



Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 05:28 PM EDT

PDB ID : 8TRZ
EMDB ID : EMD-41586
Title : Cryo-EM structure of N-glycosylated Pomacea canaliculata hemocyanin
Authors : Brola, T.R.; Chiumiento, I.R.; Gragera, M.; Carazo, J.M.; Heras, H.; Dreon, M.S.; Otero, L.H.
Deposited on : 2023-08-10
Resolution : 4.40 Å(reported)
Based on initial model : .

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

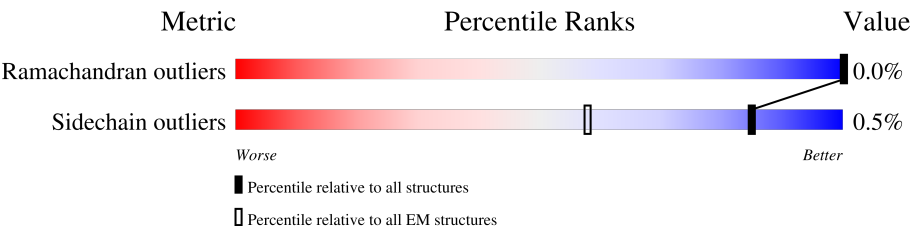
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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.



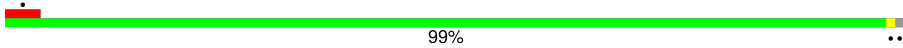
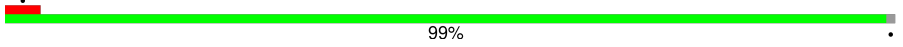
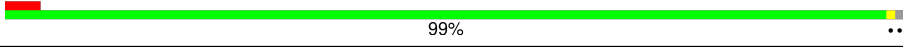
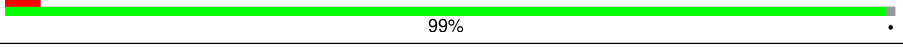
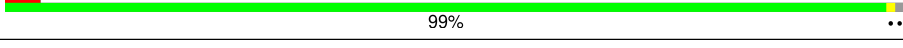
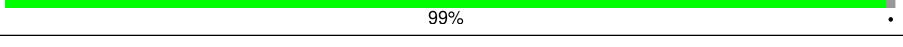
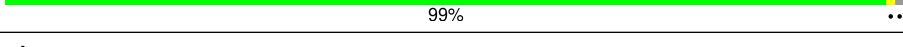
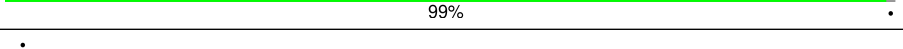
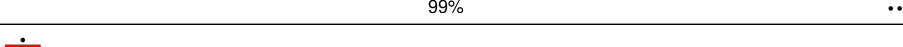
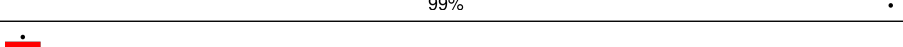
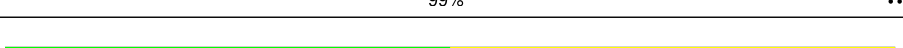

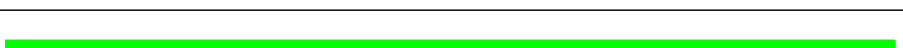

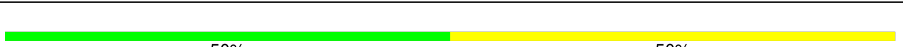
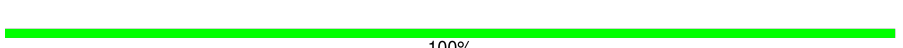





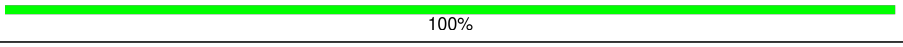

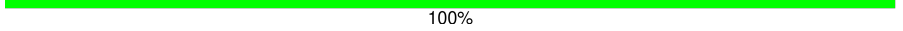

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3408	 99% .
1	B	3408	 99% ..
1	C	3408	 99% .
1	D	3408	 99% ..
1	E	3408	 99% .
1	F	3408	 99% .
1	G	3408	 99% .
1	H	3408	 99% ..
1	I	3408	 99% .

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Mol	Chain	Length	Quality of chain
1	J	3408	 99% ..
1	K	3408	 99% .
1	L	3408	 99% ..
1	M	3408	 99% .
1	N	3408	 99% ..
1	O	3408	 99% .
1	P	3408	 99% ..
1	Q	3408	 99% .
1	R	3408	 99% ..
1	S	3408	 99% .
1	T	3408	 99% ..
2	0	2	 50% 50%
2	0A	2	 100%
2	2	2	 100%
2	5A	2	 50% 50%
2	7	2	 50% 50%
2	8	2	 100%
2	AA	2	 100%
2	CA	2	 50% 50%
2	HA	2	 50% 50%
2	IA	2	 100%
2	KA	2	 50% 50%
2	MA	2	 100%
2	RA	2	 50% 50%
2	SA	2	 100%

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Mol	Chain	Length	Quality of chain
2	U	2	100%
2	UA	2	100%
2	W	2	100%
2	WA	2	50% 50%
2	Y	2	100%
2	bA	2	50% 50%
2	cA	2	100%
2	d	2	100%
2	e	2	100%
2	eA	2	100%
2	g	2	100%
2	gA	2	100%
2	i	2	50% 50%
2	lA	2	50% 50%
2	mA	2	100%
2	n	2	50% 50%
2	o	2	100%
2	oA	2	100%
2	q	2	100%
2	qA	2	100%
2	s	2	100%
2	vA	2	50% 50%
2	wA	2	100%
2	x	2	50% 50%
2	y	2	100%



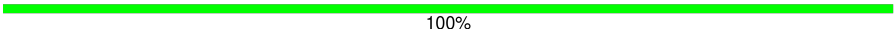
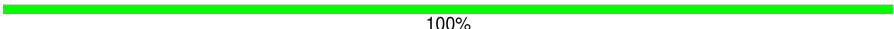
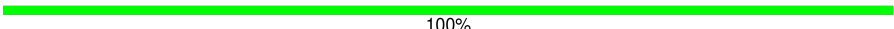
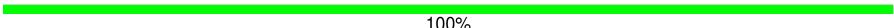

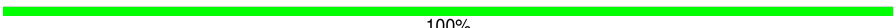

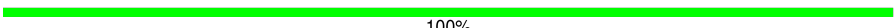
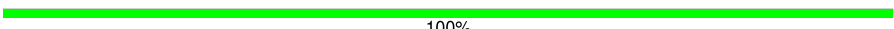
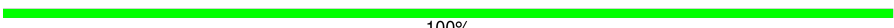

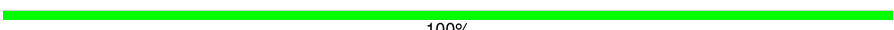
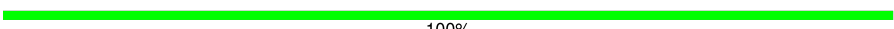
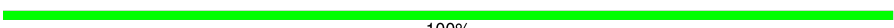
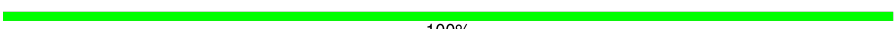
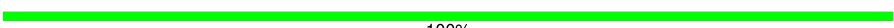
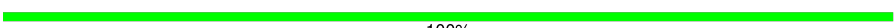
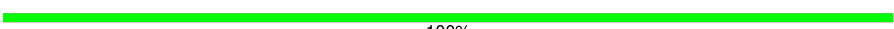


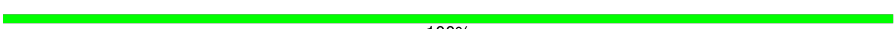


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Mol	Chain	Length	Quality of chain
2	yA	2	100%
3	1	3	67% 33%
3	1A	3	67% 33%
3	2A	3	100%
3	3	3	67% 33%
3	3A	3	100%
3	4	3	100%
3	4A	3	33% 67%
3	5	3	100%
3	6	3	67% 33%
3	9	3	67% 33%
3	BA	3	67% 33%
3	DA	3	67% 33%
3	EA	3	100%
3	FA	3	100%
3	GA	3	67% 33%
3	JA	3	100%
3	LA	3	100%
3	NA	3	67% 33%
3	OA	3	100%
3	PA	3	100%
3	QA	3	67% 33%
3	TA	3	100%
3	V	3	100%
3	VA	3	67% 33%

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Mol	Chain	Length	Quality of chain
3	X	3	 67% 33%
3	XA	3	 67% 33%
3	YA	3	 100%
3	Z	3	 100%
3	ZA	3	 100%
3	a	3	 100%
3	aA	3	 67% 33%
3	b	3	 100%
3	c	3	 67% 33%
3	dA	3	 100%
3	f	3	 100%
3	fA	3	 100%
3	h	3	 67% 33%
3	hA	3	 100%
3	iA	3	 100%
3	j	3	 100%
3	jA	3	 100%
3	k	3	 100%
3	kA	3	 100%
3	l	3	 100%
3	m	3	 67% 33%
3	nA	3	 100%
3	p	3	 100%
3	pA	3	 67% 33%
3	r	3	 67% 33%

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Mol	Chain	Length	Quality of chain
3	rA	3	 100%
3	sA	3	 100%
3	t	3	 100%
3	tA	3	 100%
3	u	3	 100%
3	uA	3	 67% 33%
3	v	3	 100%
3	w	3	 67% 33%
3	xA	3	 100%
3	z	3	 100%
3	zA	3	 33% 67% 33%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 549912 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Hemocyanin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	B	3388	Total	C	N	O	S	0	0
			27308	17387	4689	5141	91		
1	C	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	D	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	E	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	F	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	G	3387	Total	C	N	O	S	0	0
			27307	17393	4686	5137	91		
1	H	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	I	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	J	3388	Total	C	N	O	S	0	0
			27309	17388	4689	5141	91		
1	K	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	L	3388	Total	C	N	O	S	0	0
			27308	17387	4689	5141	91		
1	M	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	N	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	O	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	P	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	Q	3387	Total	C	N	O	S	0	0
			27307	17393	4686	5137	91		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	3388	Total	C	N	O	S	0	0
			27310	17389	4689	5141	91		
1	S	3387	Total	C	N	O	S	0	0
			27308	17393	4686	5138	91		
1	T	3388	Total	C	N	O	S	0	0
			27309	17388	4689	5141	91		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	W	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	e	2	Total	C	N	O	0	0
			28	16	2	10		
2	g	2	Total	C	N	O	0	0
			28	16	2	10		
2	i	2	Total	C	N	O	0	0
			28	16	2	10		
2	n	2	Total	C	N	O	0	0
			28	16	2	10		
2	o	2	Total	C	N	O	0	0
			28	16	2	10		
2	q	2	Total	C	N	O	0	0
			28	16	2	10		
2	s	2	Total	C	N	O	0	0
			28	16	2	10		
2	x	2	Total	C	N	O	0	0
			28	16	2	10		
2	y	2	Total	C	N	O	0	0
			28	16	2	10		
2	0	2	Total	C	N	O	0	0
			28	16	2	10		

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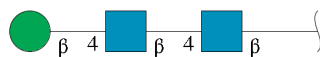
Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	2	Total	C	N	O	0	0
			28	16	2	10		
2	7	2	Total	C	N	O	0	0
			28	16	2	10		
2	8	2	Total	C	N	O	0	0
			28	16	2	10		
2	AA	2	Total	C	N	O	0	0
			28	16	2	10		
2	CA	2	Total	C	N	O	0	0
			28	16	2	10		
2	HA	2	Total	C	N	O	0	0
			28	16	2	10		
2	IA	2	Total	C	N	O	0	0
			28	16	2	10		
2	KA	2	Total	C	N	O	0	0
			28	16	2	10		
2	MA	2	Total	C	N	O	0	0
			28	16	2	10		
2	RA	2	Total	C	N	O	0	0
			28	16	2	10		
2	SA	2	Total	C	N	O	0	0
			28	16	2	10		
2	UA	2	Total	C	N	O	0	0
			28	16	2	10		
2	WA	2	Total	C	N	O	0	0
			28	16	2	10		
2	bA	2	Total	C	N	O	0	0
			28	16	2	10		
2	cA	2	Total	C	N	O	0	0
			28	16	2	10		
2	eA	2	Total	C	N	O	0	0
			28	16	2	10		
2	gA	2	Total	C	N	O	0	0
			28	16	2	10		
2	lA	2	Total	C	N	O	0	0
			28	16	2	10		
2	mA	2	Total	C	N	O	0	0
			28	16	2	10		
2	oA	2	Total	C	N	O	0	0
			28	16	2	10		
2	qA	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	vA	2	Total	C	N	O	0	0
			28	16	2	10		
2	wA	2	Total	C	N	O	0	0
			28	16	2	10		
2	yA	2	Total	C	N	O	0	0
			28	16	2	10		
2	0A	2	Total	C	N	O	0	0
			28	16	2	10		
2	5A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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				AltConf	Trace
3	V	3	Total	C	N	O	0	0
			39	22	2	15		
3	X	3	Total	C	N	O	0	0
			39	22	2	15		
3	Z	3	Total	C	N	O	0	0
			39	22	2	15		
3	a	3	Total	C	N	O	0	0
			39	22	2	15		
3	b	3	Total	C	N	O	0	0
			39	22	2	15		
3	c	3	Total	C	N	O	0	0
			39	22	2	15		
3	f	3	Total	C	N	O	0	0
			39	22	2	15		
3	h	3	Total	C	N	O	0	0
			39	22	2	15		
3	j	3	Total	C	N	O	0	0
			39	22	2	15		
3	k	3	Total	C	N	O	0	0
			39	22	2	15		
3	l	3	Total	C	N	O	0	0
			39	22	2	15		
3	m	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	p	3	Total	C	N	O	0	0
			39	22	2	15		
3	r	3	Total	C	N	O	0	0
			39	22	2	15		
3	t	3	Total	C	N	O	0	0
			39	22	2	15		
3	u	3	Total	C	N	O	0	0
			39	22	2	15		
3	v	3	Total	C	N	O	0	0
			39	22	2	15		
3	w	3	Total	C	N	O	0	0
			39	22	2	15		
3	z	3	Total	C	N	O	0	0
			39	22	2	15		
3	1	3	Total	C	N	O	0	0
			39	22	2	15		
3	3	3	Total	C	N	O	0	0
			39	22	2	15		
3	4	3	Total	C	N	O	0	0
			39	22	2	15		
3	5	3	Total	C	N	O	0	0
			39	22	2	15		
3	6	3	Total	C	N	O	0	0
			39	22	2	15		
3	9	3	Total	C	N	O	0	0
			39	22	2	15		
3	BA	3	Total	C	N	O	0	0
			39	22	2	15		
3	DA	3	Total	C	N	O	0	0
			39	22	2	15		
3	EA	3	Total	C	N	O	0	0
			39	22	2	15		
3	FA	3	Total	C	N	O	0	0
			39	22	2	15		
3	GA	3	Total	C	N	O	0	0
			39	22	2	15		
3	JA	3	Total	C	N	O	0	0
			39	22	2	15		
3	LA	3	Total	C	N	O	0	0
			39	22	2	15		
3	NA	3	Total	C	N	O	0	0
			39	22	2	15		

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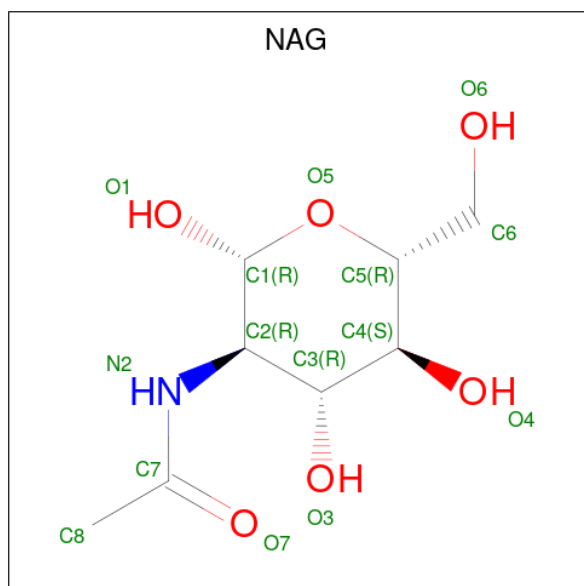
Mol	Chain	Residues	Atoms				AltConf	Trace
3	OA	3	Total	C	N	O	0	0
			39	22	2	15		
3	PA	3	Total	C	N	O	0	0
			39	22	2	15		
3	QA	3	Total	C	N	O	0	0
			39	22	2	15		
3	TA	3	Total	C	N	O	0	0
			39	22	2	15		
3	VA	3	Total	C	N	O	0	0
			39	22	2	15		
3	XA	3	Total	C	N	O	0	0
			39	22	2	15		
3	YA	3	Total	C	N	O	0	0
			39	22	2	15		
3	ZA	3	Total	C	N	O	0	0
			39	22	2	15		
3	aA	3	Total	C	N	O	0	0
			39	22	2	15		
3	dA	3	Total	C	N	O	0	0
			39	22	2	15		
3	fA	3	Total	C	N	O	0	0
			39	22	2	15		
3	hA	3	Total	C	N	O	0	0
			39	22	2	15		
3	iA	3	Total	C	N	O	0	0
			39	22	2	15		
3	jA	3	Total	C	N	O	0	0
			39	22	2	15		
3	kA	3	Total	C	N	O	0	0
			39	22	2	15		
3	nA	3	Total	C	N	O	0	0
			39	22	2	15		
3	pA	3	Total	C	N	O	0	0
			39	22	2	15		
3	rA	3	Total	C	N	O	0	0
			39	22	2	15		
3	sA	3	Total	C	N	O	0	0
			39	22	2	15		
3	tA	3	Total	C	N	O	0	0
			39	22	2	15		
3	uA	3	Total	C	N	O	0	0
			39	22	2	15		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	xA	3	Total	C	N	O	0	0
			39	22	2	15		
3	zA	3	Total	C	N	O	0	0
			39	22	2	15		
3	1A	3	Total	C	N	O	0	0
			39	22	2	15		
3	2A	3	Total	C	N	O	0	0
			39	22	2	15		
3	3A	3	Total	C	N	O	0	0
			39	22	2	15		
3	4A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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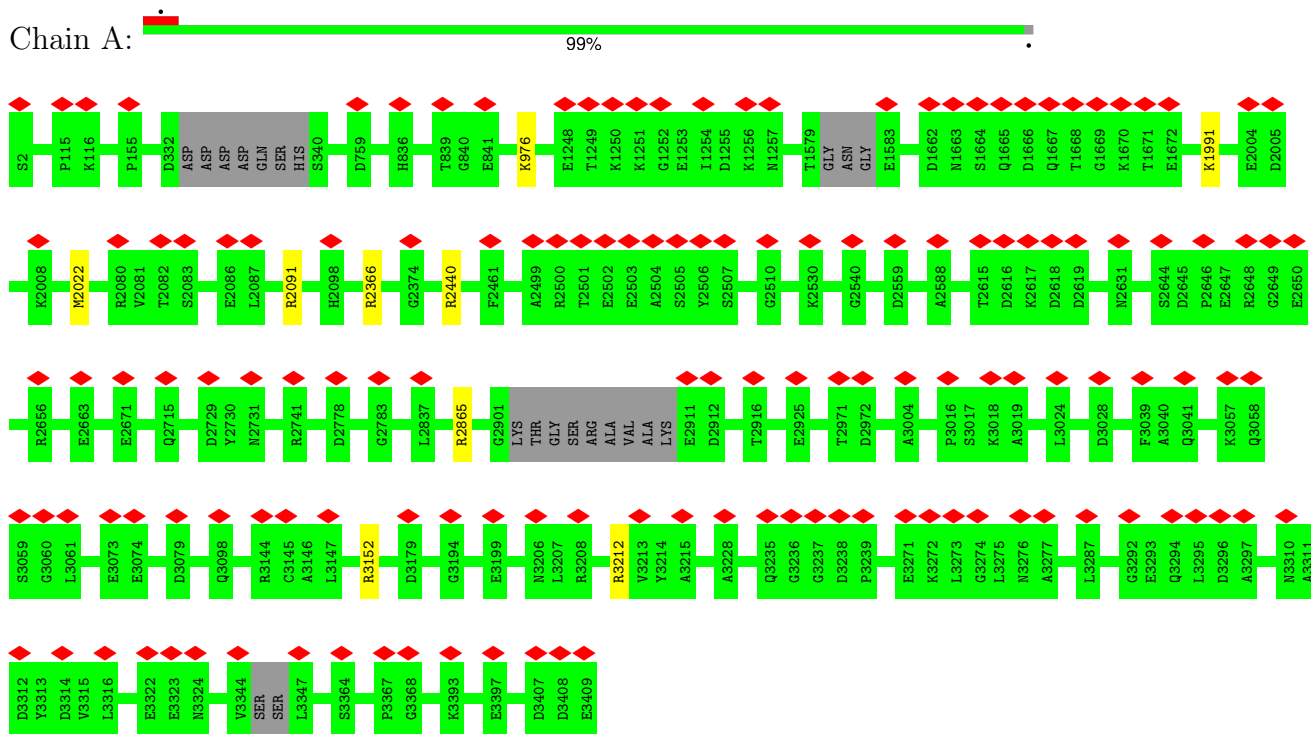
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Mol	Chain	Residues	Atoms				AltConf
4	F	1	Total 14	C 8	N 1	O 5	0
4	G	1	Total 14	C 8	N 1	O 5	0
4	H	1	Total 14	C 8	N 1	O 5	0
4	I	1	Total 14	C 8	N 1	O 5	0
4	J	1	Total 14	C 8	N 1	O 5	0
4	K	1	Total 14	C 8	N 1	O 5	0
4	L	1	Total 14	C 8	N 1	O 5	0
4	M	1	Total 14	C 8	N 1	O 5	0
4	N	1	Total 14	C 8	N 1	O 5	0
4	O	1	Total 14	C 8	N 1	O 5	0
4	P	1	Total 14	C 8	N 1	O 5	0
4	Q	1	Total 14	C 8	N 1	O 5	0
4	R	1	Total 14	C 8	N 1	O 5	0
4	S	1	Total 14	C 8	N 1	O 5	0
4	T	1	Total 14	C 8	N 1	O 5	0

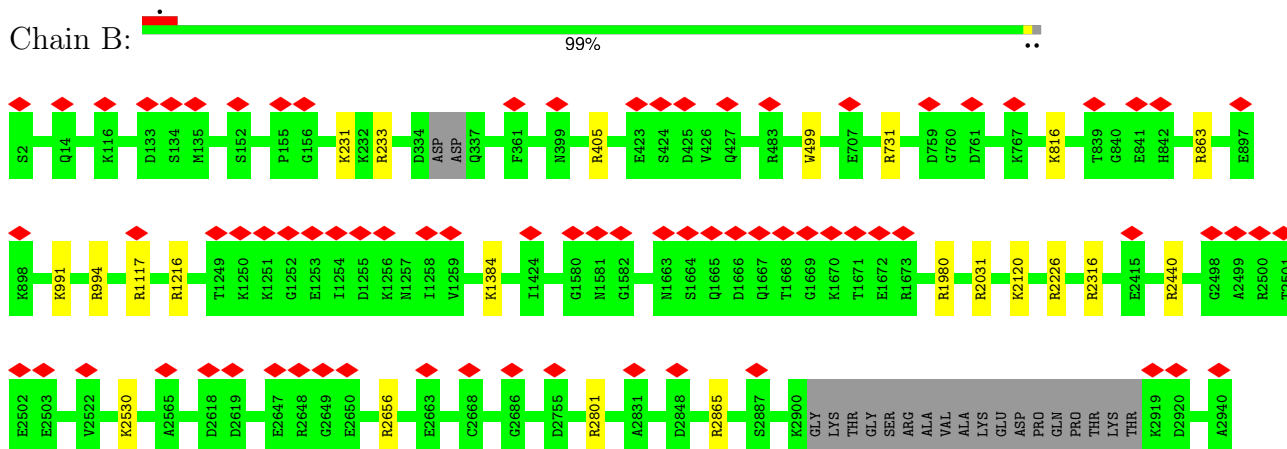
3 Residue-property plots

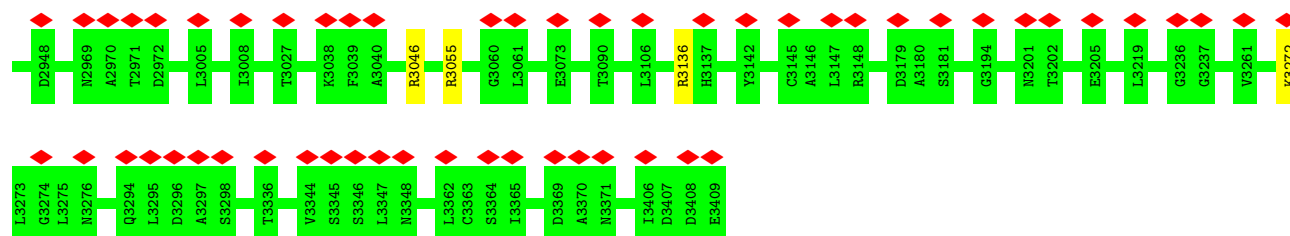
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Hemocyanin



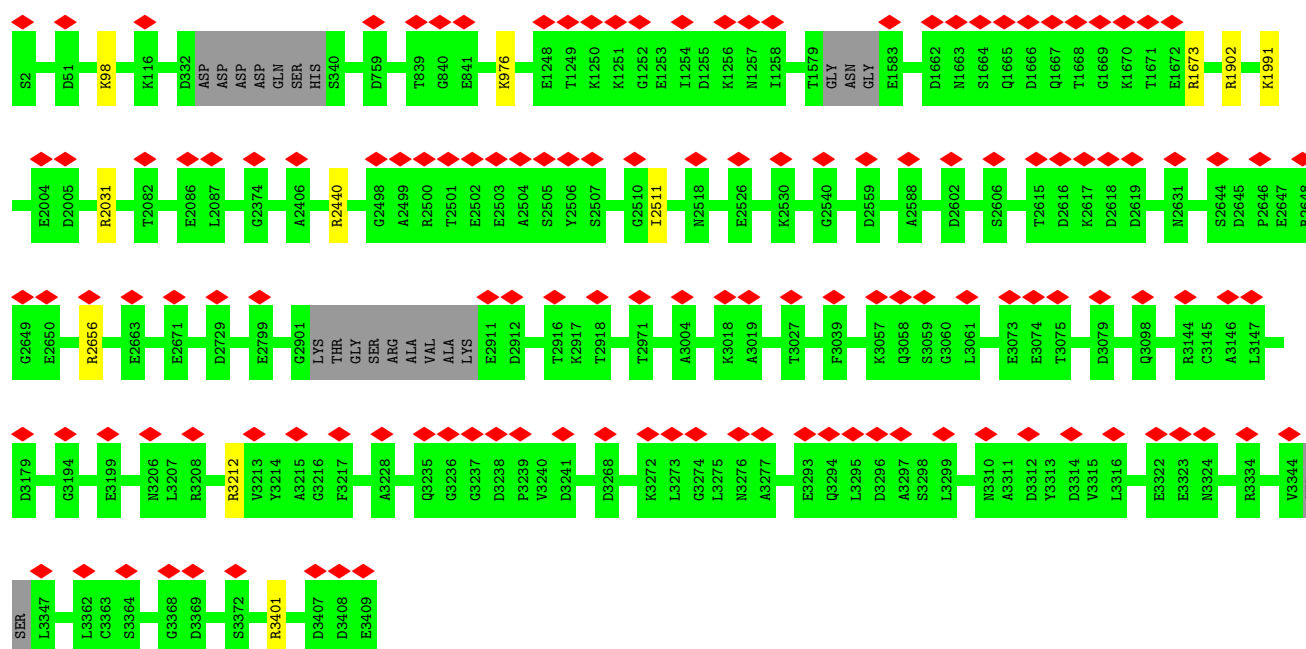
• Molecule 1: Hemocyanin





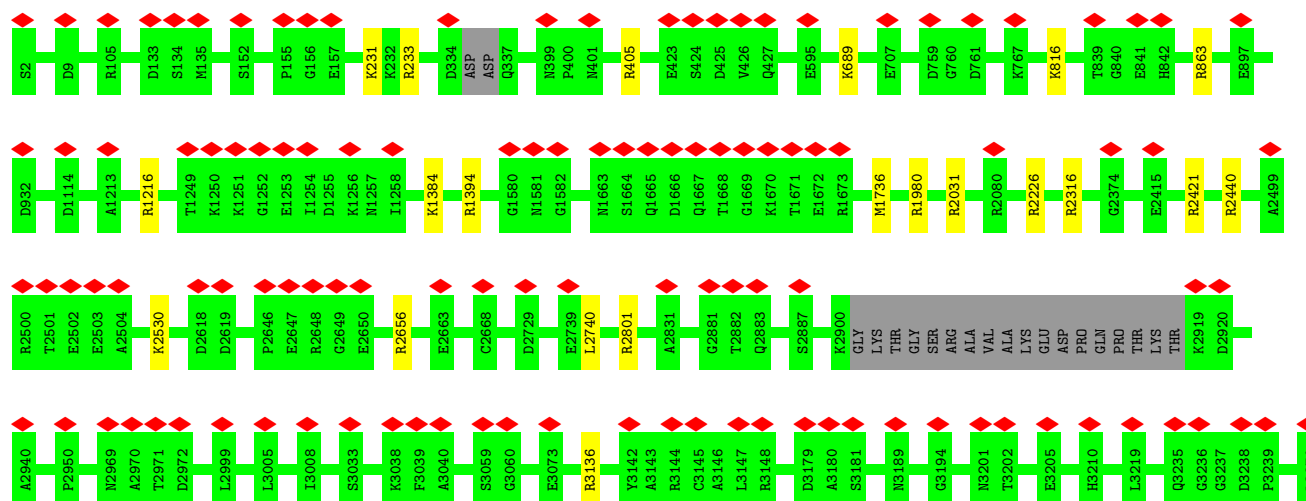
• Molecule 1: Hemocyanin

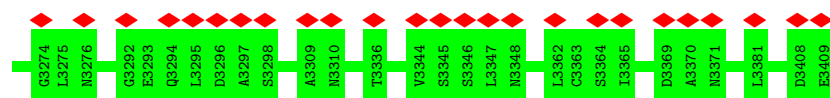
Chain C: 99%



• Molecule 1: Hemocyanin

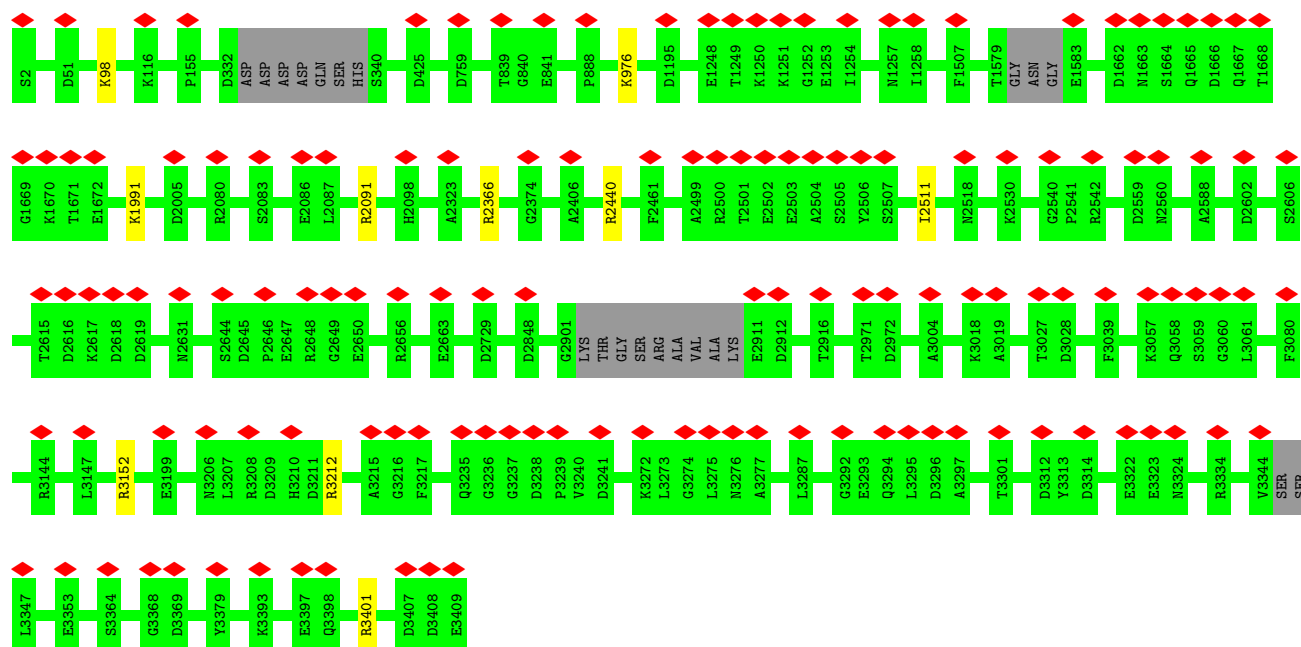
Chain D: 99%





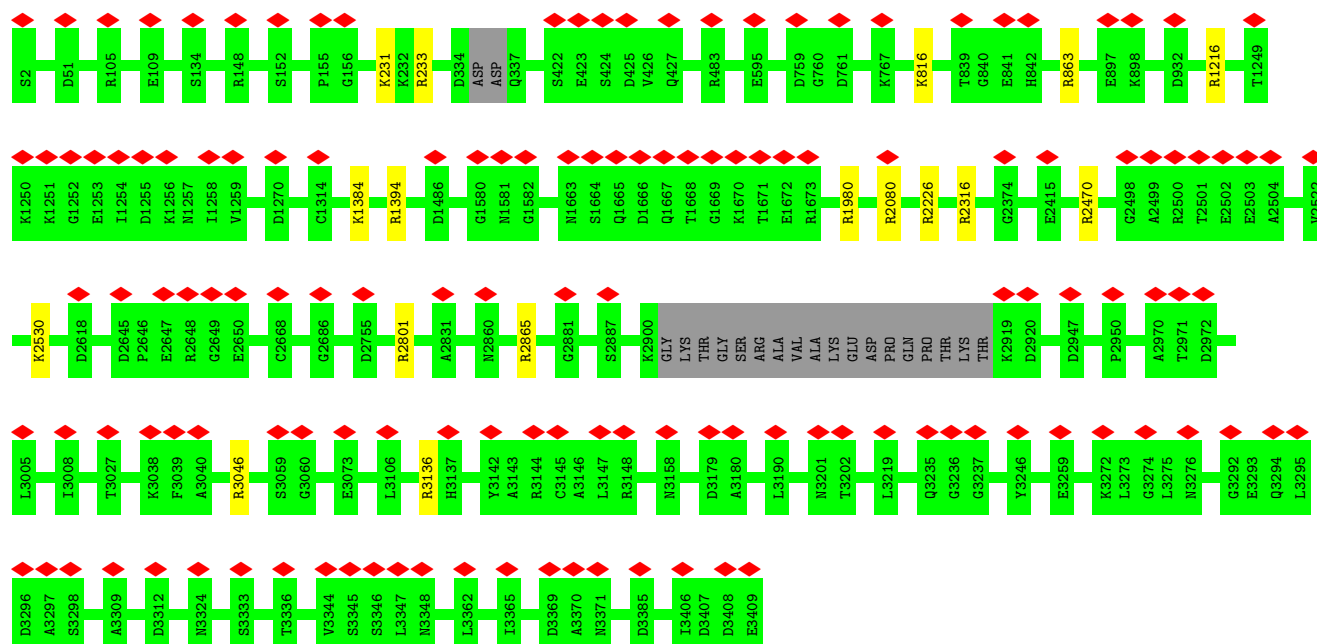
• Molecule 1: Hemocyanin

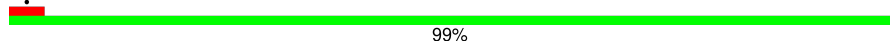
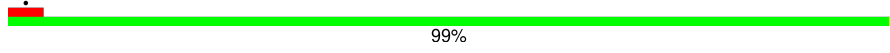
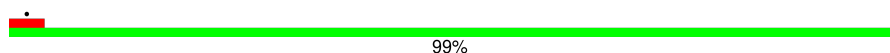
Chain E: 99%

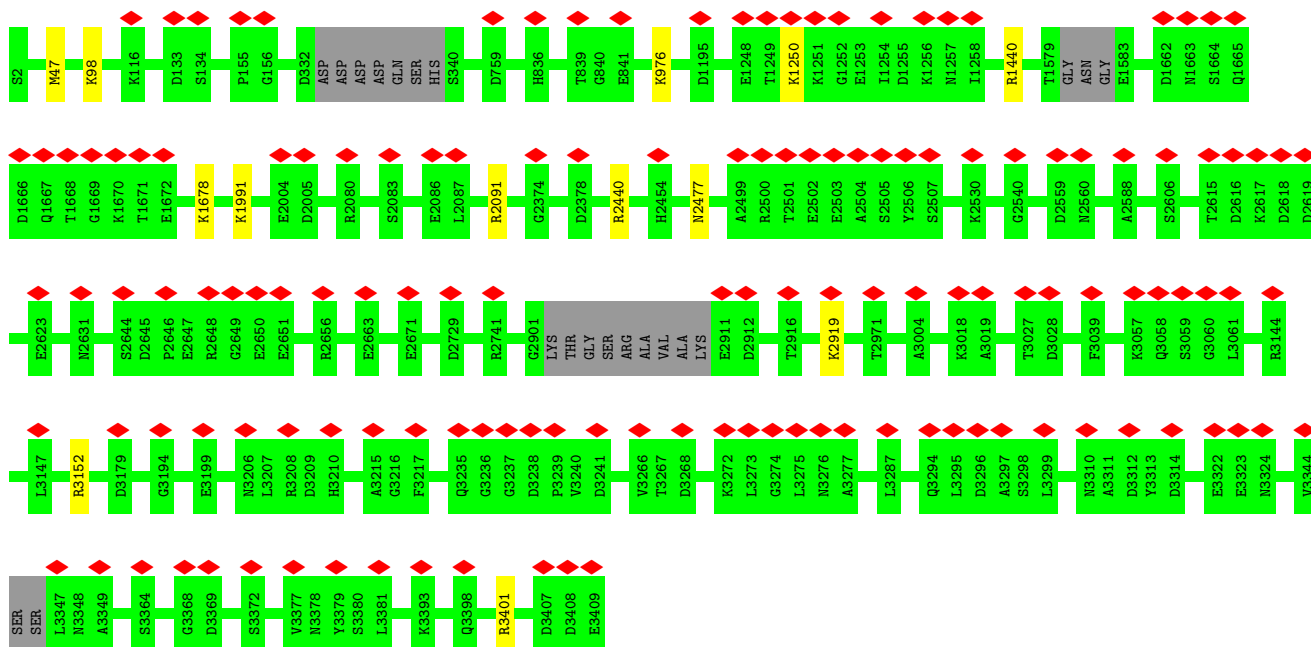


• Molecule 1: Hemocyanin

Chain F: 99%

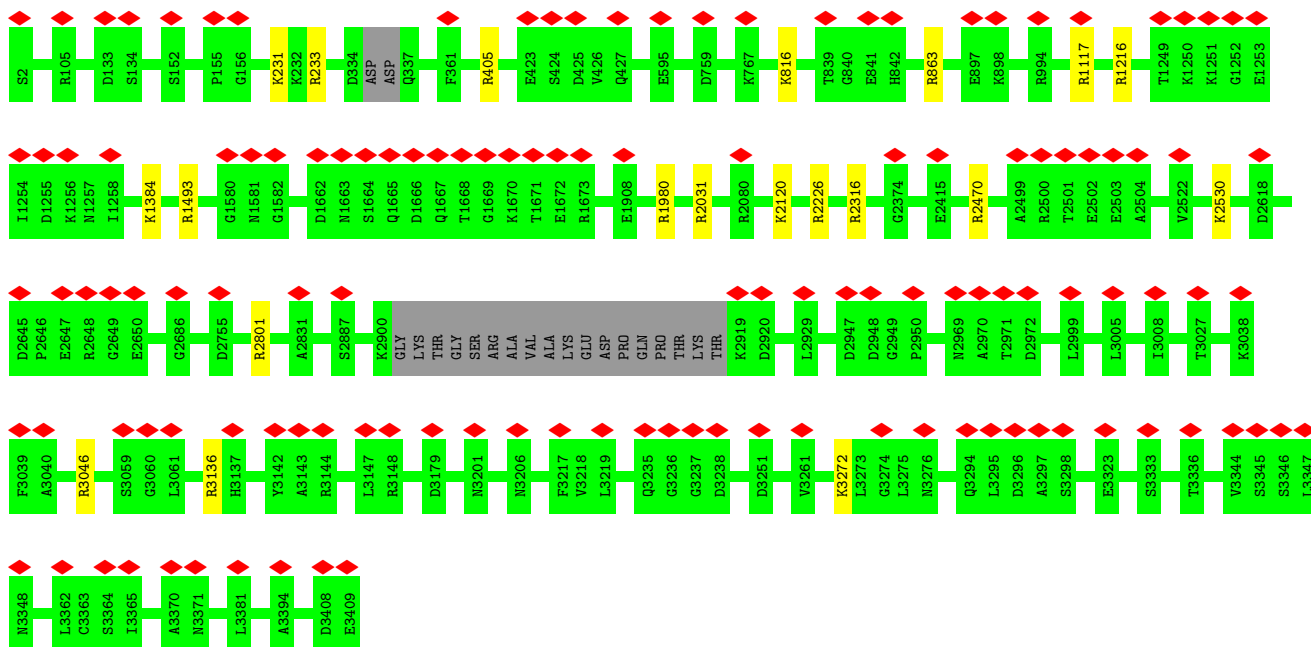






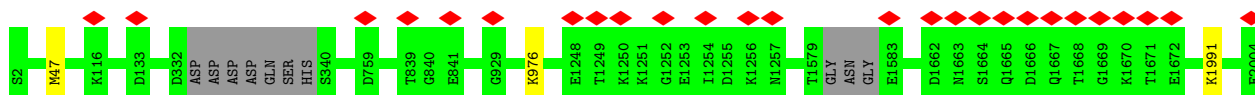
• Molecule 1: Hemocyanin

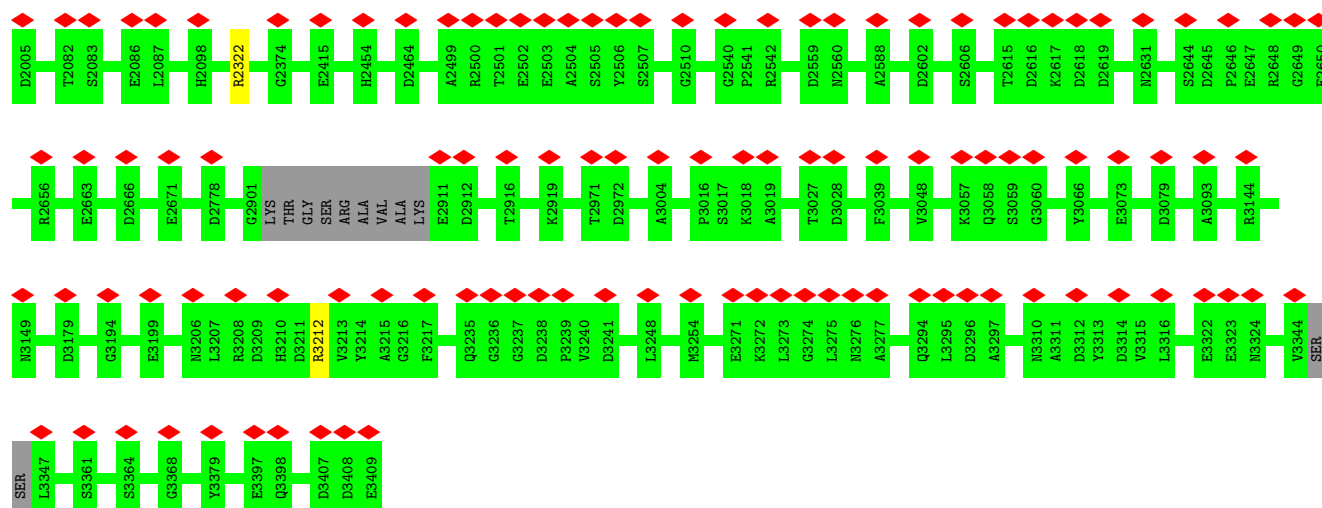
Chain J: 99%



• Molecule 1: Hemocyanin

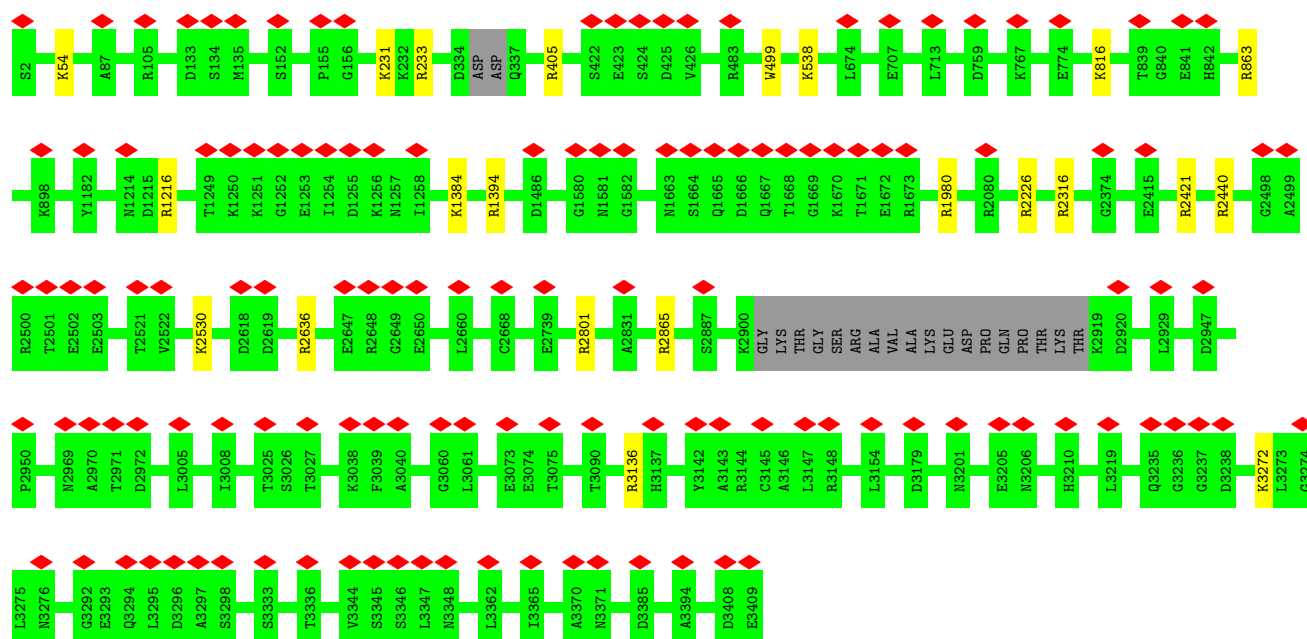
Chain K: 99%





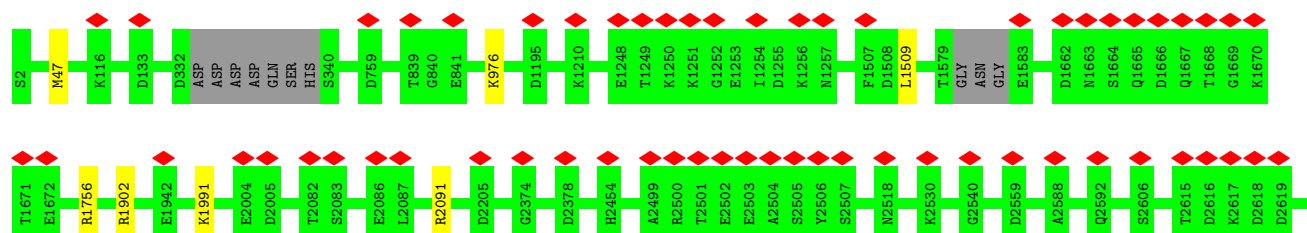
• Molecule 1: Hemocyanin

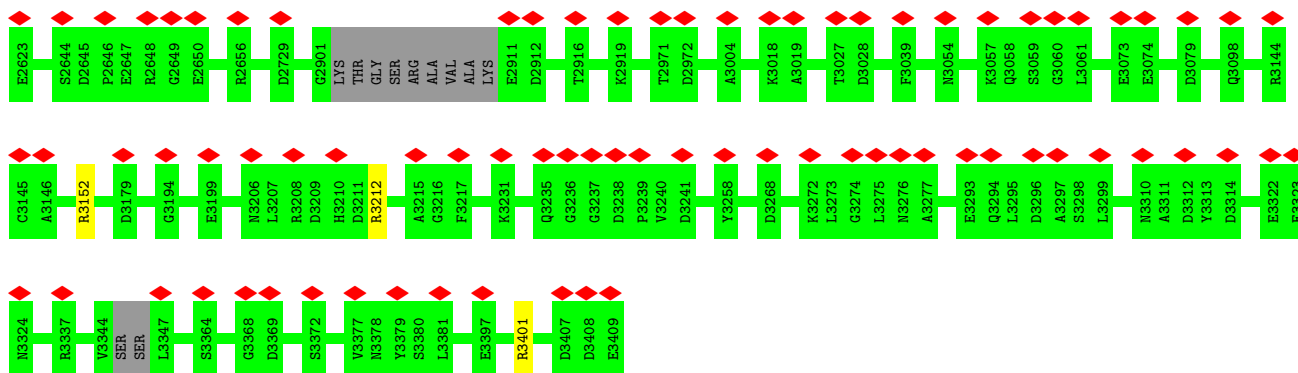
Chain L: 99%



• Molecule 1: Hemocyanin

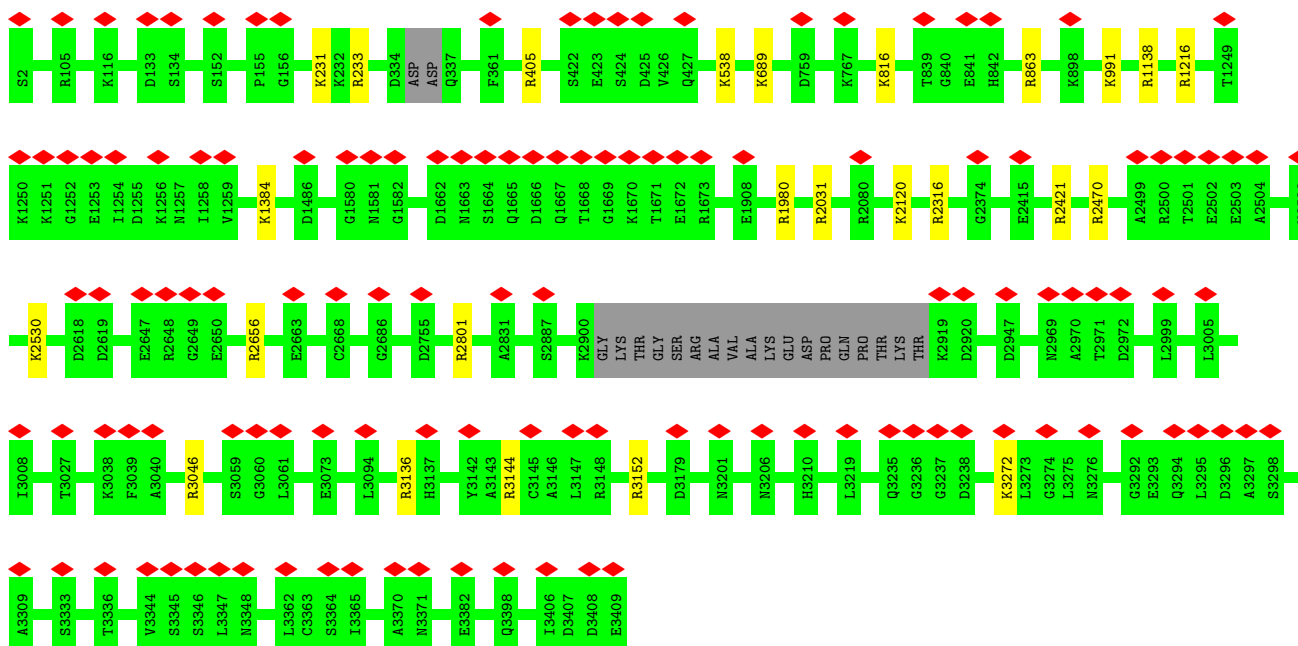
Chain M: 99%





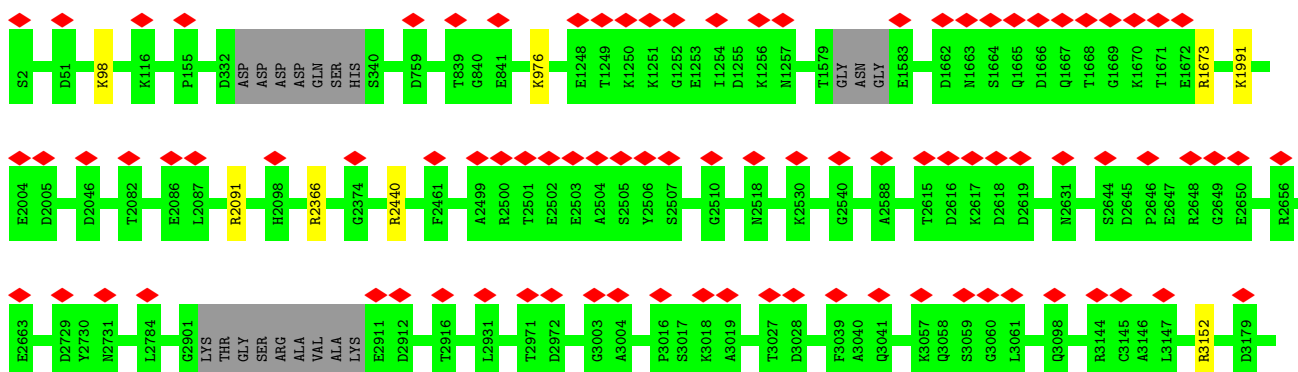
• Molecule 1: Hemocyanin

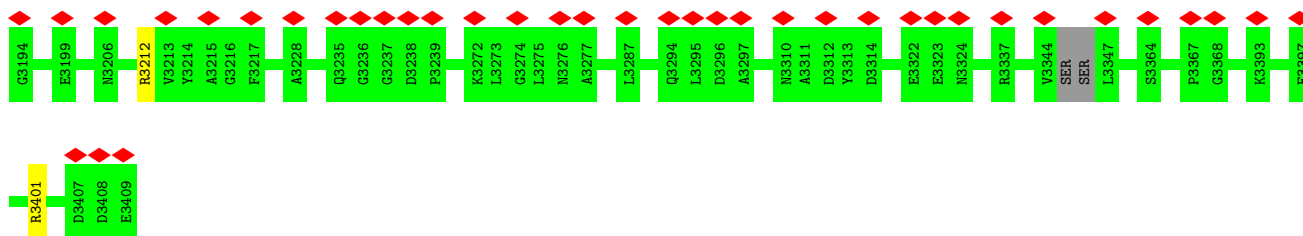
Chain N: 99%



• Molecule 1: Hemocyanin

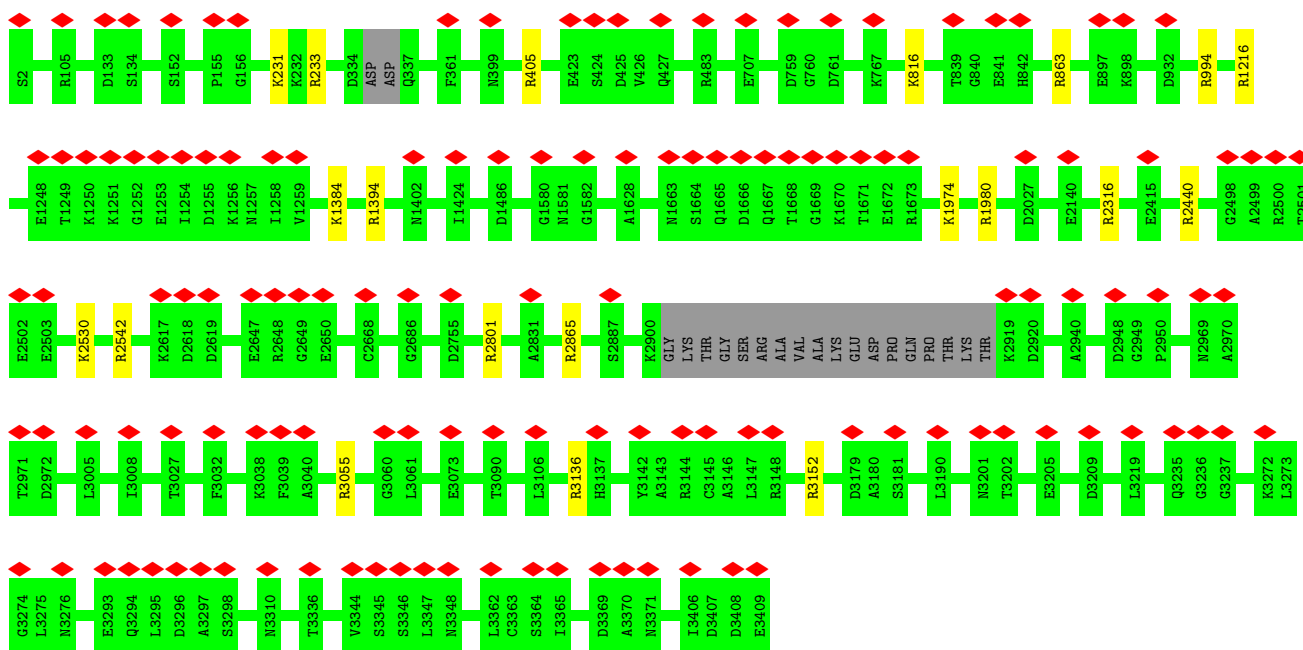
Chain O: 99%





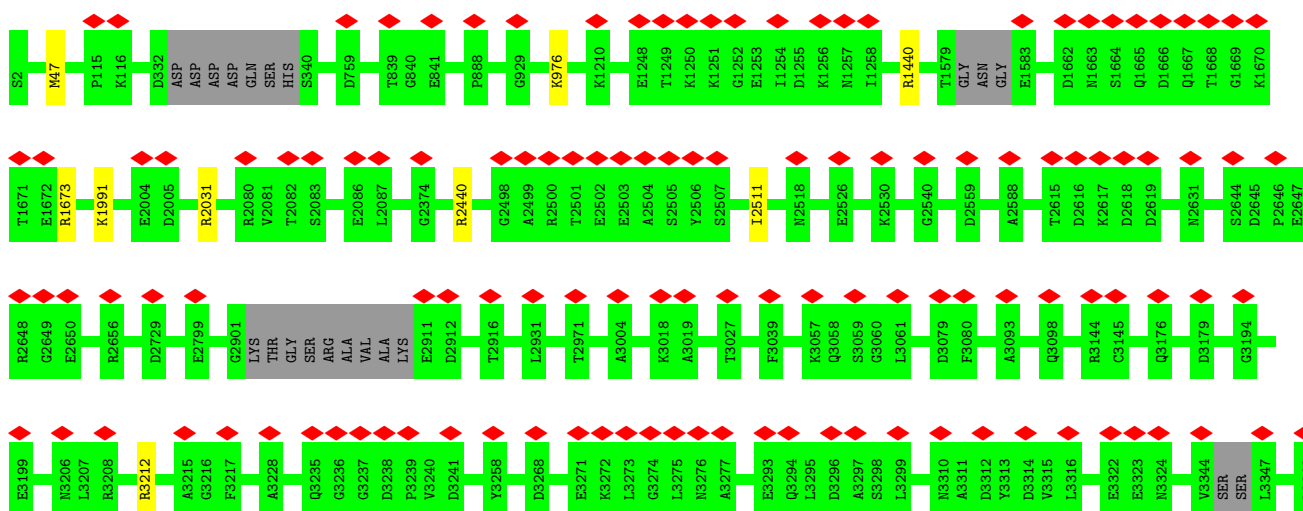
• Molecule 1: Hemocyanin

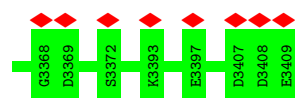
Chain P: 99%



• Molecule 1: Hemocyanin

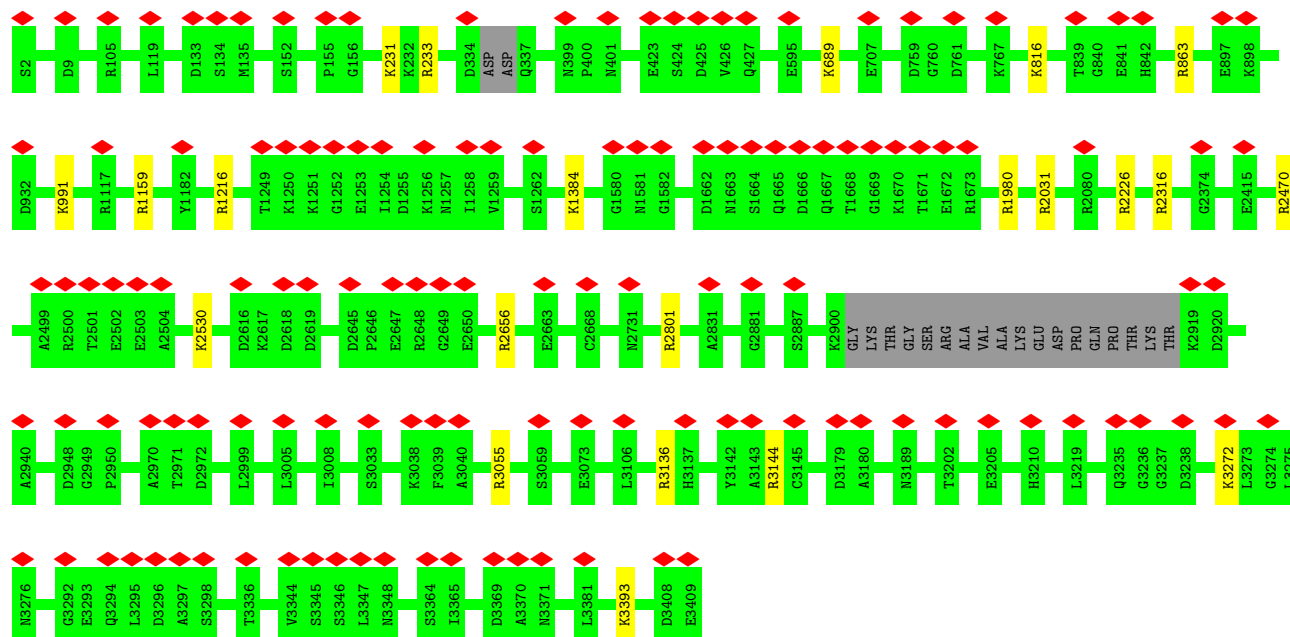
Chain Q: 99%





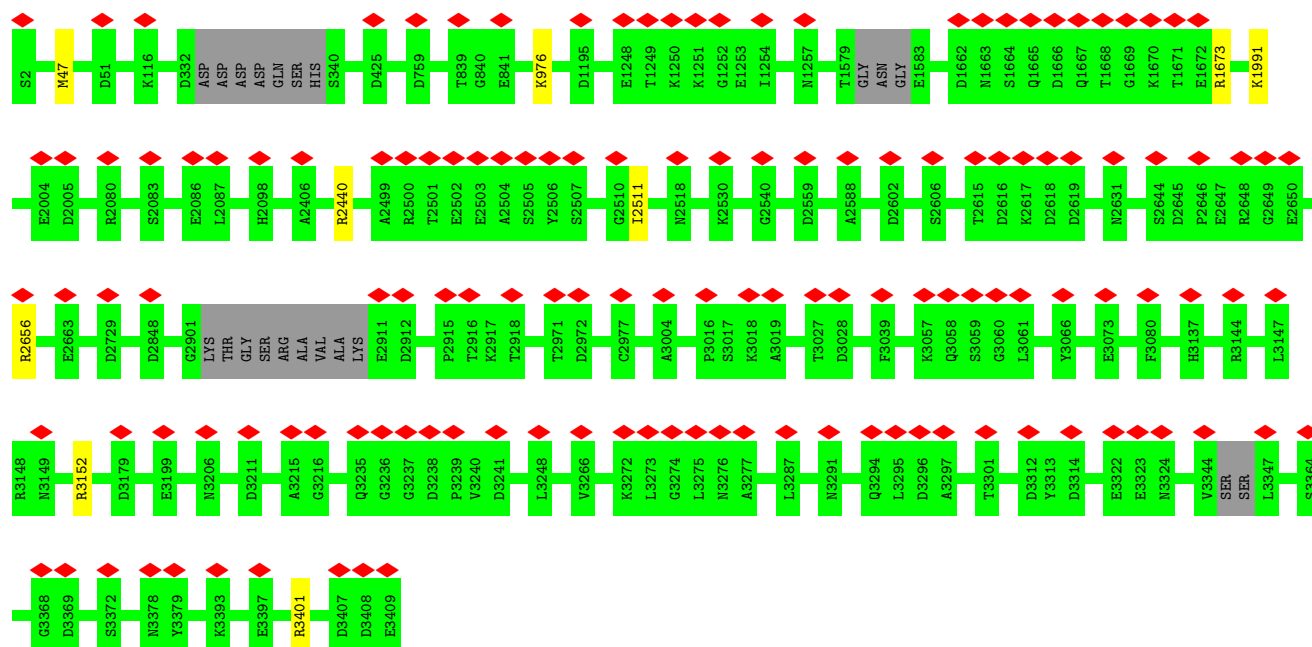
• Molecule 1: Hemocyanin

Chain R: 99%



• Molecule 1: Hemocyanin

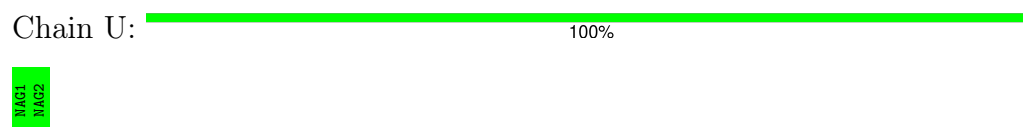
Chain S: 99%



- Molecule 1: Hemocyanin



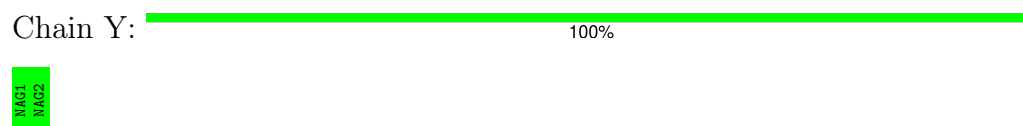
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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





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

Chain e:  100%



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

Chain g:  100%



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

Chain i:  50% 50%



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

Chain n:  50% 50% 50%



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

Chain o:  100%



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

Chain q:  100%



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

Chain s:  100%

MAG1
MAG2

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

Chain x:  50% 50%

MAG1
MAG2

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

Chain y:  100%

MAG1
MAG2

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

Chain 0:  50% 50%

MAG1
MAG2

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

Chain 2:  100%

MAG1
MAG2

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

Chain 7:  50% 50%

MAG1
MAG2

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

Chain 8:  100%



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

Chain AA:  100%



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

Chain CA:  50% 50%



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

Chain HA:  50% 50%



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

Chain IA:  100%



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

Chain KA:  50% 50%



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

Chain MA:  100%



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

Chain RA:  50% 50%



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

Chain SA:  100%



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

Chain UA:  100%



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

Chain WA:  50% 50%



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

Chain bA:  50% 50%



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

Chain cA:  100%



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

Chain eA:  100%



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

Chain gA:  100%



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

Chain lA:  50% 50%



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

Chain mA:  100%



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

Chain oA:  100%



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

Chain qA:  100%



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

Chain vA:  50% 50%



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

Chain wA:  100%

MAG1
MAG2

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

Chain yA:  100%

MAG1
MAG2

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

Chain 0A:  100%

MAG1
MAG2

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

Chain 5A:  50% 50%

MAG1
MAG2

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

Chain V:  100%

MAG1
MAG2
BMA3

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

Chain X:  67% 33%

MAG1
MAG2
BMA3

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

Chain Z:  100%



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

Chain a:  100%



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

Chain b:  100%



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

Chain c:  67% 33%



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

Chain f:  100%



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

Chain h:  67% 33%



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

Chain j:  100%



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

Chain k:  100%

MAG1
MAG2
BMA3

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

Chain l:  100%

MAG1
MAG2
BMA3

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

Chain m:  67% 33%

MAG1
MAG2
BMA3

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

Chain p:  100%

MAG1
MAG2
BMA3

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

Chain r:  67% 33%

MAG1
MAG2
BMA3

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

Chain t:  100%

MAG1
MAG2
BMA3

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

Chain u:  100%



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

Chain v:  100%



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

Chain w:  67% 33%



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

Chain z:  100%



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

Chain 1:  67% 33%



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

Chain 3:  67% 33%



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

Chain 4:  100%



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

Chain 5:  100%

MAG1
MAG2
BMA3

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

Chain 6:  67% 33%

MAG1
MAG2
BMA3

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

Chain 9:  67% 33%

MAG1
MAG2
BMA3

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

Chain BA:  67% 33%

MAG1
MAG2
BMA3

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

Chain DA:  67% 33%

MAG1
MAG2
BMA3

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

Chain EA:  100%

MAG1
MAG2
BMA3

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

Chain FA:  100%



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

Chain GA:



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

Chain JA:



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

Chain LA:



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

Chain NA:



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

Chain OA:



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

Chain PA:



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

Chain QA:  67% 33%



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

Chain TA:  100%



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

Chain VA:  67% 33%



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

Chain XA:  67% 33%



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

Chain YA:  100%



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

Chain ZA:  100%



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

Chain aA:  67% 33%



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

Chain dA:  100%



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

Chain fA:  100%



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

Chain hA:  100%



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

Chain iA:  100%



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

Chain jA:  100%



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

Chain kA:  100%



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

Chain nA:  100%

MAG1
MAG2
BMA3

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

Chain pA:  67%  33%

MAG1
MAG2
BMA3

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

Chain rA:  100%

MAG1
MAG2
BMA3

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

Chain sA:  100%

MAG1
MAG2
BMA3

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

Chain tA:  100%

MAG1
MAG2
BMA3

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

Chain uA:  67%  33%

MAG1
MAG2
BMA3

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

Chain xA:  100%



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



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



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	29935	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36.75	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.862	Depositor
Minimum map value	-2.136	Depositor
Average map value	0.033	Depositor
Map value standard deviation	0.212	Depositor
Recommended contour level	0.637	Depositor
Map size (Å)	597.77997, 597.77997, 597.77997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.9925998, 1.9925998, 1.9925998	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.29	0/28074	0.51	0/38177
1	B	0.28	0/28072	0.51	0/38172
1	C	0.29	0/28074	0.51	0/38177
1	D	0.28	0/28077	0.51	1/38182 (0.0%)
1	E	0.29	0/28074	0.51	0/38177
1	F	0.28	0/28077	0.51	0/38182
1	G	0.29	0/28073	0.51	0/38176
1	H	0.28	0/28077	0.51	2/38182 (0.0%)
1	I	0.29	0/28074	0.51	0/38177
1	J	0.28	0/28074	0.51	0/38175
1	K	0.29	0/28074	0.51	0/38177
1	L	0.28	0/28072	0.51	0/38172
1	M	0.29	0/28074	0.51	0/38177
1	N	0.28	0/28077	0.51	0/38182
1	O	0.29	0/28074	0.51	0/38177
1	P	0.28	0/28077	0.51	0/38182
1	Q	0.29	0/28073	0.51	0/38176
1	R	0.28	0/28077	0.51	0/38182
1	S	0.29	0/28074	0.51	0/38177
1	T	0.28	0/28074	0.51	0/38175
All	All	0.29	0/561492	0.51	3/763554 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	2541	PRO	CA-N-CD	-6.23	102.78	111.50
1	H	3142	TYR	CA-CB-CG	5.91	124.63	113.40
1	D	2740	LEU	CA-CB-CG	5.39	127.70	115.30

There are no chirality outliers.

There are no planarity outliers.

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 PDB entries followed by that with respect to all EM entries.

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	3377/3408 (99%)	3136 (93%)	241 (7%)	0	100	100
1	B	3382/3408 (99%)	3151 (93%)	231 (7%)	0	100	100
1	C	3377/3408 (99%)	3138 (93%)	238 (7%)	1 (0%)	100	100
1	D	3382/3408 (99%)	3141 (93%)	241 (7%)	0	100	100
1	E	3377/3408 (99%)	3143 (93%)	233 (7%)	1 (0%)	100	100
1	F	3382/3408 (99%)	3151 (93%)	231 (7%)	0	100	100
1	G	3377/3408 (99%)	3143 (93%)	234 (7%)	0	100	100
1	H	3382/3408 (99%)	3135 (93%)	247 (7%)	0	100	100
1	I	3377/3408 (99%)	3132 (93%)	244 (7%)	1 (0%)	100	100
1	J	3381/3408 (99%)	3128 (92%)	253 (8%)	0	100	100
1	K	3377/3408 (99%)	3146 (93%)	231 (7%)	0	100	100
1	L	3382/3408 (99%)	3147 (93%)	235 (7%)	0	100	100
1	M	3377/3408 (99%)	3130 (93%)	246 (7%)	1 (0%)	100	100
1	N	3382/3408 (99%)	3140 (93%)	242 (7%)	0	100	100
1	O	3377/3408 (99%)	3139 (93%)	238 (7%)	0	100	100
1	P	3382/3408 (99%)	3137 (93%)	245 (7%)	0	100	100
1	Q	3377/3408 (99%)	3139 (93%)	237 (7%)	1 (0%)	100	100
1	R	3382/3408 (99%)	3143 (93%)	239 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	3377/3408 (99%)	3135 (93%)	241 (7%)	1 (0%)	100	100
1	T	3381/3408 (99%)	3159 (93%)	222 (7%)	0	100	100
All	All	67588/68160 (99%)	62813 (93%)	4769 (7%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	1509	LEU
1	I	2477	ASN
1	E	2511	ILE
1	Q	2511	ILE
1	S	2511	ILE
1	C	2511	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 PDB entries followed by that with respect to all EM entries.

