



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 09:01 AM EST

PDB ID : 6CDE
EMDB ID : EMD-7459
Title : Cryo-EM structure at 3.8 Å resolution of vaccine-elicited antibody vFP20.01 in complex with HIV-1 Env BG505 DS-SOSIP, and antibodies VRC03 and PGT122
Authors : Acharya, P.; Xu, K.; Liu, K.; Carragher, B.; Potter, C.S.; Kwong, P.D.
Deposited on : 2018-02-08
Resolution : 3.80 Å (reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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:

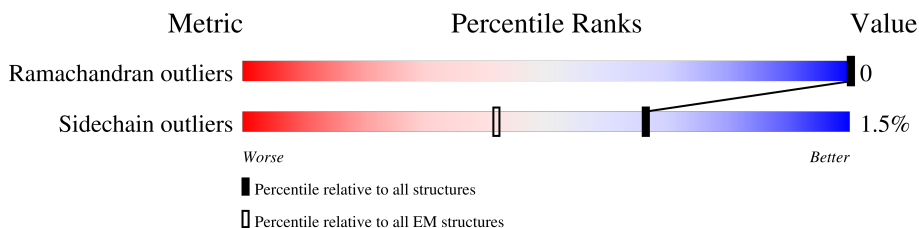
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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	154571	4023
Sidechain outliers	154315	3826

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	3	211	9% 54% 46%
1	H	211	9% 54% 46%
1	h	211	9% 54% 46%
2	4	216	30% 51% 48%
2	L	216	30% 51% 48%
2	l	216	29% 51% 48%
3	7	228	56% 42%
3	M	228	56% 42%
3	m	228	56% 42%

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Mol	Chain	Length	Quality of chain
4	8	210	51% 48%
4	N	210	51% 48%
4	n	210	51% 48%
5	6	208	49% 50%
5	R	208	50% 50%
5	r	208	49% 50%
6	5	227	56% 44%
6	Q	227	56% 44%
6	q	227	56% 44%
7	1	153	86% 14%
7	D	153	86% 14%
7	d	153	86% 14%
8	2	473	95%
8	C	473	94%
8	c	473	94%
9	A	3	33% 67%
9	B	3	33% 67%
9	HA	3	33% 67%
9	JA	3	67% 33%
9	LA	3	33% 67%
9	MA	3	33% 67%
9	T	3	33% 67%
9	V	3	67% 33%
9	X	3	33% 67%
9	Y	3	33% 67%

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Mol	Chain	Length	Quality of chain
9	Z	3	67% 33% 67%
9	a	3	100% 33% 67%
9	s	3	33% 33% 67%
9	u	3	67% 33%
9	w	3	33% 67% 33%
9	x	3	33% 67% 33%
9	y	3	67% 33% 67%
9	z	3	100% 33% 67%
10	0	2	50% 100%
10	9	2	50% 50%
10	DA	2	100%
10	E	2	50% 100%
10	F	2	50% 50%
10	GA	2	100%
10	K	2	100%
10	S	2	100%
10	b	2	50% 100%
10	e	2	50% 50%
10	j	2	100%
10	p	2	100%
11	AA	4	25% 75%
11	G	4	25% 75%
11	f	4	25% 75%
12	BA	6	17% 50% 50%
12	I	6	17% 50% 50%

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Mol	Chain	Length	Quality of chain
12	g	6	 17% 50% 50%
13	CA	8	 25% 75% 75%
13	J	8	 25% 75% 75%
13	i	8	 25% 75% 75%
14	EA	5	 40% 40% 60%
14	O	5	 20% 40% 80%
14	k	5	 20% 40% 80%
15	FA	8	 25% 25% 75%
15	P	8	 25% 25% 75%
15	o	8	 25% 25% 75%
16	IA	9	 11% 11% 89%
16	U	9	 11% 11% 89%
16	t	9	 11% 11% 89%
17	KA	4	 25% 25% 75%
17	W	4	 25% 25% 75%
17	v	4	 25% 25% 75%

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 32973 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 vFP20.01 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	h	113	882	565	143	169	5	0	0
1	H	113	882	565	143	169	5	0	0
1	3	113	882	565	143	169	5	0	0

- Molecule 2 is a protein called vFP20.01 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	113	879	559	146	170	4	0	0
2	L	113	879	559	146	170	4	0	0
2	4	113	879	559	146	170	4	0	0

- Molecule 3 is a protein called PGT122 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	M	132	1047	669	180	195	3	0	0
3	m	132	1047	669	180	195	3	0	0
3	7	132	1047	669	180	195	3	0	0

- Molecule 4 is a protein called PGT122 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	109	832	520	144	166	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	109	Total	C	N	O	S	0	0
			832	520	144	166	2		
4	8	109	Total	C	N	O	S	0	0
			832	520	144	166	2		

- Molecule 5 is a protein called VRC03 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	103	Total	C	N	O	S	0	0
			813	516	141	153	3		
5	r	103	Total	C	N	O	S	0	0
			813	516	141	153	3		
5	6	103	Total	C	N	O	S	0	0
			813	516	141	153	3		

- Molecule 6 is a protein called VRC03 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	128	Total	C	N	O	S	0	0
			1023	657	175	185	6		
6	q	128	Total	C	N	O	S	0	0
			1023	657	175	185	6		
6	5	128	Total	C	N	O	S	0	0
			1023	657	175	185	6		

- Molecule 7 is a protein called Glycoprotein 41.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
7	d	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		
7	1	132	Total	C	N	O	S	0	0
			1034	654	178	196	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	605	CYS	THR	conflict	UNP Q2N0S7
d	605	CYS	THR	conflict	UNP Q2N0S7
1	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 8 is a protein called Glycoprotein 120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	C	452	3556	2229	629	668	30	0	0
8	c	452	3556	2229	629	668	30	0	0
8	2	452	3556	2229	629	668	30	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	201	CYS	ILE	conflict	UNP Q2N0S5
C	332	ASN	THR	conflict	UNP Q2N0S5
C	433	CYS	ALA	conflict	UNP Q2N0S5
C	501	CYS	ALA	conflict	UNP Q2N0S5
c	201	CYS	ILE	conflict	UNP Q2N0S5
c	332	ASN	THR	conflict	UNP Q2N0S5
c	433	CYS	ALA	conflict	UNP Q2N0S5
c	501	CYS	ALA	conflict	UNP Q2N0S5
2	201	CYS	ILE	conflict	UNP Q2N0S5
2	332	ASN	THR	conflict	UNP Q2N0S5
2	433	CYS	ALA	conflict	UNP Q2N0S5
2	501	CYS	ALA	conflict	UNP Q2N0S5

- Molecule 9 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
			Total	C	N	O		
9	A	3	39	22	2	15	0	0
9	B	3	39	22	2	15	0	0
9	T	3	39	22	2	15	0	0
9	V	3	39	22	2	15	0	0
9	X	3	39	22	2	15	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	Y	3	Total 39	C 22	N 2	O 15	0	0
9	Z	3	Total 39	C 22	N 2	O 15	0	0
9	a	3	Total 39	C 22	N 2	O 15	0	0
9	s	3	Total 39	C 22	N 2	O 15	0	0
9	u	3	Total 39	C 22	N 2	O 15	0	0
9	w	3	Total 39	C 22	N 2	O 15	0	0
9	x	3	Total 39	C 22	N 2	O 15	0	0
9	y	3	Total 39	C 22	N 2	O 15	0	0
9	z	3	Total 39	C 22	N 2	O 15	0	0
9	HA	3	Total 39	C 22	N 2	O 15	0	0
9	JA	3	Total 39	C 22	N 2	O 15	0	0
9	LA	3	Total 39	C 22	N 2	O 15	0	0
9	MA	3	Total 39	C 22	N 2	O 15	0	0

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



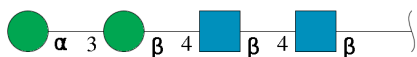
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	E	2	Total 28	C 16	N 2	O 10	0	0
10	F	2	Total 28	C 16	N 2	O 10	0	0
10	K	2	Total 28	C 16	N 2	O 10	0	0
10	S	2	Total 28	C 16	N 2	O 10	0	0

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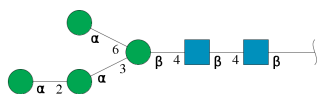
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	b	2	28	16	2	10	0	0
10	e	2	28	16	2	10	0	0
10	j	2	28	16	2	10	0	0
10	p	2	28	16	2	10	0	0
10	0	2	28	16	2	10	0	0
10	9	2	28	16	2	10	0	0
10	DA	2	28	16	2	10	0	0
10	GA	2	28	16	2	10	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



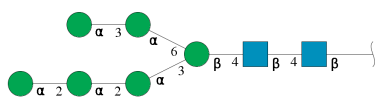
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	G	4	50	28	2	20	0	0
11	f	4	50	28	2	20	0	0
11	AA	4	50	28	2	20	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



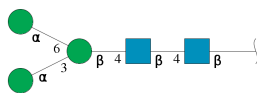
Mol	Chain	Residues	Atoms				AltConf	Trace
12	I	6	Total	C	N	O	0	0
			72	40	2	30		
12	g	6	Total	C	N	O	0	0
			72	40	2	30		
12	BA	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	J	8	Total	C	N	O	0	0
			94	52	2	40		
13	i	8	Total	C	N	O	0	0
			94	52	2	40		
13	CA	8	Total	C	N	O	0	0
			94	52	2	40		

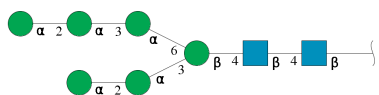
- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	5	Total	C	N	O	0	0
			61	34	2	25		
14	k	5	Total	C	N	O	0	0
			61	34	2	25		
14	EA	5	Total	C	N	O	0	0
			61	34	2	25		

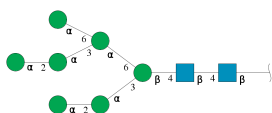
- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-

-acetamido-2-deoxy-beta-D-glucopyranose.



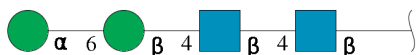
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	P	8	94	52	2	40	0	0
15	o	8	94	52	2	40	0	0
15	FA	8	94	52	2	40	0	0

- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	U	9	105	58	2	45	0	0
16	t	9	105	58	2	45	0	0
16	IA	9	105	58	2	45	0	0

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



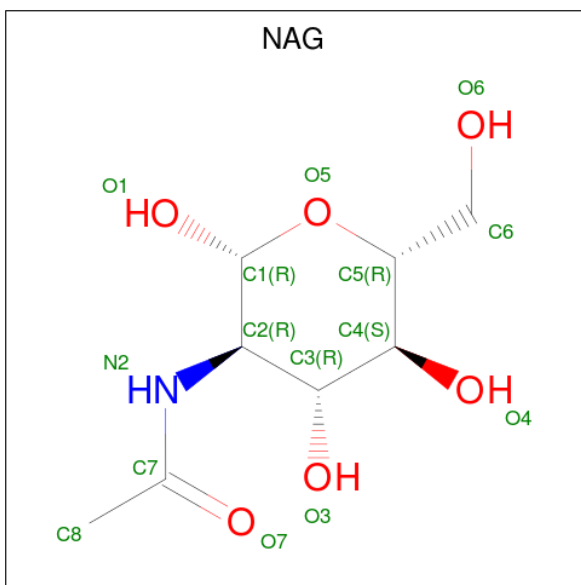
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	W	4	50	28	2	20	0	0
17	v	4	50	28	2	20	0	0

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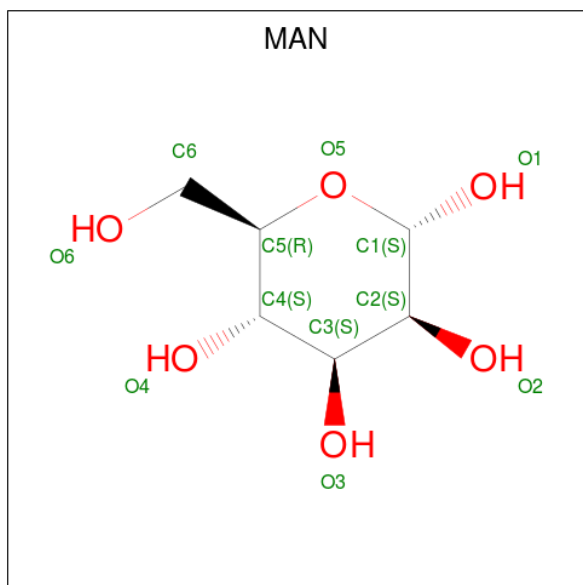
Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
17	KA	4	50	28	2	20	0	0

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
18	D	1	14	8	1	5	0
18	C	1	28	16	2	10	0
18	C	1	28	16	2	10	0
18	d	1	14	8	1	5	0
18	c	1	28	16	2	10	0
18	c	1	28	16	2	10	0
18	1	1	14	8	1	5	0
18	2	1	28	16	2	10	0
18	2	1	28	16	2	10	0

- Molecule 19 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).

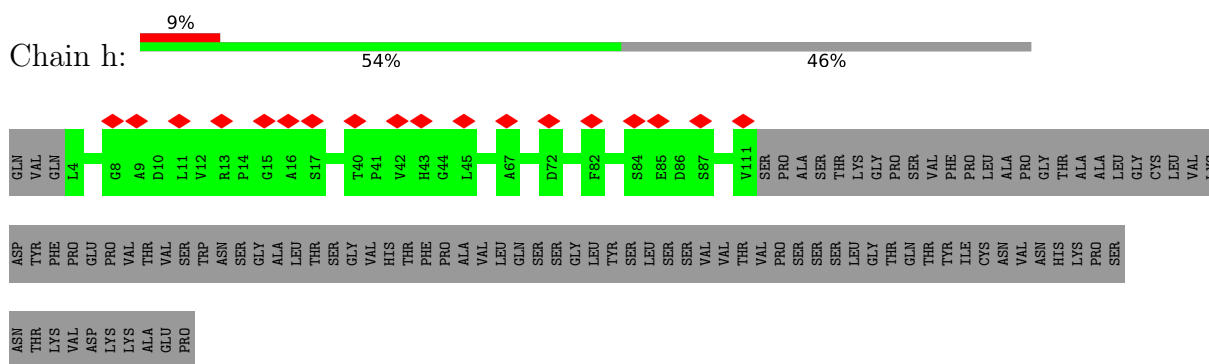


Mol	Chain	Residues	Atoms			AltConf
19	C	1	Total	C	O	0
			11	6	5	
19	c	1	Total	C	O	0
			11	6	5	
19	2	1	Total	C	O	0
			11	6	5	

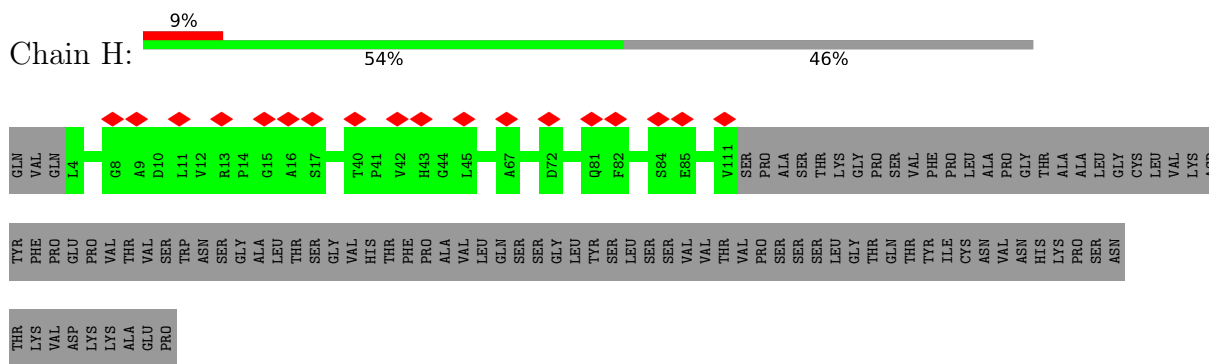
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

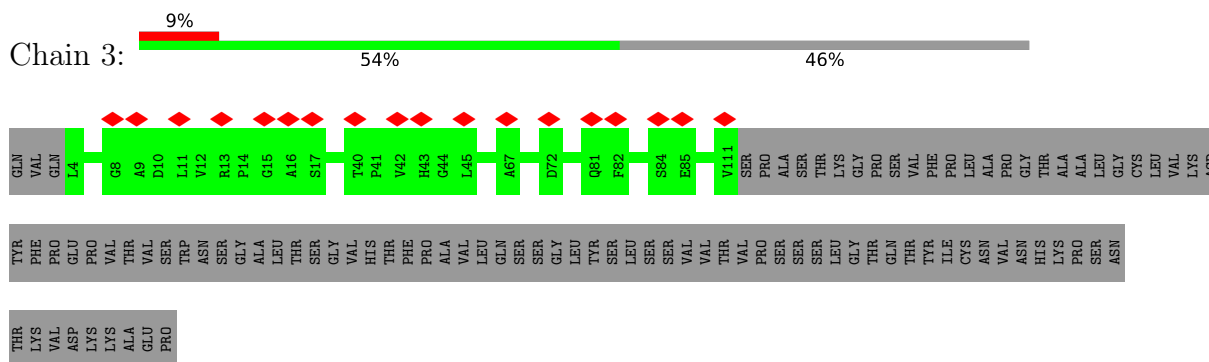
- Molecule 1: vFP20.01 Heavy Chain



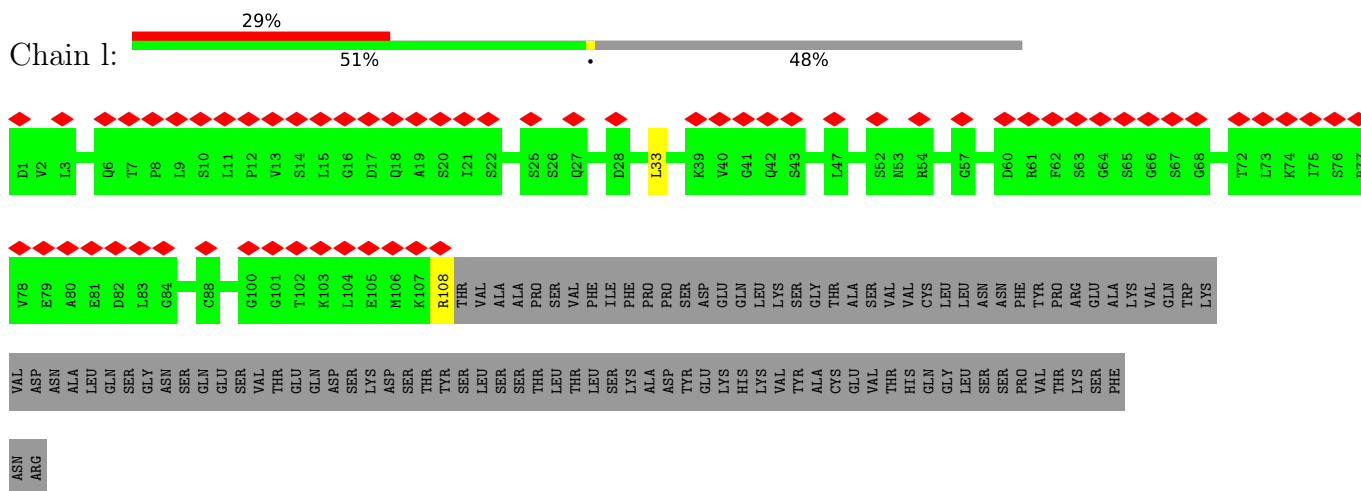
- Molecule 1: vFP20.01 Heavy Chain



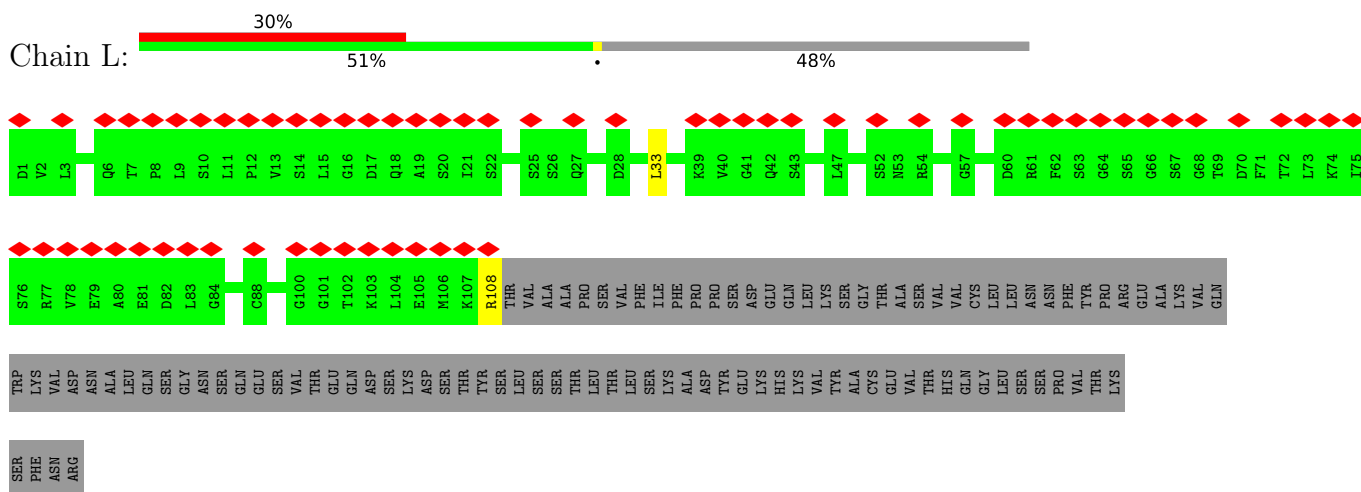
- Molecule 1: vFP20.01 Heavy Chain



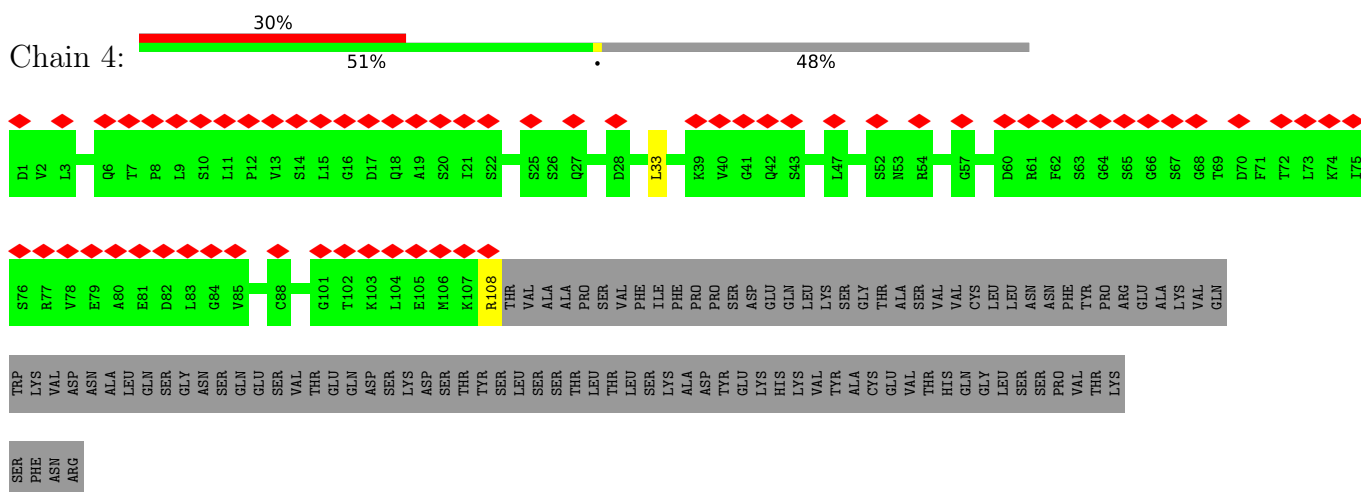
• Molecule 2: vFP20.01 Light chain



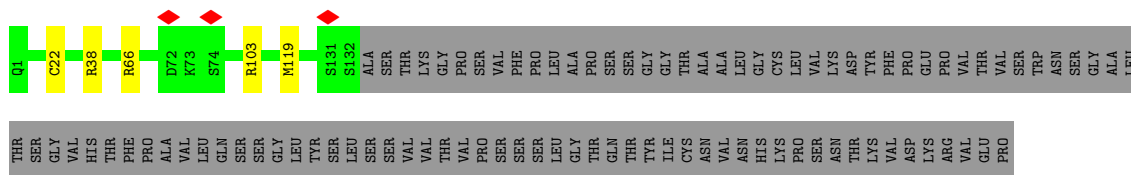
• Molecule 2: vFP20.01 Light chain



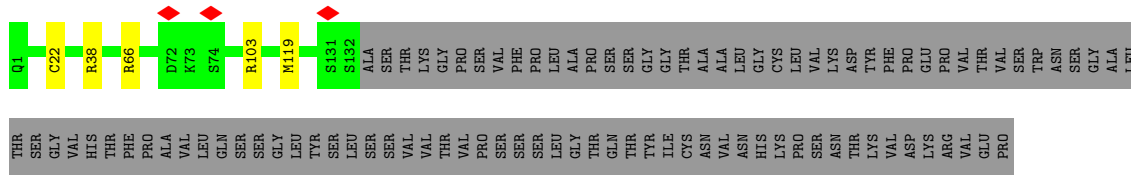
• Molecule 2: vFP20.01 Light chain



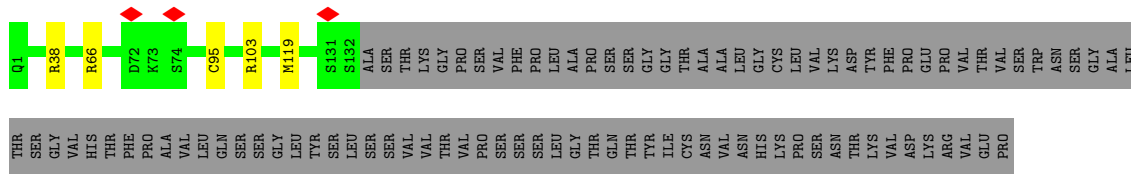
• Molecule 3: PGT122 Heavy chain



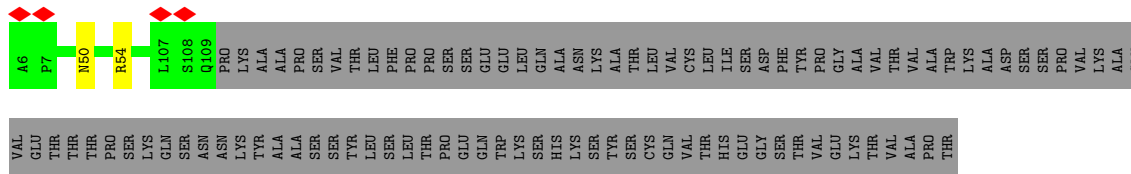
• Molecule 3: PGT122 Heavy chain



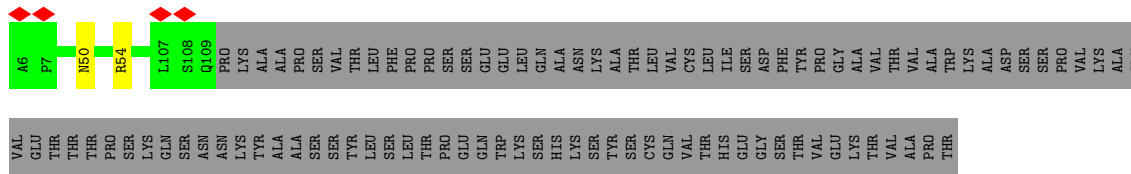
• Molecule 3: PGT122 Heavy chain



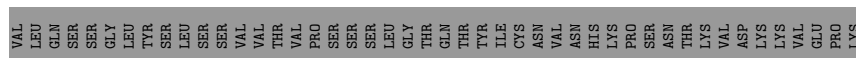
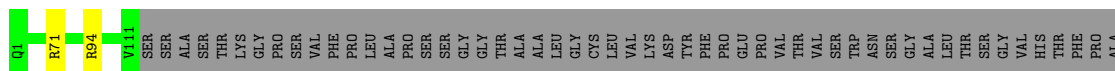
• Molecule 4: PGT122 Light Chain



