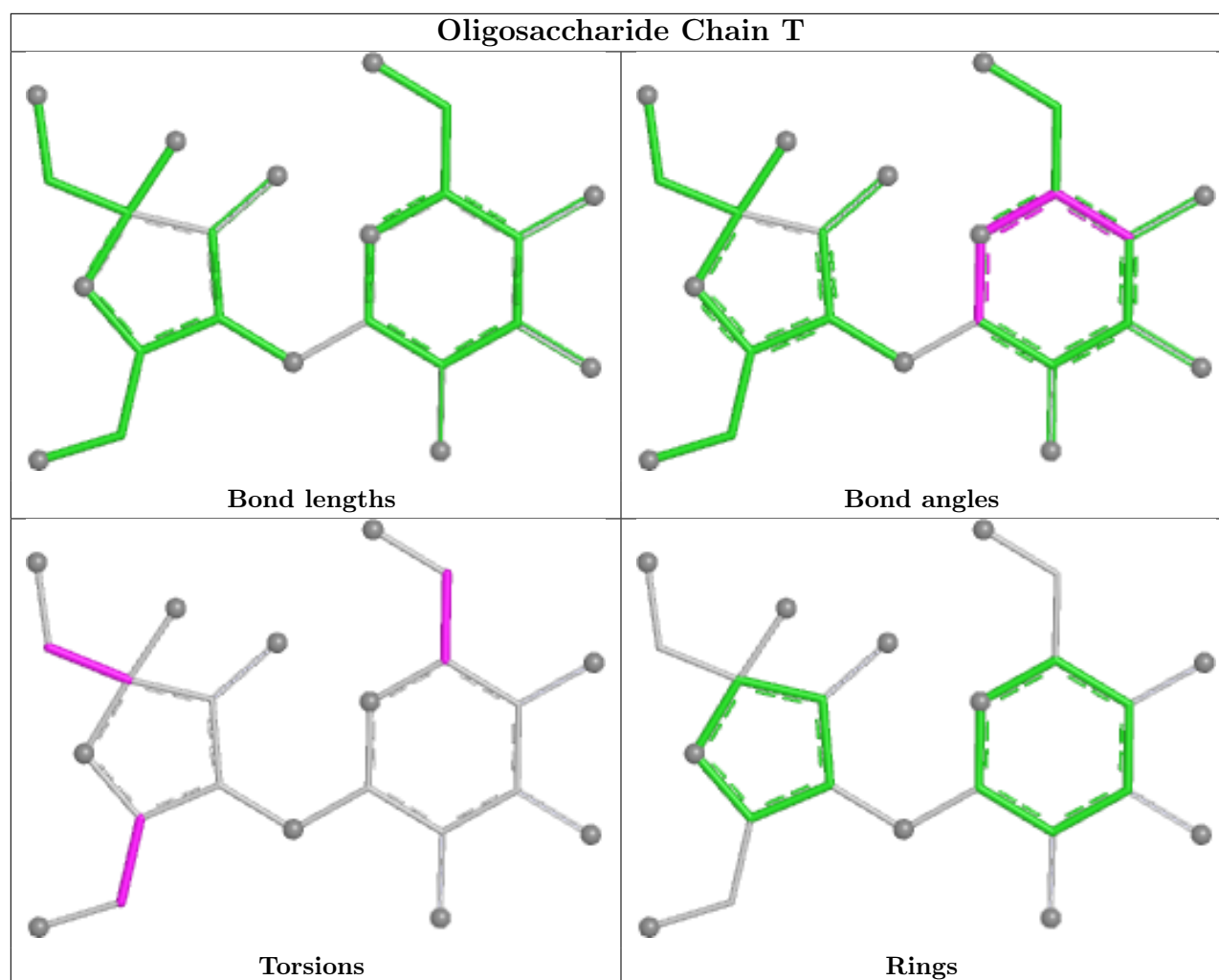


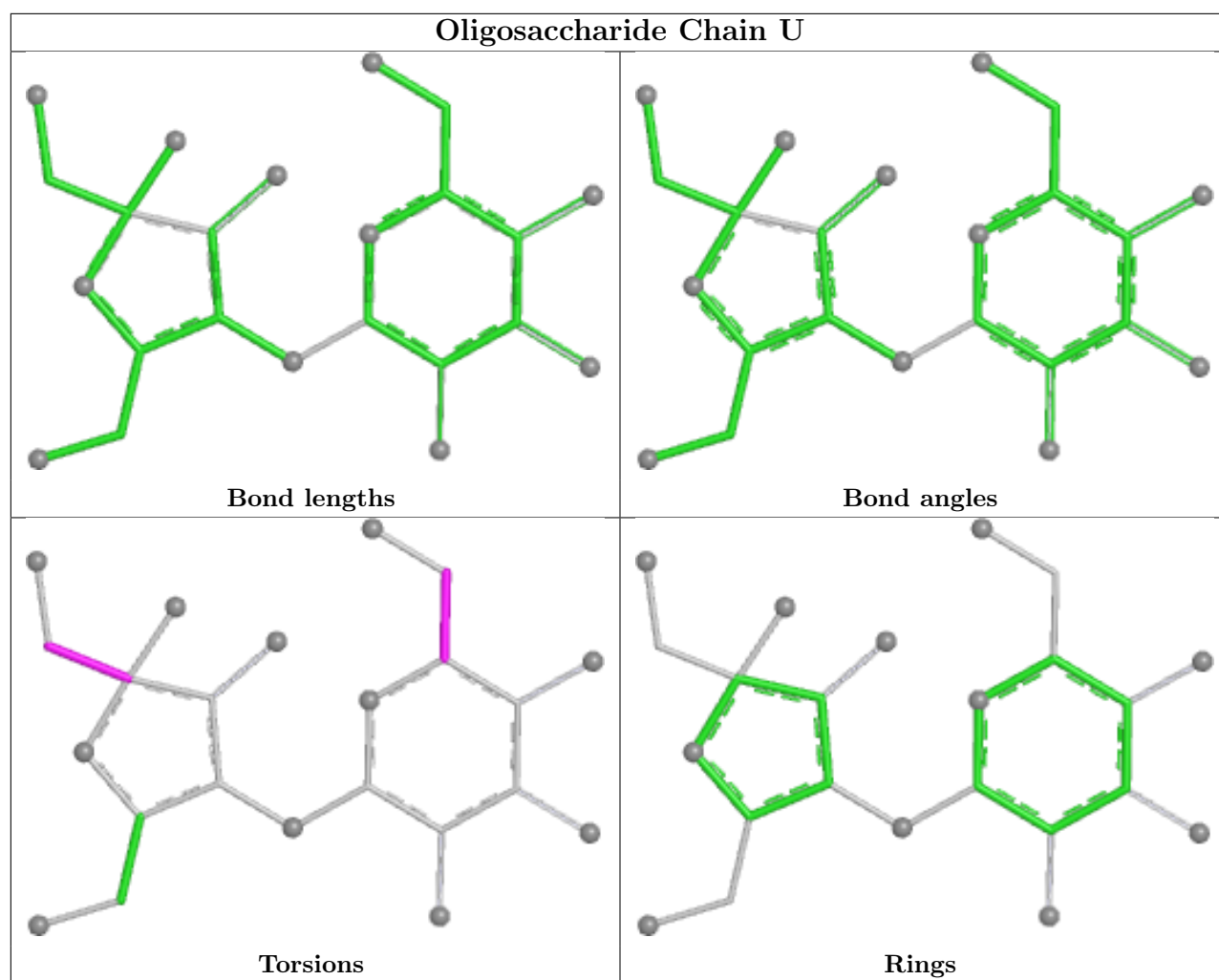


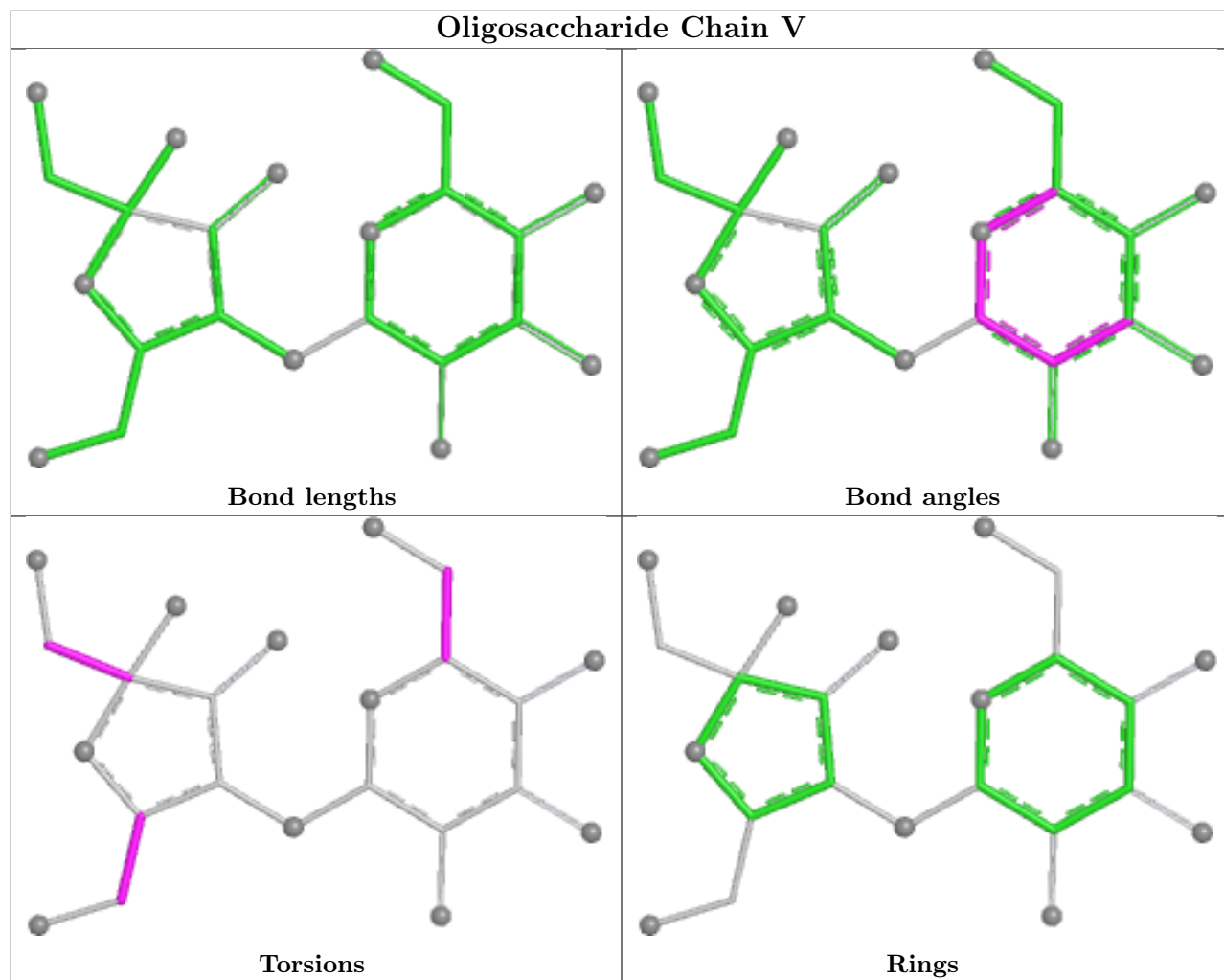


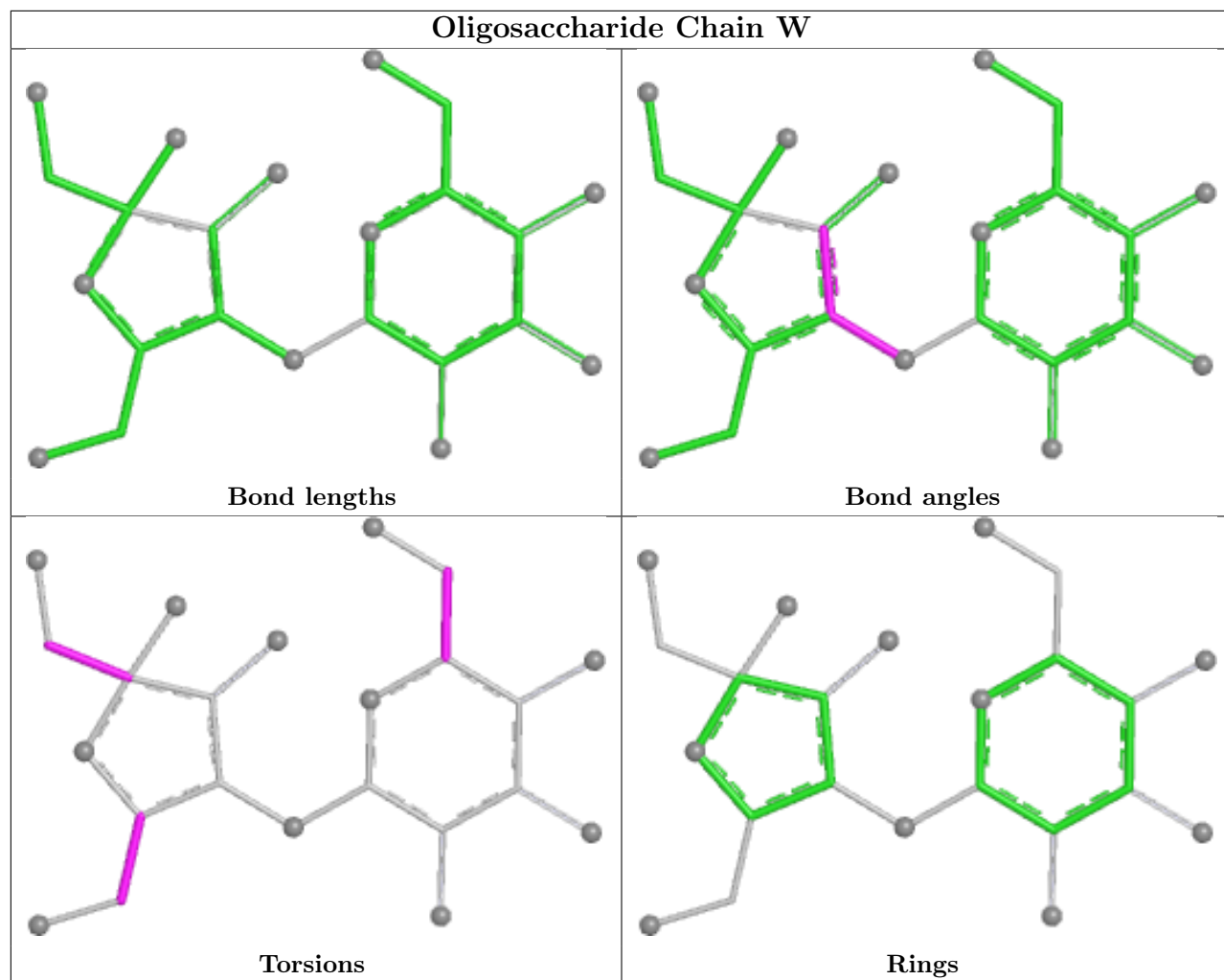


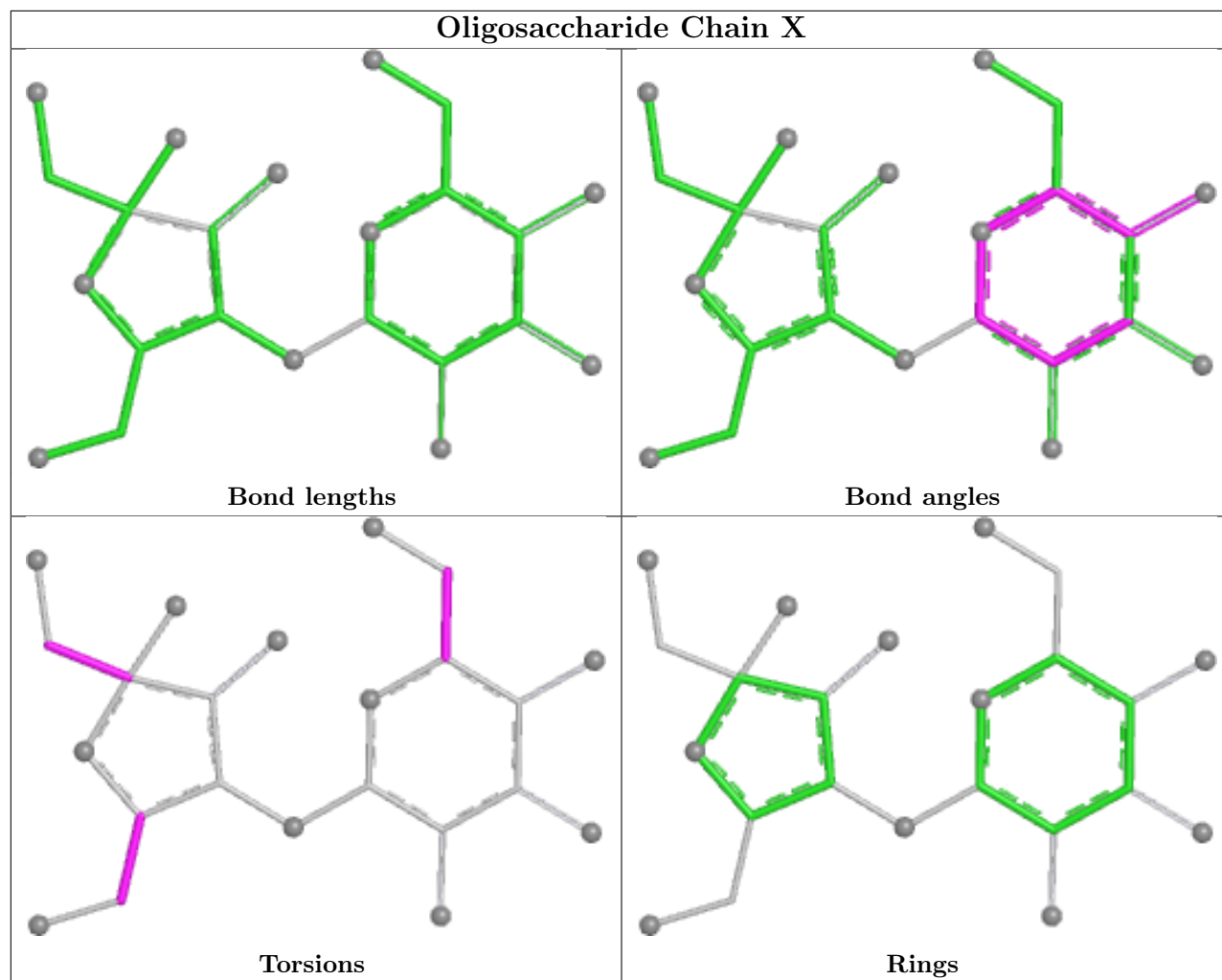


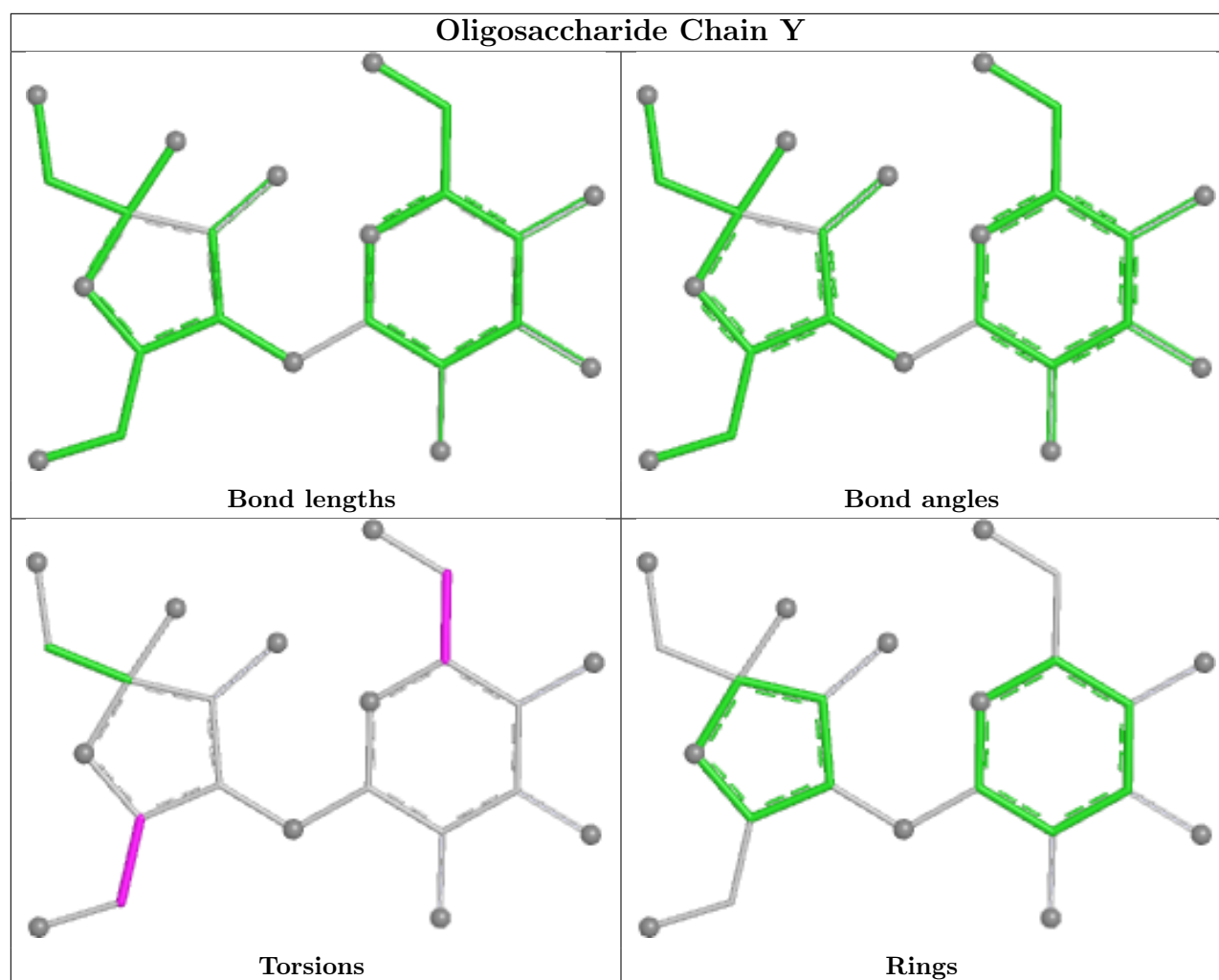


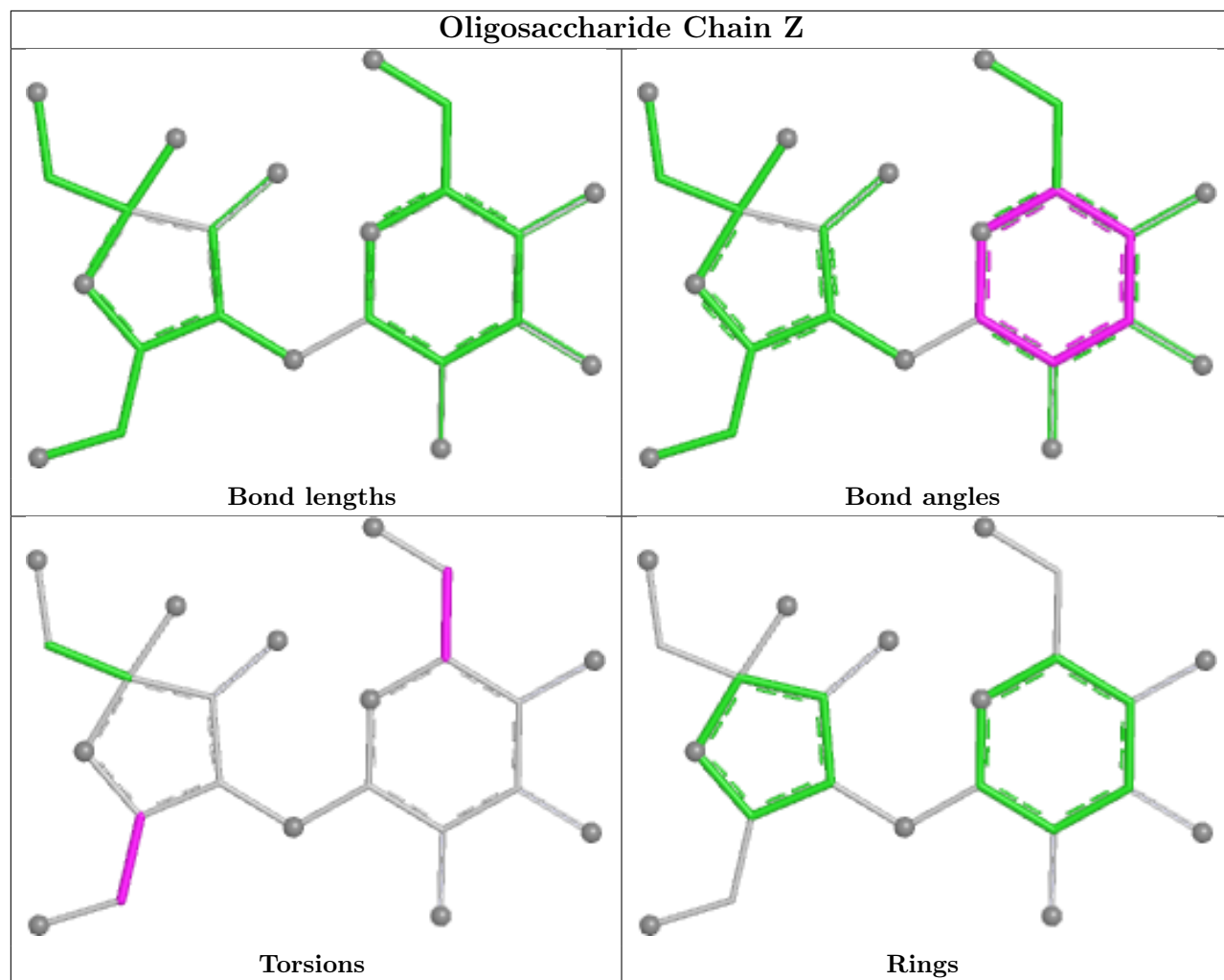


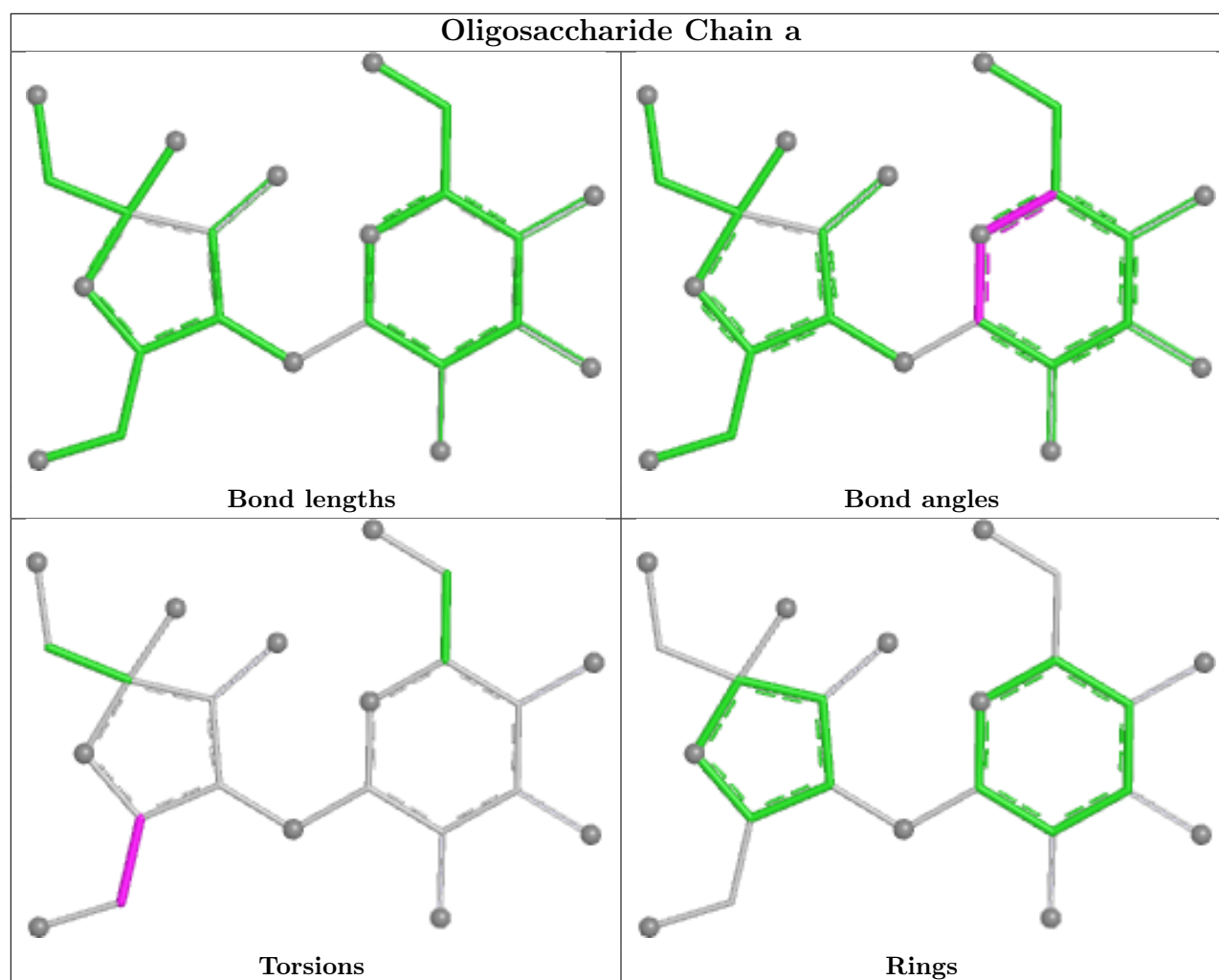


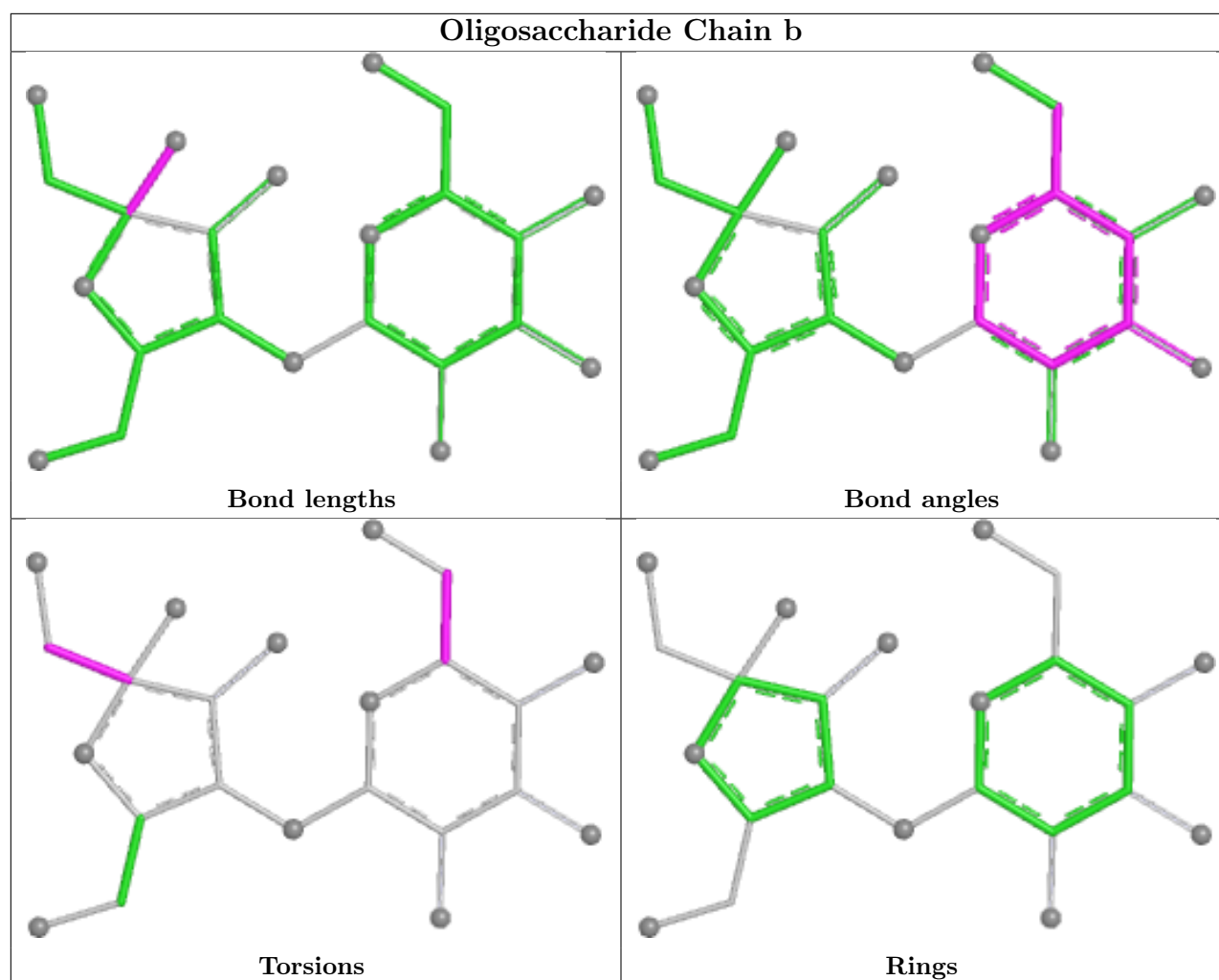


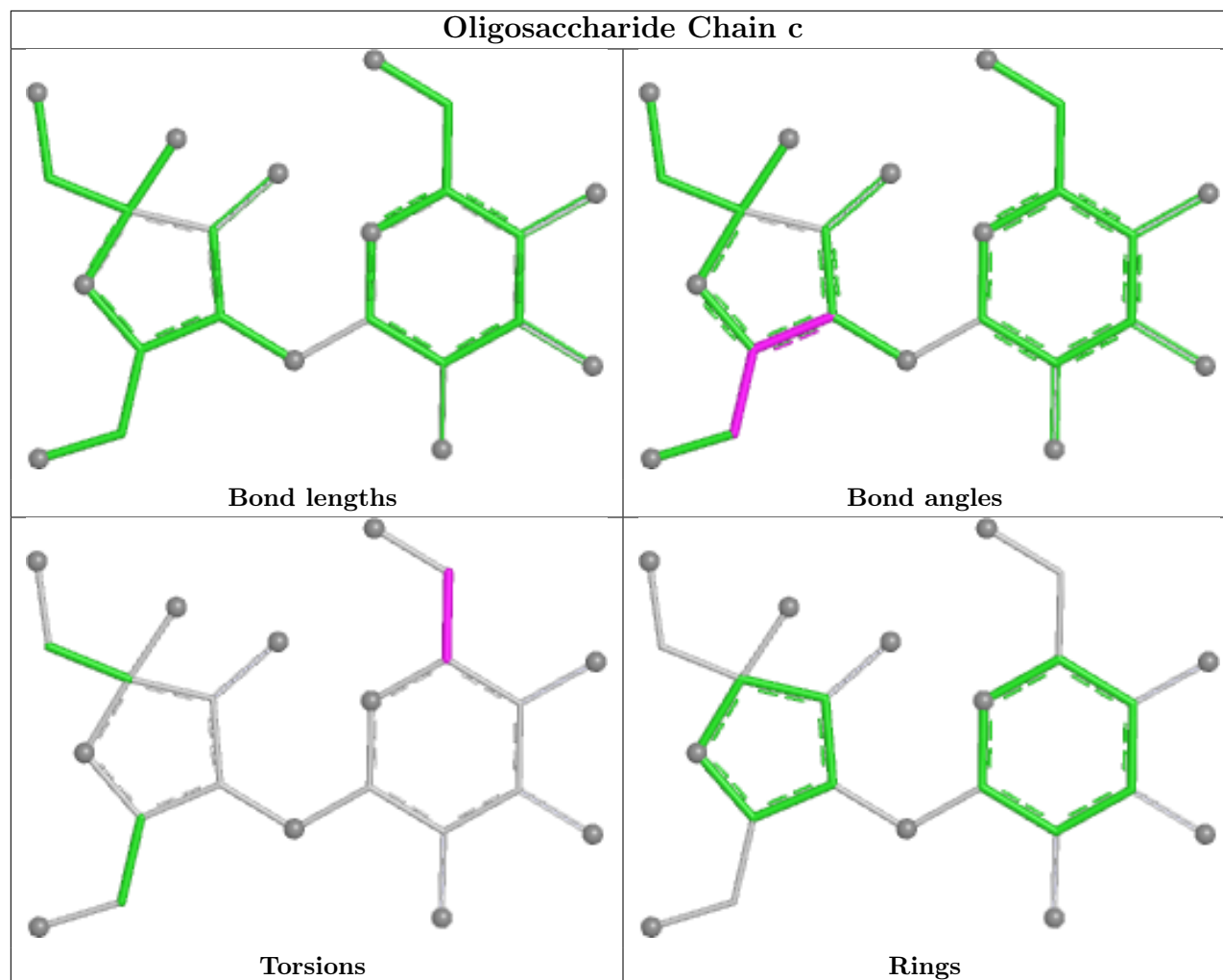


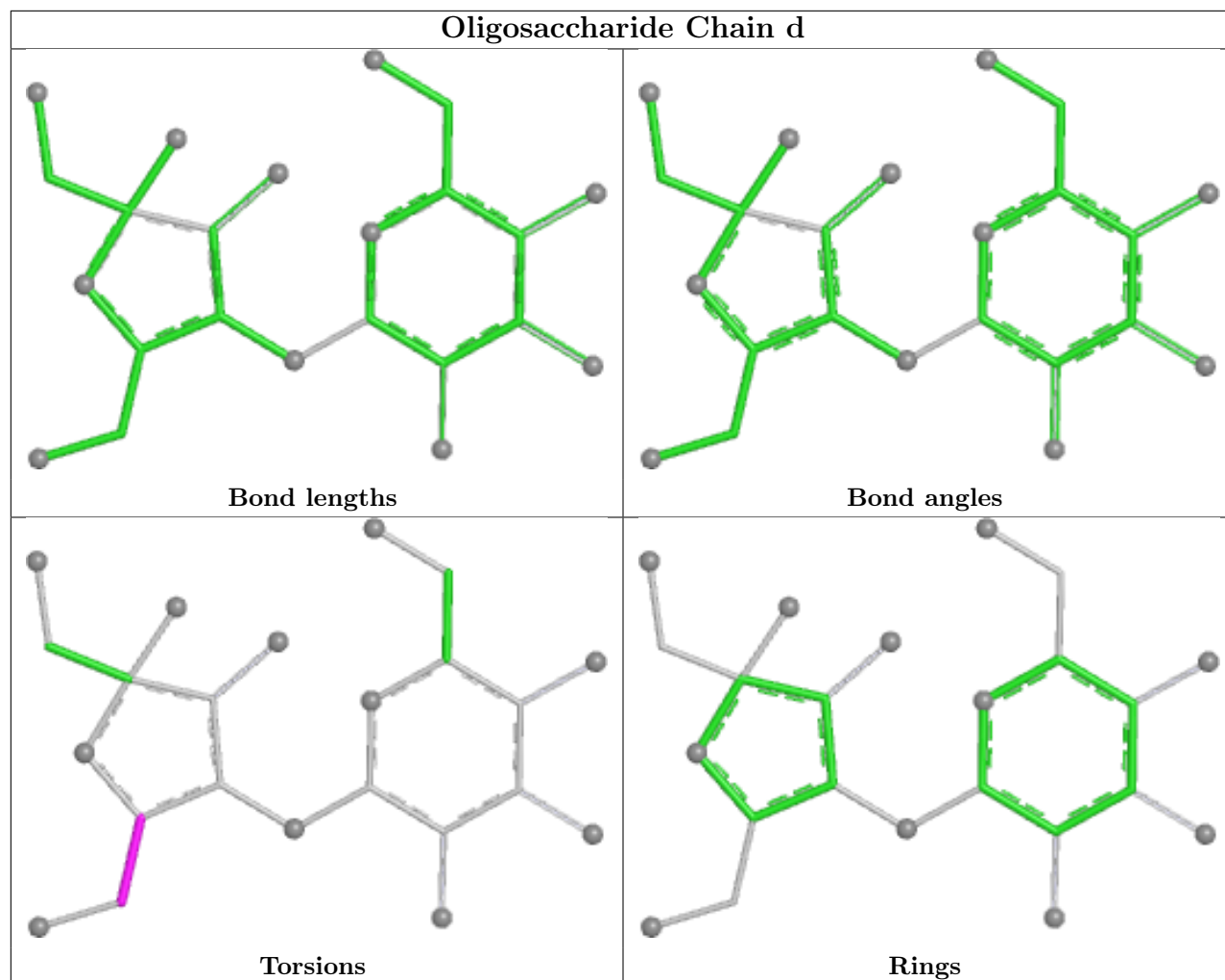


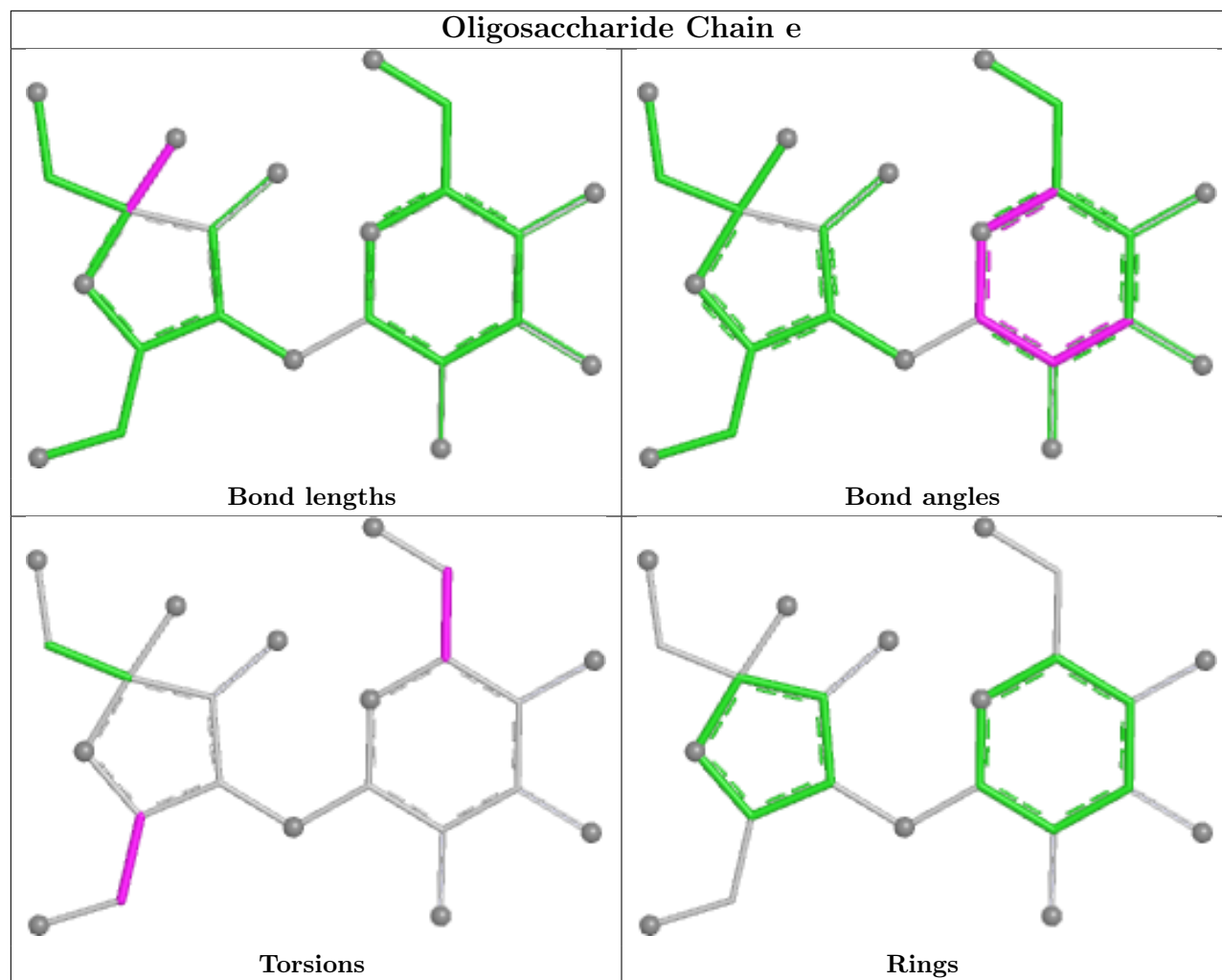


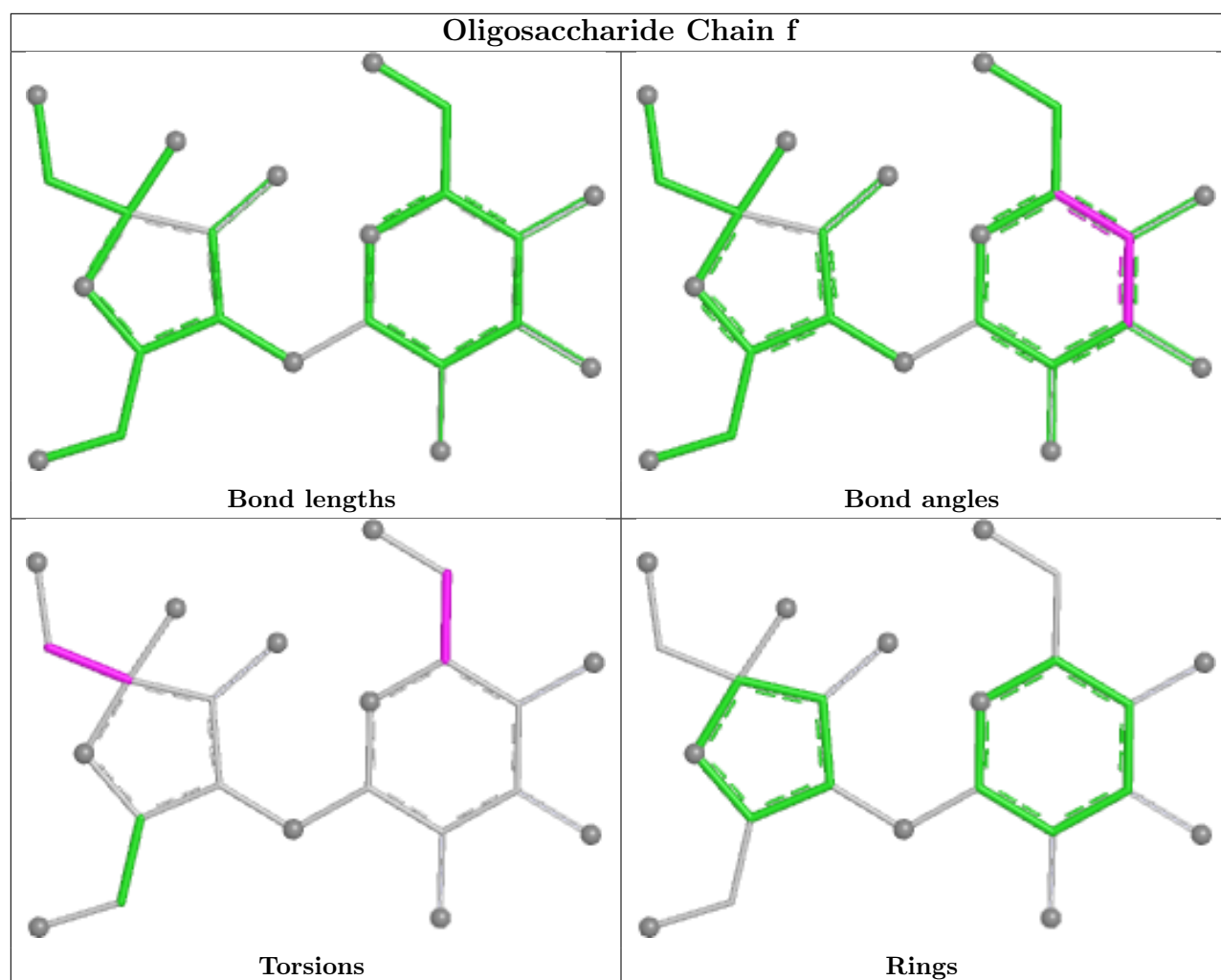


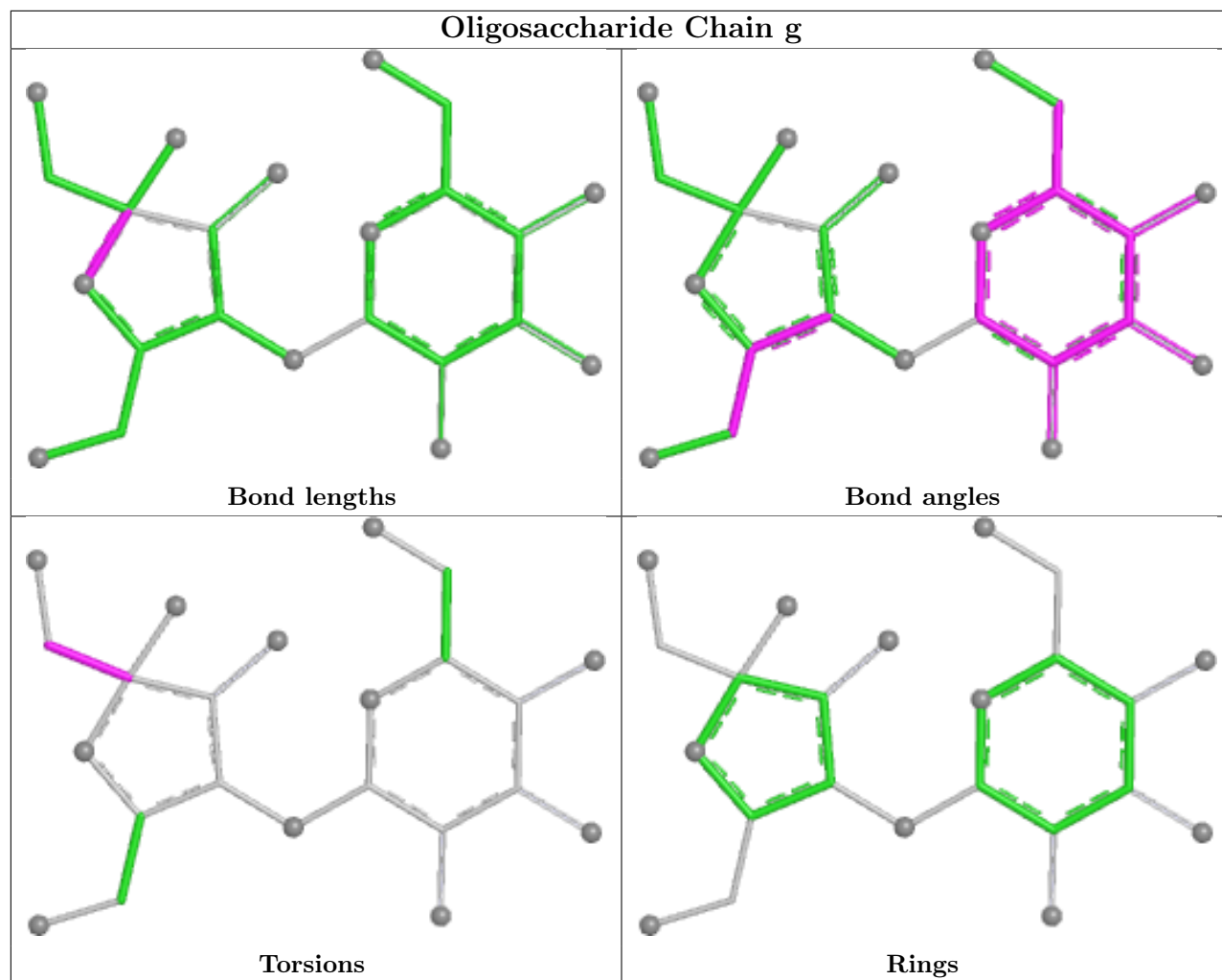


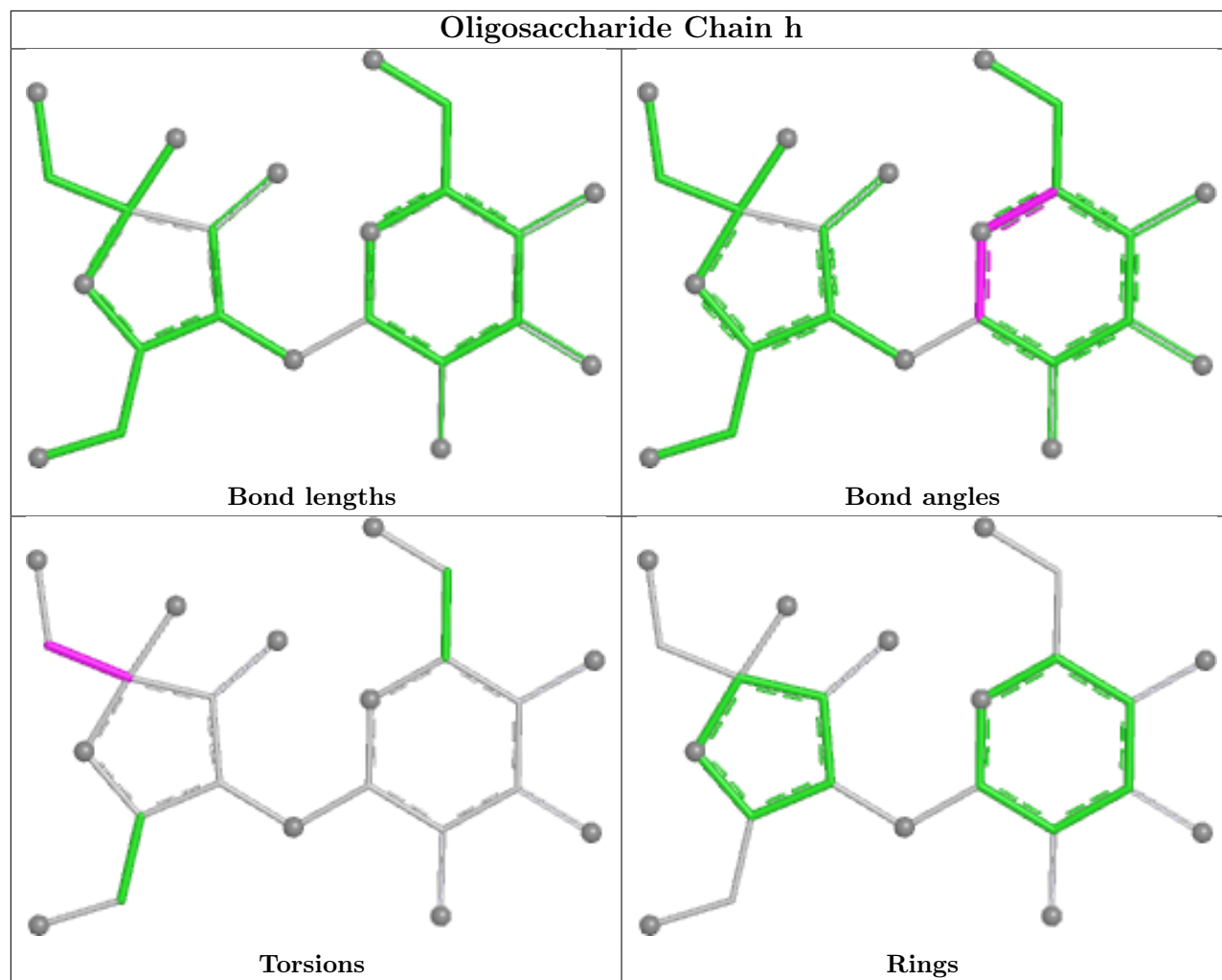


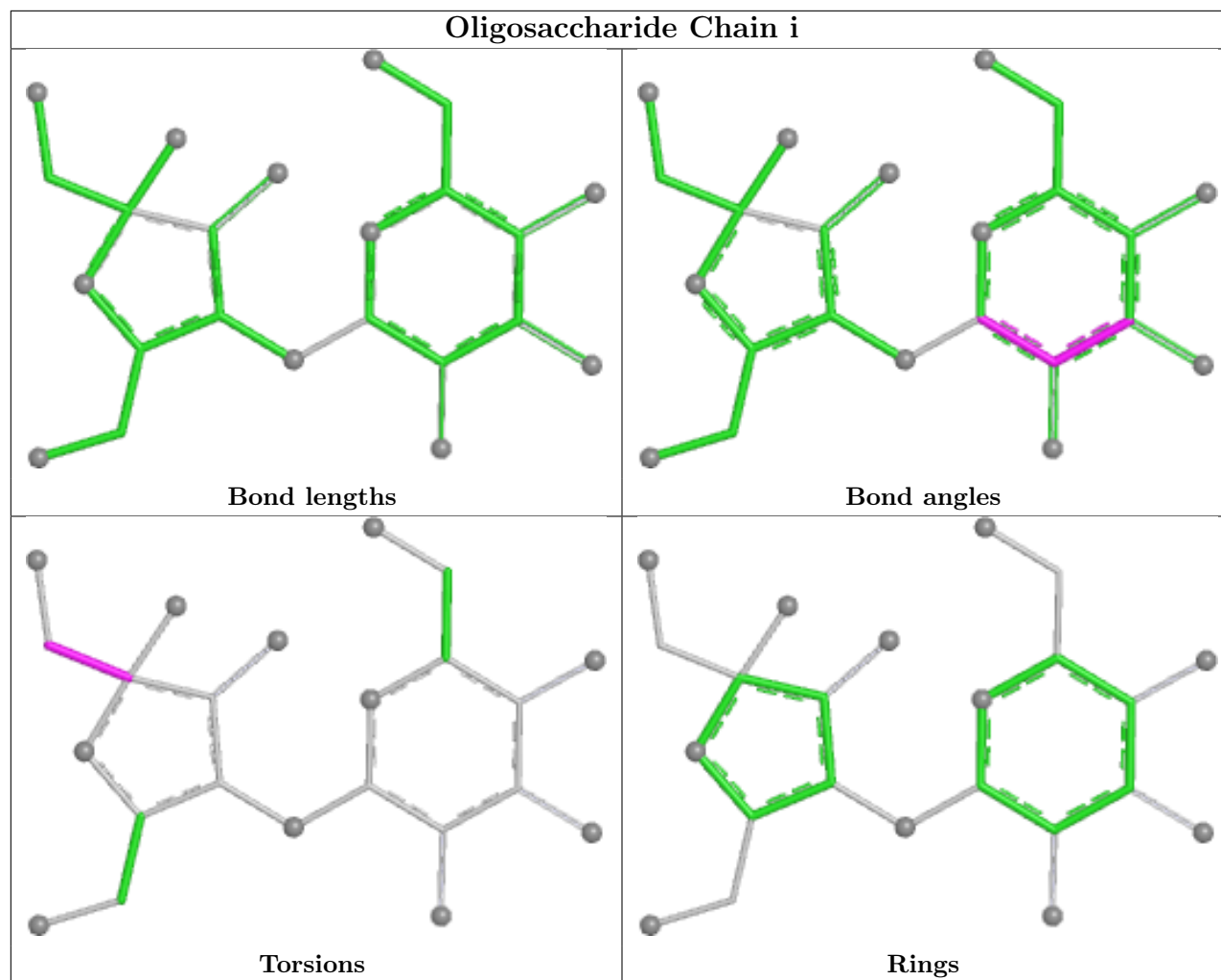


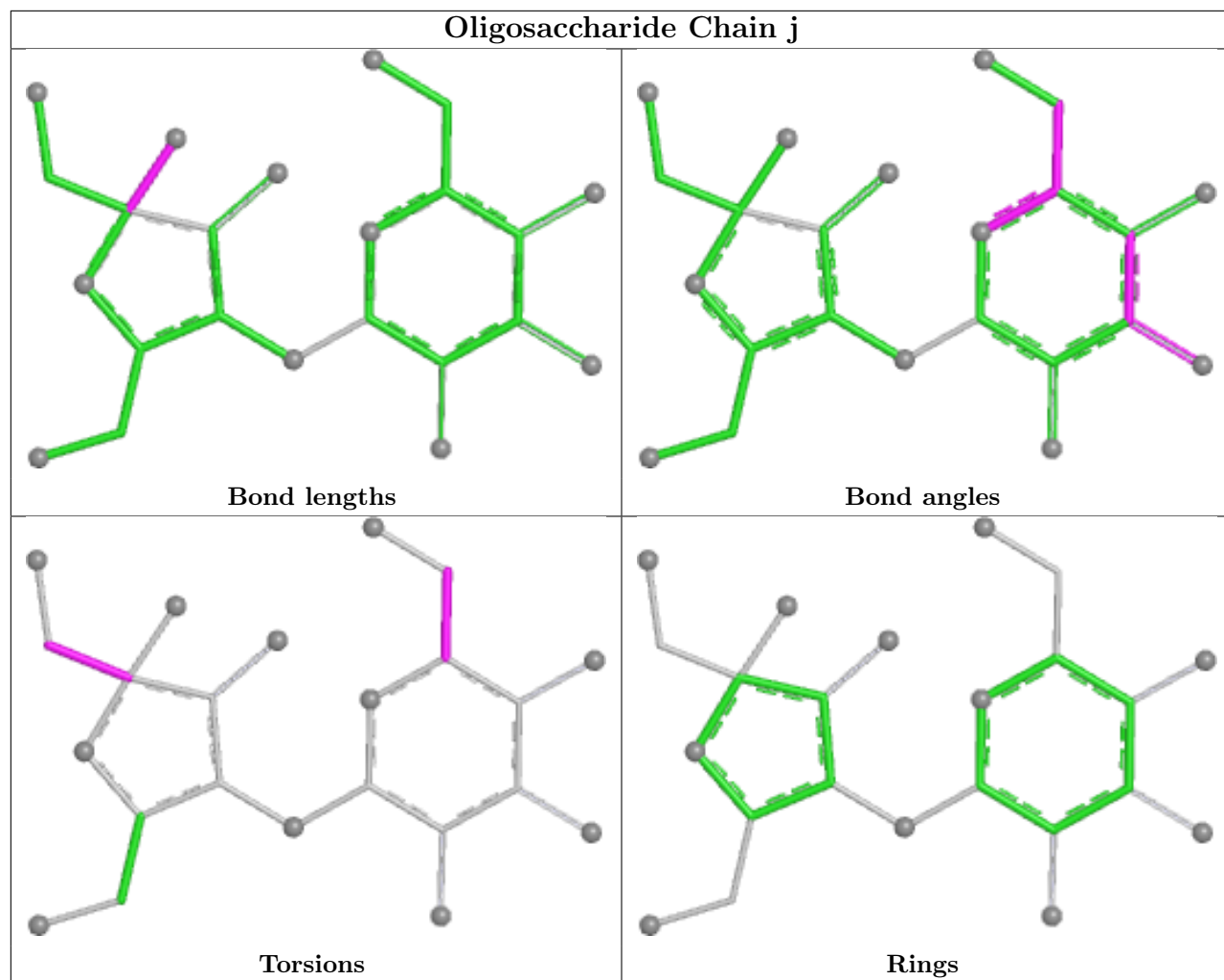


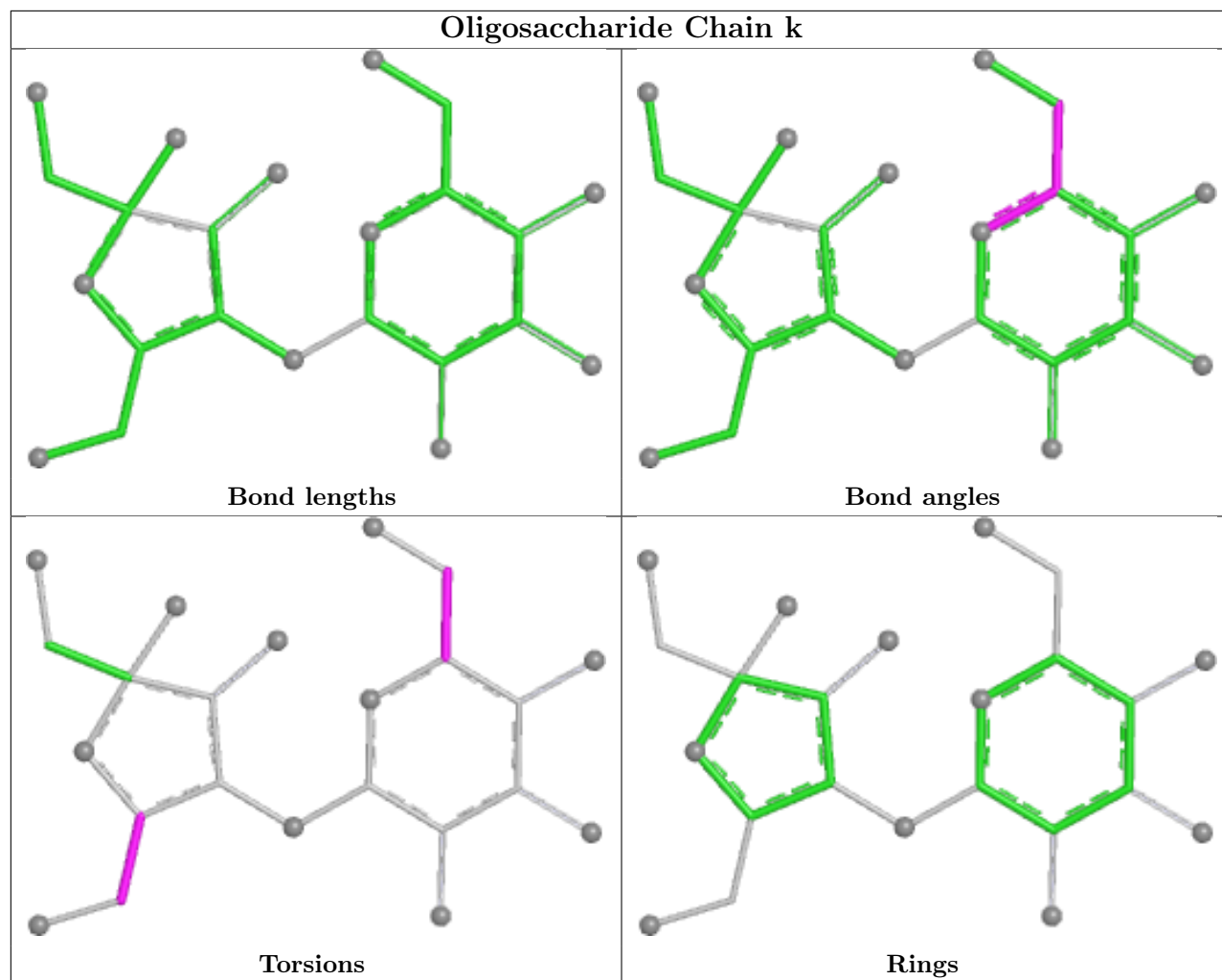


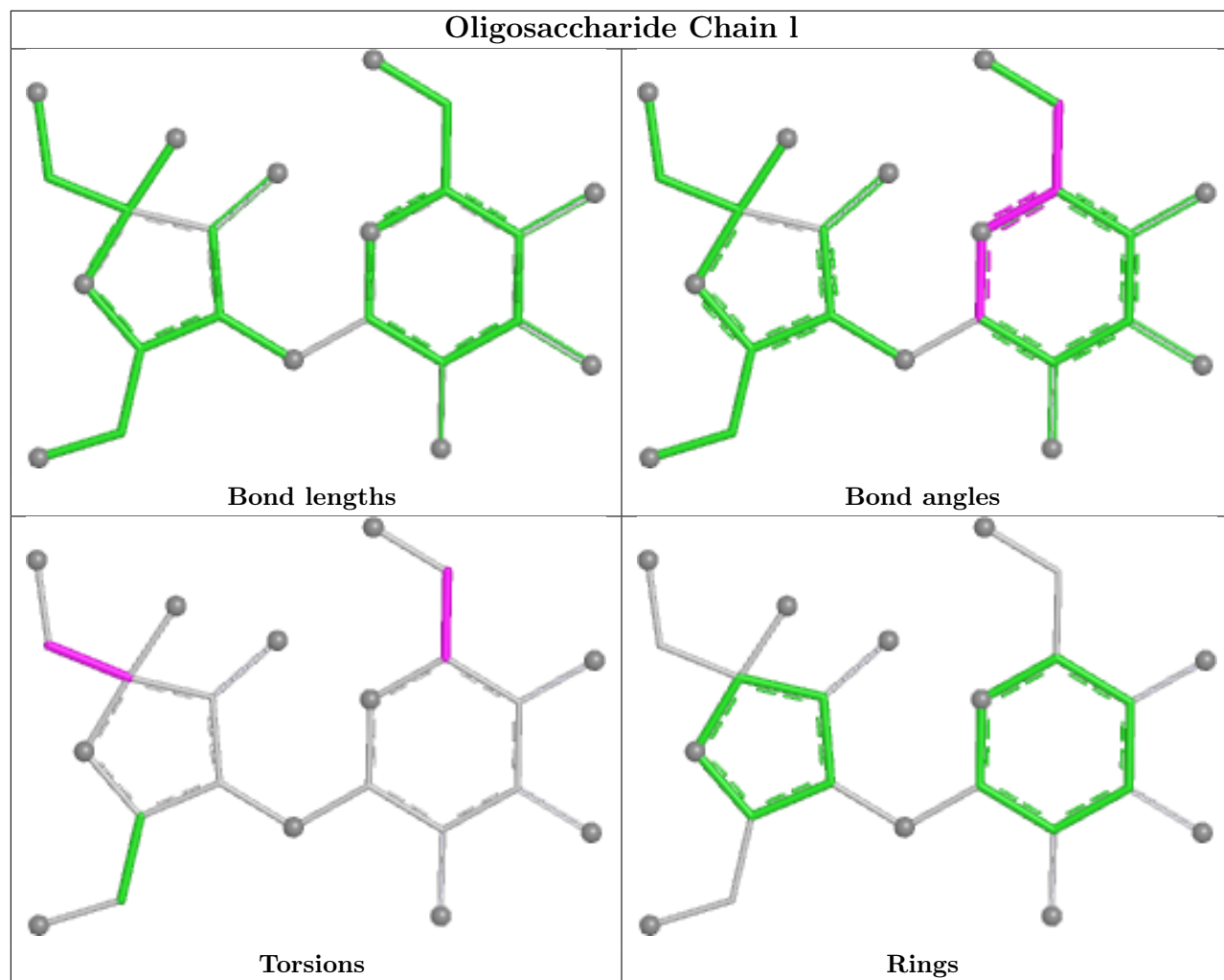


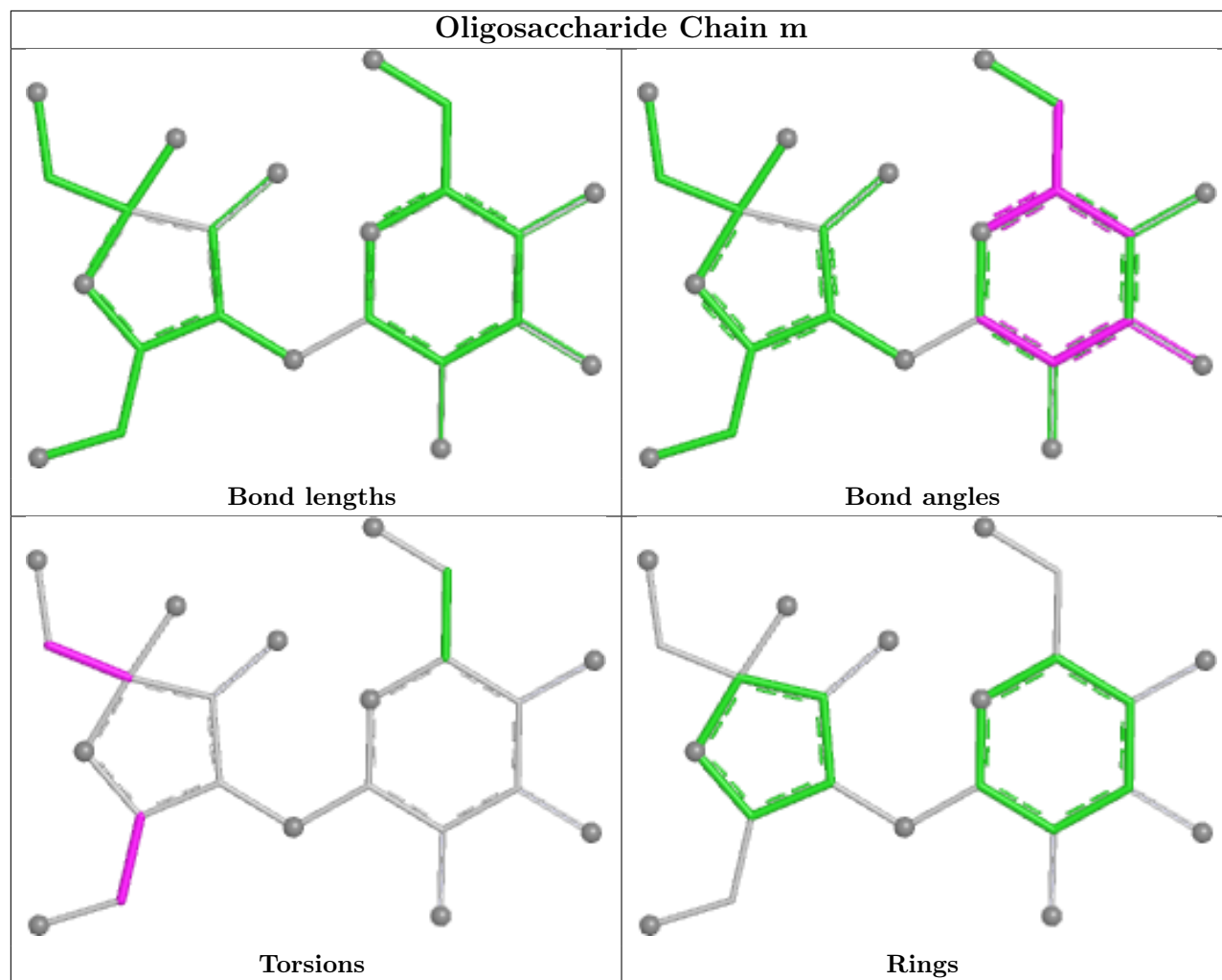


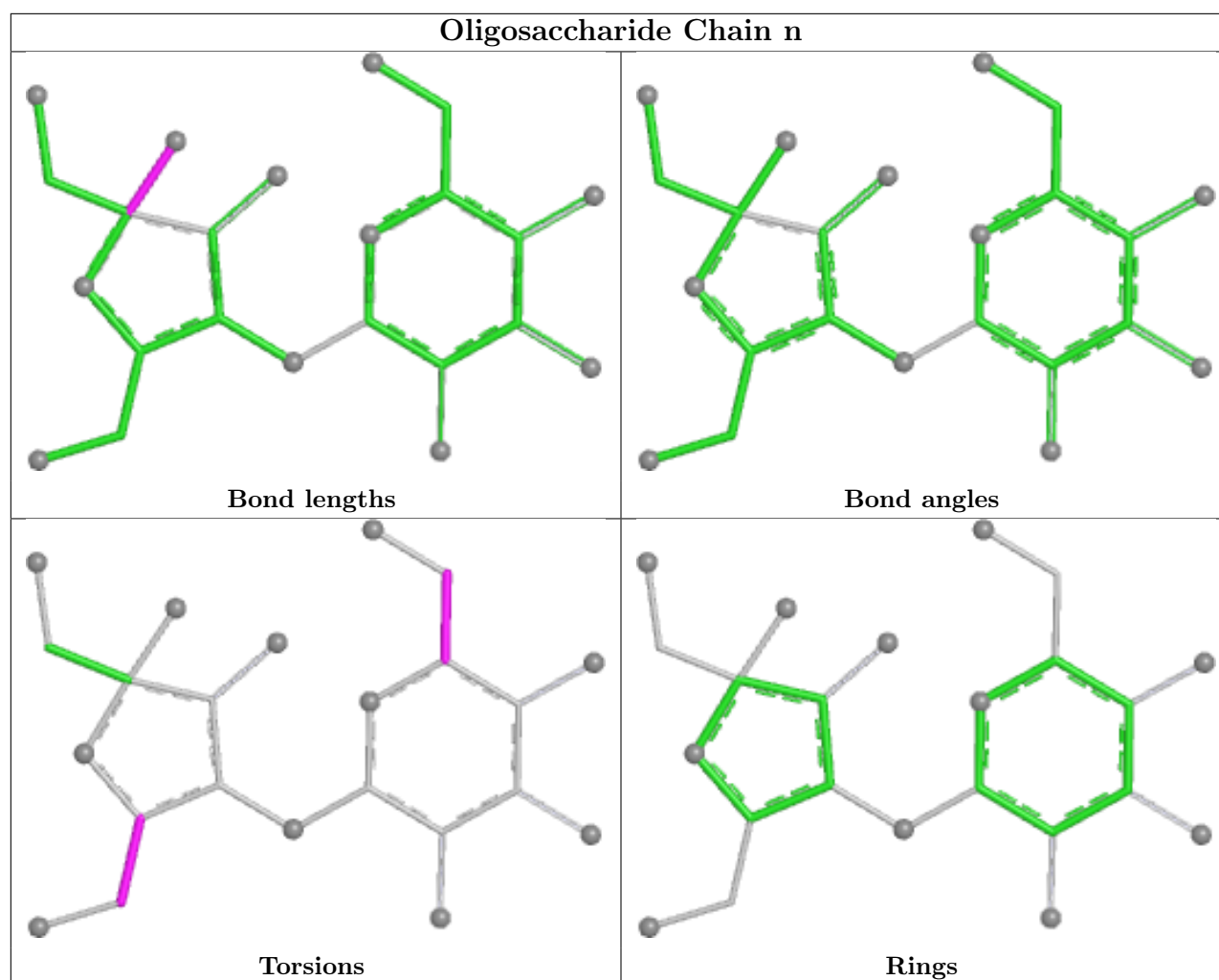


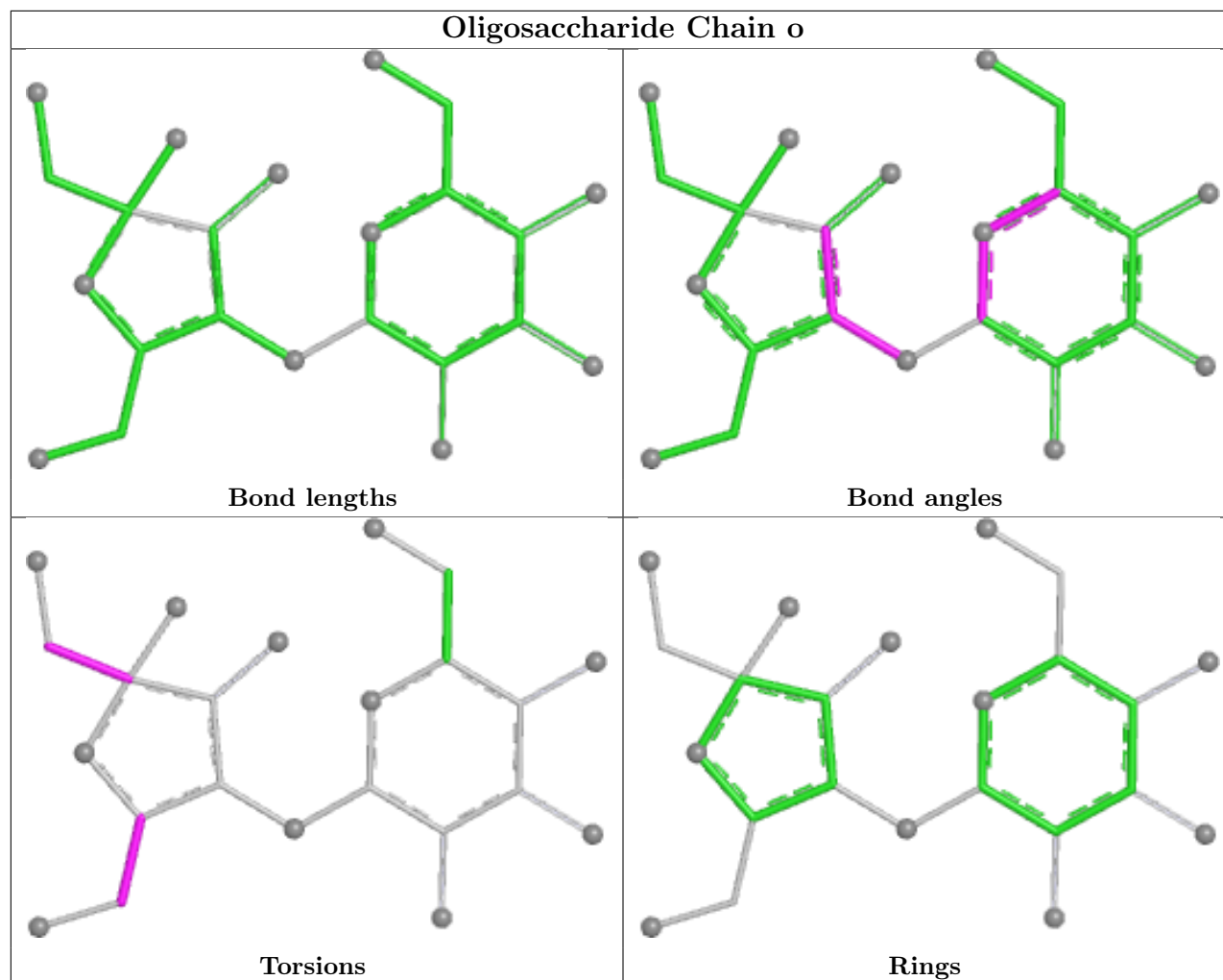


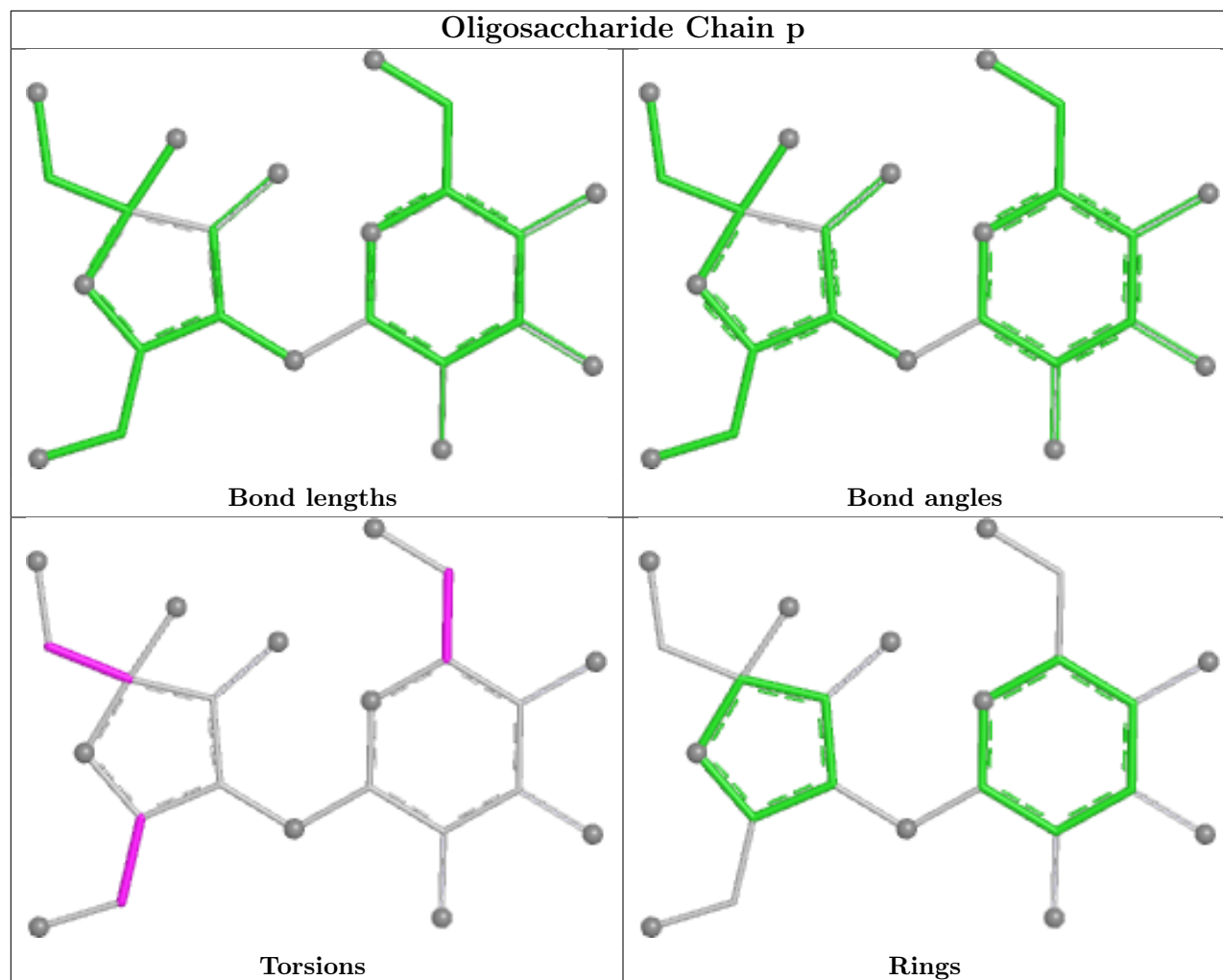


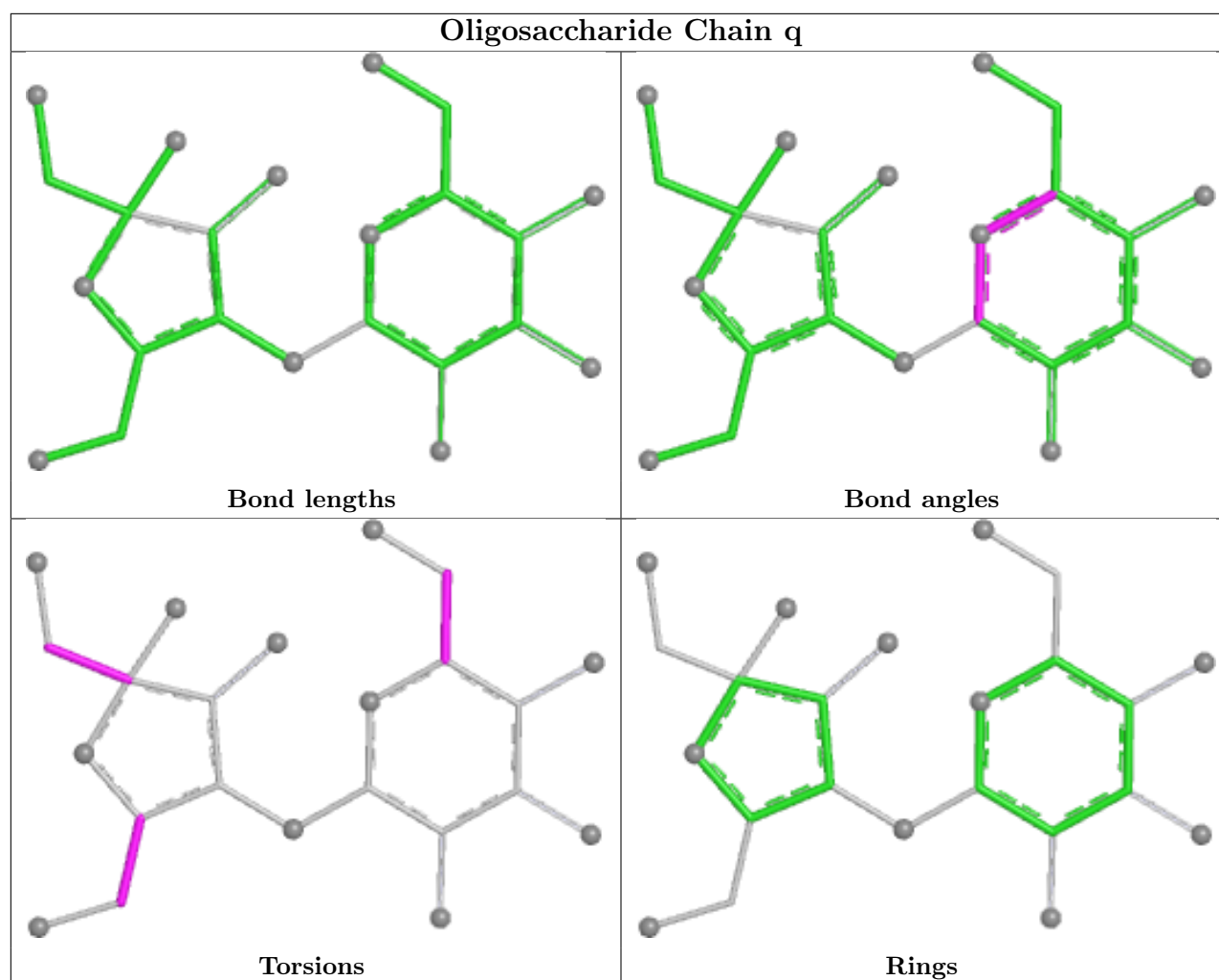


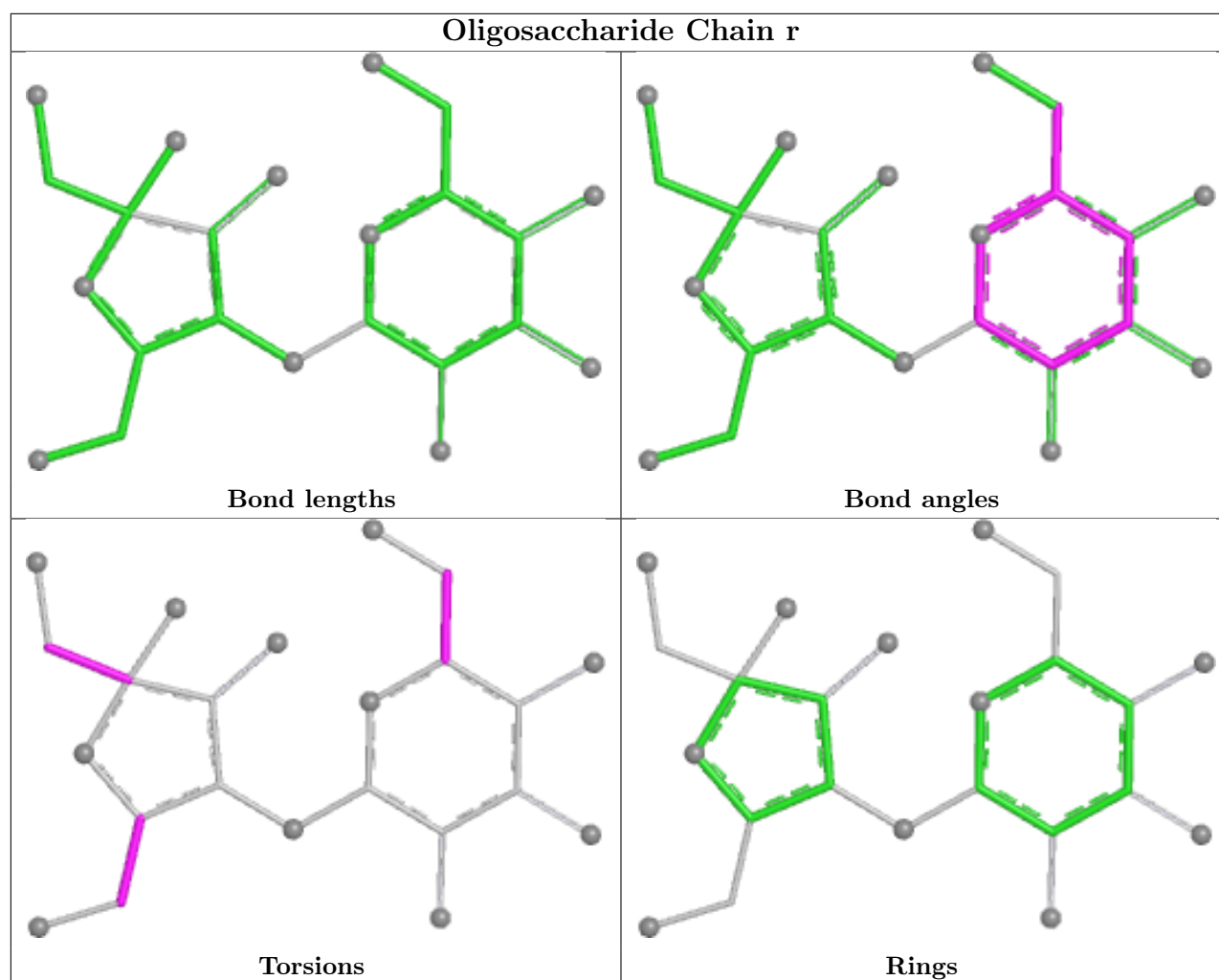