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	2965/2981 (100%)	2956 (100%)	9 (0%)	91	92
1	B	2964/2981 (99%)	2938 (99%)	26 (1%)	75	83
1	C	2965/2981 (100%)	2955 (100%)	10 (0%)	91	92
1	D	2965/2981 (100%)	2945 (99%)	20 (1%)	81	87
1	E	2965/2981 (100%)	2956 (100%)	9 (0%)	91	92
1	F	2965/2981 (100%)	2948 (99%)	17 (1%)	84	88
1	G	2964/2981 (99%)	2951 (100%)	13 (0%)	89	91
1	H	2965/2981 (100%)	2944 (99%)	21 (1%)	81	87
1	I	2965/2981 (100%)	2953 (100%)	12 (0%)	89	91
1	J	2964/2981 (99%)	2944 (99%)	20 (1%)	81	87
1	K	2965/2981 (100%)	2960 (100%)	5 (0%)	92	94
1	L	2964/2981 (99%)	2942 (99%)	22 (1%)	81	87
1	M	2965/2981 (100%)	2956 (100%)	9 (0%)	91	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	2965/2981 (100%)	2940 (99%)	25 (1%)	79	85
1	O	2965/2981 (100%)	2955 (100%)	10 (0%)	91	92
1	P	2965/2981 (100%)	2945 (99%)	20 (1%)	81	87
1	Q	2964/2981 (99%)	2956 (100%)	8 (0%)	91	92
1	R	2965/2981 (100%)	2943 (99%)	22 (1%)	81	87
1	S	2965/2981 (100%)	2957 (100%)	8 (0%)	91	92
1	T	2964/2981 (99%)	2946 (99%)	18 (1%)	84	88
All	All	59294/59620 (100%)	58990 (100%)	304 (0%)	85	90

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	976	LYS
1	A	1991	LYS
1	A	2022	MET
1	A	2091	ARG
1	A	2366	ARG
1	A	2440	ARG
1	A	2865	ARG
1	A	3152	ARG
1	A	3212	ARG
1	B	231	LYS
1	B	233	ARG
1	B	405	ARG
1	B	499	TRP
1	B	731	ARG
1	B	816	LYS
1	B	863	ARG
1	B	991	LYS
1	B	994	ARG
1	B	1117	ARG
1	B	1216	ARG
1	B	1384	LYS
1	B	1980	ARG
1	B	2031	ARG
1	B	2120	LYS
1	B	2226	ARG
1	B	2316	ARG
1	B	2440	ARG
1	B	2530	LYS

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Mol	Chain	Res	Type
1	B	2656	ARG
1	B	2801	ARG
1	B	2865	ARG
1	B	3046	ARG
1	B	3055	ARG
1	B	3136	ARG
1	B	3272	LYS
1	C	98	LYS
1	C	976	LYS
1	C	1673	ARG
1	C	1902	ARG
1	C	1991	LYS
1	C	2031	ARG
1	C	2440	ARG
1	C	2656	ARG
1	C	3212	ARG
1	C	3401	ARG
1	D	231	LYS
1	D	233	ARG
1	D	405	ARG
1	D	689	LYS
1	D	816	LYS
1	D	863	ARG
1	D	1216	ARG
1	D	1384	LYS
1	D	1394	ARG
1	D	1736	MET
1	D	1980	ARG
1	D	2031	ARG
1	D	2226	ARG
1	D	2316	ARG
1	D	2421	ARG
1	D	2440	ARG
1	D	2530	LYS
1	D	2656	ARG
1	D	2801	ARG
1	D	3136	ARG
1	E	98	LYS
1	E	976	LYS
1	E	1991	LYS
1	E	2091	ARG
1	E	2366	ARG

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Mol	Chain	Res	Type
1	E	2440	ARG
1	E	3152	ARG
1	E	3212	ARG
1	E	3401	ARG
1	F	231	LYS
1	F	233	ARG
1	F	816	LYS
1	F	863	ARG
1	F	1216	ARG
1	F	1384	LYS
1	F	1394	ARG
1	F	1980	ARG
1	F	2080	ARG
1	F	2226	ARG
1	F	2316	ARG
1	F	2470	ARG
1	F	2530	LYS
1	F	2801	ARG
1	F	2865	ARG
1	F	3046	ARG
1	F	3136	ARG
1	G	47	MET
1	G	98	LYS
1	G	405	ARG
1	G	976	LYS
1	G	994	ARG
1	G	1673	ARG
1	G	1756	ARG
1	G	1991	LYS
1	G	2226	ARG
1	G	3015	ARG
1	G	3152	ARG
1	G	3212	ARG
1	G	3401	ARG
1	H	231	LYS
1	H	233	ARG
1	H	405	ARG
1	H	689	LYS
1	H	816	LYS
1	H	863	ARG
1	H	1216	ARG
1	H	1384	LYS

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Mol	Chain	Res	Type
1	H	1394	ARG
1	H	2031	ARG
1	H	2120	LYS
1	H	2226	ARG
1	H	2316	ARG
1	H	2440	ARG
1	H	2470	ARG
1	H	2530	LYS
1	H	2542	ARG
1	H	2656	ARG
1	H	2801	ARG
1	H	2865	ARG
1	H	3136	ARG
1	I	47	MET
1	I	98	LYS
1	I	976	LYS
1	I	1250	LYS
1	I	1440	ARG
1	I	1678	LYS
1	I	1991	LYS
1	I	2091	ARG
1	I	2440	ARG
1	I	2919	LYS
1	I	3152	ARG
1	I	3401	ARG
1	J	231	LYS
1	J	233	ARG
1	J	405	ARG
1	J	816	LYS
1	J	863	ARG
1	J	1117	ARG
1	J	1216	ARG
1	J	1384	LYS
1	J	1493	ARG
1	J	1980	ARG
1	J	2031	ARG
1	J	2120	LYS
1	J	2226	ARG
1	J	2316	ARG
1	J	2470	ARG
1	J	2530	LYS
1	J	2801	ARG

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Mol	Chain	Res	Type
1	J	3046	ARG
1	J	3136	ARG
1	J	3272	LYS
1	K	47	MET
1	K	976	LYS
1	K	1991	LYS
1	K	2322	ARG
1	K	3212	ARG
1	L	54	LYS
1	L	231	LYS
1	L	233	ARG
1	L	405	ARG
1	L	499	TRP
1	L	538	LYS
1	L	816	LYS
1	L	863	ARG
1	L	1216	ARG
1	L	1384	LYS
1	L	1394	ARG
1	L	1980	ARG
1	L	2226	ARG
1	L	2316	ARG
1	L	2421	ARG
1	L	2440	ARG
1	L	2530	LYS
1	L	2636	ARG
1	L	2801	ARG
1	L	2865	ARG
1	L	3136	ARG
1	L	3272	LYS
1	M	47	MET
1	M	976	LYS
1	M	1756	ARG
1	M	1902	ARG
1	M	1991	LYS
1	M	2091	ARG
1	M	3152	ARG
1	M	3212	ARG
1	M	3401	ARG
1	N	231	LYS
1	N	233	ARG
1	N	405	ARG

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Mol	Chain	Res	Type
1	N	538	LYS
1	N	689	LYS
1	N	816	LYS
1	N	863	ARG
1	N	991	LYS
1	N	1138	ARG
1	N	1216	ARG
1	N	1384	LYS
1	N	1980	ARG
1	N	2031	ARG
1	N	2120	LYS
1	N	2316	ARG
1	N	2421	ARG
1	N	2470	ARG
1	N	2530	LYS
1	N	2656	ARG
1	N	2801	ARG
1	N	3046	ARG
1	N	3136	ARG
1	N	3144	ARG
1	N	3152	ARG
1	N	3272	LYS
1	O	98	LYS
1	O	976	LYS
1	O	1673	ARG
1	O	1991	LYS
1	O	2091	ARG
1	O	2366	ARG
1	O	2440	ARG
1	O	3152	ARG
1	O	3212	ARG
1	O	3401	ARG
1	P	231	LYS
1	P	233	ARG
1	P	405	ARG
1	P	816	LYS
1	P	863	ARG
1	P	994	ARG
1	P	1216	ARG
1	P	1384	LYS
1	P	1394	ARG
1	P	1974	LYS

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Mol	Chain	Res	Type
1	P	1980	ARG
1	P	2316	ARG
1	P	2440	ARG
1	P	2530	LYS
1	P	2542	ARG
1	P	2801	ARG
1	P	2865	ARG
1	P	3055	ARG
1	P	3136	ARG
1	P	3152	ARG
1	Q	47	MET
1	Q	976	LYS
1	Q	1440	ARG
1	Q	1673	ARG
1	Q	1991	LYS
1	Q	2031	ARG
1	Q	2440	ARG
1	Q	3212	ARG
1	R	231	LYS
1	R	233	ARG
1	R	689	LYS
1	R	816	LYS
1	R	863	ARG
1	R	991	LYS
1	R	1159	ARG
1	R	1216	ARG
1	R	1384	LYS
1	R	1980	ARG
1	R	2031	ARG
1	R	2226	ARG
1	R	2316	ARG
1	R	2470	ARG
1	R	2530	LYS
1	R	2656	ARG
1	R	2801	ARG
1	R	3055	ARG
1	R	3136	ARG
1	R	3144	ARG
1	R	3272	LYS
1	R	3393	LYS
1	S	47	MET
1	S	976	LYS

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Mol	Chain	Res	Type
1	S	1673	ARG
1	S	1991	LYS
1	S	2440	ARG
1	S	2656	ARG
1	S	3152	ARG
1	S	3401	ARG
1	T	231	LYS
1	T	233	ARG
1	T	405	ARG
1	T	816	LYS
1	T	863	ARG
1	T	1216	ARG
1	T	1384	LYS
1	T	1394	ARG
1	T	1980	ARG
1	T	2031	ARG
1	T	2080	ARG
1	T	2226	ARG
1	T	2316	ARG
1	T	2530	LYS
1	T	2656	ARG
1	T	2801	ARG
1	T	2865	ARG
1	T	3136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1059) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	61	HIS
1	A	70	HIS
1	A	158	ASN
1	A	180	GLN
1	A	187	HIS
1	A	189	HIS
1	A	216	HIS
1	A	259	ASN
1	A	331	HIS
1	A	491	HIS
1	A	610	HIS
1	A	640	HIS
1	A	860	GLN

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Mol	Chain	Res	Type
1	A	905	HIS
1	A	914	HIS
1	A	1017	GLN
1	A	1026	HIS
1	A	1052	HIS
1	A	1055	ASN
1	A	1067	GLN
1	A	1176	HIS
1	A	1307	HIS
1	A	1317	HIS
1	A	1326	HIS
1	A	1430	HIS
1	A	1460	HIS
1	A	1461	HIS
1	A	1494	GLN
1	A	1500	ASN
1	A	1505	ASN
1	A	1708	GLN
1	A	1734	HIS
1	A	1743	HIS
1	A	1749	GLN
1	A	1772	GLN
1	A	1854	HIS
1	A	1855	ASN
1	A	1884	HIS
1	A	2085	GLN
1	A	2149	HIS
1	A	2299	HIS
1	A	2345	ASN
1	A	2569	HIS
1	A	2657	GLN
1	A	2664	GLN
1	A	2679	ASN
1	A	2711	ASN
1	A	2773	ASN
1	A	2960	HIS
1	A	2979	HIS
1	A	3036	GLN
1	A	3043	GLN
1	A	3089	ASN
1	A	3141	ASN
1	A	3149	ASN

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Mol	Chain	Res	Type
1	A	3291	ASN
1	B	37	ASN
1	B	61	HIS
1	B	131	ASN
1	B	186	ASN
1	B	187	HIS
1	B	491	HIS
1	B	741	HIS
1	B	744	ASN
1	B	858	GLN
1	B	905	HIS
1	B	914	HIS
1	B	1089	GLN
1	B	1142	HIS
1	B	1317	HIS
1	B	1326	HIS
1	B	1408	ASN
1	B	1430	HIS
1	B	1475	GLN
1	B	1494	GLN
1	B	1542	GLN
1	B	1564	ASN
1	B	1663	ASN
1	B	1708	GLN
1	B	1734	HIS
1	B	1743	HIS
1	B	1884	HIS
1	B	2149	HIS
1	B	2254	GLN
1	B	2263	GLN
1	B	2298	HIS
1	B	2345	ASN
1	B	2454	HIS
1	B	2569	HIS
1	B	2679	ASN
1	B	2715	GLN
1	B	2738	GLN
1	B	2775	GLN
1	B	2951	ASN
1	B	2960	HIS
1	B	2979	HIS
1	B	3088	HIS

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Mol	Chain	Res	Type
1	B	3089	ASN
1	B	3092	HIS
1	B	3127	GLN
1	B	3206	ASN
1	B	3276	ASN
1	C	37	ASN
1	C	61	HIS
1	C	187	HIS
1	C	259	ASN
1	C	462	ASN
1	C	491	HIS
1	C	640	HIS
1	C	672	HIS
1	C	858	GLN
1	C	905	HIS
1	C	914	HIS
1	C	1023	ASN
1	C	1053	HIS
1	C	1055	ASN
1	C	1263	HIS
1	C	1317	HIS
1	C	1373	GLN
1	C	1402	ASN
1	C	1430	HIS
1	C	1476	GLN
1	C	1505	ASN
1	C	1534	ASN
1	C	1708	GLN
1	C	1734	HIS
1	C	1741	GLN
1	C	1743	HIS
1	C	1884	HIS
1	C	2085	GLN
1	C	2149	HIS
1	C	2345	ASN
1	C	2414	GLN
1	C	2538	GLN
1	C	2569	HIS
1	C	2578	HIS
1	C	2673	GLN
1	C	2678	HIS
1	C	2679	ASN

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Mol	Chain	Res	Type
1	C	2682	HIS
1	C	2708	HIS
1	C	2723	GLN
1	C	2805	ASN
1	C	2826	ASN
1	C	2852	GLN
1	C	2960	HIS
1	C	2979	HIS
1	C	3088	HIS
1	C	3176	GLN
1	C	3284	GLN
1	C	3291	ASN
1	D	37	ASN
1	D	42	HIS
1	D	61	HIS
1	D	70	HIS
1	D	123	ASN
1	D	187	HIS
1	D	259	ASN
1	D	381	ASN
1	D	462	ASN
1	D	491	HIS
1	D	498	HIS
1	D	500	HIS
1	D	610	HIS
1	D	693	HIS
1	D	741	HIS
1	D	858	GLN
1	D	905	HIS
1	D	914	HIS
1	D	1023	ASN
1	D	1026	HIS
1	D	1089	GLN
1	D	1317	HIS
1	D	1430	HIS
1	D	1431	ASN
1	D	1461	HIS
1	D	1475	GLN
1	D	1494	GLN
1	D	1564	ASN
1	D	1663	ASN
1	D	1665	GLN

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Mol	Chain	Res	Type
1	D	1727	GLN
1	D	1734	HIS
1	D	1743	HIS
1	D	1849	GLN
1	D	1854	HIS
1	D	1871	HIS
1	D	1884	HIS
1	D	1907	ASN
1	D	2149	HIS
1	D	2158	HIS
1	D	2254	GLN
1	D	2263	GLN
1	D	2299	HIS
1	D	2345	ASN
1	D	2551	HIS
1	D	2569	HIS
1	D	2669	ASN
1	D	2708	HIS
1	D	2709	HIS
1	D	2720	GLN
1	D	2752	ASN
1	D	2951	ASN
1	D	2960	HIS
1	D	2979	HIS
1	D	3067	GLN
1	D	3088	HIS
1	D	3089	ASN
1	D	3149	ASN
1	D	3184	HIS
1	D	3206	ASN
1	D	3276	ASN
1	E	37	ASN
1	E	61	HIS
1	E	70	HIS
1	E	138	HIS
1	E	189	HIS
1	E	295	GLN
1	E	331	HIS
1	E	491	HIS
1	E	640	HIS
1	E	641	HIS
1	E	880	HIS

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Mol	Chain	Res	Type
1	E	905	HIS
1	E	914	HIS
1	E	1026	HIS
1	E	1052	HIS
1	E	1055	ASN
1	E	1317	HIS
1	E	1402	ASN
1	E	1460	HIS
1	E	1494	GLN
1	E	1500	ASN
1	E	1734	HIS
1	E	1772	GLN
1	E	1854	HIS
1	E	1884	HIS
1	E	2085	GLN
1	E	2090	ASN
1	E	2098	HIS
1	E	2149	HIS
1	E	2158	HIS
1	E	2278	HIS
1	E	2299	HIS
1	E	2345	ASN
1	E	2538	GLN
1	E	2569	HIS
1	E	2578	HIS
1	E	2592	GLN
1	E	2673	GLN
1	E	2679	ASN
1	E	2708	HIS
1	E	2805	ASN
1	E	2852	GLN
1	E	2979	HIS
1	E	2988	HIS
1	E	3036	GLN
1	E	3043	GLN
1	E	3089	ASN
1	E	3119	HIS
1	E	3165	ASN
1	E	3176	GLN
1	E	3284	GLN
1	E	3291	ASN
1	F	37	ASN

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Mol	Chain	Res	Type
1	F	61	HIS
1	F	186	ASN
1	F	187	HIS
1	F	366	HIS
1	F	491	HIS
1	F	545	ASN
1	F	610	HIS
1	F	614	HIS
1	F	685	ASN
1	F	714	GLN
1	F	741	HIS
1	F	860	GLN
1	F	905	HIS
1	F	914	HIS
1	F	969	HIS
1	F	1052	HIS
1	F	1089	GLN
1	F	1098	ASN
1	F	1142	HIS
1	F	1317	HIS
1	F	1326	HIS
1	F	1430	HIS
1	F	1494	GLN
1	F	1564	ASN
1	F	1727	GLN
1	F	1734	HIS
1	F	1743	HIS
1	F	1749	GLN
1	F	1772	GLN
1	F	1854	HIS
1	F	1884	HIS
1	F	2149	HIS
1	F	2164	GLN
1	F	2254	GLN
1	F	2263	GLN
1	F	2551	HIS
1	F	2569	HIS
1	F	2709	HIS
1	F	2723	GLN
1	F	2752	ASN
1	F	2951	ASN
1	F	2960	HIS

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Mol	Chain	Res	Type
1	F	2979	HIS
1	F	2994	GLN
1	F	3089	ASN
1	F	3119	HIS
1	F	3127	GLN
1	F	3163	ASN
1	F	3206	ASN
1	F	3276	ASN
1	G	37	ASN
1	G	61	HIS
1	G	121	GLN
1	G	180	GLN
1	G	187	HIS
1	G	259	ASN
1	G	462	ASN
1	G	491	HIS
1	G	611	ASN
1	G	629	HIS
1	G	640	HIS
1	G	672	HIS
1	G	741	HIS
1	G	887	GLN
1	G	905	HIS
1	G	1026	HIS
1	G	1193	GLN
1	G	1263	HIS
1	G	1269	GLN
1	G	1307	HIS
1	G	1317	HIS
1	G	1326	HIS
1	G	1402	ASN
1	G	1431	ASN
1	G	1460	HIS
1	G	1461	HIS
1	G	1463	ASN
1	G	1494	GLN
1	G	1500	ASN
1	G	1505	ASN
1	G	1708	GLN
1	G	1734	HIS
1	G	1743	HIS
1	G	1854	HIS

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Mol	Chain	Res	Type
1	G	1884	HIS
1	G	1885	HIS
1	G	1899	GLN
1	G	2149	HIS
1	G	2189	GLN
1	G	2345	ASN
1	G	2364	ASN
1	G	2376	ASN
1	G	2414	GLN
1	G	2569	HIS
1	G	2576	GLN
1	G	2592	GLN
1	G	2664	GLN
1	G	2679	ASN
1	G	2708	HIS
1	G	2736	ASN
1	G	2805	ASN
1	G	2852	GLN
1	G	2939	ASN
1	G	2960	HIS
1	G	2979	HIS
1	G	2988	HIS
1	G	3089	ASN
1	G	3092	HIS
1	G	3284	GLN
1	G	3291	ASN
1	H	37	ASN
1	H	61	HIS
1	H	70	HIS
1	H	186	ASN
1	H	187	HIS
1	H	450	GLN
1	H	491	HIS
1	H	722	GLN
1	H	741	HIS
1	H	744	ASN
1	H	858	GLN
1	H	905	HIS
1	H	914	HIS
1	H	969	HIS
1	H	1023	ASN
1	H	1026	HIS

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Mol	Chain	Res	Type
1	H	1089	GLN
1	H	1142	HIS
1	H	1144	GLN
1	H	1317	HIS
1	H	1402	ASN
1	H	1430	HIS
1	H	1460	HIS
1	H	1494	GLN
1	H	1564	ASN
1	H	1727	GLN
1	H	1734	HIS
1	H	1743	HIS
1	H	1854	HIS
1	H	1884	HIS
1	H	2085	GLN
1	H	2149	HIS
1	H	2254	GLN
1	H	2263	GLN
1	H	2335	GLN
1	H	2569	HIS
1	H	2715	GLN
1	H	2752	ASN
1	H	2775	GLN
1	H	2939	ASN
1	H	2960	HIS
1	H	2979	HIS
1	H	3058	GLN
1	H	3089	ASN
1	H	3127	GLN
1	H	3163	ASN
1	H	3206	ASN
1	H	3276	ASN
1	I	61	HIS
1	I	180	GLN
1	I	189	HIS
1	I	491	HIS
1	I	610	HIS
1	I	614	HIS
1	I	641	HIS
1	I	693	HIS
1	I	722	GLN
1	I	836	HIS

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Mol	Chain	Res	Type
1	I	858	GLN
1	I	860	GLN
1	I	887	GLN
1	I	905	HIS
1	I	1026	HIS
1	I	1052	HIS
1	I	1055	ASN
1	I	1263	HIS
1	I	1307	HIS
1	I	1317	HIS
1	I	1402	ASN
1	I	1434	HIS
1	I	1494	GLN
1	I	1529	HIS
1	I	1708	GLN
1	I	1734	HIS
1	I	1743	HIS
1	I	1854	HIS
1	I	1885	HIS
1	I	2085	GLN
1	I	2094	HIS
1	I	2098	HIS
1	I	2115	GLN
1	I	2149	HIS
1	I	2158	HIS
1	I	2197	GLN
1	I	2272	HIS
1	I	2299	HIS
1	I	2345	ASN
1	I	2518	ASN
1	I	2569	HIS
1	I	2673	GLN
1	I	2678	HIS
1	I	2679	ASN
1	I	2682	HIS
1	I	2708	HIS
1	I	2711	ASN
1	I	2752	ASN
1	I	2773	ASN
1	I	2960	HIS
1	I	2979	HIS
1	I	3036	GLN

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Mol	Chain	Res	Type
1	I	3043	GLN
1	I	3076	ASN
1	I	3089	ASN
1	I	3119	HIS
1	I	3141	ASN
1	I	3149	ASN
1	I	3176	GLN
1	I	3284	GLN
1	J	42	HIS
1	J	61	HIS
1	J	131	ASN
1	J	186	ASN
1	J	187	HIS
1	J	259	ASN
1	J	491	HIS
1	J	610	HIS
1	J	652	GLN
1	J	741	HIS
1	J	905	HIS
1	J	1022	HIS
1	J	1026	HIS
1	J	1089	GLN
1	J	1142	HIS
1	J	1317	HIS
1	J	1324	HIS
1	J	1326	HIS
1	J	1353	GLN
1	J	1408	ASN
1	J	1430	HIS
1	J	1431	ASN
1	J	1434	HIS
1	J	1494	GLN
1	J	1564	ASN
1	J	1581	ASN
1	J	1663	ASN
1	J	1734	HIS
1	J	1743	HIS
1	J	1749	GLN
1	J	1854	HIS
1	J	1884	HIS
1	J	1896	GLN
1	J	2149	HIS

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Mol	Chain	Res	Type
1	J	2254	GLN
1	J	2263	GLN
1	J	2335	GLN
1	J	2569	HIS
1	J	2578	HIS
1	J	2624	HIS
1	J	2682	HIS
1	J	2752	ASN
1	J	2939	ASN
1	J	2951	ASN
1	J	2960	HIS
1	J	2979	HIS
1	J	3163	ASN
1	J	3184	HIS
1	J	3189	ASN
1	J	3206	ASN
1	J	3276	ASN
1	K	37	ASN
1	K	61	HIS
1	K	187	HIS
1	K	259	ASN
1	K	331	HIS
1	K	491	HIS
1	K	640	HIS
1	K	672	HIS
1	K	741	HIS
1	K	836	HIS
1	K	905	HIS
1	K	1026	HIS
1	K	1089	GLN
1	K	1193	GLN
1	K	1307	HIS
1	K	1317	HIS
1	K	1402	ASN
1	K	1434	HIS
1	K	1460	HIS
1	K	1505	ASN
1	K	1529	HIS
1	K	1708	GLN
1	K	1734	HIS
1	K	1743	HIS
1	K	1749	GLN

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Mol	Chain	Res	Type
1	K	1842	ASN
1	K	1854	HIS
1	K	1855	ASN
1	K	1884	HIS
1	K	1885	HIS
1	K	2085	GLN
1	K	2149	HIS
1	K	2158	HIS
1	K	2167	GLN
1	K	2172	HIS
1	K	2345	ASN
1	K	2414	GLN
1	K	2569	HIS
1	K	2578	HIS
1	K	2657	GLN
1	K	2679	ASN
1	K	2708	HIS
1	K	2736	ASN
1	K	2827	HIS
1	K	2863	HIS
1	K	2939	ASN
1	K	2979	HIS
1	K	2988	HIS
1	K	3043	GLN
1	K	3089	ASN
1	K	3119	HIS
1	K	3149	ASN
1	K	3176	GLN
1	K	3201	ASN
1	K	3291	ASN
1	L	37	ASN
1	L	61	HIS
1	L	70	HIS
1	L	131	ASN
1	L	186	ASN
1	L	491	HIS
1	L	506	GLN
1	L	714	GLN
1	L	741	HIS
1	L	905	HIS
1	L	914	HIS
1	L	969	HIS

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Mol	Chain	Res	Type
1	L	1023	ASN
1	L	1026	HIS
1	L	1055	ASN
1	L	1089	GLN
1	L	1098	ASN
1	L	1137	GLN
1	L	1142	HIS
1	L	1257	ASN
1	L	1307	HIS
1	L	1317	HIS
1	L	1353	GLN
1	L	1408	ASN
1	L	1430	HIS
1	L	1494	GLN
1	L	1564	ASN
1	L	1665	GLN
1	L	1727	GLN
1	L	1734	HIS
1	L	1743	HIS
1	L	1749	GLN
1	L	1884	HIS
1	L	2085	GLN
1	L	2149	HIS
1	L	2229	GLN
1	L	2254	GLN
1	L	2263	GLN
1	L	2569	HIS
1	L	2709	HIS
1	L	2752	ASN
1	L	2773	ASN
1	L	2775	GLN
1	L	2875	HIS
1	L	2939	ASN
1	L	2946	ASN
1	L	2960	HIS
1	L	2979	HIS
1	L	3058	GLN
1	L	3089	ASN
1	L	3118	HIS
1	L	3119	HIS
1	L	3149	ASN
1	L	3206	ASN

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Mol	Chain	Res	Type
1	L	3276	ASN
1	M	61	HIS
1	M	189	HIS
1	M	491	HIS
1	M	610	HIS
1	M	611	ASN
1	M	722	GLN
1	M	887	GLN
1	M	905	HIS
1	M	914	HIS
1	M	1026	HIS
1	M	1055	ASN
1	M	1137	GLN
1	M	1263	HIS
1	M	1317	HIS
1	M	1402	ASN
1	M	1430	HIS
1	M	1460	HIS
1	M	1494	GLN
1	M	1529	HIS
1	M	1708	GLN
1	M	1734	HIS
1	M	1743	HIS
1	M	1855	ASN
1	M	2085	GLN
1	M	2098	HIS
1	M	2149	HIS
1	M	2335	GLN
1	M	2345	ASN
1	M	2569	HIS
1	M	2578	HIS
1	M	2673	GLN
1	M	2678	HIS
1	M	2679	ASN
1	M	2682	HIS
1	M	2723	GLN
1	M	2979	HIS
1	M	3036	GLN
1	M	3043	GLN
1	M	3089	ASN
1	M	3092	HIS
1	M	3119	HIS

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Mol	Chain	Res	Type
1	M	3284	GLN
1	M	3403	GLN
1	N	37	ASN
1	N	42	HIS
1	N	61	HIS
1	N	70	HIS
1	N	160	GLN
1	N	186	ASN
1	N	187	HIS
1	N	491	HIS
1	N	605	GLN
1	N	610	HIS
1	N	643	ASN
1	N	698	ASN
1	N	741	HIS
1	N	860	GLN
1	N	905	HIS
1	N	920	GLN
1	N	1026	HIS
1	N	1089	GLN
1	N	1098	ASN
1	N	1142	HIS
1	N	1317	HIS
1	N	1324	HIS
1	N	1430	HIS
1	N	1434	HIS
1	N	1461	HIS
1	N	1494	GLN
1	N	1536	ASN
1	N	1564	ASN
1	N	1727	GLN
1	N	1734	HIS
1	N	1743	HIS
1	N	1749	GLN
1	N	1854	HIS
1	N	1858	HIS
1	N	1884	HIS
1	N	1907	ASN
1	N	2085	GLN
1	N	2124	GLN
1	N	2149	HIS
1	N	2263	GLN

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Mol	Chain	Res	Type
1	N	2272	HIS
1	N	2299	HIS
1	N	2551	HIS
1	N	2569	HIS
1	N	2682	HIS
1	N	2709	HIS
1	N	2720	GLN
1	N	2752	ASN
1	N	2875	HIS
1	N	2883	GLN
1	N	2939	ASN
1	N	2951	ASN
1	N	2960	HIS
1	N	2979	HIS
1	N	3067	GLN
1	N	3089	ASN
1	N	3127	GLN
1	N	3163	ASN
1	N	3206	ASN
1	N	3276	ASN
1	O	37	ASN
1	O	61	HIS
1	O	138	HIS
1	O	189	HIS
1	O	289	ASN
1	O	331	HIS
1	O	491	HIS
1	O	596	GLN
1	O	605	GLN
1	O	640	HIS
1	O	836	HIS
1	O	858	GLN
1	O	889	ASN
1	O	905	HIS
1	O	914	HIS
1	O	1053	HIS
1	O	1055	ASN
1	O	1067	GLN
1	O	1137	GLN
1	O	1176	HIS
1	O	1317	HIS
1	O	1408	ASN

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Mol	Chain	Res	Type
1	O	1476	GLN
1	O	1494	GLN
1	O	1500	ASN
1	O	1708	GLN
1	O	1734	HIS
1	O	1743	HIS
1	O	1855	ASN
1	O	1884	HIS
1	O	2085	GLN
1	O	2149	HIS
1	O	2278	HIS
1	O	2299	HIS
1	O	2345	ASN
1	O	2569	HIS
1	O	2592	GLN
1	O	2624	HIS
1	O	2657	GLN
1	O	2678	HIS
1	O	2679	ASN
1	O	2682	HIS
1	O	2708	HIS
1	O	2736	ASN
1	O	2979	HIS
1	O	2988	HIS
1	O	3036	GLN
1	O	3043	GLN
1	O	3089	ASN
1	O	3092	HIS
1	O	3119	HIS
1	O	3137	HIS
1	O	3284	GLN
1	O	3291	ASN
1	O	3324	ASN
1	P	37	ASN
1	P	42	HIS
1	P	61	HIS
1	P	381	ASN
1	P	450	GLN
1	P	491	HIS
1	P	506	GLN
1	P	687	ASN
1	P	722	GLN

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Mol	Chain	Res	Type
1	P	741	HIS
1	P	744	ASN
1	P	858	GLN
1	P	860	GLN
1	P	887	GLN
1	P	905	HIS
1	P	914	HIS
1	P	1023	ASN
1	P	1089	GLN
1	P	1317	HIS
1	P	1324	HIS
1	P	1408	ASN
1	P	1430	HIS
1	P	1434	HIS
1	P	1475	GLN
1	P	1494	GLN
1	P	1727	GLN
1	P	1734	HIS
1	P	1743	HIS
1	P	1854	HIS
1	P	1884	HIS
1	P	2149	HIS
1	P	2254	GLN
1	P	2263	GLN
1	P	2454	HIS
1	P	2569	HIS
1	P	2679	ASN
1	P	2709	HIS
1	P	2734	ASN
1	P	2775	GLN
1	P	2951	ASN
1	P	2960	HIS
1	P	2979	HIS
1	P	3089	ASN
1	P	3163	ASN
1	P	3206	ASN
1	P	3276	ASN
1	P	3280	ASN
1	P	3341	HIS
1	P	3398	GLN
1	Q	37	ASN
1	Q	61	HIS

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Mol	Chain	Res	Type
1	Q	186	ASN
1	Q	187	HIS
1	Q	189	HIS
1	Q	259	ASN
1	Q	491	HIS
1	Q	640	HIS
1	Q	858	GLN
1	Q	860	GLN
1	Q	905	HIS
1	Q	914	HIS
1	Q	1026	HIS
1	Q	1317	HIS
1	Q	1326	HIS
1	Q	1461	HIS
1	Q	1476	GLN
1	Q	1494	GLN
1	Q	1500	ASN
1	Q	1505	ASN
1	Q	1529	HIS
1	Q	1536	ASN
1	Q	1708	GLN
1	Q	1734	HIS
1	Q	1884	HIS
1	Q	2085	GLN
1	Q	2149	HIS
1	Q	2268	HIS
1	Q	2272	HIS
1	Q	2345	ASN
1	Q	2364	ASN
1	Q	2414	GLN
1	Q	2569	HIS
1	Q	2592	GLN
1	Q	2679	ASN
1	Q	2708	HIS
1	Q	2711	ASN
1	Q	2805	ASN
1	Q	2852	GLN
1	Q	2939	ASN
1	Q	2979	HIS
1	Q	2988	HIS
1	Q	3089	ASN
1	Q	3137	HIS

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Mol	Chain	Res	Type
1	Q	3284	GLN
1	R	37	ASN
1	R	61	HIS
1	R	70	HIS
1	R	187	HIS
1	R	259	ASN
1	R	366	HIS
1	R	381	ASN
1	R	491	HIS
1	R	610	HIS
1	R	714	GLN
1	R	722	GLN
1	R	741	HIS
1	R	858	GLN
1	R	905	HIS
1	R	914	HIS
1	R	923	ASN
1	R	969	HIS
1	R	1026	HIS
1	R	1089	GLN
1	R	1101	HIS
1	R	1317	HIS
1	R	1430	HIS
1	R	1461	HIS
1	R	1494	GLN
1	R	1564	ASN
1	R	1727	GLN
1	R	1734	HIS
1	R	1743	HIS
1	R	1854	HIS
1	R	1858	HIS
1	R	1884	HIS
1	R	2085	GLN
1	R	2149	HIS
1	R	2158	HIS
1	R	2164	GLN
1	R	2254	GLN
1	R	2263	GLN
1	R	2313	GLN
1	R	2345	ASN
1	R	2551	HIS
1	R	2569	HIS

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Mol	Chain	Res	Type
1	R	2669	ASN
1	R	2709	HIS
1	R	2715	GLN
1	R	2951	ASN
1	R	2960	HIS
1	R	2979	HIS
1	R	3067	GLN
1	R	3163	ASN
1	R	3195	HIS
1	R	3201	ASN
1	R	3276	ASN
1	S	36	GLN
1	S	61	HIS
1	S	79	GLN
1	S	187	HIS
1	S	189	HIS
1	S	259	ASN
1	S	295	GLN
1	S	331	HIS
1	S	366	HIS
1	S	491	HIS
1	S	610	HIS
1	S	611	ASN
1	S	641	HIS
1	S	722	GLN
1	S	741	HIS
1	S	860	GLN
1	S	887	GLN
1	S	905	HIS
1	S	1026	HIS
1	S	1055	ASN
1	S	1067	GLN
1	S	1137	GLN
1	S	1317	HIS
1	S	1326	HIS
1	S	1402	ASN
1	S	1460	HIS
1	S	1494	GLN
1	S	1714	HIS
1	S	1734	HIS
1	S	1743	HIS
1	S	1772	GLN

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Mol	Chain	Res	Type
1	S	1884	HIS
1	S	2098	HIS
1	S	2149	HIS
1	S	2197	GLN
1	S	2272	HIS
1	S	2345	ASN
1	S	2518	ASN
1	S	2569	HIS
1	S	2576	GLN
1	S	2592	GLN
1	S	2657	GLN
1	S	2673	GLN
1	S	2678	HIS
1	S	2679	ASN
1	S	2682	HIS
1	S	2708	HIS
1	S	2715	GLN
1	S	2723	GLN
1	S	2861	GLN
1	S	2979	HIS
1	S	2988	HIS
1	S	3043	GLN
1	S	3089	ASN
1	S	3119	HIS
1	S	3149	ASN
1	S	3176	GLN
1	S	3284	GLN
1	S	3324	ASN
1	S	3403	GLN
1	T	42	HIS
1	T	61	HIS
1	T	131	ASN
1	T	186	ASN
1	T	198	HIS
1	T	399	ASN
1	T	401	ASN
1	T	450	GLN
1	T	491	HIS
1	T	545	ASN
1	T	605	GLN
1	T	610	HIS
1	T	712	ASN

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Mol	Chain	Res	Type
1	T	741	HIS
1	T	905	HIS
1	T	969	HIS
1	T	1022	HIS
1	T	1052	HIS
1	T	1089	GLN
1	T	1142	HIS
1	T	1145	HIS
1	T	1317	HIS
1	T	1326	HIS
1	T	1430	HIS
1	T	1461	HIS
1	T	1494	GLN
1	T	1524	ASN
1	T	1536	ASN
1	T	1734	HIS
1	T	1743	HIS
1	T	1854	HIS
1	T	1884	HIS
1	T	2149	HIS
1	T	2263	GLN
1	T	2335	GLN
1	T	2345	ASN
1	T	2569	HIS
1	T	2752	ASN
1	T	2775	GLN
1	T	2846	HIS
1	T	2860	ASN
1	T	2939	ASN
1	T	2951	ASN
1	T	2960	HIS
1	T	2979	HIS
1	T	3089	ASN
1	T	3158	ASN
1	T	3163	ASN
1	T	3206	ASN
1	T	3276	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

260 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	0	1	1,2	14,14,15	1.05	1 (7%)	17,19,21	0.99	1 (5%)
2	NAG	0	2	2	14,14,15	0.28	0	17,19,21	0.46	0
2	NAG	0A	1	1,2	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	0A	2	2	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	1	1	1,3	14,14,15	1.06	1 (7%)	17,19,21	0.95	1 (5%)
3	NAG	1	2	3	14,14,15	0.22	0	17,19,21	0.57	0
3	BMA	1	3	3	11,11,12	0.46	0	15,15,17	0.78	0
3	NAG	1A	1	1,3	14,14,15	0.62	0	17,19,21	0.93	1 (5%)
3	NAG	1A	2	3	14,14,15	0.27	0	17,19,21	0.44	0
3	BMA	1A	3	3	11,11,12	0.59	0	15,15,17	0.73	0
2	NAG	2	1	1,2	14,14,15	0.26	0	17,19,21	0.54	0
2	NAG	2	2	2	14,14,15	0.29	0	17,19,21	0.43	0
3	NAG	2A	1	1,3	14,14,15	0.53	0	17,19,21	0.45	0
3	NAG	2A	2	3	14,14,15	0.29	0	17,19,21	0.49	0
3	BMA	2A	3	3	11,11,12	0.53	0	15,15,17	0.68	0
3	NAG	3	1	1,3	14,14,15	0.60	0	17,19,21	0.93	1 (5%)
3	NAG	3	2	3	14,14,15	0.23	0	17,19,21	0.49	0
3	BMA	3	3	3	11,11,12	0.63	0	15,15,17	0.75	0
3	NAG	3A	1	1,3	14,14,15	0.29	0	17,19,21	0.48	0
3	NAG	3A	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	BMA	3A	3	3	11,11,12	0.55	0	15,15,17	0.78	0
3	NAG	4	1	1,3	14,14,15	0.45	0	17,19,21	0.43	0
3	NAG	4	2	3	14,14,15	0.30	0	17,19,21	0.51	0
3	BMA	4	3	3	11,11,12	0.57	0	15,15,17	0.77	0
3	NAG	4A	1	1,3	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
3	NAG	4A	2	3	14,14,15	0.86	1 (7%)	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	4A	3	3	11,11,12	0.64	0	15,15,17	1.02	0
3	NAG	5	1	1,3	14,14,15	0.26	0	17,19,21	0.48	0
3	NAG	5	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	BMA	5	3	3	11,11,12	0.57	0	15,15,17	0.79	0
2	NAG	5A	1	1,2	14,14,15	0.19	0	17,19,21	0.43	0
2	NAG	5A	2	2	14,14,15	0.51	0	17,19,21	1.25	1 (5%)
3	NAG	6	1	1,3	14,14,15	0.39	0	17,19,21	0.35	0
3	NAG	6	2	3	14,14,15	0.63	1 (7%)	17,19,21	1.41	1 (5%)
3	BMA	6	3	3	11,11,12	0.67	0	15,15,17	0.77	0
2	NAG	7	1	1,2	14,14,15	0.18	0	17,19,21	0.42	0
2	NAG	7	2	2	14,14,15	0.50	0	17,19,21	1.26	1 (5%)
2	NAG	8	1	1,2	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	8	2	2	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	9	1	1,3	14,14,15	0.54	0	17,19,21	0.76	1 (5%)
3	NAG	9	2	3	14,14,15	0.20	0	17,19,21	0.39	0
3	BMA	9	3	3	11,11,12	0.54	0	15,15,17	0.78	0
2	NAG	AA	1	1,2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	AA	2	2	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	BA	1	1,3	14,14,15	1.07	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	BA	2	3	14,14,15	0.23	0	17,19,21	0.60	0
3	BMA	BA	3	3	11,11,12	0.47	0	15,15,17	0.78	0
2	NAG	CA	1	1,2	14,14,15	0.88	1 (7%)	17,19,21	1.43	1 (5%)
2	NAG	CA	2	2	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	DA	1	1,3	14,14,15	0.64	0	17,19,21	0.96	1 (5%)
3	NAG	DA	2	3	14,14,15	0.24	0	17,19,21	0.47	0
3	BMA	DA	3	3	11,11,12	0.59	0	15,15,17	0.81	0
3	NAG	EA	1	1,3	14,14,15	0.50	0	17,19,21	0.48	0
3	NAG	EA	2	3	14,14,15	0.27	0	17,19,21	0.49	0
3	BMA	EA	3	3	11,11,12	0.52	0	15,15,17	0.71	0
3	NAG	FA	1	1,3	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	FA	2	3	14,14,15	0.19	0	17,19,21	0.46	0
3	BMA	FA	3	3	11,11,12	0.51	0	15,15,17	0.81	0
3	NAG	GA	1	1,3	14,14,15	0.34	0	17,19,21	0.35	0
3	NAG	GA	2	3	14,14,15	0.60	1 (7%)	17,19,21	1.33	1 (5%)
3	BMA	GA	3	3	11,11,12	0.63	0	15,15,17	0.76	0
2	NAG	HA	1	1,2	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	HA	2	2	14,14,15	0.49	0	17,19,21	1.26	1 (5%)
2	NAG	IA	1	1,2	14,14,15	0.20	0	17,19,21	0.40	0
2	NAG	IA	2	2	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	JA	1	1,3	14,14,15	0.19	0	17,19,21	0.36	0
3	NAG	JA	2	3	14,14,15	0.20	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	JA	3	3	11,11,12	0.49	0	15,15,17	0.78	0
2	NAG	KA	1	1,2	14,14,15	0.38	0	17,19,21	0.65	1 (5%)
2	NAG	KA	2	2	14,14,15	0.27	0	17,19,21	0.47	0
3	NAG	LA	1	1,3	14,14,15	0.46	0	17,19,21	0.66	0
3	NAG	LA	2	3	14,14,15	0.18	0	17,19,21	0.49	0
3	BMA	LA	3	3	11,11,12	0.45	0	15,15,17	0.82	0
2	NAG	MA	1	1,2	14,14,15	0.26	0	17,19,21	0.53	0
2	NAG	MA	2	2	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	NA	1	1,3	14,14,15	0.61	0	17,19,21	0.95	1 (5%)
3	NAG	NA	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	BMA	NA	3	3	11,11,12	0.61	0	15,15,17	0.75	0
3	NAG	OA	1	1,3	14,14,15	0.44	0	17,19,21	0.41	0
3	NAG	OA	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	BMA	OA	3	3	11,11,12	0.58	0	15,15,17	0.77	0
3	NAG	PA	1	1,3	14,14,15	0.27	0	17,19,21	0.48	0
3	NAG	PA	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	BMA	PA	3	3	11,11,12	0.55	0	15,15,17	0.79	0
3	NAG	QA	1	1,3	14,14,15	0.28	0	17,19,21	0.40	0
3	NAG	QA	2	3	14,14,15	0.55	0	17,19,21	1.34	1 (5%)
3	BMA	QA	3	3	11,11,12	0.58	0	15,15,17	0.80	0
2	NAG	RA	1	1,2	14,14,15	0.19	0	17,19,21	0.42	0
2	NAG	RA	2	2	14,14,15	0.50	0	17,19,21	1.25	1 (5%)
2	NAG	SA	1	1,2	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	SA	2	2	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	TA	1	1,3	14,14,15	0.18	0	17,19,21	0.39	0
3	NAG	TA	2	3	14,14,15	0.22	0	17,19,21	0.42	0
3	BMA	TA	3	3	11,11,12	0.54	0	15,15,17	0.76	0
2	NAG	U	1	1,2	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	U	2	2	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	UA	1	1,2	14,14,15	0.23	0	17,19,21	0.48	0
2	NAG	UA	2	2	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	V	1	1,3	14,14,15	0.14	0	17,19,21	0.39	0
3	NAG	V	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	BMA	V	3	3	11,11,12	0.49	0	15,15,17	0.78	0
3	NAG	VA	1	1,3	14,14,15	0.43	0	17,19,21	0.65	0
3	NAG	VA	2	3	14,14,15	0.17	0	17,19,21	0.50	0
3	BMA	VA	3	3	11,11,12	0.45	0	15,15,17	0.85	1 (6%)
2	NAG	W	1	1,2	14,14,15	0.21	0	17,19,21	0.50	0
2	NAG	W	2	2	14,14,15	0.25	0	17,19,21	0.44	0
2	NAG	WA	1	1,2	14,14,15	0.60	1 (7%)	17,19,21	0.69	0
2	NAG	WA	2	2	14,14,15	0.21	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	X	1	1,3	14,14,15	1.10	1 (7%)	17,19,21	0.96	1 (5%)
3	NAG	X	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	BMA	X	3	3	11,11,12	0.47	0	15,15,17	0.76	0
3	NAG	XA	1	1,3	14,14,15	0.62	0	17,19,21	0.93	1 (5%)
3	NAG	XA	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	BMA	XA	3	3	11,11,12	0.56	0	15,15,17	0.79	0
2	NAG	Y	1	1,2	14,14,15	0.27	0	17,19,21	0.44	0
2	NAG	Y	2	2	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	YA	1	1,3	14,14,15	0.54	0	17,19,21	0.47	0
3	NAG	YA	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	BMA	YA	3	3	11,11,12	0.54	0	15,15,17	0.72	0
3	NAG	Z	1	1,3	14,14,15	0.19	0	17,19,21	0.46	0
3	NAG	Z	2	3	14,14,15	0.25	0	17,19,21	0.45	0
3	BMA	Z	3	3	11,11,12	0.61	0	15,15,17	0.74	0
3	NAG	ZA	1	1,3	14,14,15	0.27	0	17,19,21	0.46	0
3	NAG	ZA	2	3	14,14,15	0.19	0	17,19,21	0.45	0
3	BMA	ZA	3	3	11,11,12	0.51	0	15,15,17	0.83	0
3	NAG	a	1	1,3	14,14,15	0.42	0	17,19,21	0.42	0
3	NAG	a	2	3	14,14,15	0.31	0	17,19,21	0.49	0
3	BMA	a	3	3	11,11,12	0.53	0	15,15,17	0.77	0
3	NAG	aA	1	1,3	14,14,15	0.36	0	17,19,21	0.37	0
3	NAG	aA	2	3	14,14,15	0.64	1 (7%)	17,19,21	1.33	1 (5%)
3	BMA	aA	3	3	11,11,12	0.63	0	15,15,17	0.77	0
3	NAG	b	1	1,3	14,14,15	0.32	0	17,19,21	0.48	0
3	NAG	b	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	BMA	b	3	3	11,11,12	0.56	0	15,15,17	0.83	0
2	NAG	bA	1	1,2	14,14,15	0.20	0	17,19,21	0.38	0
2	NAG	bA	2	2	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
3	NAG	c	1	1,3	14,14,15	0.35	0	17,19,21	0.38	0
3	NAG	c	2	3	14,14,15	0.42	0	17,19,21	1.32	1 (5%)
3	BMA	c	3	3	11,11,12	0.62	0	15,15,17	0.78	0
2	NAG	cA	1	1,2	14,14,15	0.22	0	17,19,21	0.48	0
2	NAG	cA	2	2	14,14,15	0.26	0	17,19,21	0.47	0
2	NAG	d	1	1,2	14,14,15	0.45	0	17,19,21	0.56	0
2	NAG	d	2	2	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	dA	1	1,3	14,14,15	0.15	0	17,19,21	0.39	0
3	NAG	dA	2	3	14,14,15	0.22	0	17,19,21	0.40	0
3	BMA	dA	3	3	11,11,12	0.50	0	15,15,17	0.79	0
2	NAG	e	1	1,2	14,14,15	0.24	0	17,19,21	0.46	0
2	NAG	e	2	2	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	eA	1	1,2	14,14,15	0.21	0	17,19,21	0.48	0
2	NAG	eA	2	2	14,14,15	0.25	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	f	1	1,3	14,14,15	0.18	0	17,19,21	0.38	0
3	NAG	f	2	3	14,14,15	0.23	0	17,19,21	0.42	0
3	BMA	f	3	3	11,11,12	0.52	0	15,15,17	0.77	0
3	NAG	fA	1	1,3	14,14,15	0.44	0	17,19,21	0.64	0
3	NAG	fA	2	3	14,14,15	0.19	0	17,19,21	0.47	0
3	BMA	fA	3	3	11,11,12	0.48	0	15,15,17	0.82	0
2	NAG	g	1	1,2	14,14,15	0.21	0	17,19,21	0.49	0
2	NAG	g	2	2	14,14,15	0.28	0	17,19,21	0.44	0
2	NAG	gA	1	1,2	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	gA	2	2	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	h	1	1,3	14,14,15	0.99	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	h	2	3	14,14,15	0.22	0	17,19,21	0.58	0
3	BMA	h	3	3	11,11,12	0.47	0	15,15,17	0.76	0
3	NAG	hA	1	1,3	14,14,15	0.18	0	17,19,21	0.48	0
3	NAG	hA	2	3	14,14,15	0.24	0	17,19,21	0.44	0
3	BMA	hA	3	3	11,11,12	0.62	0	15,15,17	0.74	0
2	NAG	i	1	1,2	14,14,15	0.63	1 (7%)	17,19,21	0.70	0
2	NAG	i	2	2	14,14,15	0.26	0	17,19,21	0.49	0
3	NAG	iA	1	1,3	14,14,15	0.43	0	17,19,21	0.41	0
3	NAG	iA	2	3	14,14,15	0.29	0	17,19,21	0.49	0
3	BMA	iA	3	3	11,11,12	0.53	0	15,15,17	0.78	0
3	NAG	j	1	1,3	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	j	2	3	14,14,15	0.26	0	17,19,21	0.44	0
3	BMA	j	3	3	11,11,12	0.62	0	15,15,17	0.78	0
3	NAG	jA	1	1,3	14,14,15	0.30	0	17,19,21	0.48	0
3	NAG	jA	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	BMA	jA	3	3	11,11,12	0.56	0	15,15,17	0.81	0
3	NAG	k	1	1,3	14,14,15	0.46	0	17,19,21	0.43	0
3	NAG	k	2	3	14,14,15	0.29	0	17,19,21	0.49	0
3	BMA	k	3	3	11,11,12	0.53	0	15,15,17	0.74	0
3	NAG	kA	1	1,3	14,14,15	0.25	0	17,19,21	0.38	0
3	NAG	kA	2	3	14,14,15	0.25	0	17,19,21	0.42	0
3	BMA	kA	3	3	11,11,12	0.55	0	15,15,17	0.71	0
3	NAG	l	1	1,3	14,14,15	0.32	0	17,19,21	0.50	0
3	NAG	l	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	BMA	l	3	3	11,11,12	0.56	0	15,15,17	0.78	0
2	NAG	lA	1	1,2	14,14,15	0.44	0	17,19,21	0.65	0
2	NAG	lA	2	2	14,14,15	0.59	1 (7%)	17,19,21	1.23	1 (5%)
3	NAG	m	1	1,3	14,14,15	0.28	0	17,19,21	0.37	0
3	NAG	m	2	3	14,14,15	0.51	0	17,19,21	1.37	1 (5%)
3	BMA	m	3	3	11,11,12	0.57	0	15,15,17	0.76	0
2	NAG	mA	1	1,2	14,14,15	0.24	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	mA	2	2	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	n	1	1,2	14,14,15	0.18	0	17,19,21	0.39	0
2	NAG	n	2	2	14,14,15	0.50	0	17,19,21	1.27	1 (5%)
3	NAG	nA	1	1,3	14,14,15	0.17	0	17,19,21	0.38	0
3	NAG	nA	2	3	14,14,15	0.25	0	17,19,21	0.43	0
3	BMA	nA	3	3	11,11,12	0.53	0	15,15,17	0.78	0
2	NAG	o	1	1,2	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	o	2	2	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	oA	1	1,2	14,14,15	0.19	0	17,19,21	0.50	0
2	NAG	oA	2	2	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	p	1	1,3	14,14,15	0.15	0	17,19,21	0.42	0
3	NAG	p	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	BMA	p	3	3	11,11,12	0.55	0	15,15,17	0.75	0
3	NAG	pA	1	1,3	14,14,15	0.46	0	17,19,21	0.66	0
3	NAG	pA	2	3	14,14,15	0.19	0	17,19,21	0.48	0
3	BMA	pA	3	3	11,11,12	0.47	0	15,15,17	0.88	1 (6%)
2	NAG	q	1	1,2	14,14,15	0.29	0	17,19,21	0.49	0
2	NAG	q	2	2	14,14,15	0.26	0	17,19,21	0.43	0
2	NAG	qA	1	1,2	14,14,15	0.28	0	17,19,21	0.55	0
2	NAG	qA	2	2	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	r	1	1,3	14,14,15	1.00	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	r	2	3	14,14,15	0.23	0	17,19,21	0.55	0
3	BMA	r	3	3	11,11,12	0.52	0	15,15,17	0.78	0
3	NAG	rA	1	1,3	14,14,15	0.21	0	17,19,21	0.49	0
3	NAG	rA	2	3	14,14,15	0.22	0	17,19,21	0.46	0
3	BMA	rA	3	3	11,11,12	0.56	0	15,15,17	0.84	0
2	NAG	s	1	1,2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	s	2	2	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	sA	1	1,3	14,14,15	0.47	0	17,19,21	0.42	0
3	NAG	sA	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	BMA	sA	3	3	11,11,12	0.54	0	15,15,17	0.74	0
3	NAG	t	1	1,3	14,14,15	0.21	0	17,19,21	0.48	0
3	NAG	t	2	3	14,14,15	0.28	0	17,19,21	0.48	0
3	BMA	t	3	3	11,11,12	0.63	0	15,15,17	0.72	0
3	NAG	tA	1	1,3	14,14,15	0.33	0	17,19,21	0.49	0
3	NAG	tA	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	BMA	tA	3	3	11,11,12	0.58	0	15,15,17	0.79	0
3	NAG	u	1	1,3	14,14,15	0.49	0	17,19,21	0.44	0
3	NAG	u	2	3	14,14,15	0.31	0	17,19,21	0.50	0
3	BMA	u	3	3	11,11,12	0.58	0	15,15,17	0.75	0
3	NAG	uA	1	1,3	14,14,15	0.30	0	17,19,21	0.36	0
3	NAG	uA	2	3	14,14,15	0.53	0	17,19,21	1.37	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	uA	3	3	11,11,12	0.59	0	15,15,17	0.76	0
3	NAG	v	1	1,3	14,14,15	0.30	0	17,19,21	0.47	0
3	NAG	v	2	3	14,14,15	0.19	0	17,19,21	0.44	0
3	BMA	v	3	3	11,11,12	0.56	0	15,15,17	0.78	0
2	NAG	vA	1	1,2	14,14,15	0.18	0	17,19,21	0.43	0
2	NAG	vA	2	2	14,14,15	0.54	0	17,19,21	1.26	1 (5%)
3	NAG	w	1	1,3	14,14,15	0.38	0	17,19,21	0.86	1 (5%)
3	NAG	w	2	3	14,14,15	0.37	0	17,19,21	0.50	0
3	BMA	w	3	3	11,11,12	0.54	0	15,15,17	0.76	0
2	NAG	wA	1	1,2	14,14,15	0.25	0	17,19,21	0.49	0
2	NAG	wA	2	2	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	x	1	1,2	14,14,15	0.19	0	17,19,21	0.41	0
2	NAG	x	2	2	14,14,15	0.51	0	17,19,21	1.24	1 (5%)
3	NAG	xA	1	1,3	14,14,15	0.27	0	17,19,21	0.38	0
3	NAG	xA	2	3	14,14,15	0.16	0	17,19,21	0.47	0
3	BMA	xA	3	3	11,11,12	0.58	0	15,15,17	0.76	0
2	NAG	y	1	1,2	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	y	2	2	14,14,15	0.27	0	17,19,21	0.47	0
2	NAG	yA	1	1,2	14,14,15	0.20	0	17,19,21	0.52	0
2	NAG	yA	2	2	14,14,15	0.28	0	17,19,21	0.41	0
3	NAG	z	1	1,3	14,14,15	0.17	0	17,19,21	0.39	0
3	NAG	z	2	3	14,14,15	0.23	0	17,19,21	0.43	0
3	BMA	z	3	3	11,11,12	0.51	0	15,15,17	0.75	0
3	NAG	zA	1	1,3	14,14,15	1.04	1 (7%)	17,19,21	0.94	1 (5%)
3	NAG	zA	2	3	14,14,15	0.22	0	17,19,21	0.53	0
3	BMA	zA	3	3	11,11,12	0.49	0	15,15,17	0.78	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	1A	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	1A	2	3	-	2/6/23/26	0/1/1/1
3	BMA	1A	3	3	-	0/2/19/22	0/1/1/1
2	NAG	2	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	2	2	2	-	2/6/23/26	0/1/1/1
3	NAG	2A	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	2A	2	3	-	3/6/23/26	0/1/1/1
3	BMA	2A	3	3	-	1/2/19/22	0/1/1/1
3	NAG	3	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	3	2	3	-	3/6/23/26	0/1/1/1
3	BMA	3	3	3	-	0/2/19/22	0/1/1/1
3	NAG	3A	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	3A	2	3	-	2/6/23/26	0/1/1/1
3	BMA	3A	3	3	-	0/2/19/22	0/1/1/1
3	NAG	4	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	4	2	3	-	4/6/23/26	0/1/1/1
3	BMA	4	3	3	-	0/2/19/22	0/1/1/1
3	NAG	4A	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	4A	2	3	-	4/6/23/26	0/1/1/1
3	BMA	4A	3	3	-	2/2/19/22	0/1/1/1
3	NAG	5	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	5	2	3	-	2/6/23/26	0/1/1/1
3	BMA	5	3	3	-	0/2/19/22	0/1/1/1
2	NAG	5A	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	5A	2	2	-	2/6/23/26	0/1/1/1
3	NAG	6	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	6	2	3	-	2/6/23/26	0/1/1/1
3	BMA	6	3	3	-	1/2/19/22	0/1/1/1
2	NAG	7	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	7	2	2	-	2/6/23/26	0/1/1/1
2	NAG	8	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	8	2	2	-	0/6/23/26	0/1/1/1
3	NAG	9	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	9	2	3	-	2/6/23/26	0/1/1/1
3	BMA	9	3	3	-	0/2/19/22	0/1/1/1
2	NAG	AA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	BA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	BA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	BA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	CA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	CA	2	2	-	0/6/23/26	0/1/1/1
3	NAG	DA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	DA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	DA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	EA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	EA	2	3	-	3/6/23/26	0/1/1/1
3	BMA	EA	3	3	-	1/2/19/22	0/1/1/1
3	NAG	FA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	FA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	FA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	GA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	GA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	GA	3	3	-	1/2/19/22	0/1/1/1
2	NAG	HA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	HA	2	2	-	3/6/23/26	0/1/1/1
2	NAG	IA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	IA	2	2	-	0/6/23/26	0/1/1/1
3	NAG	JA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	JA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	JA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	KA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	KA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	LA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	LA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	LA	3	3	-	1/2/19/22	0/1/1/1
2	NAG	MA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	MA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	NA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	NA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	NA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	OA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	OA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	OA	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	PA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	PA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	PA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	QA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	QA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	QA	3	3	-	1/2/19/22	0/1/1/1
2	NAG	RA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	RA	2	2	-	3/6/23/26	0/1/1/1
2	NAG	SA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	SA	2	2	-	0/6/23/26	0/1/1/1
3	NAG	TA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	TA	2	3	-	0/6/23/26	0/1/1/1
3	BMA	TA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	U	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	U	2	2	-	1/6/23/26	0/1/1/1
2	NAG	UA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	UA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	BMA	V	3	3	-	0/2/19/22	0/1/1/1
3	NAG	VA	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	VA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	VA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	NAG	WA	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	WA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
3	BMA	X	3	3	-	0/2/19/22	0/1/1/1
3	NAG	XA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	XA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	XA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
3	NAG	YA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	YA	2	3	-	3/6/23/26	0/1/1/1
3	BMA	YA	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Z	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
3	BMA	Z	3	3	-	0/2/19/22	0/1/1/1
3	NAG	ZA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	ZA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	ZA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	a	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	a	2	3	-	4/6/23/26	0/1/1/1
3	BMA	a	3	3	-	0/2/19/22	0/1/1/1
3	NAG	aA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	aA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	aA	3	3	-	1/2/19/22	0/1/1/1
3	NAG	b	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	BMA	b	3	3	-	0/2/19/22	0/1/1/1
2	NAG	bA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	bA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	c	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	BMA	c	3	3	-	1/2/19/22	0/1/1/1
2	NAG	cA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	cA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	d	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	d	2	2	-	1/6/23/26	0/1/1/1
3	NAG	dA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	dA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	dA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	e	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	NAG	eA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	eA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	f	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	BMA	f	3	3	-	0/2/19/22	0/1/1/1
3	NAG	fA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	fA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	fA	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	g	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	NAG	gA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	gA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	h	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	BMA	h	3	3	-	0/2/19/22	0/1/1/1
3	NAG	hA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	hA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	hA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	i	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	i	2	2	-	2/6/23/26	0/1/1/1
3	NAG	iA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	iA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	iA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	j	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	j	2	3	-	2/6/23/26	0/1/1/1
3	BMA	j	3	3	-	0/2/19/22	0/1/1/1
3	NAG	jA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	jA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	jA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	k	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	k	2	3	-	4/6/23/26	0/1/1/1
3	BMA	k	3	3	-	0/2/19/22	0/1/1/1
3	NAG	kA	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	kA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	kA	3	3	-	2/2/19/22	0/1/1/1
3	NAG	l	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	l	2	3	-	2/6/23/26	0/1/1/1
3	BMA	l	3	3	-	2/2/19/22	0/1/1/1
2	NAG	lA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	lA	2	2	-	1/6/23/26	0/1/1/1
3	NAG	m	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	m	2	3	-	2/6/23/26	0/1/1/1
3	BMA	m	3	3	-	1/2/19/22	0/1/1/1
2	NAG	mA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	mA	2	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	n	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	n	2	2	-	2/6/23/26	0/1/1/1
3	NAG	nA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	nA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	nA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	o	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	o	2	2	-	1/6/23/26	0/1/1/1
2	NAG	oA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	oA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	p	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	p	2	3	-	2/6/23/26	0/1/1/1
3	BMA	p	3	3	-	0/2/19/22	0/1/1/1
3	NAG	pA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	pA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	pA	3	3	-	0/2/19/22	0/1/1/1
2	NAG	q	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	q	2	2	-	2/6/23/26	0/1/1/1
2	NAG	qA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	qA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	r	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	r	2	3	-	2/6/23/26	0/1/1/1
3	BMA	r	3	3	-	0/2/19/22	0/1/1/1
3	NAG	rA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	rA	2	3	-	3/6/23/26	0/1/1/1
3	BMA	rA	3	3	-	1/2/19/22	0/1/1/1
2	NAG	s	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	s	2	2	-	2/6/23/26	0/1/1/1
3	NAG	sA	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	sA	2	3	-	4/6/23/26	0/1/1/1
3	BMA	sA	3	3	-	0/2/19/22	0/1/1/1
3	NAG	t	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	t	2	3	-	2/6/23/26	0/1/1/1
3	BMA	t	3	3	-	0/2/19/22	0/1/1/1
3	NAG	tA	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	tA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	tA	3	3	-	2/2/19/22	0/1/1/1
3	NAG	u	1	1,3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	u	2	3	-	4/6/23/26	0/1/1/1
3	BMA	u	3	3	-	0/2/19/22	0/1/1/1
3	NAG	uA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	uA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	uA	3	3	-	1/2/19/22	0/1/1/1
3	NAG	v	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	v	2	3	-	2/6/23/26	0/1/1/1
3	BMA	v	3	3	-	0/2/19/22	0/1/1/1
2	NAG	vA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	vA	2	2	-	4/6/23/26	0/1/1/1
3	NAG	w	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	w	2	3	-	2/6/23/26	0/1/1/1
3	BMA	w	3	3	-	1/2/19/22	0/1/1/1
2	NAG	wA	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	wA	2	2	-	1/6/23/26	0/1/1/1
2	NAG	x	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	x	2	2	-	2/6/23/26	0/1/1/1
3	NAG	xA	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	xA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	xA	3	3	-	2/2/19/22	0/1/1/1
2	NAG	y	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	y	2	2	-	0/6/23/26	0/1/1/1
2	NAG	yA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	yA	2	2	-	2/6/23/26	0/1/1/1
3	NAG	z	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	z	2	3	-	2/6/23/26	0/1/1/1
3	BMA	z	3	3	-	0/2/19/22	0/1/1/1
3	NAG	zA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	zA	2	3	-	2/6/23/26	0/1/1/1
3	BMA	zA	3	3	-	0/2/19/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	1	NAG	O5-C1	-3.78	1.37	1.43
3	1	1	NAG	O5-C1	-3.68	1.37	1.43
3	BA	1	NAG	O5-C1	-3.66	1.37	1.43
3	zA	1	NAG	O5-C1	-3.57	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	1	NAG	O5-C1	-3.53	1.37	1.43
3	r	1	NAG	O5-C1	-3.41	1.38	1.43
3	h	1	NAG	O5-C1	-3.39	1.38	1.43
3	4A	2	NAG	C1-C2	2.87	1.56	1.52
2	CA	1	NAG	C1-C2	2.32	1.55	1.52
3	aA	2	NAG	O5-C1	2.23	1.47	1.43
3	6	2	NAG	O5-C1	2.15	1.47	1.43
2	i	1	NAG	O5-C1	-2.15	1.40	1.43
3	GA	2	NAG	O5-C1	2.08	1.47	1.43
2	WA	1	NAG	O5-C1	-2.03	1.40	1.43
2	lA	2	NAG	O5-C1	2.01	1.47	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	2	NAG	C1-O5-C5	5.32	119.32	112.19
3	m	2	NAG	C1-O5-C5	5.16	119.10	112.19
2	CA	1	NAG	C1-O5-C5	5.15	119.09	112.19
3	uA	2	NAG	C1-O5-C5	5.14	119.08	112.19
3	QA	2	NAG	C1-O5-C5	5.12	119.04	112.19
3	c	2	NAG	C1-O5-C5	5.05	118.96	112.19
3	GA	2	NAG	C1-O5-C5	5.03	118.93	112.19
3	aA	2	NAG	C1-O5-C5	5.03	118.93	112.19
2	bA	2	NAG	C1-O5-C5	4.85	118.68	112.19
2	n	2	NAG	C1-O5-C5	4.83	118.66	112.19
2	RA	2	NAG	C1-O5-C5	4.79	118.60	112.19
2	vA	2	NAG	C1-O5-C5	4.78	118.59	112.19
2	HA	2	NAG	C1-O5-C5	4.78	118.59	112.19
2	7	2	NAG	C1-O5-C5	4.77	118.58	112.19
2	5A	2	NAG	C1-O5-C5	4.76	118.56	112.19
2	lA	2	NAG	C1-O5-C5	4.72	118.51	112.19
2	x	2	NAG	C1-O5-C5	4.72	118.51	112.19
3	DA	1	NAG	C1-O5-C5	3.37	116.70	112.19
3	w	1	NAG	C1-O5-C5	3.15	116.40	112.19
3	NA	1	NAG	C1-O5-C5	3.15	116.40	112.19
3	lA	1	NAG	C1-O5-C5	3.11	116.35	112.19
3	3	1	NAG	C1-O5-C5	3.07	116.31	112.19
3	XA	1	NAG	C1-O5-C5	3.06	116.28	112.19
3	4A	2	NAG	C1-O5-C5	2.89	116.06	112.19
2	0	1	NAG	C3-C4-C5	2.67	115.08	110.23
3	X	1	NAG	C3-C4-C5	2.53	114.82	110.23
3	BA	1	NAG	C3-C4-C5	2.47	114.70	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1	1	NAG	C3-C4-C5	2.44	114.66	110.23
3	9	1	NAG	C1-O5-C5	2.42	115.44	112.19
3	zA	1	NAG	C3-C4-C5	2.42	114.62	110.23
3	h	1	NAG	C3-C4-C5	2.35	114.49	110.23
3	r	1	NAG	C3-C4-C5	2.34	114.47	110.23
3	4A	1	NAG	C1-O5-C5	2.30	115.27	112.19
2	KA	1	NAG	C1-O5-C5	2.22	115.16	112.19
3	VA	3	BMA	C1-O5-C5	2.06	114.95	112.19
3	pA	3	BMA	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (421) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	pA	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	C4-C5-C6-O6
2	i	2	NAG	C4-C5-C6-O6
2	WA	2	NAG	C4-C5-C6-O6
3	fA	2	NAG	C4-C5-C6-O6
3	BA	1	NAG	O5-C5-C6-O6
3	FA	2	NAG	O5-C5-C6-O6
3	ZA	2	NAG	O5-C5-C6-O6
3	tA	2	NAG	O5-C5-C6-O6
2	s	2	NAG	C4-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	l	2	NAG	O5-C5-C6-O6
3	GA	1	NAG	O5-C5-C6-O6
3	PA	2	NAG	O5-C5-C6-O6
3	QA	1	NAG	O5-C5-C6-O6
2	0A	2	NAG	C4-C5-C6-O6
3	LA	2	NAG	C4-C5-C6-O6
3	VA	2	NAG	C4-C5-C6-O6
2	AA	2	NAG	O5-C5-C6-O6
2	WA	1	NAG	C4-C5-C6-O6
2	0	2	NAG	O5-C5-C6-O6
2	UA	2	NAG	O5-C5-C6-O6
3	5	2	NAG	O5-C5-C6-O6
3	aA	1	NAG	O5-C5-C6-O6
3	jA	2	NAG	O5-C5-C6-O6
2	i	2	NAG	O5-C5-C6-O6
2	qA	2	NAG	C4-C5-C6-O6
2	Y	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	q	2	NAG	O5-C5-C6-O6
2	KA	2	NAG	O5-C5-C6-O6
3	VA	2	NAG	O5-C5-C6-O6
3	fA	2	NAG	O5-C5-C6-O6
2	gA	2	NAG	C4-C5-C6-O6
2	WA	1	NAG	O5-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6
3	LA	2	NAG	O5-C5-C6-O6
2	x	2	NAG	C4-C5-C6-O6
2	2	2	NAG	C4-C5-C6-O6
2	HA	2	NAG	C4-C5-C6-O6
2	RA	2	NAG	C4-C5-C6-O6
2	bA	2	NAG	C4-C5-C6-O6
2	5A	2	NAG	C4-C5-C6-O6
2	n	2	NAG	O5-C5-C6-O6
2	oA	2	NAG	O5-C5-C6-O6
2	yA	2	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
3	v	2	NAG	O5-C5-C6-O6
3	1	1	NAG	O5-C5-C6-O6
3	XA	1	NAG	O5-C5-C6-O6
3	kA	2	NAG	O5-C5-C6-O6
3	pA	2	NAG	O5-C5-C6-O6
3	uA	1	NAG	O5-C5-C6-O6
3	3A	2	NAG	O5-C5-C6-O6
2	0	1	NAG	C4-C5-C6-O6
2	7	2	NAG	C4-C5-C6-O6
2	AA	2	NAG	C4-C5-C6-O6
3	NA	2	NAG	C4-C5-C6-O6
2	W	2	NAG	O5-C5-C6-O6
2	g	2	NAG	O5-C5-C6-O6
2	eA	2	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	r	1	NAG	O5-C5-C6-O6
3	w	2	NAG	O5-C5-C6-O6
3	zA	1	NAG	O5-C5-C6-O6
3	1A	1	NAG	O5-C5-C6-O6
2	n	2	NAG	C4-C5-C6-O6
2	UA	2	NAG	C4-C5-C6-O6
3	BA	1	NAG	C4-C5-C6-O6
3	QA	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	7	2	NAG	O5-C5-C6-O6
2	MA	2	NAG	O5-C5-C6-O6
3	3	1	NAG	O5-C5-C6-O6
3	DA	1	NAG	O5-C5-C6-O6
3	nA	2	NAG	O5-C5-C6-O6
3	p	1	NAG	C4-C5-C6-O6
3	uA	1	NAG	C4-C5-C6-O6
2	WA	2	NAG	O5-C5-C6-O6
3	m	1	NAG	O5-C5-C6-O6
2	KA	2	NAG	C4-C5-C6-O6
2	oA	2	NAG	C4-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
3	FA	2	NAG	C4-C5-C6-O6
3	ZA	2	NAG	C4-C5-C6-O6
3	aA	1	NAG	C4-C5-C6-O6
2	RA	2	NAG	O5-C5-C6-O6
2	q	2	NAG	C4-C5-C6-O6
2	yA	2	NAG	C4-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	nA	2	NAG	C4-C5-C6-O6
3	tA	2	NAG	C4-C5-C6-O6
2	s	2	NAG	O5-C5-C6-O6
2	x	2	NAG	O5-C5-C6-O6
2	HA	2	NAG	O5-C5-C6-O6
2	bA	2	NAG	O5-C5-C6-O6
2	gA	2	NAG	O5-C5-C6-O6
2	0A	2	NAG	O5-C5-C6-O6
2	5A	2	NAG	O5-C5-C6-O6
2	g	2	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	c	1	NAG	C4-C5-C6-O6
3	w	2	NAG	C4-C5-C6-O6
3	5	2	NAG	C4-C5-C6-O6
3	JA	1	NAG	C4-C5-C6-O6
3	jA	2	NAG	C4-C5-C6-O6
3	p	1	NAG	O5-C5-C6-O6
2	eA	2	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	GA	1	NAG	C4-C5-C6-O6
3	PA	2	NAG	C4-C5-C6-O6
2	2	2	NAG	O5-C5-C6-O6
3	NA	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	iA	2	NAG	O5-C5-C6-O6
3	tA	3	BMA	O5-C5-C6-O6
3	xA	2	NAG	O5-C5-C6-O6
3	l	2	NAG	C4-C5-C6-O6
2	qA	2	NAG	O5-C5-C6-O6
2	0	2	NAG	C4-C5-C6-O6
3	NA	1	NAG	C4-C5-C6-O6
3	FA	1	NAG	O5-C5-C6-O6
3	JA	1	NAG	O5-C5-C6-O6
2	W	2	NAG	C4-C5-C6-O6
3	r	1	NAG	C4-C5-C6-O6
3	z	1	NAG	C4-C5-C6-O6
3	ZA	1	NAG	O5-C5-C6-O6
3	v	2	NAG	C4-C5-C6-O6
3	FA	1	NAG	C4-C5-C6-O6
3	ZA	1	NAG	C4-C5-C6-O6
3	kA	2	NAG	C4-C5-C6-O6
3	3A	2	NAG	C4-C5-C6-O6
3	1	1	NAG	C4-C5-C6-O6
3	DA	1	NAG	C4-C5-C6-O6
2	0	1	NAG	O5-C5-C6-O6
3	NA	2	NAG	O5-C5-C6-O6
3	4A	3	BMA	O5-C5-C6-O6
3	3	1	NAG	C4-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
3	l	3	BMA	O5-C5-C6-O6
3	v	1	NAG	O5-C5-C6-O6
3	sA	2	NAG	O5-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6
3	kA	3	BMA	C4-C5-C6-O6
3	3A	1	NAG	O5-C5-C6-O6
3	zA	2	NAG	C4-C5-C6-O6
3	zA	1	NAG	C4-C5-C6-O6
3	3A	1	NAG	C4-C5-C6-O6
2	vA	2	NAG	C8-C7-N2-C2
2	vA	2	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	Z	1	NAG	C8-C7-N2-C2
3	Z	1	NAG	O7-C7-N2-C2
3	Z	2	NAG	C8-C7-N2-C2
3	Z	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	a	1	NAG	C8-C7-N2-C2
3	a	1	NAG	O7-C7-N2-C2
3	c	2	NAG	C8-C7-N2-C2
3	c	2	NAG	O7-C7-N2-C2
3	f	1	NAG	C8-C7-N2-C2
3	f	1	NAG	O7-C7-N2-C2
3	j	1	NAG	C8-C7-N2-C2
3	j	1	NAG	O7-C7-N2-C2
3	j	2	NAG	C8-C7-N2-C2
3	j	2	NAG	O7-C7-N2-C2
3	k	1	NAG	C8-C7-N2-C2
3	k	1	NAG	O7-C7-N2-C2
3	m	2	NAG	C8-C7-N2-C2
3	m	2	NAG	O7-C7-N2-C2
3	p	1	NAG	C8-C7-N2-C2
3	p	1	NAG	O7-C7-N2-C2
3	t	1	NAG	C8-C7-N2-C2
3	t	1	NAG	O7-C7-N2-C2
3	t	2	NAG	C8-C7-N2-C2
3	t	2	NAG	O7-C7-N2-C2
3	u	1	NAG	C8-C7-N2-C2
3	u	1	NAG	O7-C7-N2-C2
3	z	1	NAG	C8-C7-N2-C2
3	z	1	NAG	O7-C7-N2-C2
3	3	1	NAG	C8-C7-N2-C2
3	3	1	NAG	O7-C7-N2-C2
3	3	2	NAG	C8-C7-N2-C2
3	3	2	NAG	O7-C7-N2-C2
3	4	1	NAG	C8-C7-N2-C2
3	4	1	NAG	O7-C7-N2-C2
3	6	2	NAG	C8-C7-N2-C2
3	6	2	NAG	O7-C7-N2-C2
3	9	1	NAG	C8-C7-N2-C2
3	9	1	NAG	O7-C7-N2-C2
3	DA	1	NAG	C8-C7-N2-C2
3	DA	1	NAG	O7-C7-N2-C2
3	DA	2	NAG	C8-C7-N2-C2
3	DA	2	NAG	O7-C7-N2-C2
3	EA	1	NAG	C8-C7-N2-C2
3	EA	1	NAG	O7-C7-N2-C2
3	GA	2	NAG	C8-C7-N2-C2
3	GA	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	JA	1	NAG	C8-C7-N2-C2
3	JA	1	NAG	O7-C7-N2-C2
3	NA	1	NAG	C8-C7-N2-C2
3	NA	1	NAG	O7-C7-N2-C2
3	NA	2	NAG	C8-C7-N2-C2
3	NA	2	NAG	O7-C7-N2-C2
3	OA	1	NAG	C8-C7-N2-C2
3	OA	1	NAG	O7-C7-N2-C2
3	QA	2	NAG	C8-C7-N2-C2
3	QA	2	NAG	O7-C7-N2-C2
3	TA	1	NAG	C8-C7-N2-C2
3	TA	1	NAG	O7-C7-N2-C2
3	XA	1	NAG	C8-C7-N2-C2
3	XA	1	NAG	O7-C7-N2-C2
3	XA	2	NAG	C8-C7-N2-C2
3	XA	2	NAG	O7-C7-N2-C2
3	YA	1	NAG	C8-C7-N2-C2
3	YA	1	NAG	O7-C7-N2-C2
3	aA	2	NAG	C8-C7-N2-C2
3	aA	2	NAG	O7-C7-N2-C2
3	dA	1	NAG	C8-C7-N2-C2
3	dA	1	NAG	O7-C7-N2-C2
3	hA	1	NAG	C8-C7-N2-C2
3	hA	1	NAG	O7-C7-N2-C2
3	hA	2	NAG	C8-C7-N2-C2
3	hA	2	NAG	O7-C7-N2-C2
3	iA	1	NAG	C8-C7-N2-C2
3	iA	1	NAG	O7-C7-N2-C2
3	nA	1	NAG	C8-C7-N2-C2
3	nA	1	NAG	O7-C7-N2-C2
3	rA	1	NAG	C8-C7-N2-C2
3	rA	1	NAG	O7-C7-N2-C2
3	rA	2	NAG	C8-C7-N2-C2
3	rA	2	NAG	O7-C7-N2-C2
3	sA	1	NAG	C8-C7-N2-C2
3	sA	1	NAG	O7-C7-N2-C2
3	uA	2	NAG	C8-C7-N2-C2
3	uA	2	NAG	O7-C7-N2-C2
3	xA	1	NAG	C8-C7-N2-C2
3	xA	1	NAG	O7-C7-N2-C2
3	1A	1	NAG	C8-C7-N2-C2
3	1A	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	1A	2	NAG	C8-C7-N2-C2
3	1A	2	NAG	O7-C7-N2-C2
3	2A	1	NAG	C8-C7-N2-C2
3	2A	1	NAG	O7-C7-N2-C2
3	z	1	NAG	O5-C5-C6-O6
3	v	1	NAG	C4-C5-C6-O6
3	XA	1	NAG	C4-C5-C6-O6
3	tA	3	BMA	C4-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	4A	2	NAG	O5-C5-C6-O6
3	m	1	NAG	C4-C5-C6-O6
3	TA	1	NAG	C4-C5-C6-O6
2	vA	2	NAG	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	9	2	NAG	O5-C5-C6-O6
3	xA	3	BMA	O5-C5-C6-O6
2	MA	2	NAG	C4-C5-C6-O6
3	1A	1	NAG	C4-C5-C6-O6
3	p	2	NAG	C4-C5-C6-O6
2	wA	1	NAG	O5-C5-C6-O6
3	u	2	NAG	O5-C5-C6-O6
3	kA	3	BMA	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	xA	2	NAG	C4-C5-C6-O6
2	d	2	NAG	O5-C5-C6-O6
3	QA	3	BMA	O5-C5-C6-O6
3	z	2	NAG	C4-C5-C6-O6
3	6	3	BMA	O5-C5-C6-O6
2	vA	1	NAG	C4-C5-C6-O6
3	4A	3	BMA	C4-C5-C6-O6
2	CA	1	NAG	O5-C5-C6-O6
3	OA	2	NAG	O5-C5-C6-O6
3	xA	3	BMA	C4-C5-C6-O6
3	dA	2	NAG	C4-C5-C6-O6
3	4A	1	NAG	O5-C5-C6-O6
3	4	2	NAG	O5-C5-C6-O6
2	lA	1	NAG	O5-C5-C6-O6
2	n	1	NAG	C4-C5-C6-O6
3	TA	1	NAG	O5-C5-C6-O6
3	p	2	NAG	O5-C5-C6-O6
3	l	3	BMA	C4-C5-C6-O6
3	zA	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	bA	1	NAG	C4-C5-C6-O6
3	hA	1	NAG	O5-C5-C6-O6
3	1	2	NAG	C4-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	4A	1	NAG	C4-C5-C6-O6
3	z	2	NAG	O5-C5-C6-O6
3	6	1	NAG	O5-C5-C6-O6
3	JA	2	NAG	C4-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
2	vA	1	NAG	O5-C5-C6-O6
2	lA	1	NAG	C4-C5-C6-O6
2	o	1	NAG	O5-C5-C6-O6
2	CA	1	NAG	C4-C5-C6-O6
3	EA	1	NAG	C4-C5-C6-O6
2	i	1	NAG	O5-C5-C6-O6
2	cA	1	NAG	O5-C5-C6-O6
3	dA	2	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	pA	1	NAG	C4-C5-C6-O6
3	3	2	NAG	O5-C5-C6-O6
3	jA	1	NAG	C4-C5-C6-O6
3	iA	2	NAG	C4-C5-C6-O6
2	SA	1	NAG	O5-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
3	kA	1	NAG	O5-C5-C6-O6
3	rA	1	NAG	O5-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
2	n	1	NAG	O5-C5-C6-O6
2	lA	1	NAG	O5-C5-C6-O6
2	mA	1	NAG	O5-C5-C6-O6
3	2A	2	NAG	O5-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	4A	2	NAG	C4-C5-C6-O6
2	8	1	NAG	O5-C5-C6-O6
3	YA	2	NAG	O5-C5-C6-O6
3	aA	3	BMA	O5-C5-C6-O6
3	dA	1	NAG	C4-C5-C6-O6
3	GA	3	BMA	O5-C5-C6-O6
2	HA	1	NAG	C4-C5-C6-O6
3	YA	1	NAG	C4-C5-C6-O6
2	U	1	NAG	O5-C5-C6-O6
2	lA	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	j	1	NAG	O5-C5-C6-O6
3	l	3	BMA	O5-C5-C6-O6
3	EA	1	NAG	O5-C5-C6-O6
3	fA	1	NAG	C4-C5-C6-O6
2	bA	1	NAG	O5-C5-C6-O6
3	l	2	NAG	O5-C5-C6-O6
2	y	1	NAG	O5-C5-C6-O6
3	m	3	BMA	O5-C5-C6-O6
3	EA	2	NAG	O5-C5-C6-O6
3	uA	3	BMA	O5-C5-C6-O6
3	c	3	BMA	O5-C5-C6-O6
3	t	1	NAG	O5-C5-C6-O6
3	rA	2	NAG	O5-C5-C6-O6
3	pA	1	NAG	O5-C5-C6-O6
3	sA	2	NAG	C4-C5-C6-O6
3	k	2	NAG	C4-C5-C6-O6
3	jA	1	NAG	O5-C5-C6-O6
2	vA	2	NAG	C4-C5-C6-O6
3	JA	2	NAG	O5-C5-C6-O6
3	9	2	NAG	C4-C5-C6-O6
3	YA	1	NAG	O5-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	2A	3	BMA	O5-C5-C6-O6
3	xA	1	NAG	O5-C5-C6-O6
3	r	2	NAG	C4-C5-C6-O6
3	w	1	NAG	C4-C5-C6-O6
3	a	2	NAG	C1-C2-N2-C7
3	k	2	NAG	C1-C2-N2-C7
3	4	2	NAG	C1-C2-N2-C7
3	EA	2	NAG	C1-C2-N2-C7
3	OA	2	NAG	C1-C2-N2-C7
3	YA	2	NAG	C1-C2-N2-C7
3	iA	2	NAG	C1-C2-N2-C7
3	sA	2	NAG	C1-C2-N2-C7
3	4A	2	NAG	C1-C2-N2-C7
3	V	1	NAG	O5-C5-C6-O6
3	4	1	NAG	C4-C5-C6-O6
2	HA	1	NAG	O5-C5-C6-O6
3	fA	1	NAG	O5-C5-C6-O6
3	dA	1	NAG	O5-C5-C6-O6
3	OA	1	NAG	C4-C5-C6-O6
3	rA	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	k	1	NAG	C4-C5-C6-O6
3	BA	2	NAG	C4-C5-C6-O6
3	iA	1	NAG	C4-C5-C6-O6
3	9	1	NAG	O5-C5-C6-O6
3	sA	1	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	u	2	NAG	C4-C5-C6-O6
2	cA	2	NAG	O5-C5-C6-O6
3	r	2	NAG	O5-C5-C6-O6
2	CA	1	NAG	C3-C2-N2-C7
3	a	2	NAG	C3-C2-N2-C7
3	k	2	NAG	C3-C2-N2-C7
3	u	2	NAG	C3-C2-N2-C7
3	4	2	NAG	C3-C2-N2-C7
3	EA	2	NAG	C3-C2-N2-C7
3	OA	2	NAG	C3-C2-N2-C7
3	YA	2	NAG	C3-C2-N2-C7
3	iA	2	NAG	C3-C2-N2-C7
3	sA	2	NAG	C3-C2-N2-C7
3	2A	2	NAG	C3-C2-N2-C7
3	f	1	NAG	C4-C5-C6-O6
3	LA	3	BMA	O5-C5-C6-O6
2	x	1	NAG	C4-C5-C6-O6
2	RA	1	NAG	C4-C5-C6-O6
3	4	1	NAG	O5-C5-C6-O6
3	BA	2	NAG	O5-C5-C6-O6
3	OA	1	NAG	O5-C5-C6-O6
3	k	1	NAG	O5-C5-C6-O6
2	U	2	NAG	O5-C5-C6-O6
2	o	2	NAG	O5-C5-C6-O6
3	sA	1	NAG	O5-C5-C6-O6
3	iA	1	NAG	O5-C5-C6-O6
2	wA	2	NAG	O5-C5-C6-O6
3	w	3	BMA	C4-C5-C6-O6
3	w	1	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
2	HA	2	NAG	C1-C2-N2-C7
2	RA	2	NAG	C1-C2-N2-C7
2	WA	1	NAG	C1-C2-N2-C7
3	u	2	NAG	C1-C2-N2-C7
3	GA	1	NAG	C1-C2-N2-C7
3	2A	2	NAG	C1-C2-N2-C7