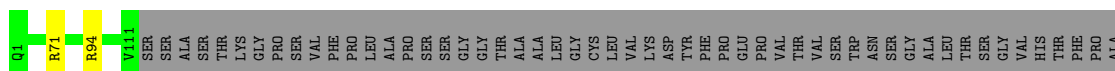
• Molecule 4: PGT122 Light Chain



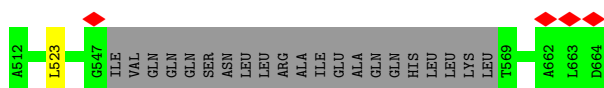
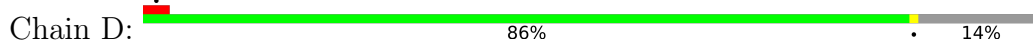
• Molecule 4: PGT122 Light Chain



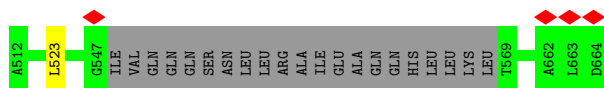
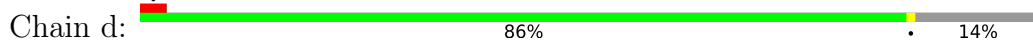
• Molecule 6: VRC03 Heavy Chain



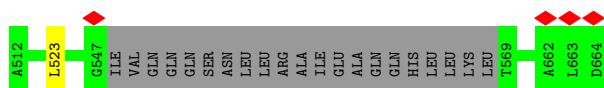
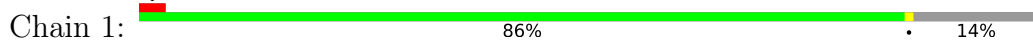
• Molecule 7: Glycoprotein 41



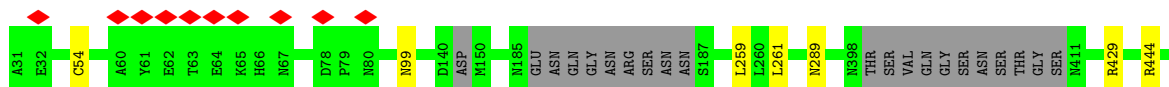
• Molecule 7: Glycoprotein 41



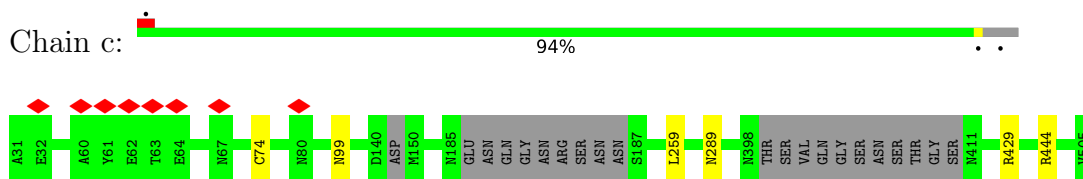
• Molecule 7: Glycoprotein 41



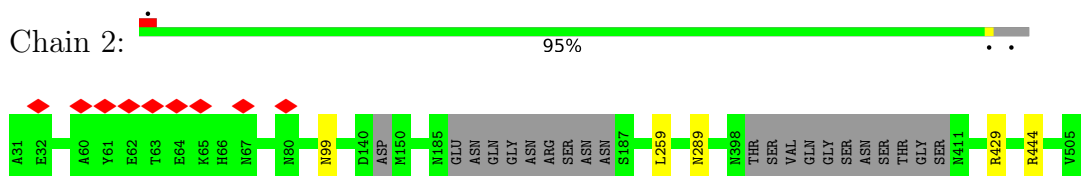
• Molecule 8: Glycoprotein 120



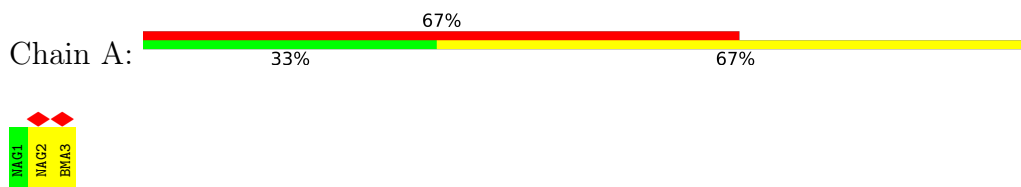
• Molecule 8: Glycoprotein 120



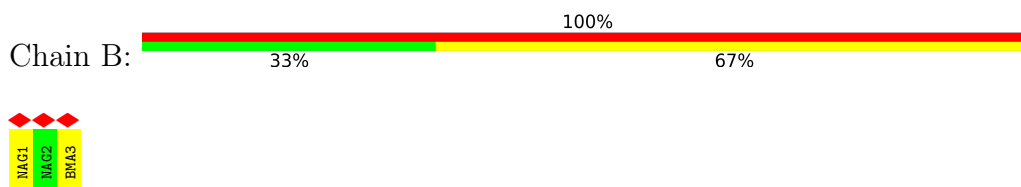
- Molecule 8: Glycoprotein 120



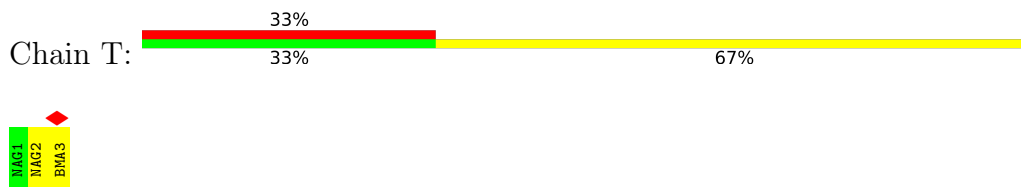
- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



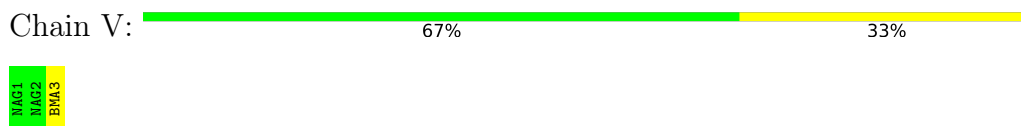
- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:  50% 100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:  100%

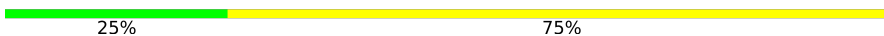


- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:  100%

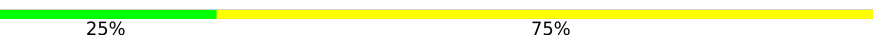
MAG1
MAG2

- Molecule 11: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 11: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 11: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  17% 50% 50%

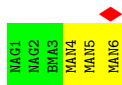
MAG1
MAG2
BMA3
MAN4
MAN5
MANG

- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

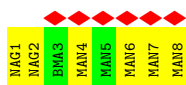
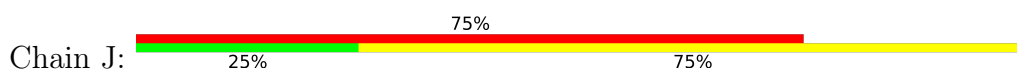
Chain g:  17% 50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
MANG

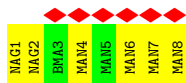
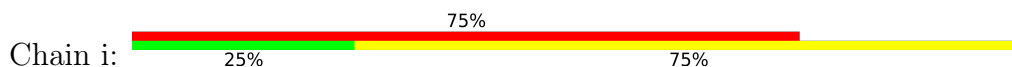
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



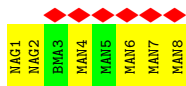
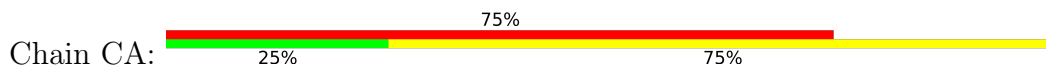
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



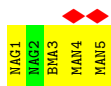
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



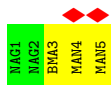
- Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



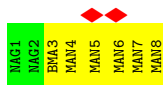
- Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



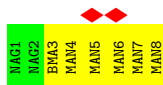
- Molecule 14: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



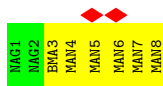
- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



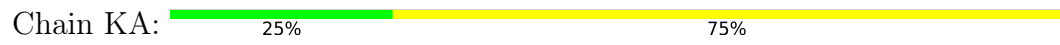
- Molecule 17: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	48248	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 ($e^-/\text{\AA}^2$)	70.70	Depositor
Minimum defocus (nm)	-1800	Depositor
Maximum defocus (nm)	-2800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.066	Depositor
Minimum map value	-1.398	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.544	Depositor
Map size (Å)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, 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	3	0.37	0/904	0.59	0/1228
1	H	0.37	0/904	0.59	0/1228
1	h	0.37	0/904	0.59	0/1228
2	4	0.38	0/898	0.61	0/1212
2	L	0.38	0/898	0.61	0/1212
2	l	0.38	0/898	0.61	0/1212
3	7	0.33	0/1076	0.59	0/1465
3	M	0.33	0/1076	0.59	0/1465
3	m	0.33	0/1076	0.59	0/1465
4	8	0.33	0/854	0.53	0/1169
4	N	0.33	0/854	0.53	0/1169
4	n	0.34	0/854	0.53	0/1169
5	6	0.37	0/831	0.57	0/1121
5	R	0.37	0/831	0.57	0/1121
5	r	0.37	0/831	0.57	0/1121
6	5	0.42	0/1056	0.58	0/1439
6	Q	0.42	0/1056	0.58	0/1439
6	q	0.42	0/1056	0.58	0/1439
7	1	0.35	0/1052	0.56	1/1427 (0.1%)
7	D	0.35	0/1052	0.56	1/1427 (0.1%)
7	d	0.35	0/1052	0.56	1/1427 (0.1%)
8	2	0.41	0/3629	0.59	1/4925 (0.0%)
8	C	0.41	0/3629	0.59	1/4925 (0.0%)
8	c	0.41	0/3629	0.59	1/4925 (0.0%)
All	All	0.38	0/30900	0.58	6/41958 (0.0%)

There are no bond length outliers.

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	d	523	LEU	CA-CB-CG	5.28	127.44	115.30
7	D	523	LEU	CA-CB-CG	5.28	127.44	115.30
7	1	523	LEU	CA-CB-CG	5.28	127.44	115.30
8	C	259	LEU	CA-CB-CG	5.11	127.05	115.30
8	c	259	LEU	CA-CB-CG	5.11	127.05	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	3	111/211 (53%)	107 (96%)	4 (4%)	0	100	100
1	H	111/211 (53%)	107 (96%)	4 (4%)	0	100	100
1	h	111/211 (53%)	107 (96%)	4 (4%)	0	100	100
2	4	111/216 (51%)	96 (86%)	15 (14%)	0	100	100
2	L	111/216 (51%)	96 (86%)	15 (14%)	0	100	100
2	l	111/216 (51%)	96 (86%)	15 (14%)	0	100	100
3	7	130/228 (57%)	122 (94%)	8 (6%)	0	100	100
3	M	130/228 (57%)	122 (94%)	8 (6%)	0	100	100
3	m	130/228 (57%)	122 (94%)	8 (6%)	0	100	100
4	8	107/210 (51%)	100 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	N	107/210 (51%)	100 (94%)	7 (6%)	0	100	100
4	n	107/210 (51%)	100 (94%)	7 (6%)	0	100	100
5	6	101/208 (49%)	97 (96%)	4 (4%)	0	100	100
5	R	101/208 (49%)	96 (95%)	5 (5%)	0	100	100
5	r	101/208 (49%)	97 (96%)	4 (4%)	0	100	100
6	5	126/227 (56%)	123 (98%)	3 (2%)	0	100	100
6	Q	126/227 (56%)	123 (98%)	3 (2%)	0	100	100
6	q	126/227 (56%)	123 (98%)	3 (2%)	0	100	100
7	1	128/153 (84%)	124 (97%)	4 (3%)	0	100	100
7	D	128/153 (84%)	124 (97%)	4 (3%)	0	100	100
7	d	128/153 (84%)	124 (97%)	4 (3%)	0	100	100
8	2	444/473 (94%)	414 (93%)	30 (7%)	0	100	100
8	C	444/473 (94%)	414 (93%)	30 (7%)	0	100	100
8	c	444/473 (94%)	414 (93%)	30 (7%)	0	100	100
All	All	3774/5778 (65%)	3548 (94%)	226 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	3	95/179 (53%)	95 (100%)	0	100	100
1	H	95/179 (53%)	95 (100%)	0	100	100
1	h	95/179 (53%)	95 (100%)	0	100	100
2	4	99/192 (52%)	97 (98%)	2 (2%)	55	75
2	L	99/192 (52%)	97 (98%)	2 (2%)	55	75
2	l	99/192 (52%)	97 (98%)	2 (2%)	55	75
3	7	116/198 (59%)	111 (96%)	5 (4%)	29	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	116/198 (59%)	111 (96%)	5 (4%)	29	58
3	m	116/198 (59%)	111 (96%)	5 (4%)	29	58
4	8	91/178 (51%)	89 (98%)	2 (2%)	52	72
4	N	91/178 (51%)	89 (98%)	2 (2%)	52	72
4	n	91/178 (51%)	89 (98%)	2 (2%)	52	72
5	6	87/181 (48%)	86 (99%)	1 (1%)	73	85
5	R	87/181 (48%)	87 (100%)	0	100	100
5	r	87/181 (48%)	86 (99%)	1 (1%)	73	85
6	5	108/193 (56%)	106 (98%)	2 (2%)	57	76
6	Q	108/193 (56%)	106 (98%)	2 (2%)	57	76
6	q	108/193 (56%)	106 (98%)	2 (2%)	57	76
7	1	110/129 (85%)	110 (100%)	0	100	100
7	D	110/129 (85%)	110 (100%)	0	100	100
7	d	110/129 (85%)	110 (100%)	0	100	100
8	2	404/422 (96%)	400 (99%)	4 (1%)	76	86
8	C	404/422 (96%)	398 (98%)	6 (2%)	65	81
8	c	404/422 (96%)	399 (99%)	5 (1%)	71	84
All	All	3330/5016 (66%)	3280 (98%)	50 (2%)	66	81

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	q	94	ARG
3	7	66	ARG
2	4	108	ARG
8	c	74	CYS
8	c	429	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	m	100	HIS
2	4	90	GLN
5	r	89	GLN
2	4	93	HIS

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Mol	Chain	Res	Type
5	6	89	GLN

5.3.3 RNA [i](#)

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](#)