5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 58 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	431/432 (99%)	0.60	38 (8%) 17 15	42, 73, 121, 211	0
1	B	431/432 (99%)	0.52	28 (6%) 26 22	44, 73, 111, 196	0
1	C	431/432 (99%)	0.50	30 (6%) 24 20	47, 75, 114, 165	0
1	D	431/432 (99%)	0.49	36 (8%) 18 16	43, 77, 119, 218	0
1	E	431/432 (99%)	0.47	29 (6%) 25 21	45, 73, 123, 193	0
1	F	431/432 (99%)	0.88	55 (12%) 9 7	46, 74, 137, 209	0
1	G	431/432 (99%)	0.85	63 (14%) 7 6	43, 77, 138, 211	0
All	All	3017/3024 (99%)	0.62	279 (9%) 16 14	42, 75, 124, 218	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	389	THR	6.3
1	B	126	ASP	6.2
1	F	141	ASP	6.1
1	A	134	TYR	6.0
1	G	326	VAL	5.9
1	C	126	ASP	5.8
1	F	128	THR	5.7
1	B	141	ASP	5.6
1	F	142	GLN	5.6
1	A	142	GLN	5.5
1	F	170	GLU	5.2
1	G	328	SER	5.2
1	G	125	SER	5.1
1	A	126	ASP	5.0
1	E	128	THR	4.9
1	D	226	ASP	4.9
1	A	329	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	G	327	SER	4.7
1	G	324	VAL	4.7
1	D	126	ASP	4.7
1	F	123	GLU	4.7
1	A	334	VAL	4.7
1	B	139	LEU	4.6
1	F	334	VAL	4.6
1	D	337	ALA	4.6
1	F	126	ASP	4.5
1	B	335	ILE	4.5
1	A	133	VAL	4.5
1	F	127	GLY	4.5
1	G	330	ILE	4.5
1	G	329	THR	4.4
1	G	339	ALA	4.4
1	C	211	GLU	4.4
1	E	339	ALA	4.3
1	D	249	LYS	4.3
1	C	335	ILE	4.2