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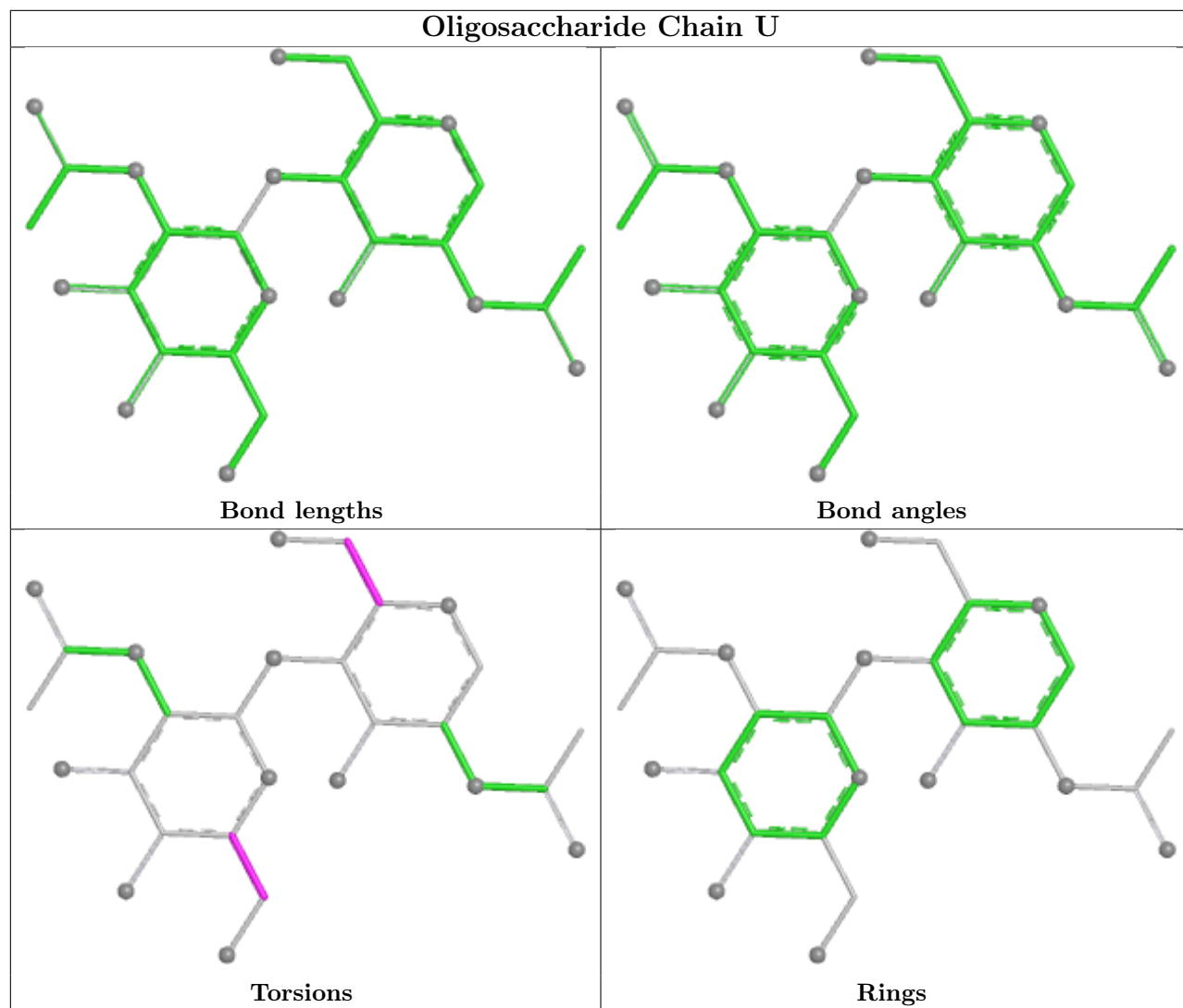
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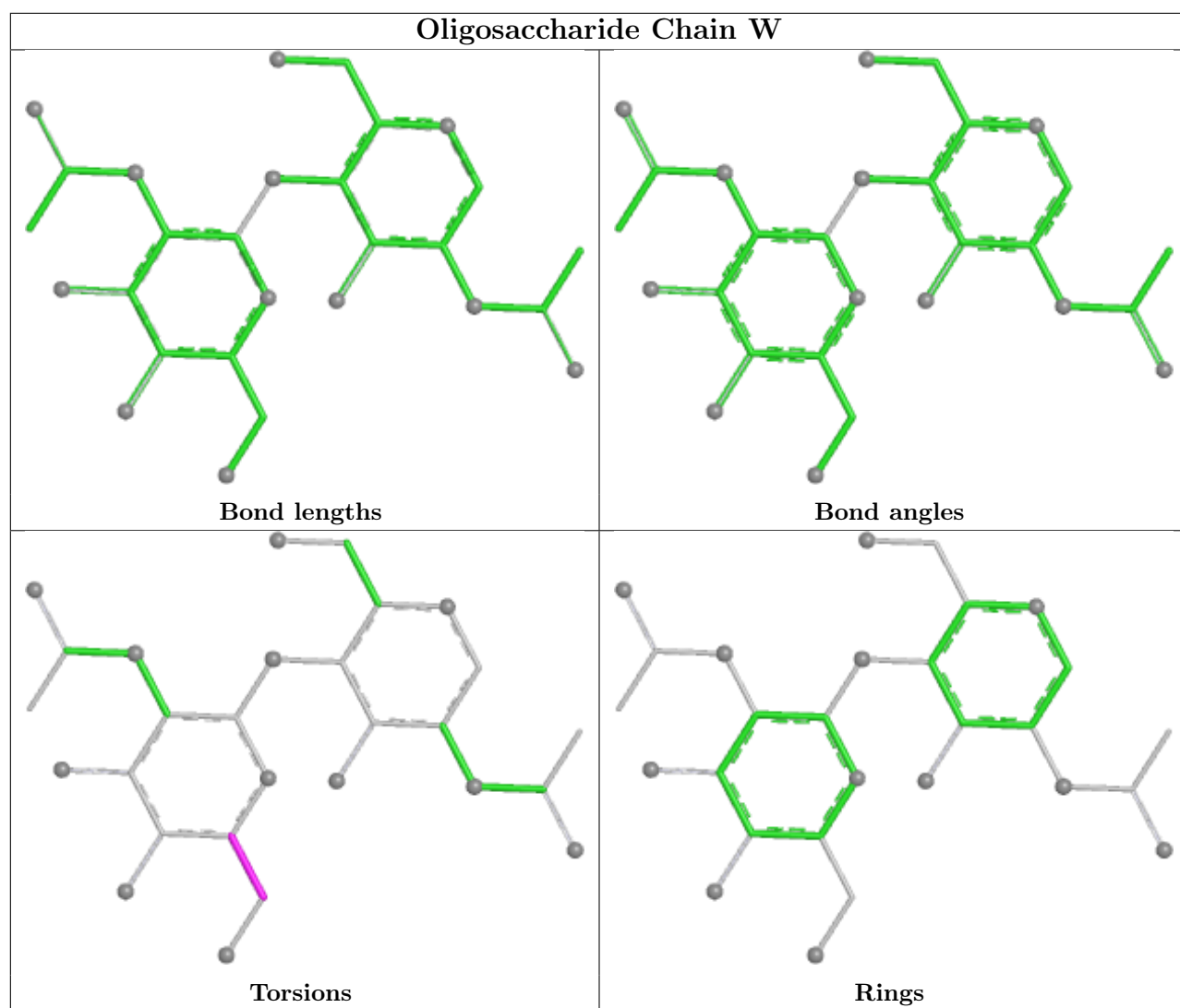
Mol	Chain	Res	Type	Atoms
3	4A	2	NAG	C3-C2-N2-C7
2	x	1	NAG	O5-C5-C6-O6
3	nA	1	NAG	C4-C5-C6-O6
3	OA	2	NAG	C4-C5-C6-O6
3	EA	3	BMA	O5-C5-C6-O6
2	RA	1	NAG	O5-C5-C6-O6
3	6	1	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
2	KA	1	NAG	C4-C5-C6-O6
2	5A	1	NAG	C4-C5-C6-O6
3	1	3	BMA	C4-C5-C6-O6
2	AA	1	NAG	C4-C5-C6-O6
3	4	2	NAG	C4-C5-C6-O6
3	u	1	NAG	C4-C5-C6-O6
3	VA	1	NAG	C4-C5-C6-O6

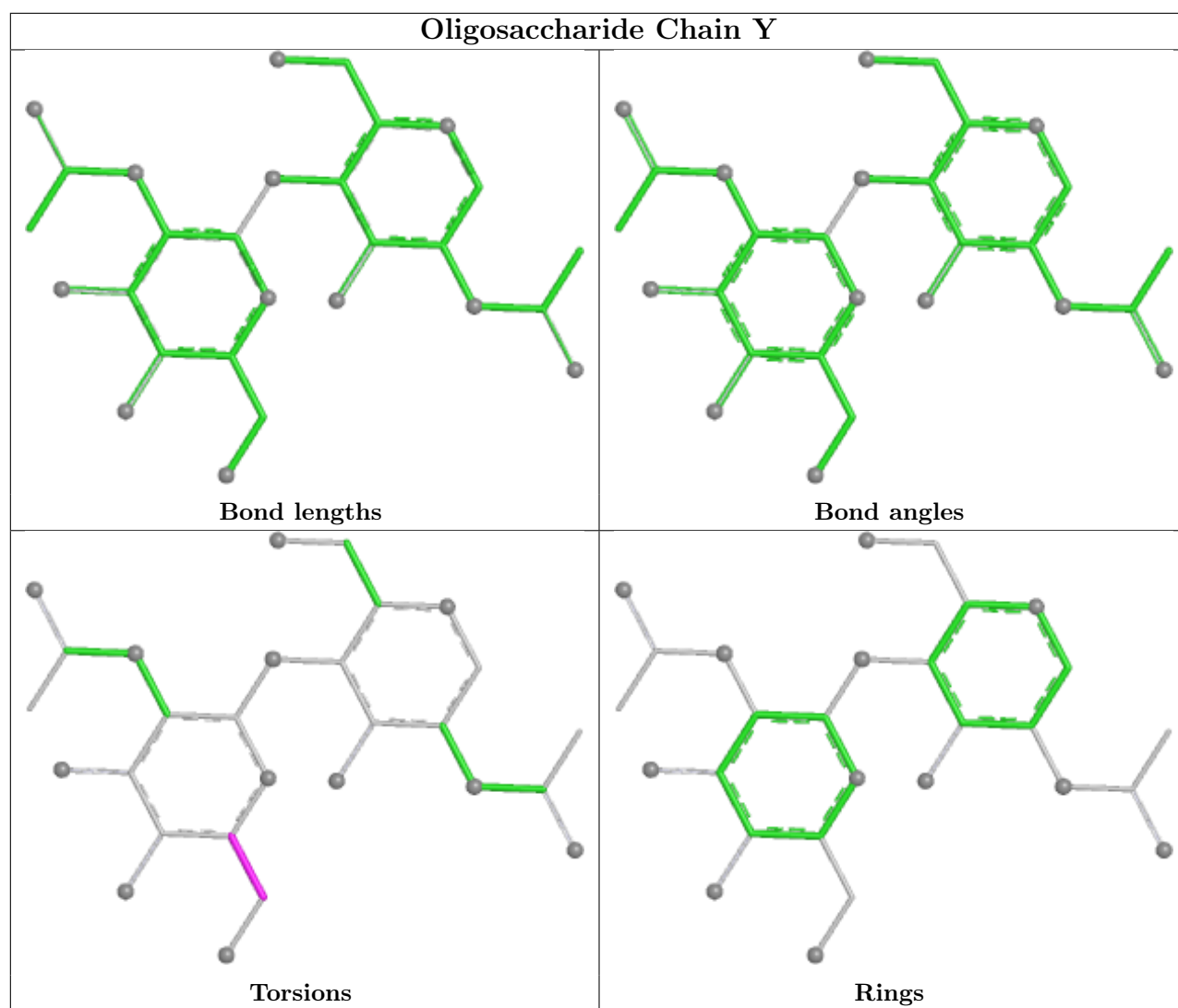
There are no ring outliers.

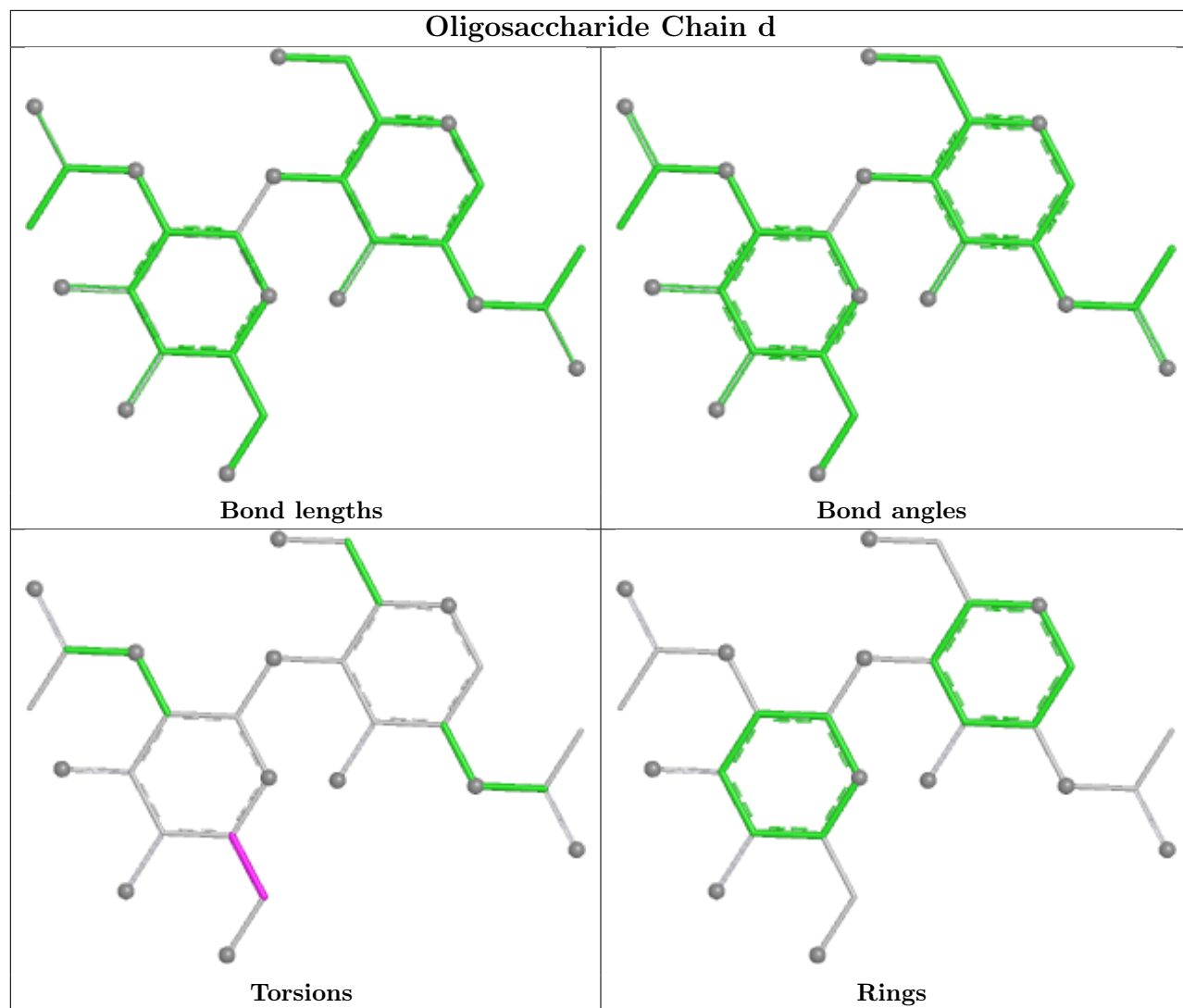
No monomer is involved in short contacts.

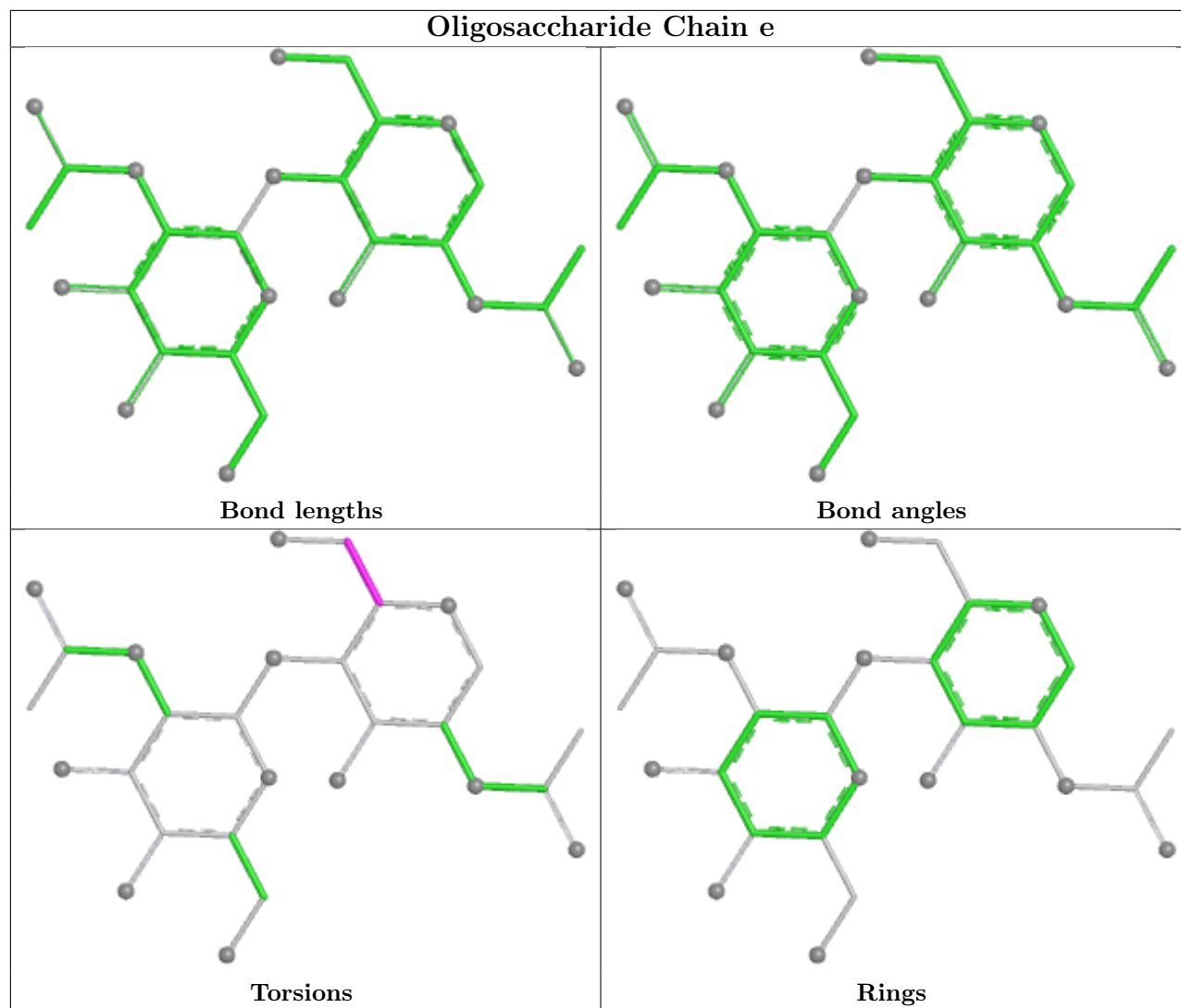
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