210 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
10	NAG	0	1	10,8	14,14,15	0.25	0	17,19,21	0.53	0
10	NAG	0	2	10	14,14,15	0.49	0	17,19,21	0.50	0
10	NAG	9	1	10,8	14,14,15	0.62	1 (7%)	17,19,21	1.12	1 (5%)
10	NAG	9	2	10,8	14,14,15	0.52	0	17,19,21	0.38	0
9	NAG	A	1	7,9	14,14,15	0.23	0	17,19,21	0.51	0
9	NAG	A	2	9	14,14,15	0.32	0	17,19,21	0.61	1 (5%)
9	BMA	A	3	9	11,11,12	0.78	0	15,15,17	0.95	1 (6%)
11	NAG	AA	1	8,11	14,14,15	0.27	0	17,19,21	0.48	0
11	NAG	AA	2	11	14,14,15	0.34	0	17,19,21	0.74	1 (5%)
11	BMA	AA	3	11	11,11,12	1.52	4 (36%)	15,15,17	1.76	1 (6%)
11	MAN	AA	4	11	11,11,12	0.66	0	15,15,17	1.18	2 (13%)
9	NAG	B	1	9	14,14,15	0.62	0	17,19,21	0.71	1 (5%)
9	NAG	B	2	9	14,14,15	0.50	0	17,19,21	0.55	0
9	BMA	B	3	9	11,11,12	0.71	0	15,15,17	0.96	1 (6%)
12	NAG	BA	1	12,8	14,14,15	0.20	0	17,19,21	0.55	0
12	NAG	BA	2	12	14,14,15	0.19	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	BMA	BA	3	12	11,11,12	0.75	0	15,15,17	0.90	0
12	MAN	BA	4	12	11,11,12	0.92	1 (9%)	15,15,17	1.19	2 (13%)
12	MAN	BA	5	12	11,11,12	0.75	0	15,15,17	1.10	2 (13%)
12	MAN	BA	6	12	11,11,12	0.85	1 (9%)	15,15,17	1.26	2 (13%)
13	NAG	CA	1	8,13	14,14,15	0.41	0	17,19,21	1.01	1 (5%)
13	NAG	CA	2	13	14,14,15	0.27	0	17,19,21	0.63	1 (5%)
13	BMA	CA	3	13	11,11,12	0.87	0	15,15,17	0.91	0
13	MAN	CA	4	13	11,11,12	1.59	3 (27%)	15,15,17	2.56	3 (20%)
13	MAN	CA	5	13	11,11,12	1.01	0	15,15,17	0.92	0
13	MAN	CA	6	13	11,11,12	0.91	1 (9%)	15,15,17	1.39	2 (13%)
13	MAN	CA	7	13	11,11,12	0.77	0	15,15,17	1.24	2 (13%)
13	MAN	CA	8	13	11,11,12	0.89	1 (9%)	15,15,17	1.49	2 (13%)
10	NAG	DA	1	10,8	14,14,15	0.34	0	17,19,21	0.49	0
10	NAG	DA	2	10	14,14,15	0.28	0	17,19,21	0.44	0
10	NAG	E	1	10,8	14,14,15	0.26	0	17,19,21	0.53	0
10	NAG	E	2	10	14,14,15	0.49	0	17,19,21	0.50	0
14	NAG	EA	1	14,8	14,14,15	0.58	0	17,19,21	0.59	0
14	NAG	EA	2	14	14,14,15	0.23	0	17,19,21	0.62	0
14	BMA	EA	3	14	11,11,12	0.75	0	15,15,17	1.22	1 (6%)
14	MAN	EA	4	14	11,11,12	0.75	0	15,15,17	1.13	2 (13%)
14	MAN	EA	5	14	11,11,12	0.77	0	15,15,17	1.19	2 (13%)
10	NAG	F	1	10,8	14,14,15	0.63	1 (7%)	17,19,21	1.11	1 (5%)
10	NAG	F	2	10,8	14,14,15	0.52	0	17,19,21	0.38	0
15	NAG	FA	1	15,8	14,14,15	0.26	0	17,19,21	0.57	0
15	NAG	FA	2	15	14,14,15	0.20	0	17,19,21	0.49	0
15	BMA	FA	3	15	11,11,12	1.09	1 (9%)	15,15,17	1.03	1 (6%)
15	MAN	FA	4	15	11,11,12	1.71	4 (36%)	15,15,17	1.93	5 (33%)
15	MAN	FA	5	15	11,11,12	0.87	0	15,15,17	1.08	2 (13%)
15	MAN	FA	6	15	11,11,12	0.88	0	15,15,17	1.00	2 (13%)
15	MAN	FA	7	15	11,11,12	0.68	0	15,15,17	1.30	2 (13%)
15	MAN	FA	8	15	11,11,12	0.71	0	15,15,17	1.22	2 (13%)
11	NAG	G	1	8,11	14,14,15	0.27	0	17,19,21	0.48	0
11	NAG	G	2	11	14,14,15	0.34	0	17,19,21	0.74	1 (5%)
11	BMA	G	3	11	11,11,12	1.51	4 (36%)	15,15,17	1.76	1 (6%)
11	MAN	G	4	11	11,11,12	0.66	0	15,15,17	1.18	2 (13%)
10	NAG	GA	1	10,8	14,14,15	0.26	0	17,19,21	0.53	0
10	NAG	GA	2	10	14,14,15	0.35	0	17,19,21	0.45	0
9	NAG	HA	1	8,9	14,14,15	0.32	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	HA	2	9	14,14,15	0.38	0	17,19,21	1.12	1 (5%)
9	BMA	HA	3	9	11,11,12	0.78	0	15,15,17	1.16	1 (6%)
12	NAG	I	1	12,8	14,14,15	0.21	0	17,19,21	0.55	0
12	NAG	I	2	12	14,14,15	0.19	0	17,19,21	0.53	0
12	BMA	I	3	12	11,11,12	0.74	0	15,15,17	0.91	0
12	MAN	I	4	12	11,11,12	0.92	1 (9%)	15,15,17	1.20	2 (13%)
12	MAN	I	5	12	11,11,12	0.75	0	15,15,17	1.11	2 (13%)
12	MAN	I	6	12	11,11,12	0.85	1 (9%)	15,15,17	1.26	2 (13%)
16	NAG	IA	1	16,8	14,14,15	0.29	0	17,19,21	0.57	0
16	NAG	IA	2	16	14,14,15	0.20	0	17,19,21	1.19	2 (11%)
16	BMA	IA	3	16	11,11,12	1.10	1 (9%)	15,15,17	1.05	1 (6%)
16	MAN	IA	4	16	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
16	MAN	IA	5	16	11,11,12	0.67	0	15,15,17	1.22	2 (13%)
16	MAN	IA	6	16	11,11,12	0.83	0	15,15,17	0.92	1 (6%)
16	MAN	IA	7	16	11,11,12	0.80	0	15,15,17	1.10	2 (13%)
16	MAN	IA	8	16	11,11,12	0.70	0	15,15,17	1.35	2 (13%)
16	MAN	IA	9	16	11,11,12	0.85	1 (9%)	15,15,17	1.01	1 (6%)
13	NAG	J	1	8,13	14,14,15	0.42	0	17,19,21	1.01	1 (5%)
13	NAG	J	2	13	14,14,15	0.28	0	17,19,21	0.62	1 (5%)
13	BMA	J	3	13	11,11,12	0.87	0	15,15,17	0.91	0
13	MAN	J	4	13	11,11,12	1.60	3 (27%)	15,15,17	2.56	3 (20%)
13	MAN	J	5	13	11,11,12	1.01	0	15,15,17	0.92	0
13	MAN	J	6	13	11,11,12	0.92	1 (9%)	15,15,17	1.39	2 (13%)
13	MAN	J	7	13	11,11,12	0.76	0	15,15,17	1.25	2 (13%)
13	MAN	J	8	13	11,11,12	0.90	1 (9%)	15,15,17	1.48	2 (13%)
9	NAG	JA	1	8,9	14,14,15	0.27	0	17,19,21	0.59	0
9	NAG	JA	2	9	14,14,15	0.22	0	17,19,21	0.72	0
9	BMA	JA	3	9	11,11,12	0.81	0	15,15,17	1.01	1 (6%)
10	NAG	K	1	10,8	14,14,15	0.34	0	17,19,21	0.50	0
10	NAG	K	2	10	14,14,15	0.28	0	17,19,21	0.44	0
17	NAG	KA	1	8,17	14,14,15	0.23	0	17,19,21	0.58	0
17	NAG	KA	2	17	14,14,15	0.54	0	17,19,21	1.06	2 (11%)
17	BMA	KA	3	17	11,11,12	0.75	0	15,15,17	0.87	1 (6%)
17	MAN	KA	4	17	11,11,12	0.88	1 (9%)	15,15,17	1.20	2 (13%)
9	NAG	LA	1	8,9	14,14,15	0.24	0	17,19,21	0.53	0
9	NAG	LA	2	9	14,14,15	0.42	0	17,19,21	0.55	0
9	BMA	LA	3	9	11,11,12	1.09	1 (9%)	15,15,17	1.19	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	MA	1	8,9	14,14,15	0.38	0	17,19,21	0.96	1 (5%)
9	NAG	MA	2	9	14,14,15	0.31	0	17,19,21	0.51	0
9	BMA	MA	3	9	11,11,12	0.78	0	15,15,17	0.81	0
14	NAG	O	1	14,8	14,14,15	0.60	1 (7%)	17,19,21	0.59	0
14	NAG	O	2	14	14,14,15	0.24	0	17,19,21	0.62	0
14	BMA	O	3	14	11,11,12	0.75	0	15,15,17	1.23	1 (6%)
14	MAN	O	4	14	11,11,12	0.75	0	15,15,17	1.13	2 (13%)
14	MAN	O	5	14	11,11,12	0.76	0	15,15,17	1.18	2 (13%)
15	NAG	P	1	15,8	14,14,15	0.25	0	17,19,21	0.57	0
15	NAG	P	2	15	14,14,15	0.20	0	17,19,21	0.50	0
15	BMA	P	3	15	11,11,12	1.08	1 (9%)	15,15,17	1.03	1 (6%)
15	MAN	P	4	15	11,11,12	1.71	4 (36%)	15,15,17	1.92	5 (33%)
15	MAN	P	5	15	11,11,12	0.87	0	15,15,17	1.08	2 (13%)
15	MAN	P	6	15	11,11,12	0.87	0	15,15,17	1.00	2 (13%)
15	MAN	P	7	15	11,11,12	0.68	0	15,15,17	1.30	2 (13%)
15	MAN	P	8	15	11,11,12	0.72	0	15,15,17	1.22	2 (13%)
10	NAG	S	1	10,8	14,14,15	0.26	0	17,19,21	0.53	0
10	NAG	S	2	10	14,14,15	0.34	0	17,19,21	0.45	0
9	NAG	T	1	8,9	14,14,15	0.33	0	17,19,21	0.52	0
9	NAG	T	2	9	14,14,15	0.38	0	17,19,21	1.11	1 (5%)
9	BMA	T	3	9	11,11,12	0.78	0	15,15,17	1.16	1 (6%)
16	NAG	U	1	16,8	14,14,15	0.29	0	17,19,21	0.57	0
16	NAG	U	2	16	14,14,15	0.20	0	17,19,21	1.19	2 (11%)
16	BMA	U	3	16	11,11,12	1.10	1 (9%)	15,15,17	1.05	1 (6%)
16	MAN	U	4	16	11,11,12	0.66	0	15,15,17	1.01	2 (13%)
16	MAN	U	5	16	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
16	MAN	U	6	16	11,11,12	0.82	0	15,15,17	0.92	1 (6%)
16	MAN	U	7	16	11,11,12	0.80	0	15,15,17	1.10	2 (13%)
16	MAN	U	8	16	11,11,12	0.70	0	15,15,17	1.34	2 (13%)
16	MAN	U	9	16	11,11,12	0.85	1 (9%)	15,15,17	1.00	1 (6%)
9	NAG	V	1	8,9	14,14,15	0.27	0	17,19,21	0.58	0
9	NAG	V	2	9	14,14,15	0.22	0	17,19,21	0.71	0
9	BMA	V	3	9	11,11,12	0.82	0	15,15,17	1.02	1 (6%)
17	NAG	W	1	8,17	14,14,15	0.22	0	17,19,21	0.58	0
17	NAG	W	2	17	14,14,15	0.54	0	17,19,21	1.06	2 (11%)
17	BMA	W	3	17	11,11,12	0.75	0	15,15,17	0.87	1 (6%)
17	MAN	W	4	17	11,11,12	0.89	1 (9%)	15,15,17	1.20	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	X	1	8,9	14,14,15	0.24	0	17,19,21	0.53	0
9	NAG	X	2	9	14,14,15	0.42	0	17,19,21	0.55	0
9	BMA	X	3	9	11,11,12	1.09	1 (9%)	15,15,17	1.19	1 (6%)
9	NAG	Y	1	8,9	14,14,15	0.37	0	17,19,21	0.96	1 (5%)
9	NAG	Y	2	9	14,14,15	0.33	0	17,19,21	0.51	0
9	BMA	Y	3	9	11,11,12	0.78	0	15,15,17	0.81	0
9	NAG	Z	1	7,9	14,14,15	0.24	0	17,19,21	0.51	0
9	NAG	Z	2	9	14,14,15	0.31	0	17,19,21	0.61	1 (5%)
9	BMA	Z	3	9	11,11,12	0.77	0	15,15,17	0.95	1 (6%)
9	NAG	a	1	9	14,14,15	0.60	0	17,19,21	0.72	1 (5%)
9	NAG	a	2	9	14,14,15	0.52	0	17,19,21	0.56	0
9	BMA	a	3	9	11,11,12	0.71	0	15,15,17	0.96	1 (6%)
10	NAG	b	1	10,8	14,14,15	0.26	0	17,19,21	0.53	0
10	NAG	b	2	10	14,14,15	0.48	0	17,19,21	0.49	0
10	NAG	e	1	10,8	14,14,15	0.62	1 (7%)	17,19,21	1.11	1 (5%)
10	NAG	e	2	10,8	14,14,15	0.52	0	17,19,21	0.38	0
11	NAG	f	1	8,11	14,14,15	0.26	0	17,19,21	0.48	0
11	NAG	f	2	11	14,14,15	0.33	0	17,19,21	0.74	1 (5%)
11	BMA	f	3	11	11,11,12	1.51	3 (27%)	15,15,17	1.76	1 (6%)
11	MAN	f	4	11	11,11,12	0.66	0	15,15,17	1.17	2 (13%)
12	NAG	g	1	12,8	14,14,15	0.22	0	17,19,21	0.56	0
12	NAG	g	2	12	14,14,15	0.19	0	17,19,21	0.53	0
12	BMA	g	3	12	11,11,12	0.74	0	15,15,17	0.91	0
12	MAN	g	4	12	11,11,12	0.92	1 (9%)	15,15,17	1.19	2 (13%)
12	MAN	g	5	12	11,11,12	0.76	0	15,15,17	1.11	2 (13%)
12	MAN	g	6	12	11,11,12	0.85	1 (9%)	15,15,17	1.25	2 (13%)
13	NAG	i	1	8,13	14,14,15	0.41	0	17,19,21	1.01	1 (5%)
13	NAG	i	2	13	14,14,15	0.28	0	17,19,21	0.63	1 (5%)
13	BMA	i	3	13	11,11,12	0.87	0	15,15,17	0.91	0
13	MAN	i	4	13	11,11,12	1.60	3 (27%)	15,15,17	2.56	3 (20%)
13	MAN	i	5	13	11,11,12	1.00	0	15,15,17	0.93	0
13	MAN	i	6	13	11,11,12	0.92	1 (9%)	15,15,17	1.40	2 (13%)
13	MAN	i	7	13	11,11,12	0.76	0	15,15,17	1.25	2 (13%)
13	MAN	i	8	13	11,11,12	0.90	1 (9%)	15,15,17	1.48	2 (13%)
10	NAG	j	1	10,8	14,14,15	0.33	0	17,19,21	0.49	0
10	NAG	j	2	10	14,14,15	0.28	0	17,19,21	0.44	0
14	NAG	k	1	14,8	14,14,15	0.60	1 (7%)	17,19,21	0.59	0
14	NAG	k	2	14	14,14,15	0.24	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BMA	k	3	14	11,11,12	0.75	0	15,15,17	1.23	1 (6%)
14	MAN	k	4	14	11,11,12	0.75	0	15,15,17	1.13	2 (13%)
14	MAN	k	5	14	11,11,12	0.77	0	15,15,17	1.18	2 (13%)
15	NAG	o	1	15,8	14,14,15	0.25	0	17,19,21	0.57	0
15	NAG	o	2	15	14,14,15	0.19	0	17,19,21	0.50	0
15	BMA	o	3	15	11,11,12	1.09	1 (9%)	15,15,17	1.03	1 (6%)
15	MAN	o	4	15	11,11,12	1.70	4 (36%)	15,15,17	1.92	5 (33%)
15	MAN	o	5	15	11,11,12	0.87	0	15,15,17	1.08	2 (13%)
15	MAN	o	6	15	11,11,12	0.87	0	15,15,17	1.00	2 (13%)
15	MAN	o	7	15	11,11,12	0.68	0	15,15,17	1.31	2 (13%)
15	MAN	o	8	15	11,11,12	0.72	0	15,15,17	1.22	2 (13%)
10	NAG	p	1	10,8	14,14,15	0.26	0	17,19,21	0.53	0
10	NAG	p	2	10	14,14,15	0.34	0	17,19,21	0.45	0
9	NAG	s	1	8,9	14,14,15	0.33	0	17,19,21	0.52	0
9	NAG	s	2	9	14,14,15	0.39	0	17,19,21	1.11	1 (5%)
9	BMA	s	3	9	11,11,12	0.78	0	15,15,17	1.16	1 (6%)
16	NAG	t	1	16,8	14,14,15	0.29	0	17,19,21	0.56	0
16	NAG	t	2	16	14,14,15	0.19	0	17,19,21	1.19	2 (11%)
16	BMA	t	3	16	11,11,12	1.10	1 (9%)	15,15,17	1.04	1 (6%)
16	MAN	t	4	16	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
16	MAN	t	5	16	11,11,12	0.68	0	15,15,17	1.22	2 (13%)
16	MAN	t	6	16	11,11,12	0.81	0	15,15,17	0.92	1 (6%)
16	MAN	t	7	16	11,11,12	0.79	0	15,15,17	1.11	2 (13%)
16	MAN	t	8	16	11,11,12	0.70	0	15,15,17	1.34	2 (13%)
16	MAN	t	9	16	11,11,12	0.86	1 (9%)	15,15,17	1.00	1 (6%)
9	NAG	u	1	8,9	14,14,15	0.26	0	17,19,21	0.58	0
9	NAG	u	2	9	14,14,15	0.22	0	17,19,21	0.72	0
9	BMA	u	3	9	11,11,12	0.82	0	15,15,17	1.01	1 (6%)
17	NAG	v	1	8,17	14,14,15	0.22	0	17,19,21	0.58	0
17	NAG	v	2	17	14,14,15	0.54	0	17,19,21	1.06	2 (11%)
17	BMA	v	3	17	11,11,12	0.76	0	15,15,17	0.87	1 (6%)
17	MAN	v	4	17	11,11,12	0.89	1 (9%)	15,15,17	1.20	2 (13%)
9	NAG	w	1	8,9	14,14,15	0.25	0	17,19,21	0.53	0
9	NAG	w	2	9	14,14,15	0.42	0	17,19,21	0.55	0
9	BMA	w	3	9	11,11,12	1.09	1 (9%)	15,15,17	1.20	1 (6%)
9	NAG	x	1	8,9	14,14,15	0.37	0	17,19,21	0.95	1 (5%)
9	NAG	x	2	9	14,14,15	0.33	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BMA	x	3	9	11,11,12	0.78	0	15,15,17	0.81	0
9	NAG	y	1	7,9	14,14,15	0.23	0	17,19,21	0.51	0
9	NAG	y	2	9	14,14,15	0.31	0	17,19,21	0.62	1 (5%)
9	BMA	y	3	9	11,11,12	0.77	0	15,15,17	0.95	1 (6%)
9	NAG	z	1	9	14,14,15	0.63	1 (7%)	17,19,21	0.71	1 (5%)
9	NAG	z	2	9	14,14,15	0.51	0	17,19,21	0.55	0
9	BMA	z	3	9	11,11,12	0.71	0	15,15,17	0.96	1 (6%)

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
10	NAG	0	1	10,8	-	0/6/23/26	0/1/1/1
10	NAG	0	2	10	-	2/6/23/26	0/1/1/1
10	NAG	9	1	10,8	-	1/6/23/26	0/1/1/1
10	NAG	9	2	10,8	-	1/6/23/26	0/1/1/1
9	NAG	A	1	7,9	-	2/6/23/26	0/1/1/1
9	NAG	A	2	9	-	2/6/23/26	0/1/1/1
9	BMA	A	3	9	-	1/2/19/22	0/1/1/1
11	NAG	AA	1	8,11	-	2/6/23/26	0/1/1/1
11	NAG	AA	2	11	-	2/6/23/26	0/1/1/1
11	BMA	AA	3	11	-	1/2/19/22	0/1/1/1
11	MAN	AA	4	11	-	2/2/19/22	0/1/1/1
9	NAG	B	1	9	-	2/6/23/26	0/1/1/1
9	NAG	B	2	9	-	0/6/23/26	0/1/1/1
9	BMA	B	3	9	-	1/2/19/22	0/1/1/1
12	NAG	BA	1	12,8	-	0/6/23/26	0/1/1/1
12	NAG	BA	2	12	-	0/6/23/26	0/1/1/1
12	BMA	BA	3	12	-	0/2/19/22	0/1/1/1
12	MAN	BA	4	12	-	1/2/19/22	0/1/1/1
12	MAN	BA	5	12	-	0/2/19/22	0/1/1/1
12	MAN	BA	6	12	-	1/2/19/22	0/1/1/1
13	NAG	CA	1	8,13	-	3/6/23/26	0/1/1/1
13	NAG	CA	2	13	-	0/6/23/26	0/1/1/1
13	BMA	CA	3	13	-	0/2/19/22	0/1/1/1
13	MAN	CA	4	13	-	0/2/19/22	0/1/1/1
13	MAN	CA	5	13	-	0/2/19/22	0/1/1/1
13	MAN	CA	6	13	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MAN	CA	7	13	-	0/2/19/22	0/1/1/1
13	MAN	CA	8	13	-	2/2/19/22	0/1/1/1
10	NAG	DA	1	10,8	-	0/6/23/26	0/1/1/1
10	NAG	DA	2	10	-	2/6/23/26	0/1/1/1
10	NAG	E	1	10,8	-	0/6/23/26	0/1/1/1
10	NAG	E	2	10	-	2/6/23/26	0/1/1/1
14	NAG	EA	1	14,8	-	0/6/23/26	0/1/1/1
14	NAG	EA	2	14	-	2/6/23/26	0/1/1/1
14	BMA	EA	3	14	-	1/2/19/22	0/1/1/1
14	MAN	EA	4	14	-	2/2/19/22	0/1/1/1
14	MAN	EA	5	14	-	0/2/19/22	0/1/1/1
10	NAG	F	1	10,8	-	1/6/23/26	0/1/1/1
10	NAG	F	2	10,8	-	1/6/23/26	0/1/1/1
15	NAG	FA	1	15,8	-	2/6/23/26	0/1/1/1
15	NAG	FA	2	15	-	2/6/23/26	0/1/1/1
15	BMA	FA	3	15	-	2/2/19/22	0/1/1/1
15	MAN	FA	4	15	-	2/2/19/22	0/1/1/1
15	MAN	FA	5	15	-	2/2/19/22	0/1/1/1
15	MAN	FA	6	15	-	0/2/19/22	0/1/1/1
15	MAN	FA	7	15	-	1/2/19/22	0/1/1/1
15	MAN	FA	8	15	-	0/2/19/22	0/1/1/1
11	NAG	G	1	8,11	-	2/6/23/26	0/1/1/1
11	NAG	G	2	11	-	2/6/23/26	0/1/1/1
11	BMA	G	3	11	-	1/2/19/22	0/1/1/1
11	MAN	G	4	11	-	2/2/19/22	0/1/1/1
10	NAG	GA	1	10,8	-	0/6/23/26	0/1/1/1
10	NAG	GA	2	10	-	0/6/23/26	0/1/1/1
9	NAG	HA	1	8,9	-	1/6/23/26	0/1/1/1
9	NAG	HA	2	9	-	2/6/23/26	0/1/1/1
9	BMA	HA	3	9	-	1/2/19/22	0/1/1/1
12	NAG	I	1	12,8	-	0/6/23/26	0/1/1/1
12	NAG	I	2	12	-	0/6/23/26	0/1/1/1
12	BMA	I	3	12	-	0/2/19/22	0/1/1/1
12	MAN	I	4	12	-	1/2/19/22	0/1/1/1
12	MAN	I	5	12	-	0/2/19/22	0/1/1/1
12	MAN	I	6	12	-	1/2/19/22	0/1/1/1
16	NAG	IA	1	16,8	-	2/6/23/26	0/1/1/1
16	NAG	IA	2	16	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BMA	IA	3	16	-	0/2/19/22	0/1/1/1
16	MAN	IA	4	16	-	0/2/19/22	0/1/1/1
16	MAN	IA	5	16	-	2/2/19/22	0/1/1/1
16	MAN	IA	6	16	-	2/2/19/22	0/1/1/1
16	MAN	IA	7	16	-	2/2/19/22	0/1/1/1
16	MAN	IA	8	16	-	1/2/19/22	0/1/1/1
16	MAN	IA	9	16	-	0/2/19/22	0/1/1/1
13	NAG	J	1	8,13	-	3/6/23/26	0/1/1/1
13	NAG	J	2	13	-	0/6/23/26	0/1/1/1
13	BMA	J	3	13	-	0/2/19/22	0/1/1/1
13	MAN	J	4	13	-	0/2/19/22	0/1/1/1
13	MAN	J	5	13	-	0/2/19/22	0/1/1/1
13	MAN	J	6	13	-	1/2/19/22	0/1/1/1
13	MAN	J	7	13	-	0/2/19/22	0/1/1/1
13	MAN	J	8	13	-	2/2/19/22	0/1/1/1
9	NAG	JA	1	8,9	-	2/6/23/26	0/1/1/1
9	NAG	JA	2	9	-	2/6/23/26	0/1/1/1
9	BMA	JA	3	9	-	0/2/19/22	0/1/1/1
10	NAG	K	1	10,8	-	0/6/23/26	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1
17	NAG	KA	1	8,17	-	1/6/23/26	0/1/1/1
17	NAG	KA	2	17	-	1/6/23/26	0/1/1/1
17	BMA	KA	3	17	-	0/2/19/22	0/1/1/1
17	MAN	KA	4	17	-	0/2/19/22	0/1/1/1
9	NAG	LA	1	8,9	-	2/6/23/26	0/1/1/1
9	NAG	LA	2	9	-	2/6/23/26	0/1/1/1
9	BMA	LA	3	9	-	2/2/19/22	0/1/1/1
9	NAG	MA	1	8,9	-	3/6/23/26	0/1/1/1
9	NAG	MA	2	9	-	2/6/23/26	0/1/1/1
9	BMA	MA	3	9	-	1/2/19/22	0/1/1/1
14	NAG	O	1	14,8	-	0/6/23/26	0/1/1/1
14	NAG	O	2	14	-	2/6/23/26	0/1/1/1
14	BMA	O	3	14	-	1/2/19/22	0/1/1/1
14	MAN	O	4	14	-	2/2/19/22	0/1/1/1
14	MAN	O	5	14	-	0/2/19/22	0/1/1/1
15	NAG	P	1	15,8	-	2/6/23/26	0/1/1/1
15	NAG	P	2	15	-	2/6/23/26	0/1/1/1
15	BMA	P	3	15	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	MAN	P	4	15	-	2/2/19/22	0/1/1/1
15	MAN	P	5	15	-	2/2/19/22	0/1/1/1
15	MAN	P	6	15	-	0/2/19/22	0/1/1/1
15	MAN	P	7	15	-	1/2/19/22	0/1/1/1
15	MAN	P	8	15	-	0/2/19/22	0/1/1/1
10	NAG	S	1	10,8	-	0/6/23/26	0/1/1/1
10	NAG	S	2	10	-	0/6/23/26	0/1/1/1
9	NAG	T	1	8,9	-	1/6/23/26	0/1/1/1
9	NAG	T	2	9	-	2/6/23/26	0/1/1/1
9	BMA	T	3	9	-	1/2/19/22	0/1/1/1
16	NAG	U	1	16,8	-	2/6/23/26	0/1/1/1
16	NAG	U	2	16	-	3/6/23/26	0/1/1/1
16	BMA	U	3	16	-	0/2/19/22	0/1/1/1
16	MAN	U	4	16	-	0/2/19/22	0/1/1/1
16	MAN	U	5	16	-	2/2/19/22	0/1/1/1
16	MAN	U	6	16	-	2/2/19/22	0/1/1/1
16	MAN	U	7	16	-	2/2/19/22	0/1/1/1
16	MAN	U	8	16	-	1/2/19/22	0/1/1/1
16	MAN	U	9	16	-	0/2/19/22	0/1/1/1
9	NAG	V	1	8,9	-	2/6/23/26	0/1/1/1
9	NAG	V	2	9	-	2/6/23/26	0/1/1/1
9	BMA	V	3	9	-	0/2/19/22	0/1/1/1
17	NAG	W	1	8,17	-	1/6/23/26	0/1/1/1
17	NAG	W	2	17	-	1/6/23/26	0/1/1/1
17	BMA	W	3	17	-	0/2/19/22	0/1/1/1
17	MAN	W	4	17	-	0/2/19/22	0/1/1/1
9	NAG	X	1	8,9	-	2/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
9	BMA	X	3	9	-	2/2/19/22	0/1/1/1
9	NAG	Y	1	8,9	-	3/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Y	3	9	-	1/2/19/22	0/1/1/1
9	NAG	Z	1	7,9	-	2/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	1/2/19/22	0/1/1/1
9	NAG	a	1	9	-	2/6/23/26	0/1/1/1
9	NAG	a	2	9	-	0/6/23/26	0/1/1/1
9	BMA	a	3	9	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	b	1	10,8	-	0/6/23/26	0/1/1/1
10	NAG	b	2	10	-	2/6/23/26	0/1/1/1
10	NAG	e	1	10,8	-	1/6/23/26	0/1/1/1
10	NAG	e	2	10,8	-	1/6/23/26	0/1/1/1
11	NAG	f	1	8,11	-	2/6/23/26	0/1/1/1
11	NAG	f	2	11	-	2/6/23/26	0/1/1/1
11	BMA	f	3	11	-	1/2/19/22	0/1/1/1
11	MAN	f	4	11	-	2/2/19/22	0/1/1/1
12	NAG	g	1	12,8	-	0/6/23/26	0/1/1/1
12	NAG	g	2	12	-	0/6/23/26	0/1/1/1
12	BMA	g	3	12	-	0/2/19/22	0/1/1/1
12	MAN	g	4	12	-	1/2/19/22	0/1/1/1
12	MAN	g	5	12	-	0/2/19/22	0/1/1/1
12	MAN	g	6	12	-	1/2/19/22	0/1/1/1
13	NAG	i	1	8,13	-	3/6/23/26	0/1/1/1
13	NAG	i	2	13	-	0/6/23/26	0/1/1/1
13	BMA	i	3	13	-	0/2/19/22	0/1/1/1
13	MAN	i	4	13	-	0/2/19/22	0/1/1/1
13	MAN	i	5	13	-	0/2/19/22	0/1/1/1
13	MAN	i	6	13	-	1/2/19/22	0/1/1/1
13	MAN	i	7	13	-	0/2/19/22	0/1/1/1
13	MAN	i	8	13	-	2/2/19/22	0/1/1/1
10	NAG	j	1	10,8	-	0/6/23/26	0/1/1/1
10	NAG	j	2	10	-	2/6/23/26	0/1/1/1
14	NAG	k	1	14,8	-	0/6/23/26	0/1/1/1
14	NAG	k	2	14	-	2/6/23/26	0/1/1/1
14	BMA	k	3	14	-	1/2/19/22	0/1/1/1
14	MAN	k	4	14	-	2/2/19/22	0/1/1/1
14	MAN	k	5	14	-	0/2/19/22	0/1/1/1
15	NAG	o	1	15,8	-	2/6/23/26	0/1/1/1
15	NAG	o	2	15	-	2/6/23/26	0/1/1/1
15	BMA	o	3	15	-	2/2/19/22	0/1/1/1
15	MAN	o	4	15	-	2/2/19/22	0/1/1/1
15	MAN	o	5	15	-	2/2/19/22	0/1/1/1
15	MAN	o	6	15	-	0/2/19/22	0/1/1/1
15	MAN	o	7	15	-	1/2/19/22	0/1/1/1
15	MAN	o	8	15	-	0/2/19/22	0/1/1/1
10	NAG	p	1	10,8	-	0/6/23/26	0/1/1/1
10	NAG	p	2	10	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	s	1	8,9	-	1/6/23/26	0/1/1/1
9	NAG	s	2	9	-	2/6/23/26	0/1/1/1
9	BMA	s	3	9	-	1/2/19/22	0/1/1/1
16	NAG	t	1	16,8	-	2/6/23/26	0/1/1/1
16	NAG	t	2	16	-	3/6/23/26	0/1/1/1
16	BMA	t	3	16	-	0/2/19/22	0/1/1/1
16	MAN	t	4	16	-	0/2/19/22	0/1/1/1
16	MAN	t	5	16	-	2/2/19/22	0/1/1/1
16	MAN	t	6	16	-	2/2/19/22	0/1/1/1
16	MAN	t	7	16	-	2/2/19/22	0/1/1/1
16	MAN	t	8	16	-	1/2/19/22	0/1/1/1
16	MAN	t	9	16	-	0/2/19/22	0/1/1/1
9	NAG	u	1	8,9	-	2/6/23/26	0/1/1/1
9	NAG	u	2	9	-	2/6/23/26	0/1/1/1
9	BMA	u	3	9	-	0/2/19/22	0/1/1/1
17	NAG	v	1	8,17	-	1/6/23/26	0/1/1/1
17	NAG	v	2	17	-	1/6/23/26	0/1/1/1
17	BMA	v	3	17	-	0/2/19/22	0/1/1/1
17	MAN	v	4	17	-	0/2/19/22	0/1/1/1
9	NAG	w	1	8,9	-	2/6/23/26	0/1/1/1
9	NAG	w	2	9	-	2/6/23/26	0/1/1/1
9	BMA	w	3	9	-	2/2/19/22	0/1/1/1
9	NAG	x	1	8,9	-	3/6/23/26	0/1/1/1
9	NAG	x	2	9	-	2/6/23/26	0/1/1/1
9	BMA	x	3	9	-	1/2/19/22	0/1/1/1
9	NAG	y	1	7,9	-	2/6/23/26	0/1/1/1
9	NAG	y	2	9	-	2/6/23/26	0/1/1/1
9	BMA	y	3	9	-	1/2/19/22	0/1/1/1
9	NAG	z	1	9	-	2/6/23/26	0/1/1/1
9	NAG	z	2	9	-	0/6/23/26	0/1/1/1
9	BMA	z	3	9	-	1/2/19/22	0/1/1/1

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	4	MAN	C2-C3	3.35	1.57	1.52
15	FA	4	MAN	C2-C3	3.33	1.57	1.52
15	o	4	MAN	C2-C3	3.32	1.57	1.52
11	AA	3	BMA	O5-C5	3.13	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	f	3	BMA	O5-C5	3.10	1.49	1.43

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	CA	4	MAN	C1-O5-C5	8.20	123.30	112.19
13	i	4	MAN	C1-O5-C5	8.18	123.27	112.19
13	J	4	MAN	C1-O5-C5	8.17	123.26	112.19
11	AA	3	BMA	C1-O5-C5	6.07	120.41	112.19
11	G	3	BMA	C1-O5-C5	6.06	120.40	112.19

There are no chirality outliers.