1	A	130	ASP	4.2
1	E	136	CYS	4.2
1	C	128	THR	4.2
1	F	388	THR	4.2
1	G	127	GLY	4.2
1	G	337	ALA	4.2
1	G	123	GLU	4.1
1	G	335	ILE	4.1
1	B	127	GLY	4.1
1	G	334	VAL	4.1
1	G	342	SER	4.0
1	F	335	ILE	4.0
1	E	334	VAL	4.0
1	D	334	VAL	4.0
1	F	314	PHE	4.0
1	E	335	ILE	4.0
1	F	134	TYR	4.0
1	C	127	GLY	4.0
1	A	128	THR	3.9
1	F	124	GLY	3.9
1	D	336	PHE	3.8
1	A	141	ASP	3.8
1	F	336	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	3.8
1	B	226	ASP	3.8
1	G	336	PHE	3.7
1	A	67	GLY	3.7
1	G	343	VAL	3.7
1	G	224	CYS	3.6
1	F	340	THR	3.6
1	B	142	GLN	3.6
1	C	339	ALA	3.6
1	D	125	SER	3.6
1	C	222	TYR	3.6
1	D	335	ILE	3.5
1	G	141	ASP	3.5
1	E	329	THR	3.5
1	F	337	ALA	3.5
1	B	128	THR	3.5
1	F	122	ILE	3.5
1	D	213	SER	3.4
1	C	333	GLY	3.4
1	G	323	ALA	3.4
1	A	228	ARG	3.3
1	G	333	GLY	3.3
1	G	347	ALA	3.3
1	B	329	THR	3.3
1	E	389	THR	3.3
1	G	133	VAL	3.3
1	F	133	VAL	3.3
1	A	74	MET	3.3
1	F	186	ASN	3.3
1	B	134	TYR	3.3
1	C	347	ALA	3.3
1	F	125	SER	3.2
1	F	181	TYR	3.2
1	E	142	GLN	3.2
1	B	228	ARG	3.2
1	G	340	THR	3.2
1	A	139	LEU	3.2
1	E	127	GLY	3.2
1	B	123	GLU	3.2
1	B	136	CYS	3.2
1	F	355	ASN	3.1
1	F	329	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	74	MET	3.1
1	A	214	ASP	3.1