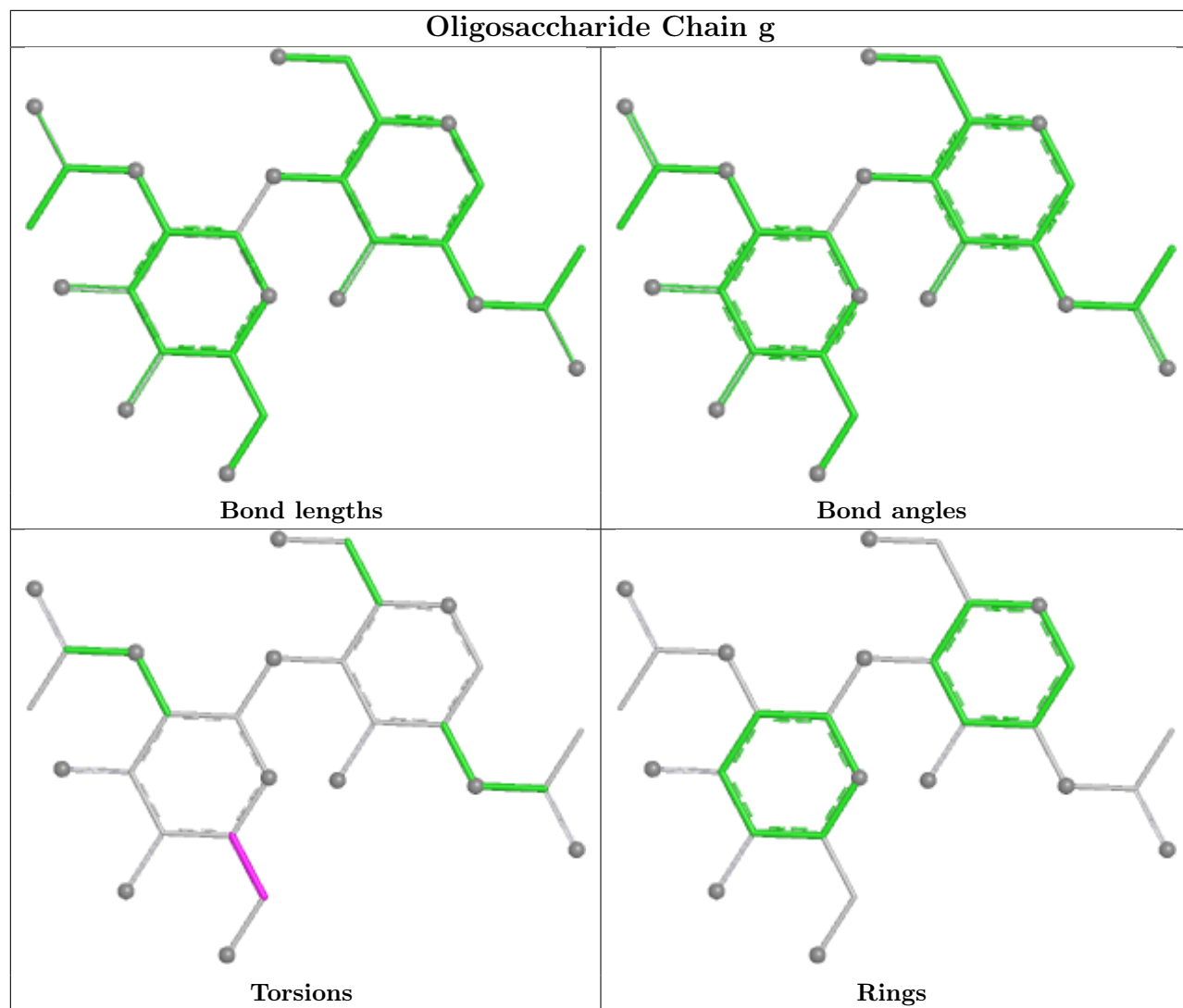


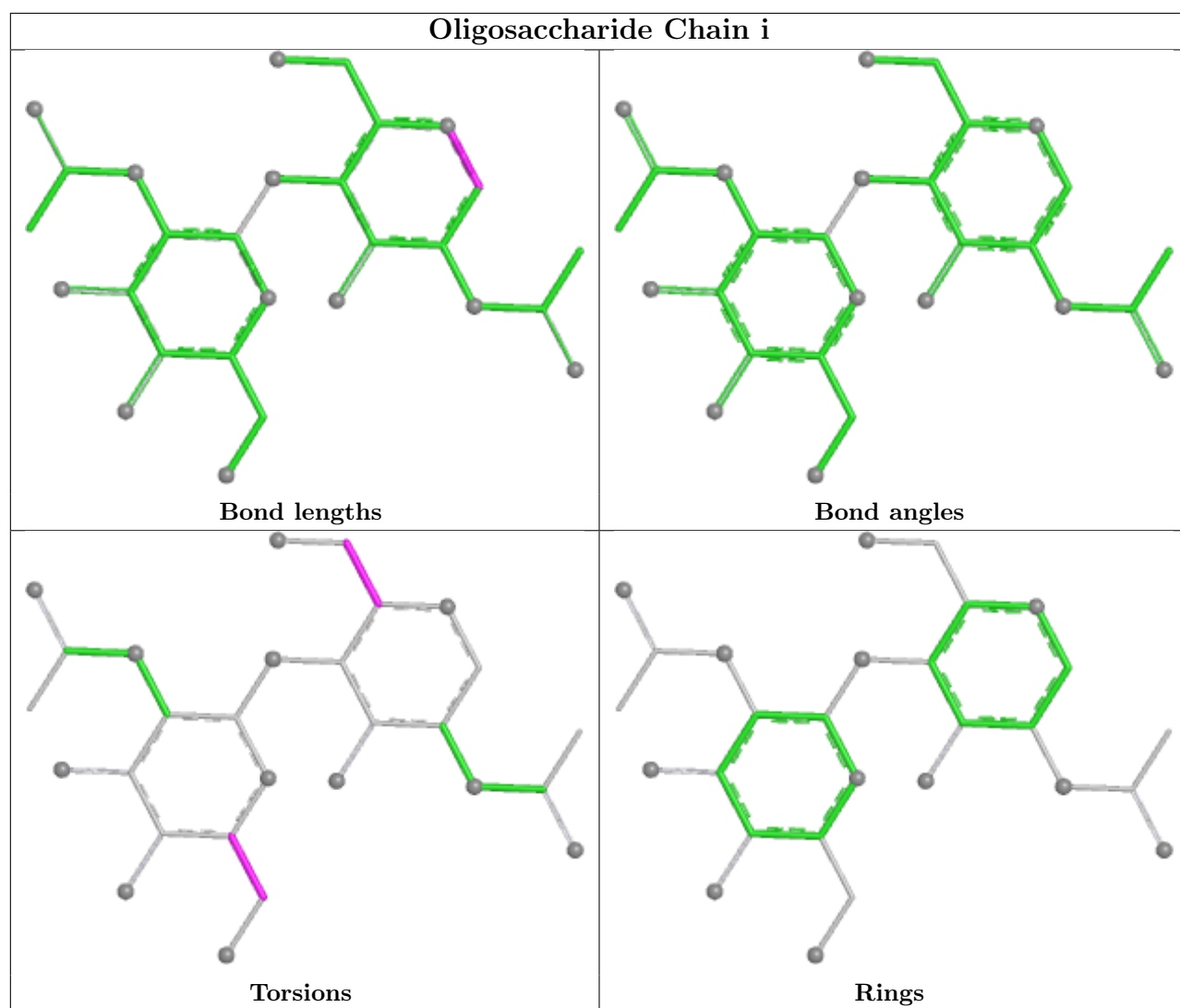


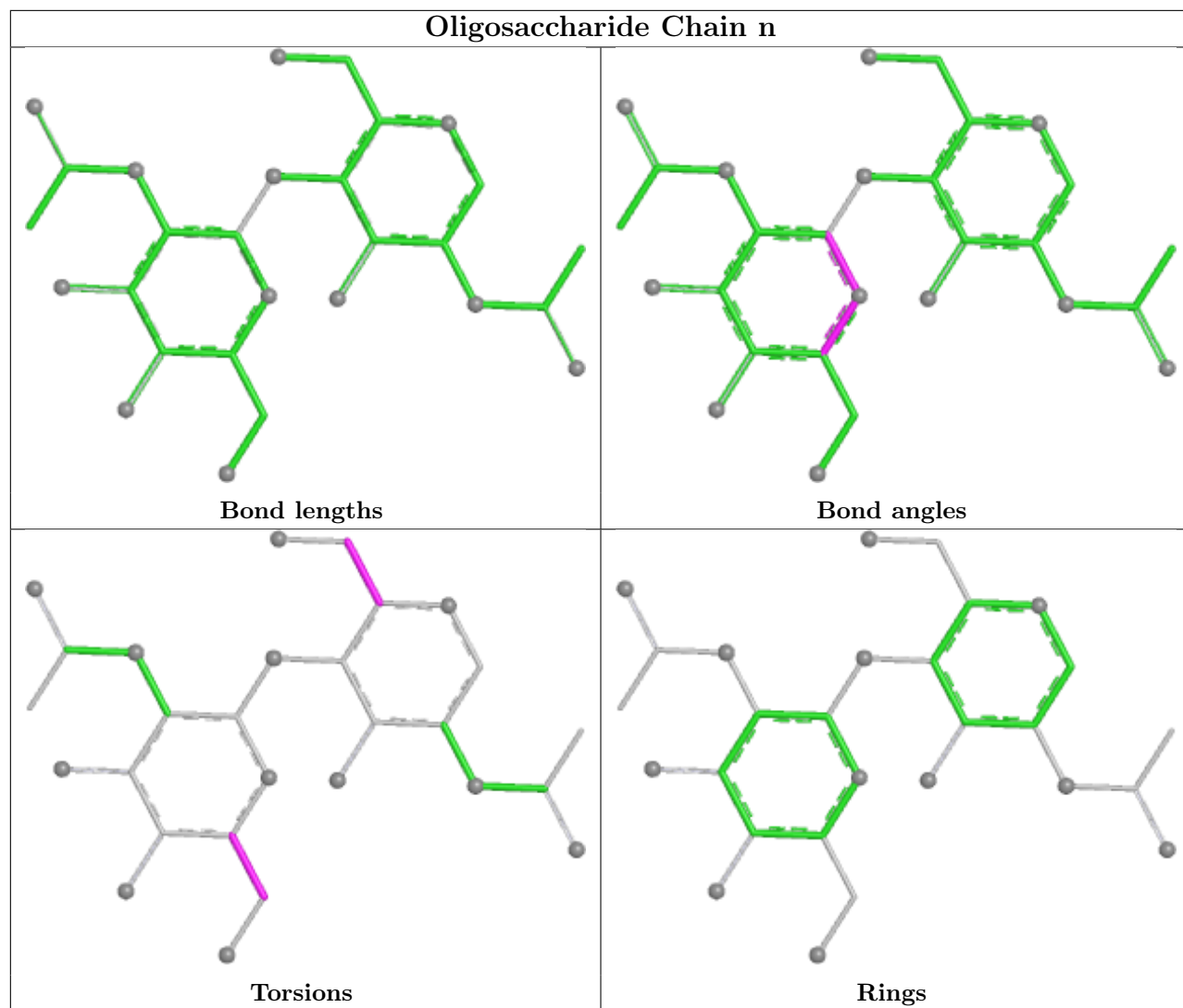


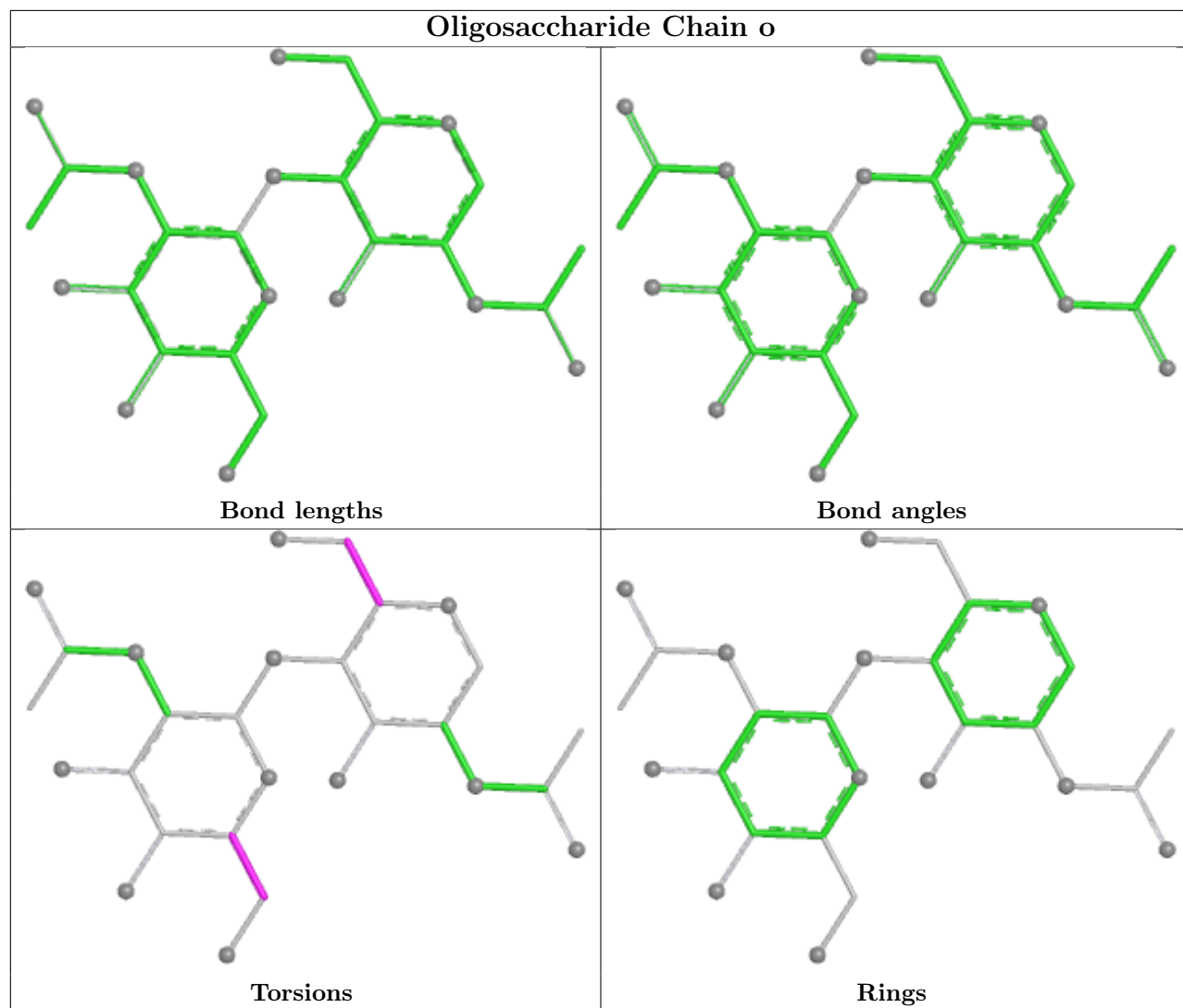


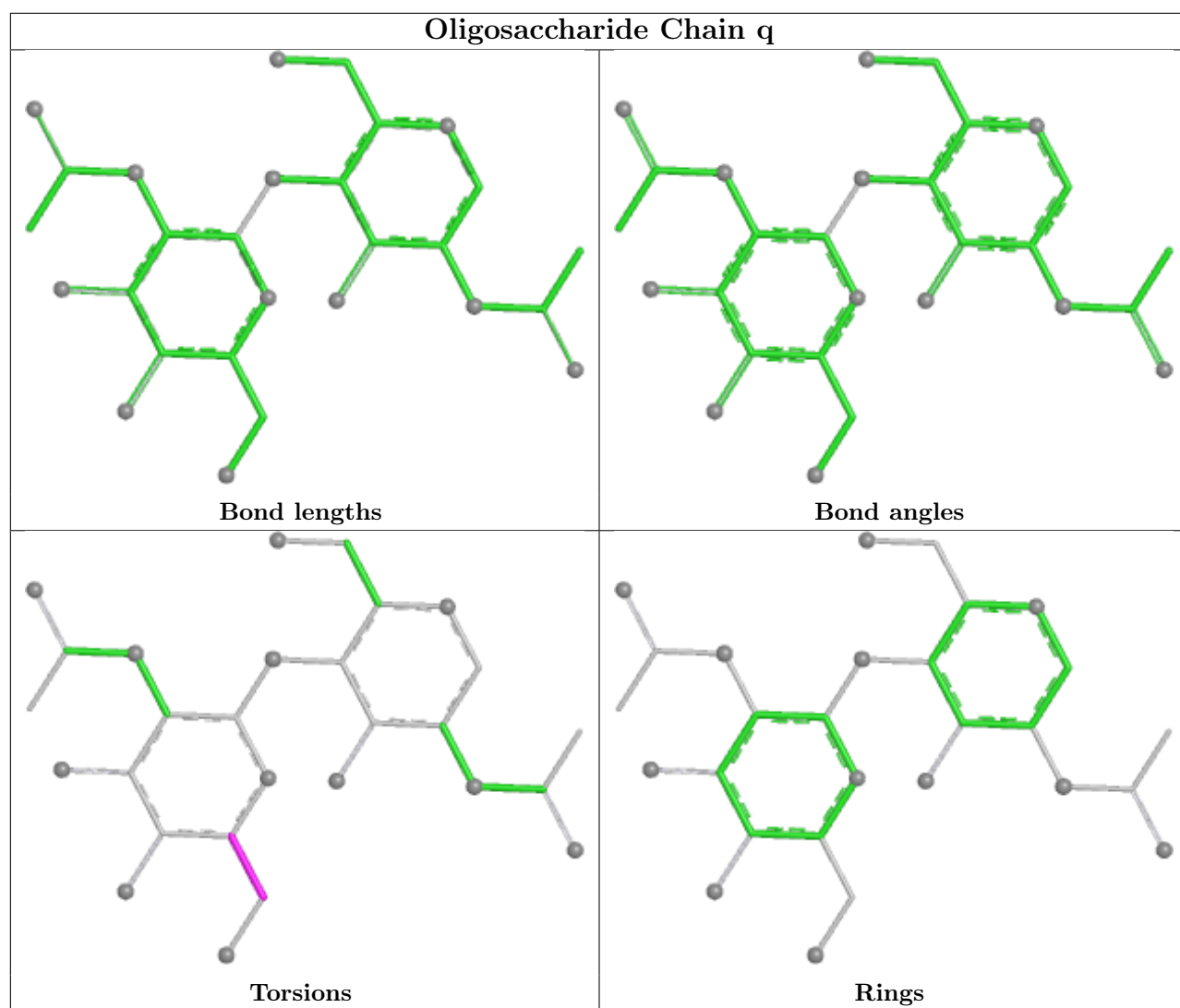


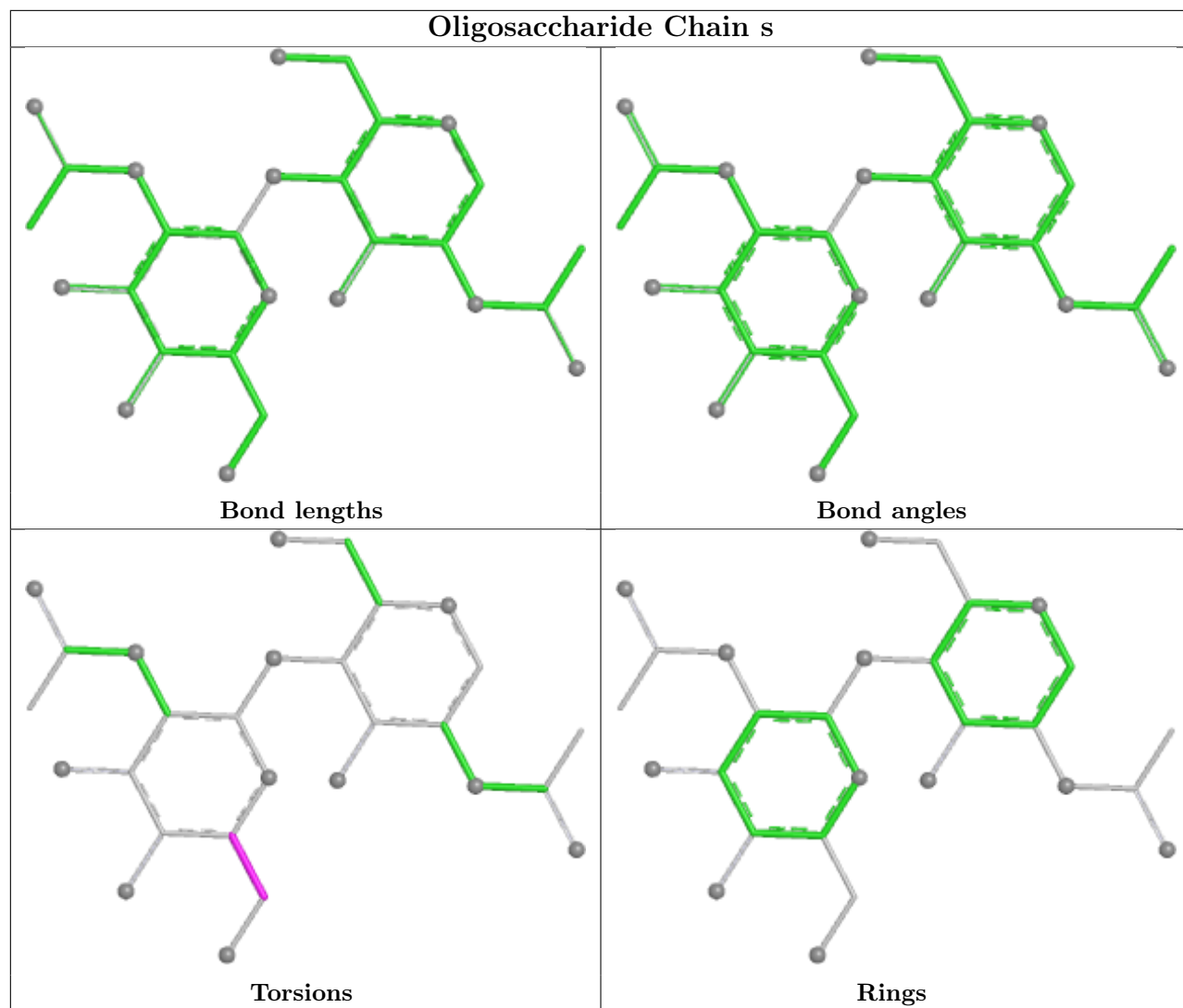


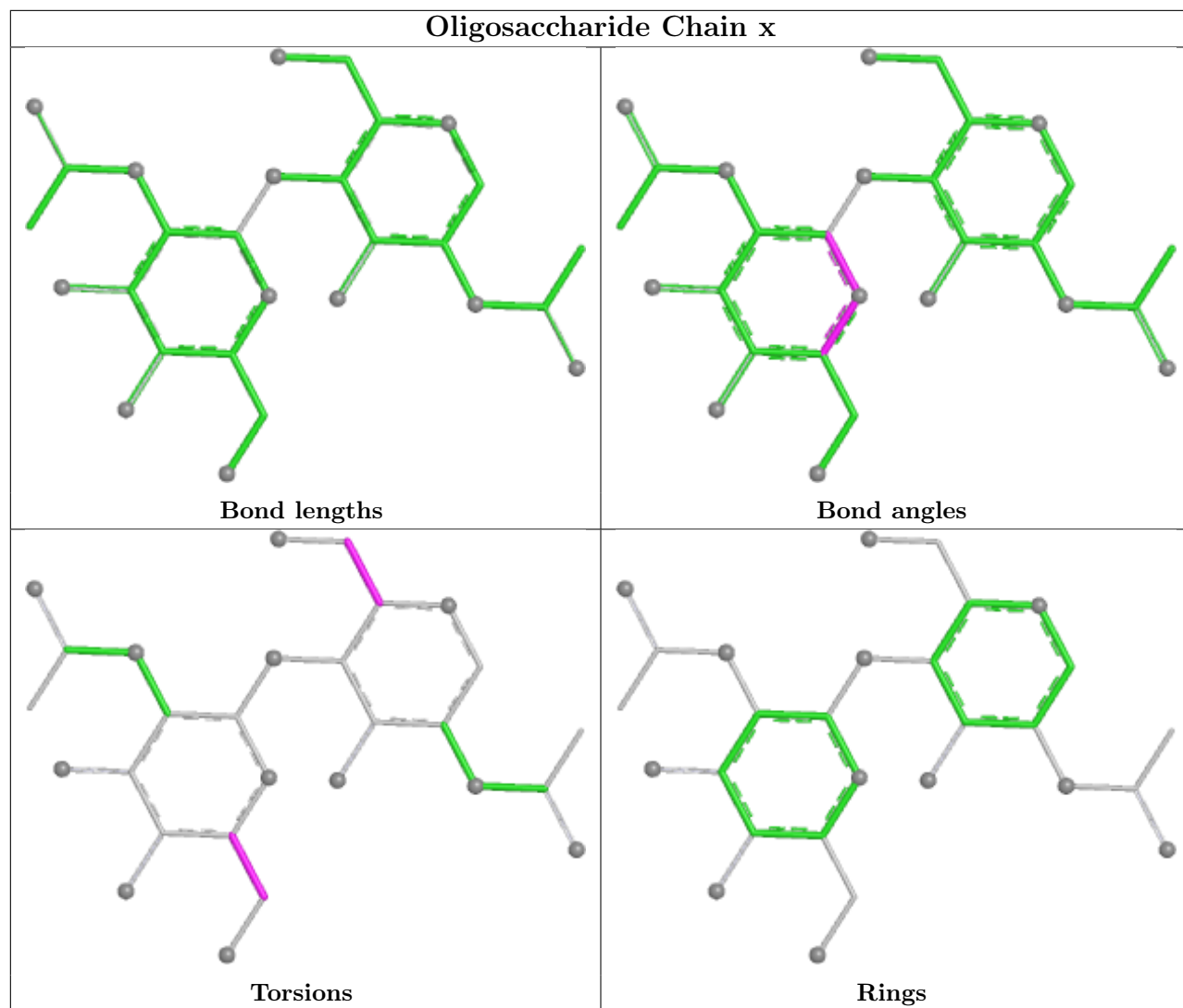


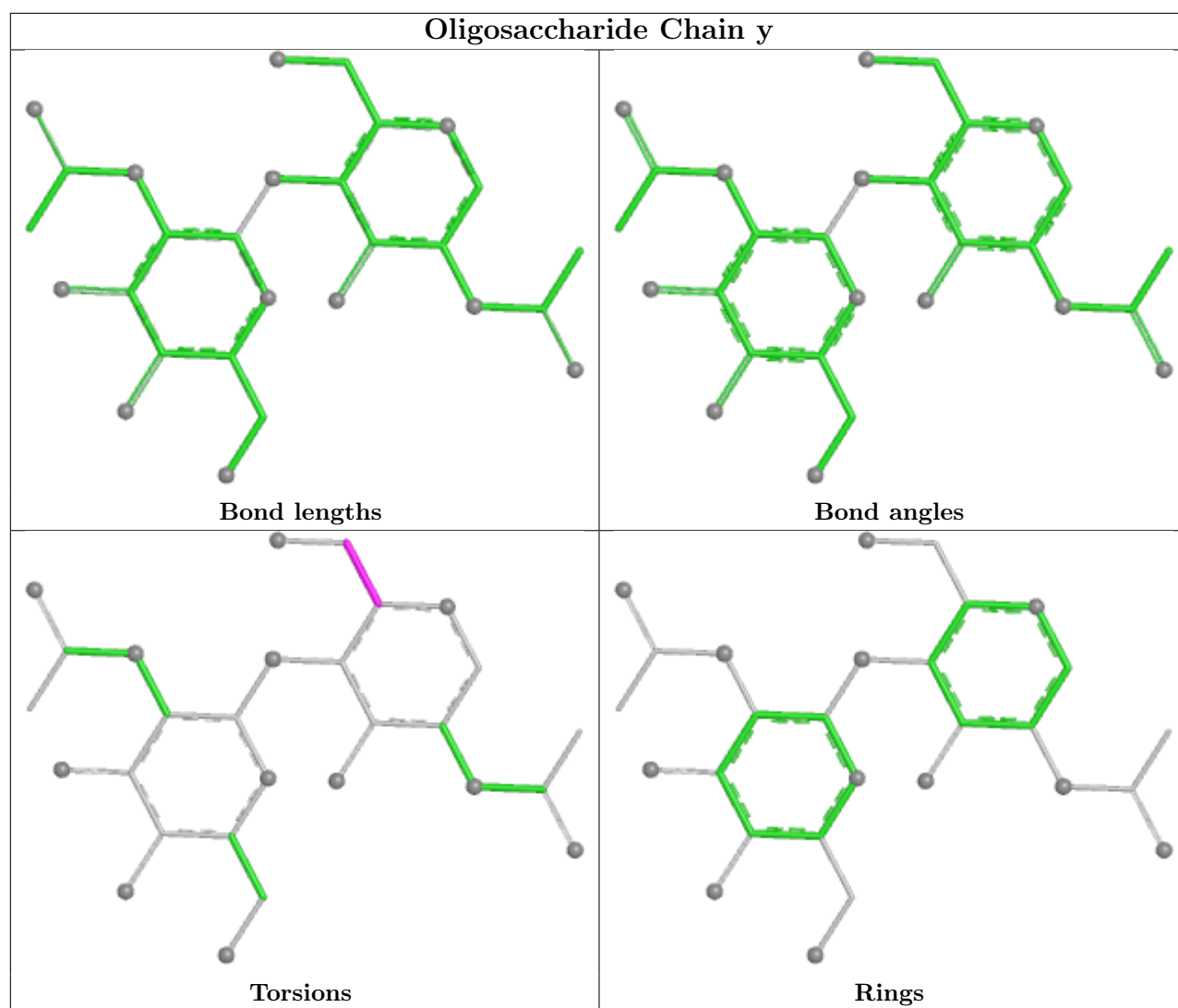


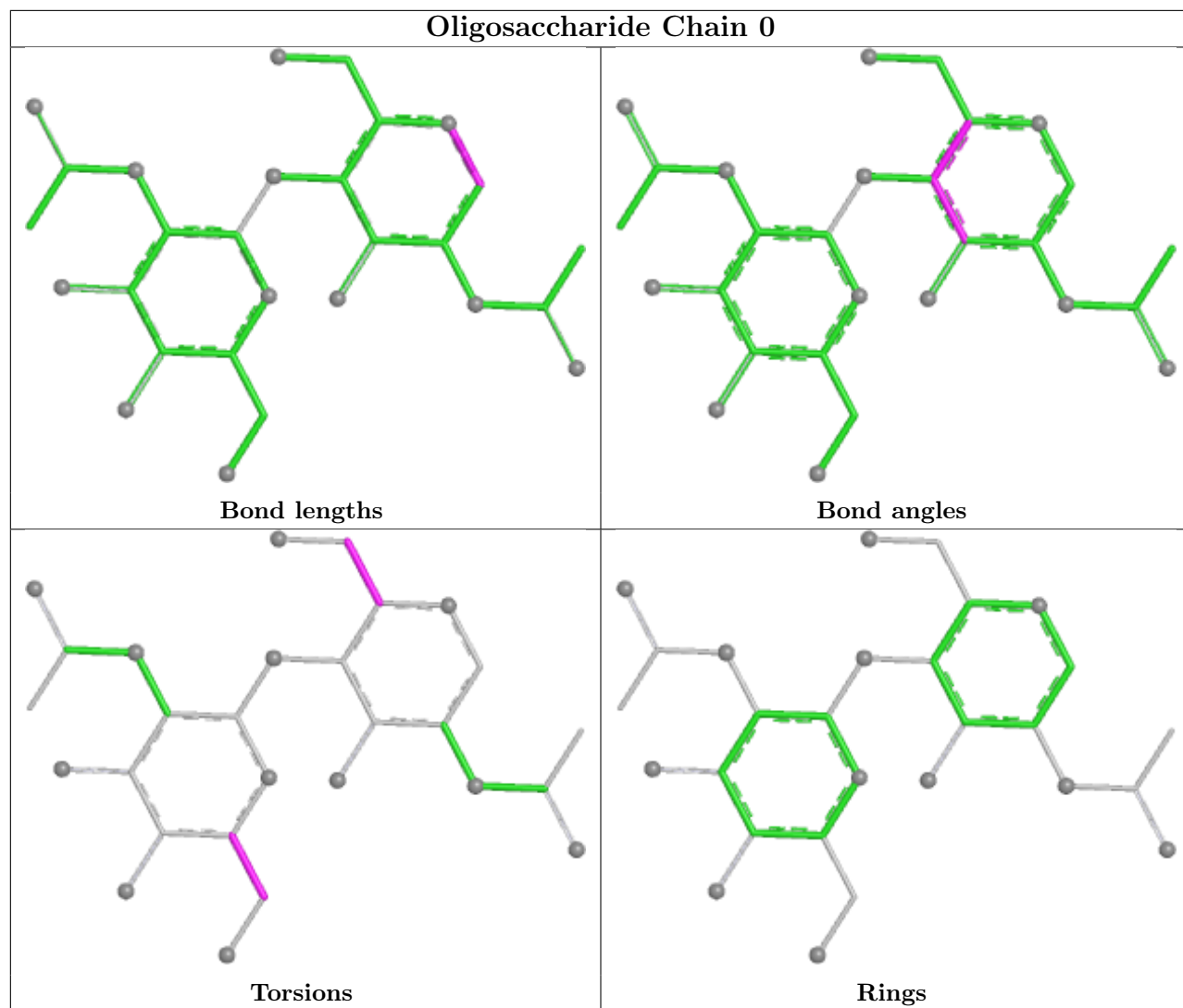


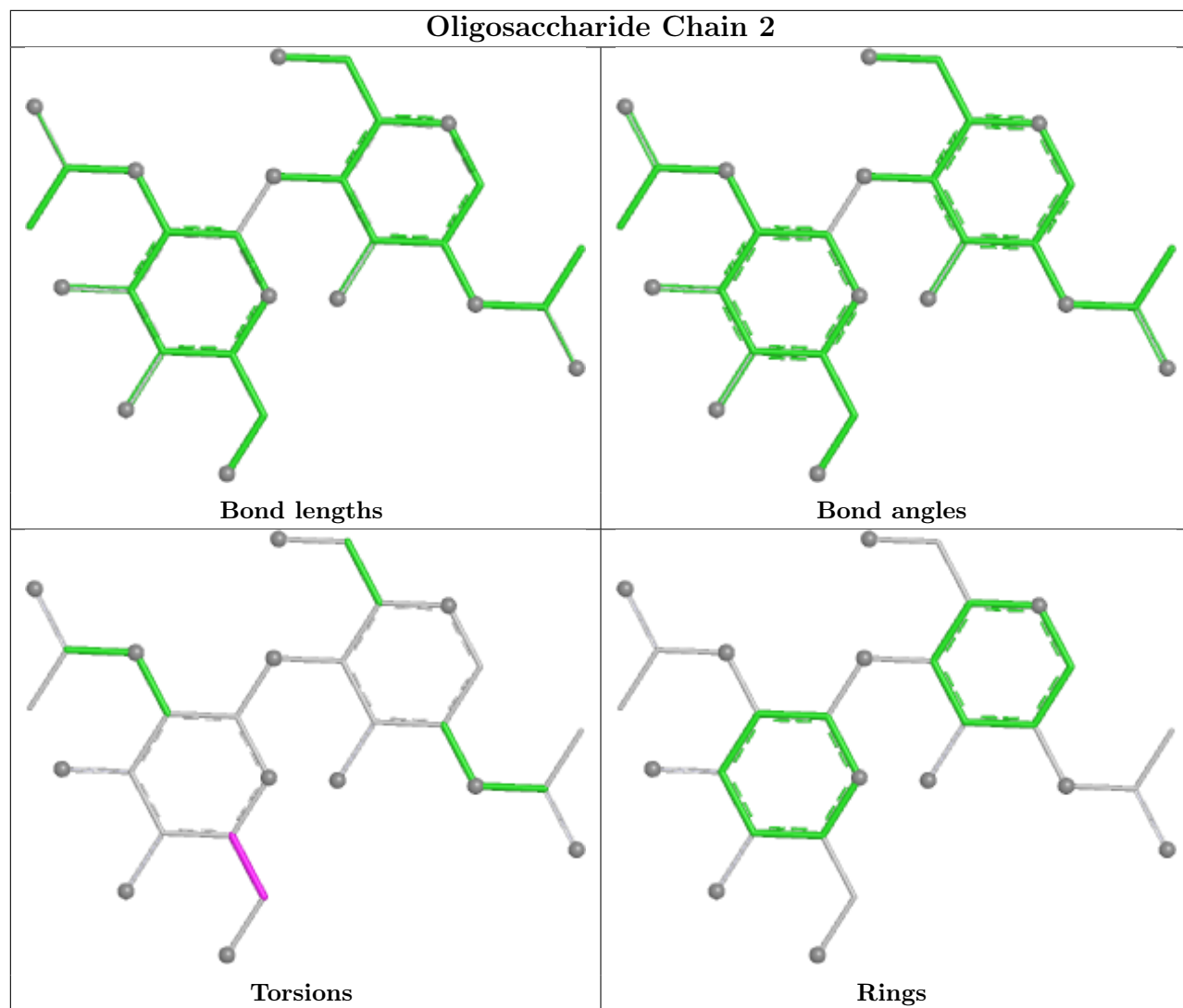


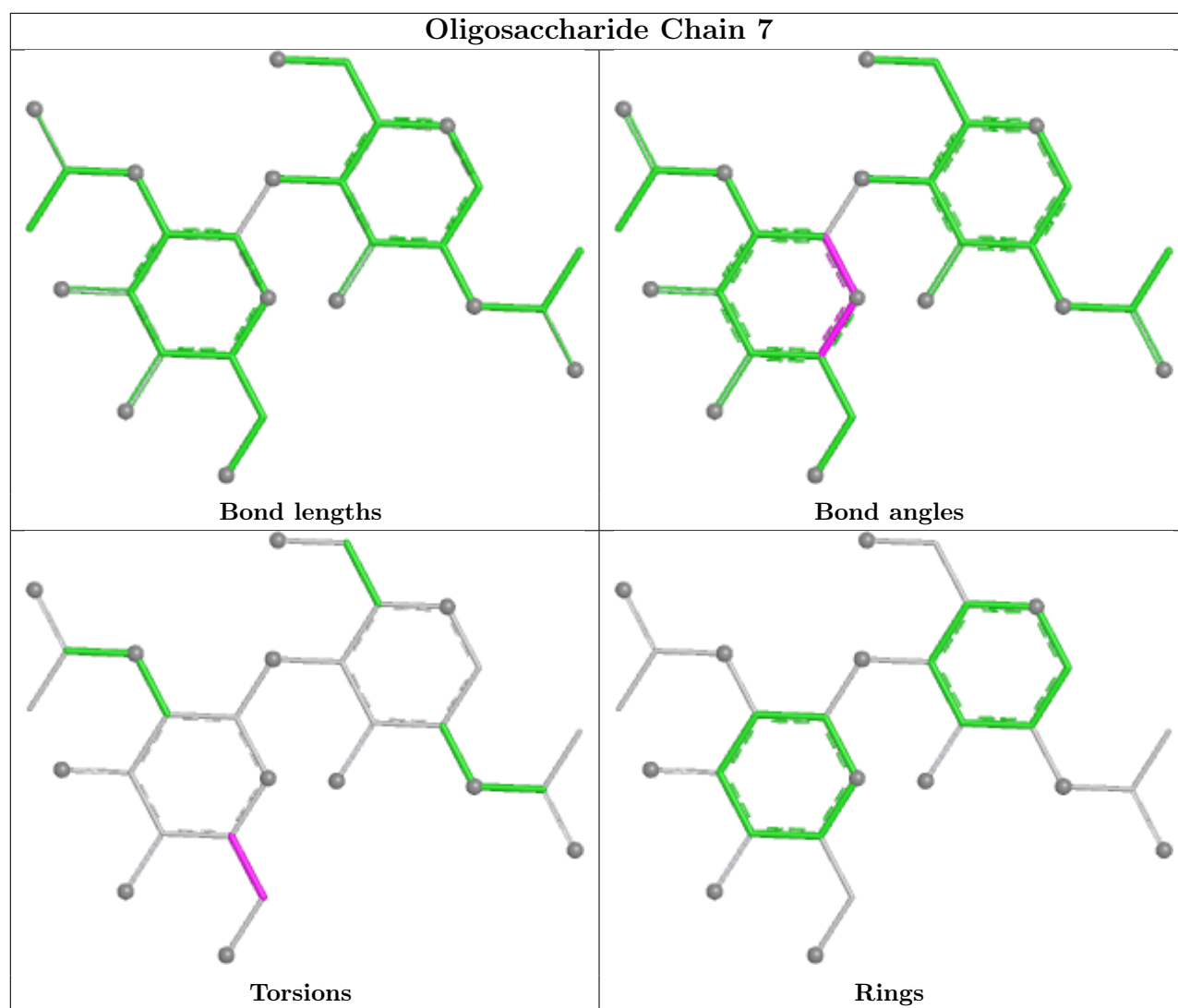


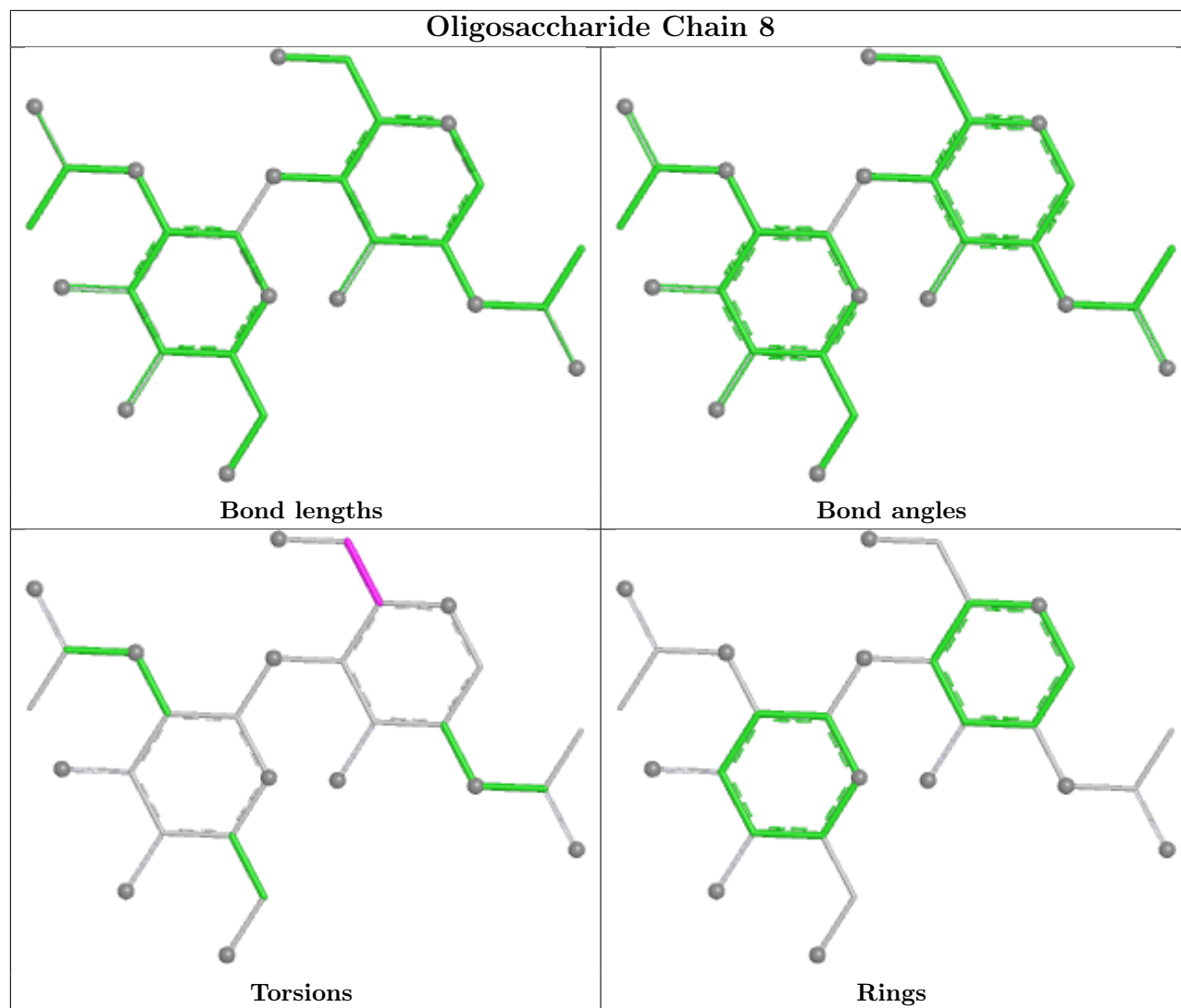


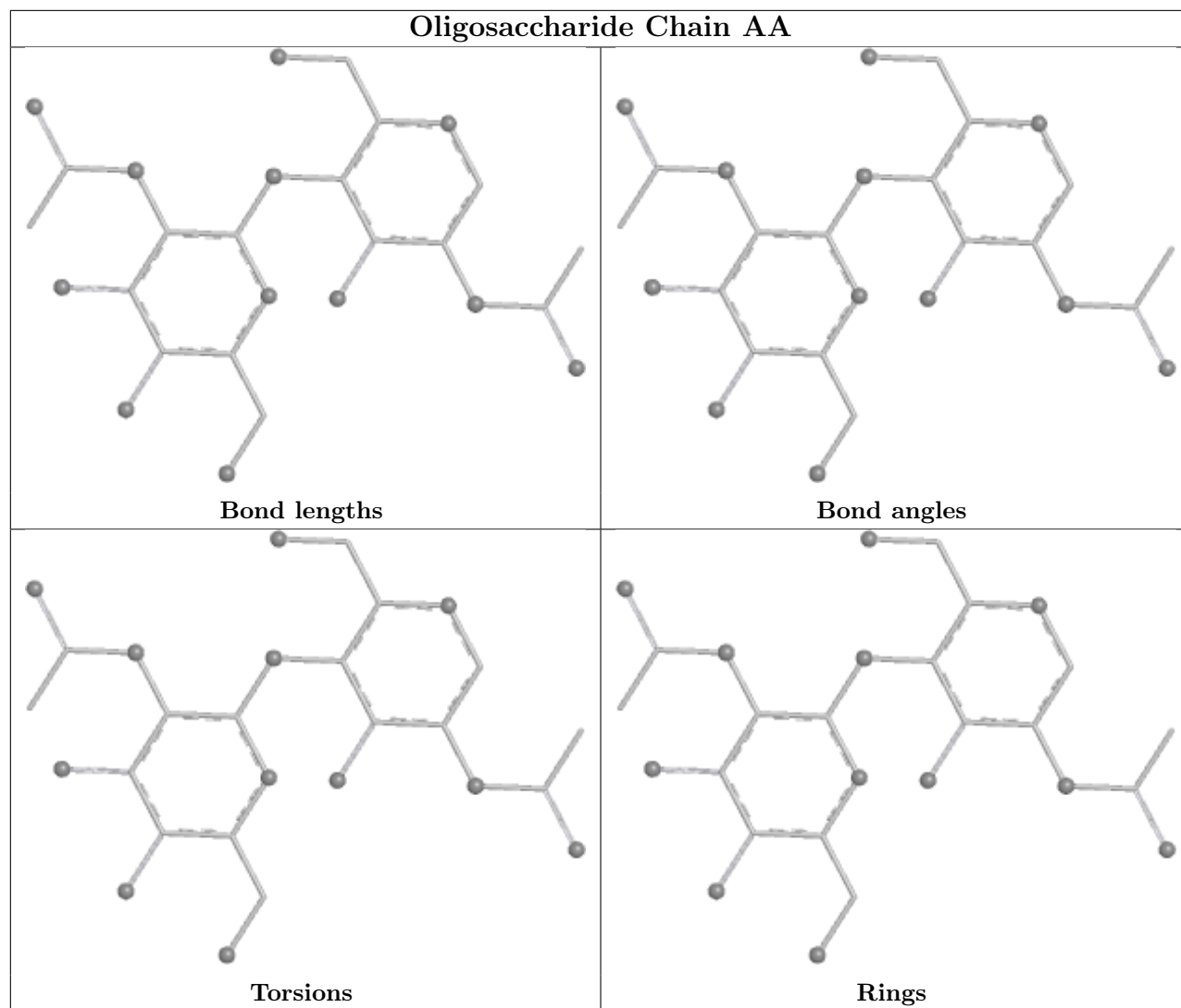


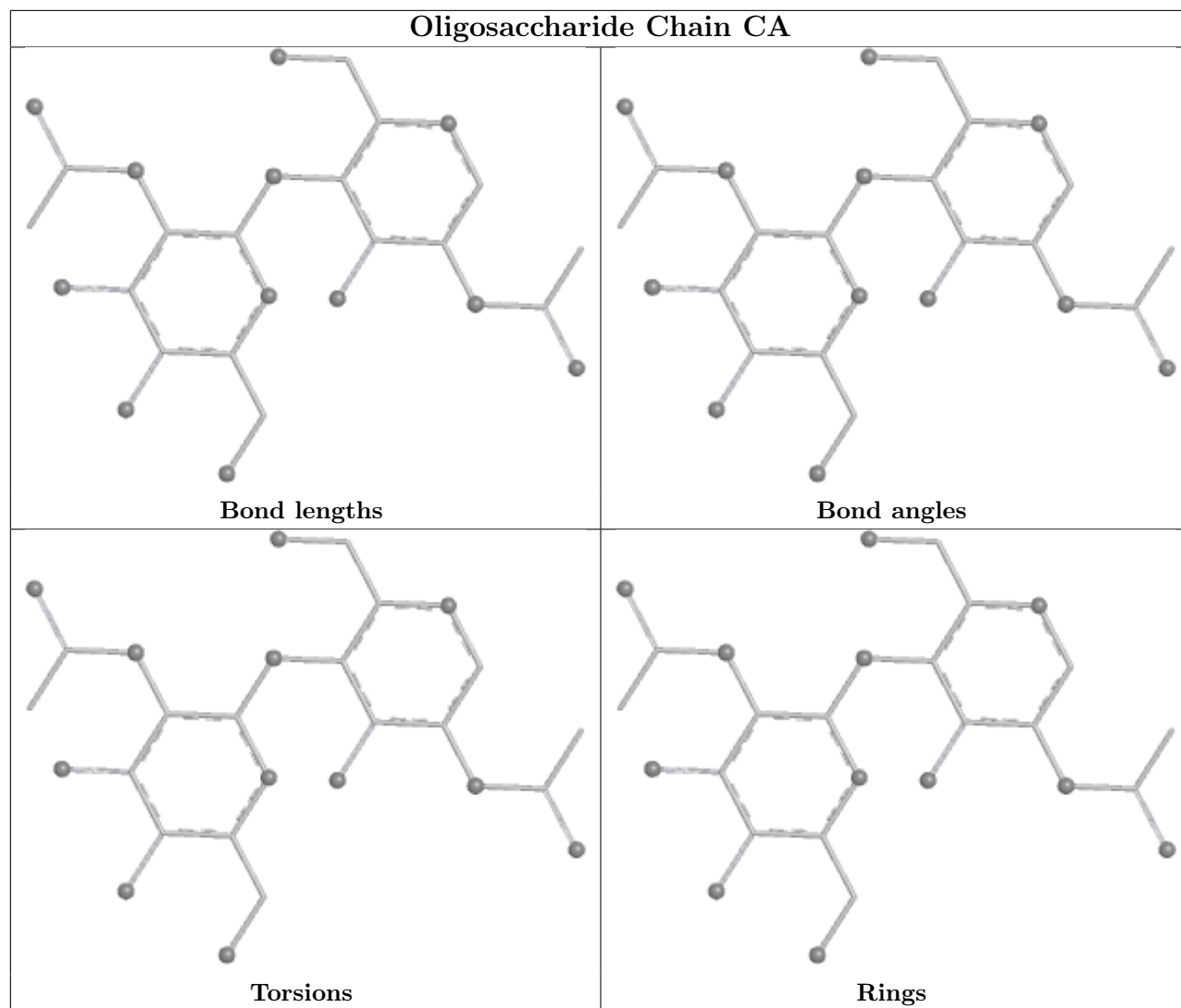


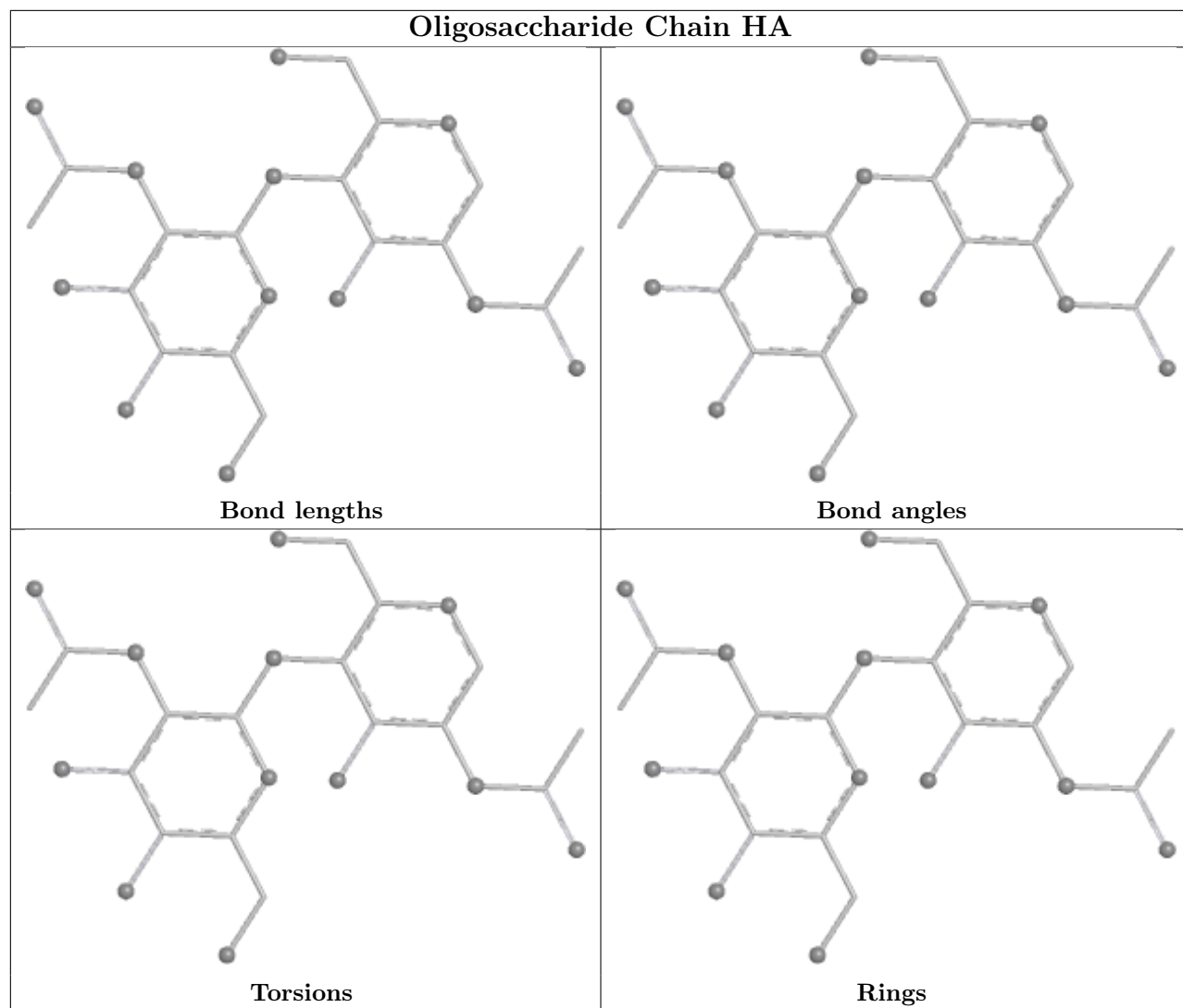


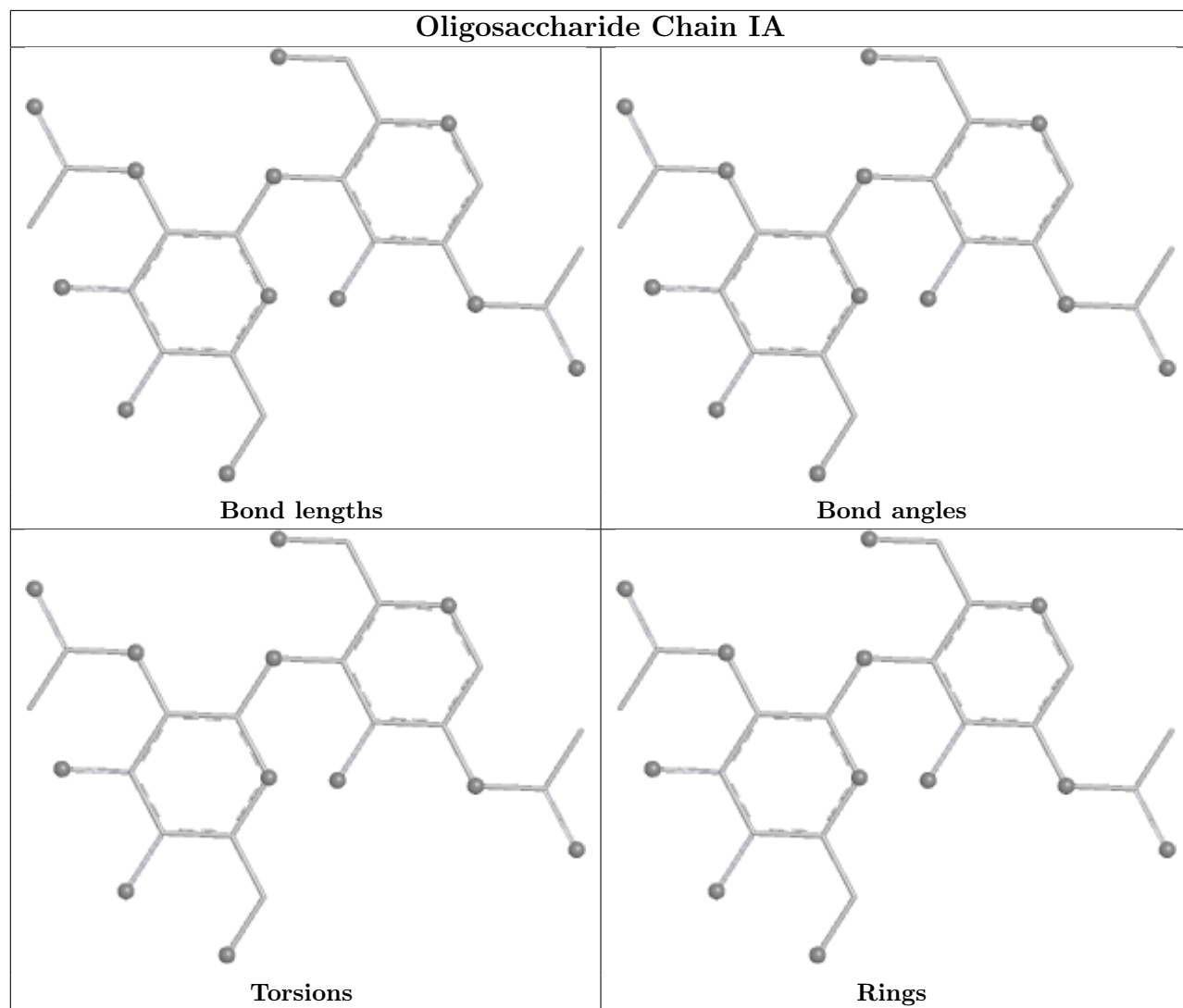


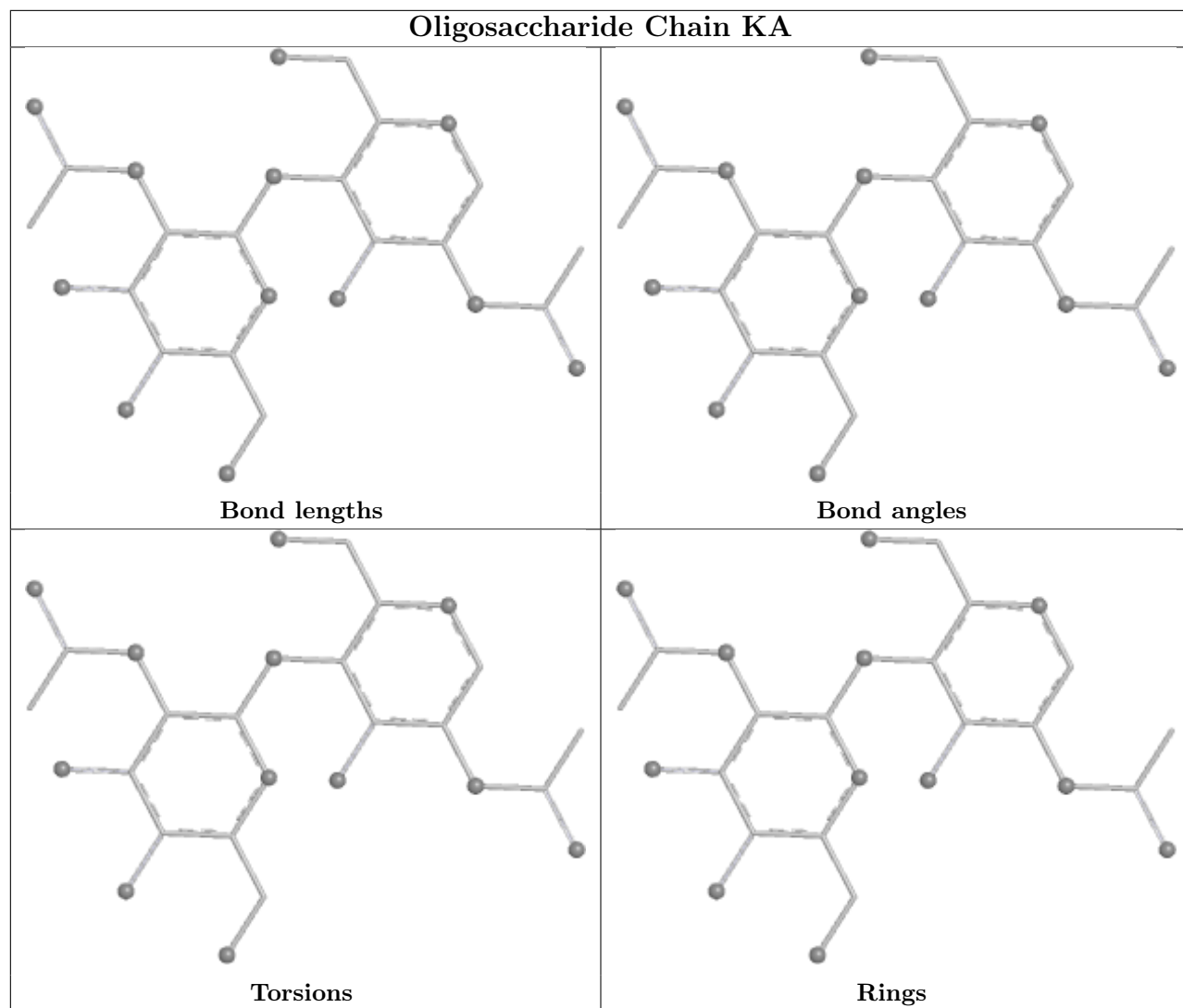


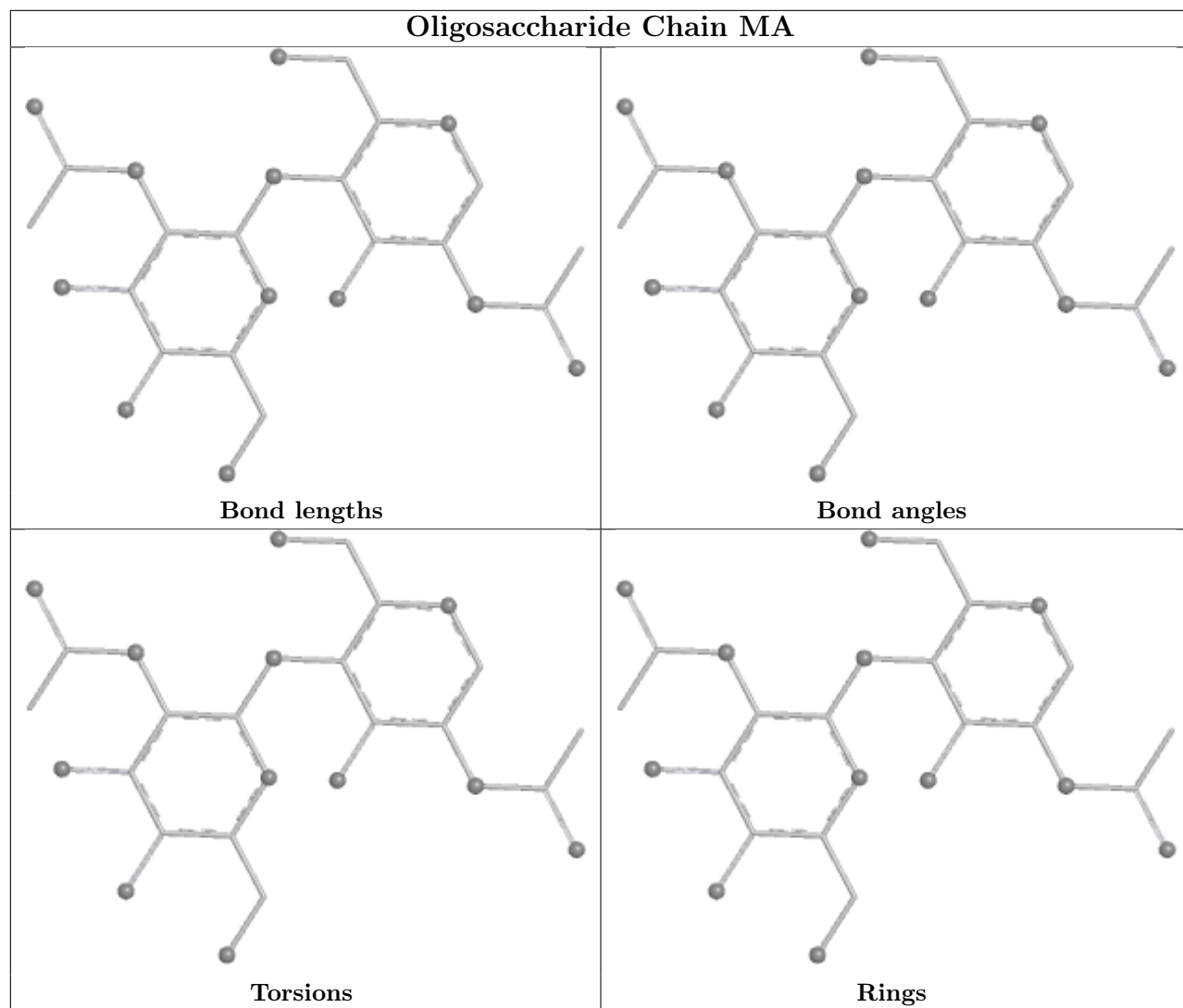


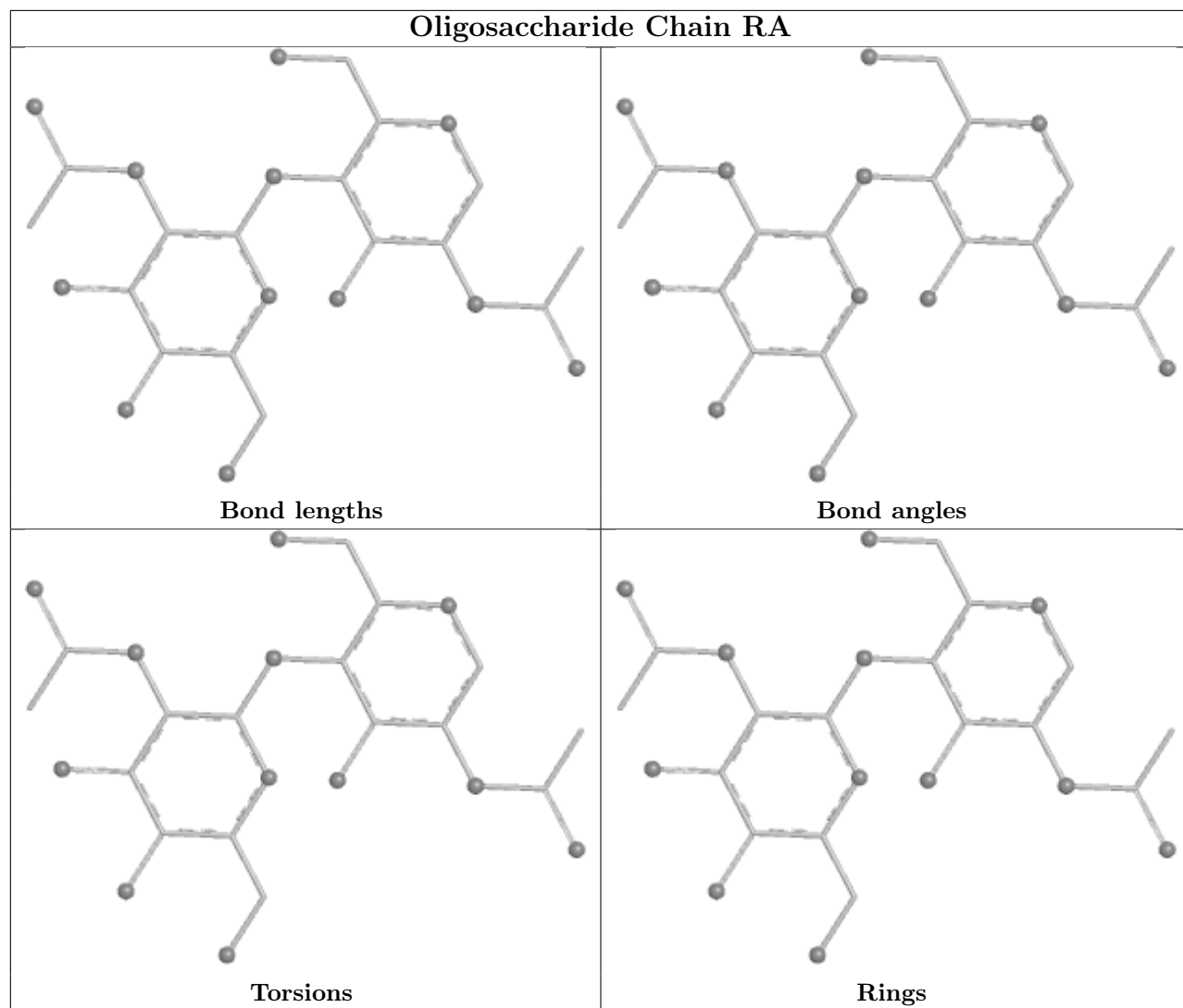


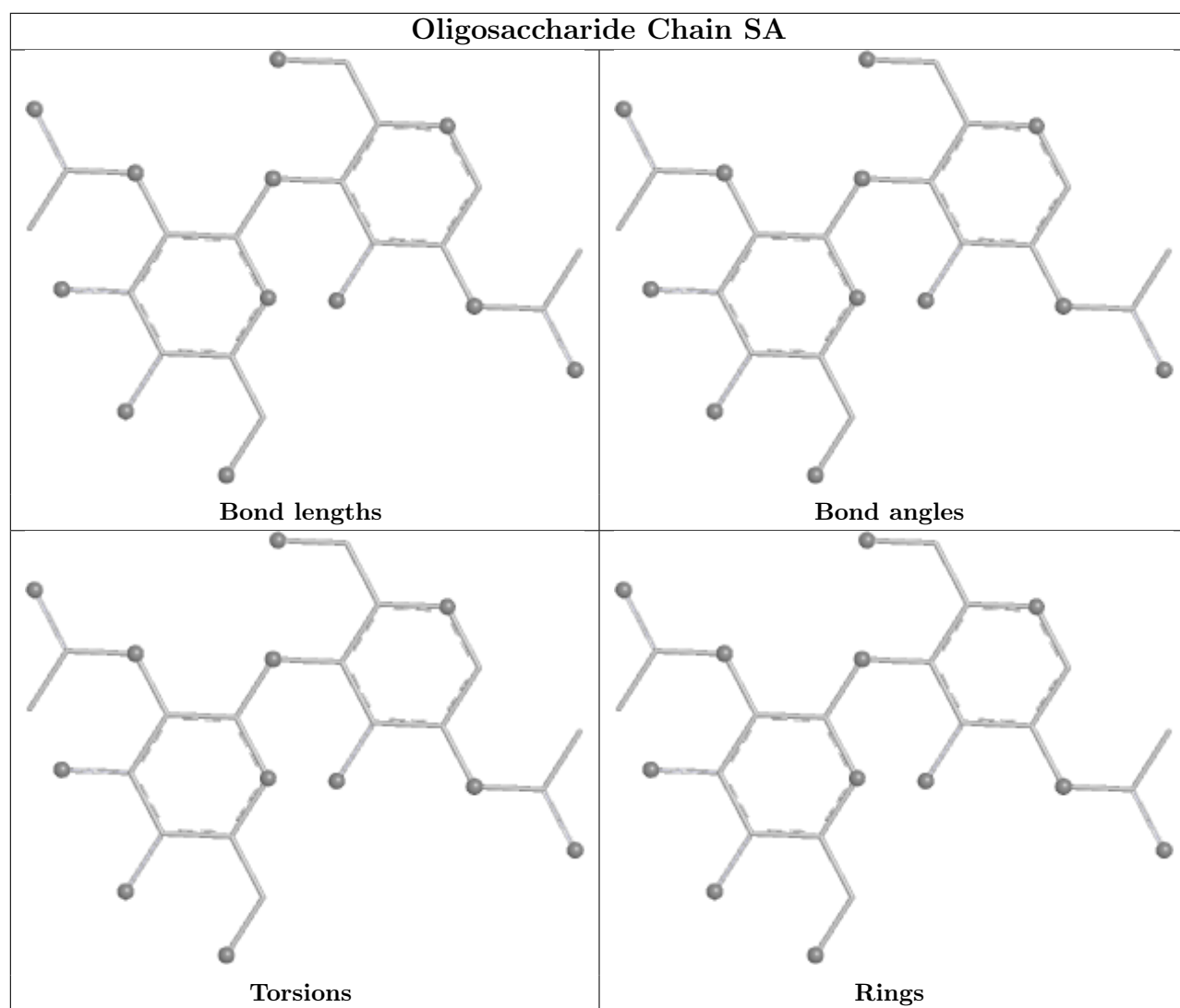


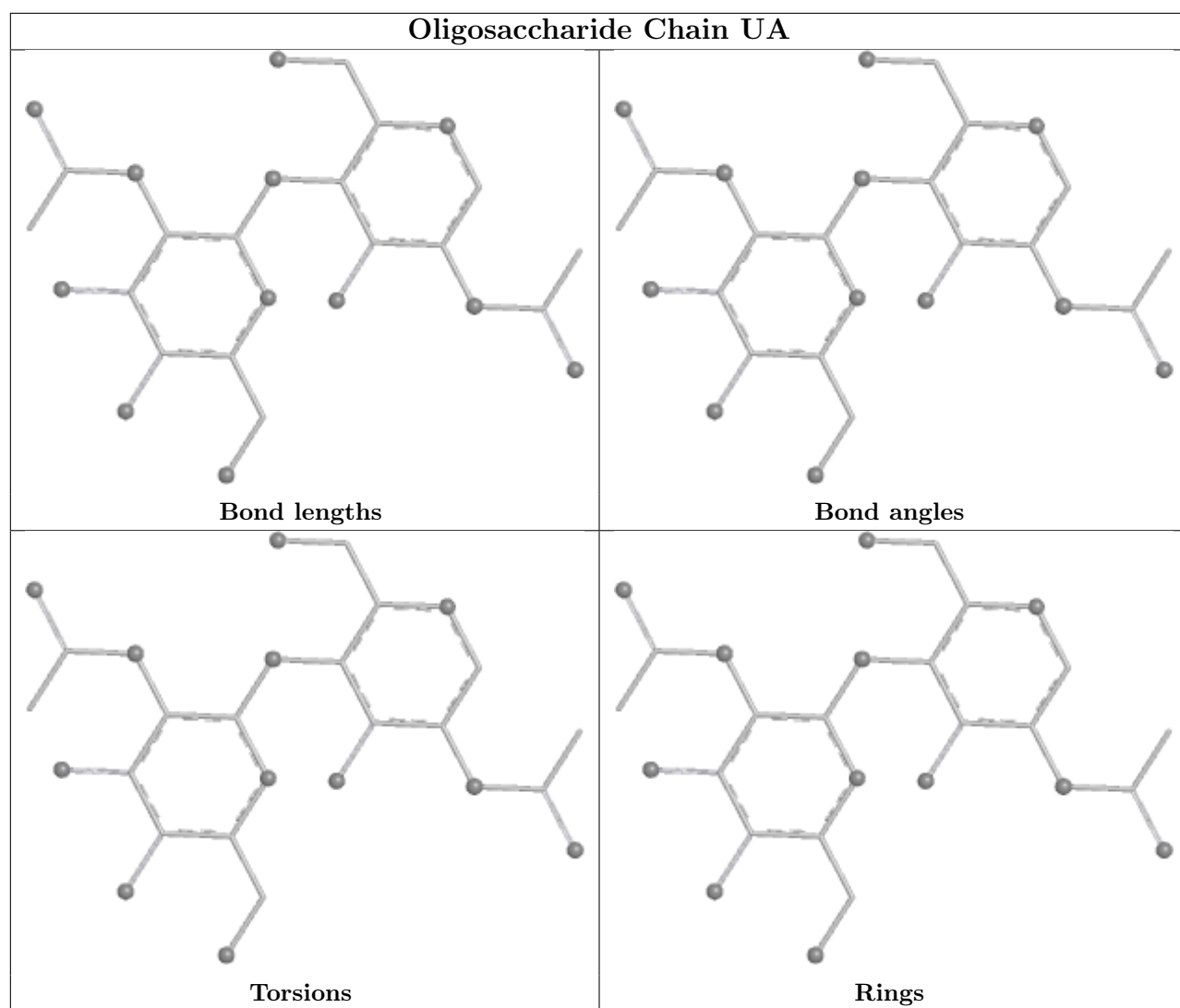


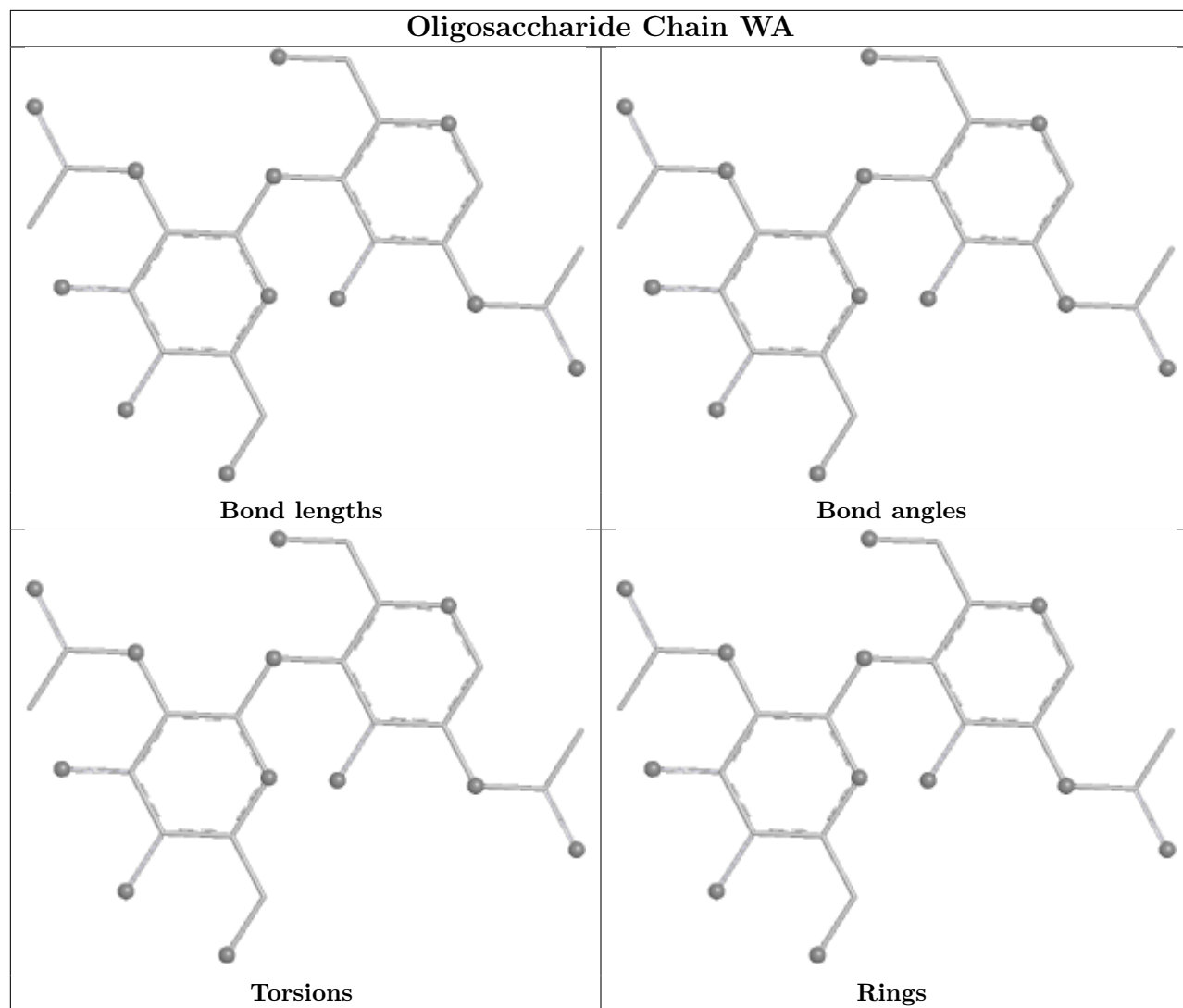


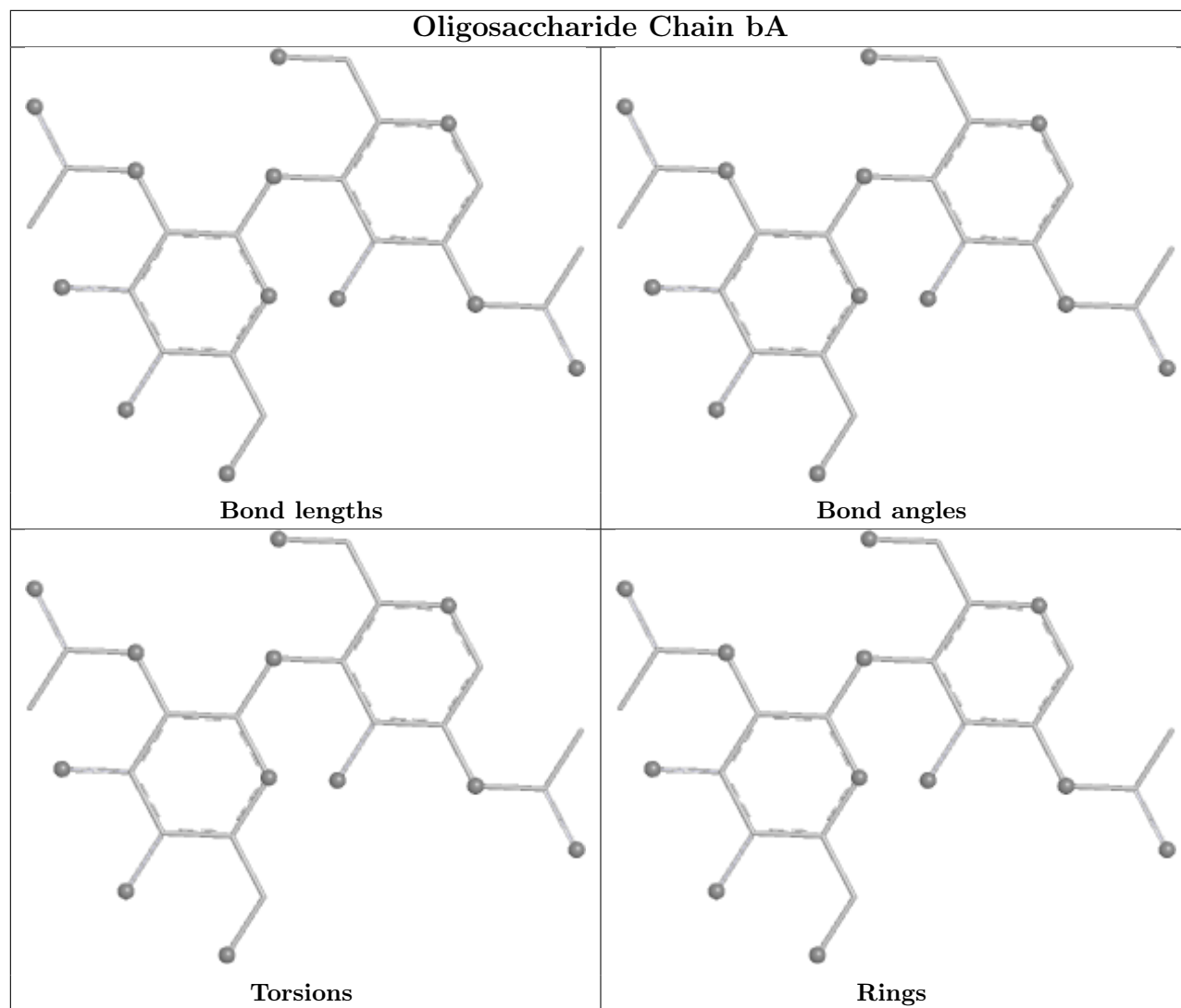


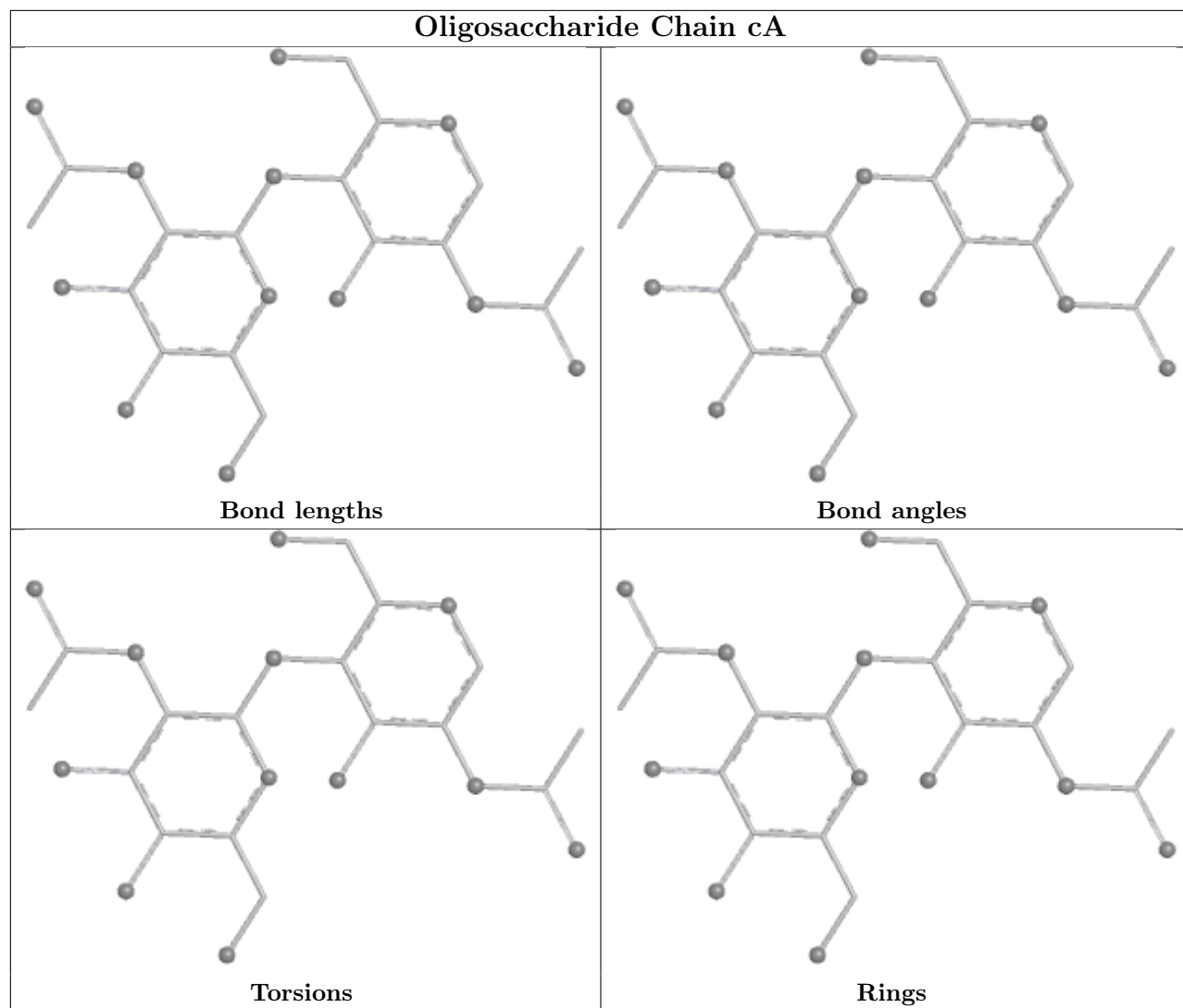


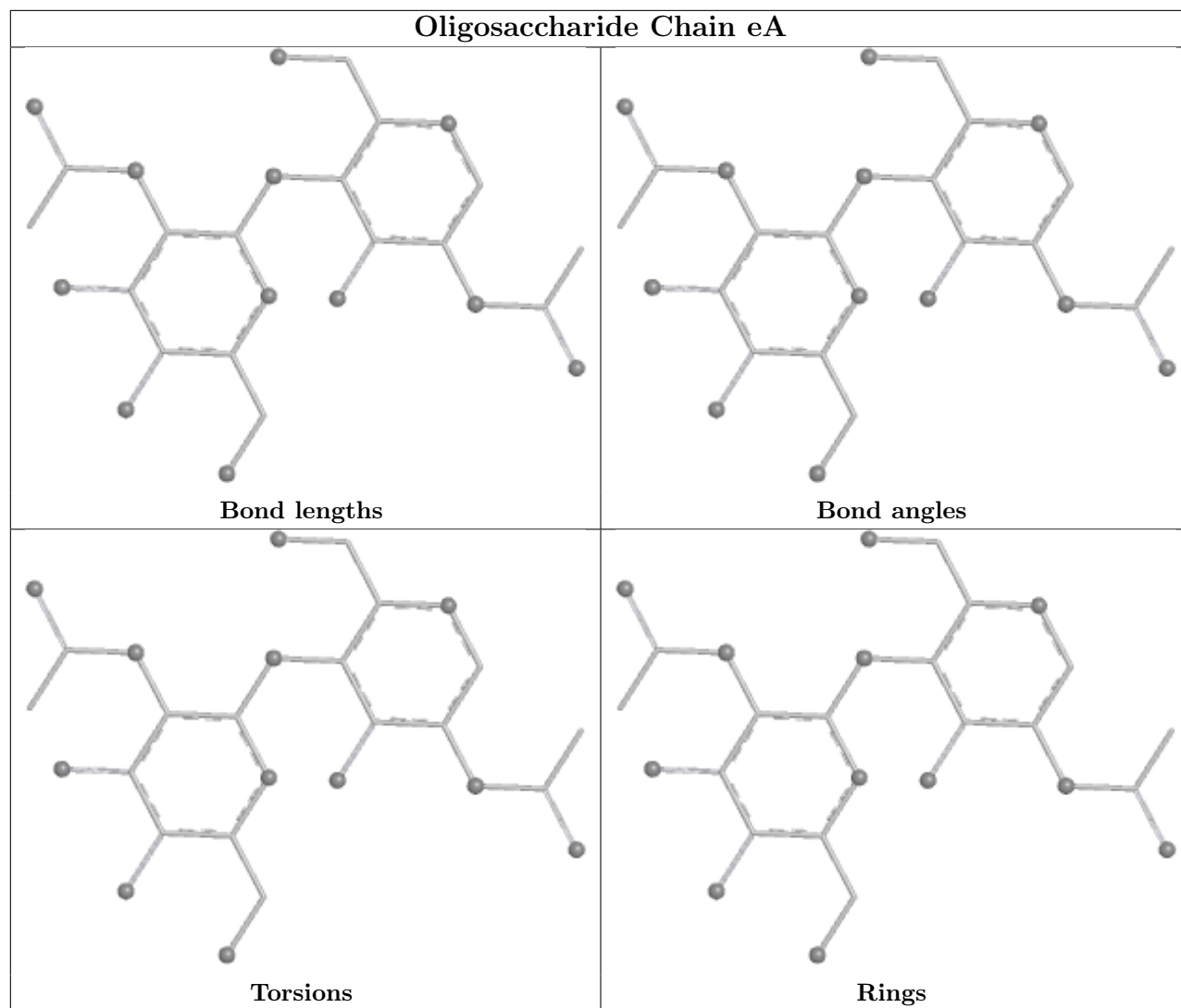


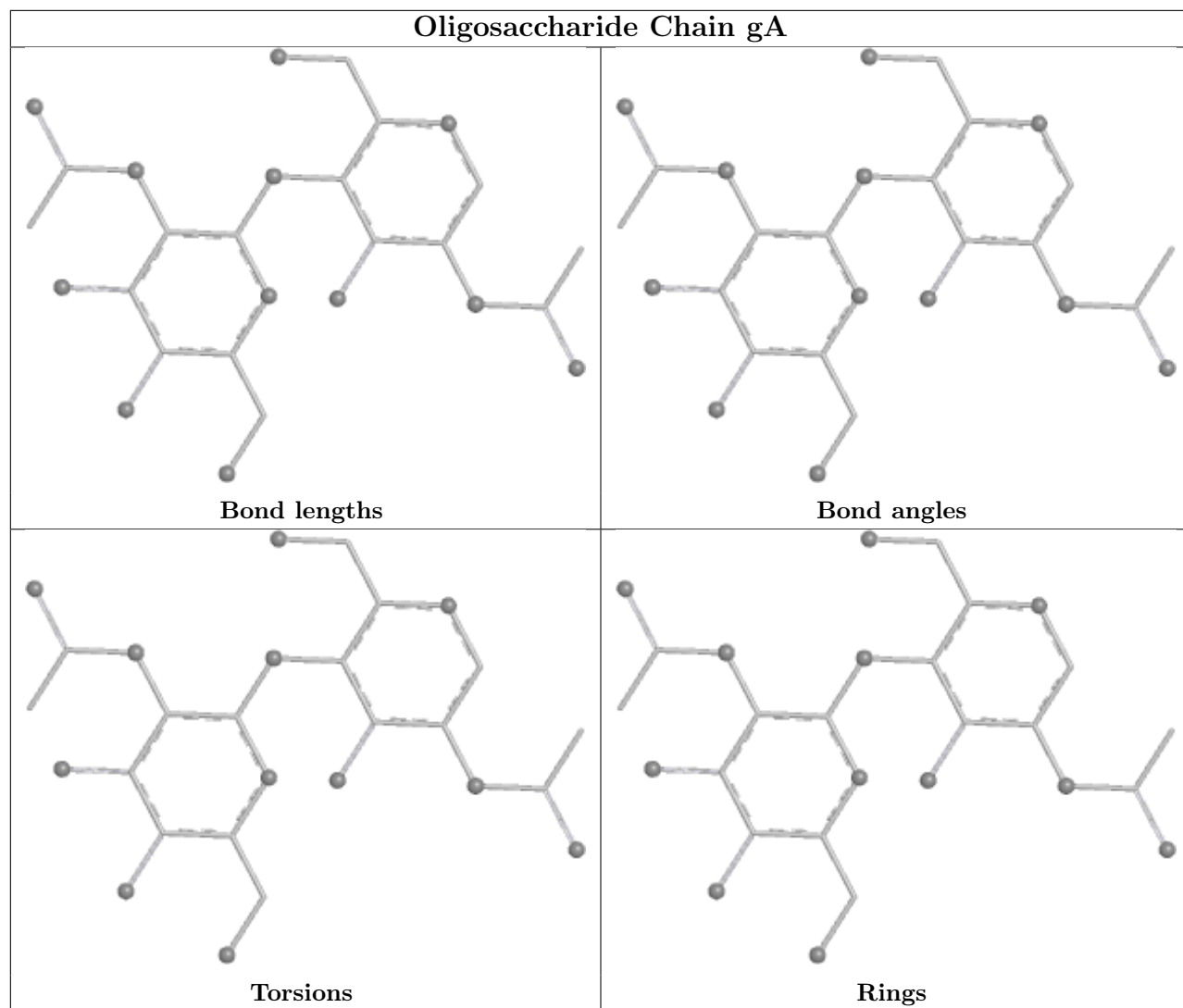


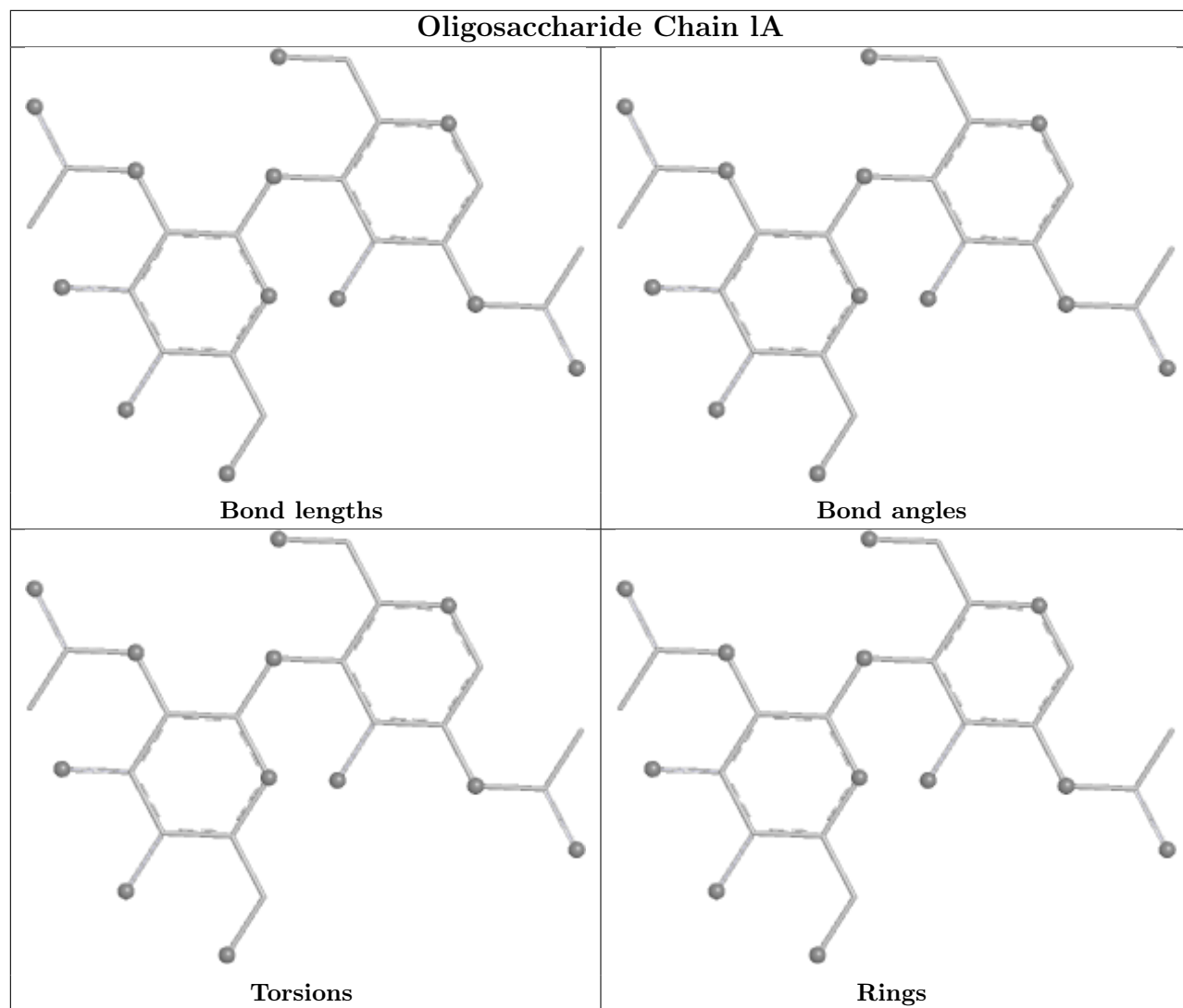


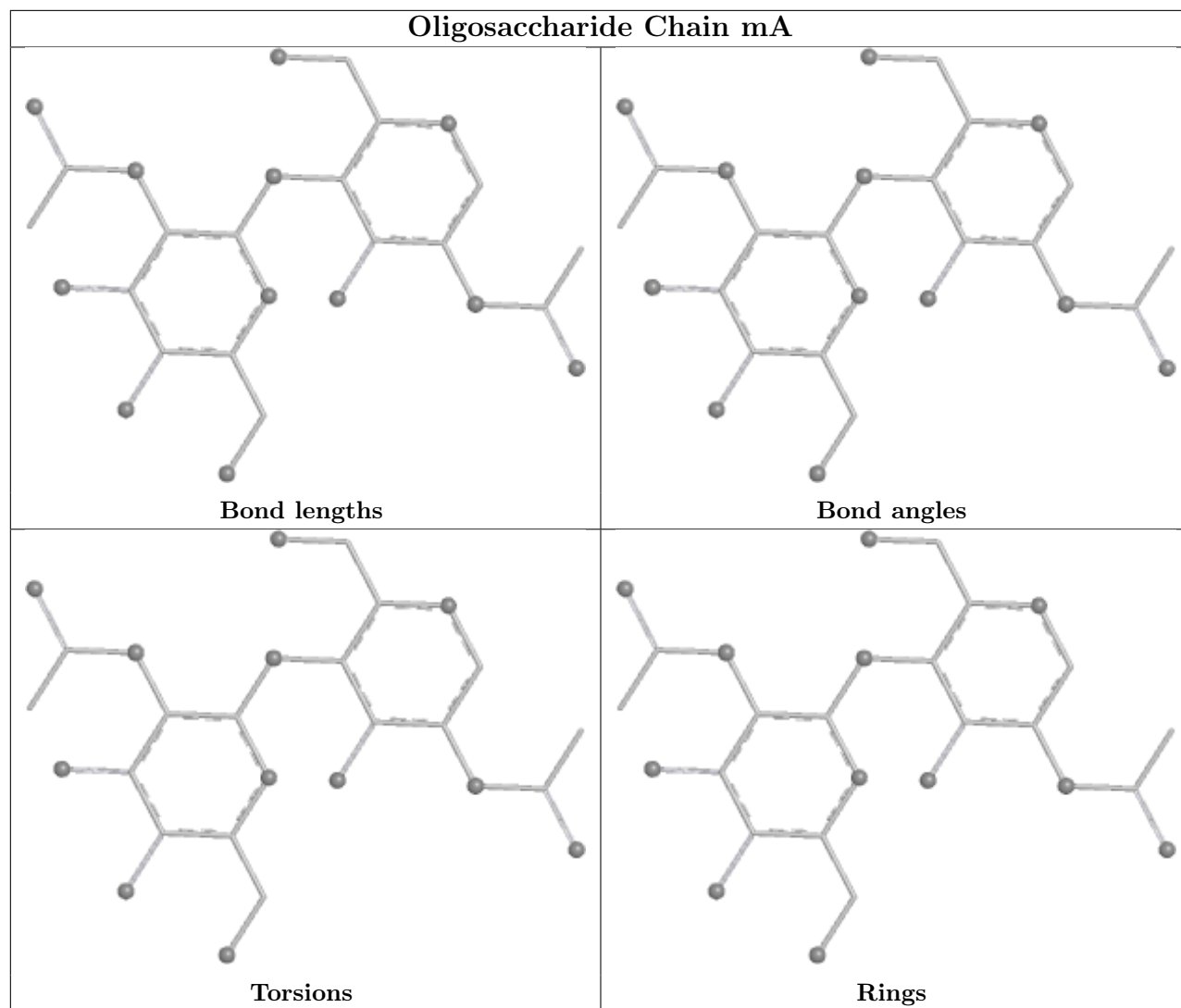


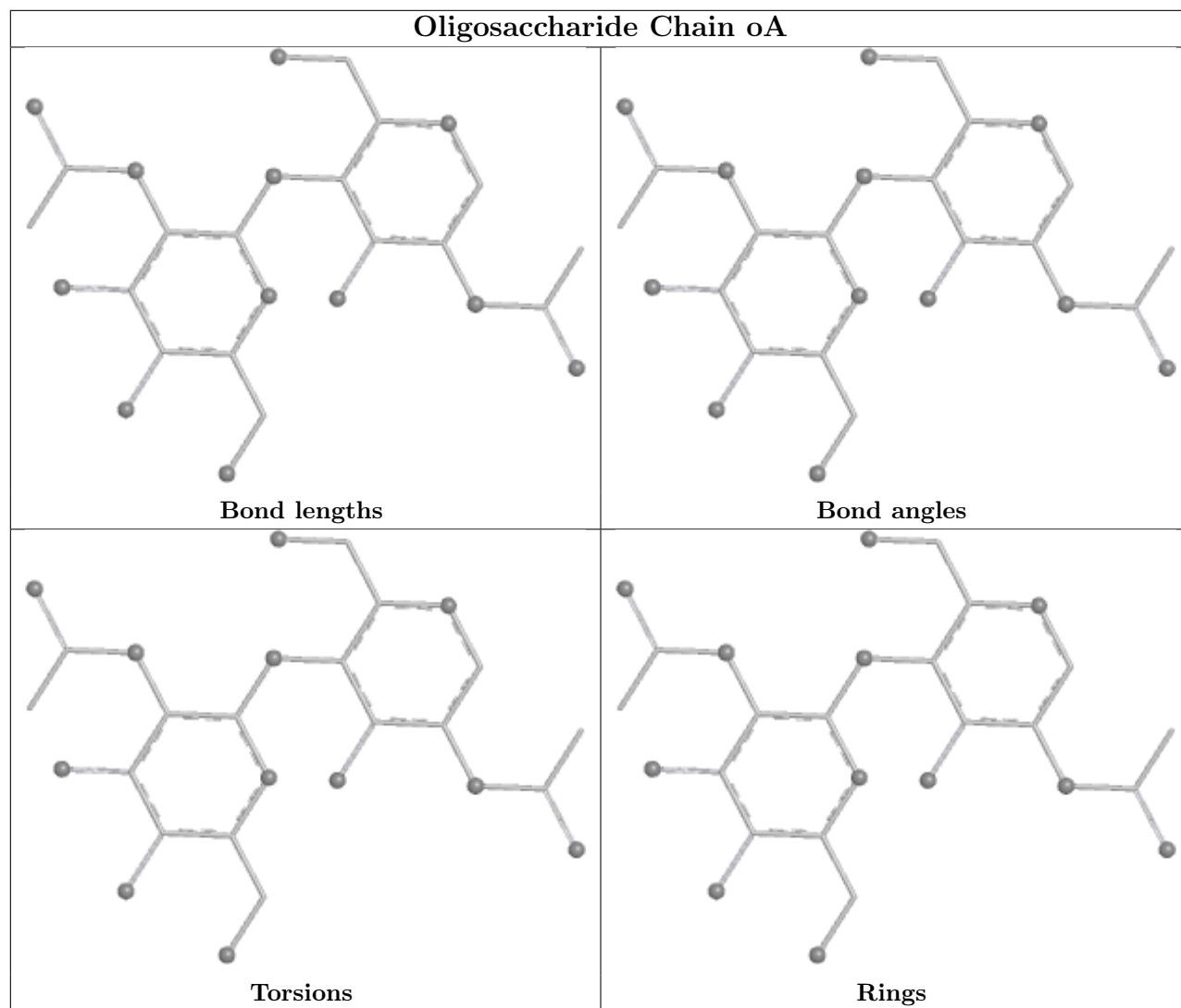


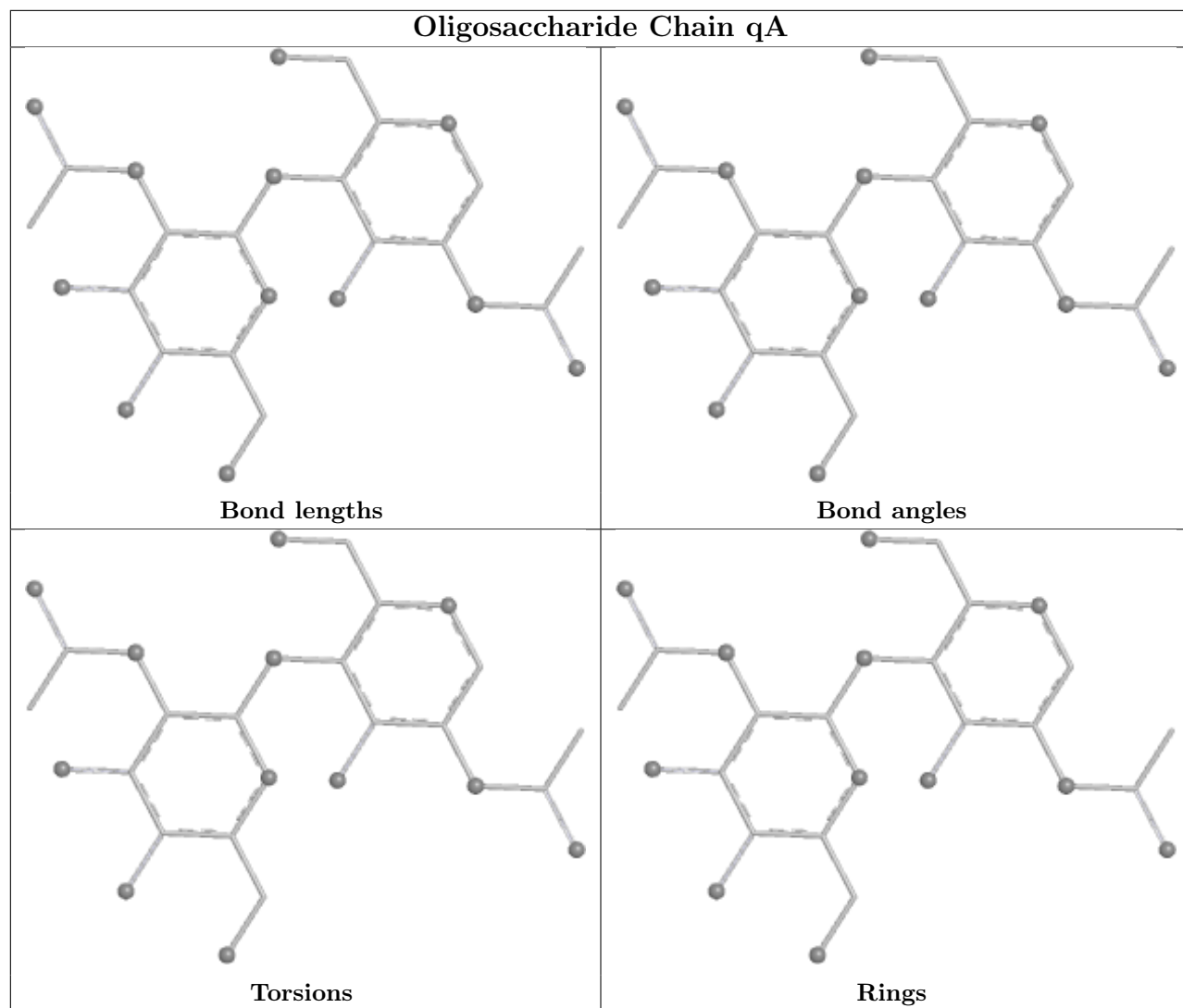


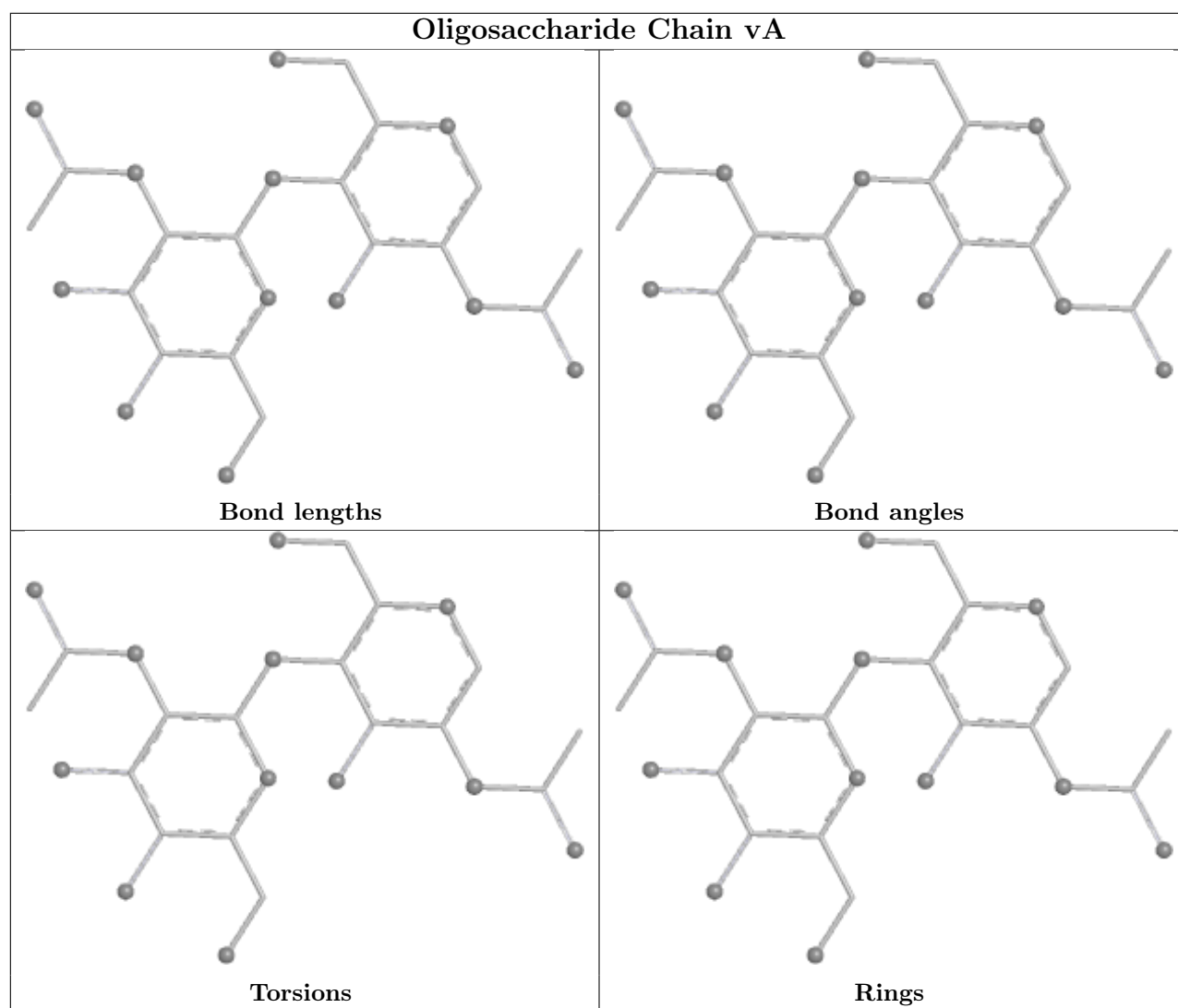


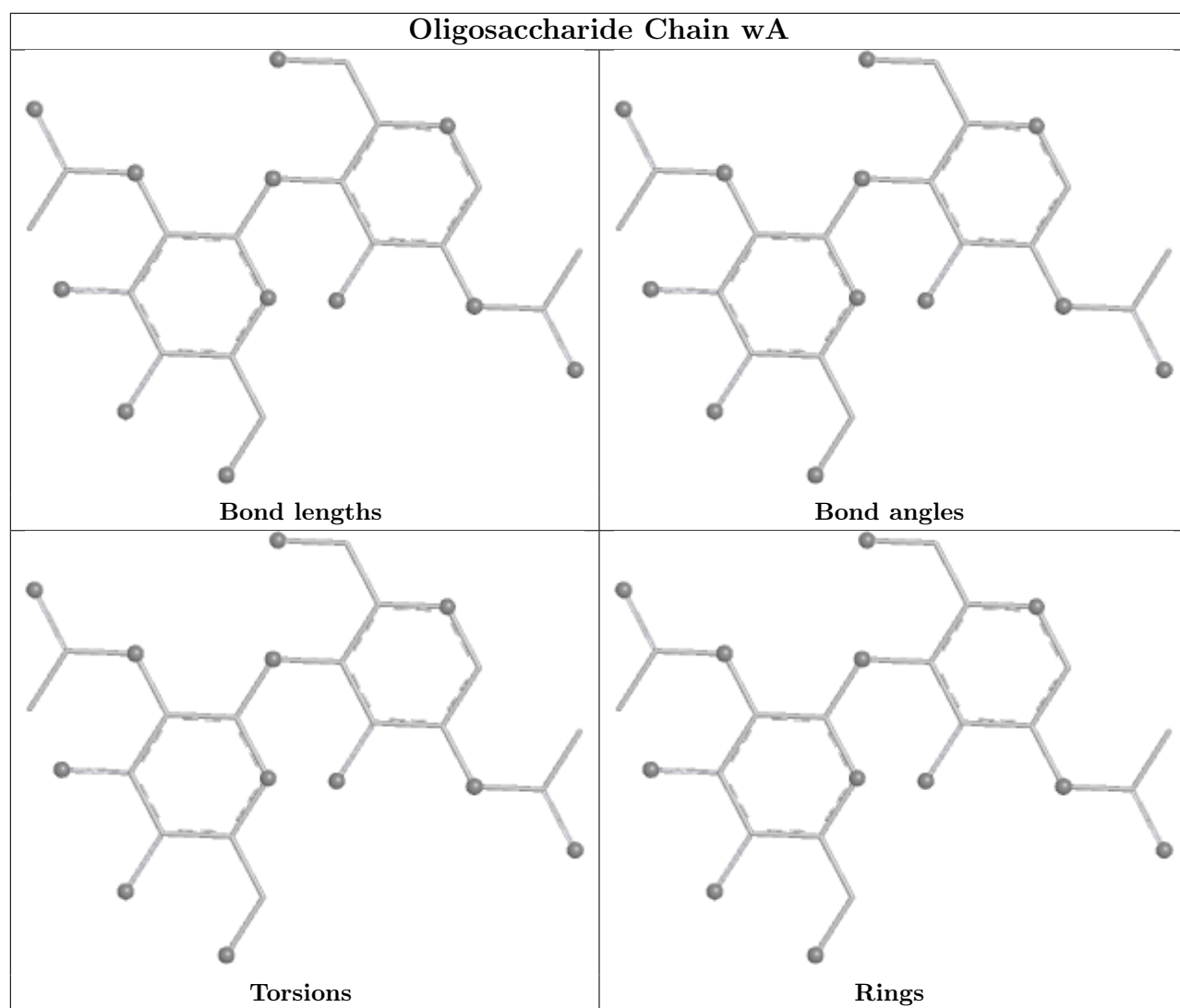


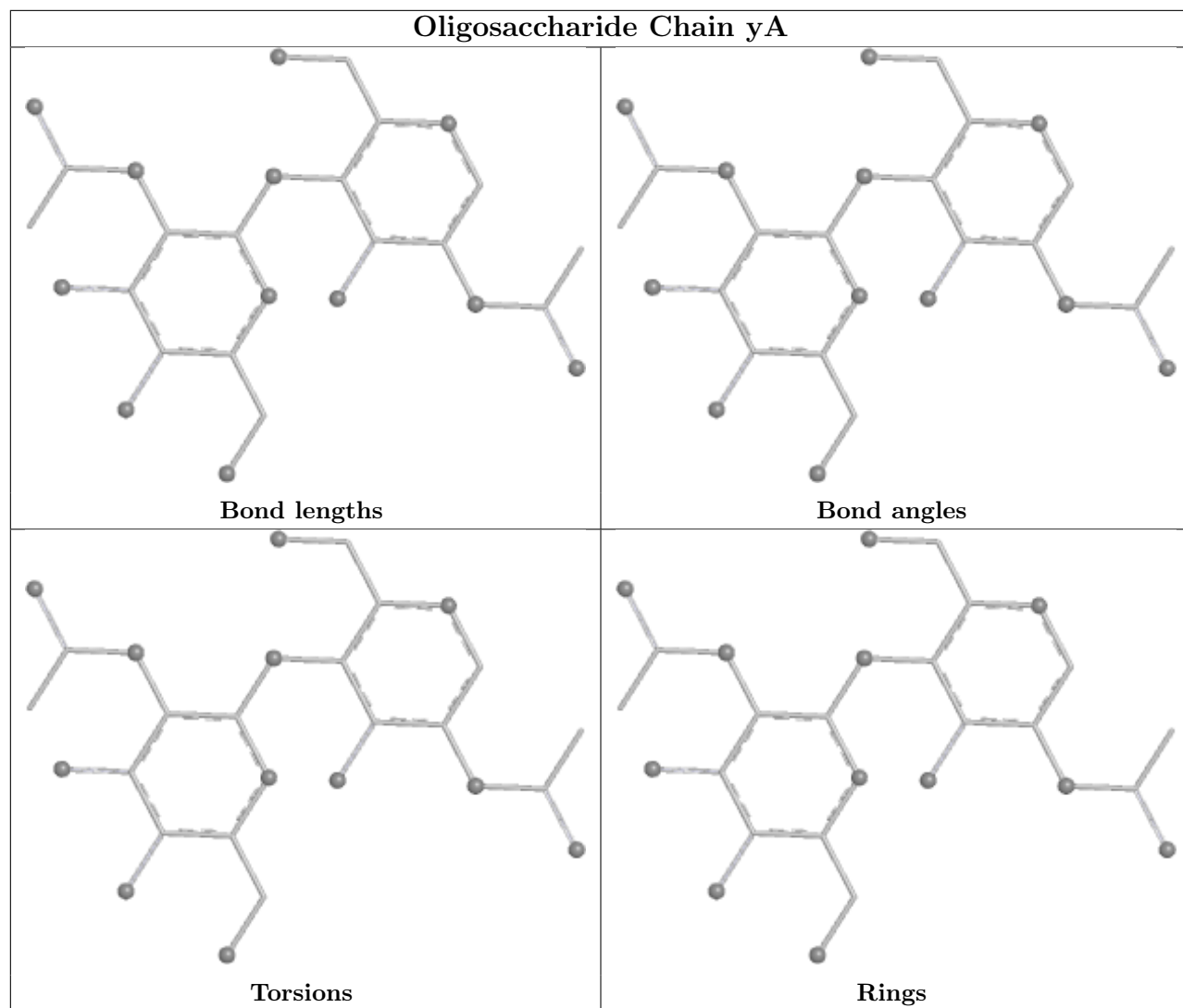


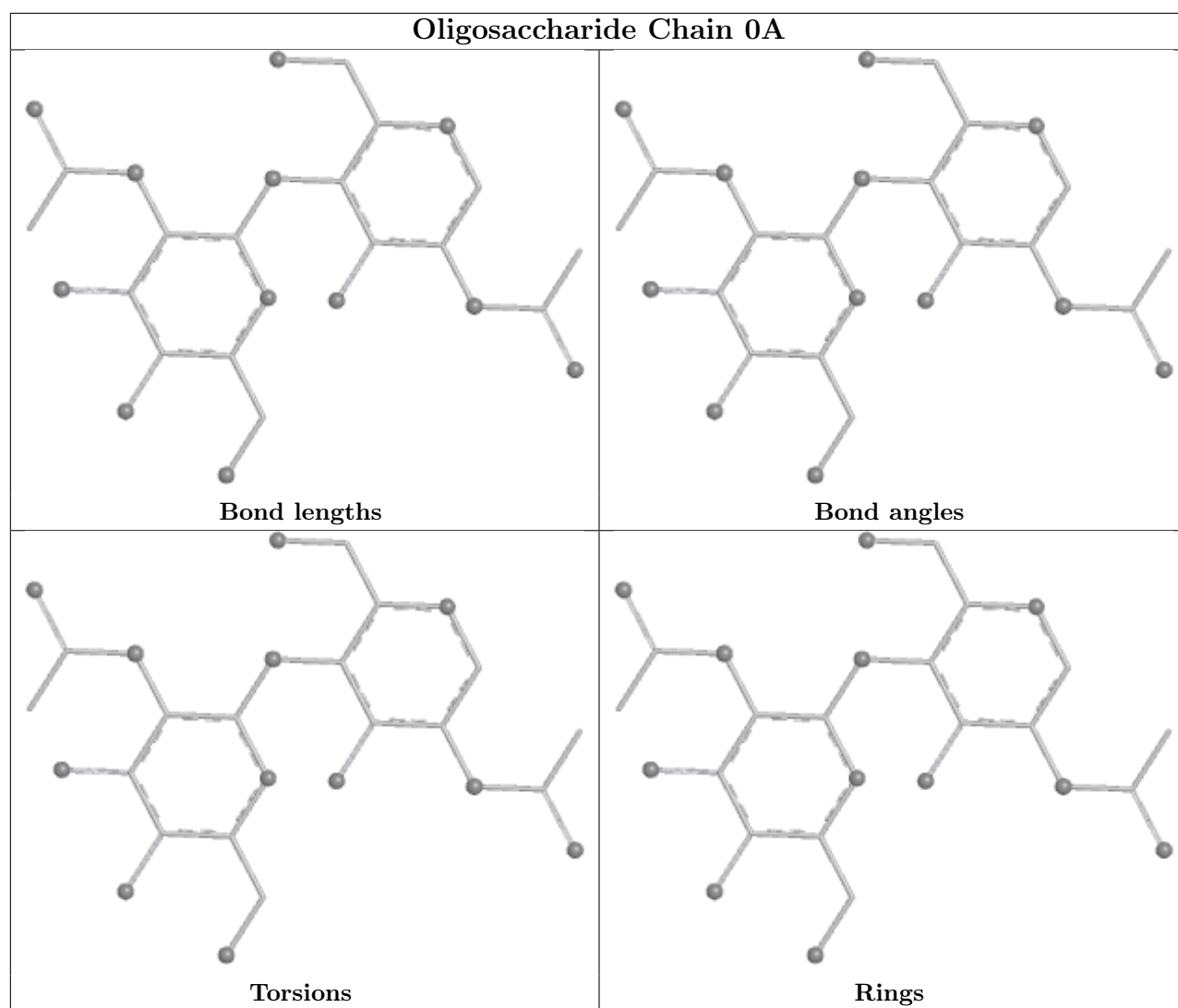


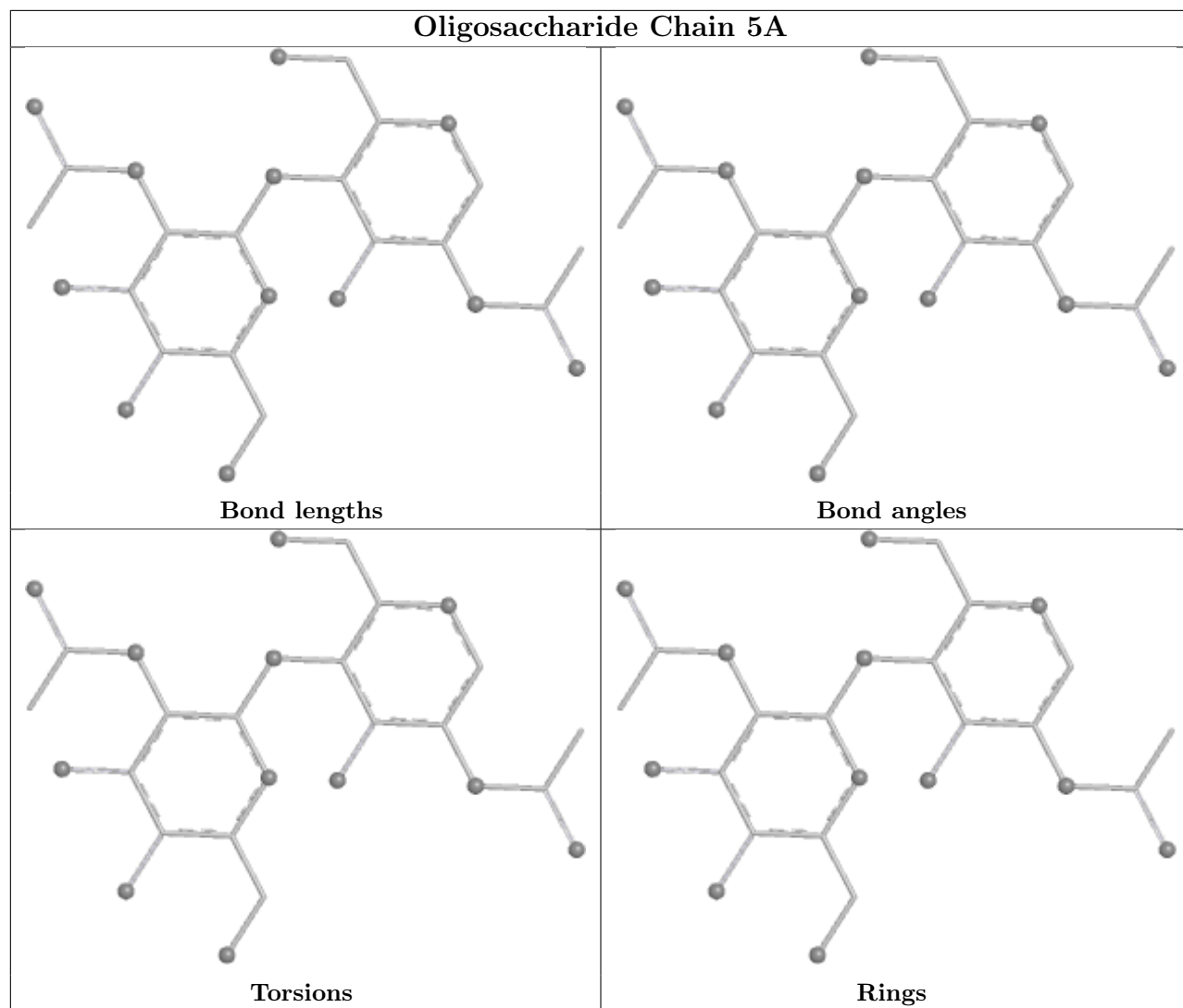


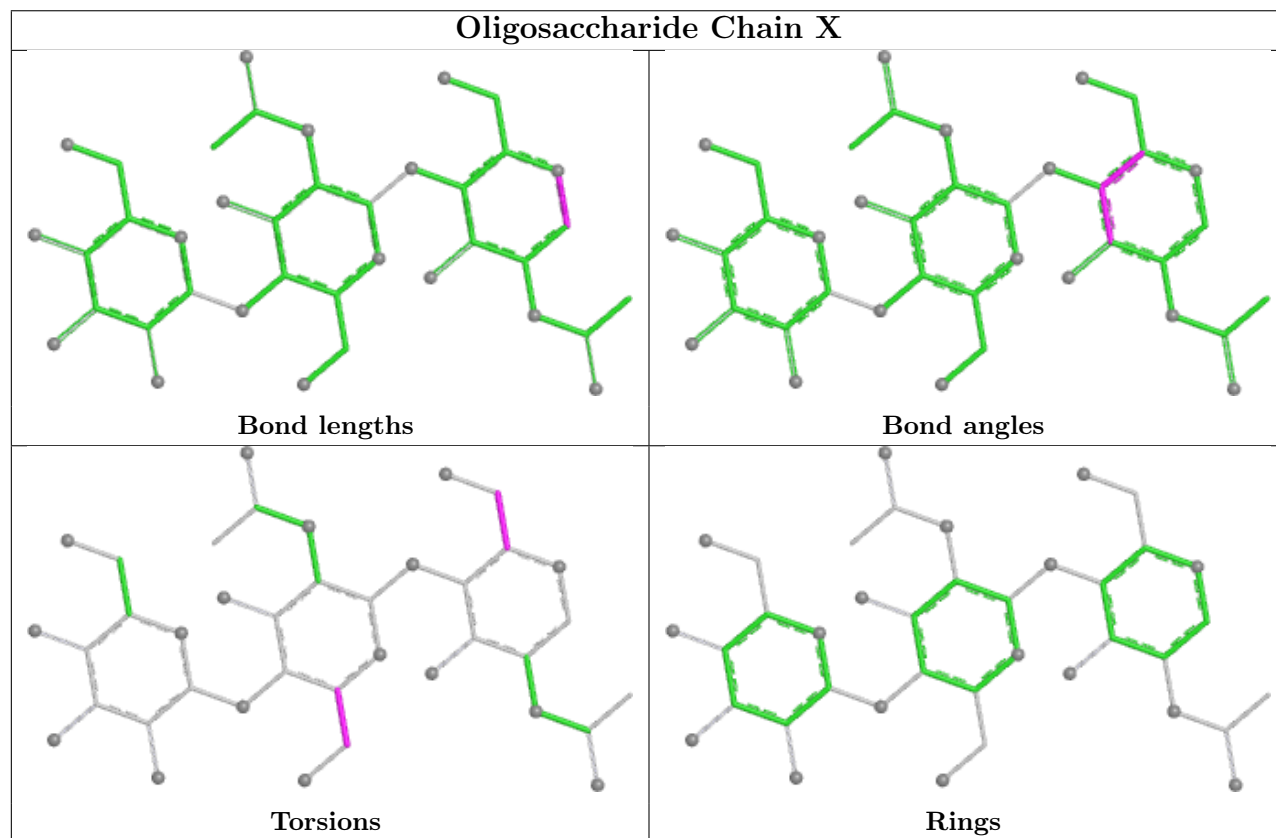
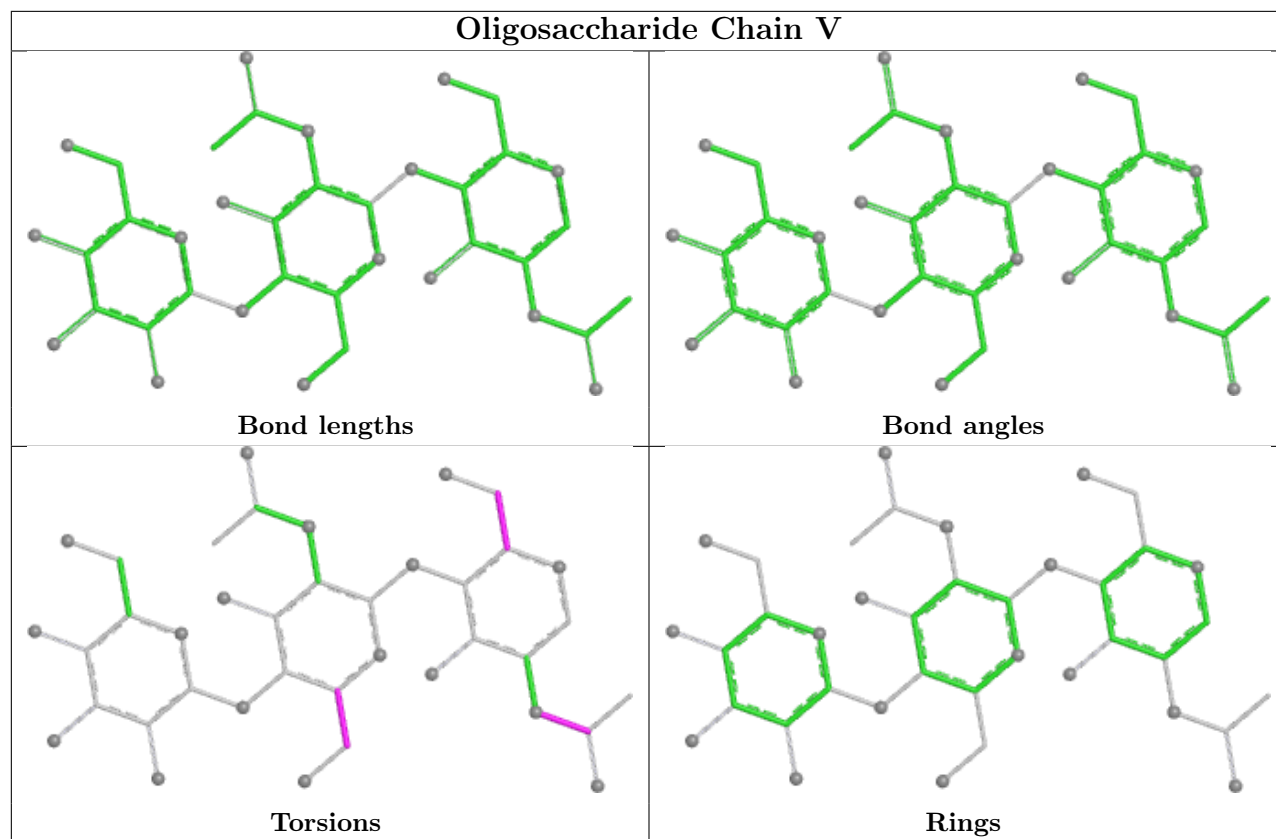