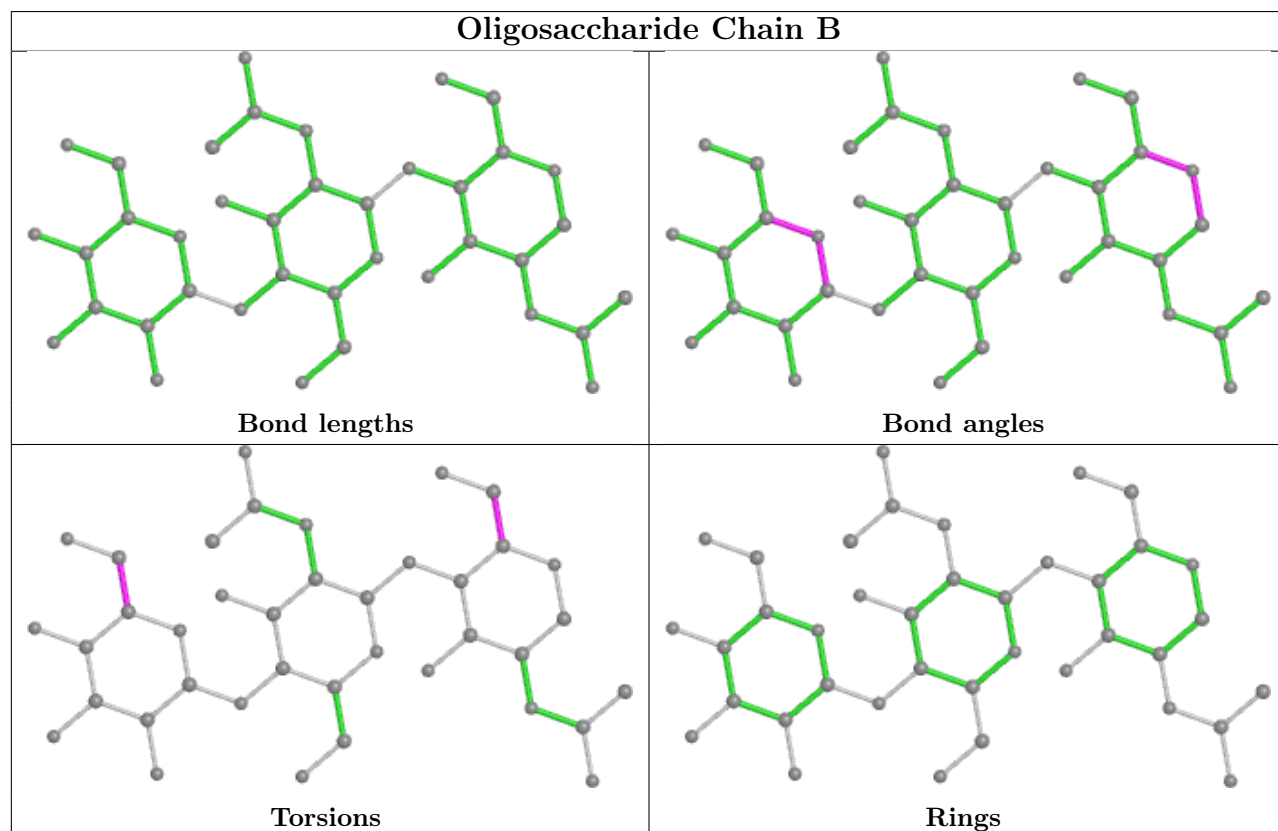
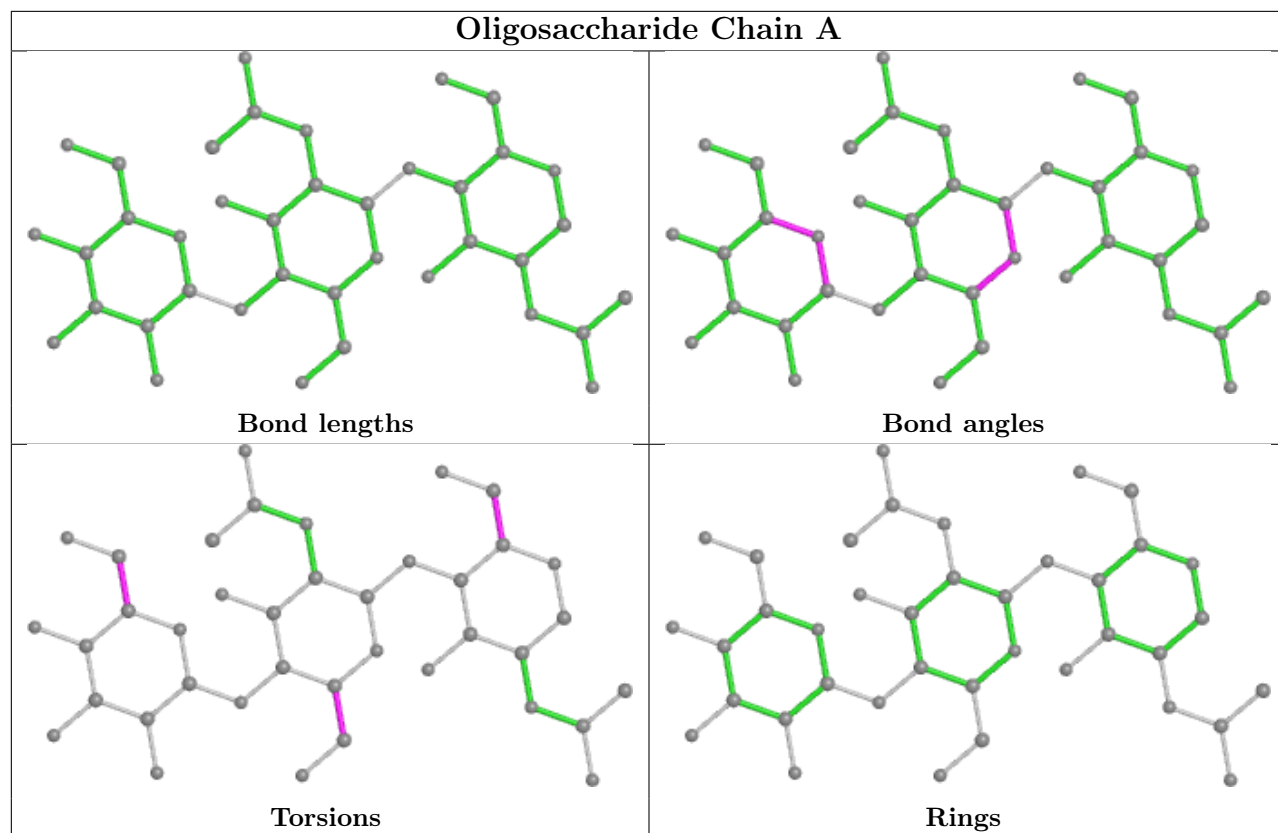
5 of 237 torsion outliers are listed below:

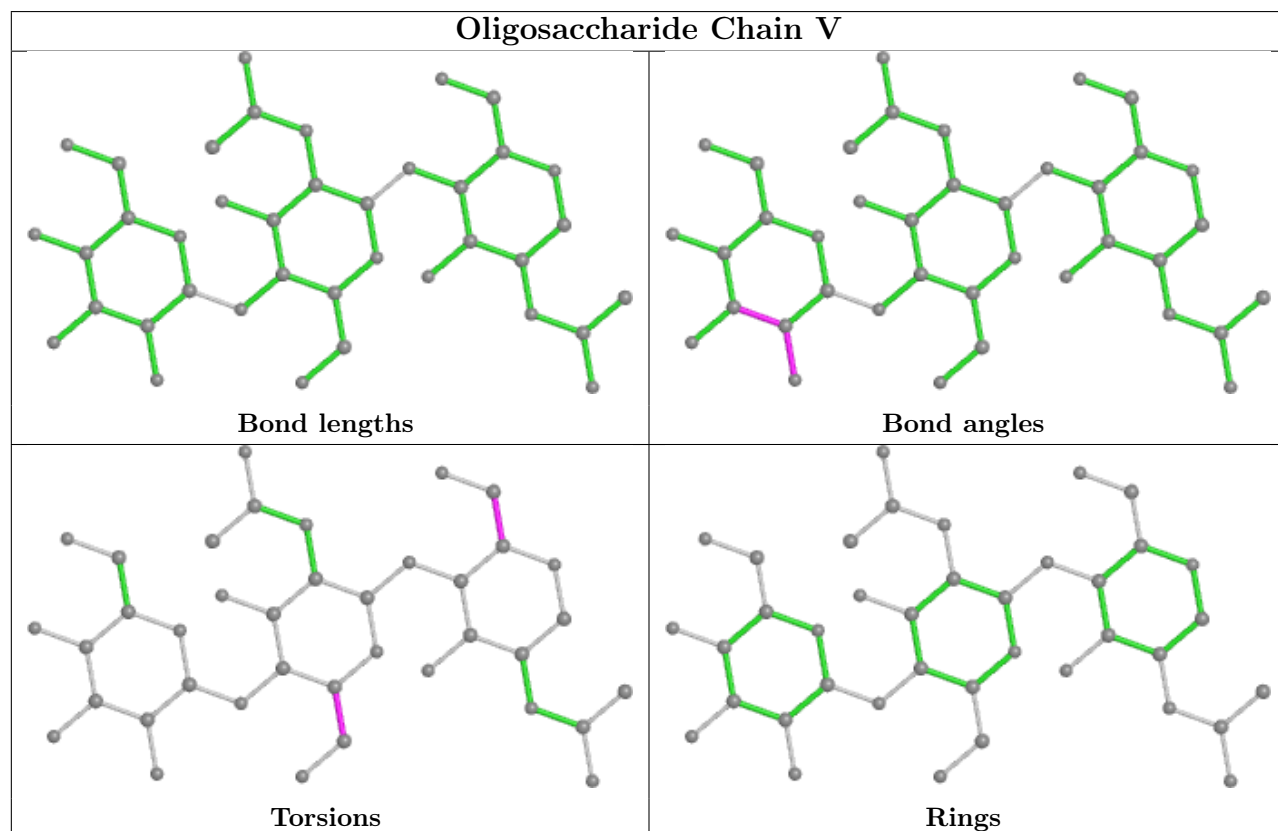
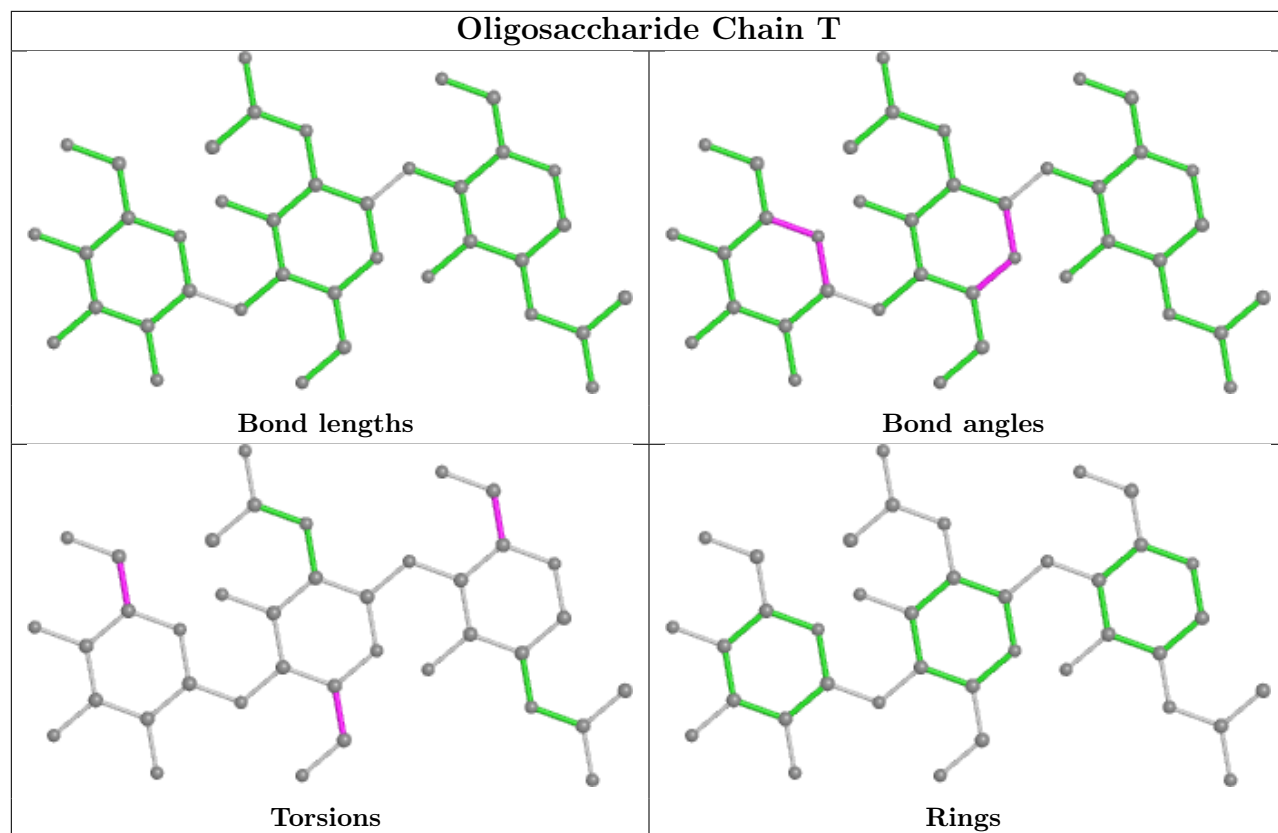
Mol	Chain	Res	Type	Atoms
16	U	2	NAG	O5-C5-C6-O6
16	t	2	NAG	O5-C5-C6-O6
16	IA	2	NAG	O5-C5-C6-O6
9	Y	2	NAG	O5-C5-C6-O6
9	x	2	NAG	O5-C5-C6-O6

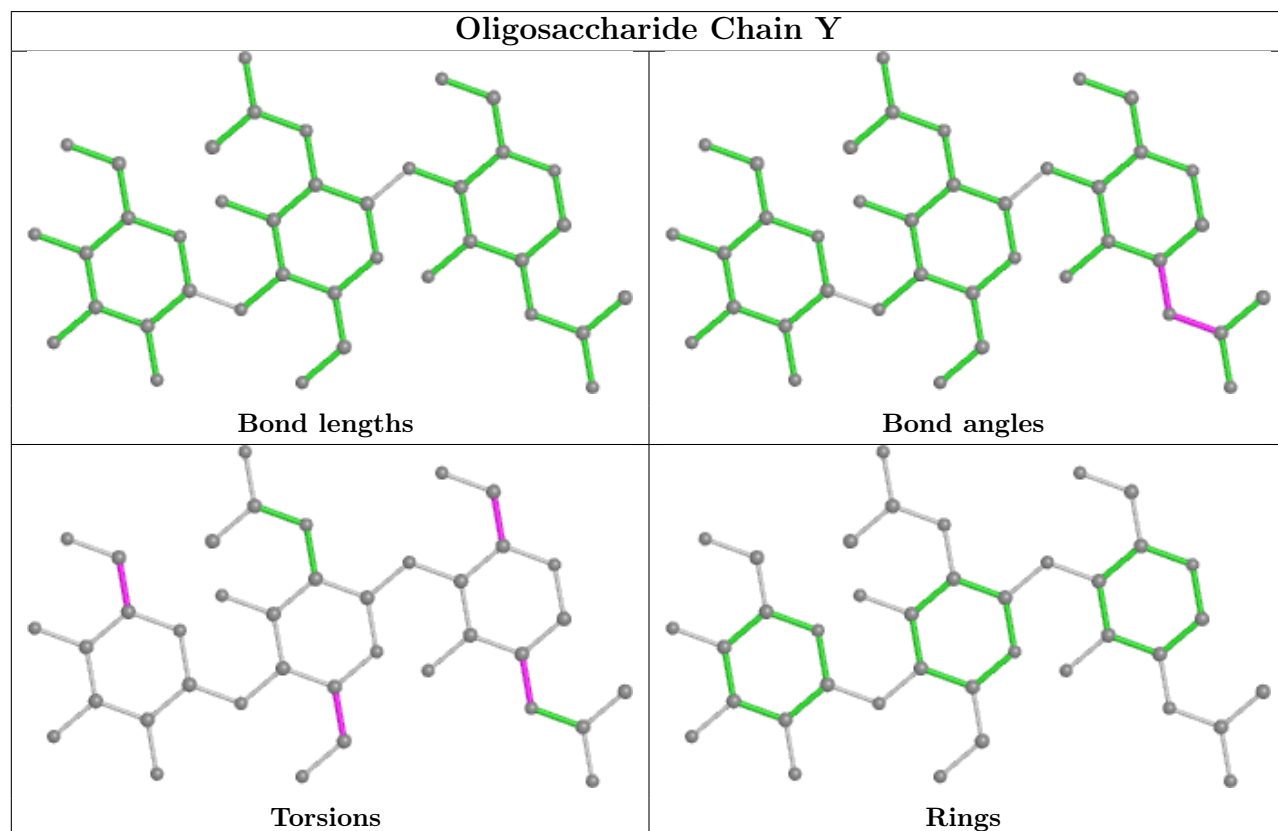
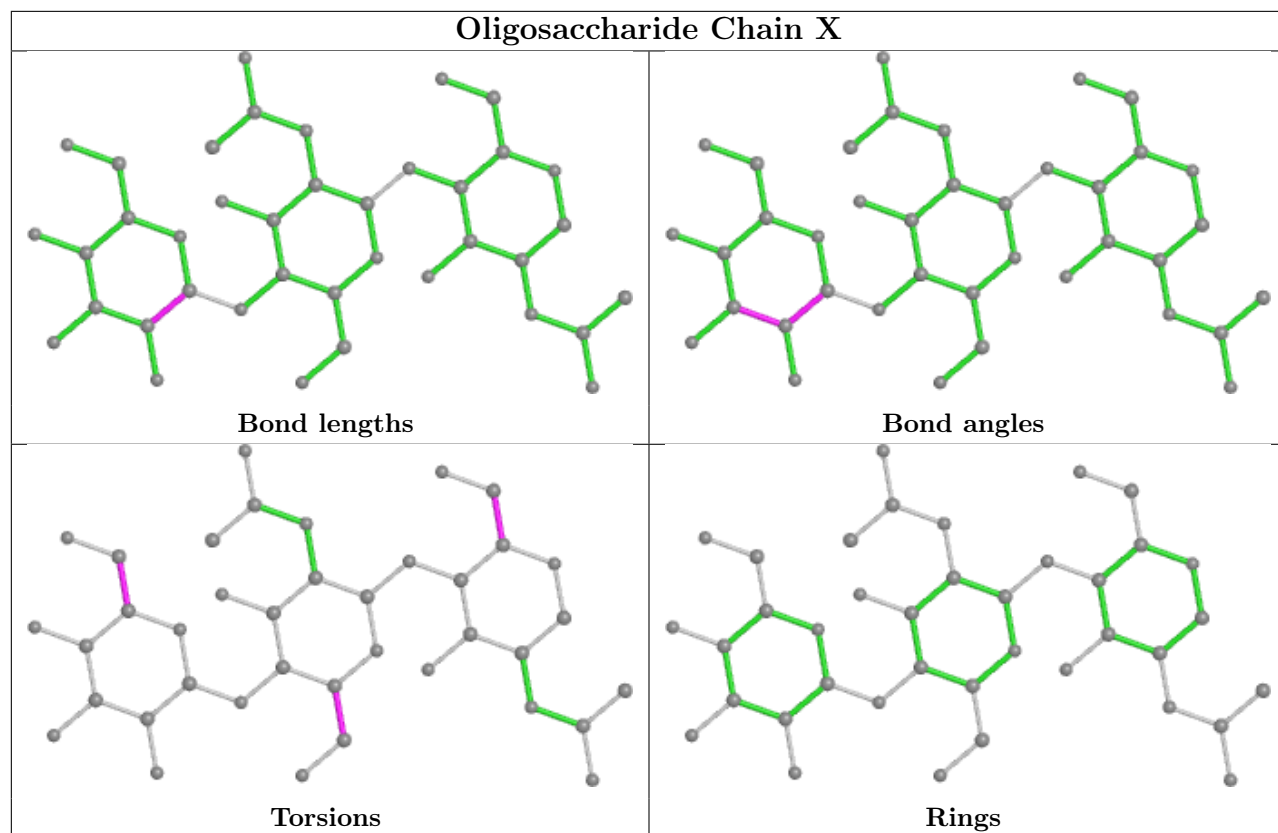
There are no ring outliers.

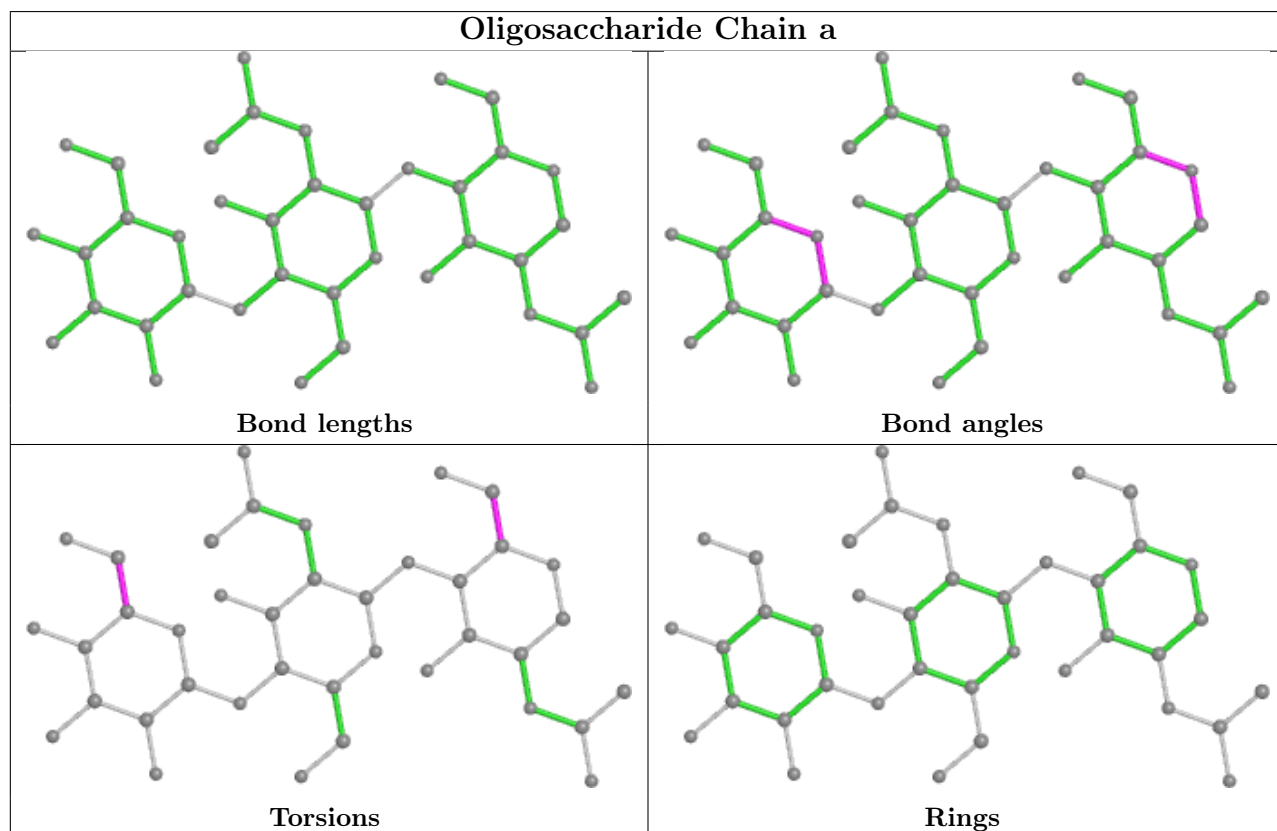
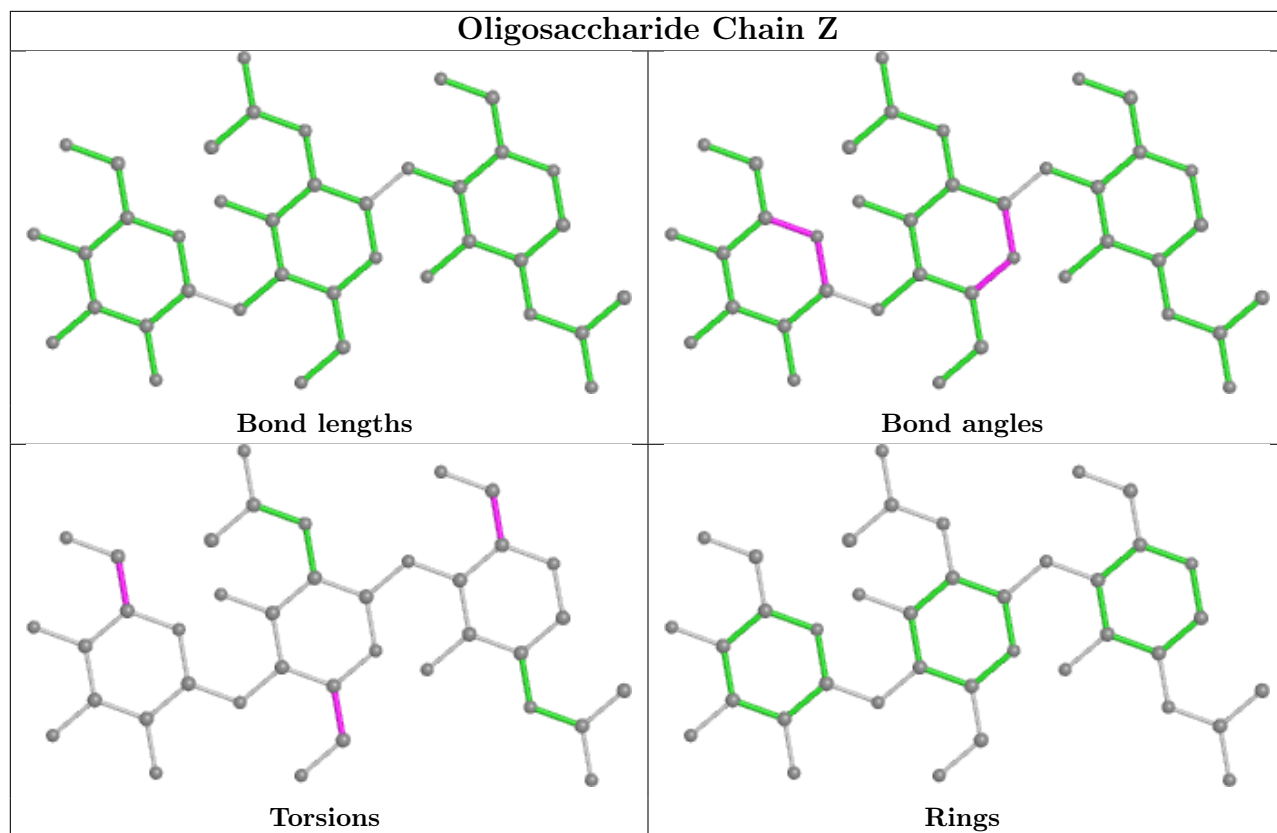
No monomer is involved in short contacts.