1	C	331	GLU	3.1
1	G	237	ALA	3.1
1	B	133	VAL	3.1
1	G	128	THR	3.1
1	F	211	GLU	3.1
1	F	260	ASP	3.1
1	D	327	SER	3.0
1	F	110	GLU	3.0
1	E	126	ASP	3.0
1	A	115	ALA	3.0
1	B	140	ASP	3.0
1	B	336	PHE	3.0
1	C	224	CYS	3.0
1	D	388	THR	3.0
1	F	320	ALA	3.0
1	D	136	CYS	2.9
1	F	173	ASP	2.9
1	G	136	CYS	2.9
1	F	339	ALA	2.9
1	C	74	MET	2.9
1	D	133	VAL	2.9
1	A	129	GLY	2.9
1	B	334	VAL	2.9
1	F	338	LYS	2.8
1	A	326	VAL	2.8
1	G	134	TYR	2.8
1	C	338	LYS	2.8
1	B	213	SER	2.8
1	B	314	PHE	2.8
1	F	129	GLY	2.8
1	C	334	VAL	2.8
1	G	115	ALA	2.8
1	F	327	SER	2.8
1	A	425	ASP	2.8
1	B	143	TYR	2.8
1	B	224	CYS	2.8
1	F	330	ILE	2.8
1	G	142	GLN	2.7
1	C	125	SER	2.7
1	D	224	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	74	MET	2.7
1	D	345	VAL	2.7
1	F	332	LYS	2.7
1	C	336	PHE	2.7
1	F	139	LEU	2.7
1	G	260	ASP	2.7
1	E	51	ASP	2.7
1	C	340	THR	2.7
1	F	333	GLY	2.7
1	G	119	CYS	2.7
1	F	17	LYS	2.6
1	E	249	LYS	2.6
1	C	215	GLY	2.6
1	C	241	GLY	2.6
1	E	328	SER	2.6
1	E	314	PHE	2.6
1	C	6	ASN	2.6
1	F	326	VAL	2.6
1	D	227	LEU	2.6
1	G	240	ASN	2.6
1	C	249	LYS	2.6
1	G	118	LYS	2.6
1	F	325	GLU	2.6
1	F	387	GLU	2.6
1	E	333	GLY	2.6
1	D	132	GLY	2.6
1	D	128	THR	2.6
1	G	322	VAL	2.6
1	B	211	GLU	2.5
1	E	123	GLU	2.5