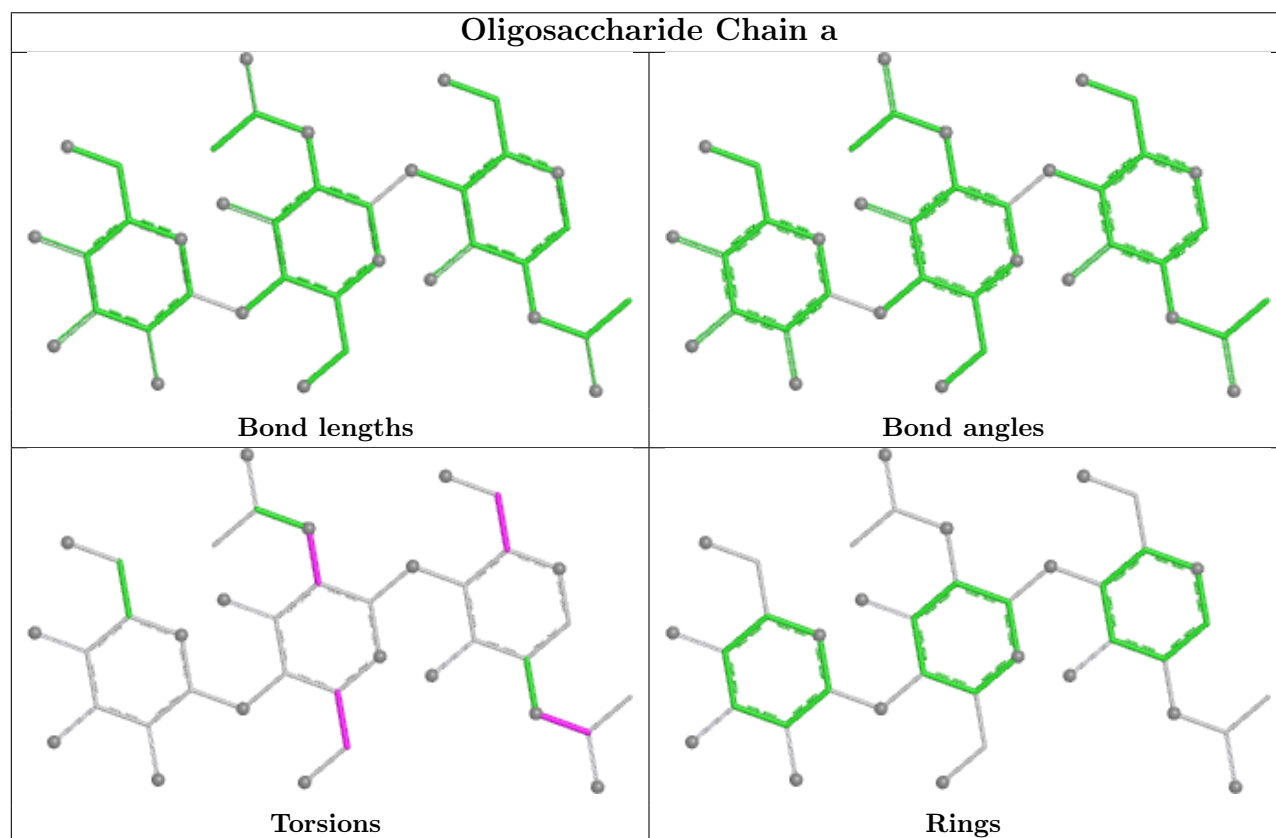
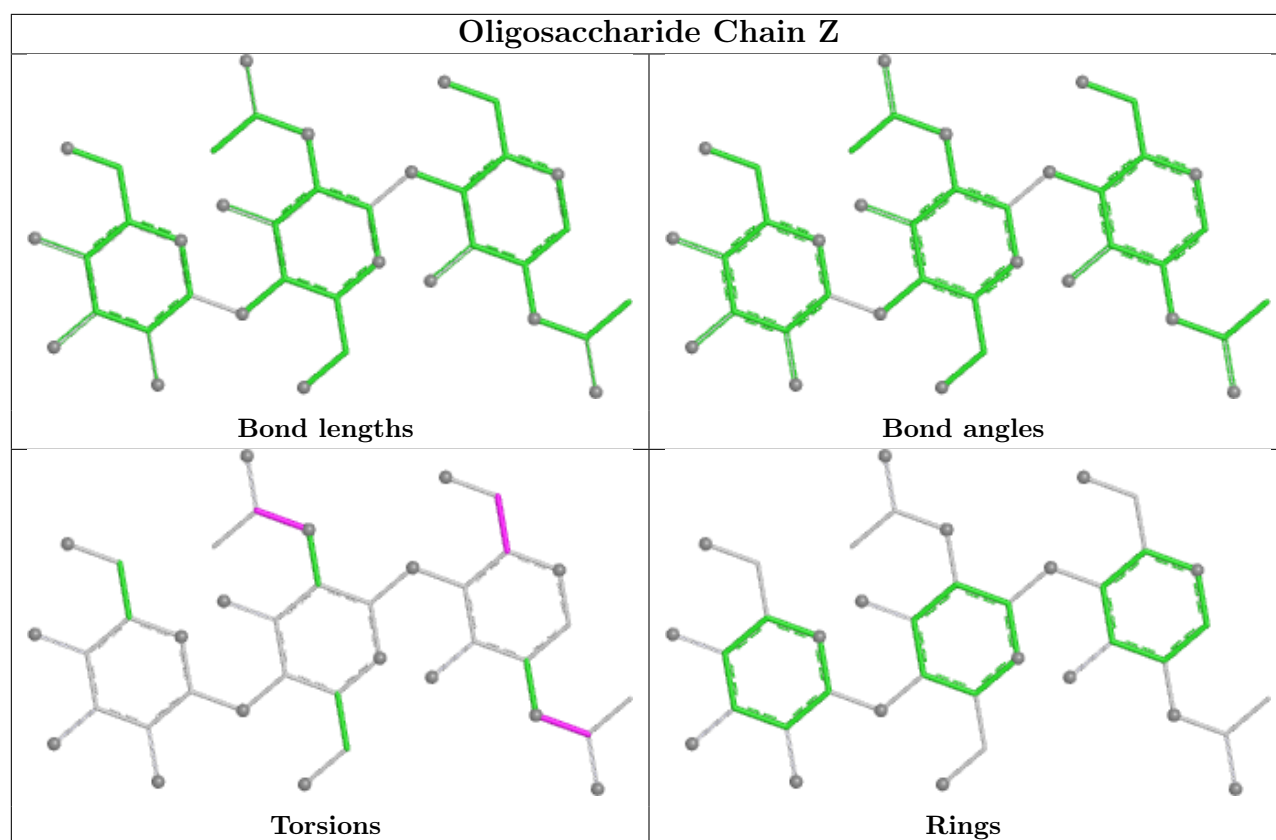


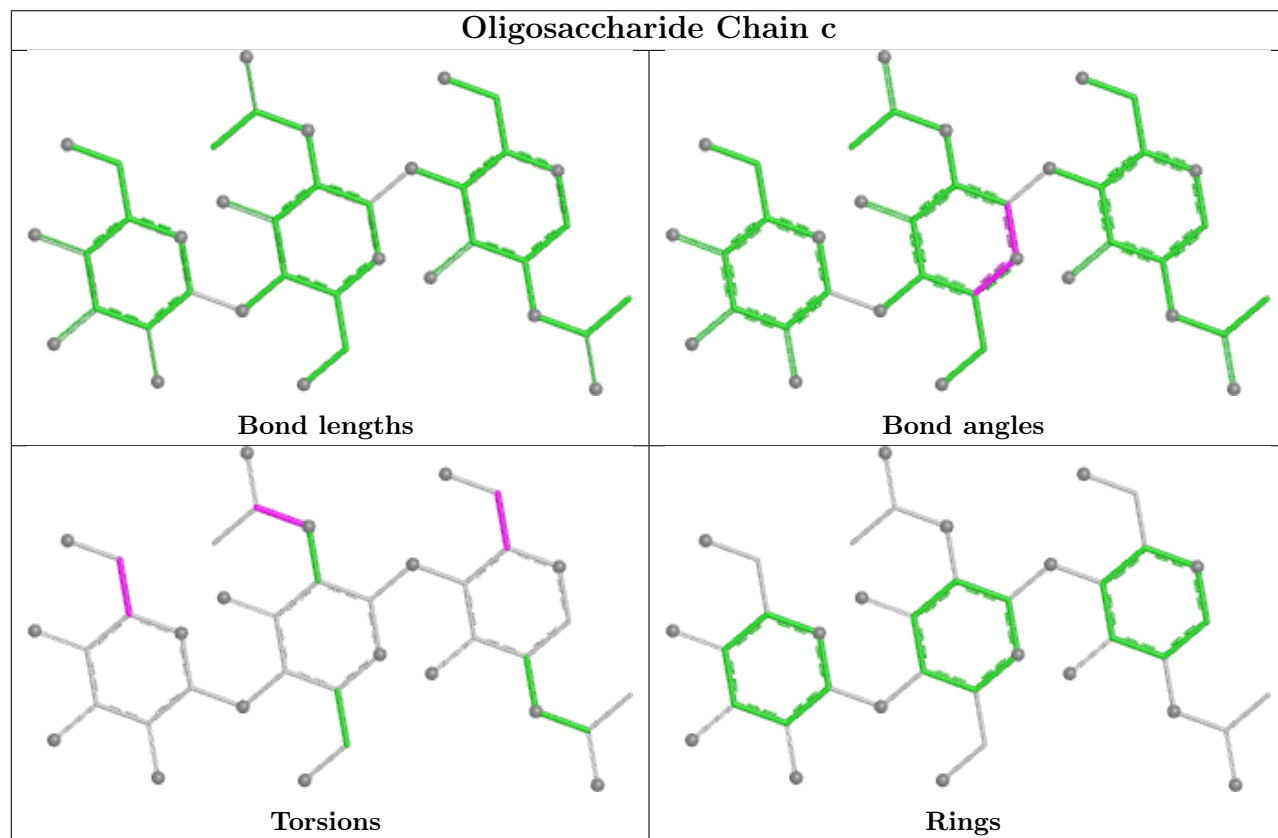
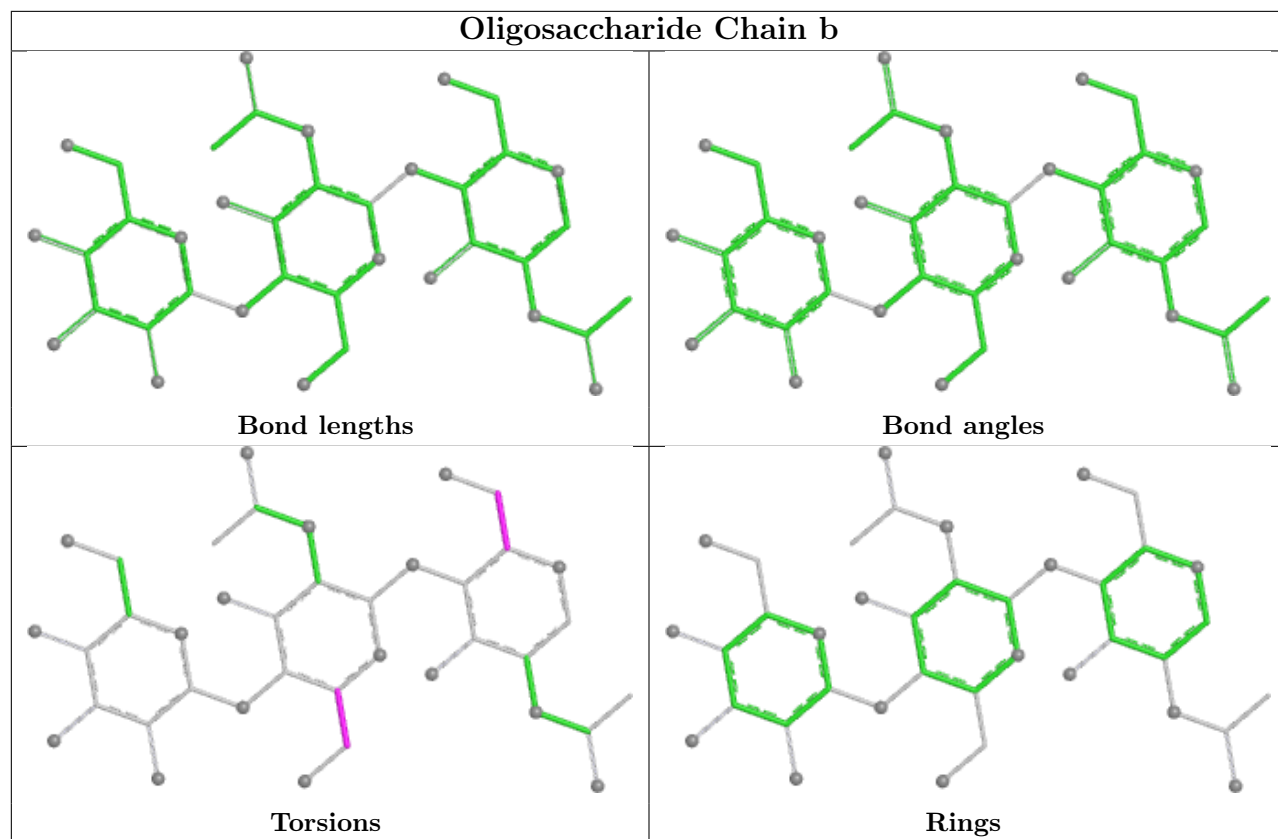


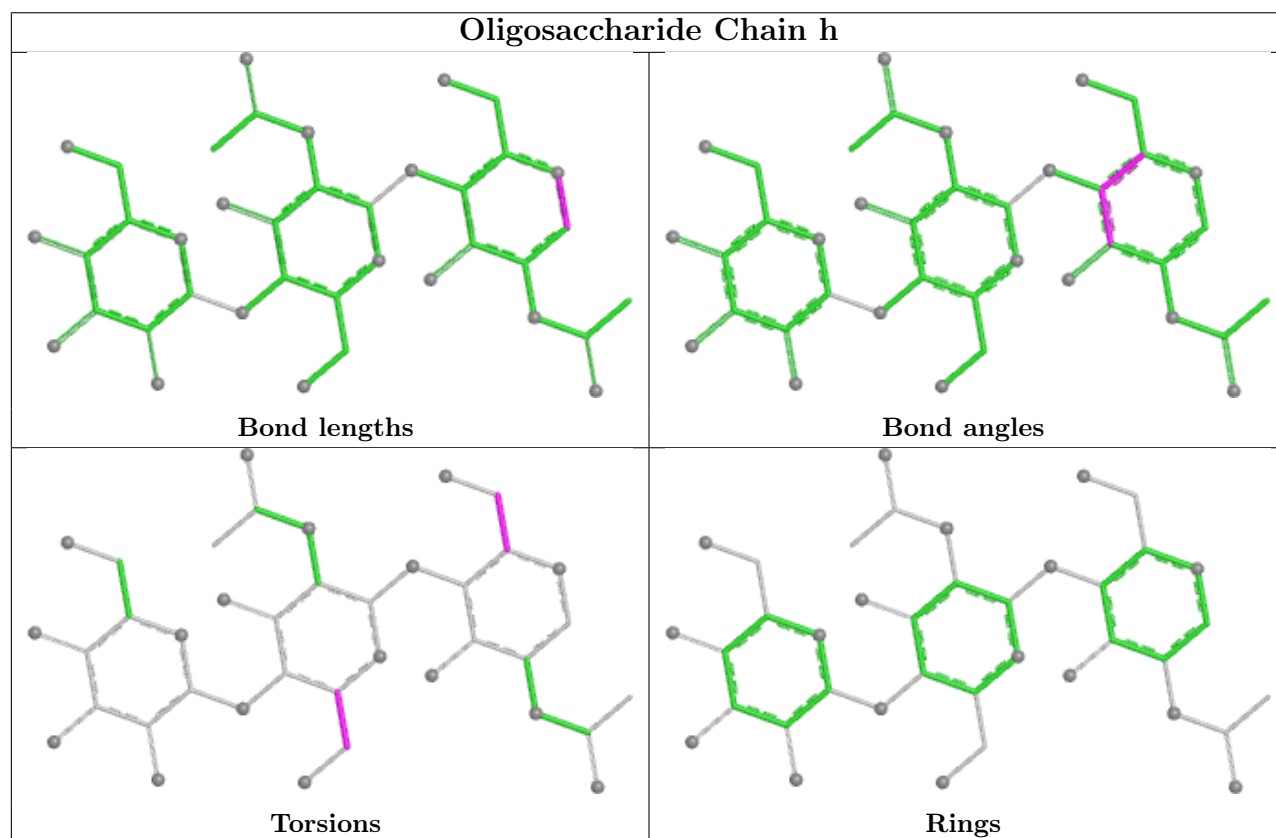
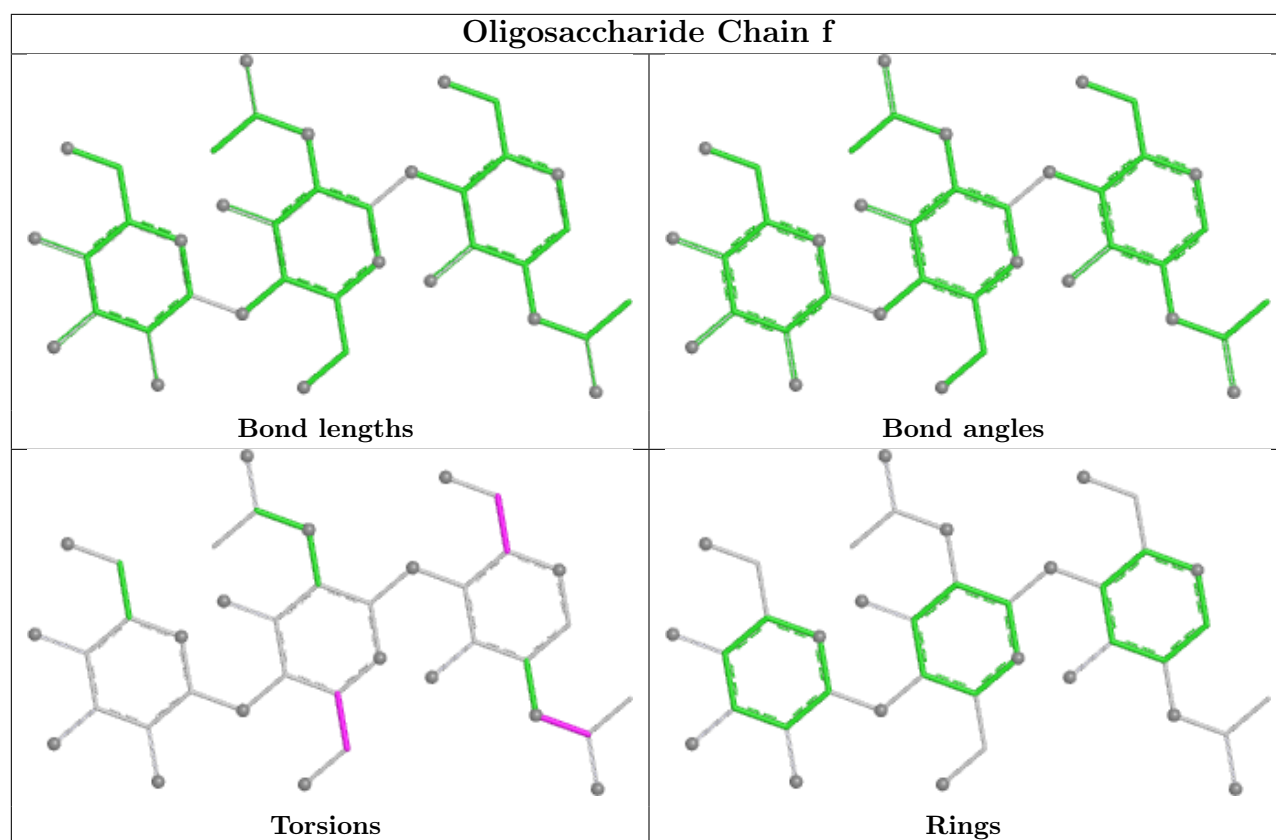


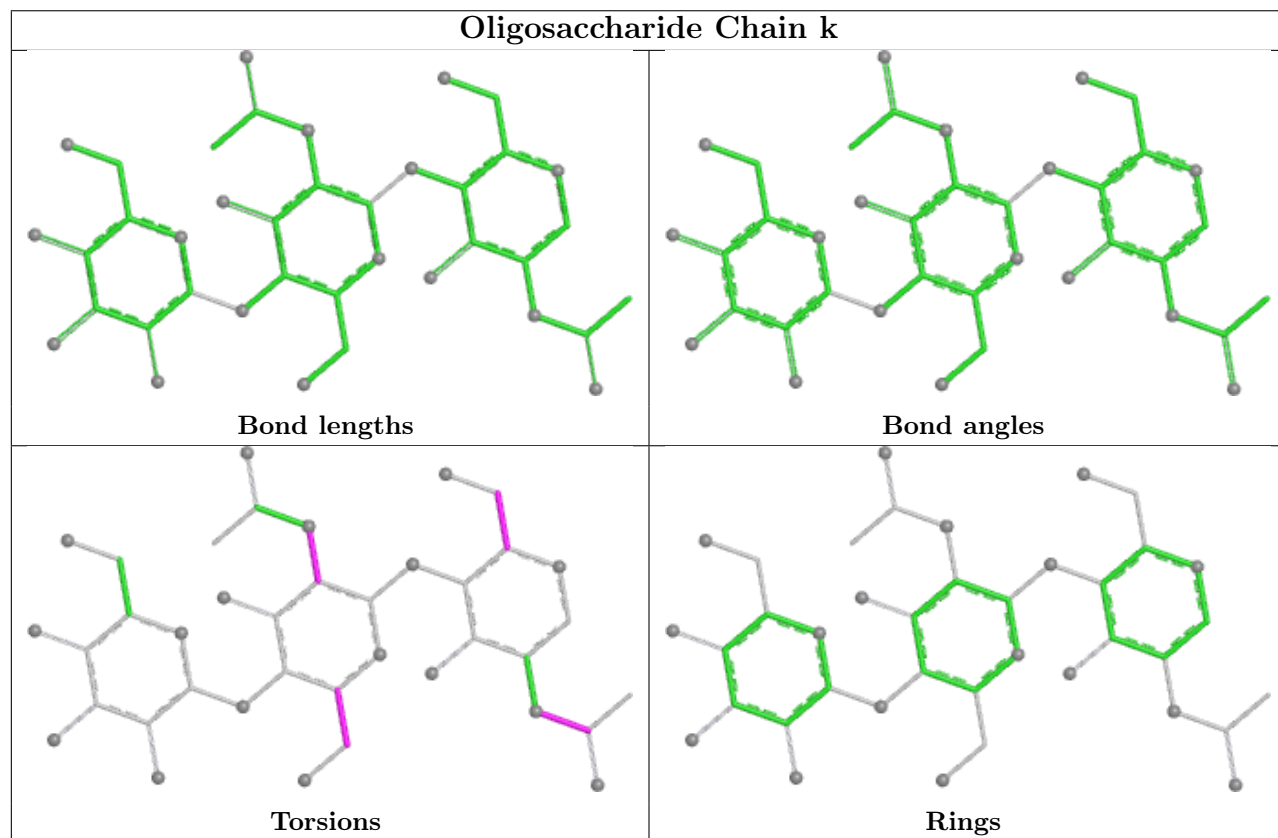
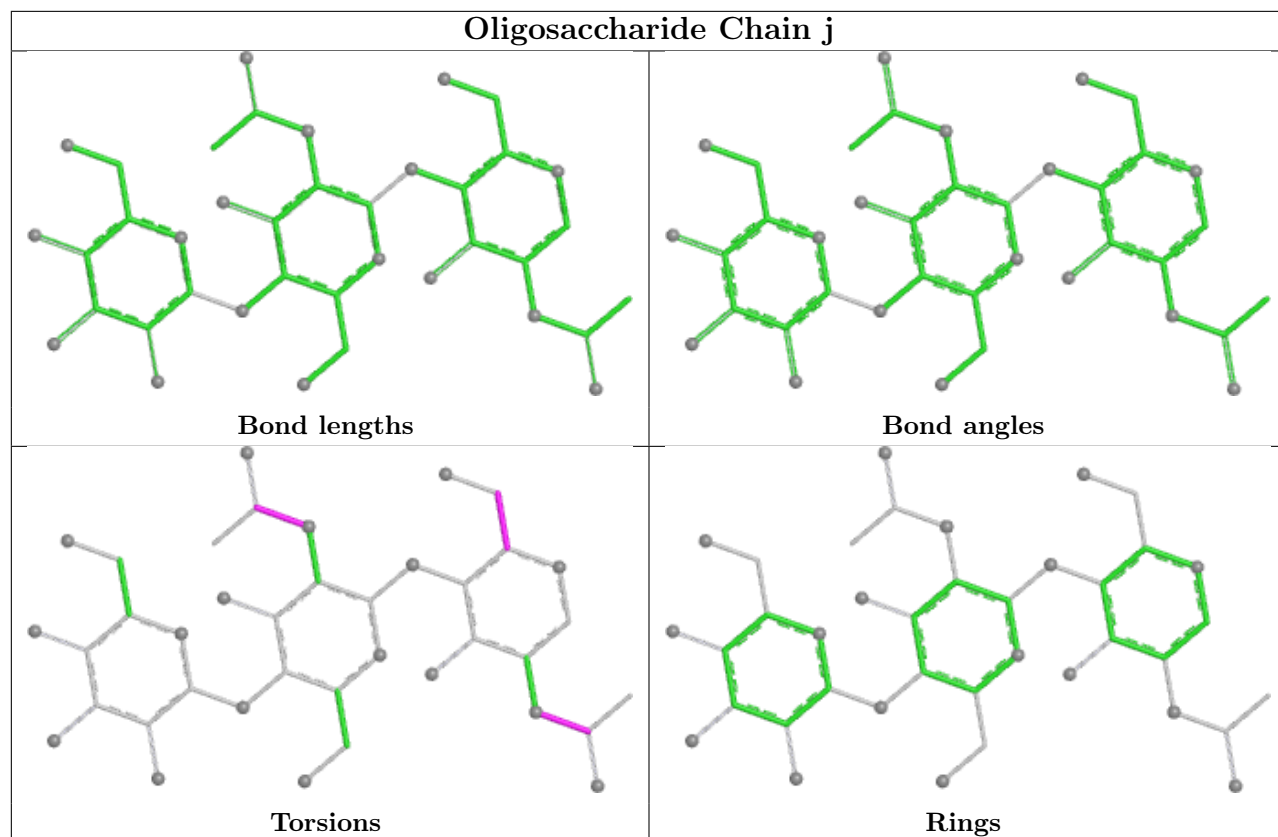


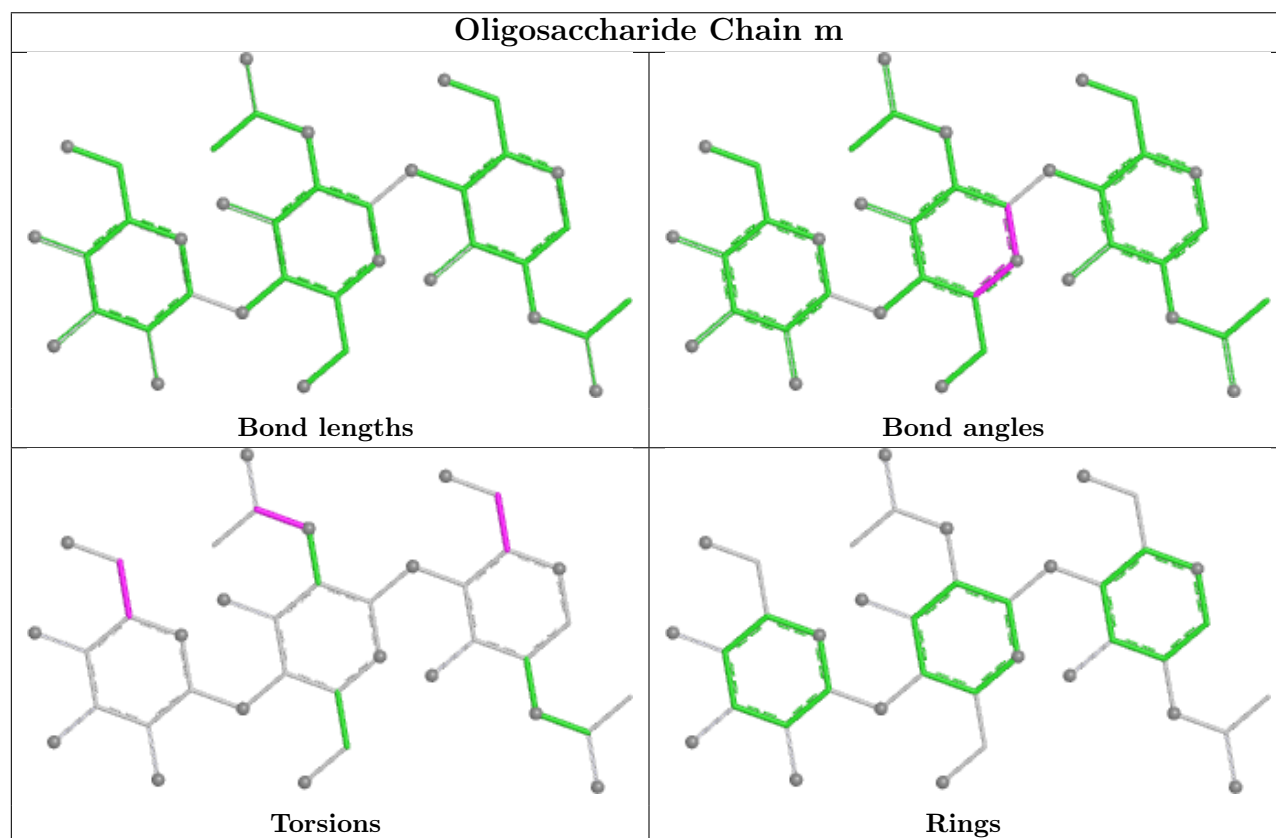
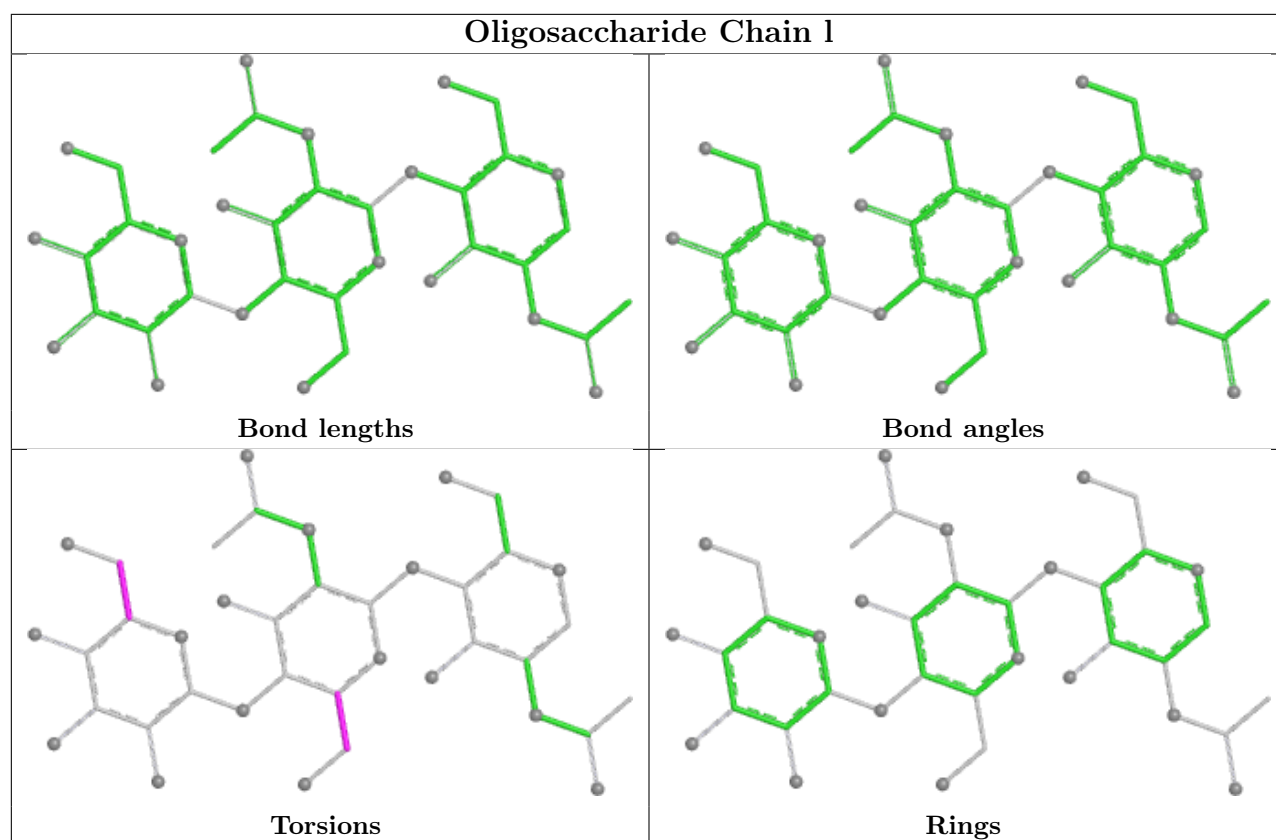


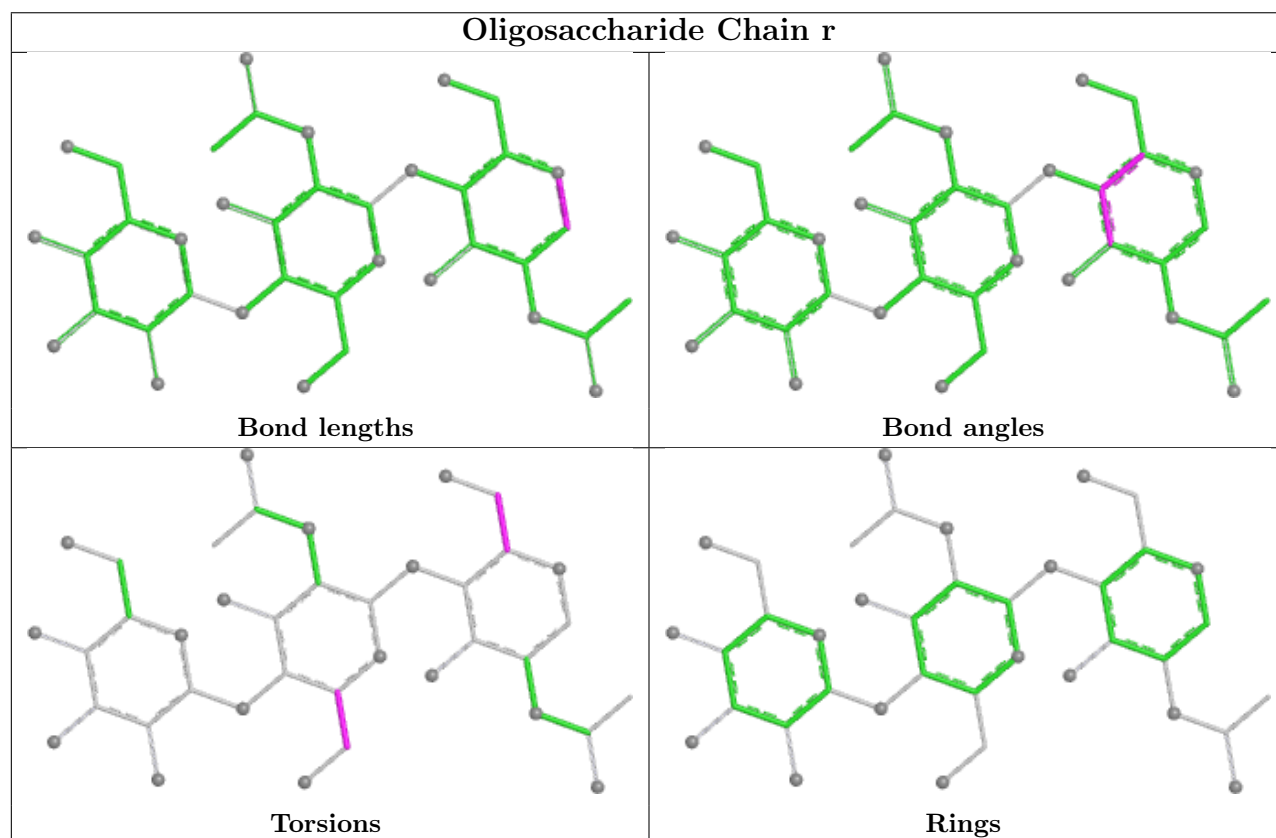
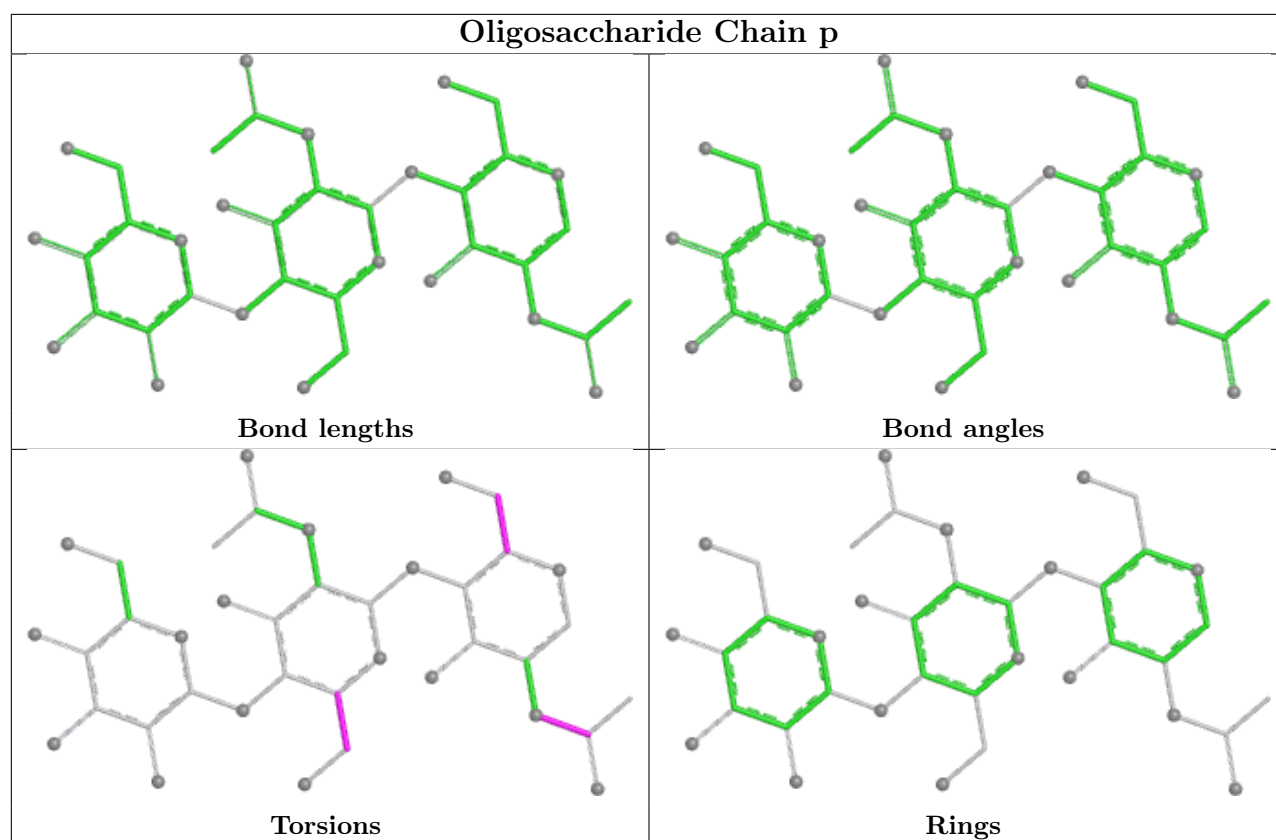


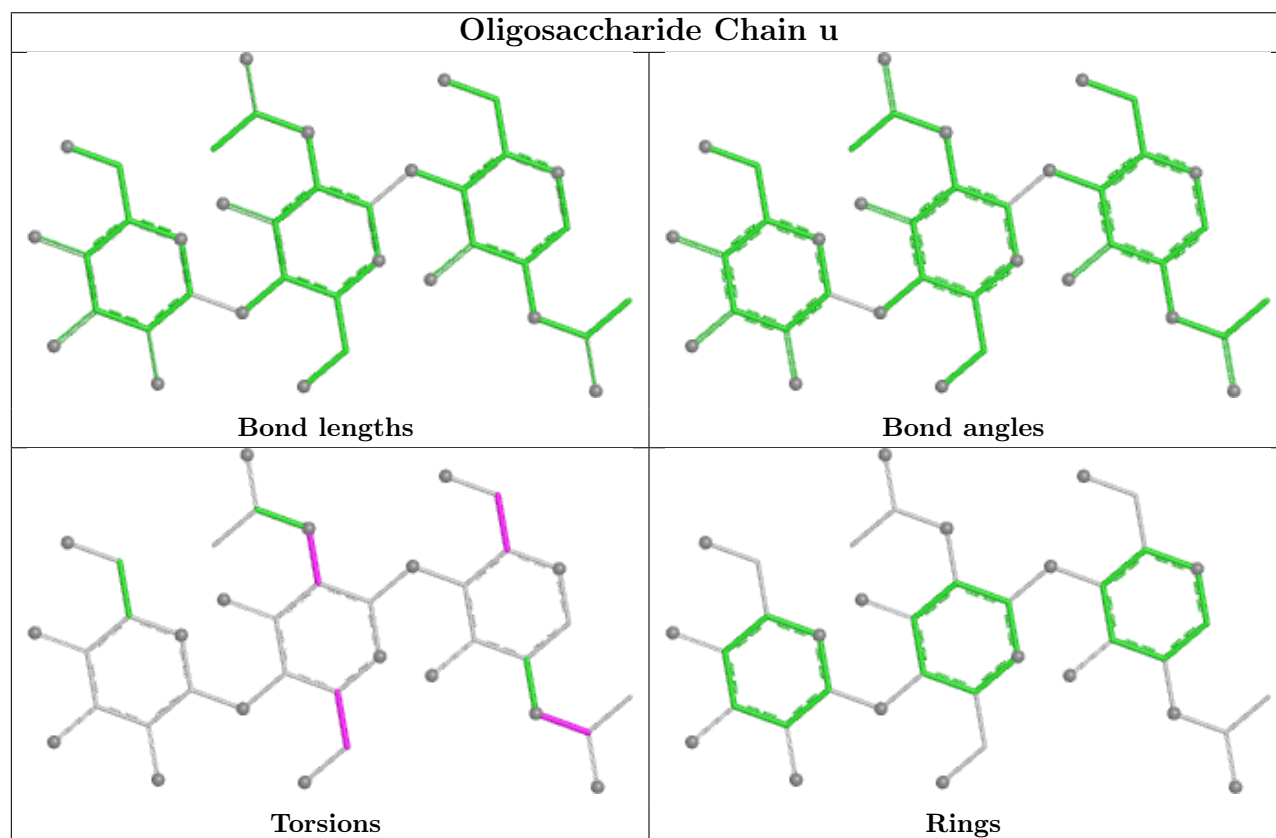
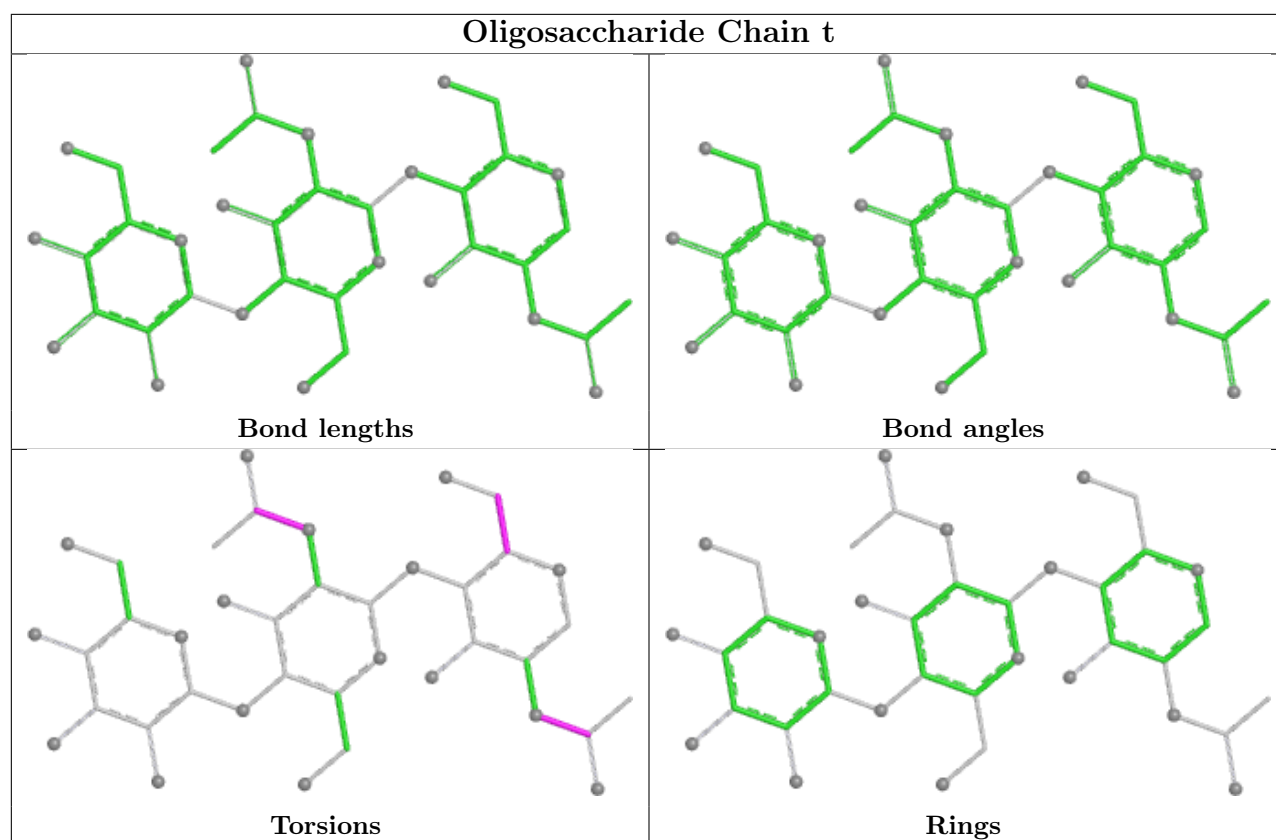


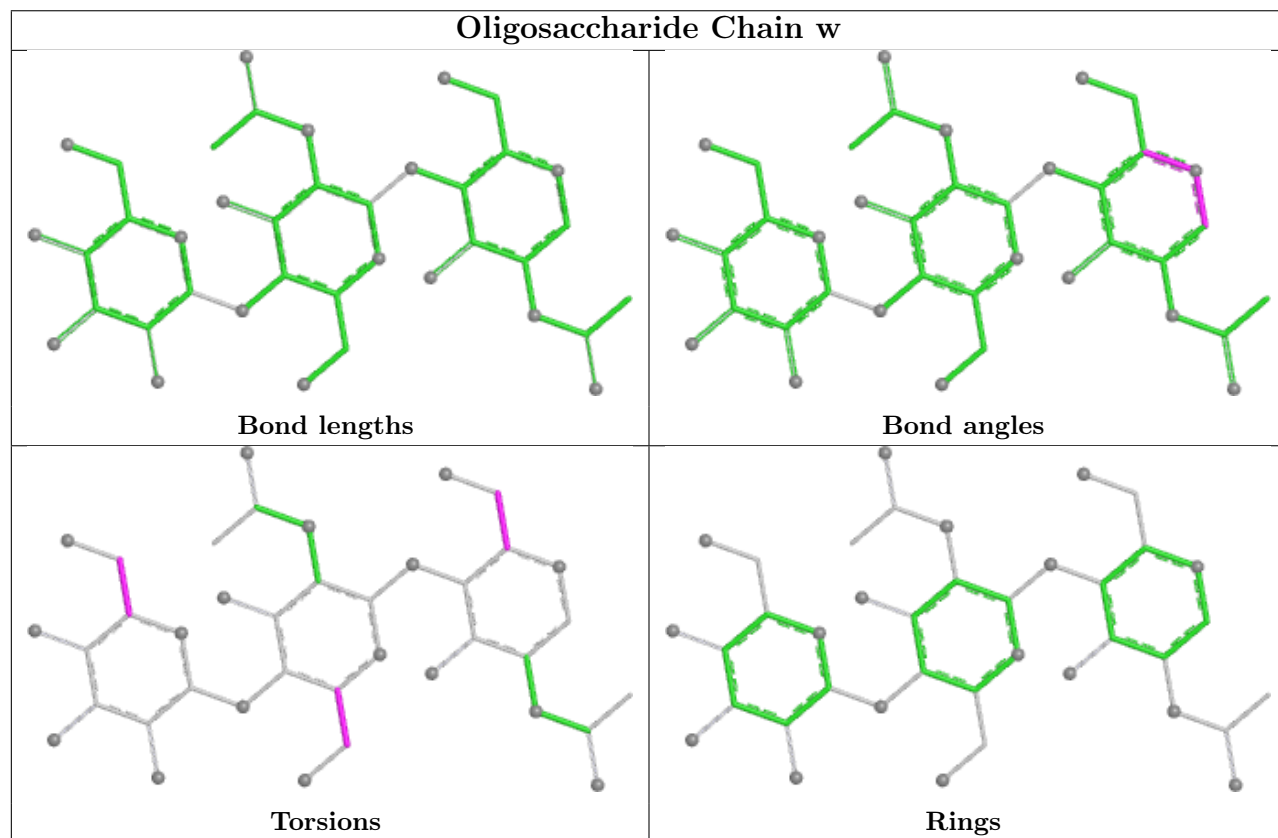
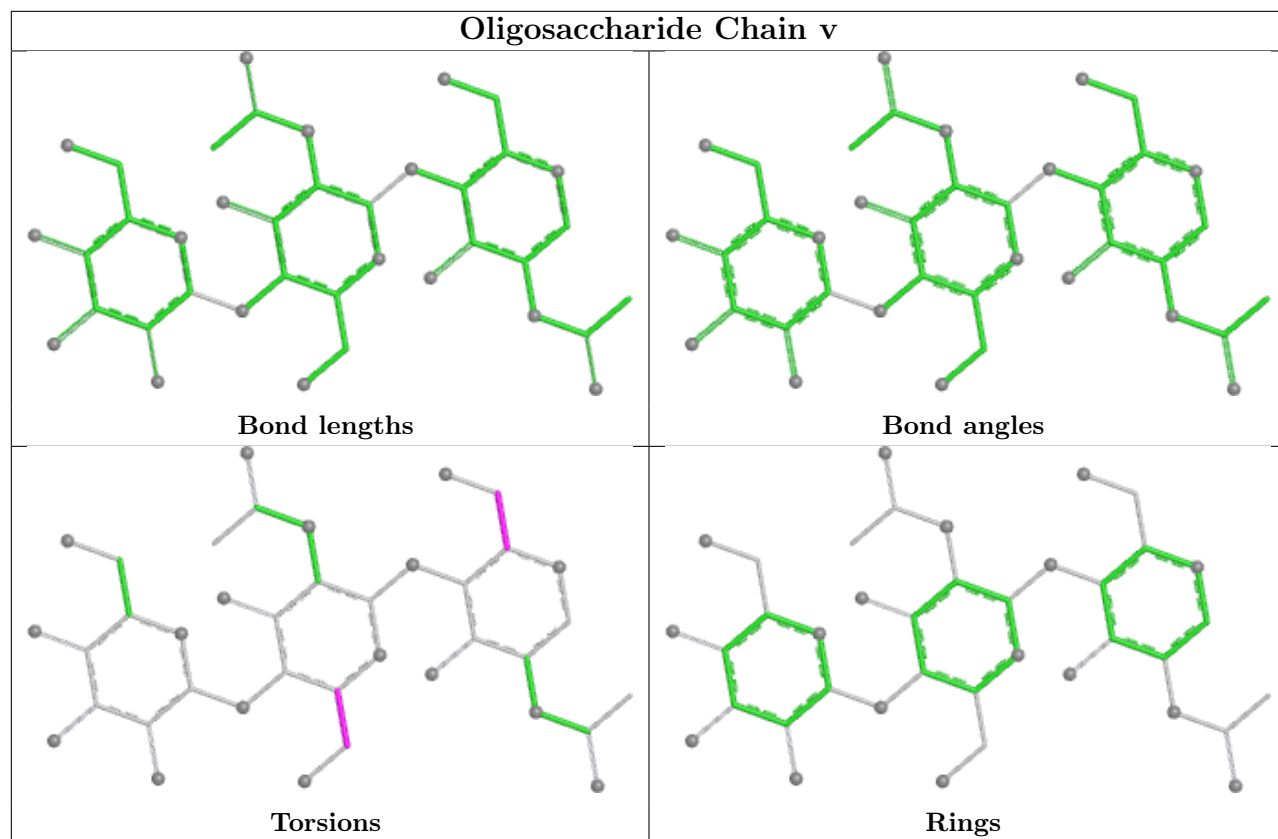


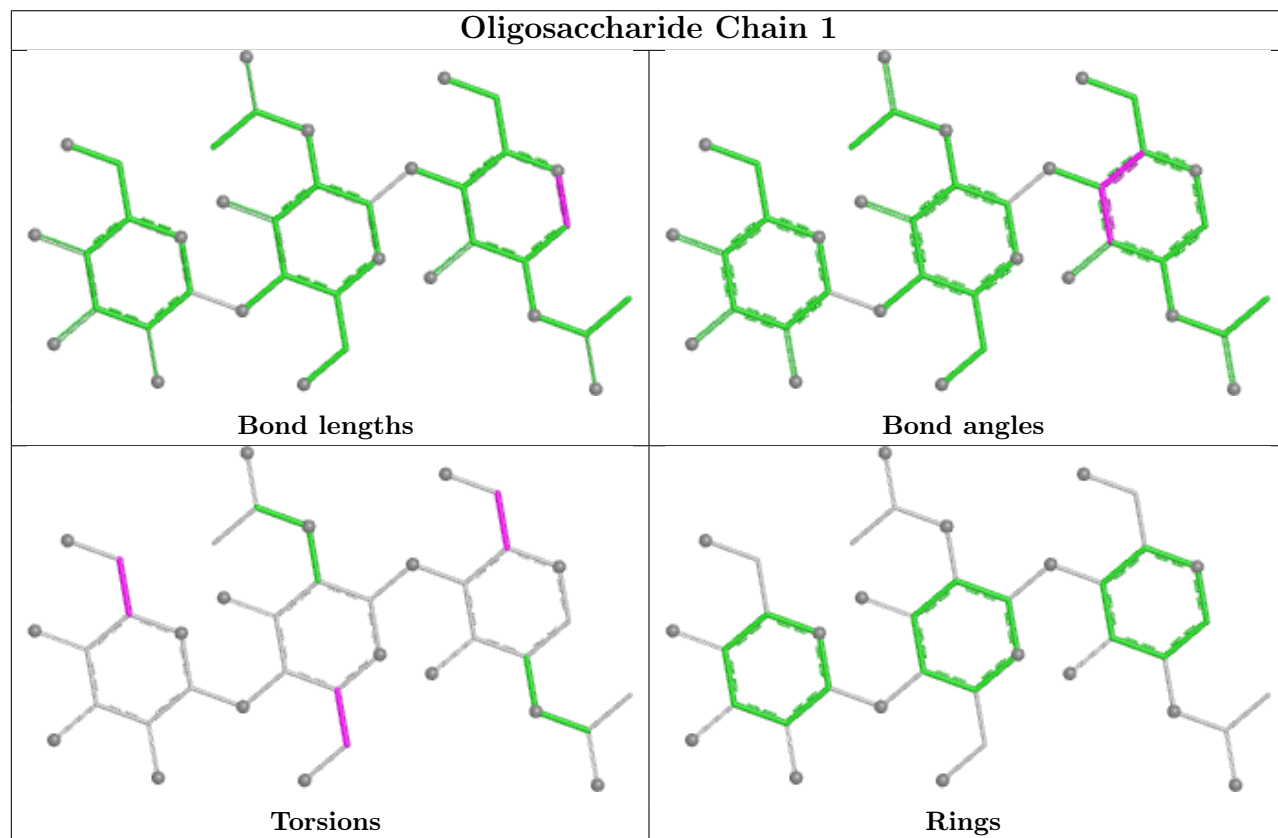
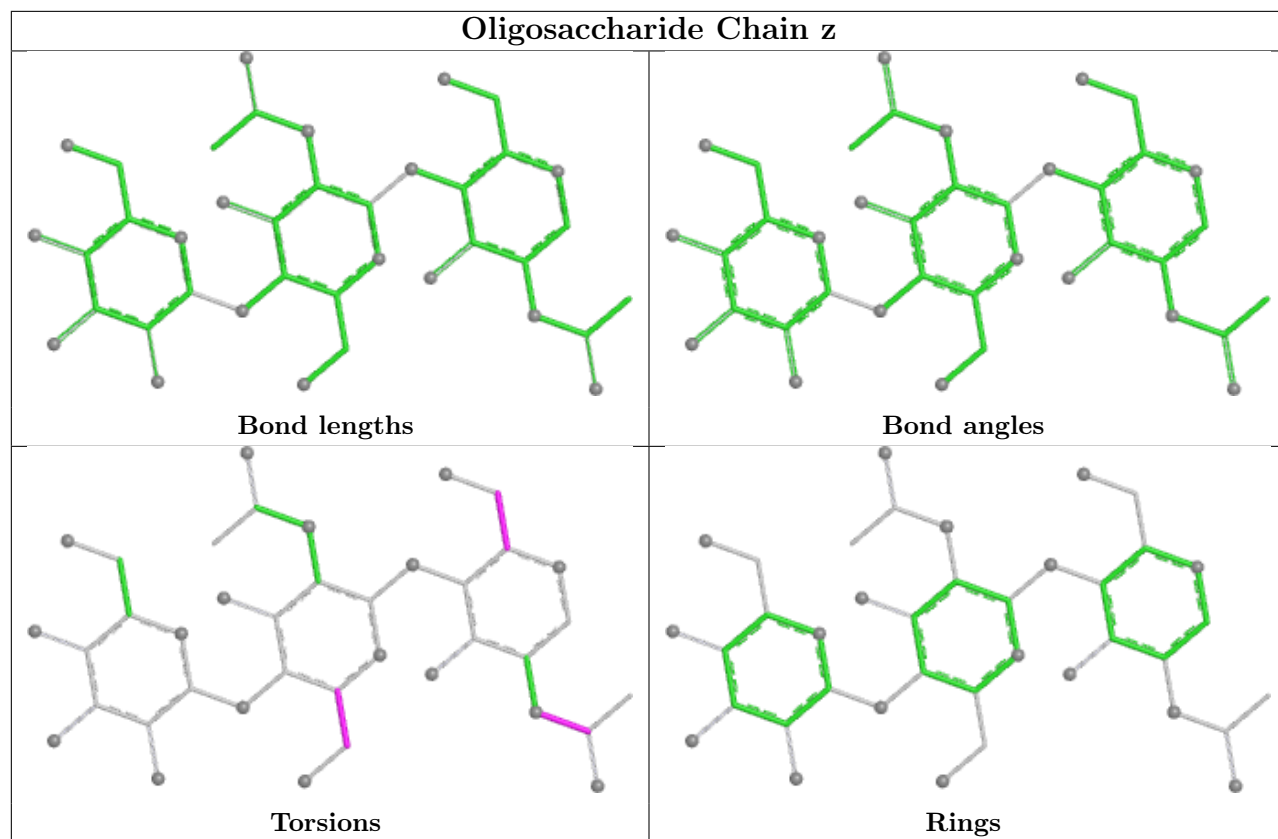


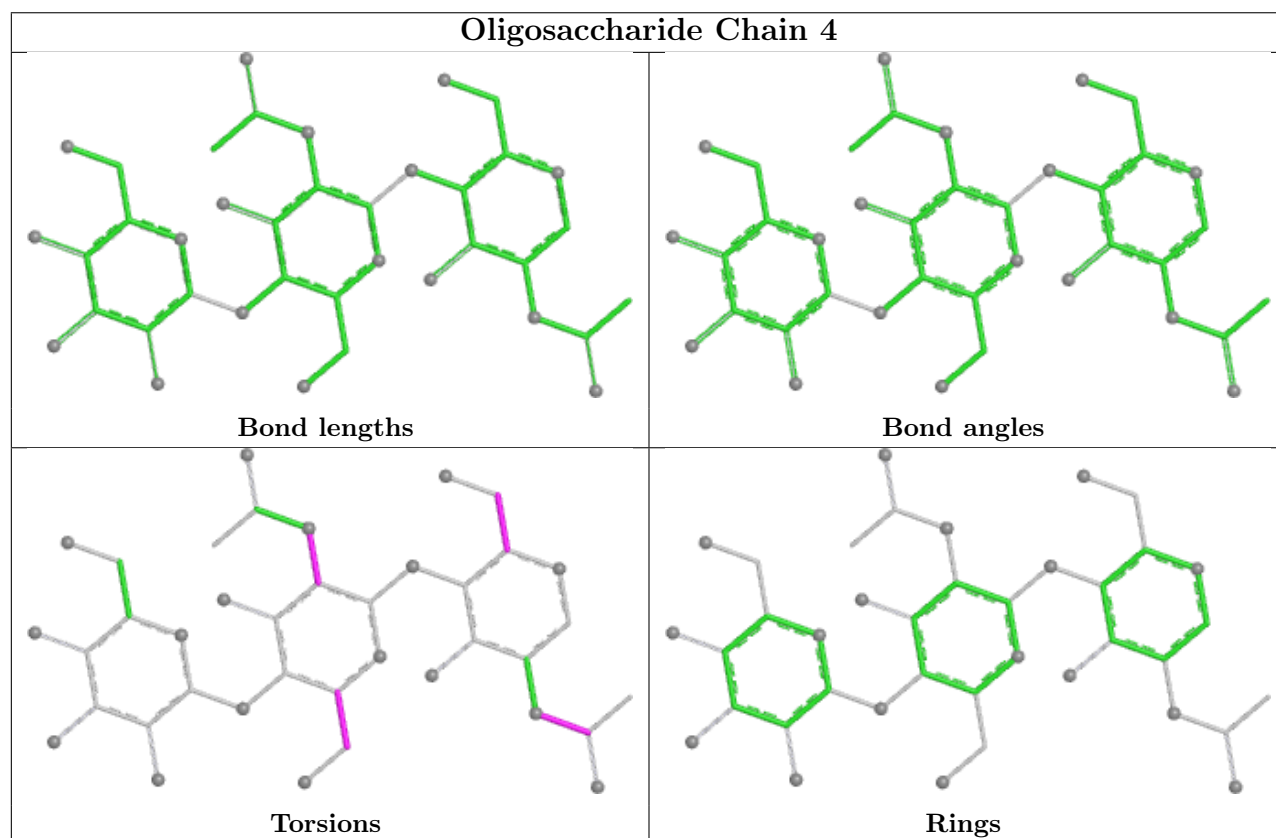
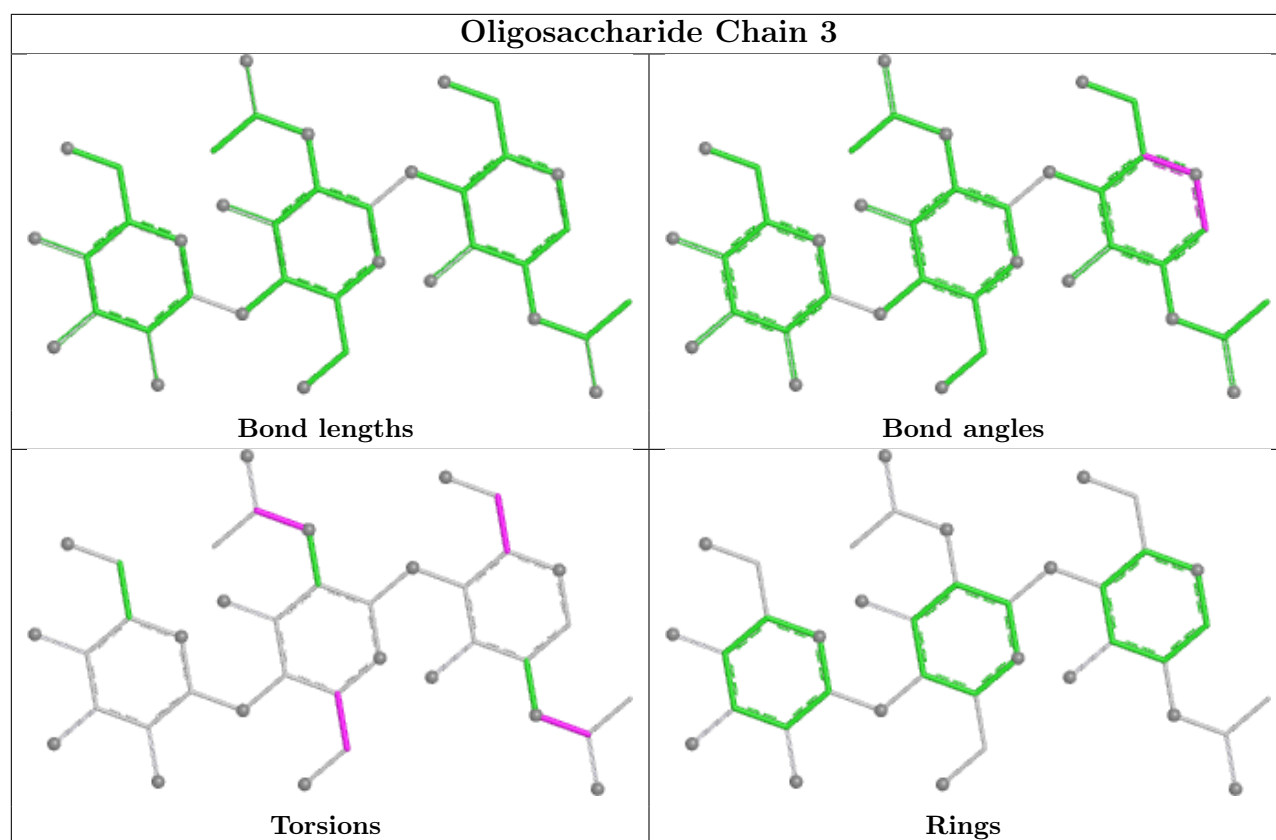




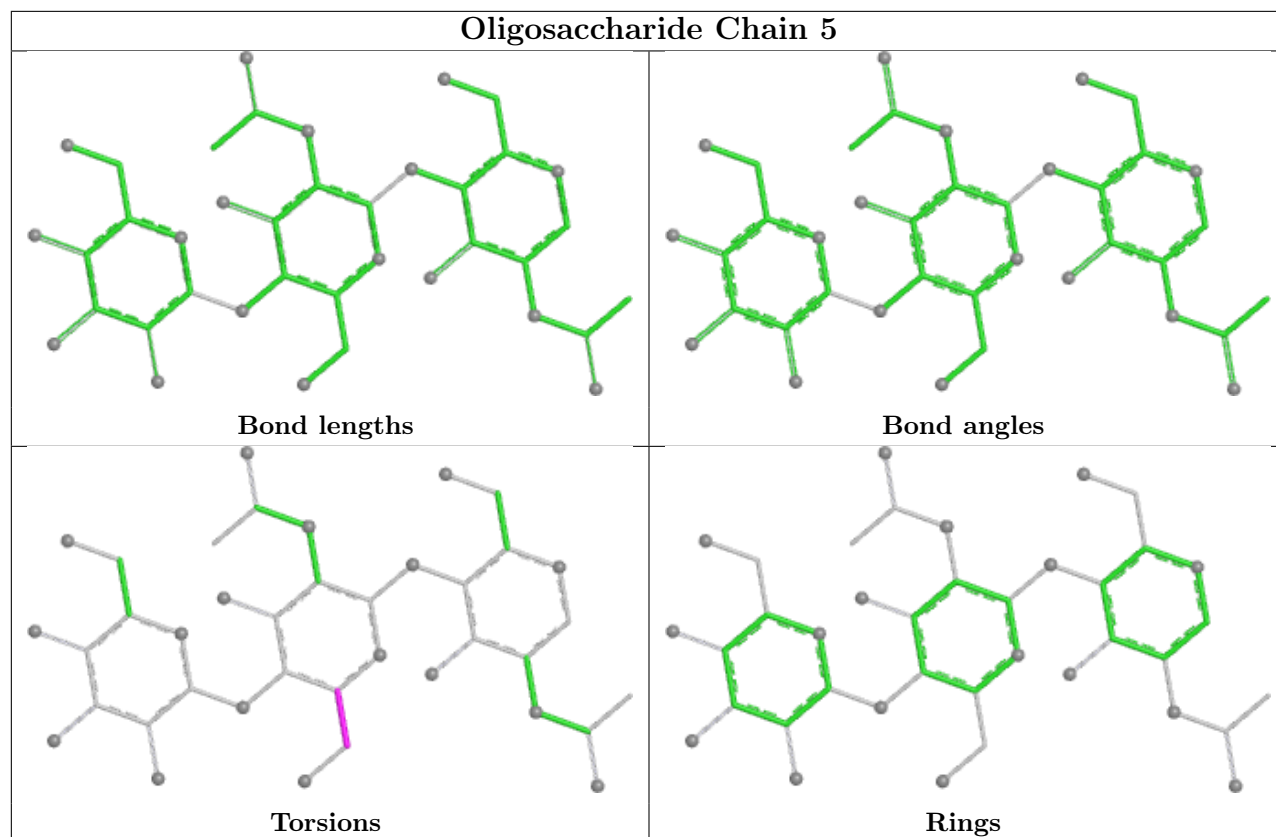




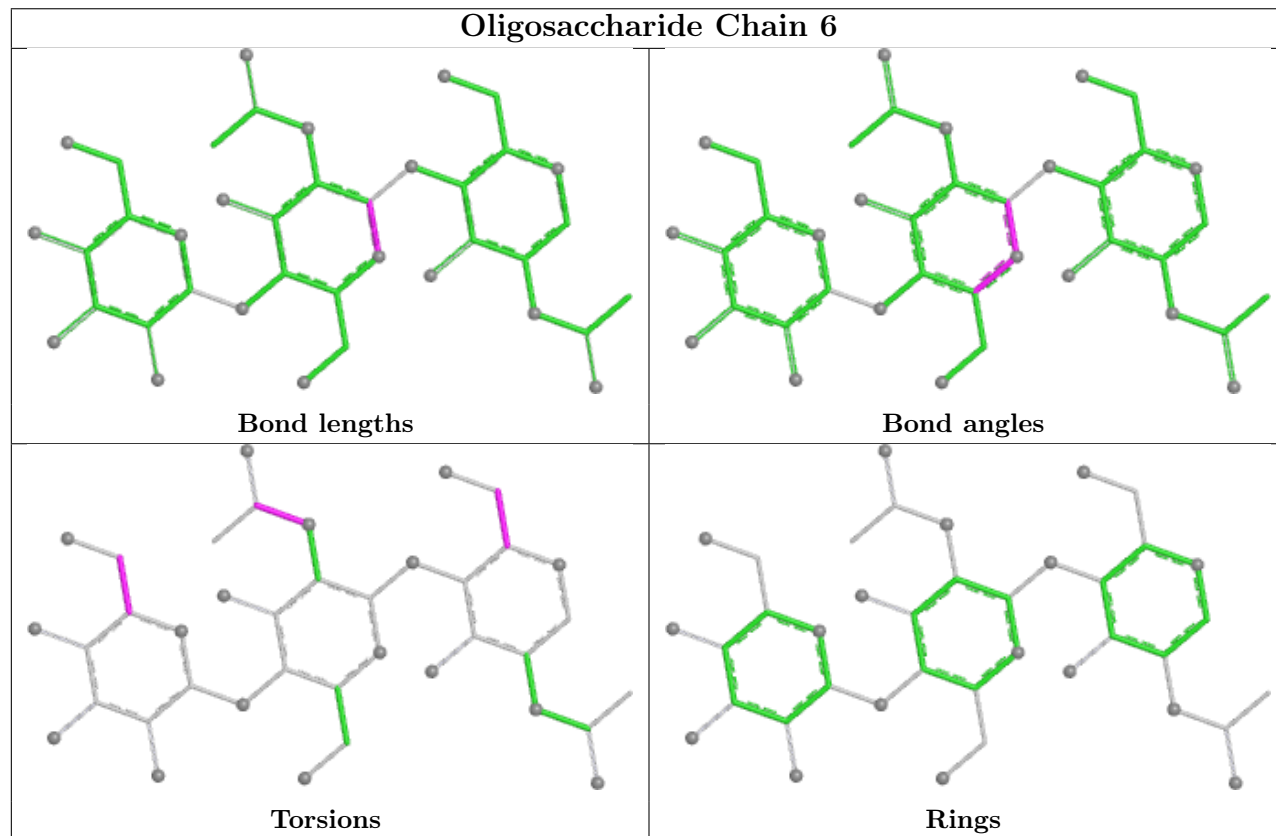


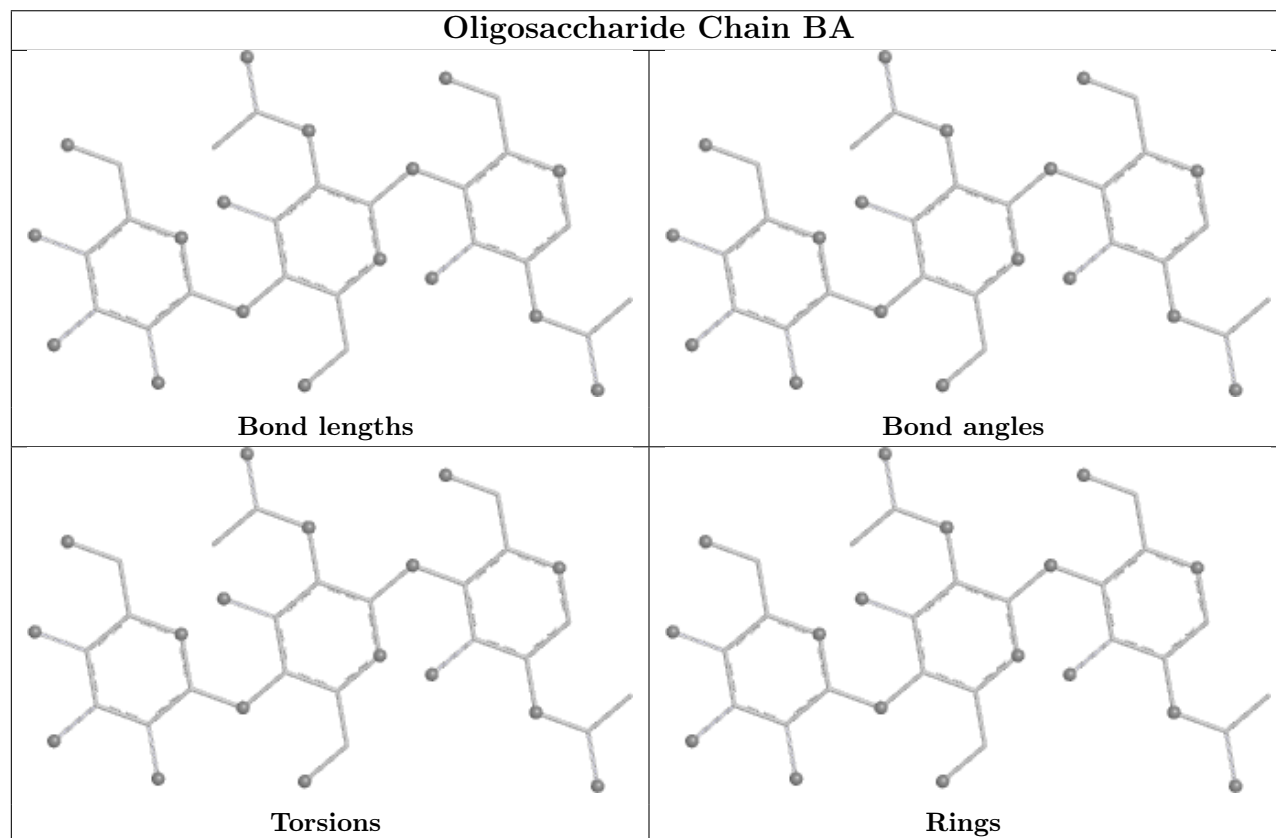
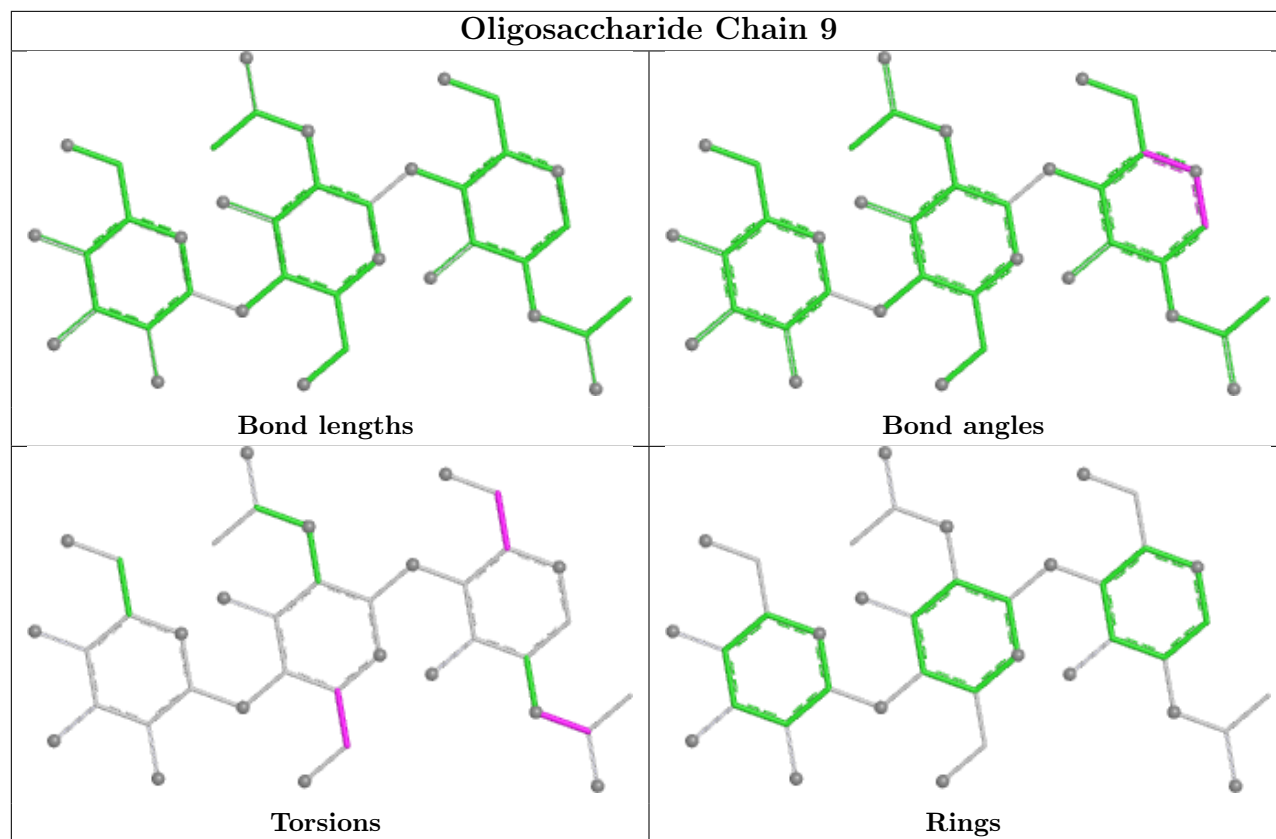