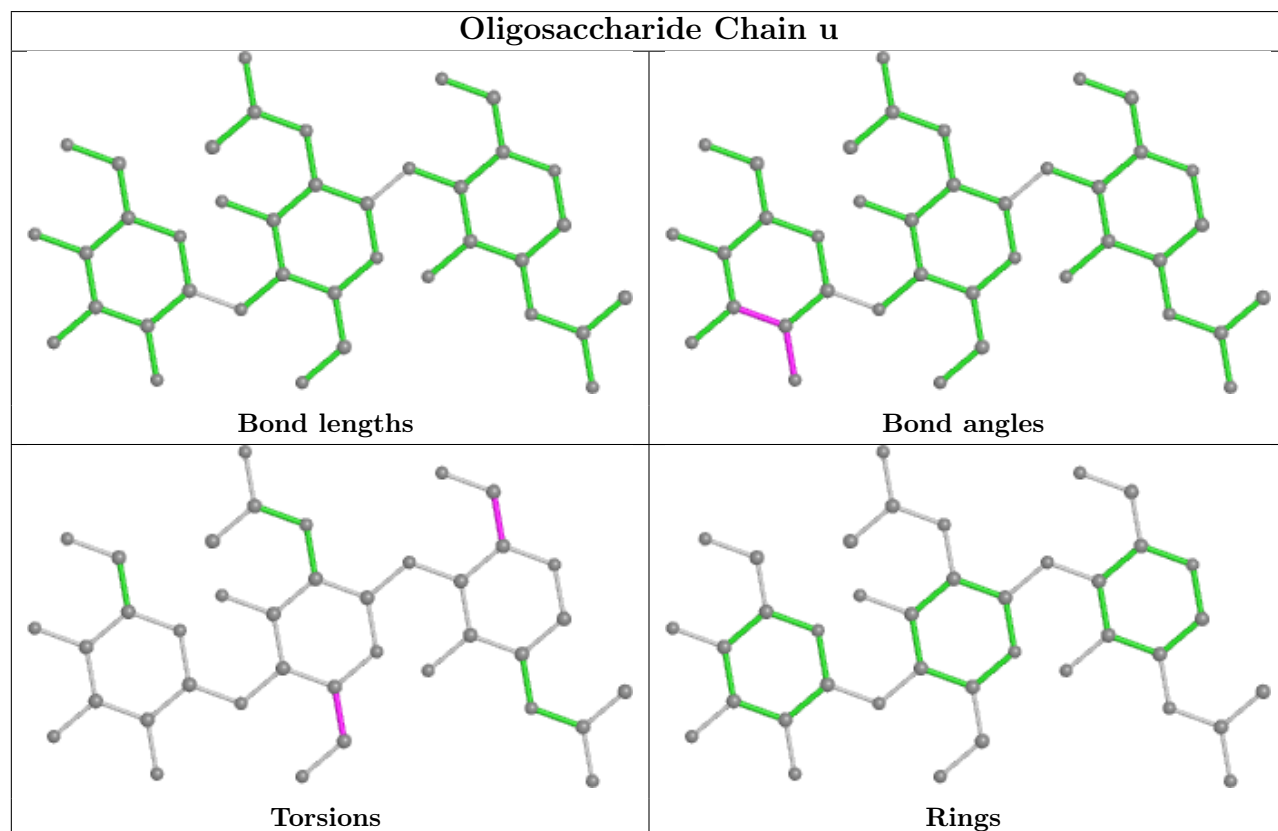
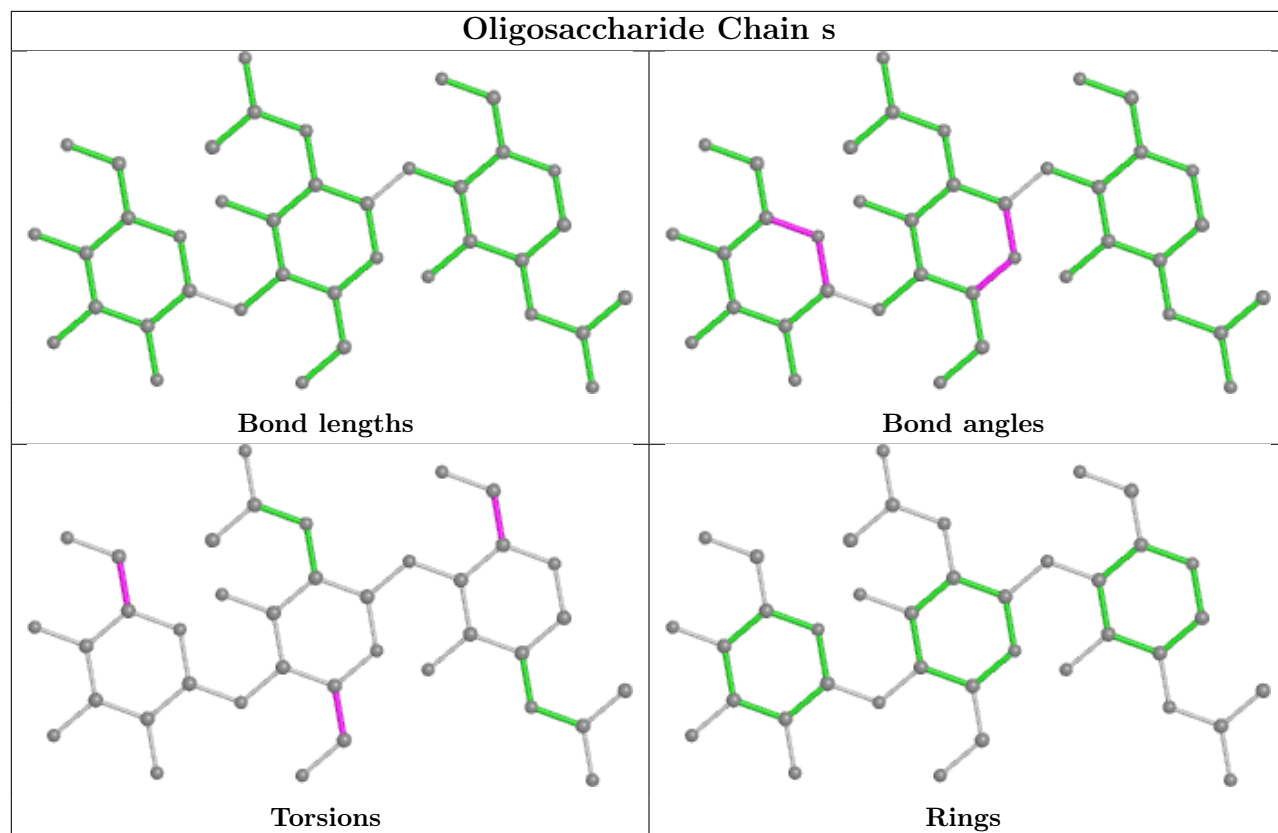
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

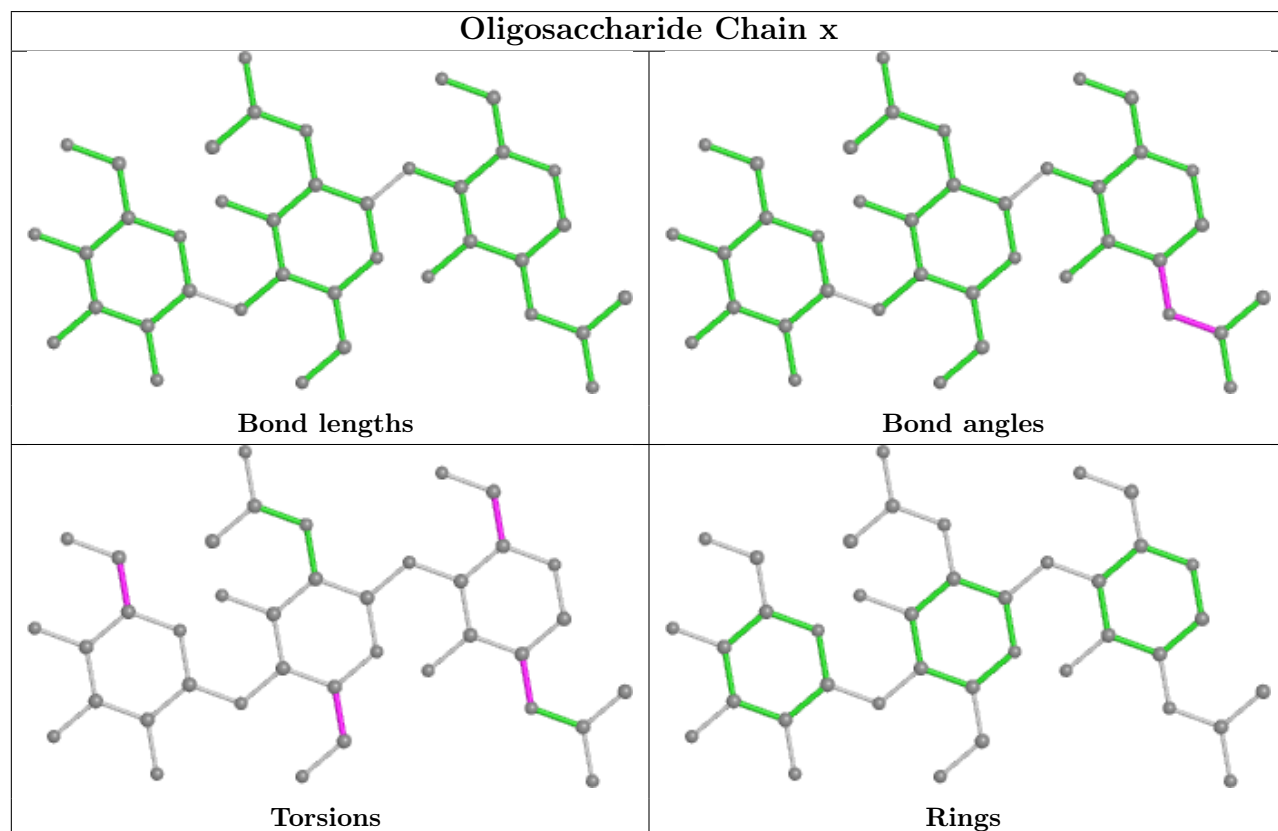
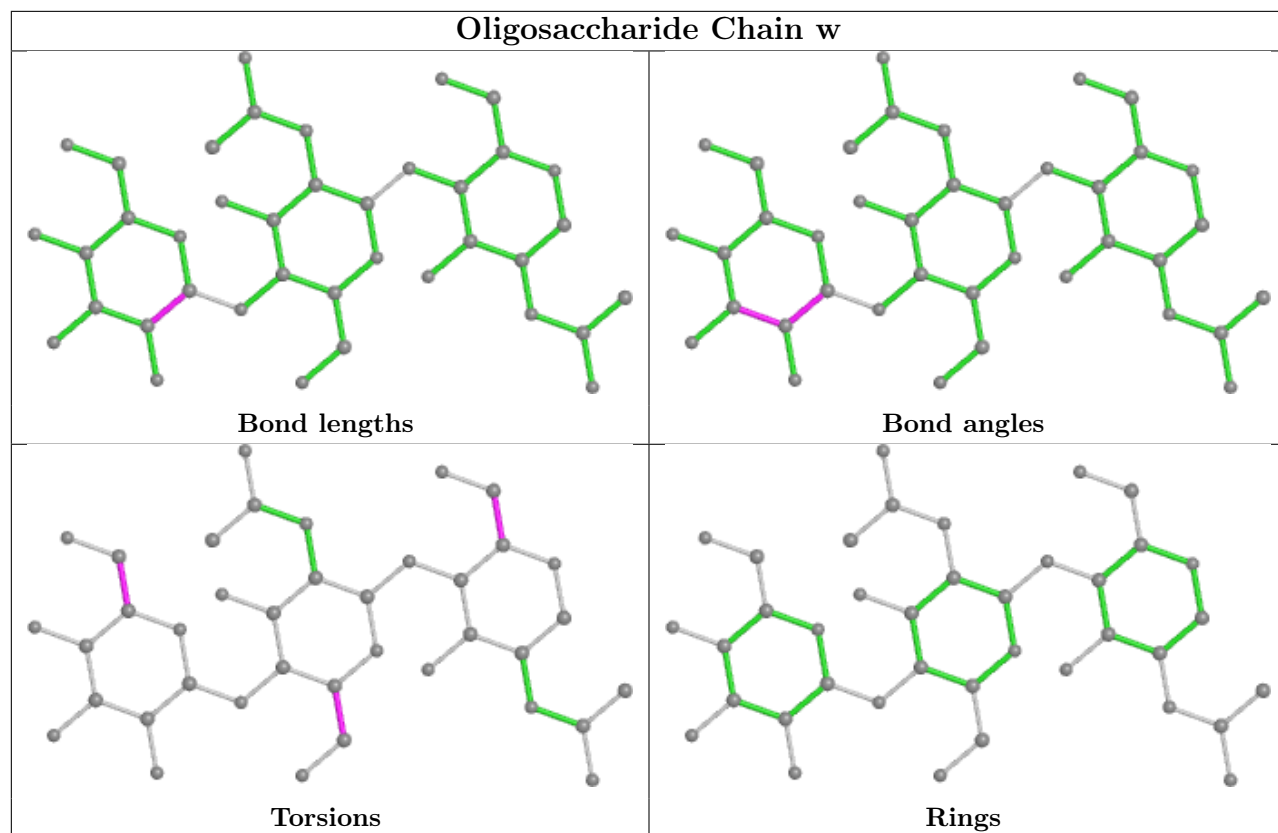


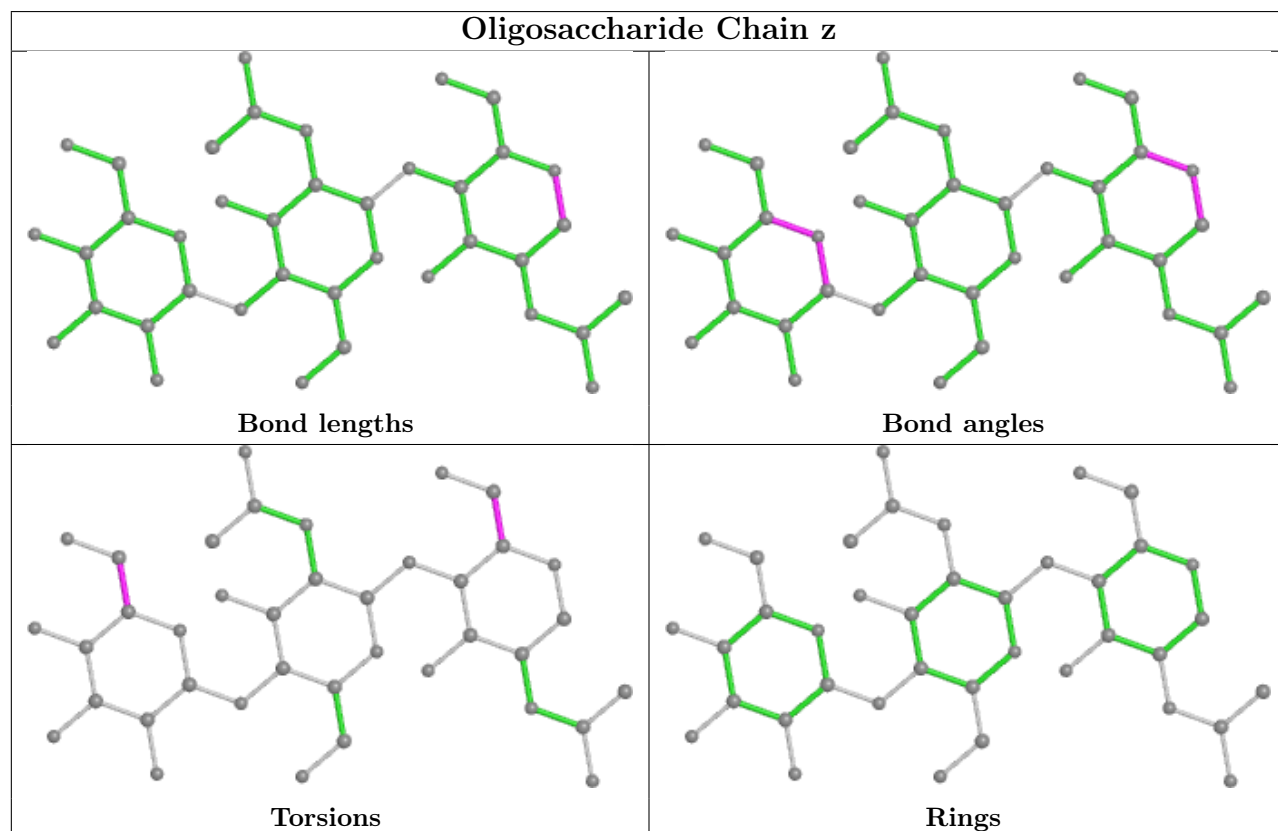
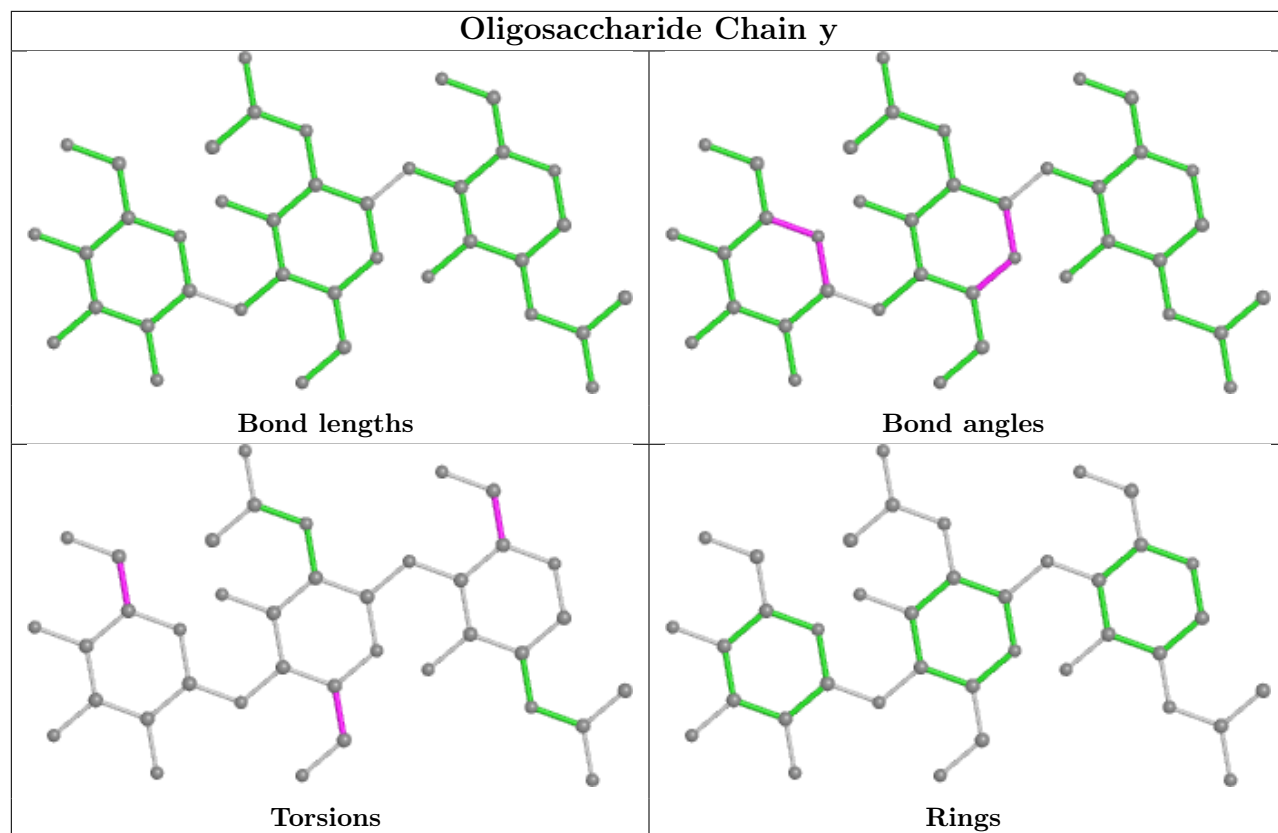


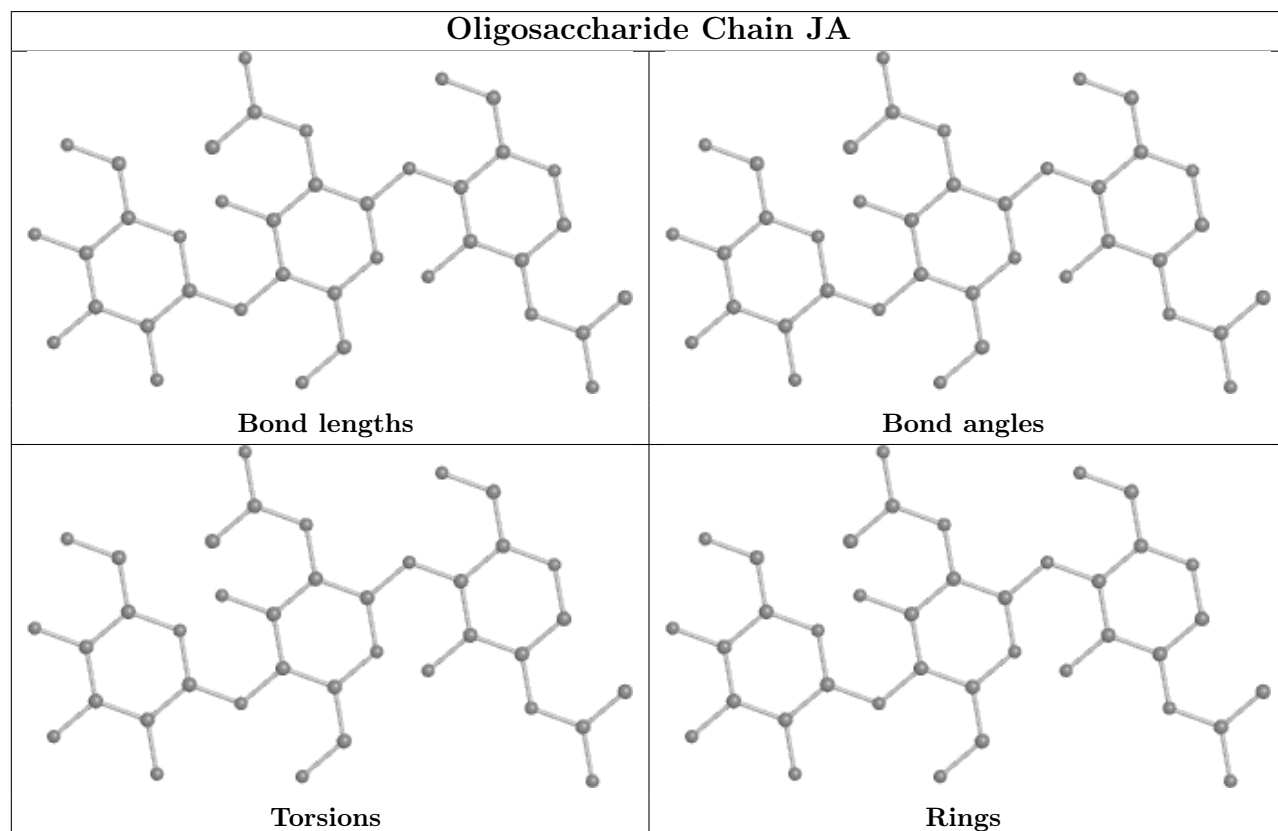
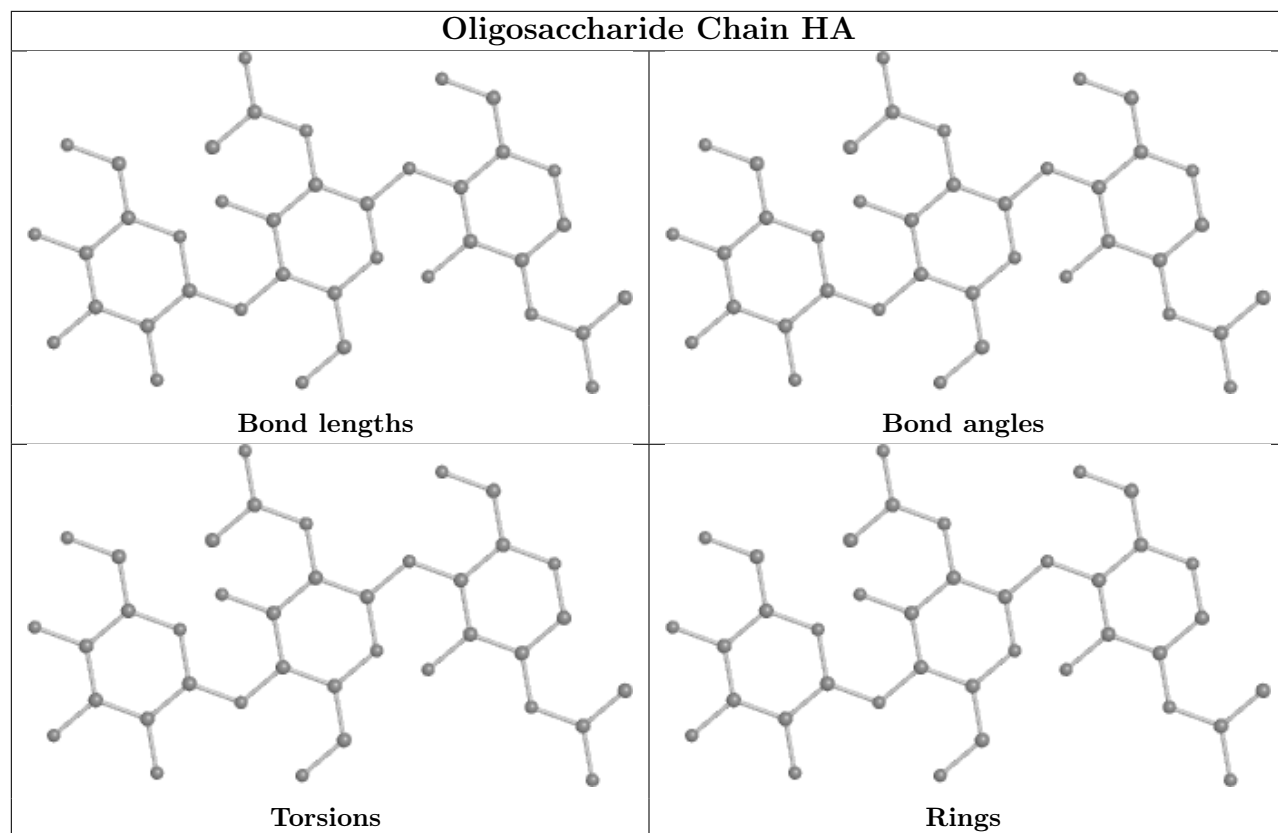