1	G	332	LYS	2.5
1	D	228	ARG	2.5
1	G	387	GLU	2.5
1	E	145	TYR	2.5
1	F	323	ALA	2.5
1	F	328	SER	2.5
1	A	338	LYS	2.5
1	G	212	GLY	2.5
1	D	330	ILE	2.5
1	A	342	SER	2.5
1	C	225	ASP	2.5
1	A	123	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	331	GLU	2.5
1	A	389	THR	2.5
1	G	71	ALA	2.5
1	G	325	GLU	2.4
1	A	426	CYS	2.4
1	C	172	SER	2.4
1	G	20	GLN	2.4
1	G	126	ASP	2.4
1	G	431	ASP	2.4
1	F	225	ASP	2.4
1	A	136	CYS	2.4
1	F	119	CYS	2.4
1	E	134	TYR	2.4
1	G	42	SER	2.4
1	E	226	ASP	2.4
1	F	341	VAL	2.4
1	G	211	GLU	2.4
1	C	330	ILE	2.4
1	G	249	LYS	2.4
1	D	250	GLU	2.4
1	F	94	ARG	2.4
1	F	136	CYS	2.4
1	D	6	ASN	2.4
1	D	145	TYR	2.3
1	A	211	GLU	2.3
1	G	331	GLU	2.3
1	G	320	ALA	2.3
1	E	6	ASN	2.3
1	B	222	TYR	2.3
1	E	139	LEU	2.3
1	A	140	ASP	2.3
1	G	346	THR	2.3
1	F	28	GLN	2.3
1	D	123	GLU	2.3
1	C	337	ALA	2.3
1	D	66	ASP	2.3
1	A	6	ASN	2.3
1	C	355	ASN	2.3
1	A	81	TYR	2.3
1	G	205	GLY	2.3
1	E	71	ALA	2.3
1	D	339	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	139	LEU	2.3
1	B	237	ALA	2.2
1	G	213	SER	2.2
1	G	348	SER	2.2
1	C	346	THR	2.2
1	D	389	THR	2.2
1	A	138	ASN	2.2
1	D	200	VAL	2.2
1	E	337	ALA	2.2
1	B	135	ASP	2.2
1	E	431	ASP	2.2
1	G	25	VAL	2.2
1	C	139	LEU	2.2
1	A	135	ASP	2.2