Oligosaccharide Chain 5

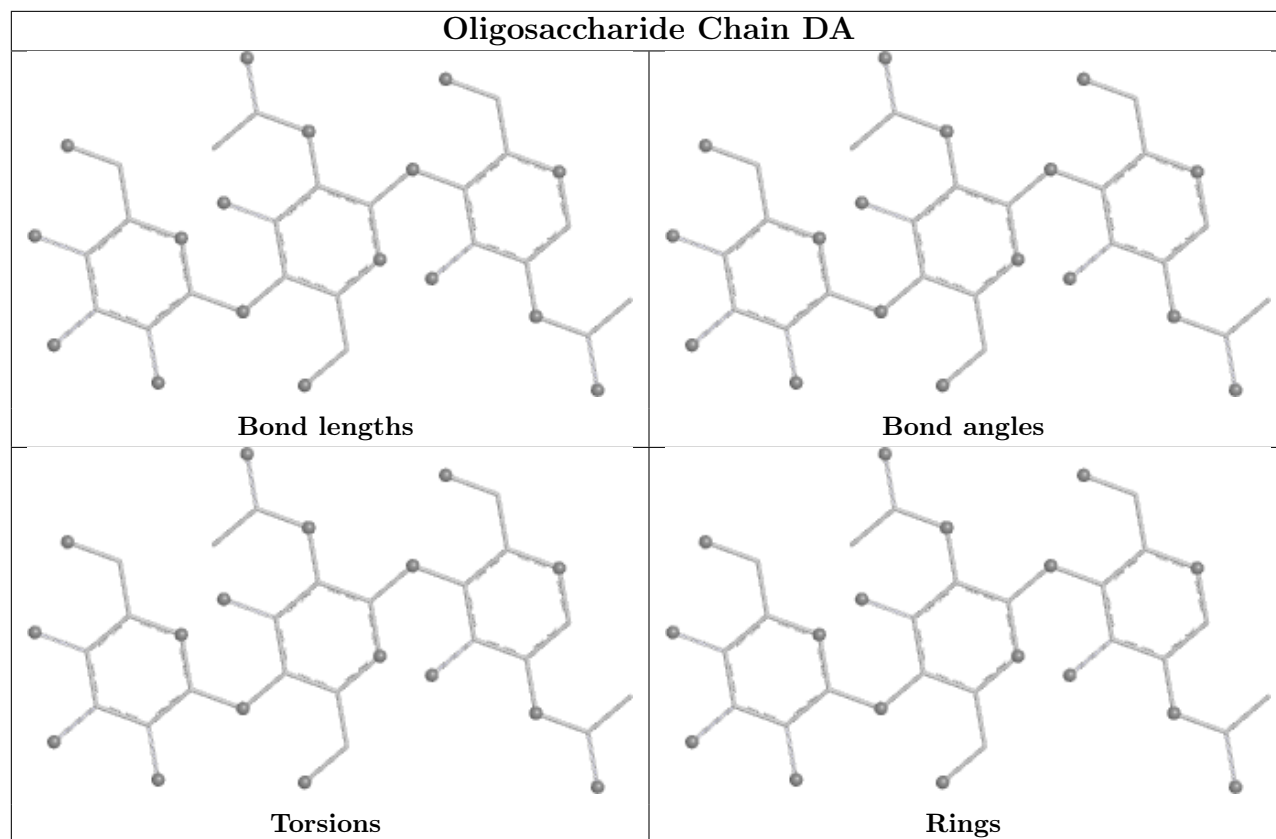


Oligosaccharide Chain 6

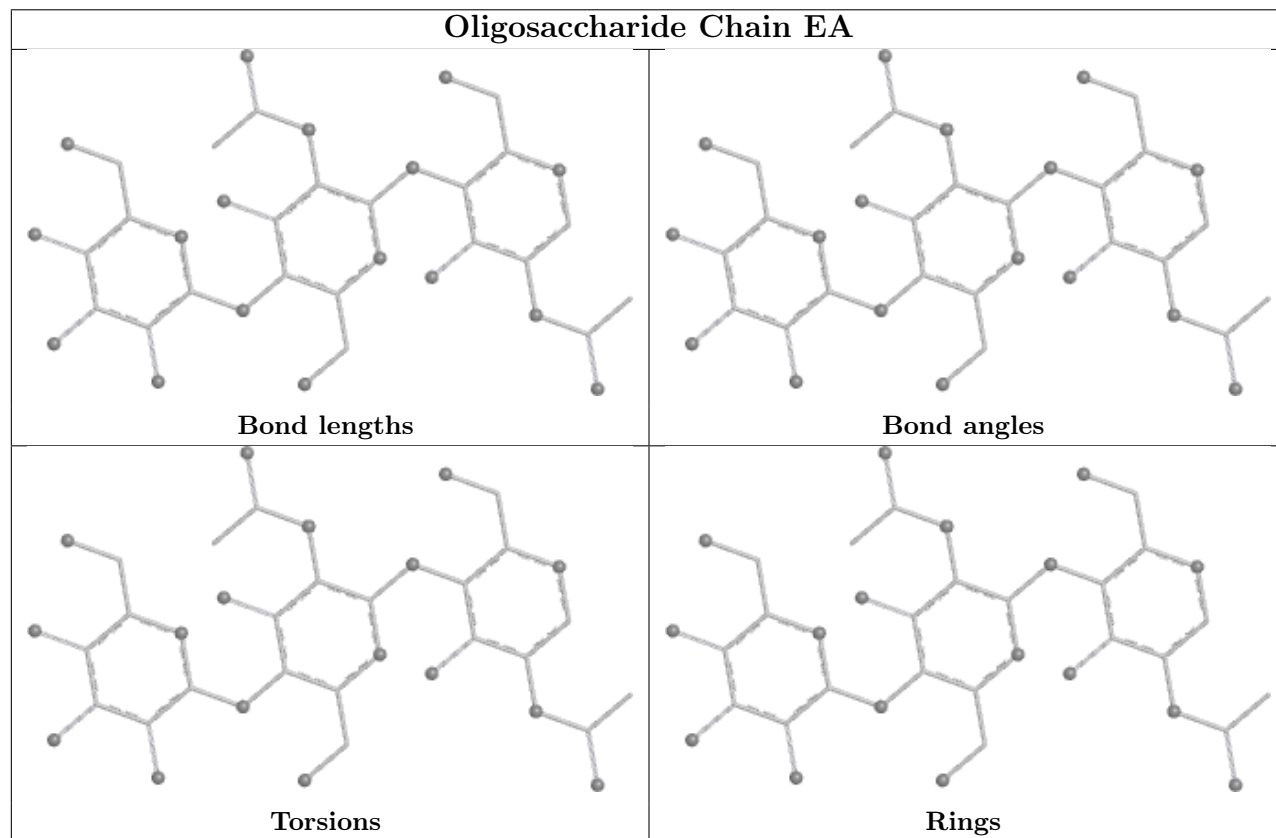


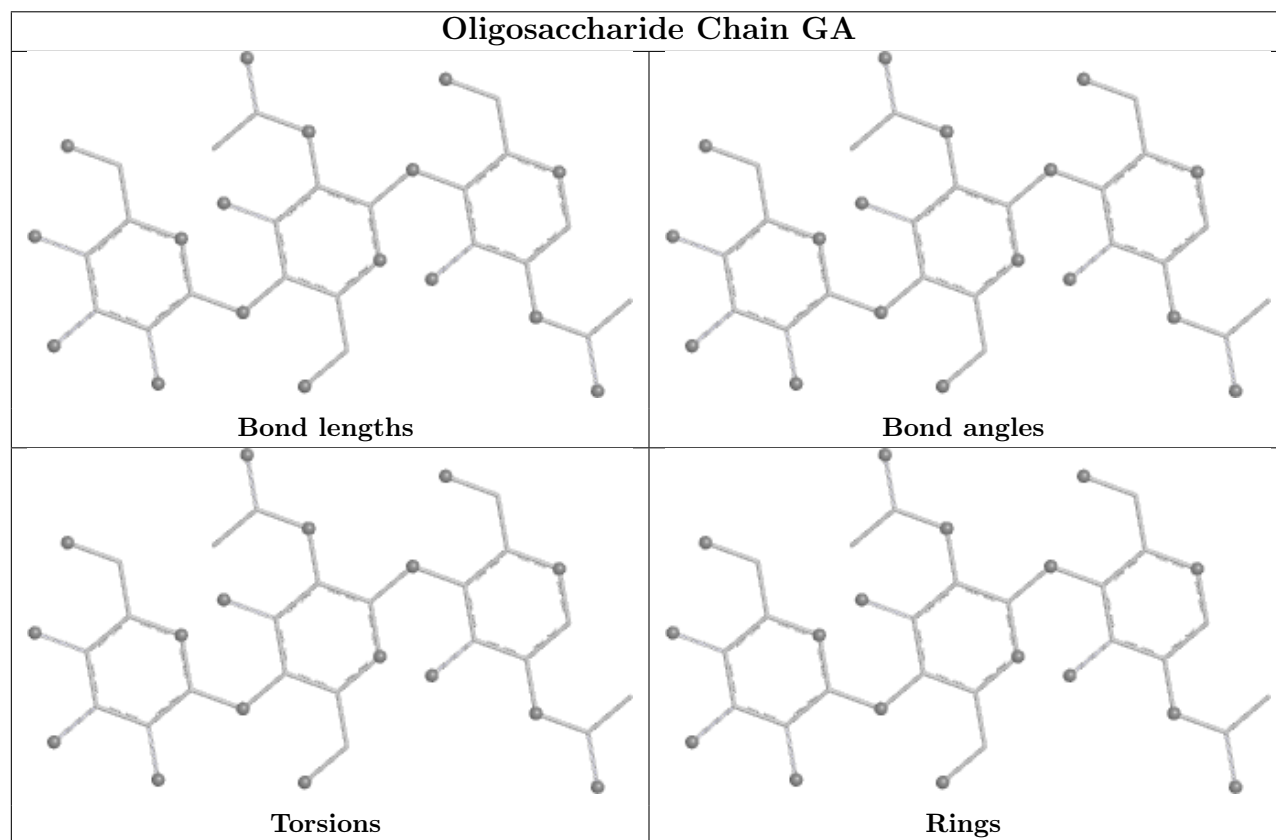
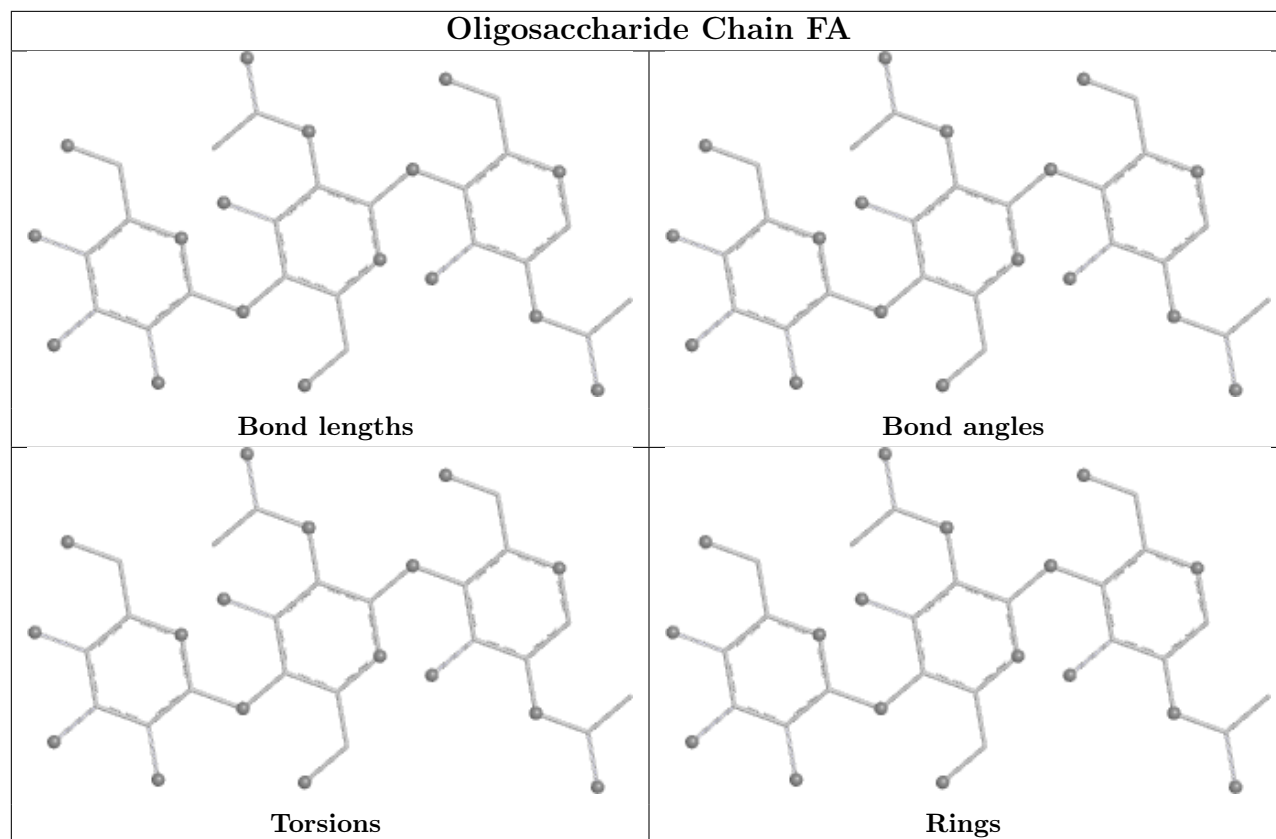


Oligosaccharide Chain DA

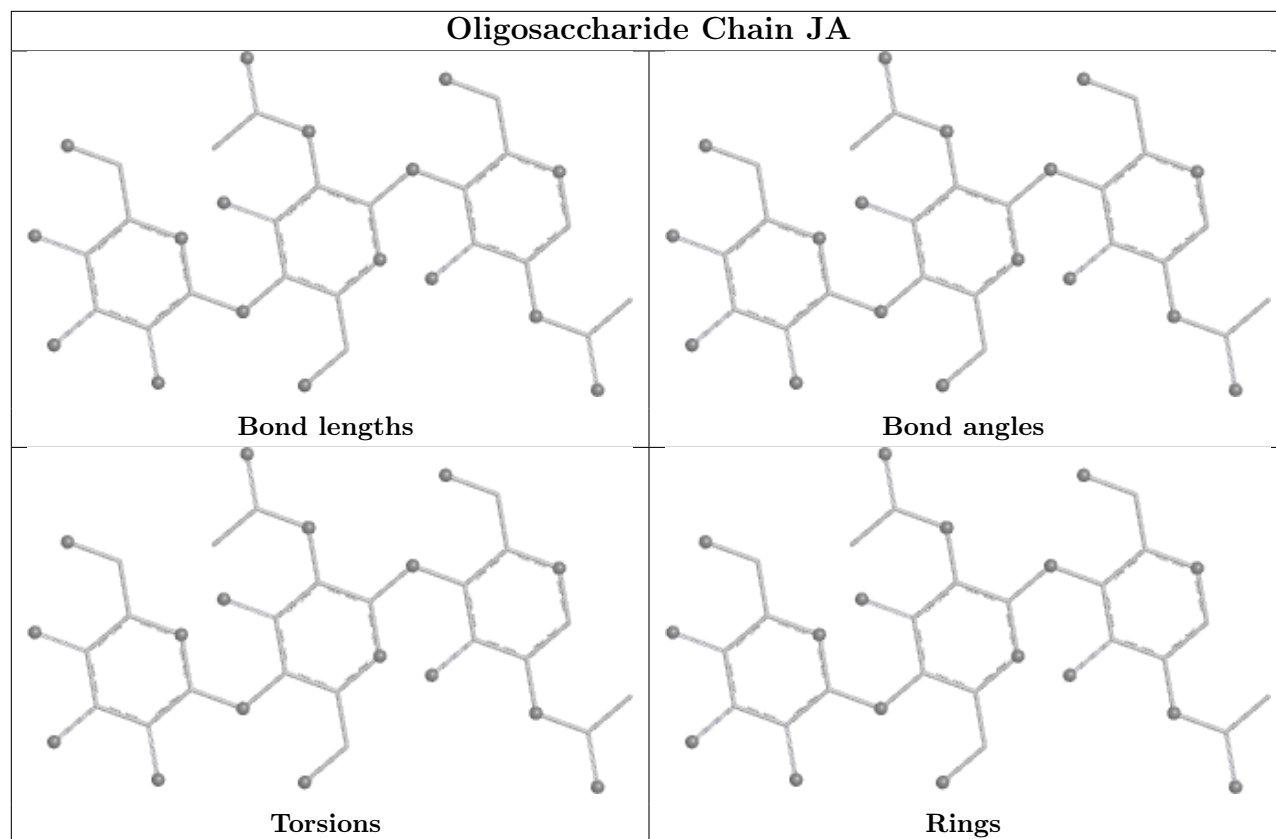


Oligosaccharide Chain EA

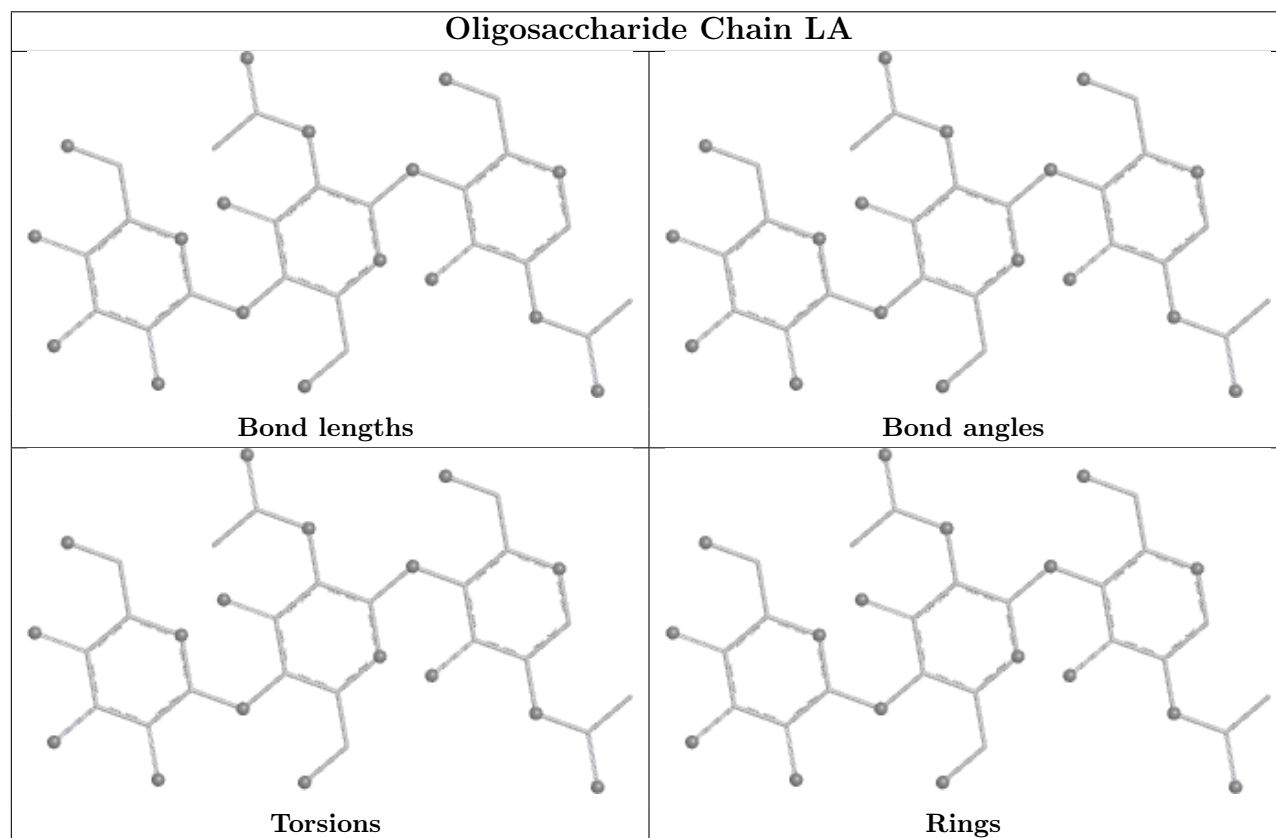




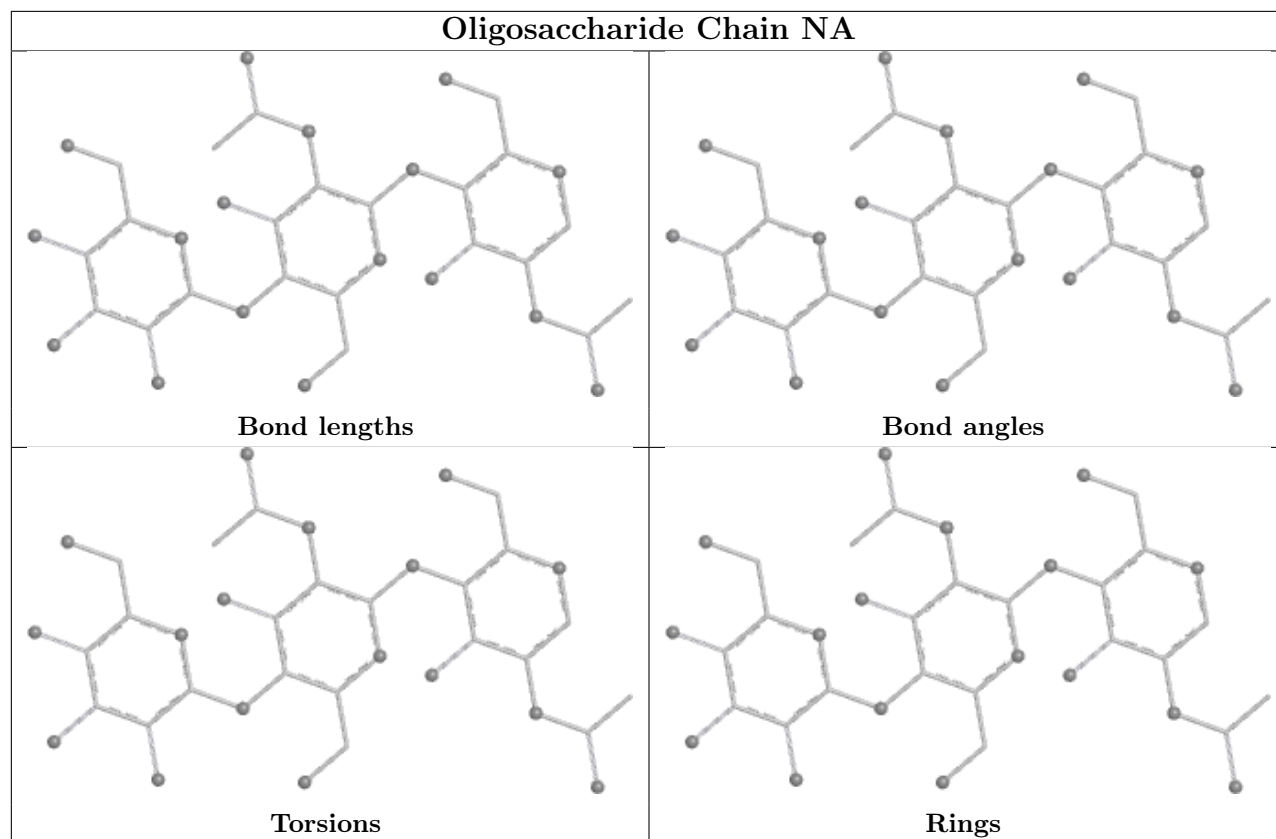
Oligosaccharide Chain JA



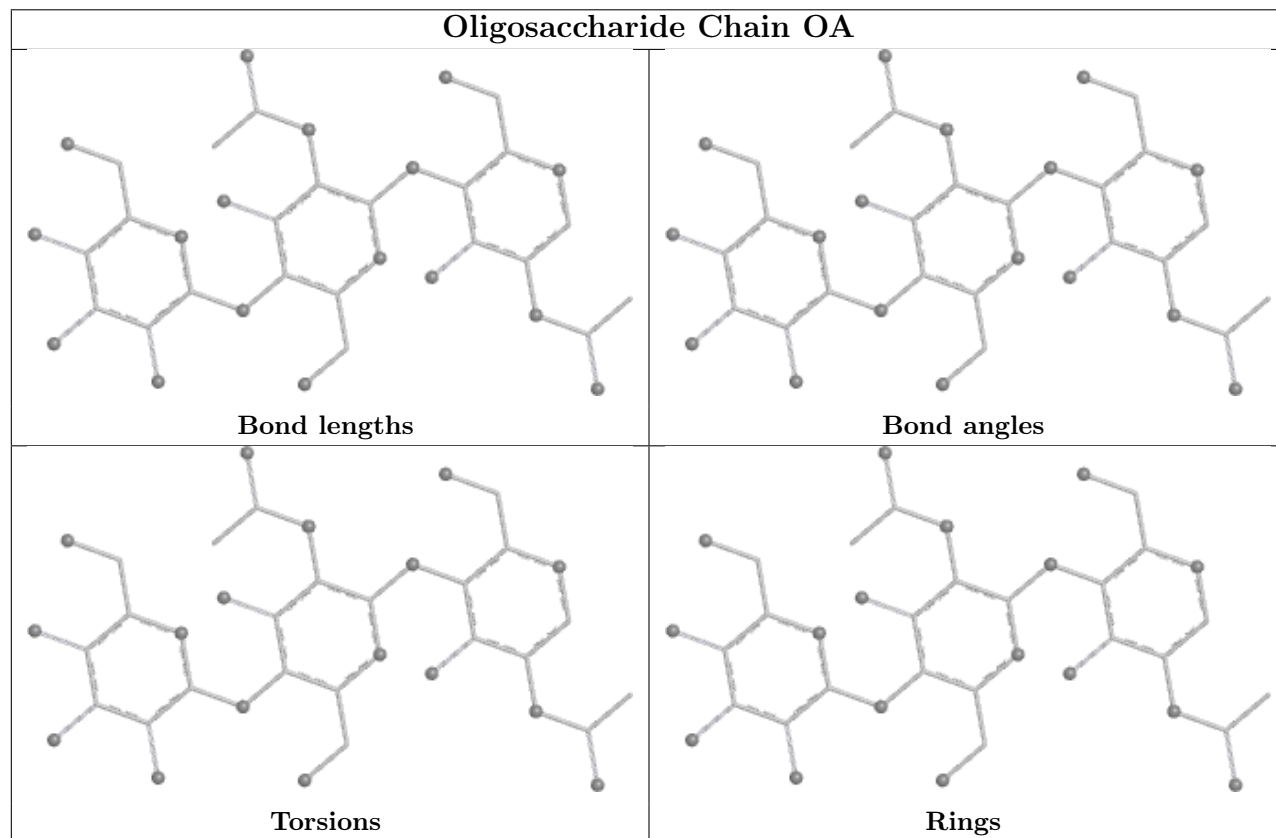
Oligosaccharide Chain LA



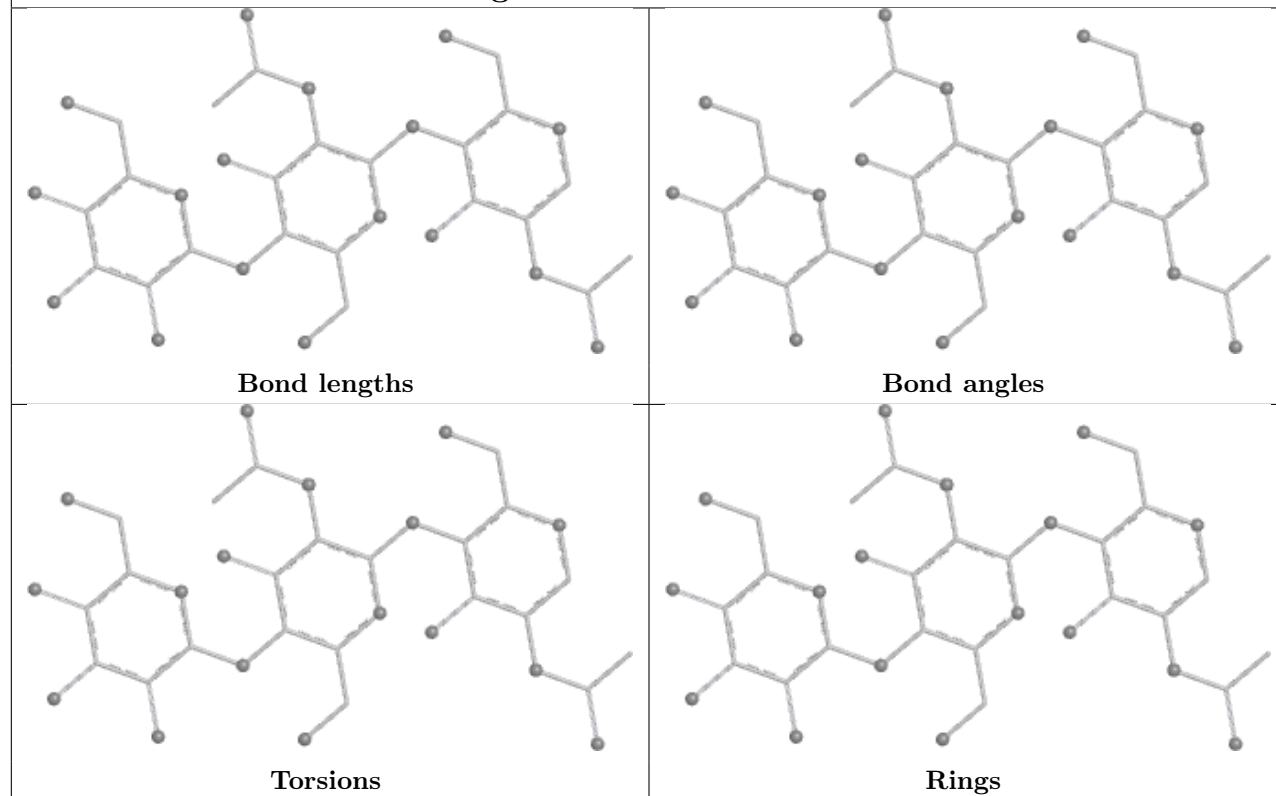
Oligosaccharide Chain NA



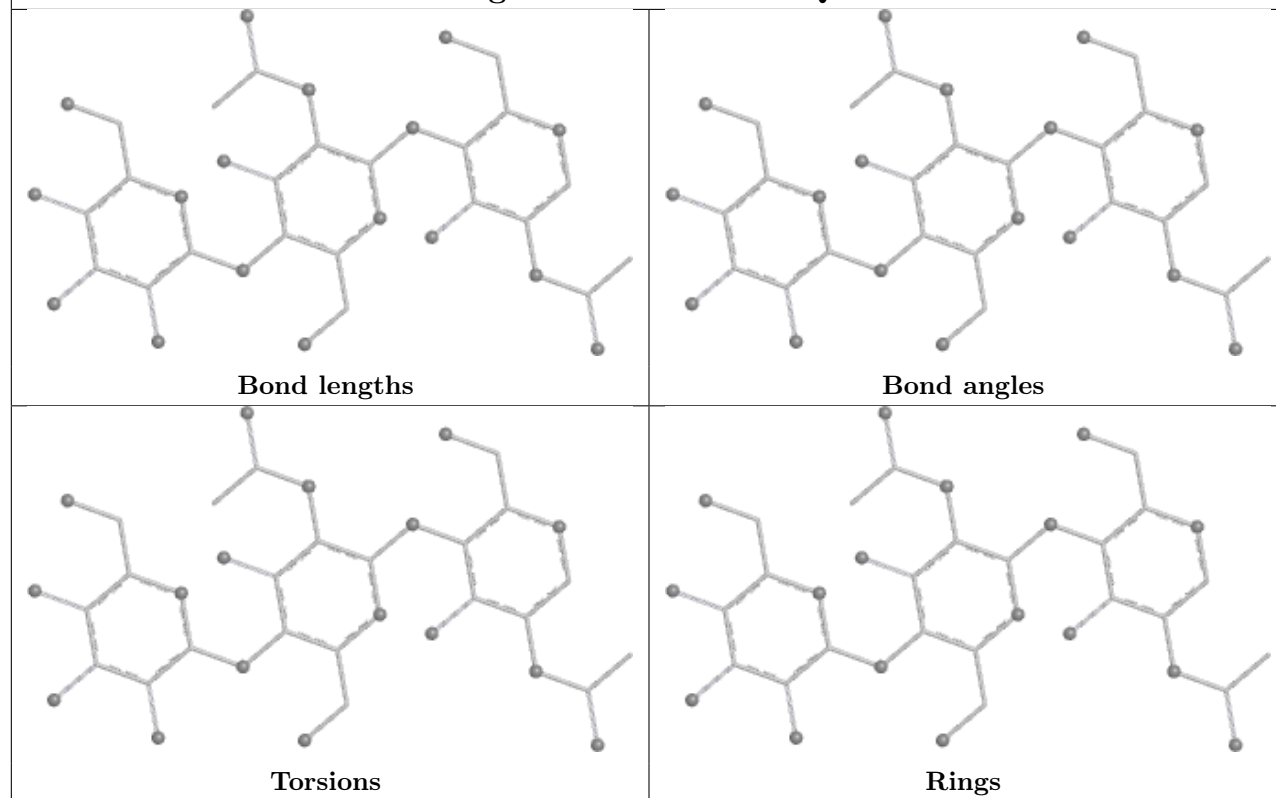
Oligosaccharide Chain OA

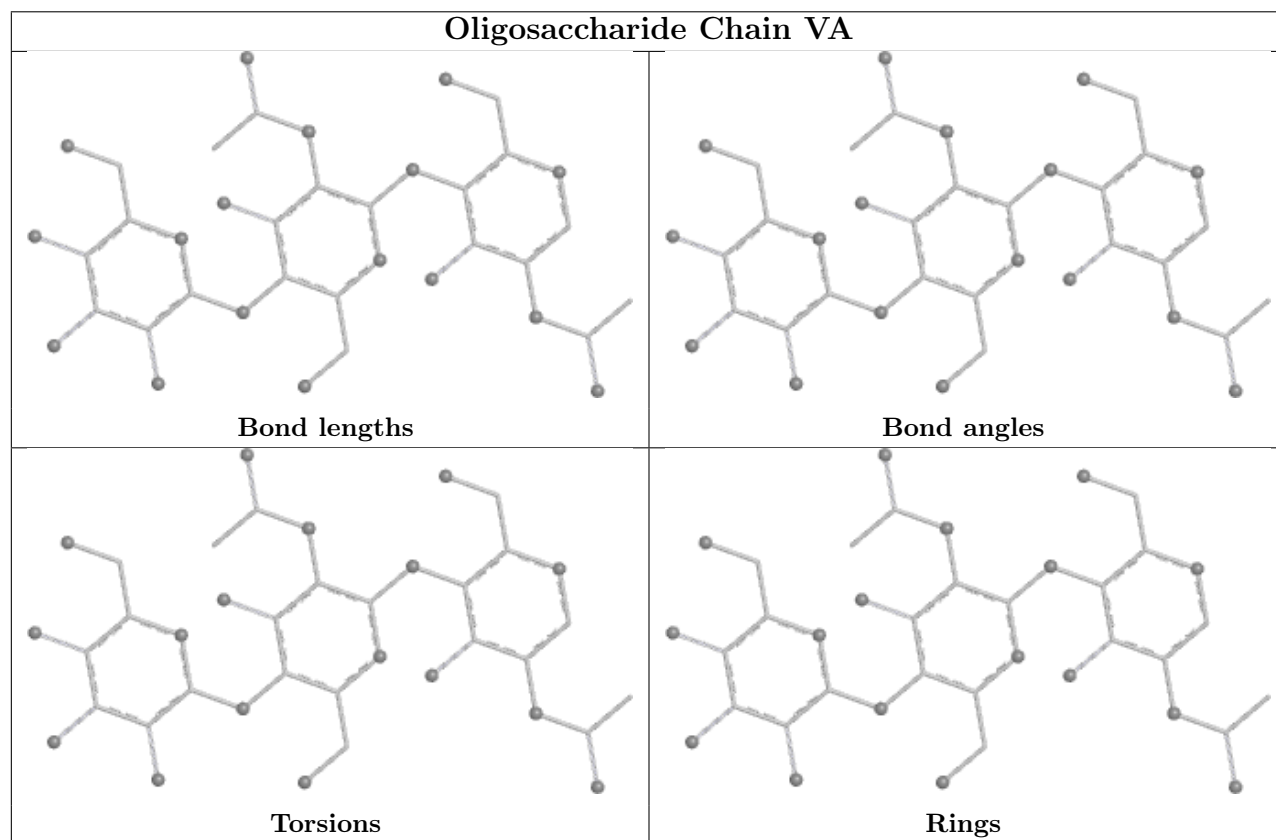
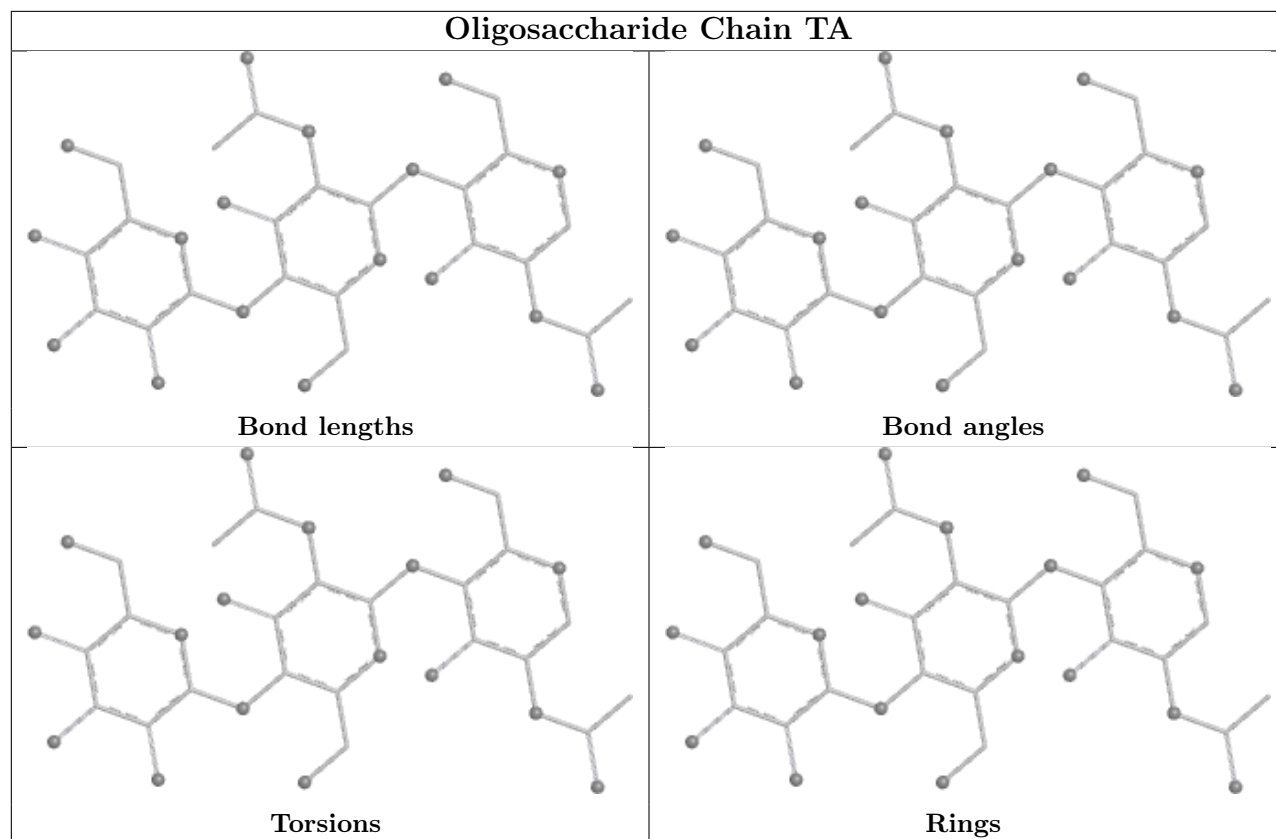


Oligosaccharide Chain PA

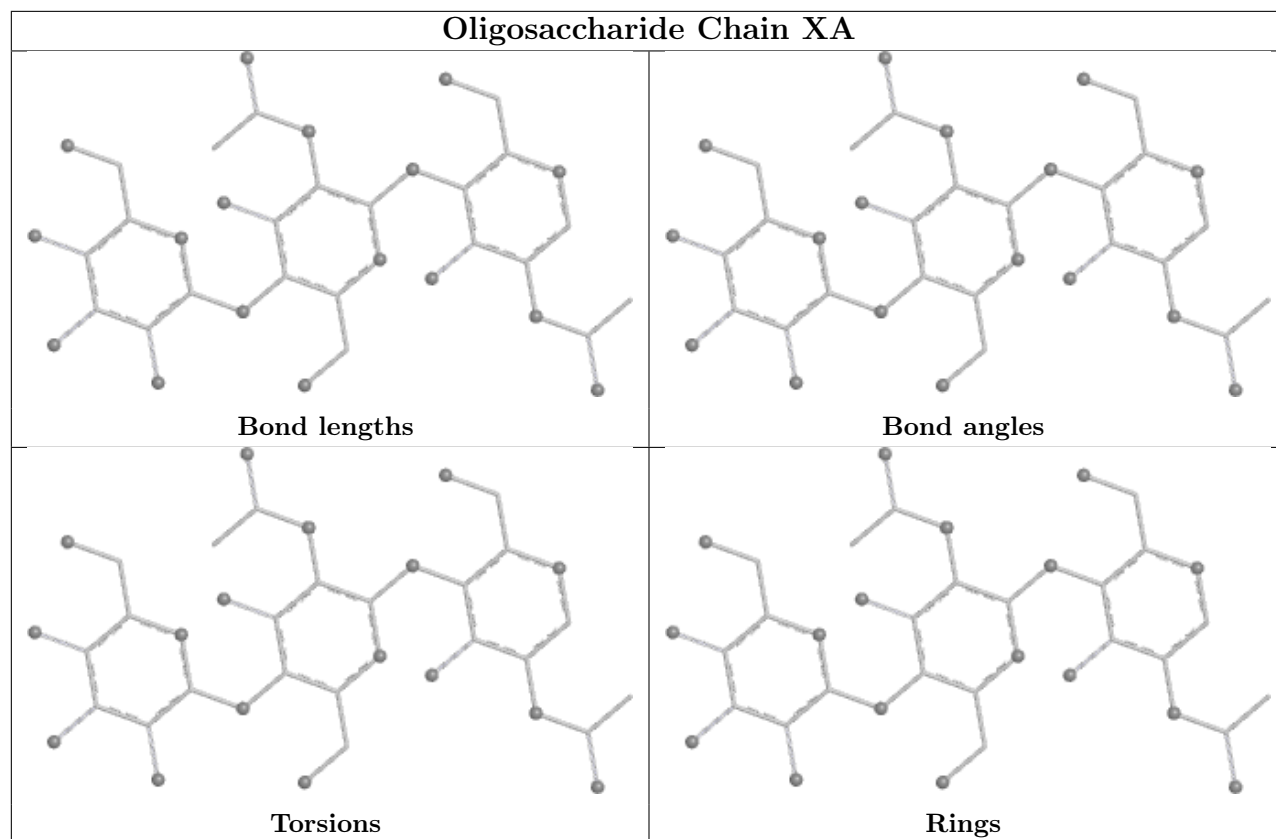


Oligosaccharide Chain QA

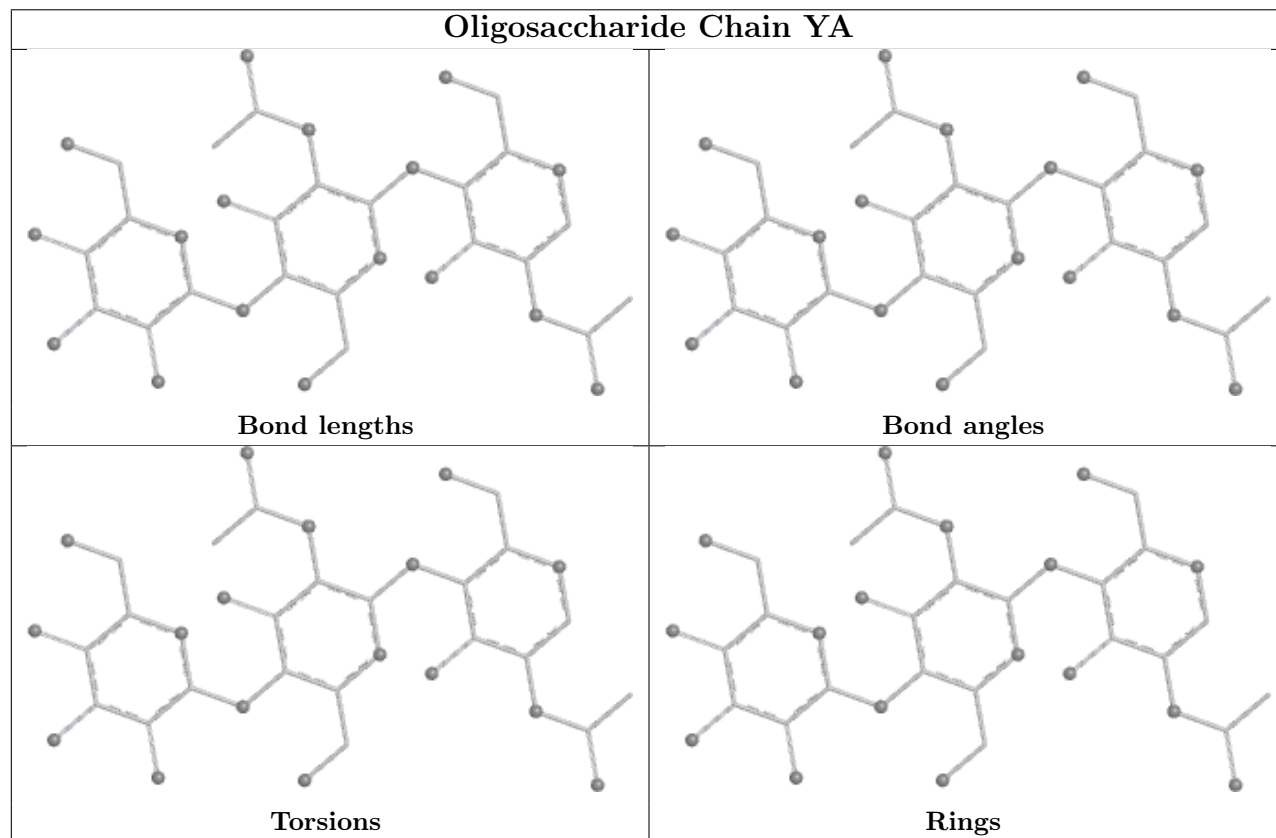


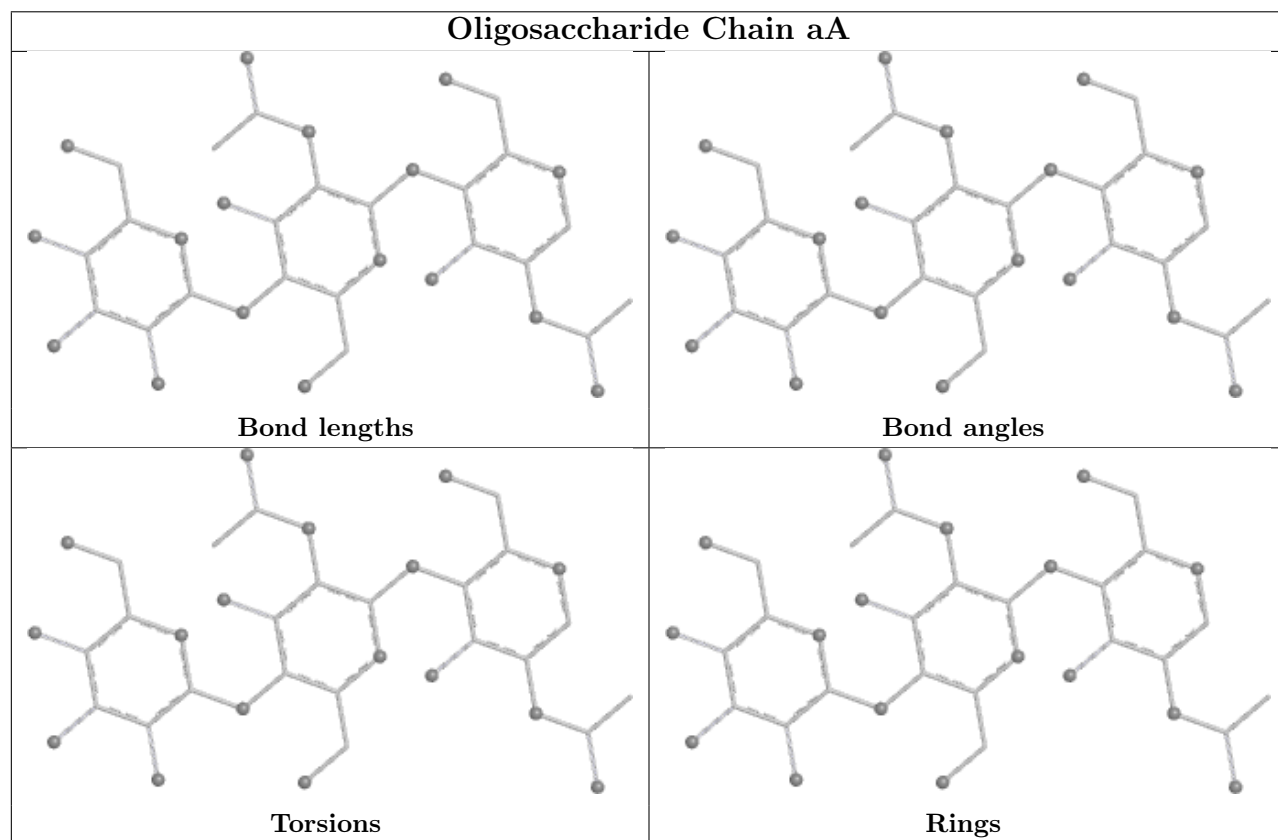
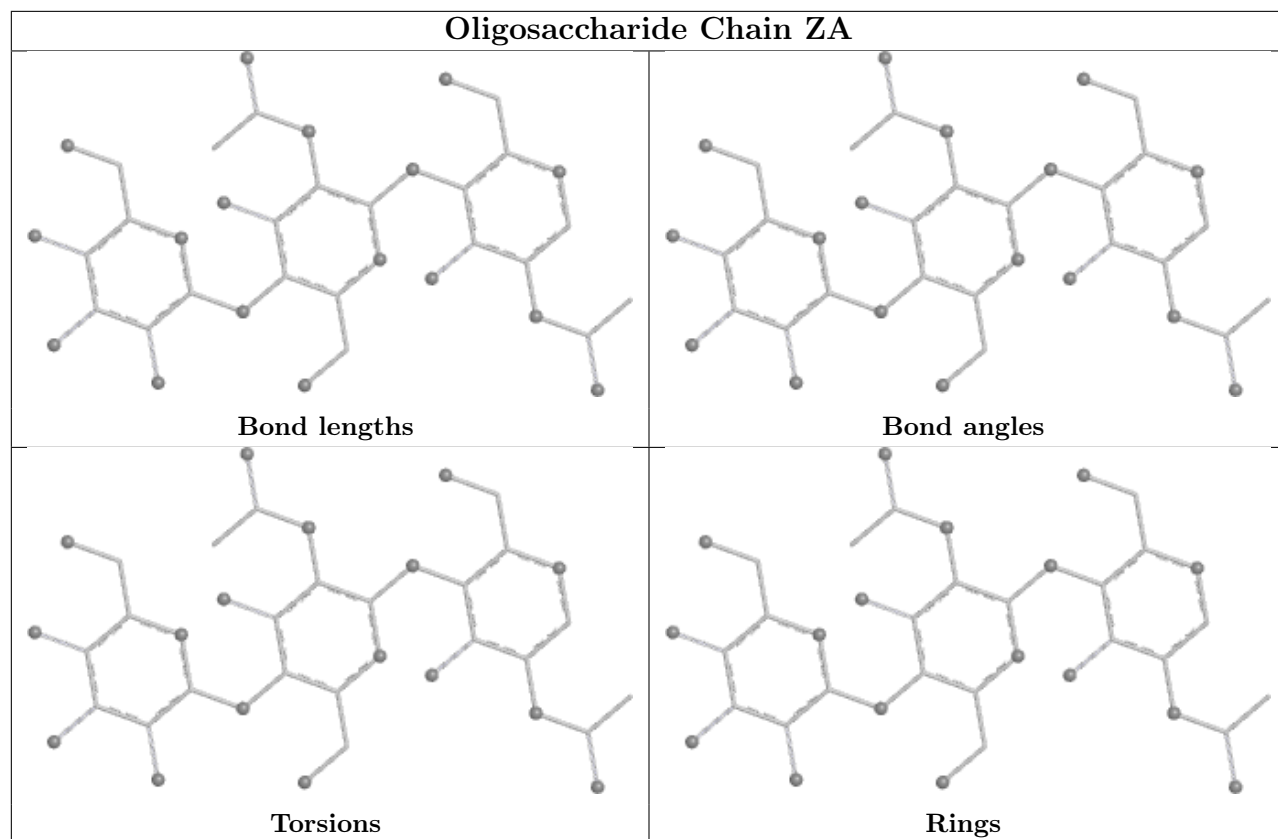


Oligosaccharide Chain XA

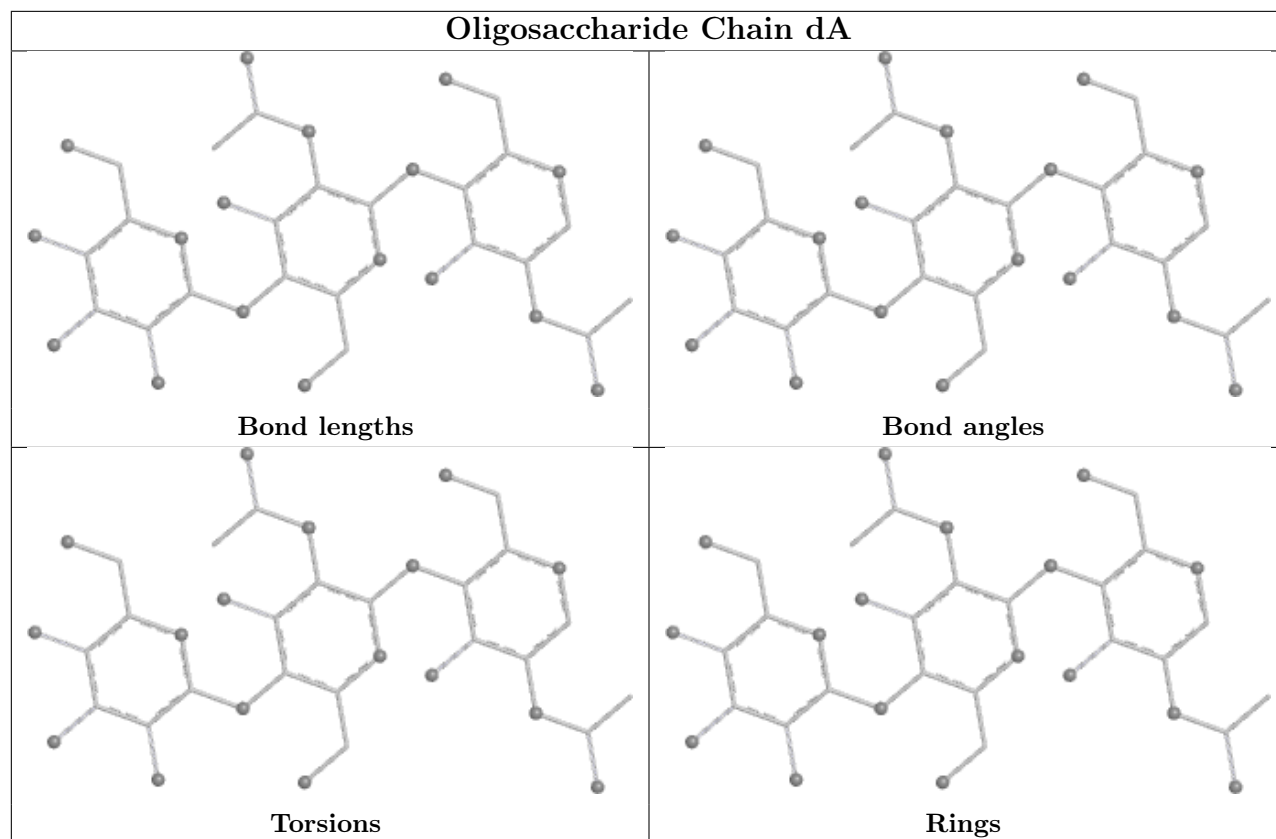


Oligosaccharide Chain YA

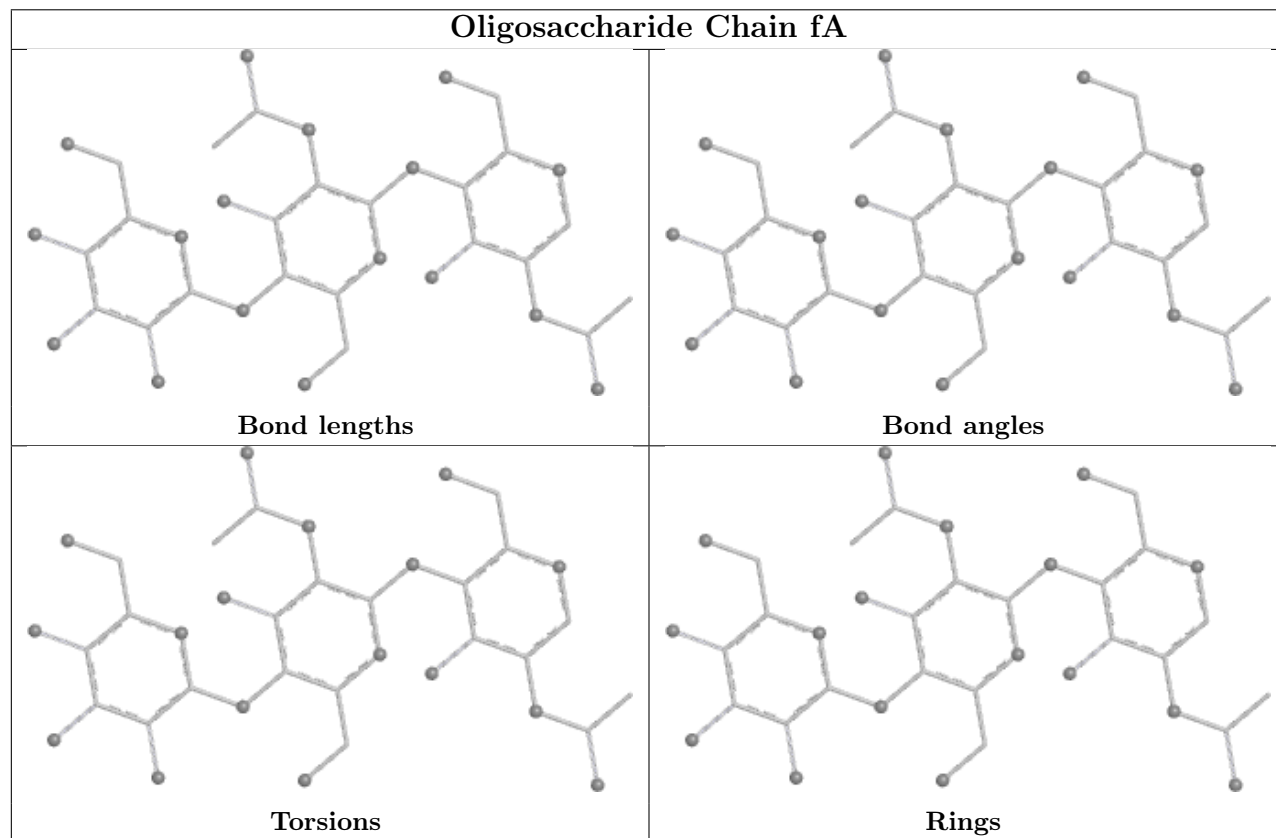




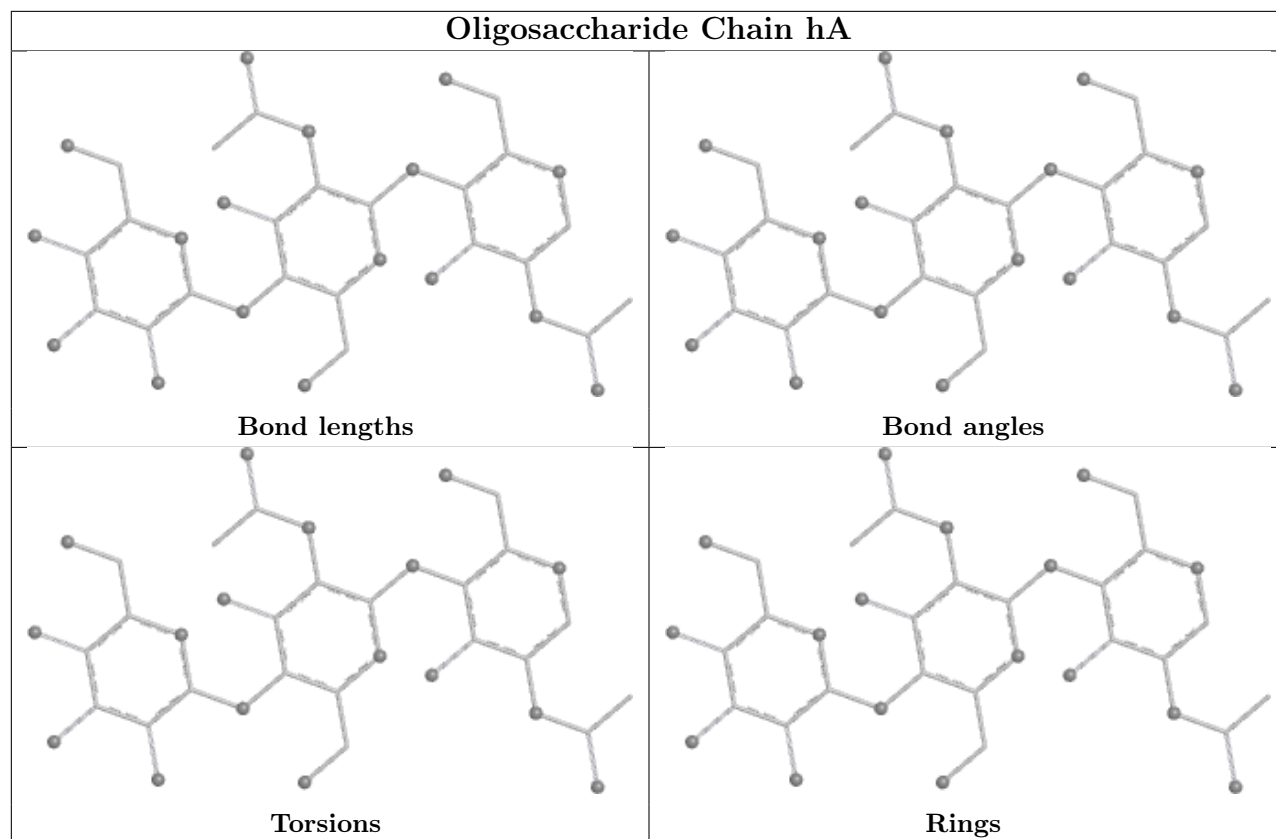
Oligosaccharide Chain dA



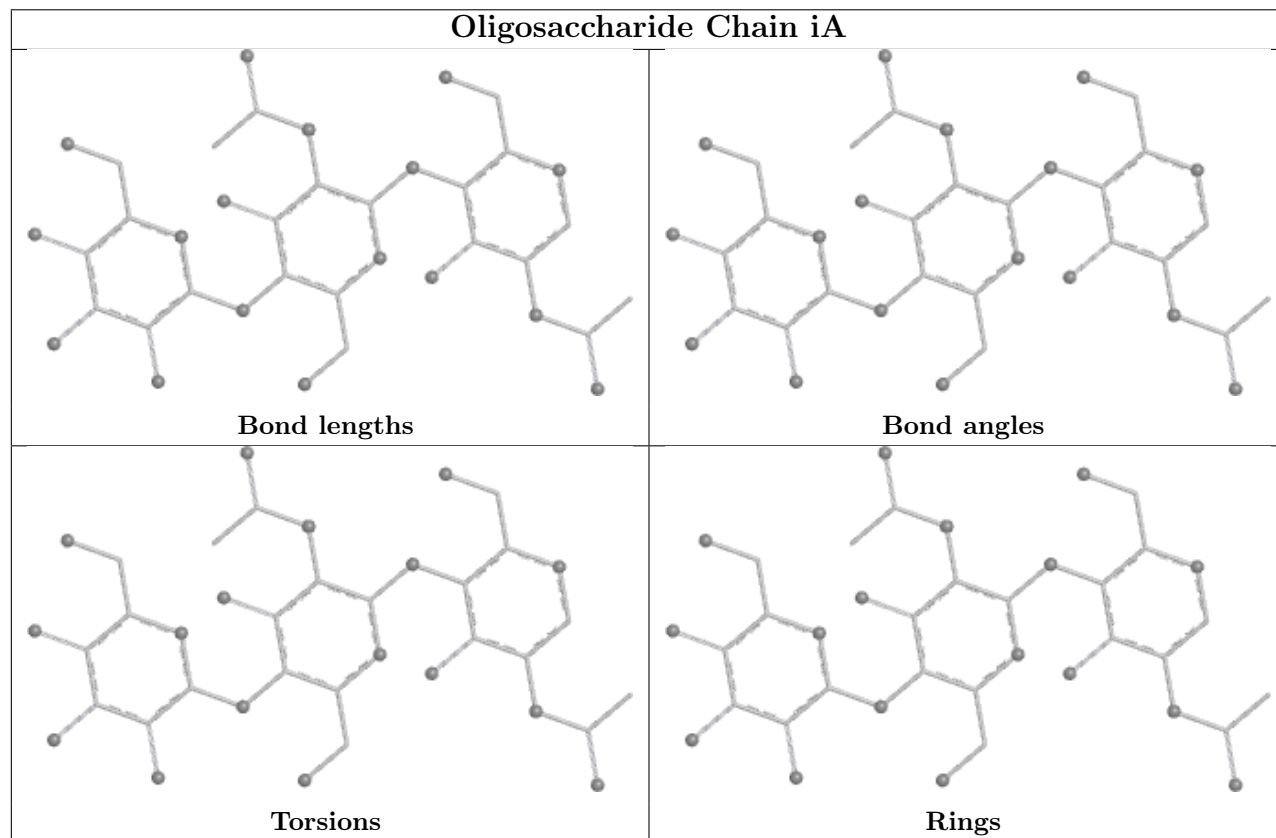
Oligosaccharide Chain fA



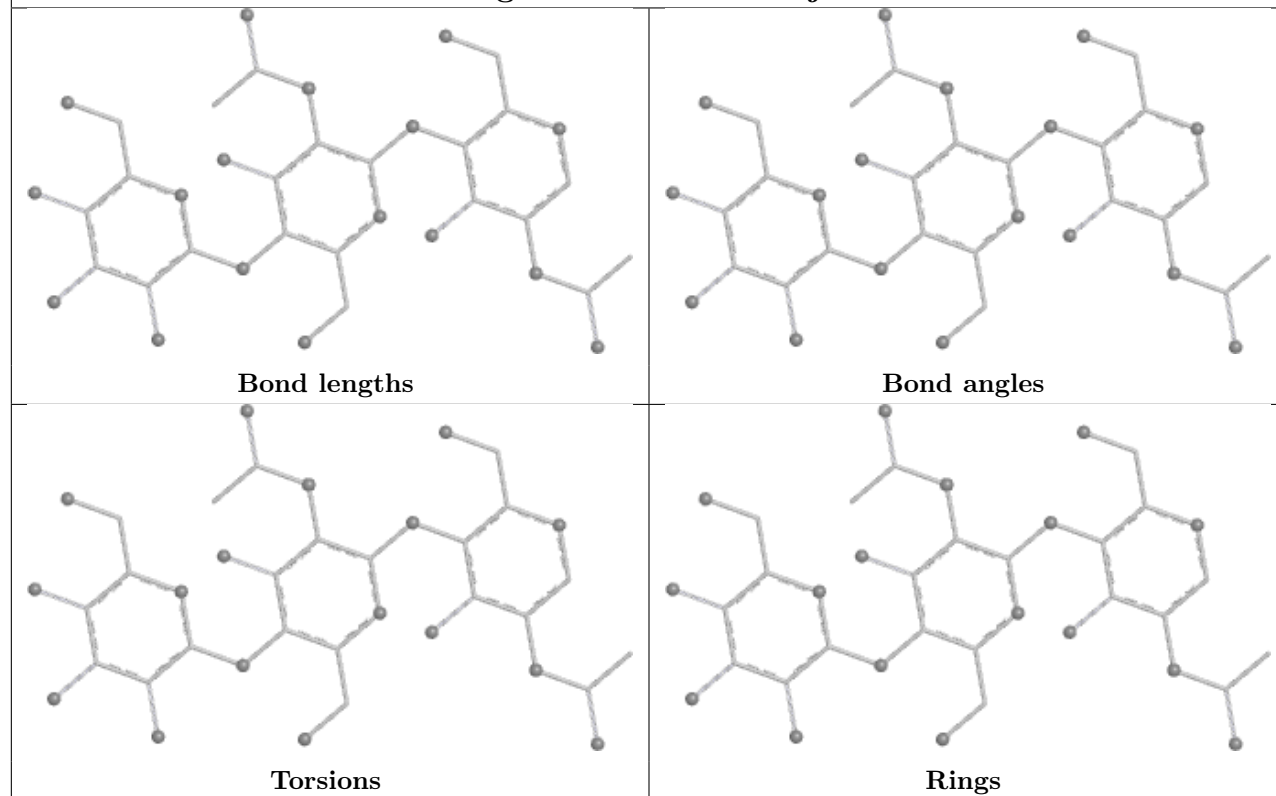
Oligosaccharide Chain hA



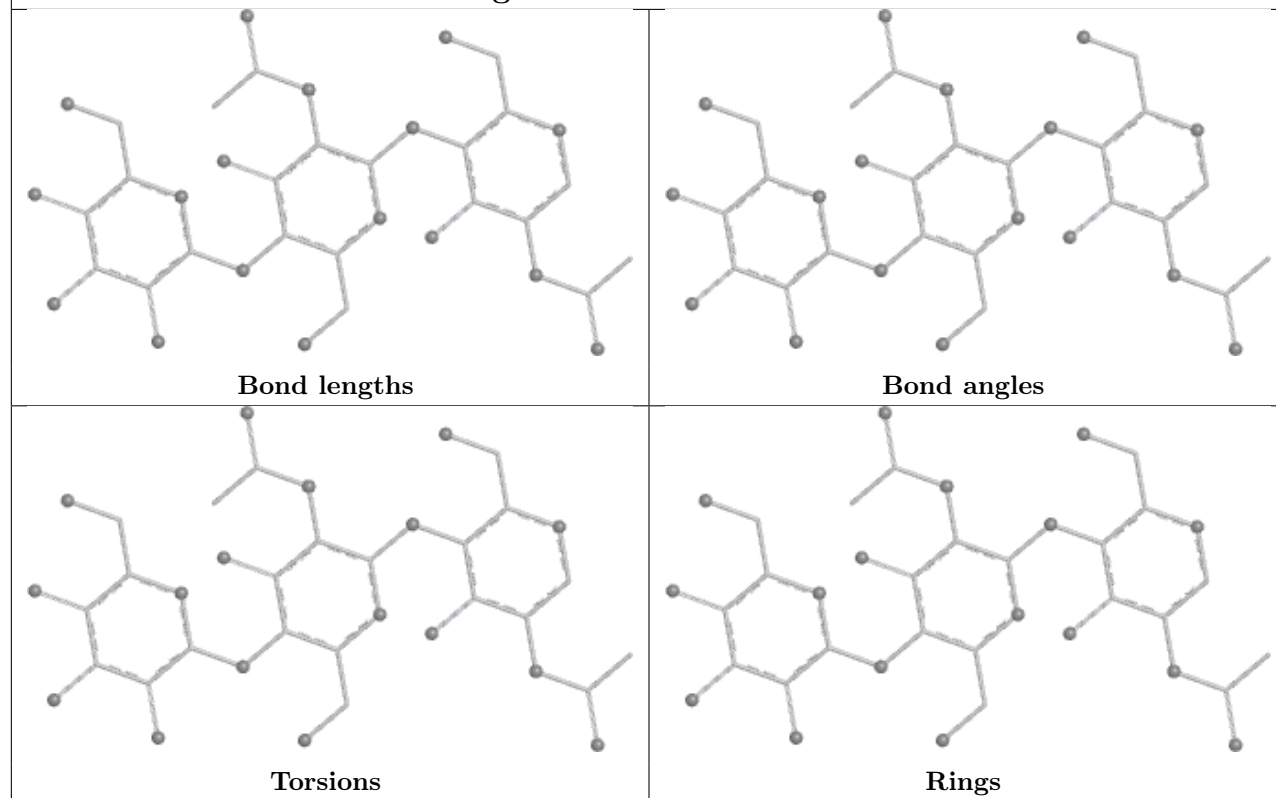
Oligosaccharide Chain iA

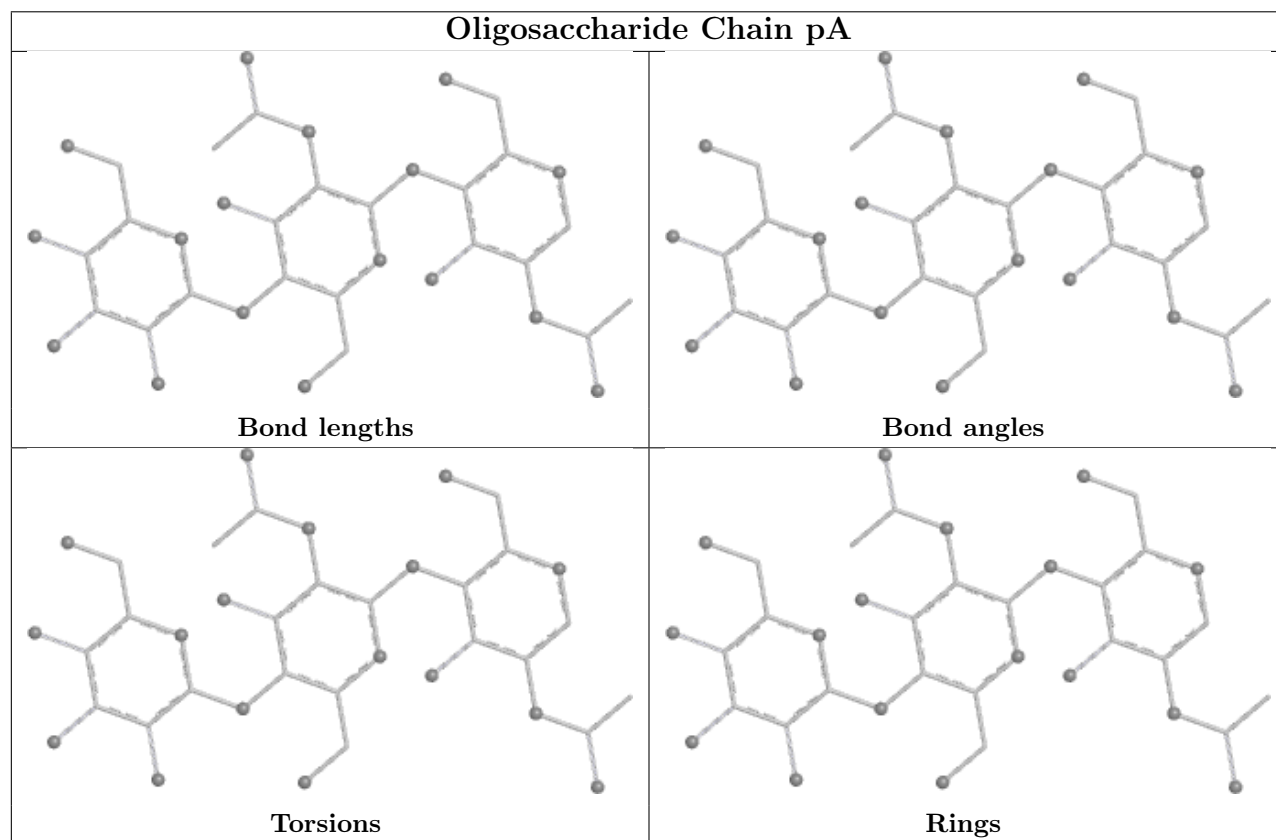
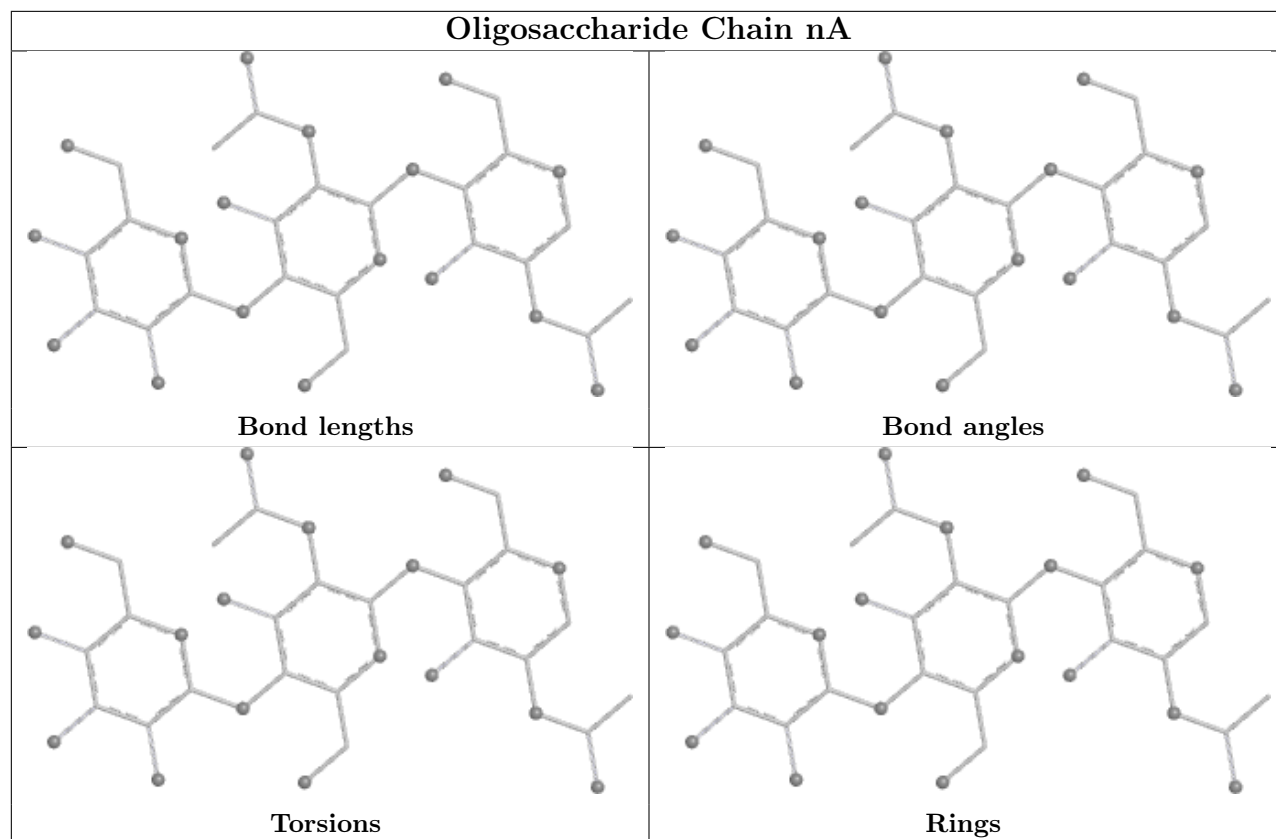