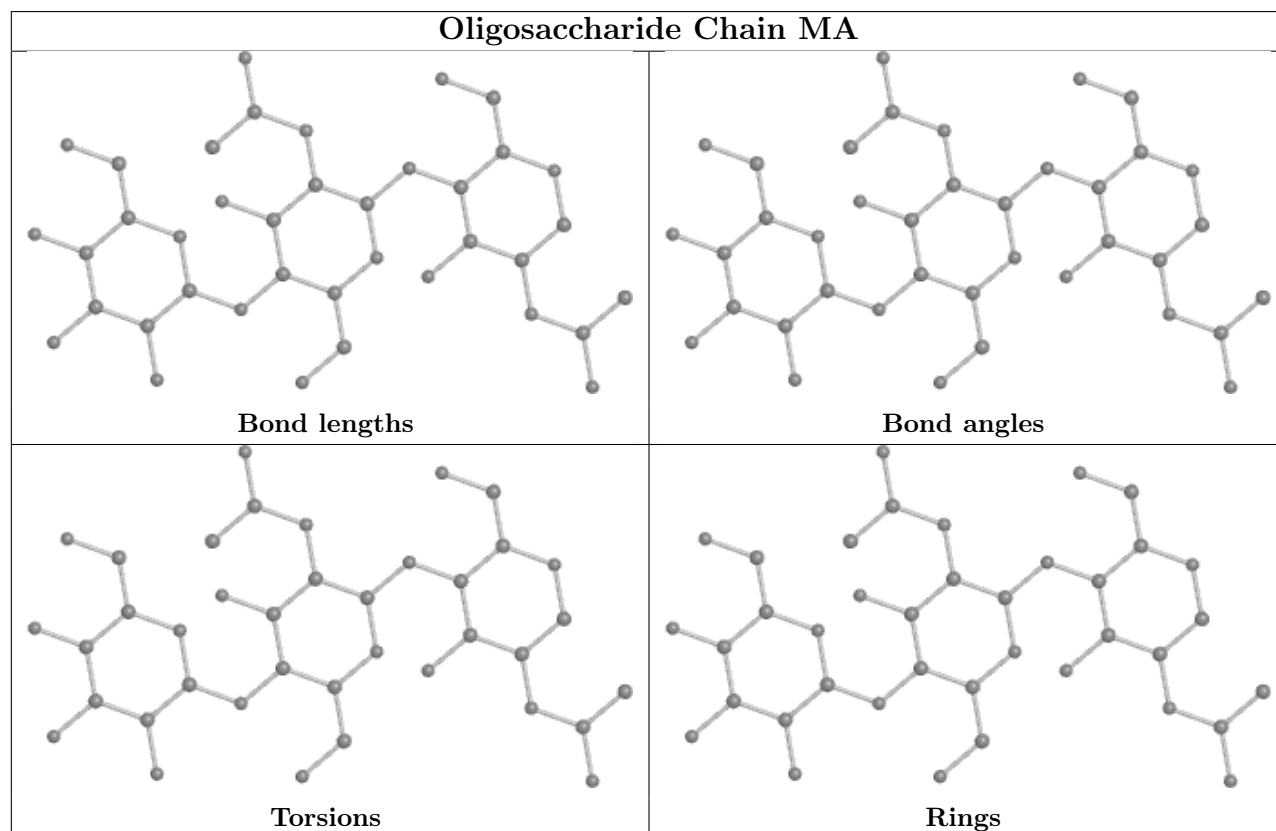
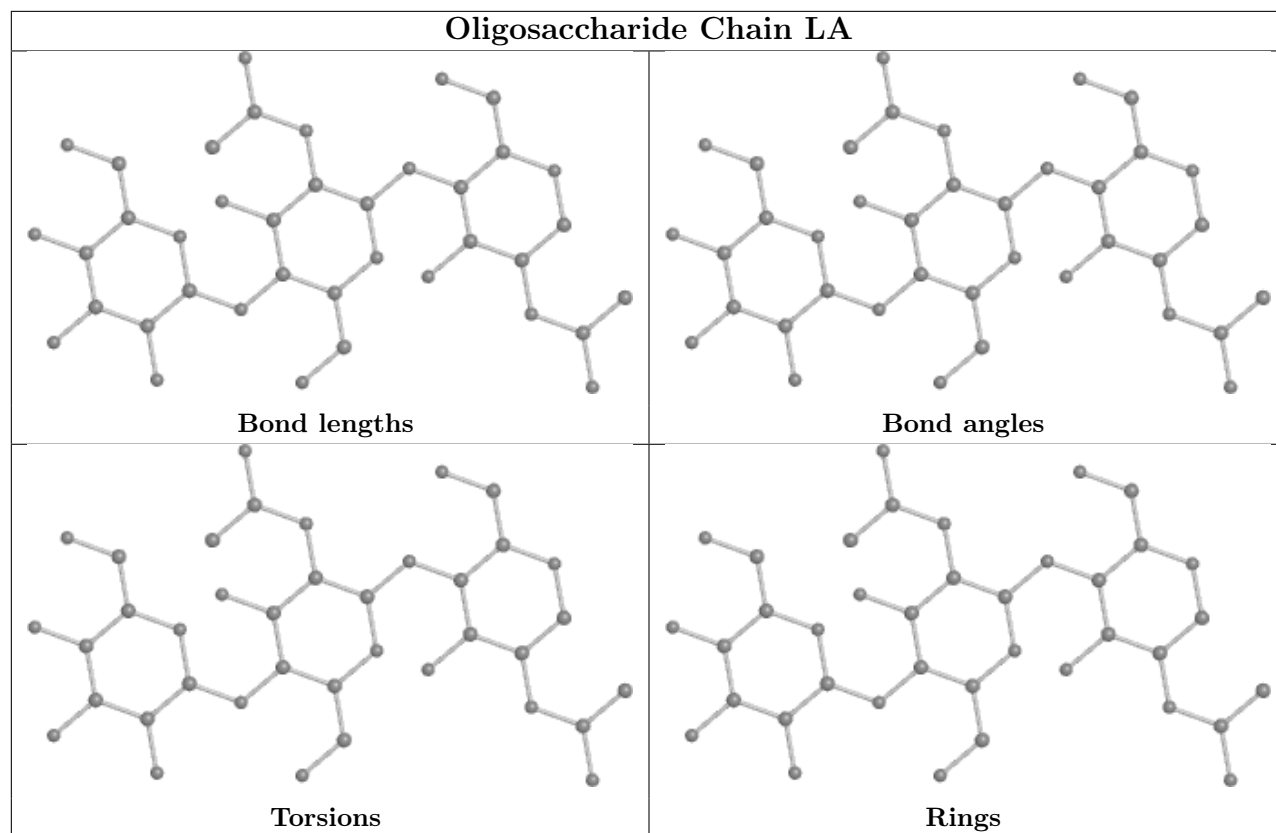