1	B	214	ASP	2.2
1	A	70	ASN	2.2
1	E	347	ALA	2.2
1	G	247	LEU	2.2
1	F	390	GLU	2.2
1	D	8	LEU	2.2
1	A	431	ASP	2.2
1	C	341	VAL	2.2
1	B	230	GLN	2.1
1	G	36	TYR	2.1
1	F	206	MET	2.1
1	D	222	TYR	2.1
1	F	331	GLU	2.1
1	G	135	ASP	2.1
1	F	324	VAL	2.1
1	D	343	VAL	2.1
1	A	340	THR	2.1
1	B	326	VAL	2.1
1	D	341	VAL	2.1
1	E	141	ASP	2.1
1	A	137	GLN	2.1
1	G	105	GLU	2.1
1	D	74	MET	2.1
1	D	314	PHE	2.1
1	C	260	ASP	2.1
1	A	68	SER	2.1
1	F	36	TYR	2.1
1	G	170	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	271	CYS	2.1
1	D	207	CYS	2.1
1	D	127	GLY	2.1
1	G	226	ASP	2.0
1	G	290	THR	2.0
1	G	172	SER	2.0
1	E	332	LYS	2.0
1	E	93	GLY	2.0
1	A	38	CYS	2.0
1	G	207	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	F	1	8/9	0.79	0.18	65,67,70,72	0
1	PCA	A	1	8/9	0.81	0.19	83,87,93,93	0
1	PCA	E	1	8/9	0.83	0.23	86,95,99,101	0
1	PCA	C	1	8/9	0.90	0.21	76,88,94,96	0
1	PCA	G	1	8/9	0.90	0.18	74,76,80,81	0
1	PCA	B	1	8/9	0.91	0.17	68,77,80,82	0
1	PCA	D	1	8/9	0.92	0.15	76,82,87,88	0

6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

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
3	CA	F	511	1/1	0.85	0.12	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	D	513	1/1	0.89	0.08	93,93,93,93	0