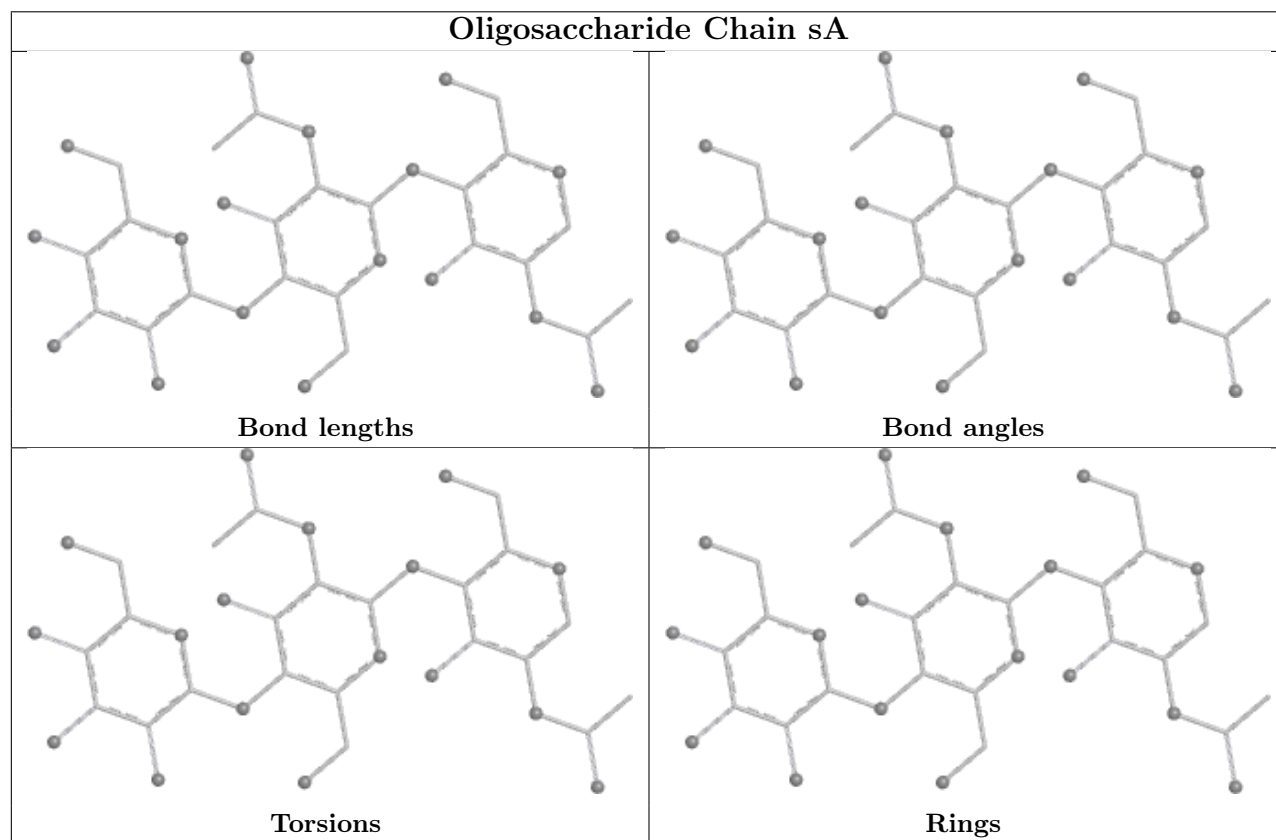
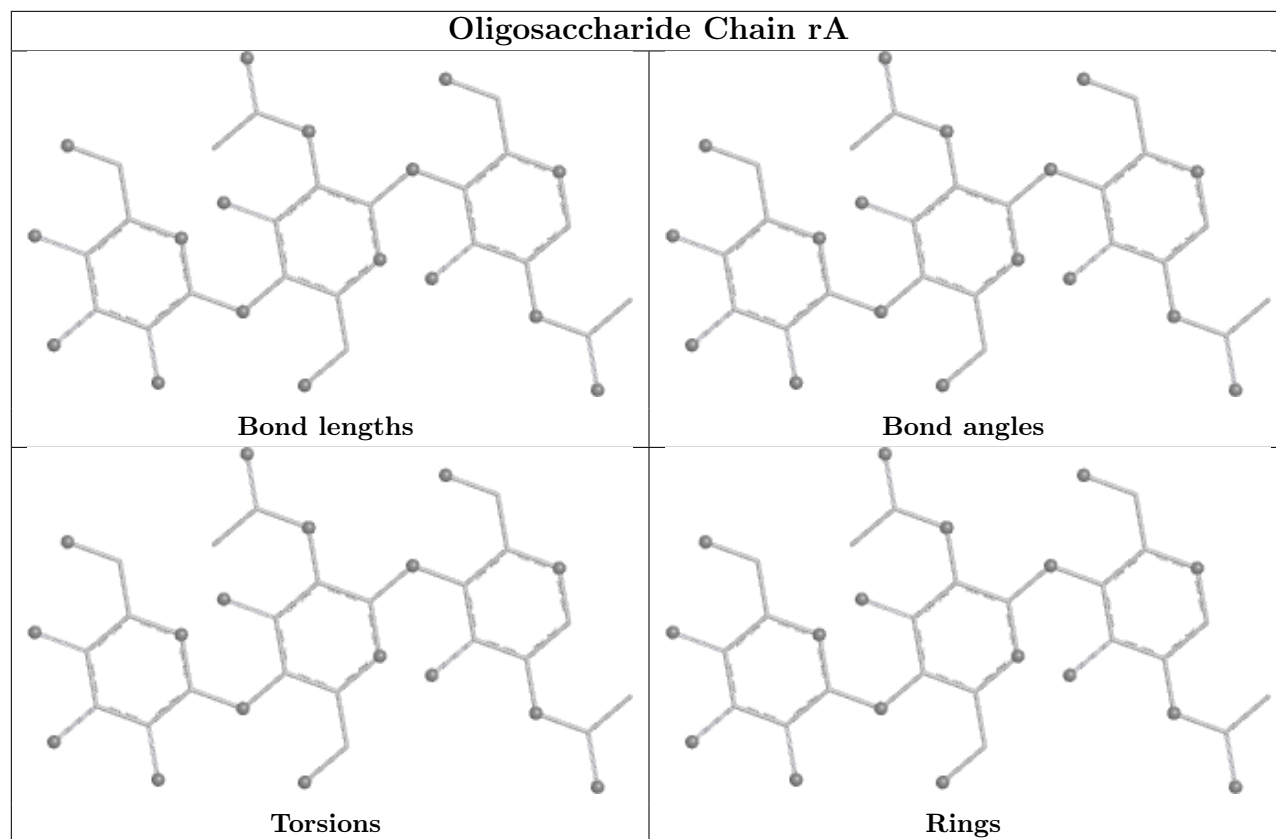
Oligosaccharide Chain jA



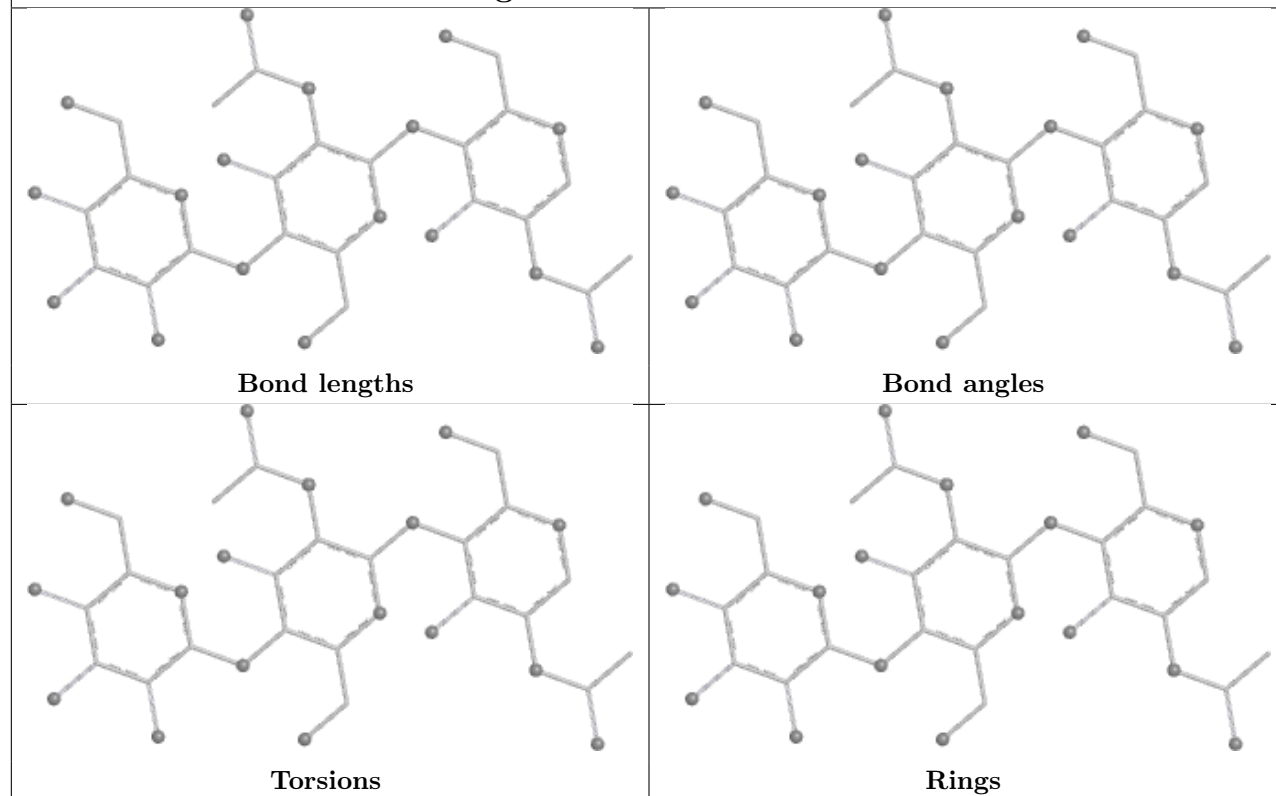
Oligosaccharide Chain kA



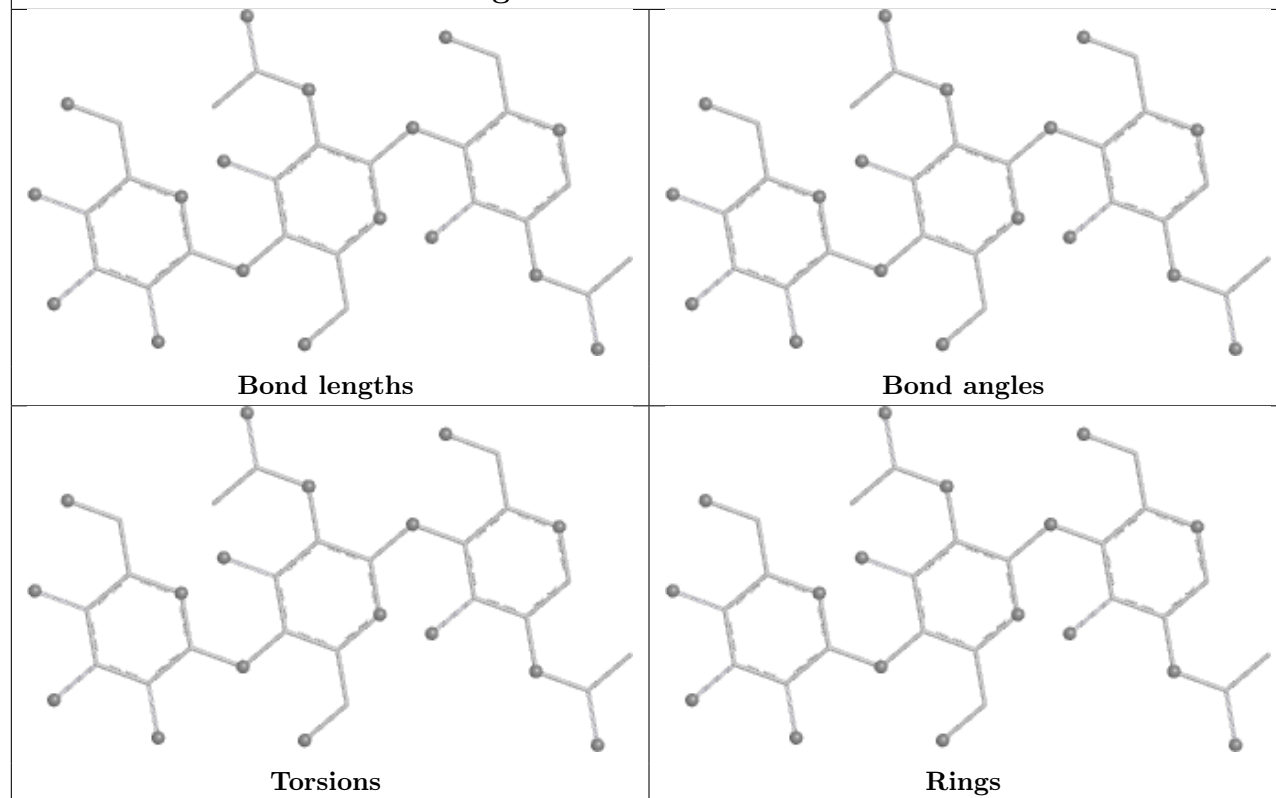


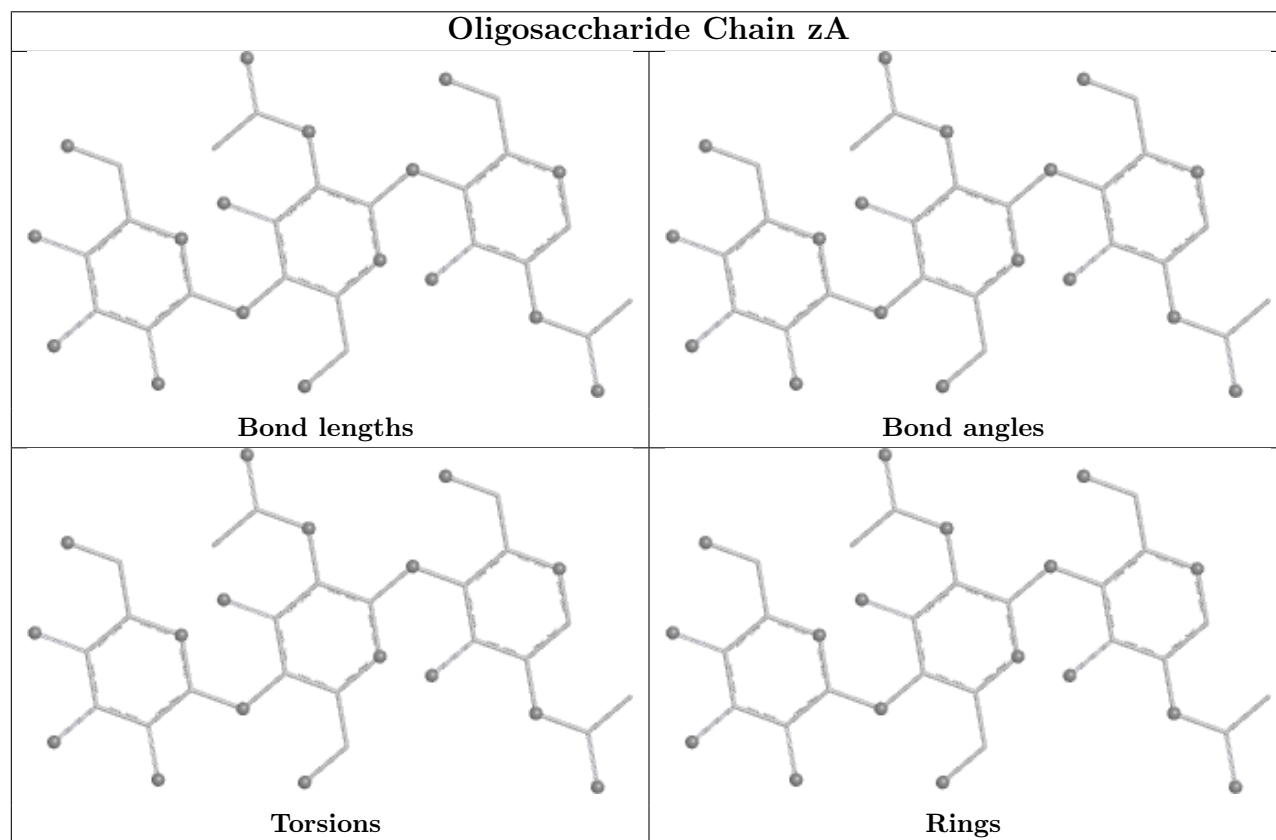
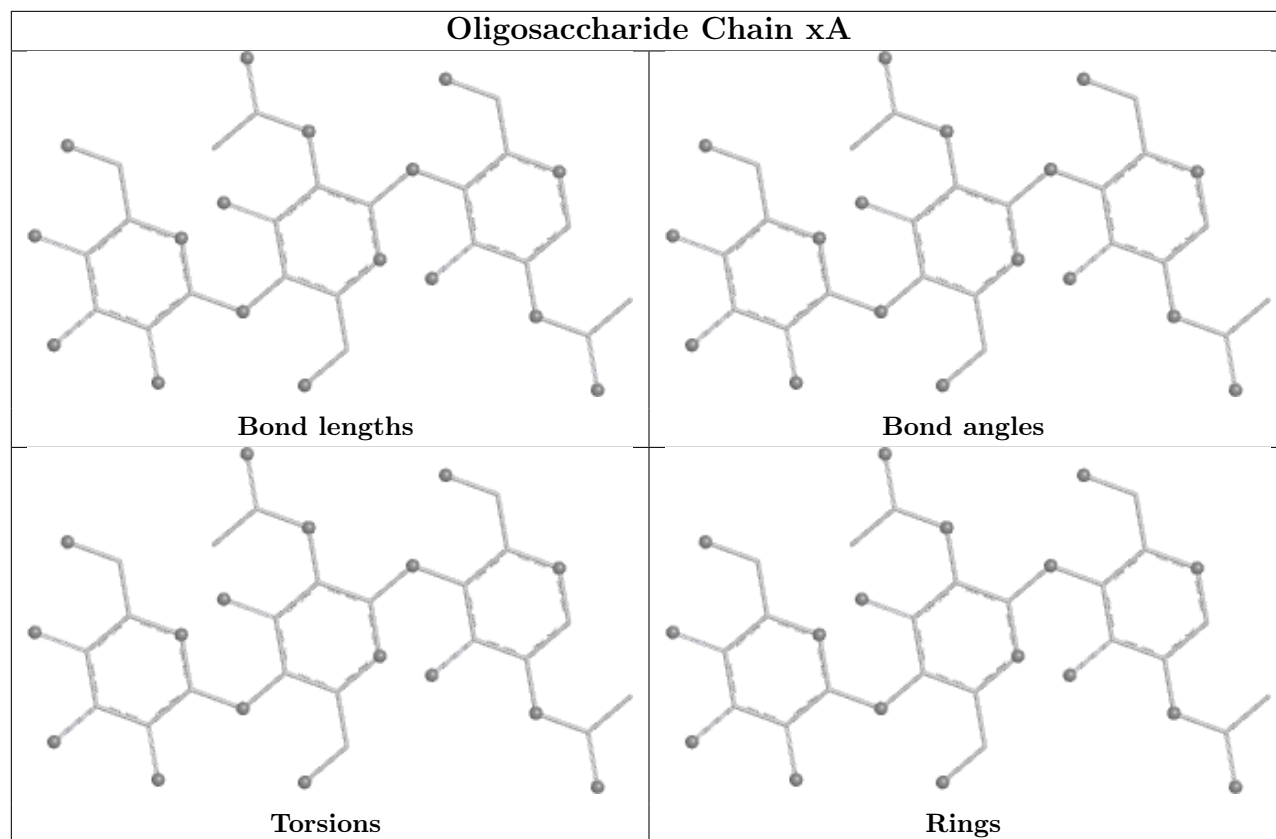


Oligosaccharide Chain tA

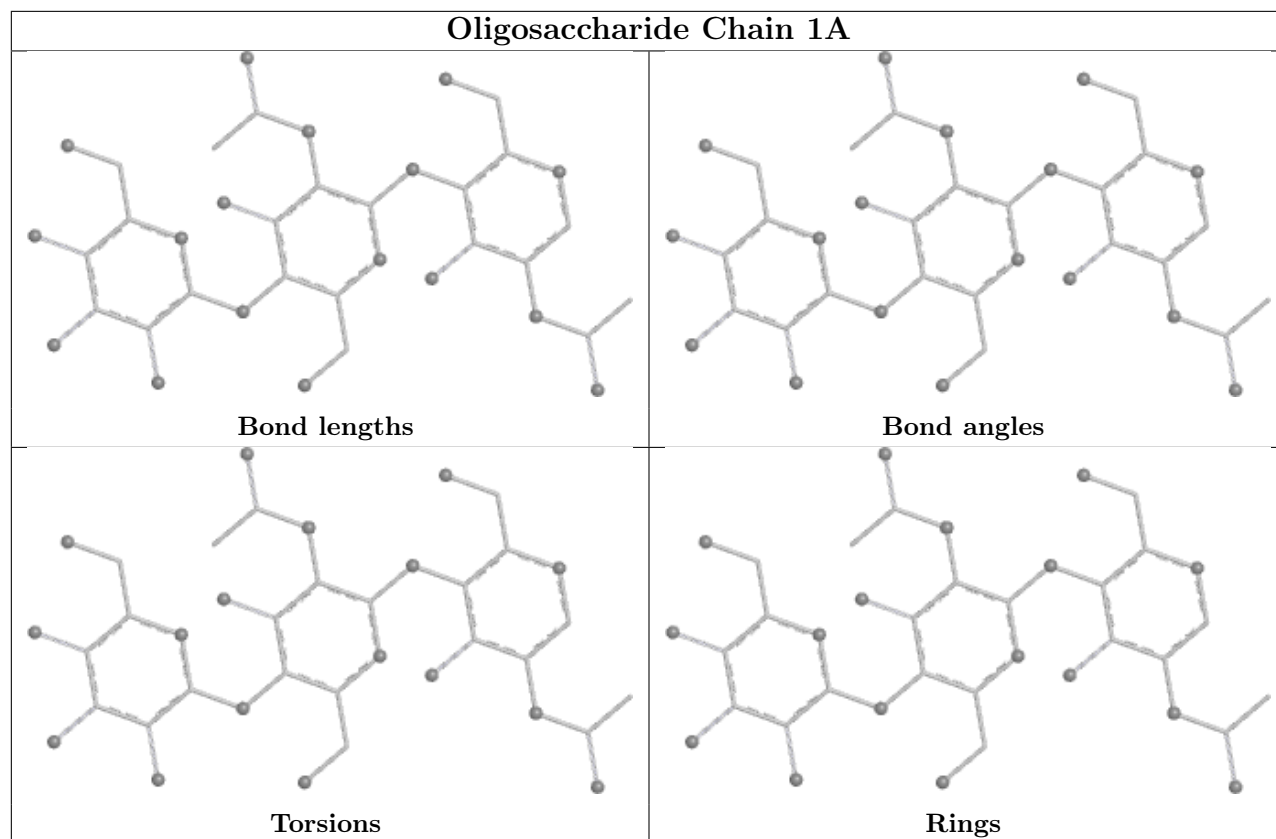


Oligosaccharide Chain uA

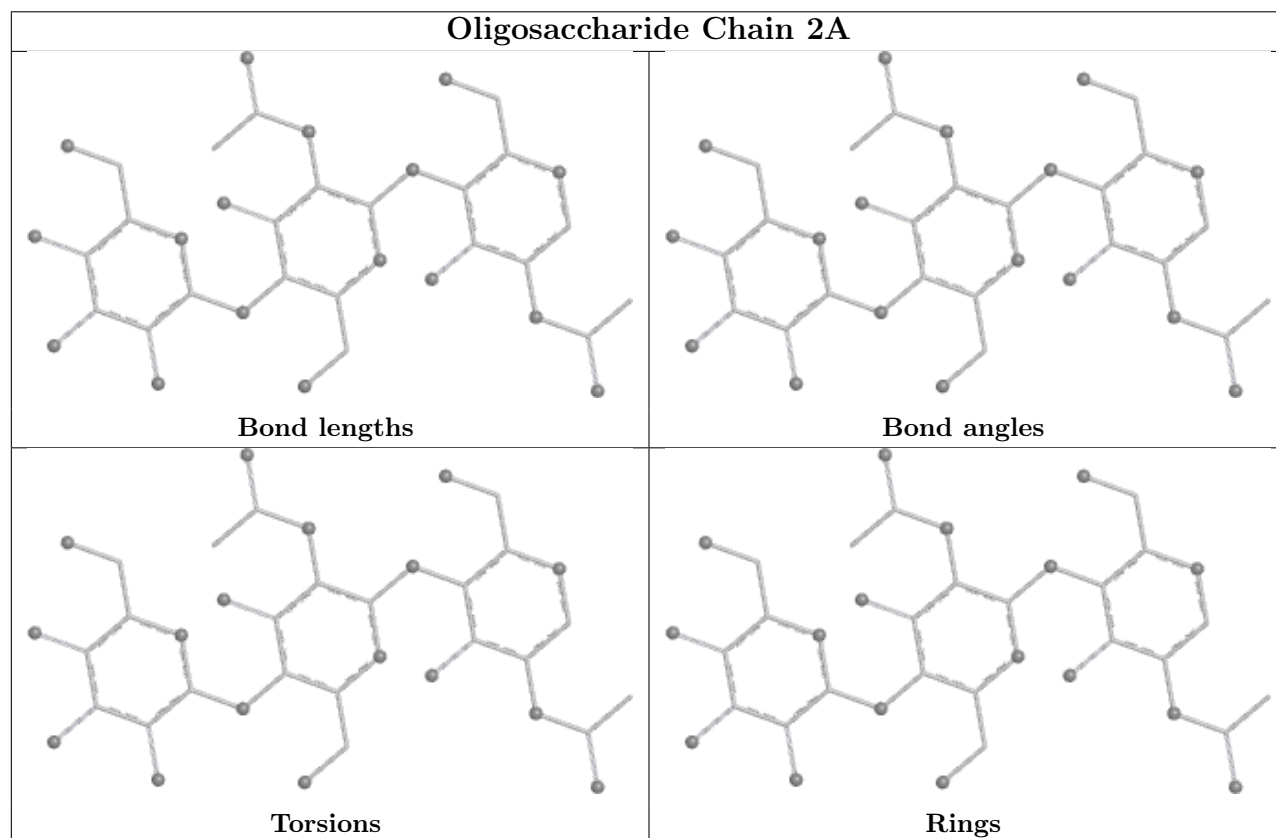




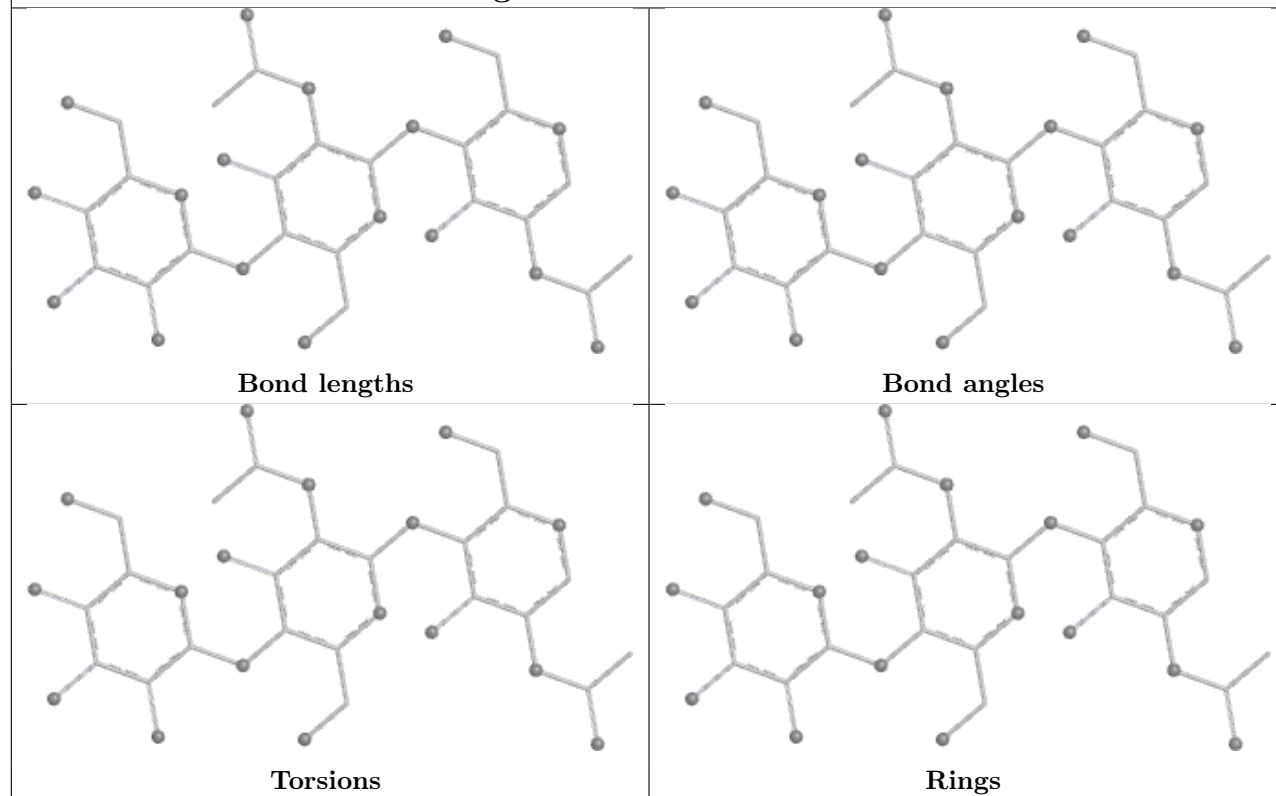
Oligosaccharide Chain 1A



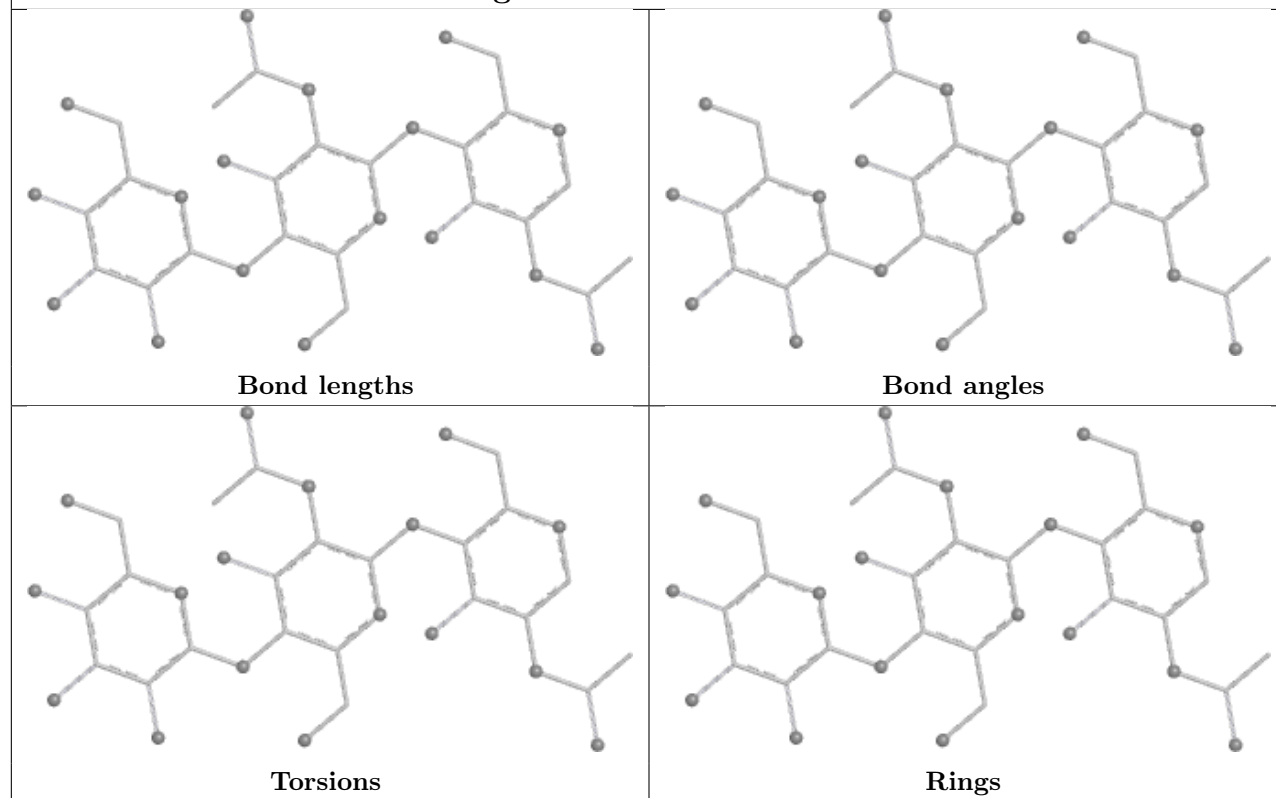
Oligosaccharide Chain 2A



Oligosaccharide Chain 3A



Oligosaccharide Chain 4A



5.6 Ligand geometry

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	F	3501	1	14,14,15	0.25	0	17,19,21	0.36	0
4	NAG	H	3501	1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	P	3501	1	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	B	3501	1	14,14,15	0.30	0	17,19,21	0.41	0
4	NAG	R	3501	1	14,14,15	0.21	0	17,19,21	0.35	0
4	NAG	D	3501	1	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	T	3501	1	14,14,15	0.24	0	17,19,21	0.65	0
4	NAG	K	3501	1	14,14,15	0.15	0	17,19,21	0.42	0
4	NAG	G	3501	1	14,14,15	0.15	0	17,19,21	0.41	0
4	NAG	I	3501	1	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	N	3501	1	14,14,15	0.21	0	17,19,21	0.36	0
4	NAG	E	3501	1	14,14,15	0.16	0	17,19,21	0.44	0
4	NAG	M	3501	1	14,14,15	0.35	0	17,19,21	0.50	0
4	NAG	J	3501	1	14,14,15	0.24	0	17,19,21	0.36	0
4	NAG	A	3501	1	14,14,15	0.21	0	17,19,21	0.41	0
4	NAG	O	3501	1	14,14,15	0.35	0	17,19,21	0.46	0
4	NAG	S	3501	1	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	L	3501	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	Q	3501	1	14,14,15	0.36	0	17,19,21	0.50	0
4	NAG	C	3501	1	14,14,15	0.18	0	17,19,21	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	H	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	P	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	B	3501	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	R	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	D	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	T	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	K	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	G	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	I	3501	1	-	1/6/23/26	0/1/1/1
4	NAG	N	3501	1	-	3/6/23/26	0/1/1/1
4	NAG	E	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	M	3501	1	-	3/6/23/26	0/1/1/1
4	NAG	J	3501	1	-	2/6/23/26	0/1/1/1
4	NAG	A	3501	1	-	1/6/23/26	0/1/1/1
4	NAG	O	3501	1	-	1/6/23/26	0/1/1/1
4	NAG	S	3501	1	-	1/6/23/26	0/1/1/1
4	NAG	L	3501	1	-	4/6/23/26	0/1/1/1
4	NAG	Q	3501	1	-	1/6/23/26	0/1/1/1
4	NAG	C	3501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	3501	NAG	O5-C5-C6-O6
4	K	3501	NAG	C4-C5-C6-O6
4	G	3501	NAG	C4-C5-C6-O6
4	C	3501	NAG	C4-C5-C6-O6
4	E	3501	NAG	C4-C5-C6-O6
4	H	3501	NAG	O5-C5-C6-O6
4	L	3501	NAG	C4-C5-C6-O6
4	P	3501	NAG	C4-C5-C6-O6
4	D	3501	NAG	O5-C5-C6-O6
4	R	3501	NAG	O5-C5-C6-O6
4	R	3501	NAG	C4-C5-C6-O6
4	B	3501	NAG	O5-C5-C6-O6
4	M	3501	NAG	O5-C5-C6-O6
4	K	3501	NAG	O5-C5-C6-O6
4	C	3501	NAG	O5-C5-C6-O6

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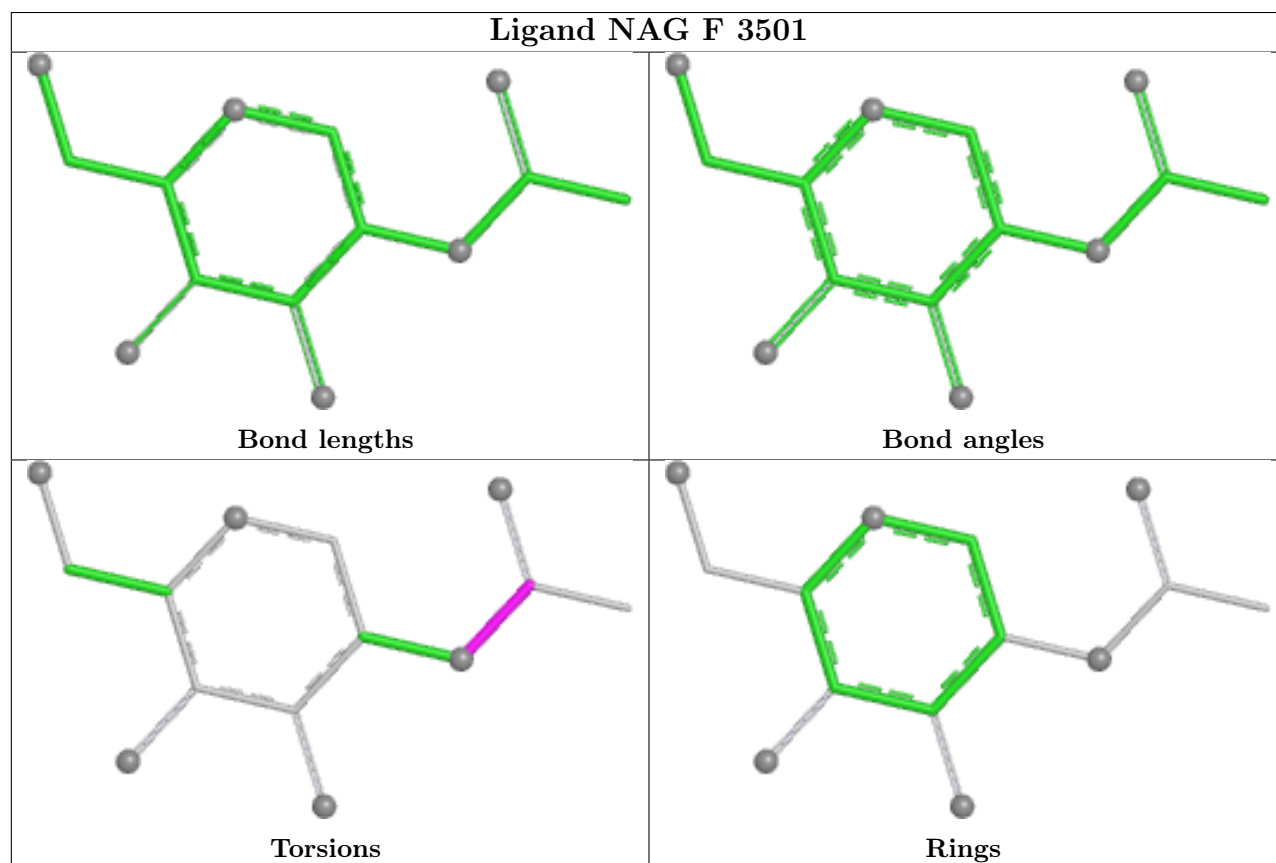
Mol	Chain	Res	Type	Atoms
4	E	3501	NAG	O5-C5-C6-O6
4	G	3501	NAG	O5-C5-C6-O6
4	L	3501	NAG	O5-C5-C6-O6
4	B	3501	NAG	C4-C5-C6-O6
4	D	3501	NAG	C4-C5-C6-O6
4	H	3501	NAG	C4-C5-C6-O6
4	B	3501	NAG	C8-C7-N2-C2
4	B	3501	NAG	O7-C7-N2-C2
4	D	3501	NAG	C8-C7-N2-C2
4	D	3501	NAG	O7-C7-N2-C2
4	F	3501	NAG	C8-C7-N2-C2
4	F	3501	NAG	O7-C7-N2-C2
4	H	3501	NAG	C8-C7-N2-C2
4	H	3501	NAG	O7-C7-N2-C2
4	J	3501	NAG	C8-C7-N2-C2
4	J	3501	NAG	O7-C7-N2-C2
4	L	3501	NAG	C8-C7-N2-C2
4	L	3501	NAG	O7-C7-N2-C2
4	N	3501	NAG	C8-C7-N2-C2
4	N	3501	NAG	O7-C7-N2-C2
4	P	3501	NAG	C8-C7-N2-C2
4	P	3501	NAG	O7-C7-N2-C2
4	R	3501	NAG	C8-C7-N2-C2
4	R	3501	NAG	O7-C7-N2-C2
4	T	3501	NAG	C8-C7-N2-C2
4	T	3501	NAG	O7-C7-N2-C2
4	T	3501	NAG	O5-C5-C6-O6
4	S	3501	NAG	O5-C5-C6-O6
4	A	3501	NAG	O5-C5-C6-O6
4	M	3501	NAG	C4-C5-C6-O6
4	Q	3501	NAG	O5-C5-C6-O6
4	I	3501	NAG	O5-C5-C6-O6
4	O	3501	NAG	O5-C5-C6-O6
4	T	3501	NAG	C4-C5-C6-O6
4	N	3501	NAG	O5-C5-C6-O6
4	M	3501	NAG	C1-C2-N2-C7

There are no ring outliers.

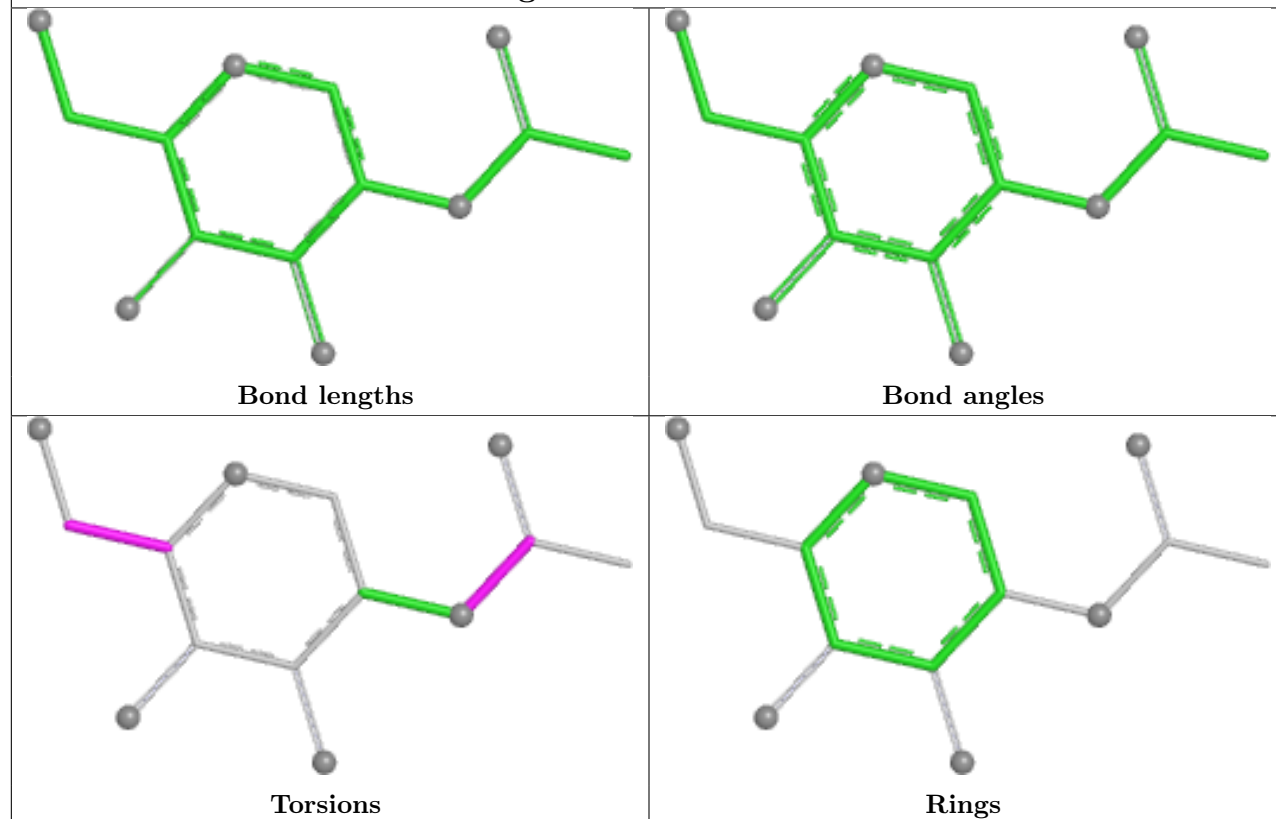
No monomer is involved in short contacts.

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

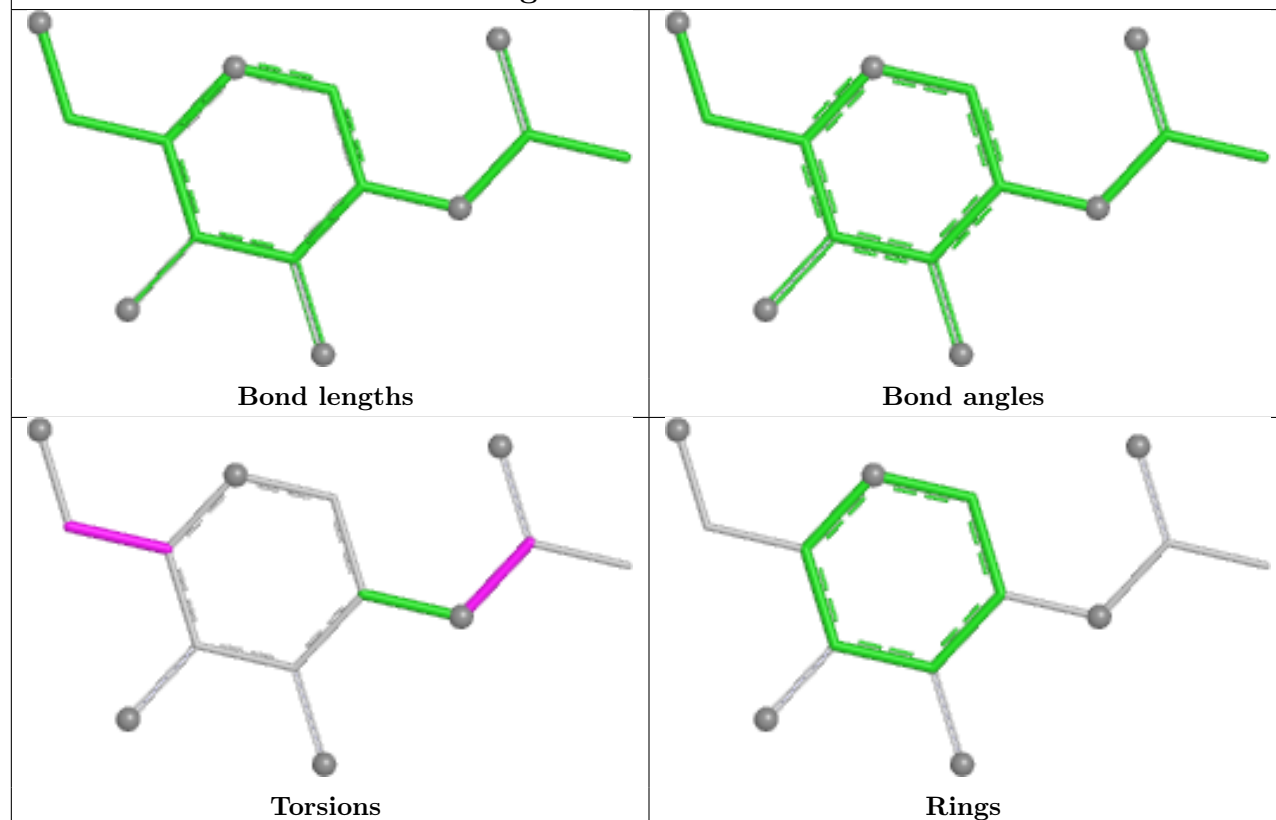
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



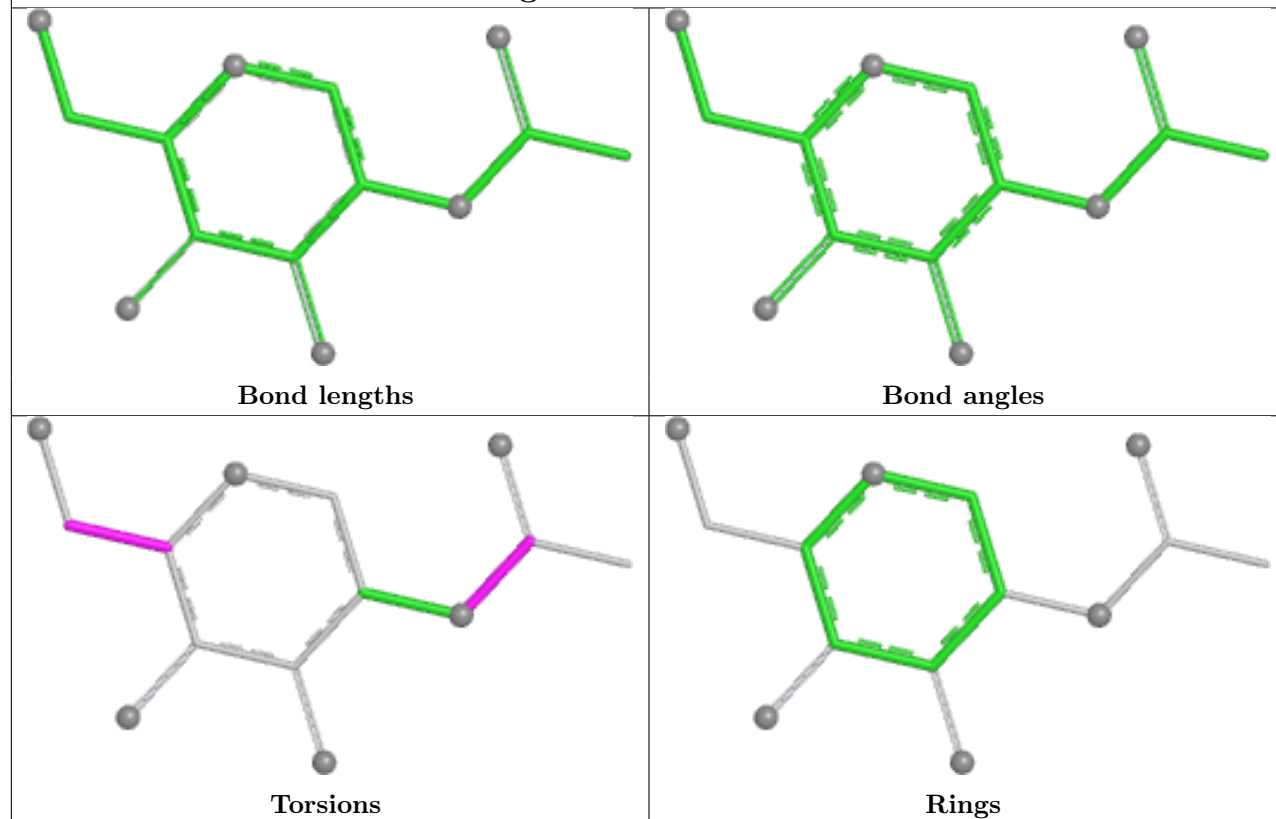
Ligand NAG H 3501



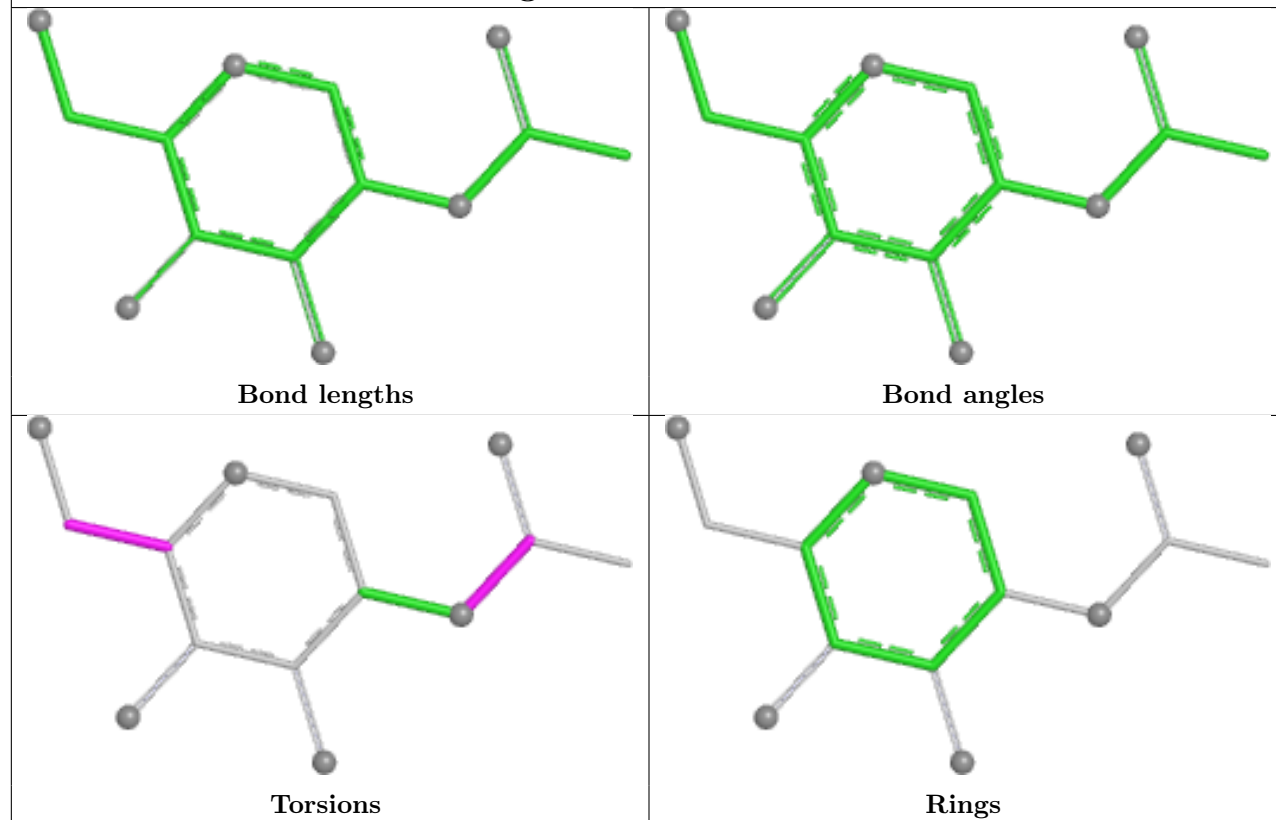
Ligand NAG P 3501



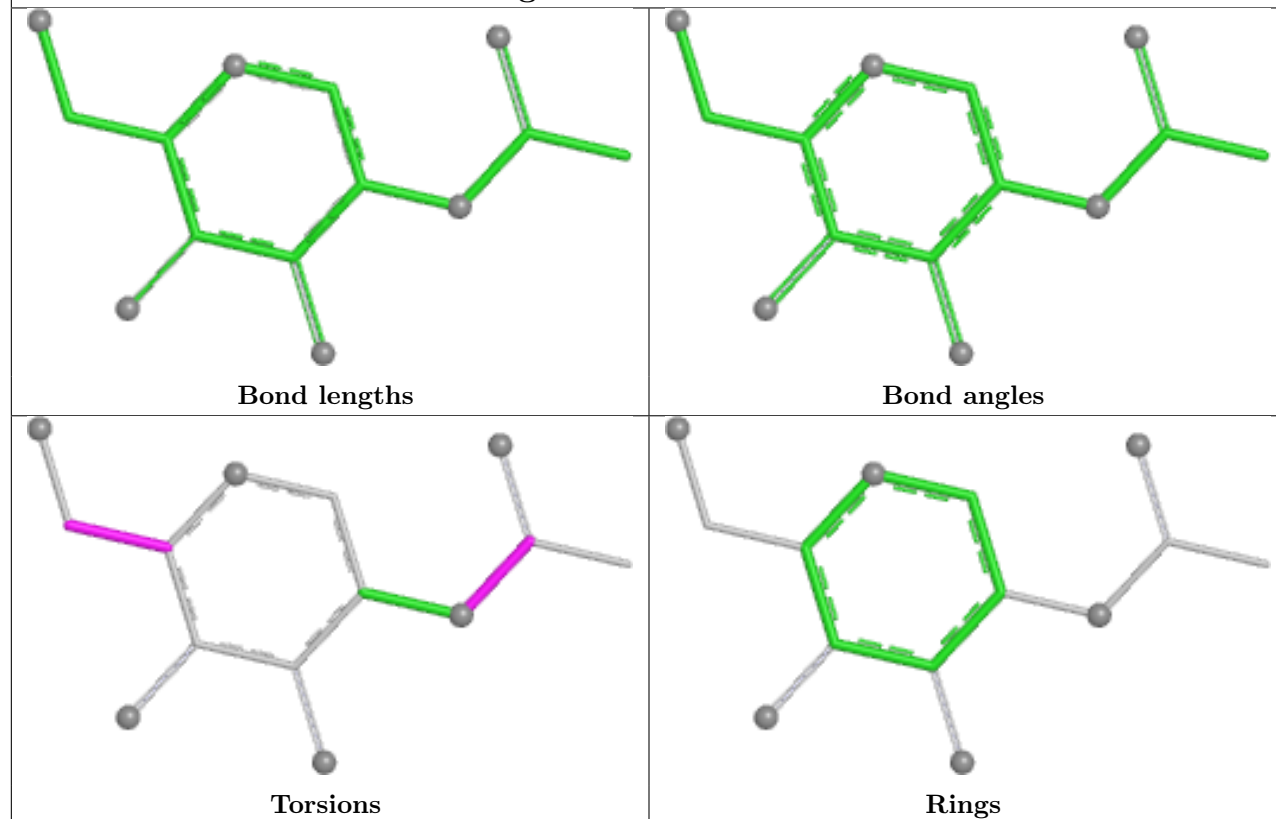
Ligand NAG B 3501



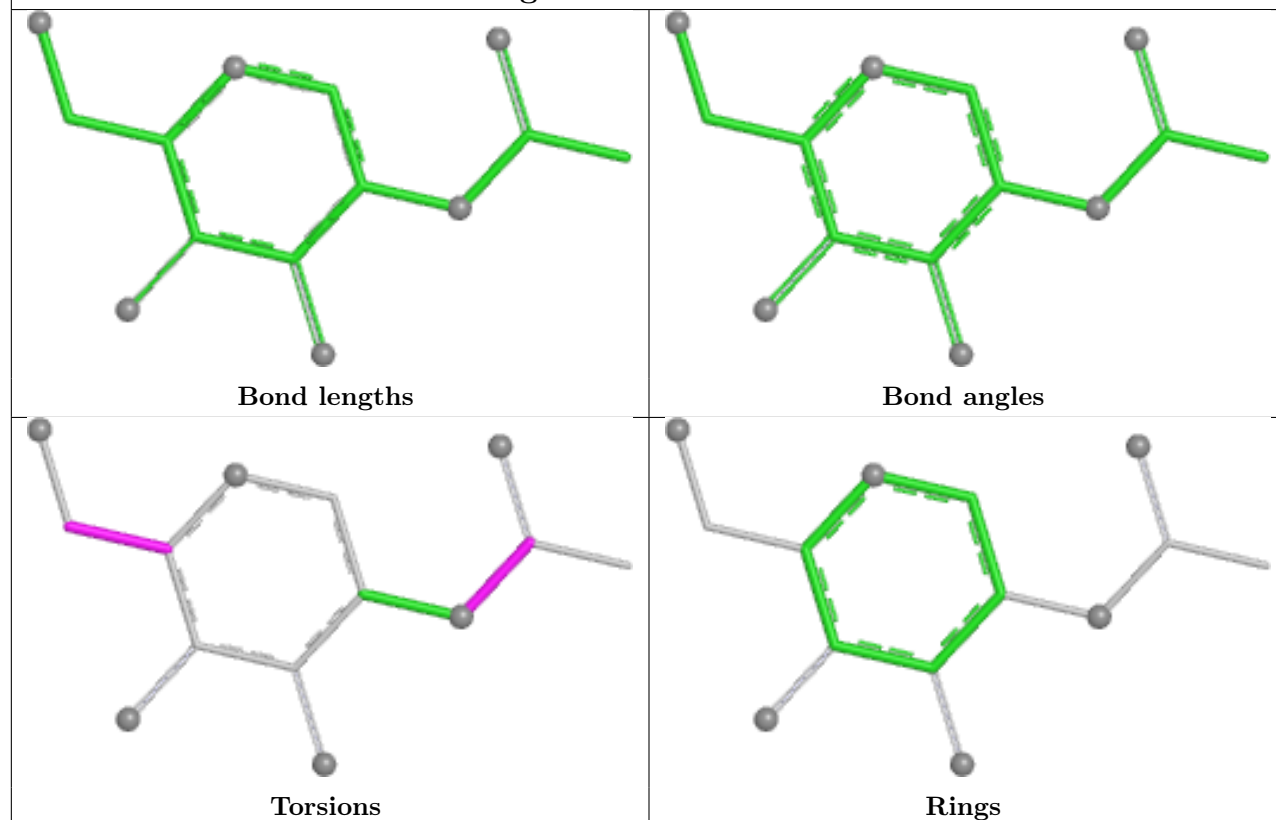
Ligand NAG R 3501



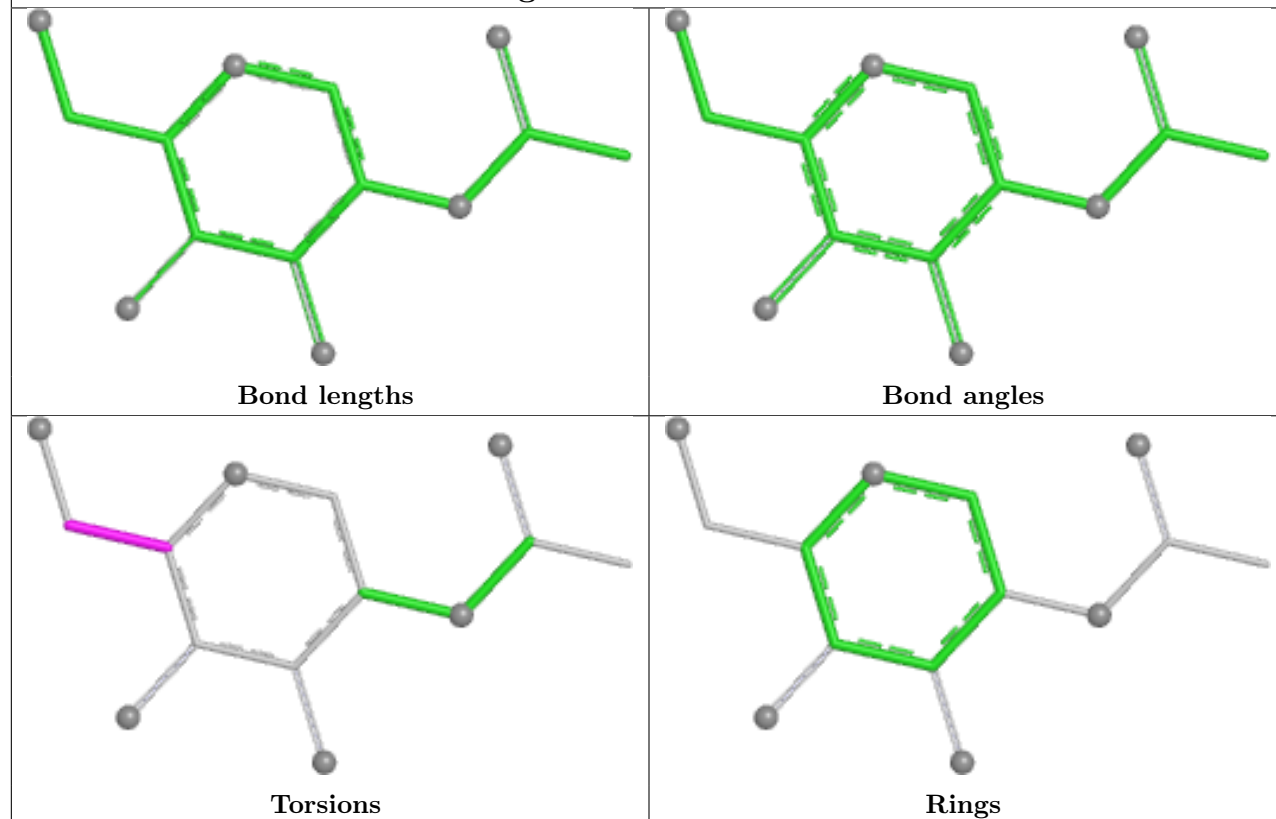
Ligand NAG D 3501



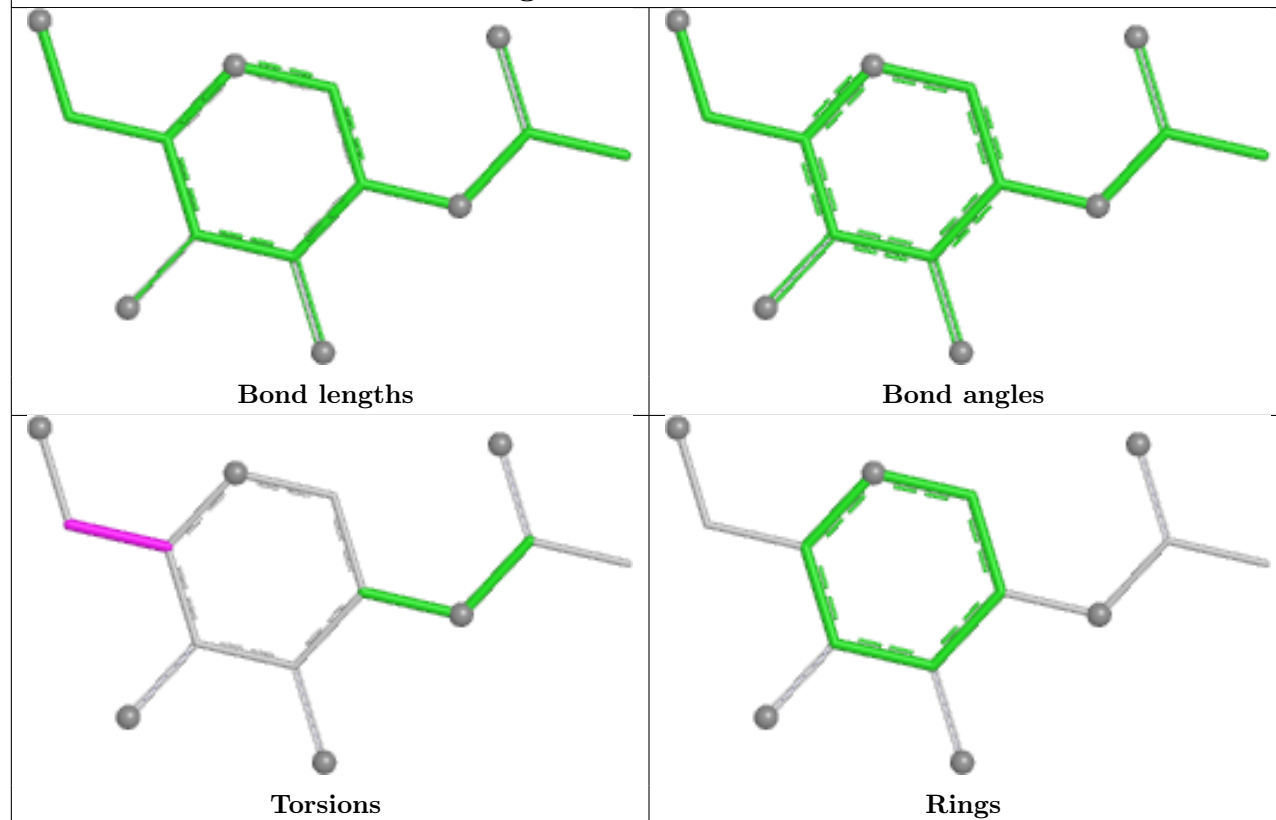
Ligand NAG T 3501

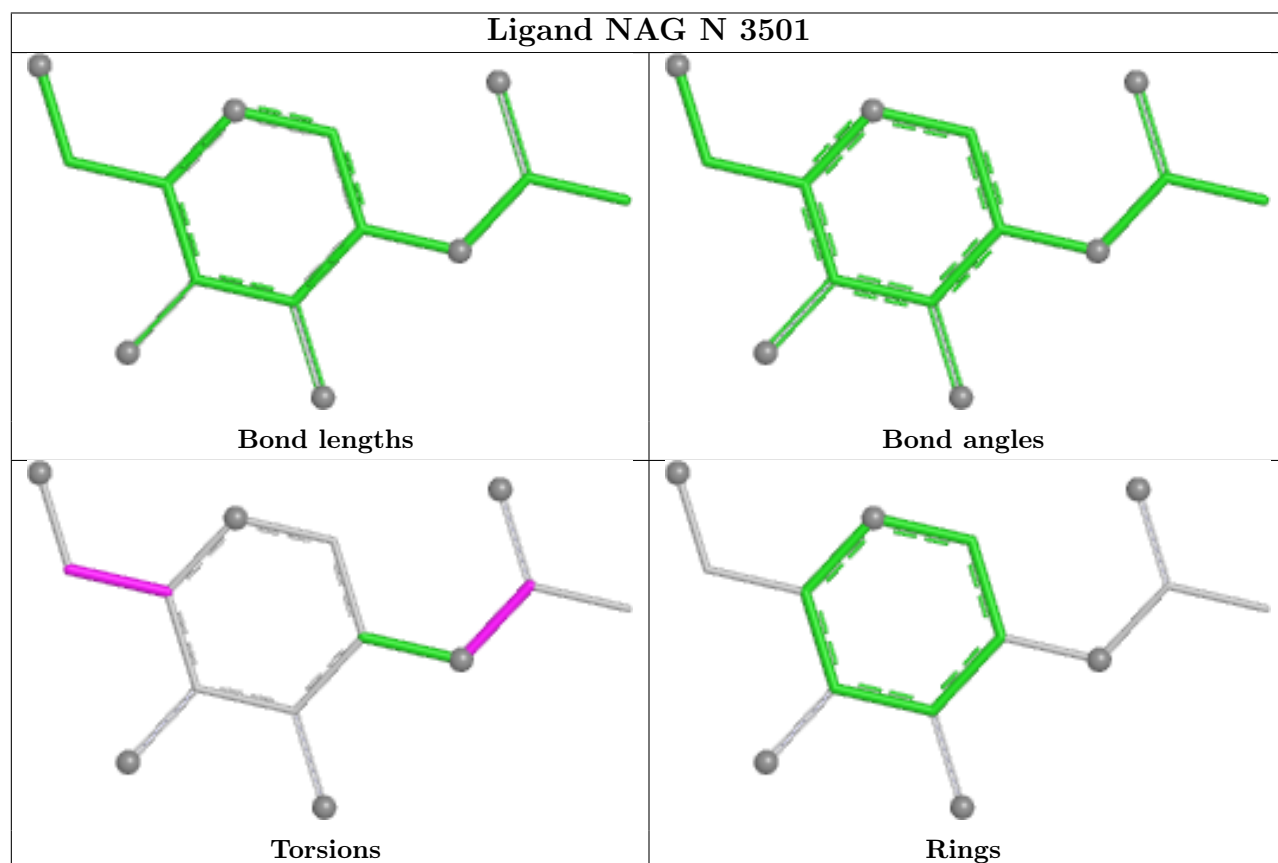
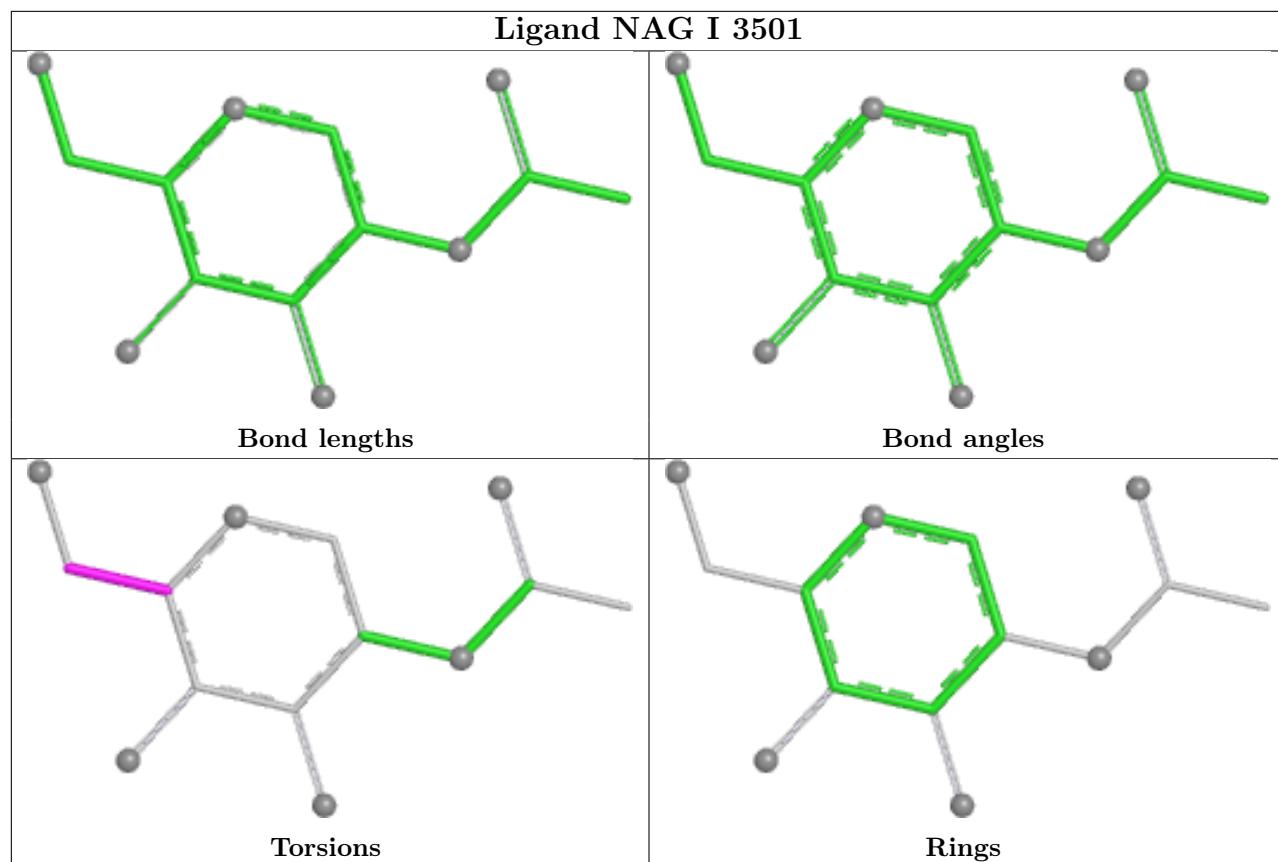