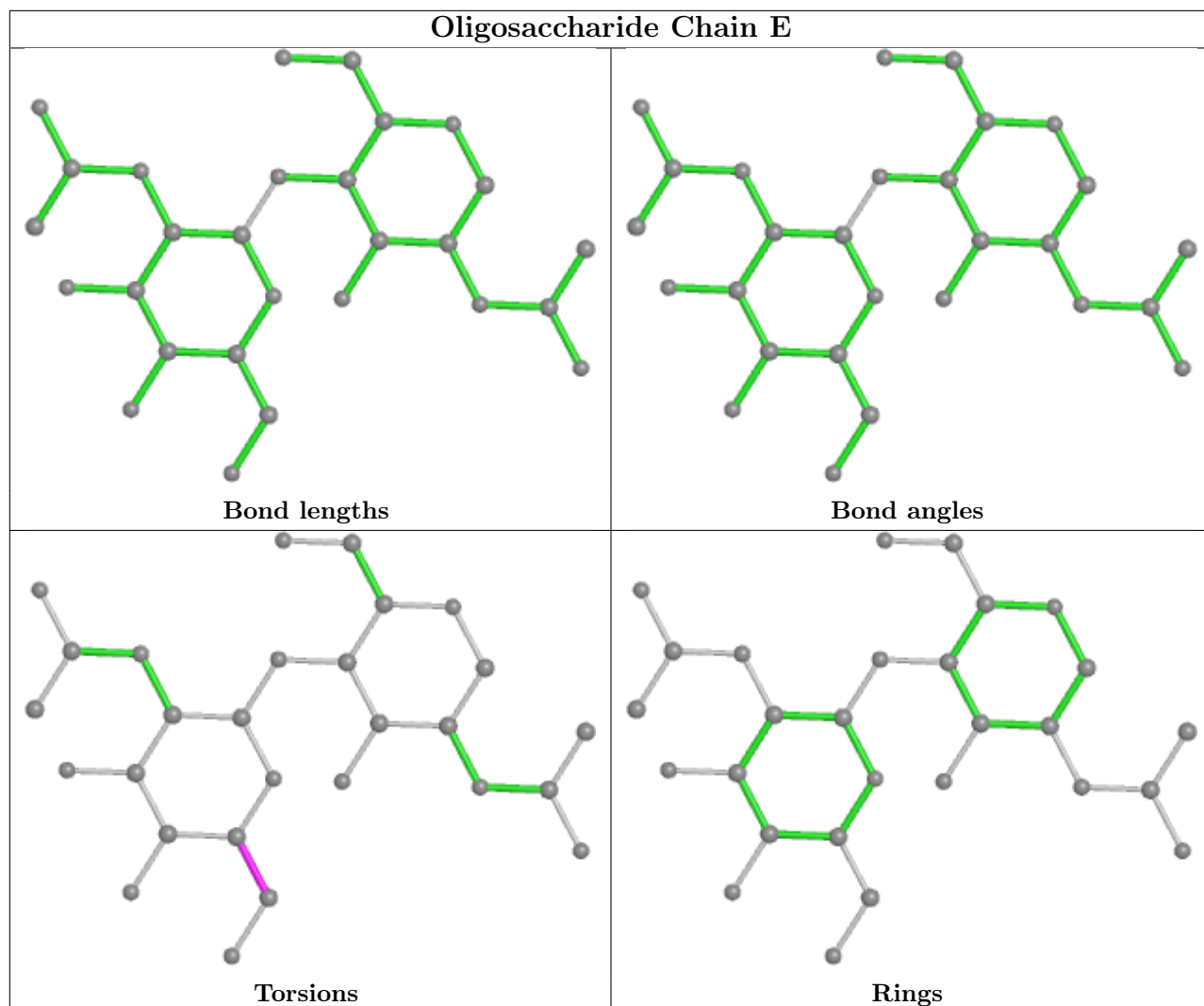


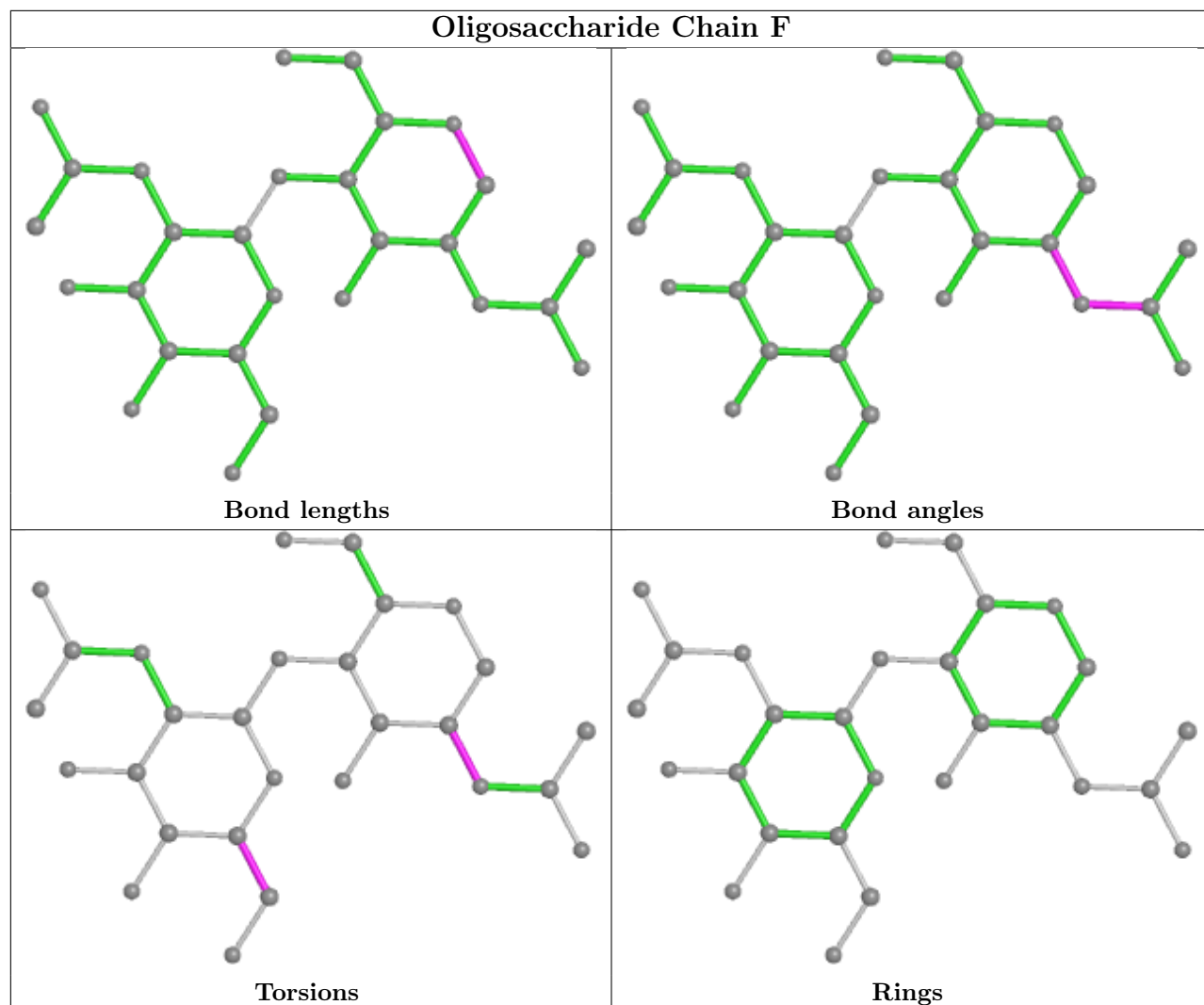


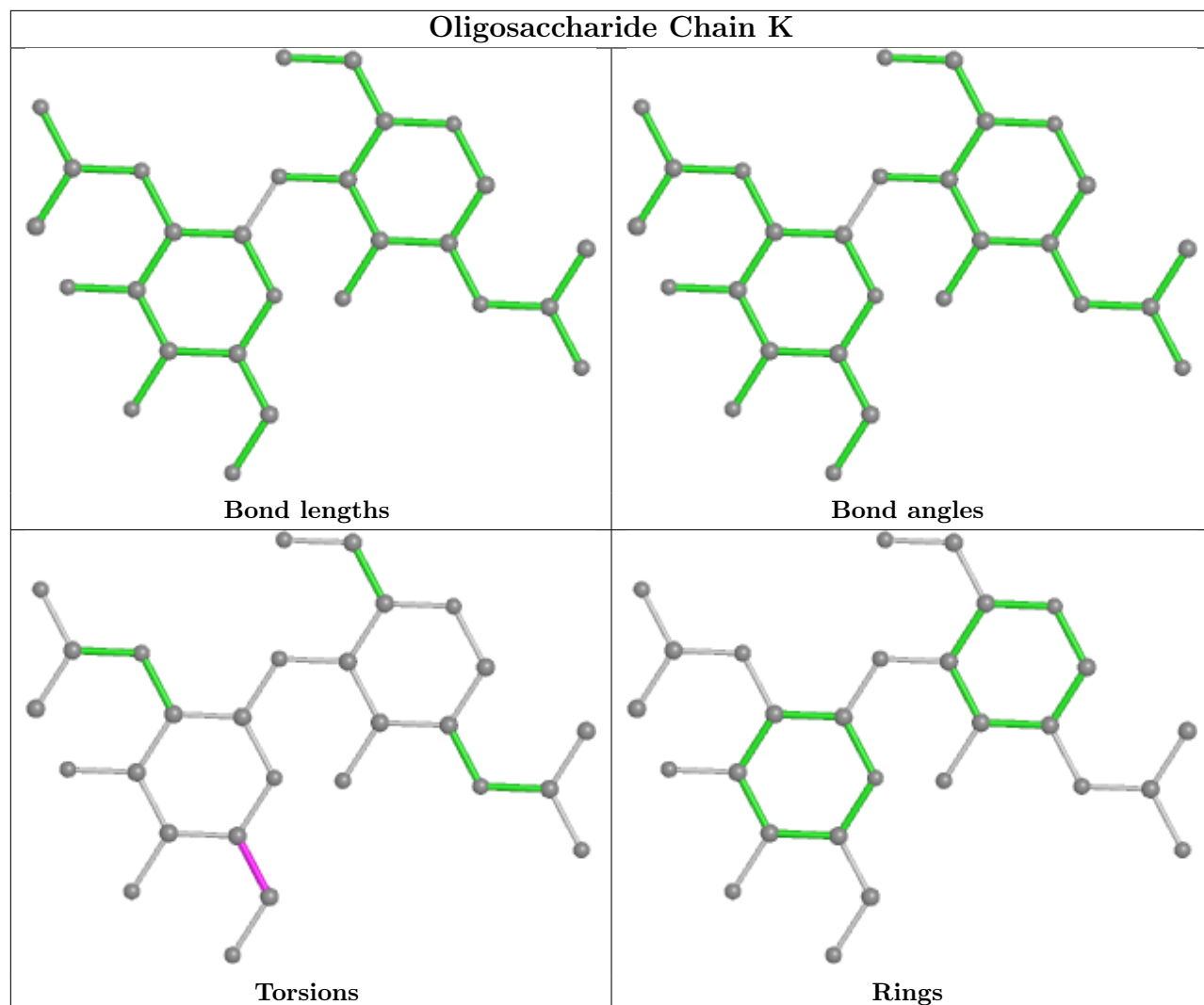


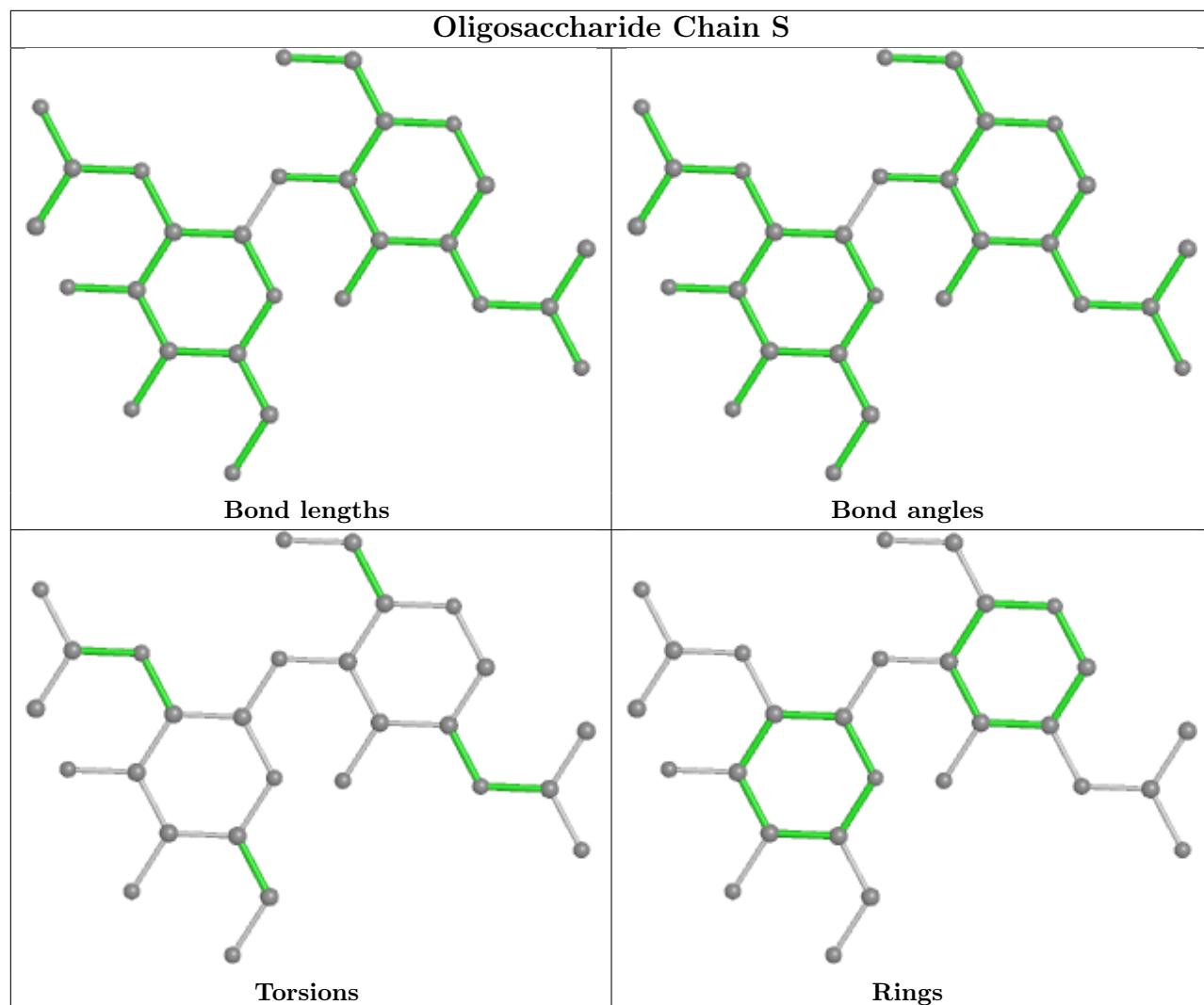


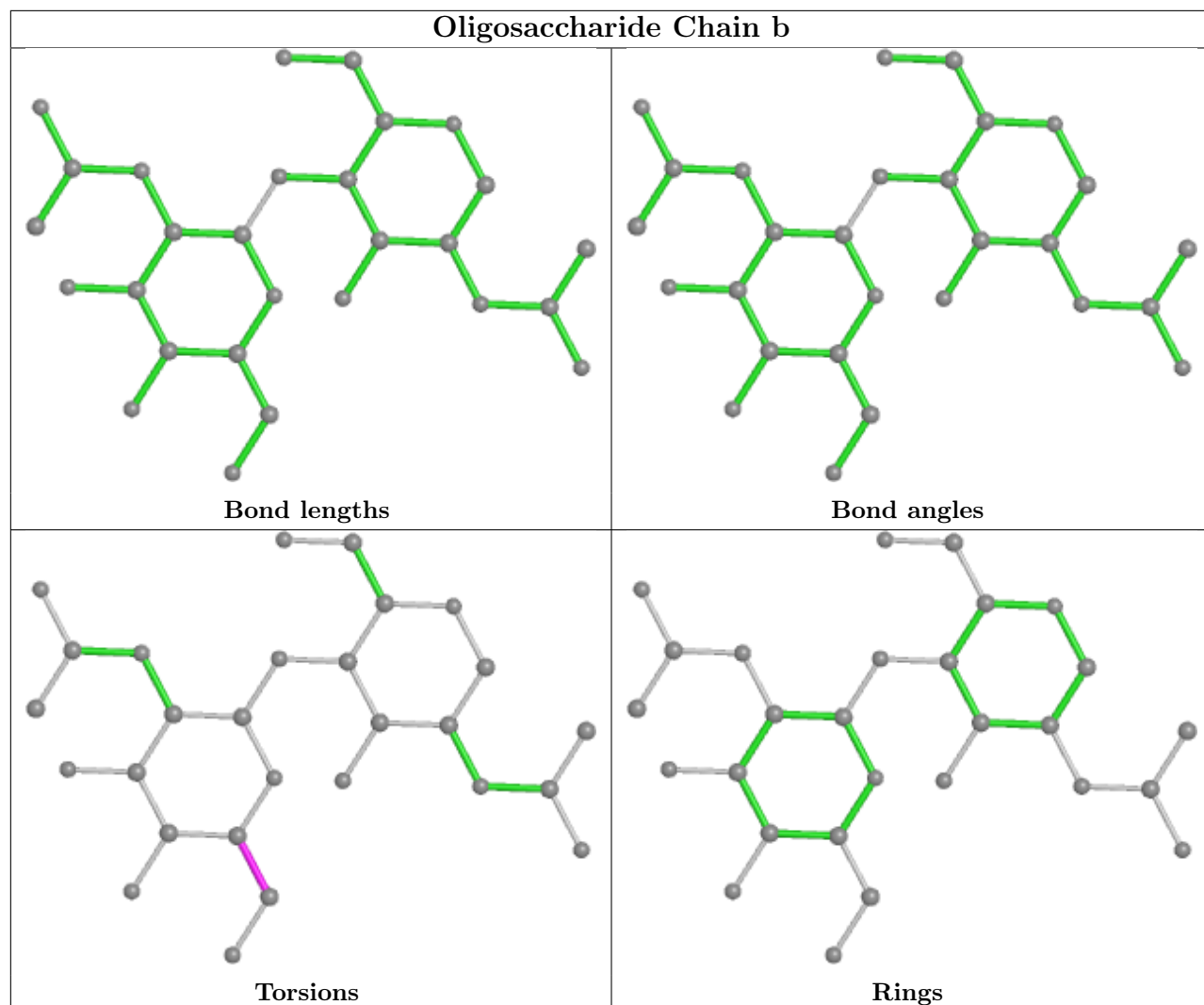


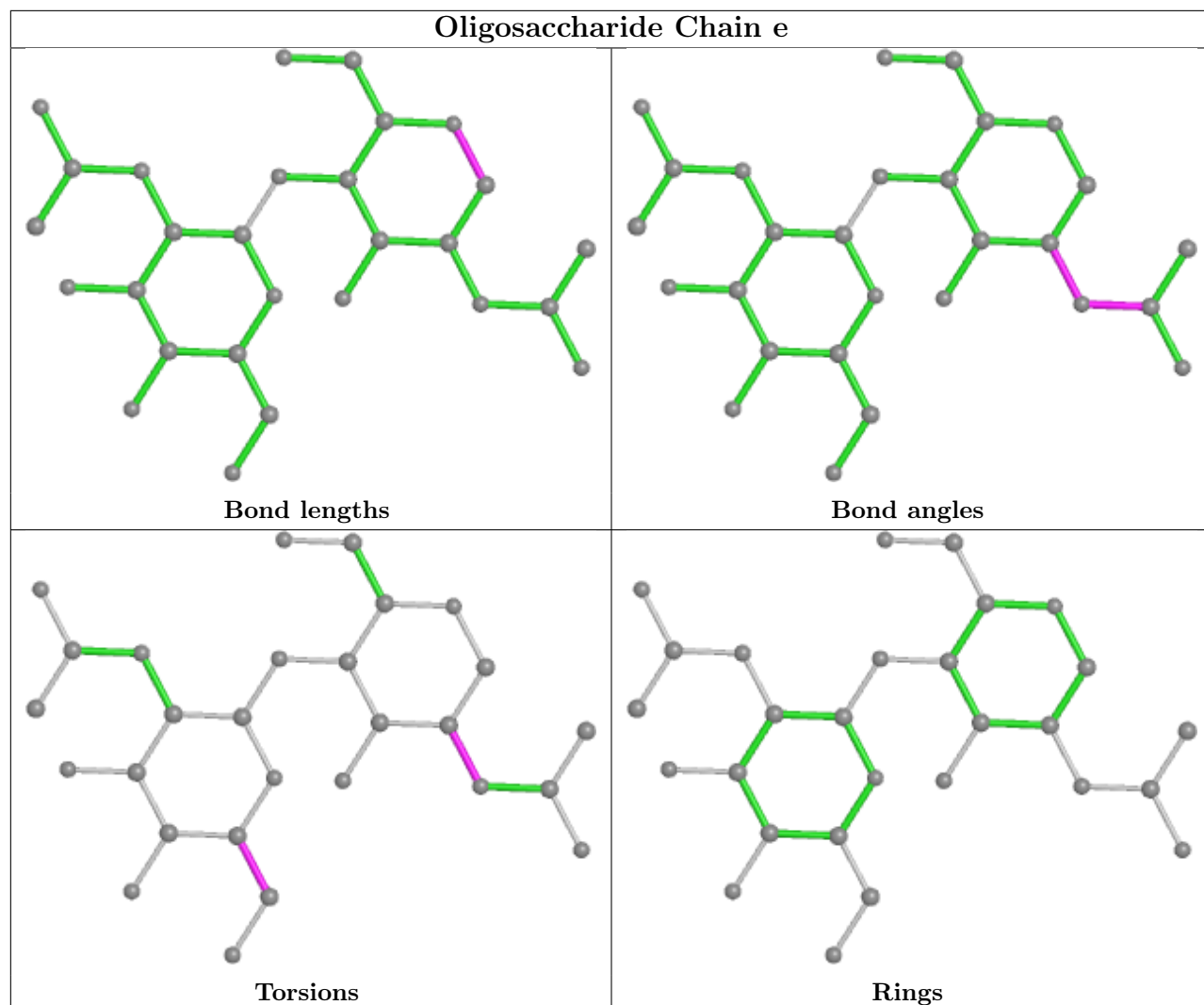


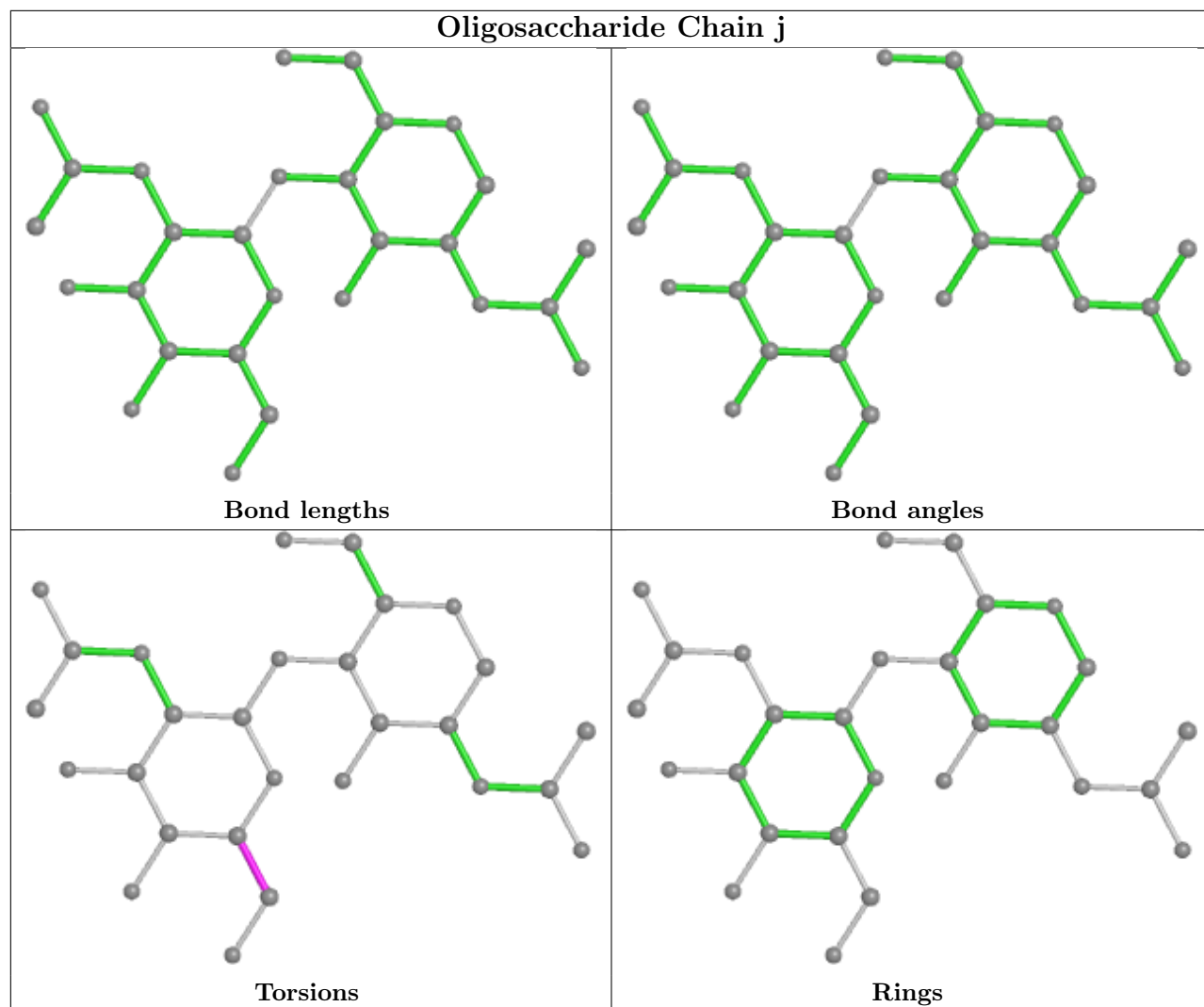


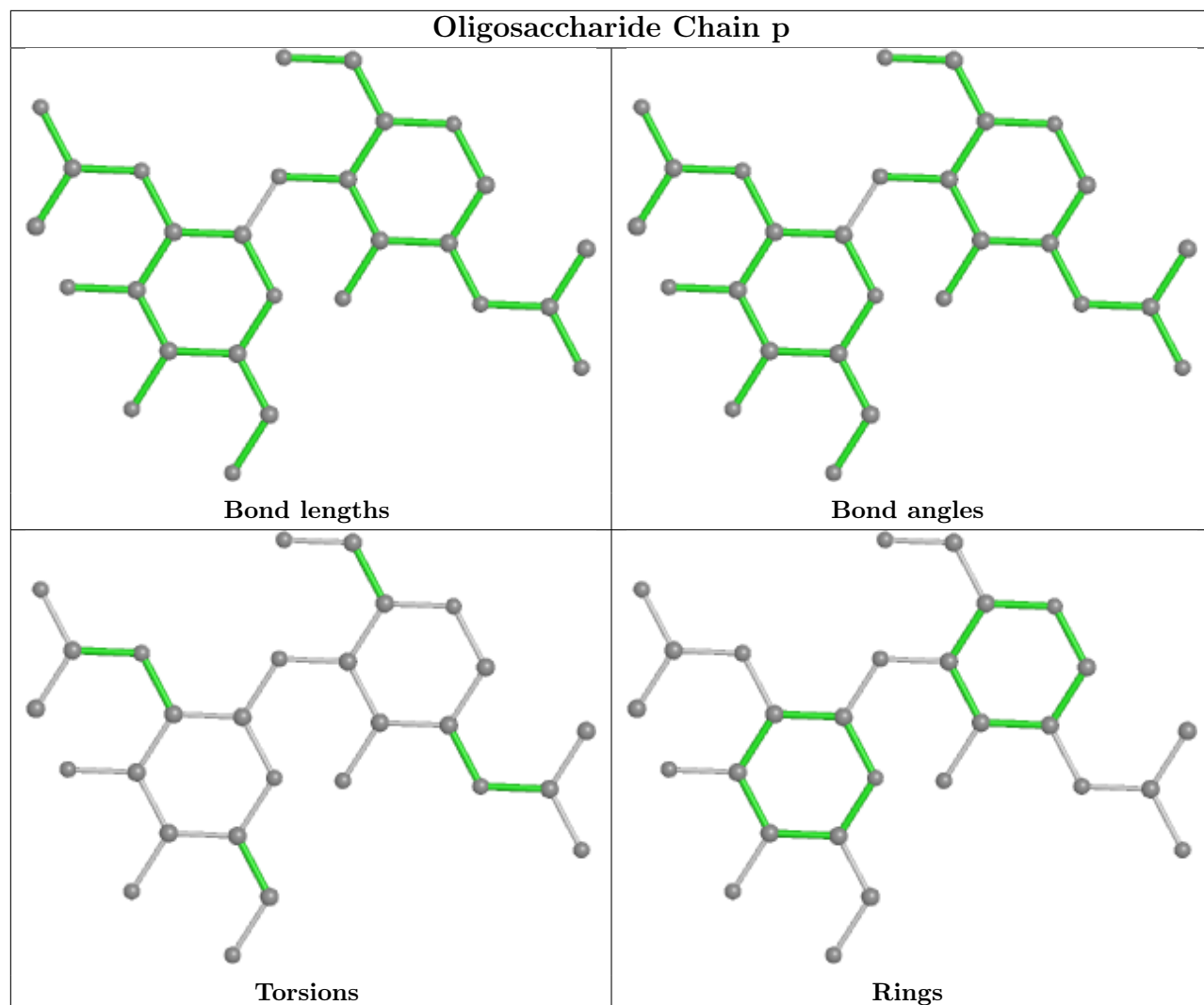


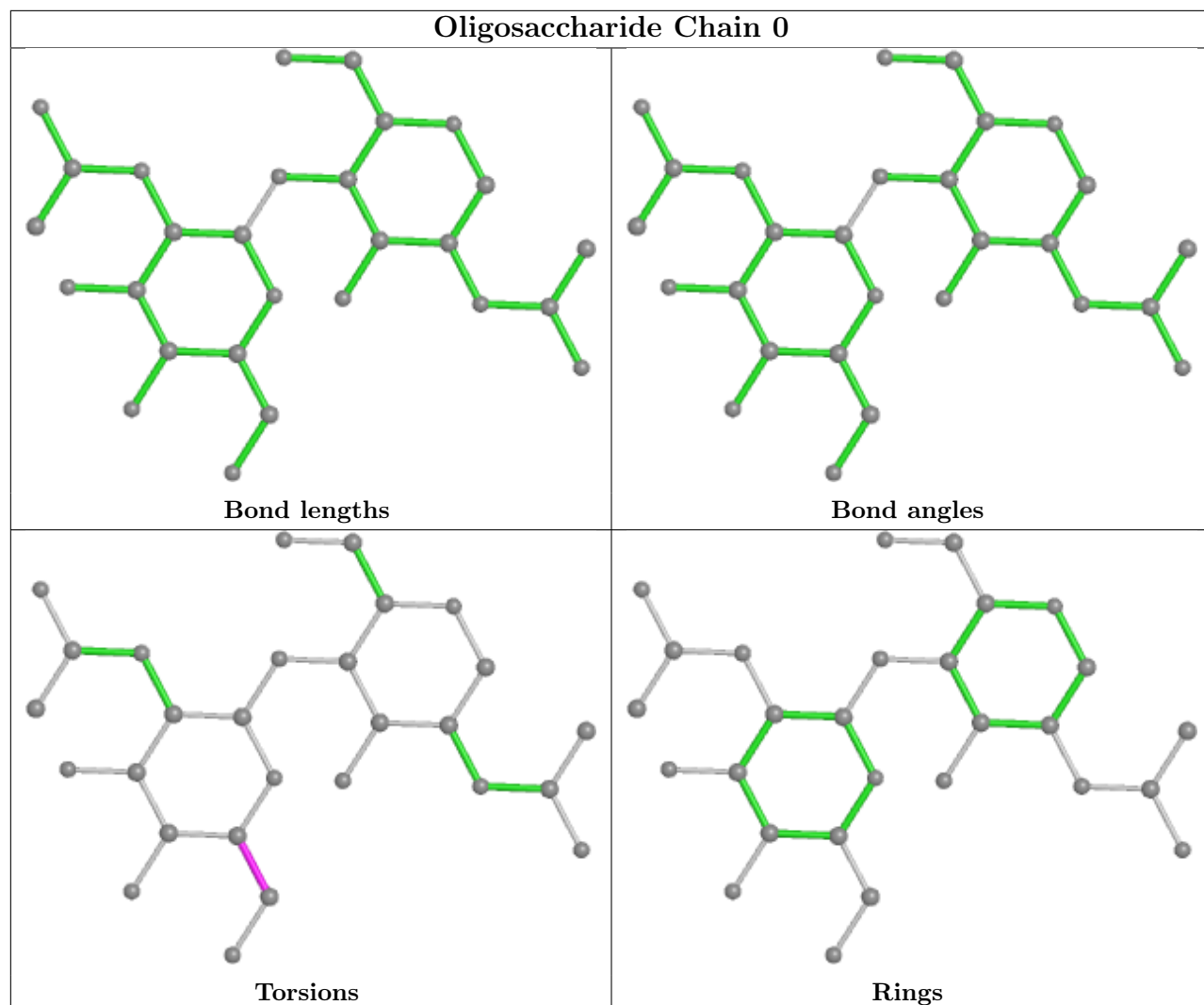


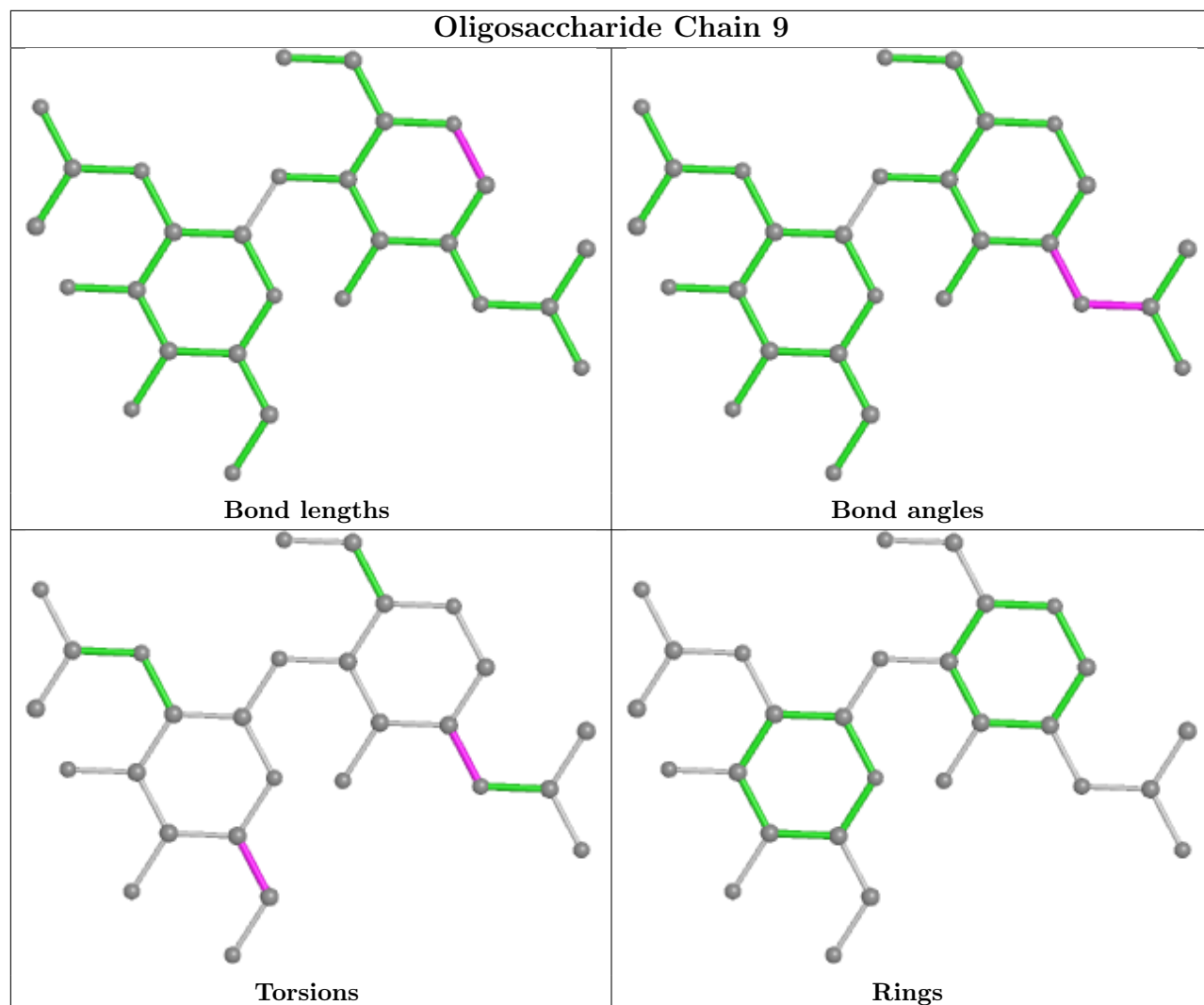


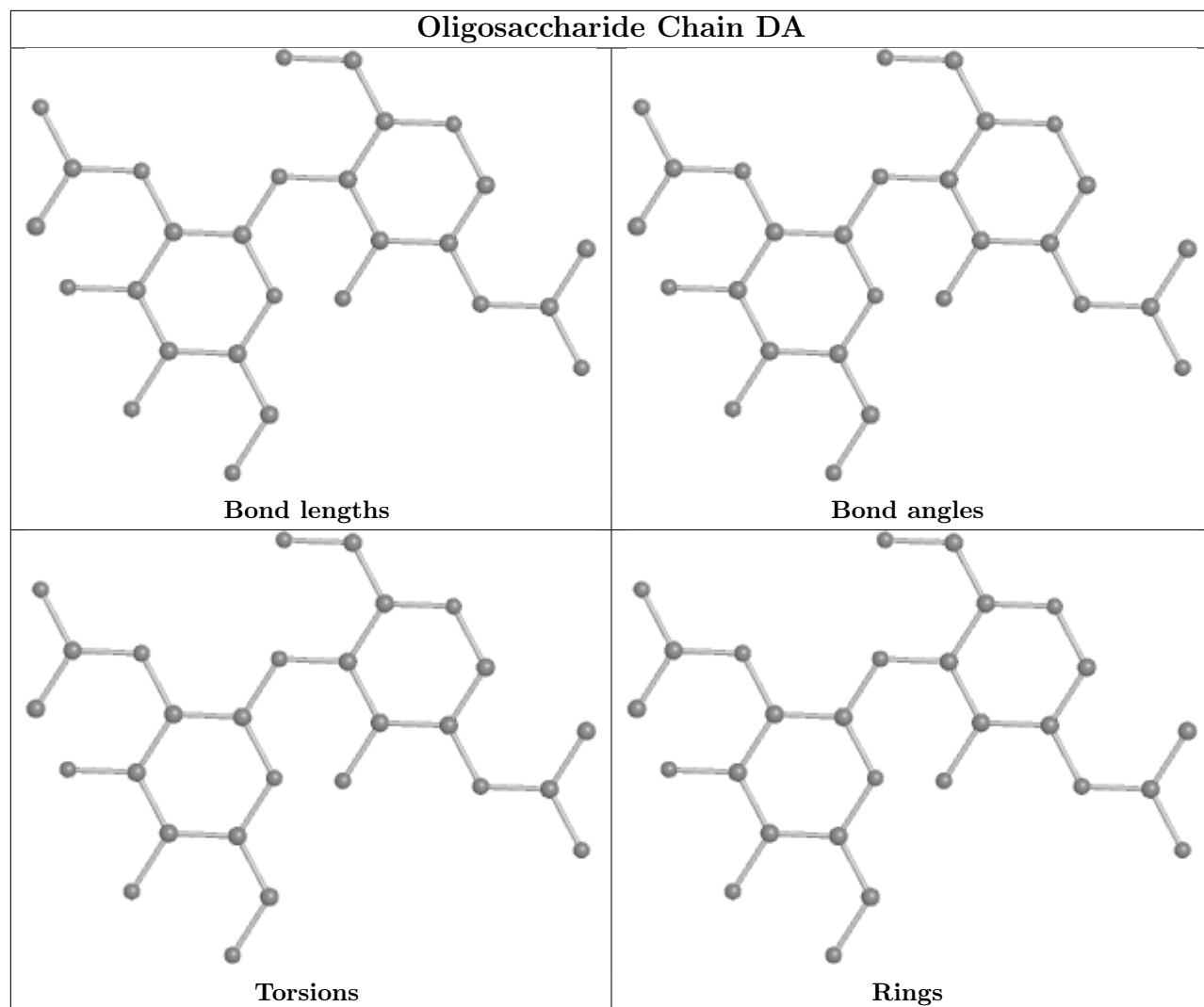


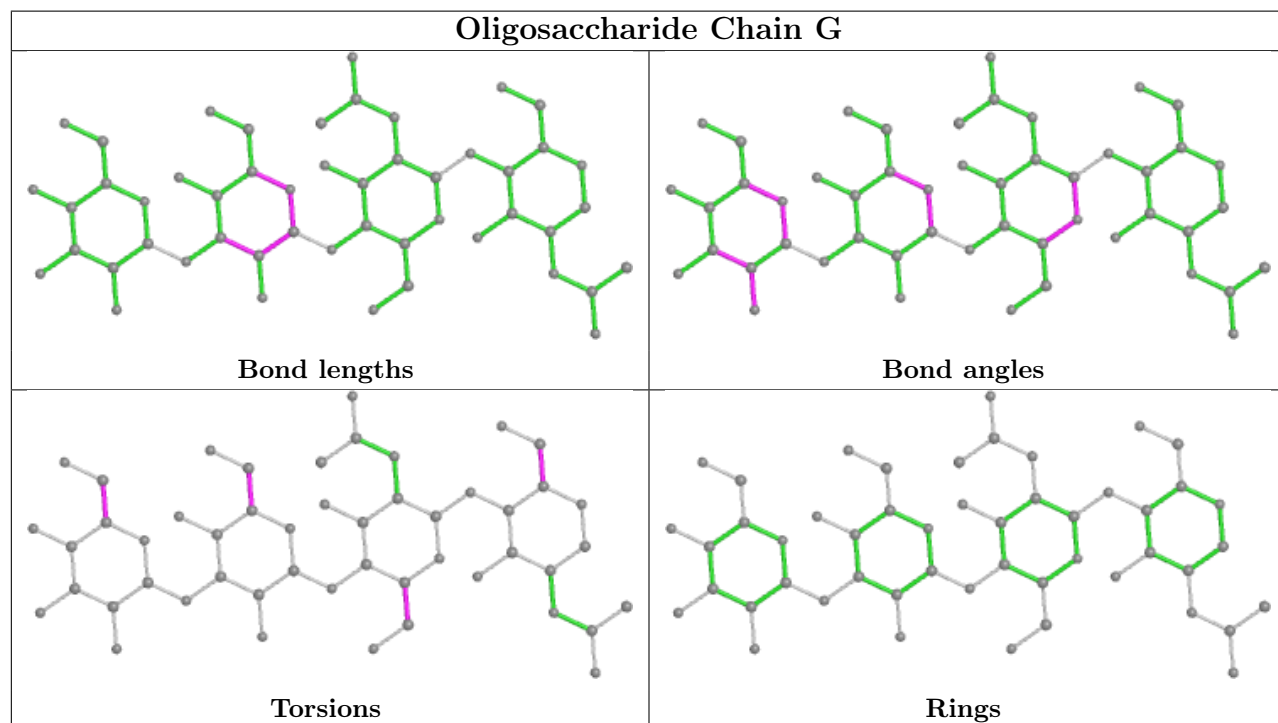
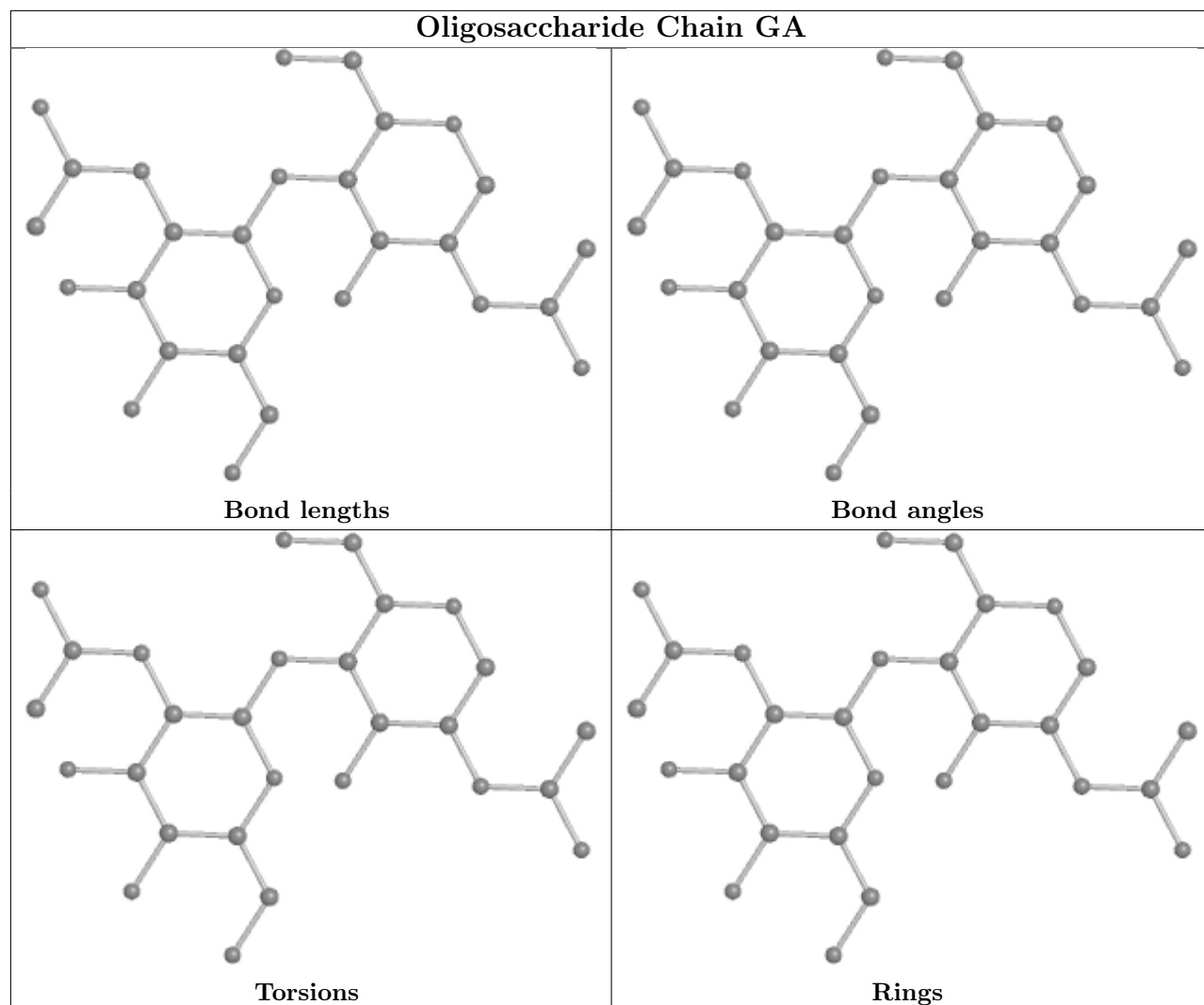