3	CA	F	513	1/1	0.91	0.06	93,93,93,93	0
3	CA	A	1013	1/1	0.91	0.11	96,96,96,96	0
3	CA	C	1013	1/1	0.92	0.09	94,94,94,94	0
3	CA	B	510	1/1	0.93	0.07	85,85,85,85	0
4	MG	G	512	1/1	0.93	0.07	108,108,108,108	0
3	CA	B	514	1/1	0.94	0.06	88,88,88,88	0
4	MG	A	1011	1/1	0.94	0.07	72,72,72,72	0
3	CA	E	514	1/1	0.94	0.06	88,88,88,88	0
3	CA	C	1008	1/1	0.95	0.09	69,69,69,69	0
3	CA	B	509	1/1	0.95	0.07	96,96,96,96	0
3	CA	E	510	1/1	0.95	0.06	95,95,95,95	0
3	CA	E	511	1/1	0.95	0.09	123,123,123,123	0
4	MG	E	513	1/1	0.95	0.06	109,109,109,109	0
3	CA	C	1007	1/1	0.96	0.06	64,64,64,64	0
3	CA	G	506	1/1	0.96	0.07	116,116,116,116	0
3	CA	G	508	1/1	0.96	0.07	84,84,84,84	0
4	MG	B	511	1/1	0.96	0.05	84,84,84,84	0
4	MG	F	510	1/1	0.96	0.06	68,68,68,68	0
3	CA	G	509	1/1	0.96	0.10	66,66,66,66	0
3	CA	G	513	1/1	0.97	0.06	87,87,87,87	0
3	CA	D	505	1/1	0.97	0.08	68,68,68,68	0
3	CA	D	508	1/1	0.97	0.06	80,80,80,80	0
3	CA	D	509	1/1	0.97	0.06	97,97,97,97	0
3	CA	F	505	1/1	0.97	0.05	61,61,61,61	0
3	CA	F	506	1/1	0.97	0.08	92,92,92,92	0
4	MG	C	1011	1/1	0.97	0.04	86,86,86,86	0
3	CA	B	505	1/1	0.97	0.06	64,64,64,64	0
3	CA	B	506	1/1	0.97	0.06	75,75,75,75	0
3	CA	A	1007	1/1	0.97	0.06	67,67,67,67	0