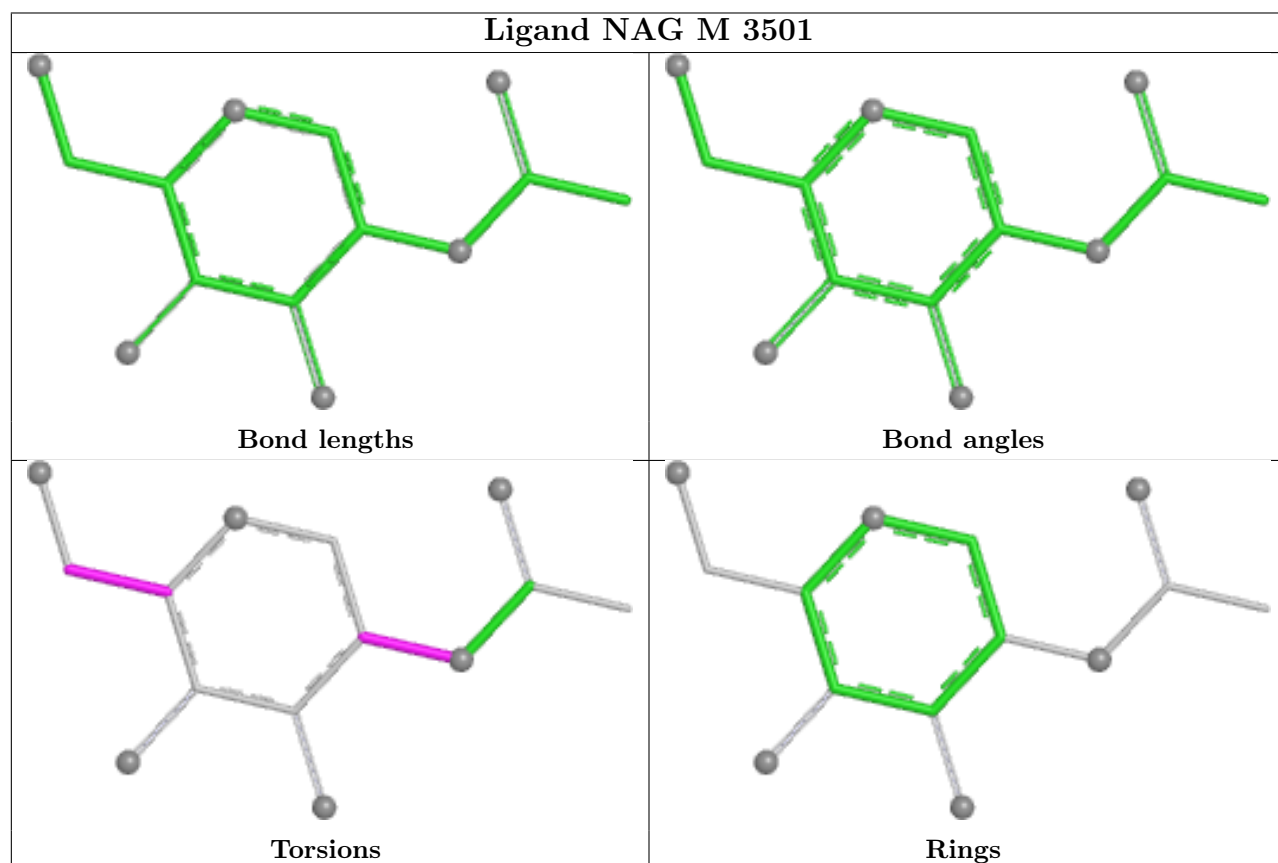
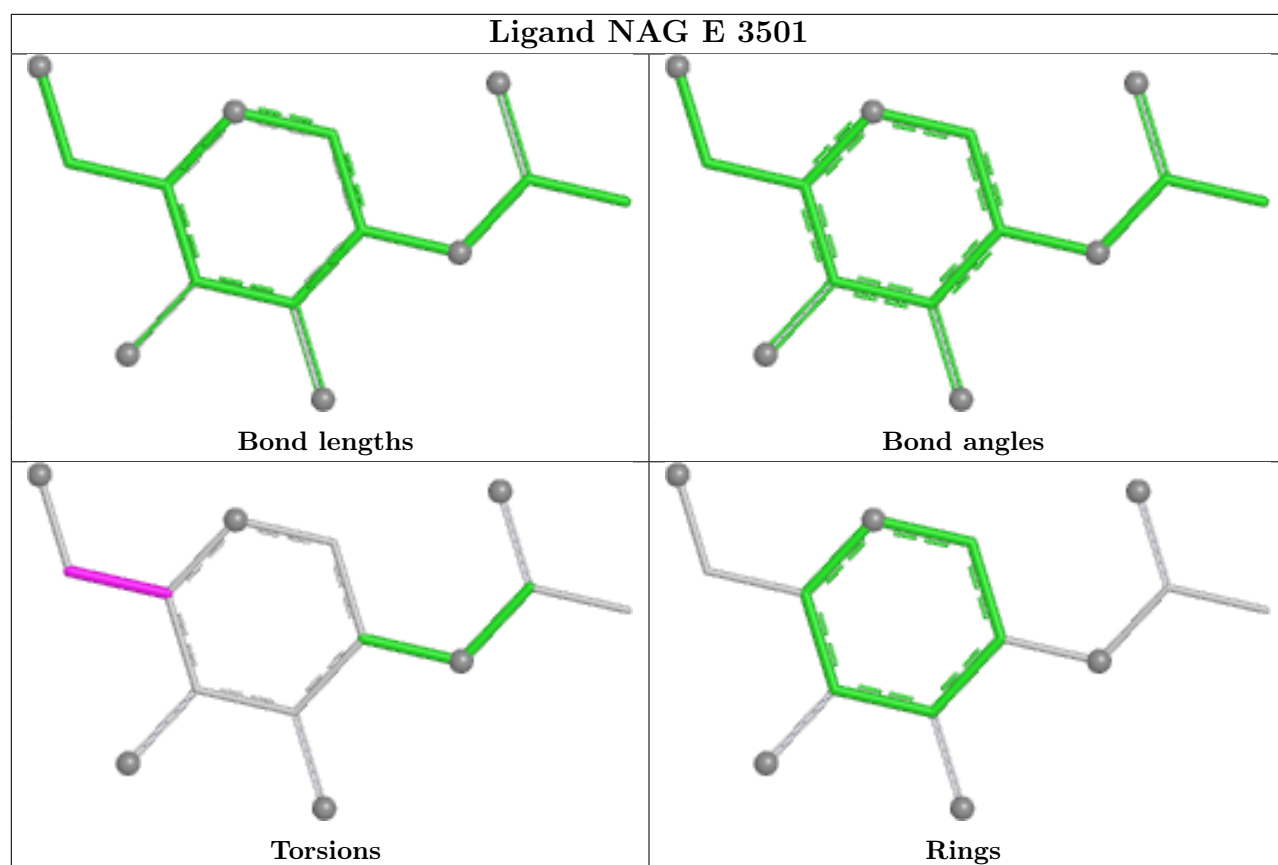
Ligand NAG K 3501



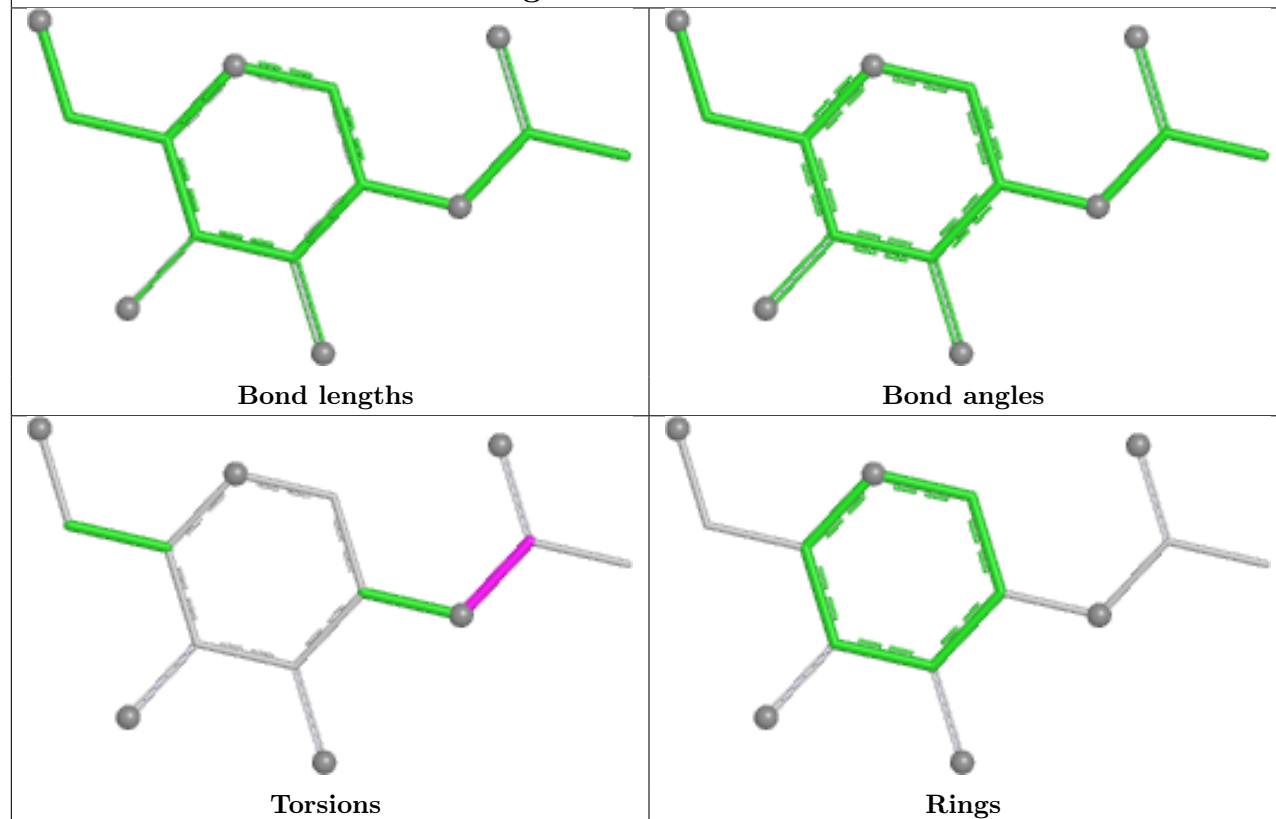
Ligand NAG G 3501



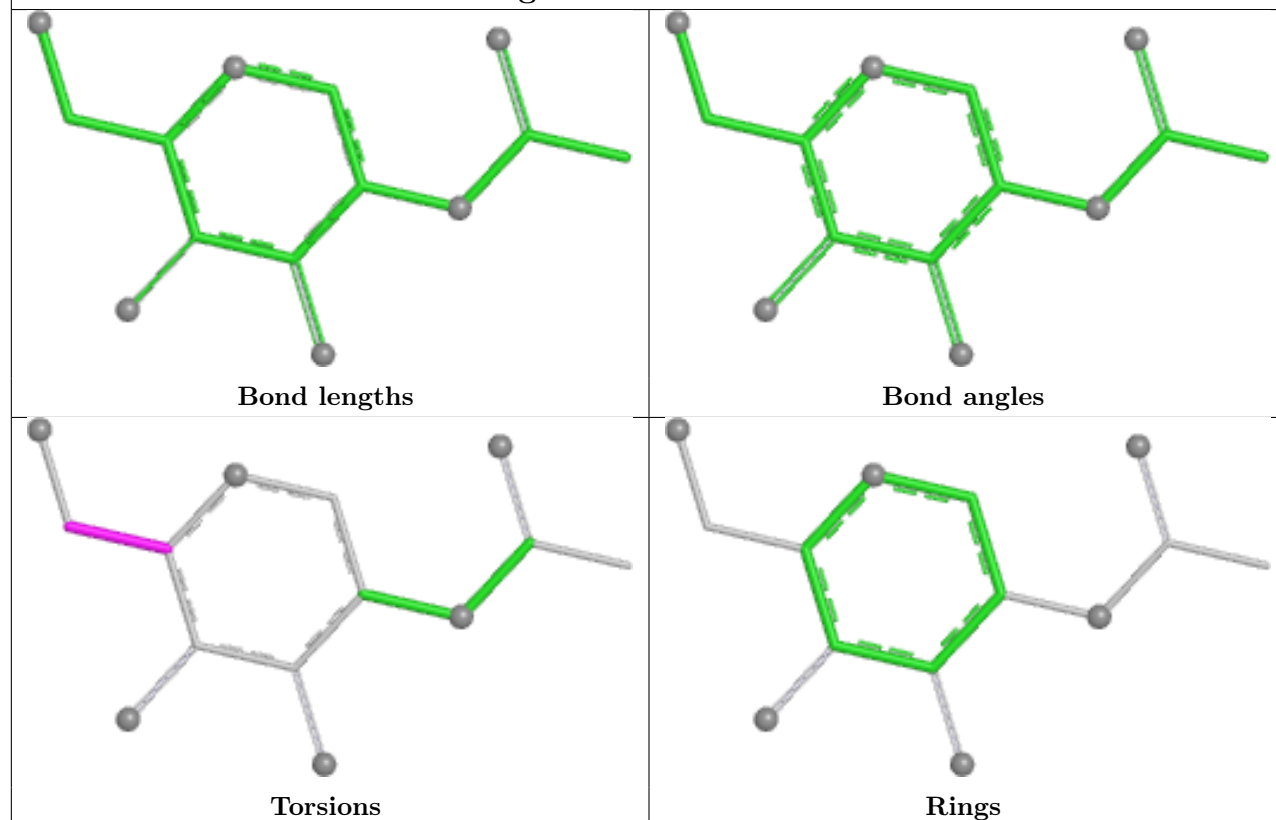




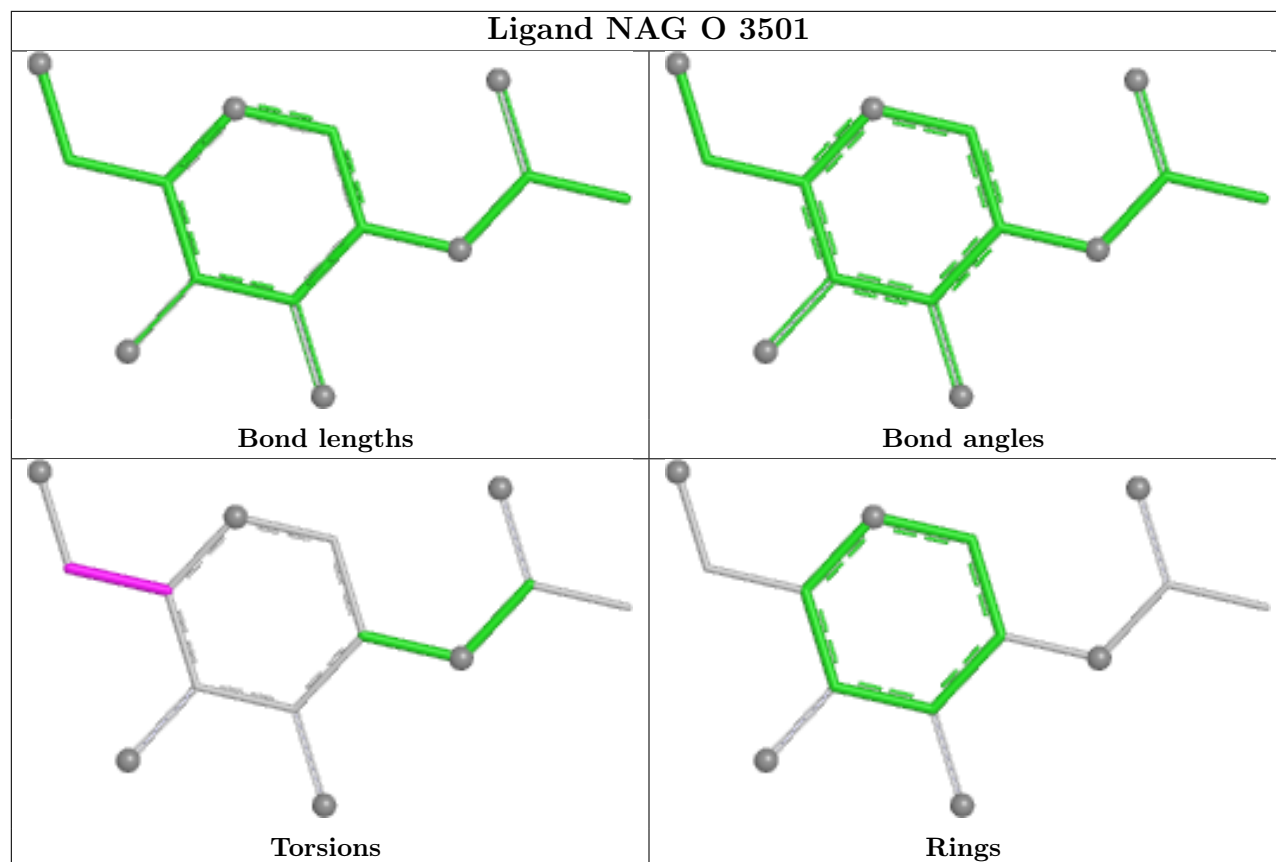
Ligand NAG J 3501



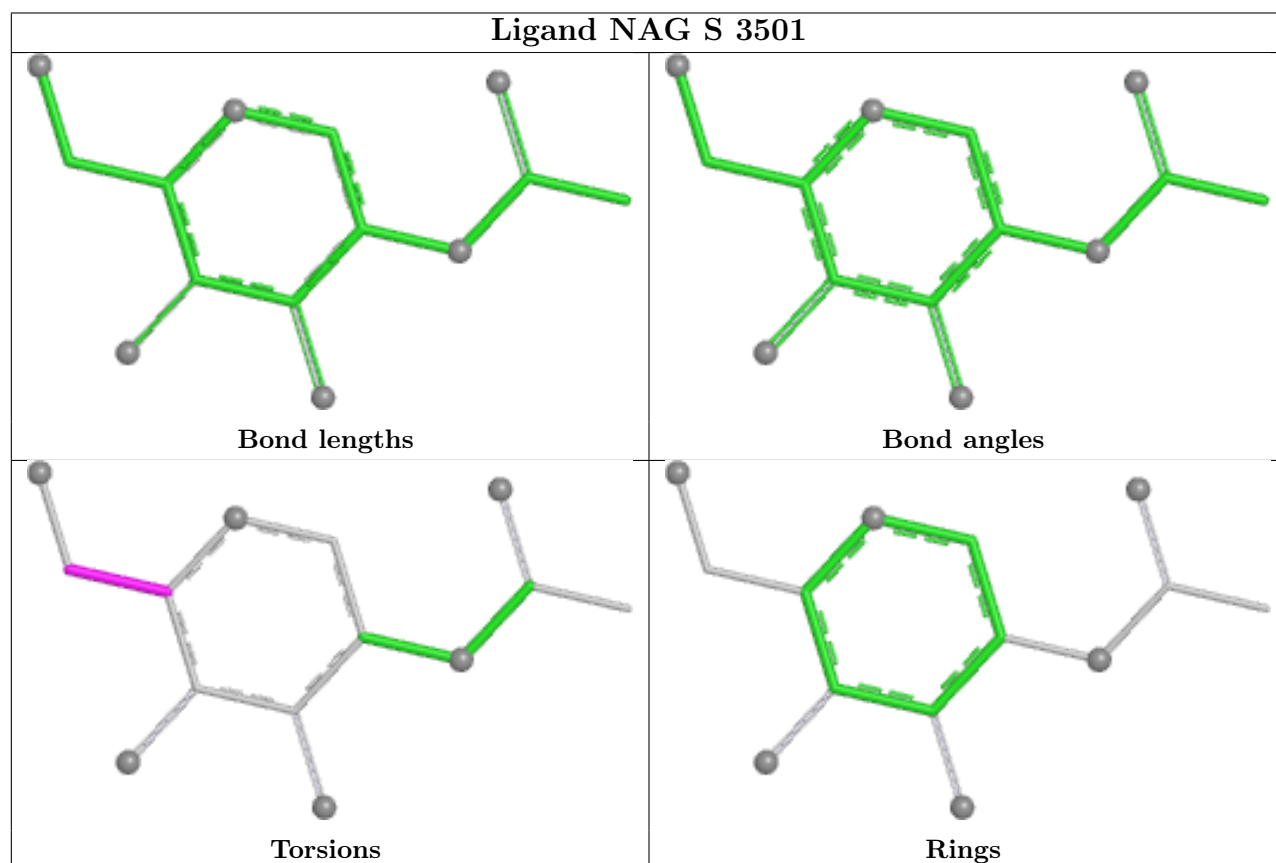
Ligand NAG A 3501

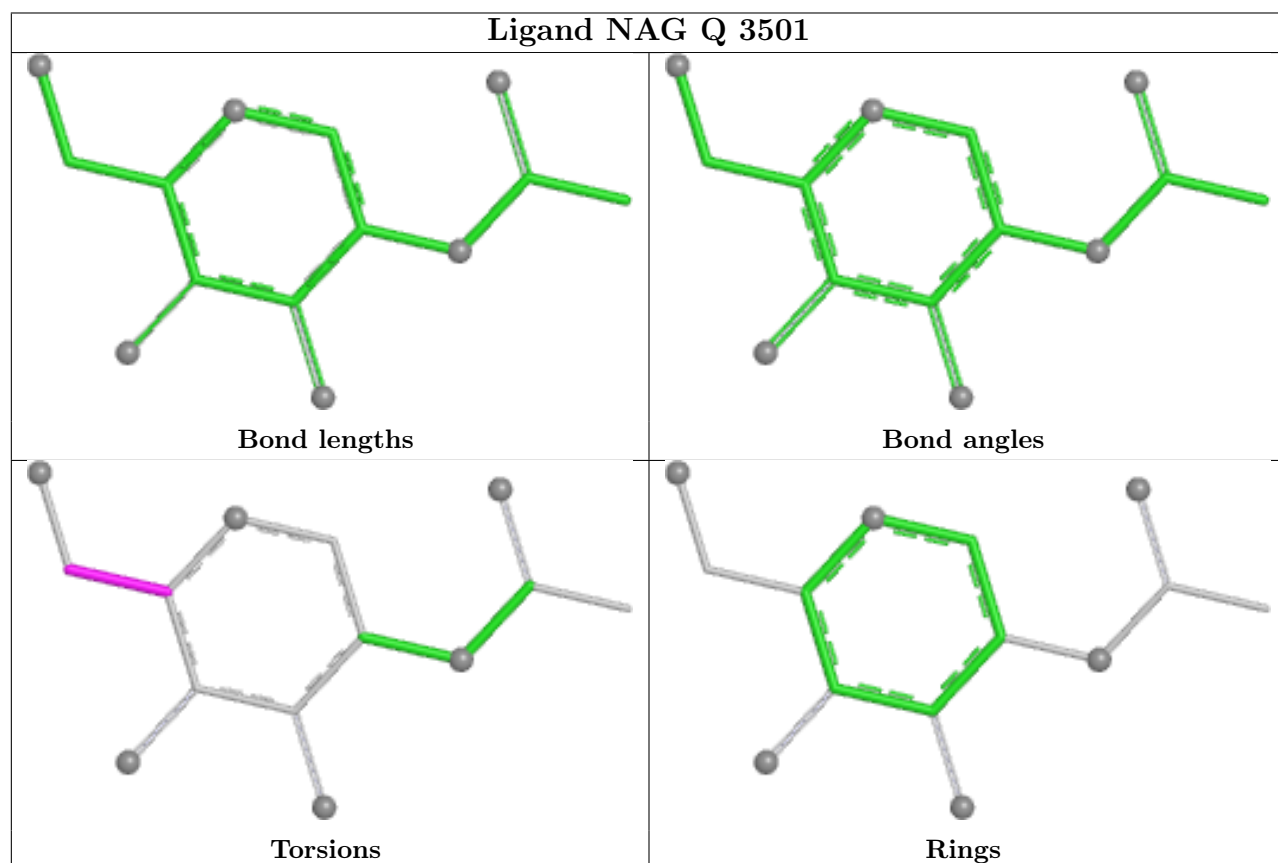
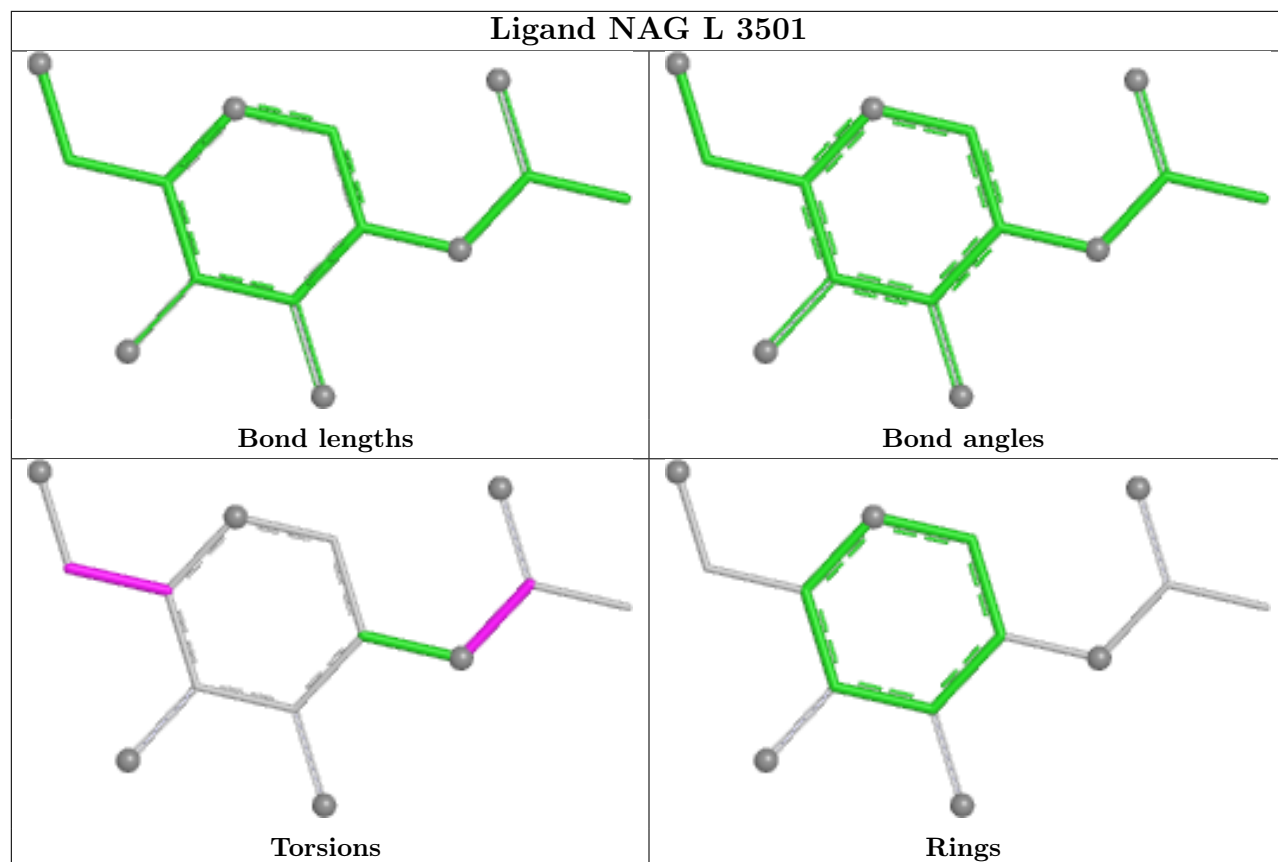


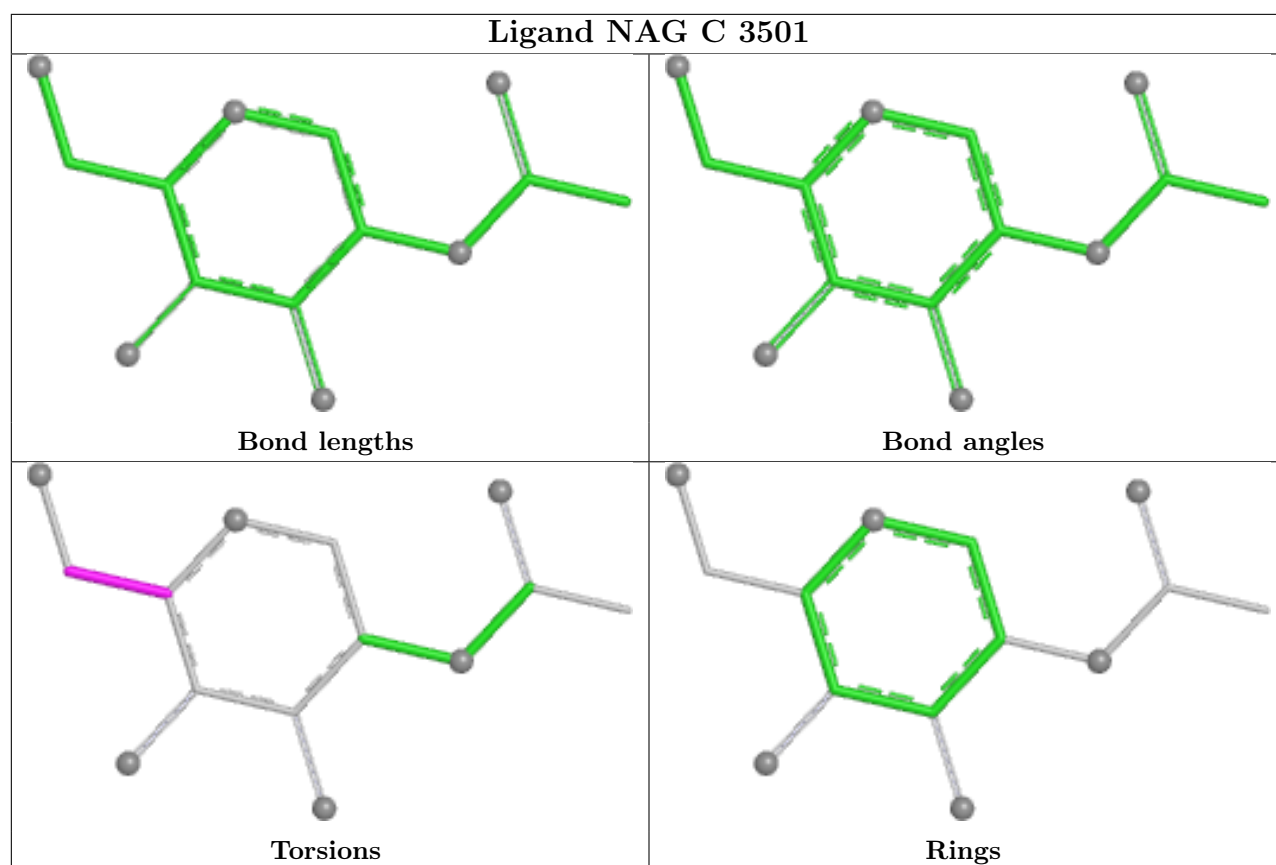
Ligand NAG O 3501



Ligand NAG S 3501







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.

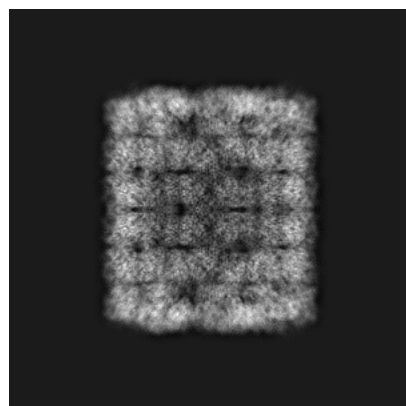
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41586. These allow visual inspection of the internal detail of the map and identification of artifacts.

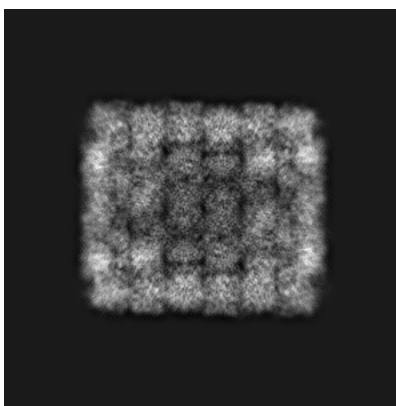
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

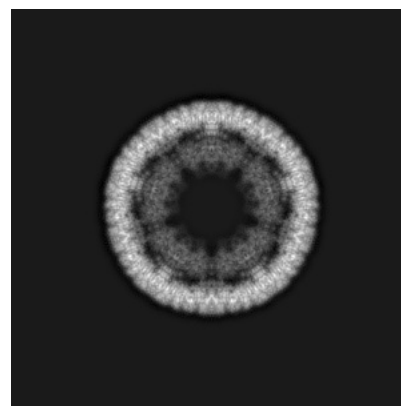
6.1.1 Primary map



X

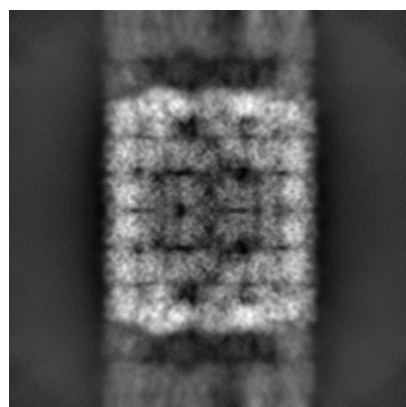


Y

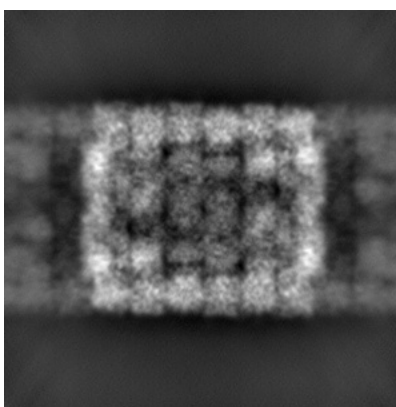


Z

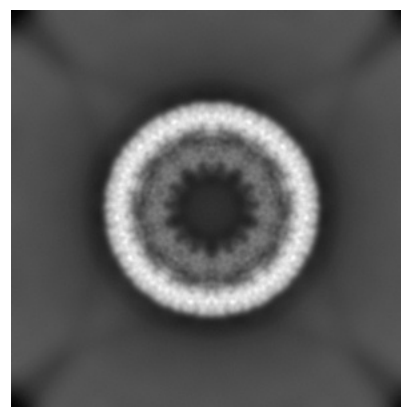
6.1.2 Raw map



X



Y

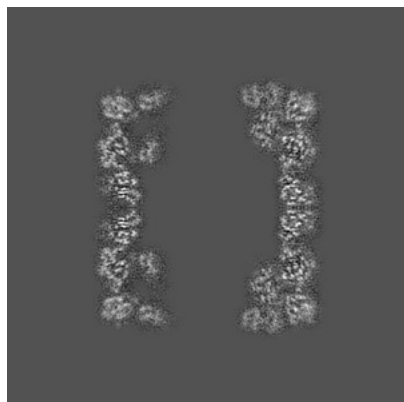


Z

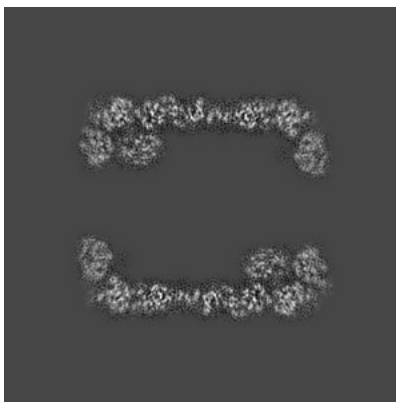
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

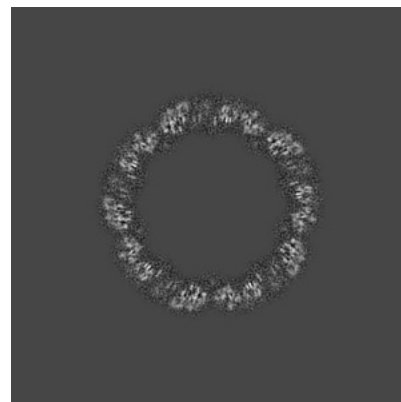
6.2.1 Primary map



X Index: 150

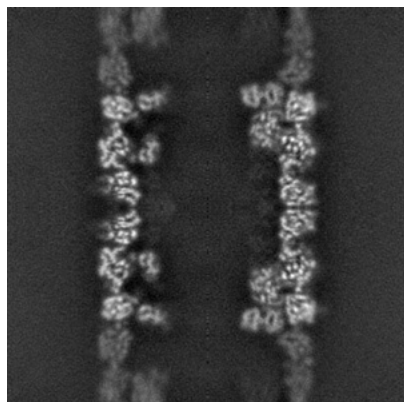


Y Index: 150

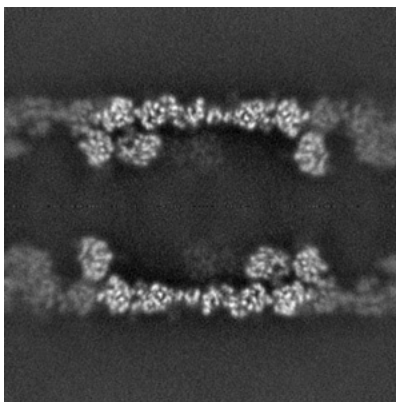


Z Index: 150

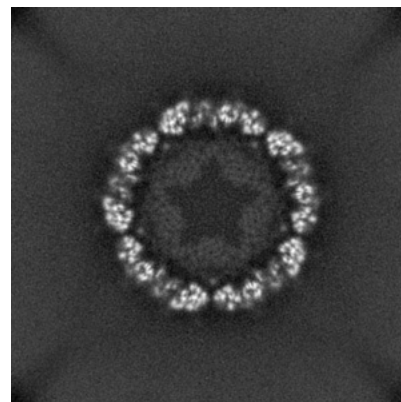
6.2.2 Raw map



X Index: 150



Y Index: 150

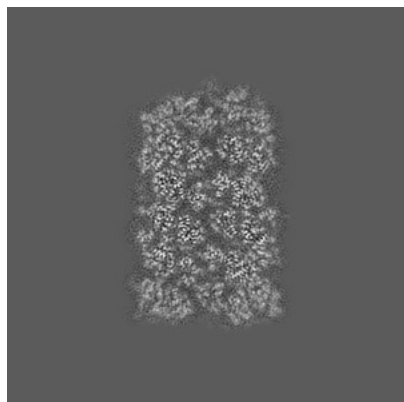


Z Index: 150

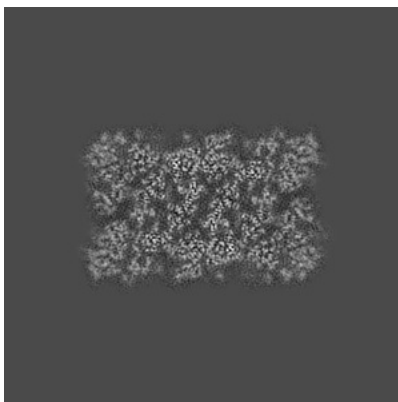
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 89

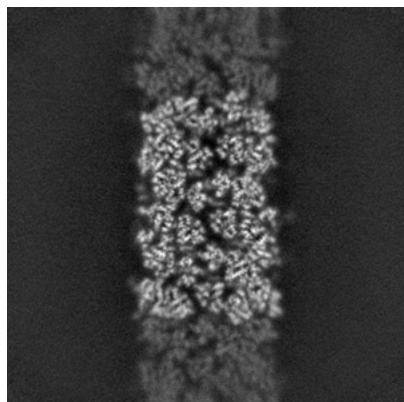


Y Index: 90

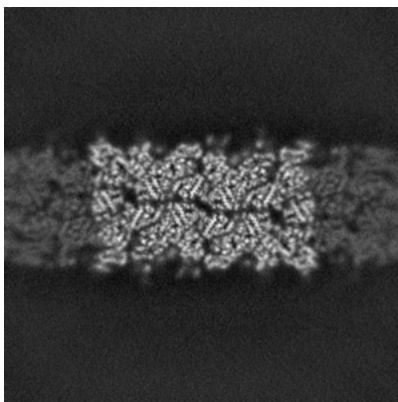


Z Index: 165

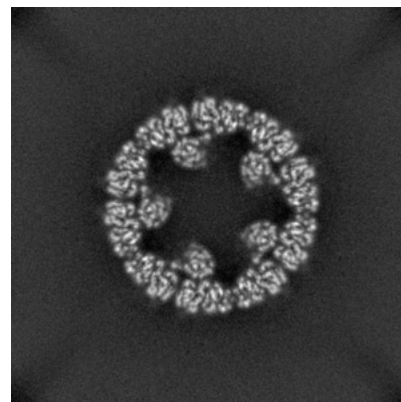
6.3.2 Raw map



X Index: 89



Y Index: 85

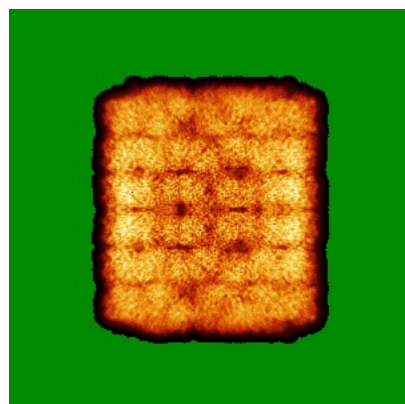


Z Index: 191

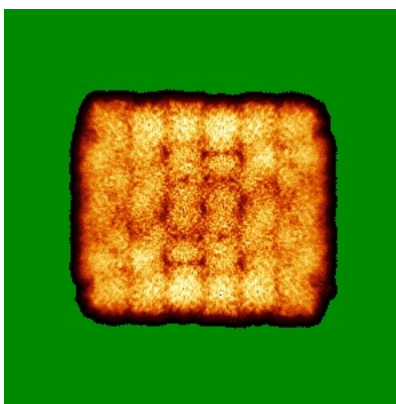
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

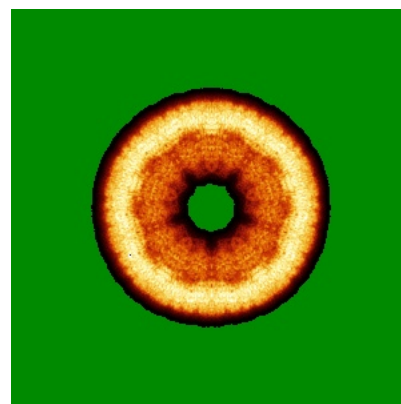
6.4.1 Primary map



X

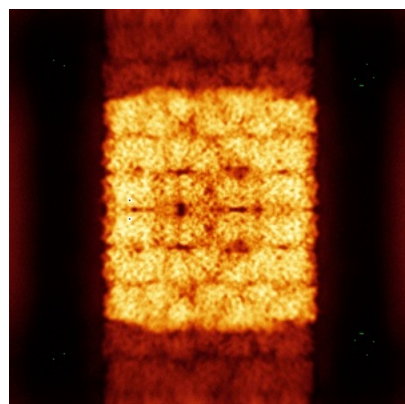


Y

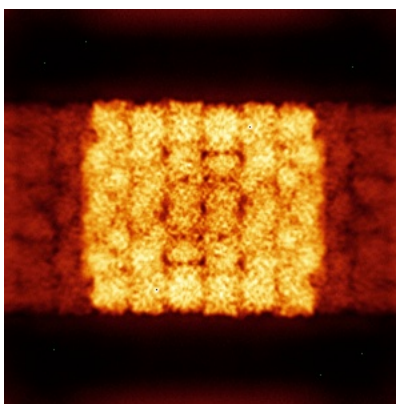


Z

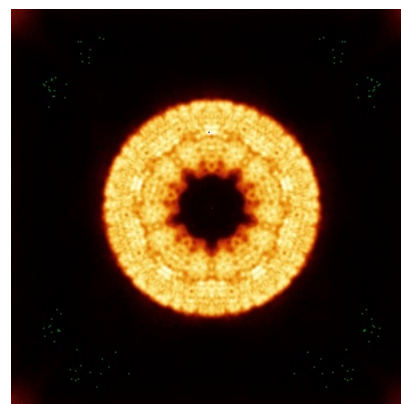
6.4.2 Raw map



X



Y

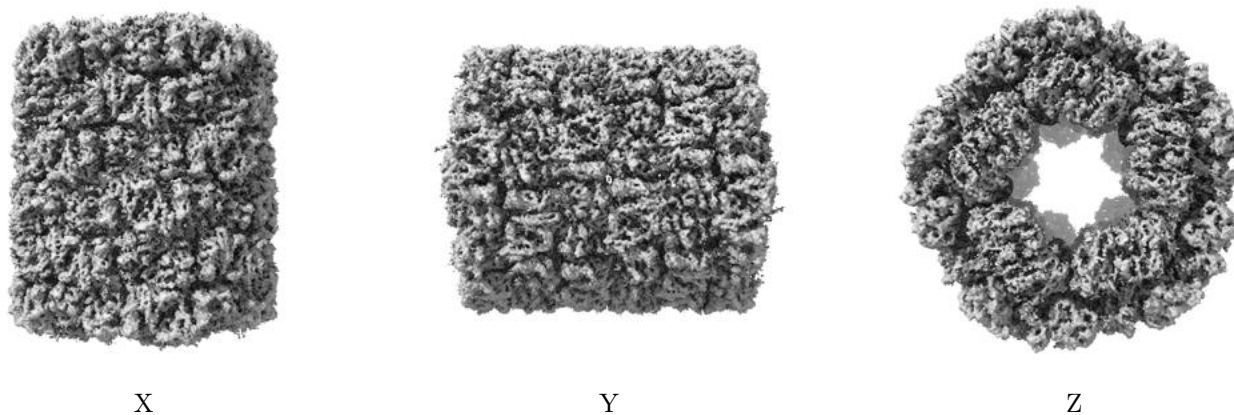


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

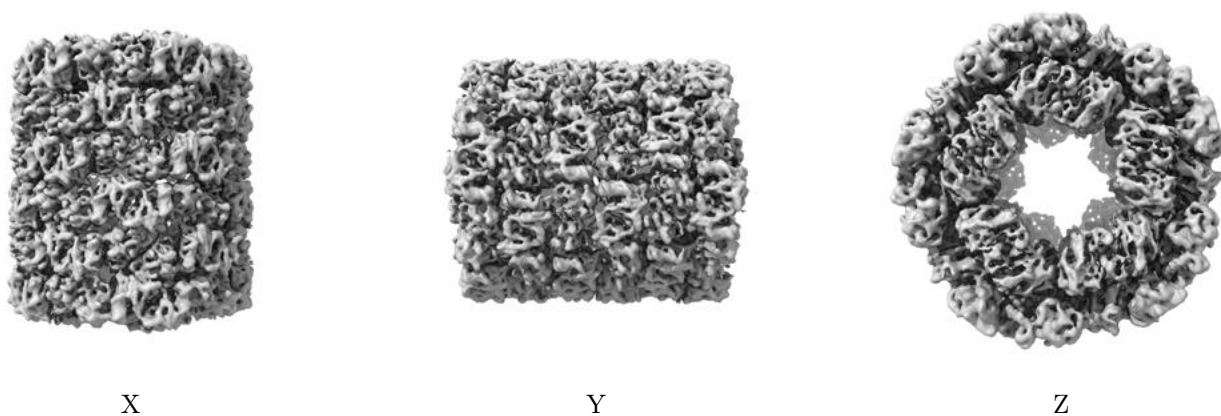
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.637. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

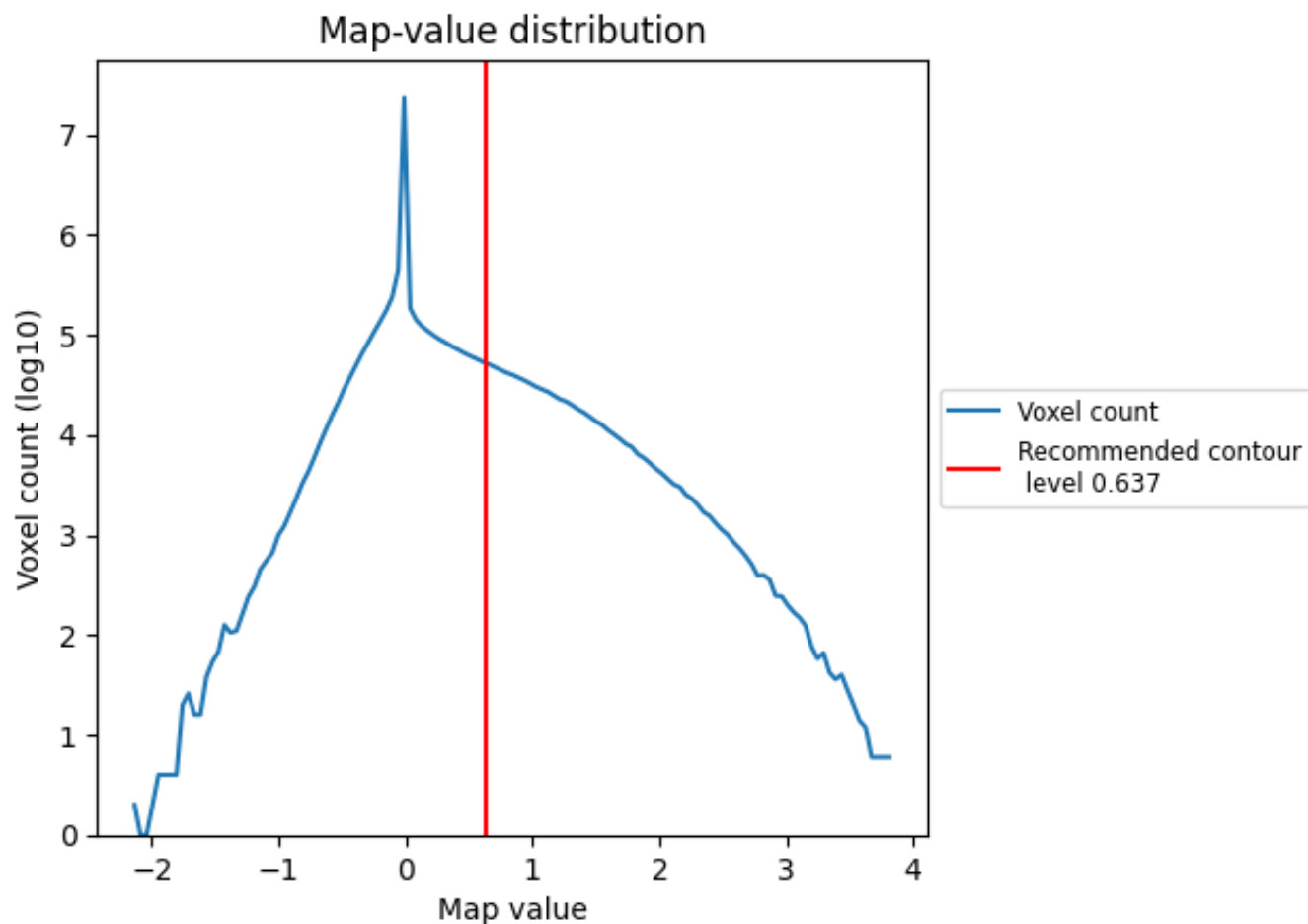
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

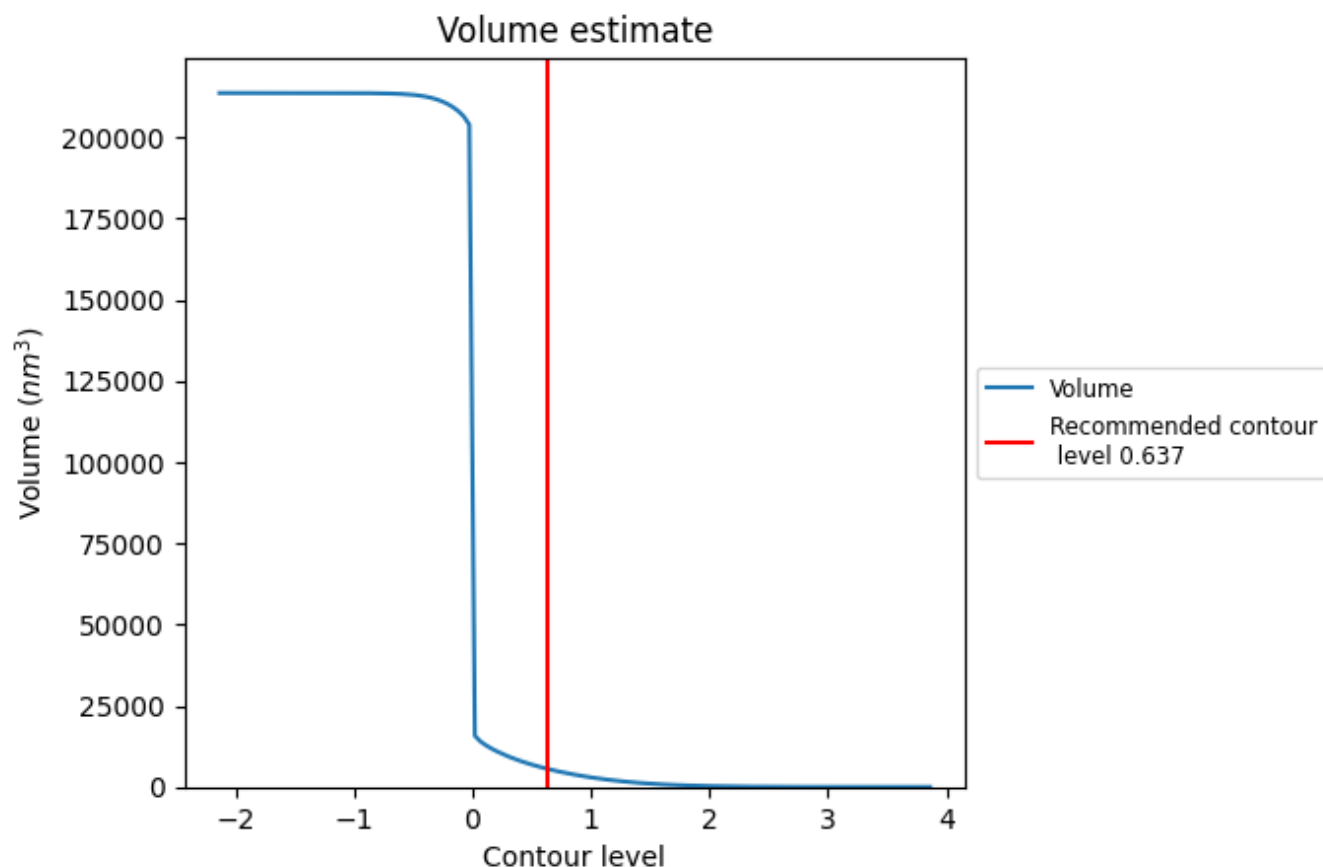
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

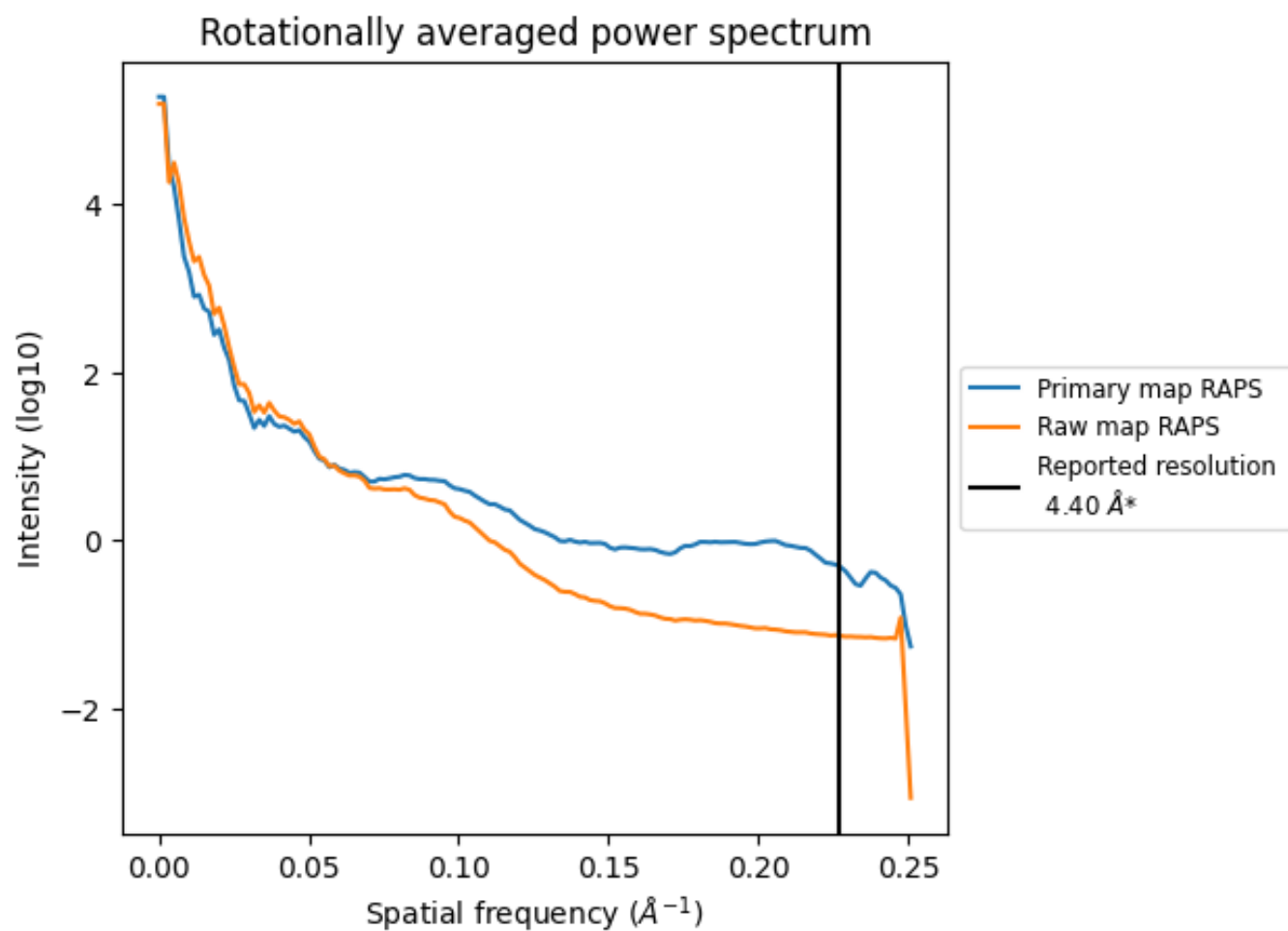
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5531 nm^3 ; this corresponds to an approximate mass of 4996 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

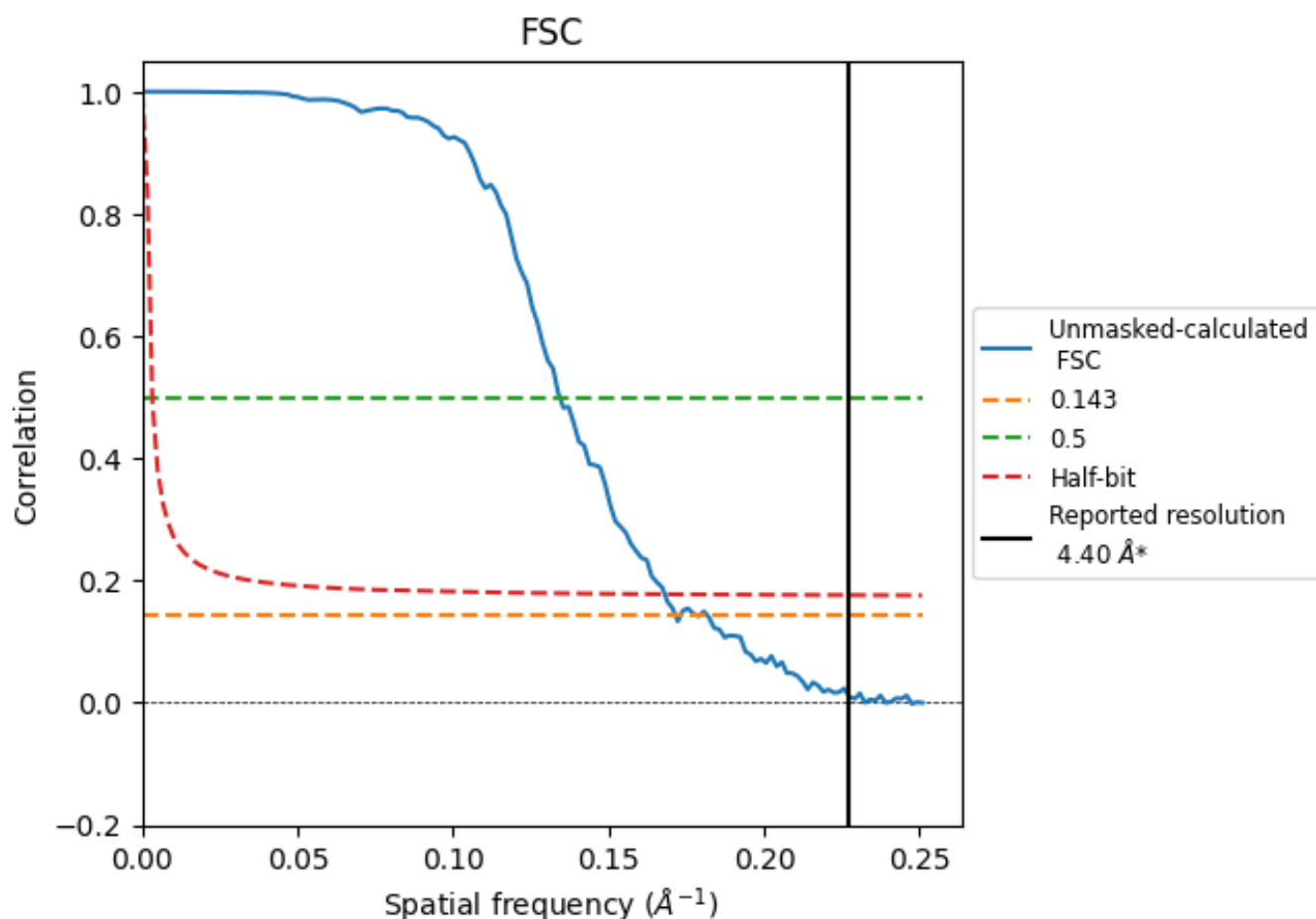


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 \AA^{-1}

8.2 Resolution estimates [i](#)

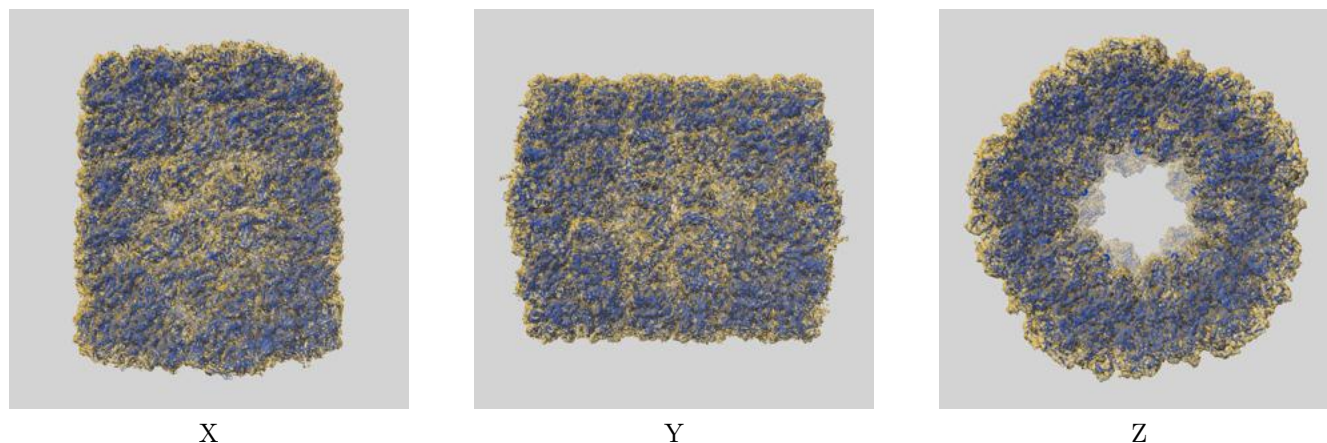
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.83	7.45	5.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.83 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

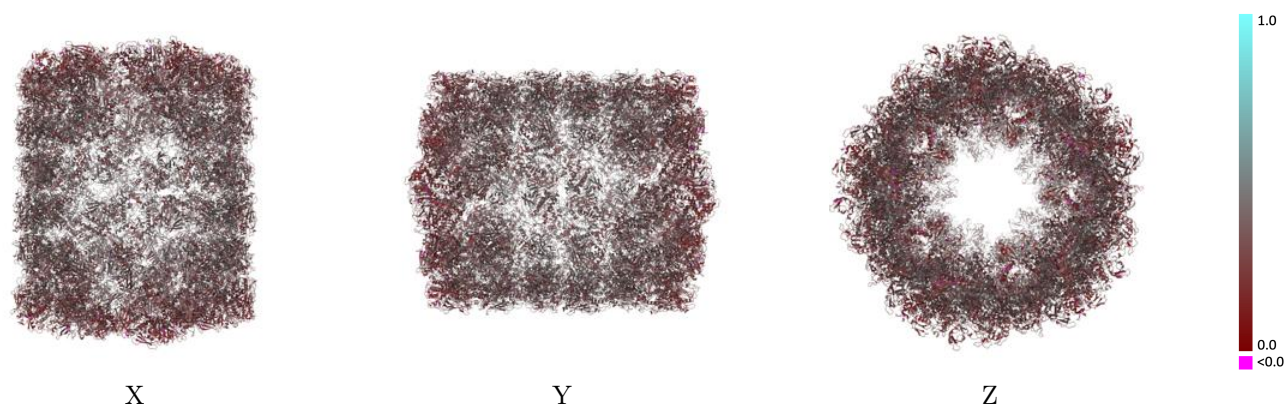
This section contains information regarding the fit between EMDB map EMD-41586 and PDB model 8TRZ. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



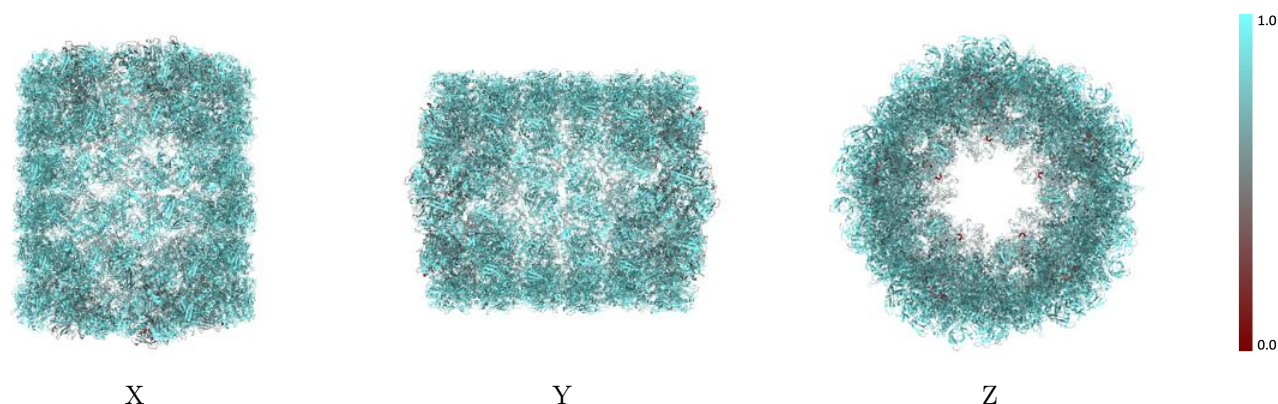
The images above show the 3D surface view of the map at the recommended contour level 0.637 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



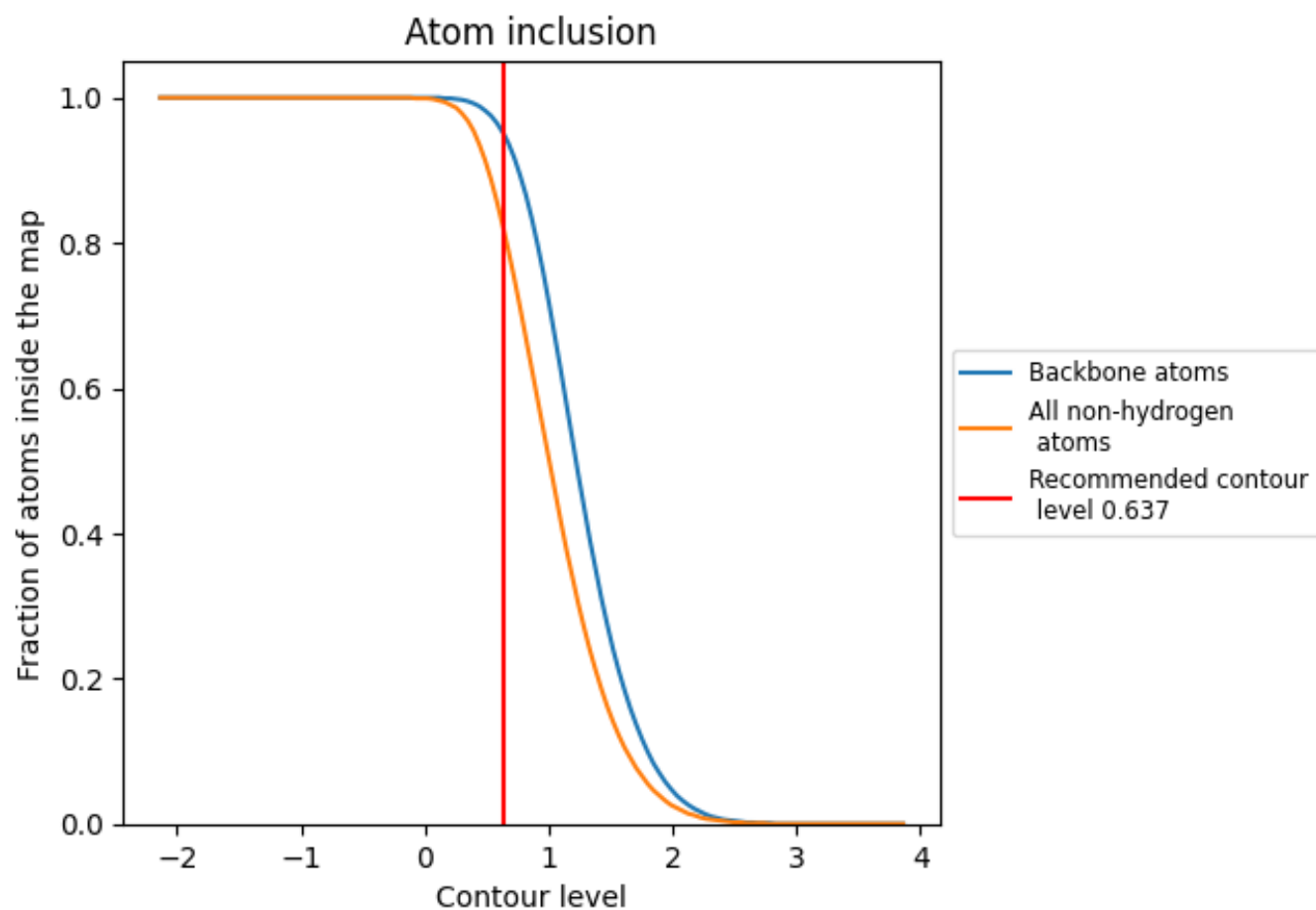
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.637).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.637) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.3460
0	 0.8570	 0.4210
0A	 0.6430	 0.2730
1	 0.8460	 0.4420
1A	 0.9490	 0.4190
2	 0.7140	 0.3260
2A	 0.7440	 0.3960
3	 0.9490	 0.4180
3A	 0.8210	 0.4200
4	 0.7440	 0.3860
4A	 0.8460	 0.3690
5	 0.8210	 0.4350
5A	 0.7500	 0.4130
6	 0.8460	 0.4270
7	 0.7500	 0.4250
8	 0.9640	 0.4330
9	 0.9490	 0.4620
A	 0.8210	 0.3590
AA	 0.8570	 0.4470
B	 0.8180	 0.3320
BA	 0.8460	 0.4330
C	 0.8210	 0.3580
CA	 0.6070	 0.2600
D	 0.8160	 0.3330
DA	 0.9490	 0.4330
E	 0.8220	 0.3590
EA	 0.7950	 0.4410
F	 0.8140	 0.3320
FA	 0.8460	 0.4350
G	 0.8200	 0.3580
GA	 0.8210	 0.4590
H	 0.8150	 0.3320
HA	 0.7140	 0.4060
I	 0.8200	 0.3580
IA	 0.9290	 0.4410























































































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Chain	Atom inclusion	Q-score
J	 0.8190	 0.3320
JA	 0.9490	 0.4600
K	 0.8210	 0.3570
KA	 0.8570	 0.3900
L	 0.8140	 0.3300
LA	 0.8210	 0.4390
M	 0.8190	 0.3580
MA	 0.7500	 0.3090
N	 0.8160	 0.3310
NA	 0.9230	 0.3900
O	 0.8220	 0.3600
OA	 0.7440	 0.3850
P	 0.8180	 0.3320
PA	 0.8210	 0.4320
Q	 0.8210	 0.3580
QA	 0.8210	 0.4470
R	 0.8180	 0.3330
RA	 0.7500	 0.4130
S	 0.8210	 0.3590
SA	 0.8570	 0.4200
T	 0.8120	 0.3320
TA	 0.9490	 0.4490
U	 0.8930	 0.4440
UA	 0.8570	 0.4460
V	 0.9230	 0.4860
VA	 0.8460	 0.4280
W	 0.7860	 0.4330
WA	 0.7140	 0.2600
X	 0.8460	 0.4110
XA	 0.9490	 0.4060
Y	 0.6430	 0.3080
YA	 0.7950	 0.4560
Z	 0.9740	 0.4590
ZA	 0.8460	 0.4390
a	 0.7950	 0.4010
aA	 0.8460	 0.4480
b	 0.8460	 0.4570
bA	 0.7140	 0.4030
c	 0.7440	 0.4650
cA	 0.8930	 0.4500
d	 0.7500	 0.4180
dA	 0.9230	 0.4750





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Chain	Atom inclusion	Q-score
e	 0.8930	 0.4480
eA	 0.8570	 0.4410
f	 0.9490	 0.4660
fA	 0.8970	 0.4330
g	 0.7860	 0.4400
gA	 0.6430	 0.2960
h	 0.8720	 0.4100
hA	 0.9740	 0.4690
i	 0.6790	 0.3330
iA	 0.8210	 0.4000
j	 0.9230	 0.4420
jA	 0.8210	 0.4460
k	 0.7440	 0.3850
kA	 0.6920	 0.4030
l	 0.8210	 0.4490
lA	 0.6430	 0.4200
m	 0.7690	 0.4140
mA	 0.8930	 0.4500
n	 0.2860	 0.3940
nA	 0.9490	 0.4720
o	 0.8210	 0.4050
oA	 0.8570	 0.4370
p	 0.9230	 0.4790
pA	 0.7950	 0.4200
q	 0.8570	 0.4090
qA	 0.7860	 0.3180
r	 0.8720	 0.4200
rA	 0.8970	 0.4090
s	 0.6790	 0.2760
sA	 0.7440	 0.3860
t	 0.9230	 0.4560
tA	 0.8210	 0.4520
u	 0.7440	 0.3950
uA	 0.7690	 0.4040
v	 0.8210	 0.4270
vA	 0.7860	 0.3800
w	 0.7690	 0.4100
wA	 0.7860	 0.4140
x	 0.7140	 0.4100
xA	 0.9230	 0.4420
y	 0.8930	 0.4310
yA	 0.8570	 0.4120

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Chain	Atom inclusion	Q-score
z	 0.9490	 0.4510
zA	 0.7440	 0.4040