3	CA	C	1010	1/1	0.97	0.05	91,91,91,91	0
4	MG	D	510	1/1	0.97	0.06	85,85,85,85	0
3	CA	D	503	1/1	0.98	0.04	73,73,73,73	0
3	CA	C	1014	1/1	0.98	0.07	60,60,60,60	0
3	CA	C	1006	1/1	0.98	0.08	65,65,65,65	0
3	CA	G	507	1/1	0.98	0.05	72,72,72,72	0
3	CA	A	1005	1/1	0.98	0.04	70,70,70,70	0
4	MG	A	1010	1/1	0.98	0.05	59,59,59,59	0
3	CA	A	1008	1/1	0.98	0.07	66,66,66,66	0
3	CA	G	510	1/1	0.98	0.05	83,83,83,83	0
4	MG	C	1012	1/1	0.98	0.04	67,67,67,67	0
3	CA	C	1009	1/1	0.98	0.04	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	E	509	1/1	0.98	0.04	65,65,65,65	0
4	MG	B	512	1/1	0.98	0.04	70,70,70,70	0
4	MG	F	509	1/1	0.98	0.04	53,53,53,53	0
3	CA	A	1009	1/1	0.98	0.06	68,68,68,68	0
3	CA	A	1006	1/1	0.98	0.05	92,92,92,92	0
3	CA	B	508	1/1	0.98	0.08	79,79,79,79	0
4	MG	D	511	1/1	0.98	0.03	83,83,83,83	0
3	CA	E	515	1/1	0.99	0.08	37,37,37,37	1
3	CA	F	507	1/1	0.99	0.04	76,76,76,76	0
3	CA	D	504	1/1	0.99	0.04	84,84,84,84	0
3	CA	F	508	1/1	0.99	0.06	70,70,70,70	0
4	MG	E	512	1/1	0.99	0.03	54,54,54,54	0
3	CA	E	507	1/1	0.99	0.04	60,60,60,60	0
4	MG	G	511	1/1	0.99	0.05	74,74,74,74	0
3	CA	E	508	1/1	0.99	0.04	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.