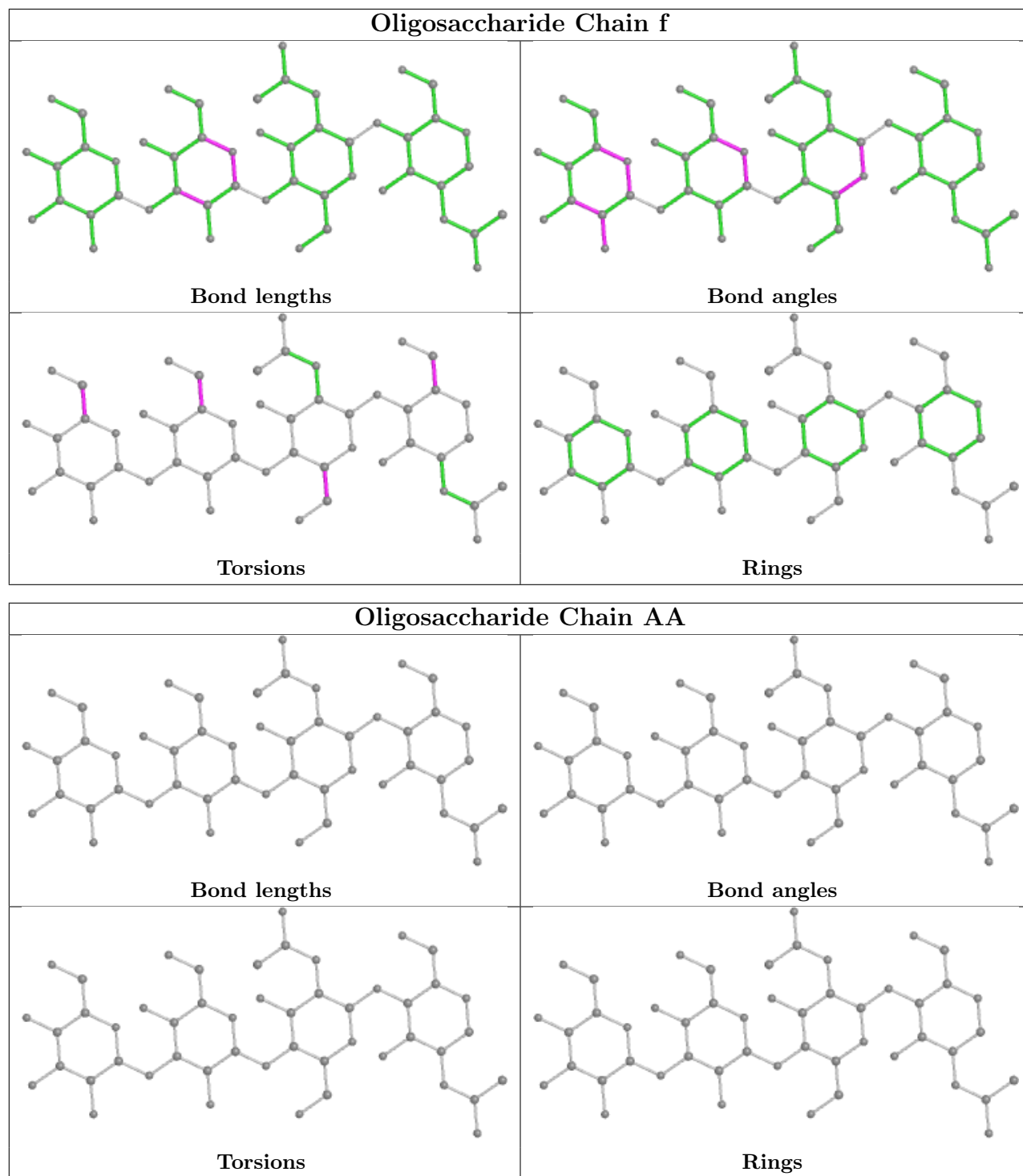


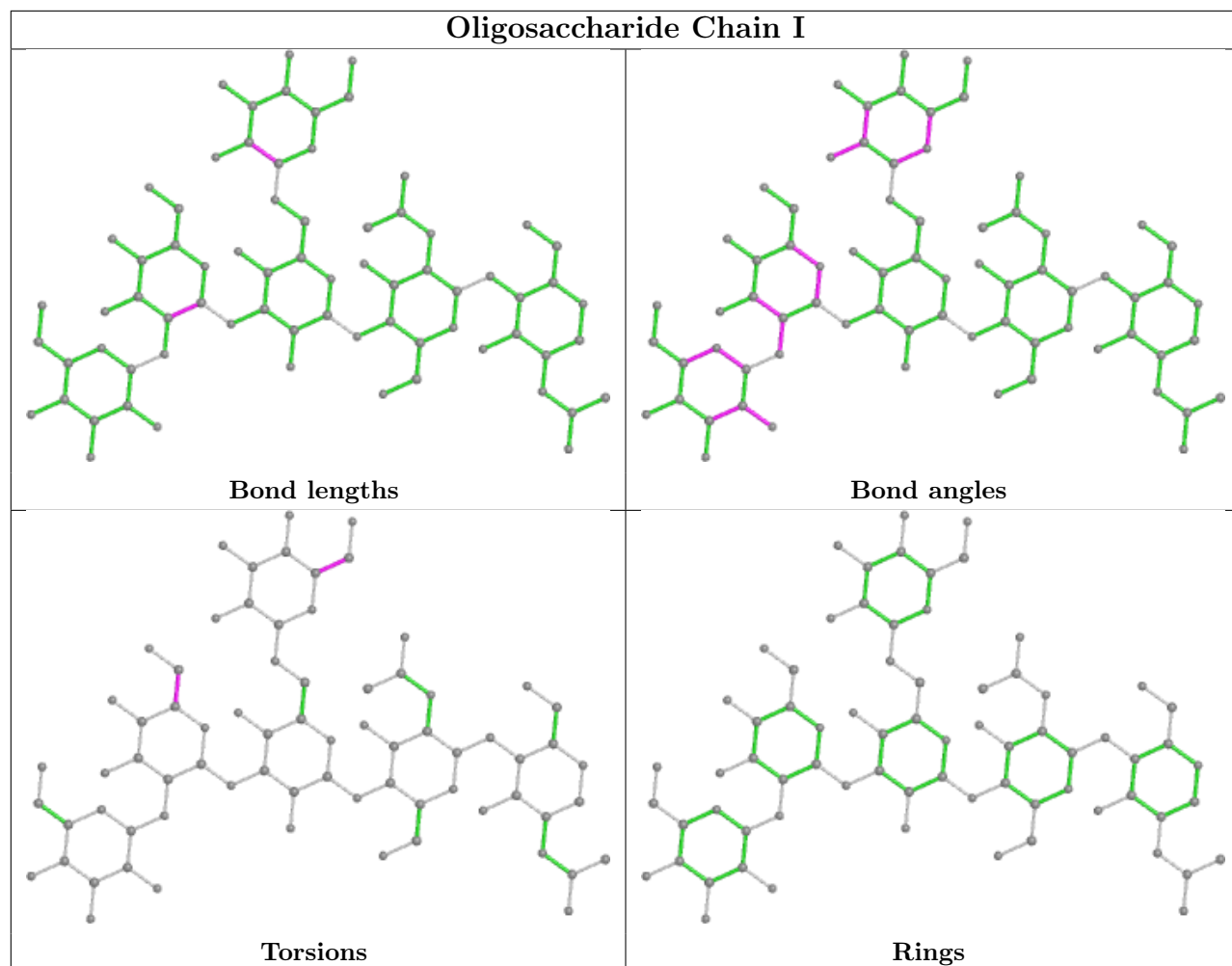


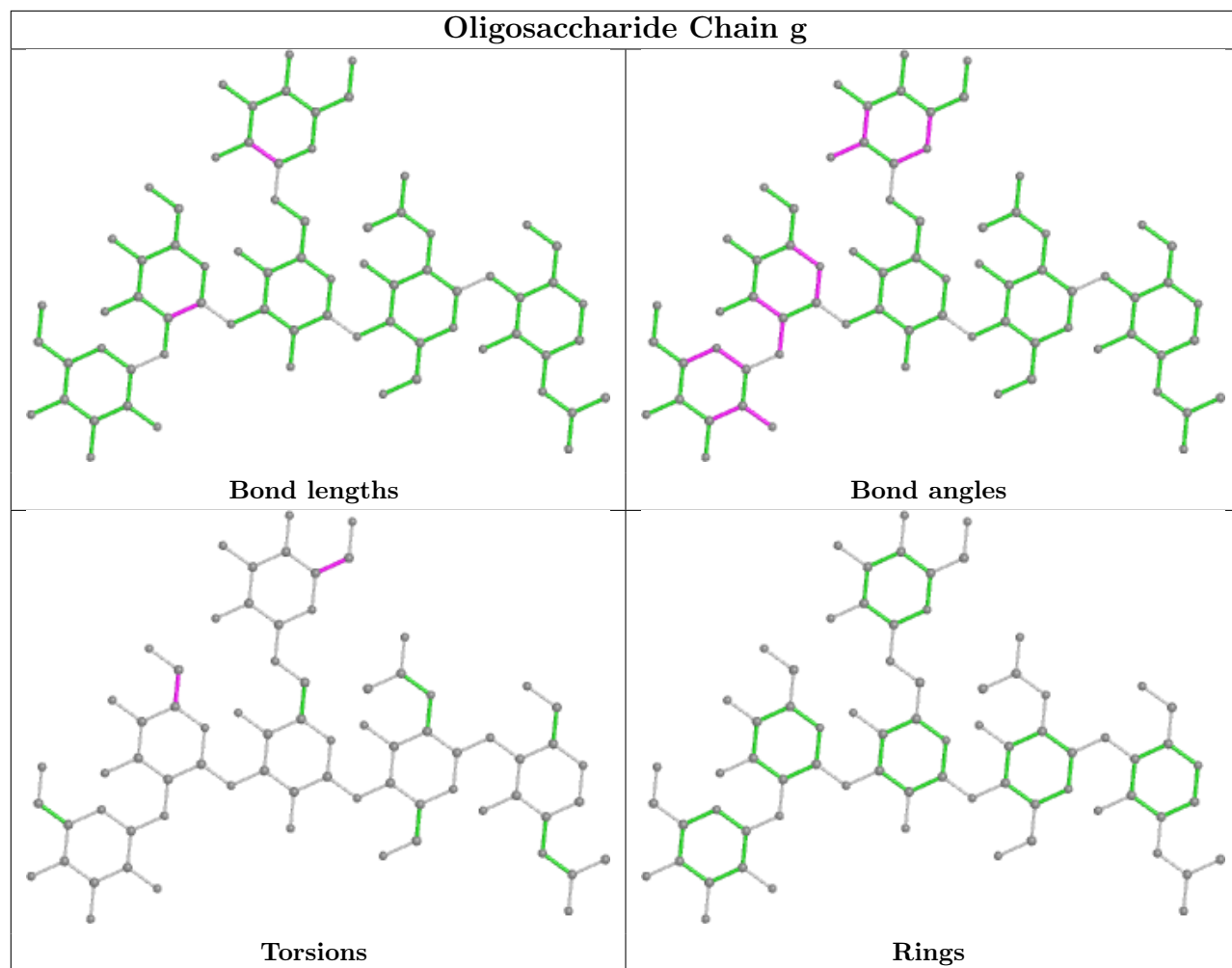


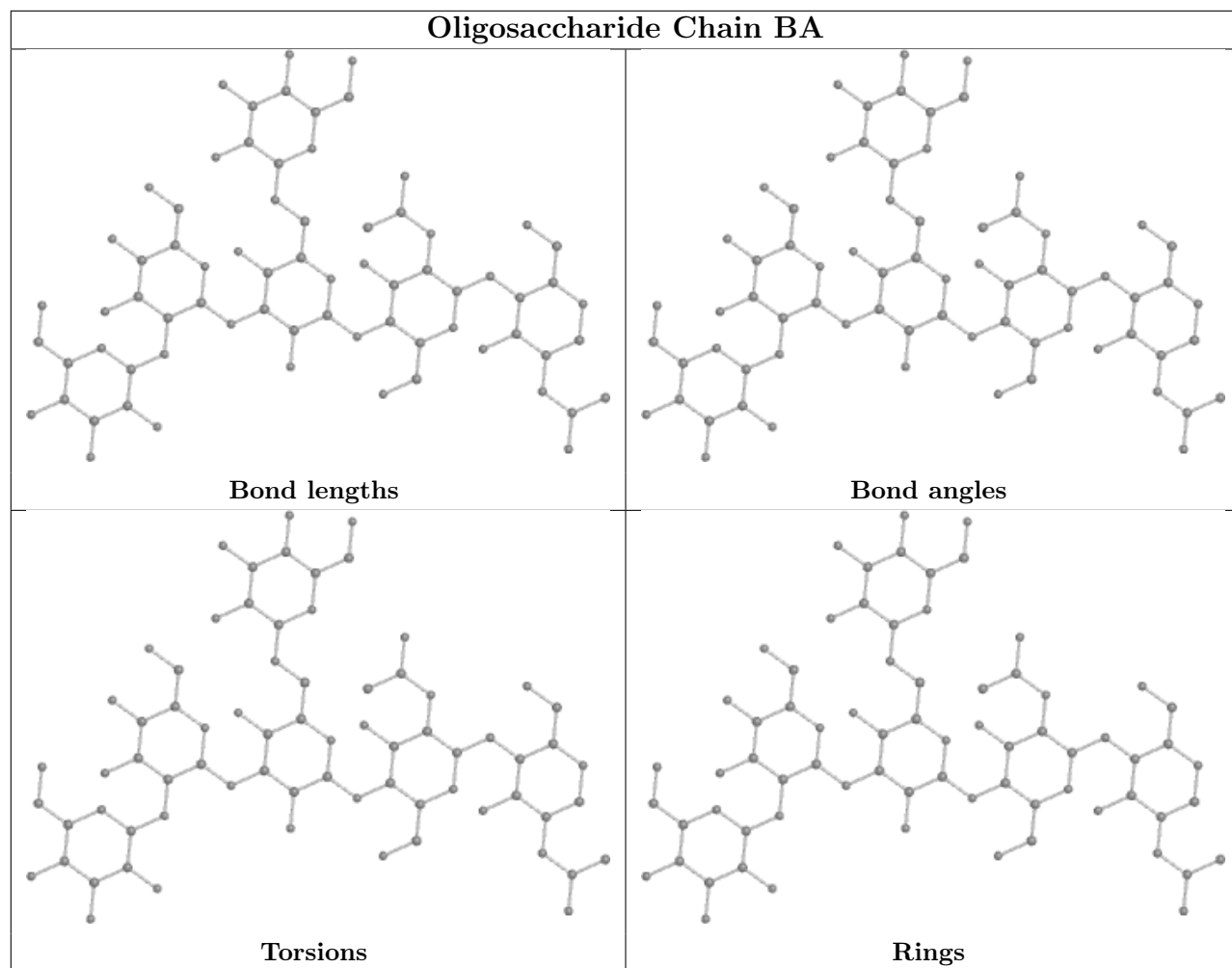


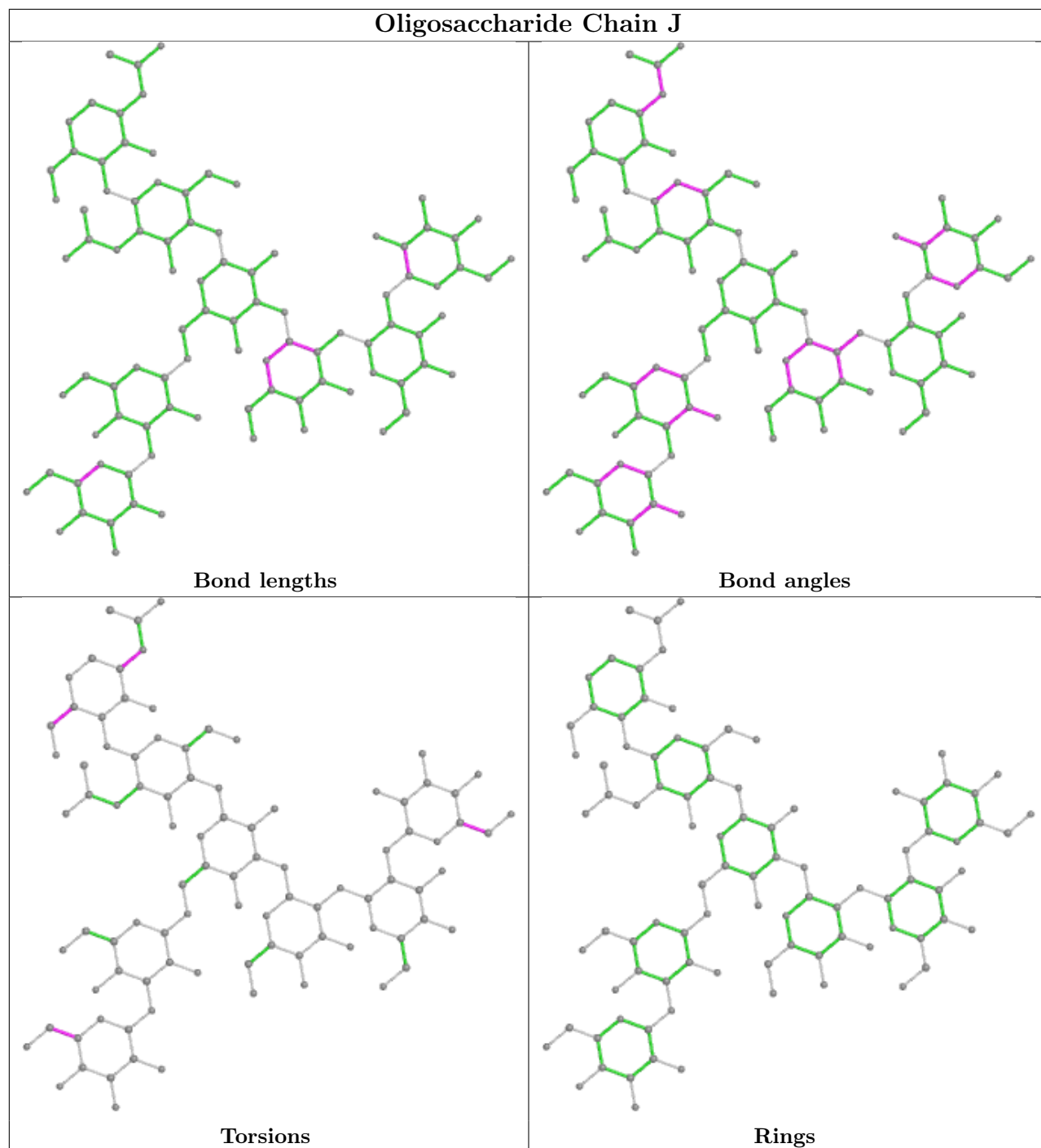


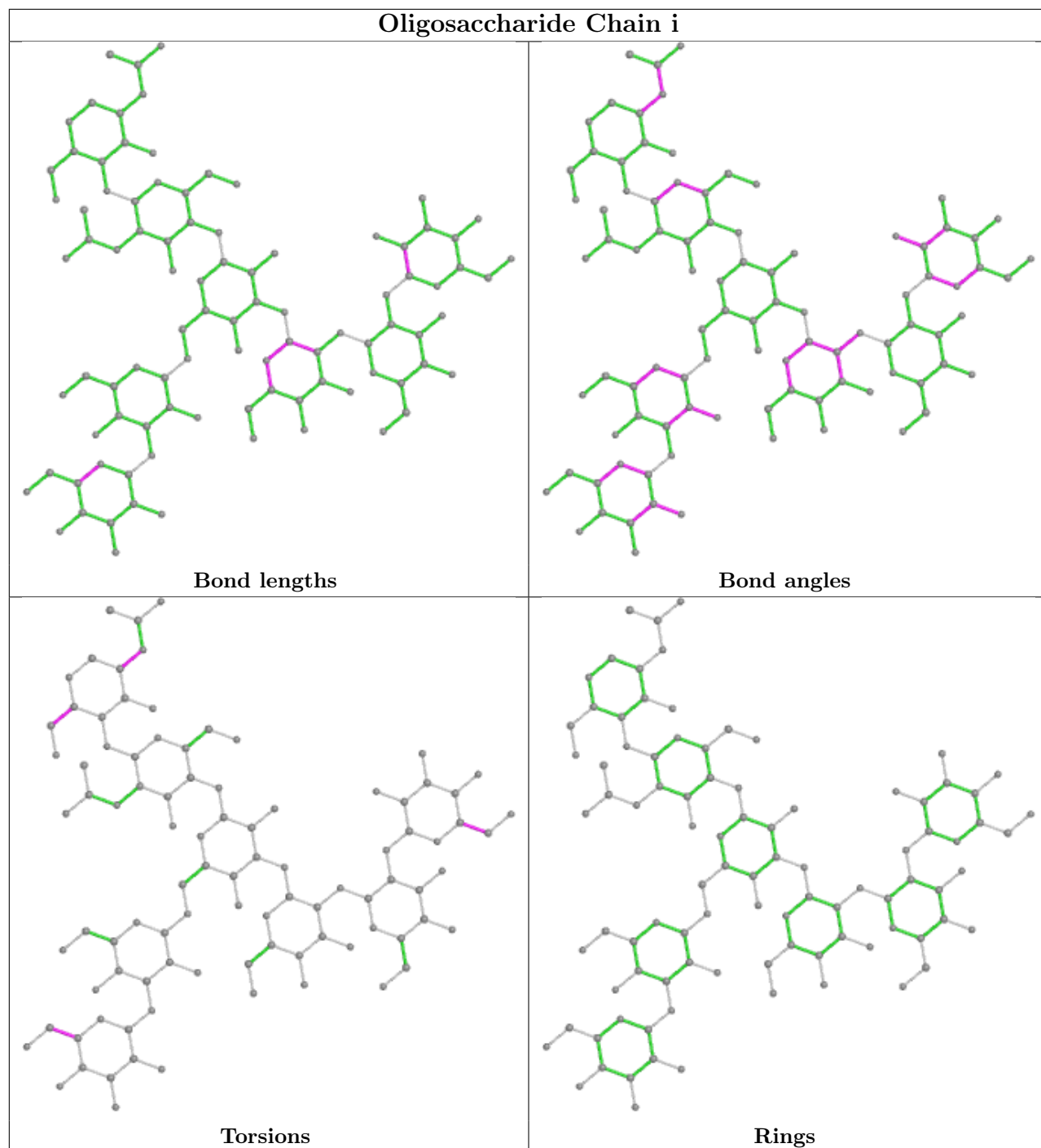


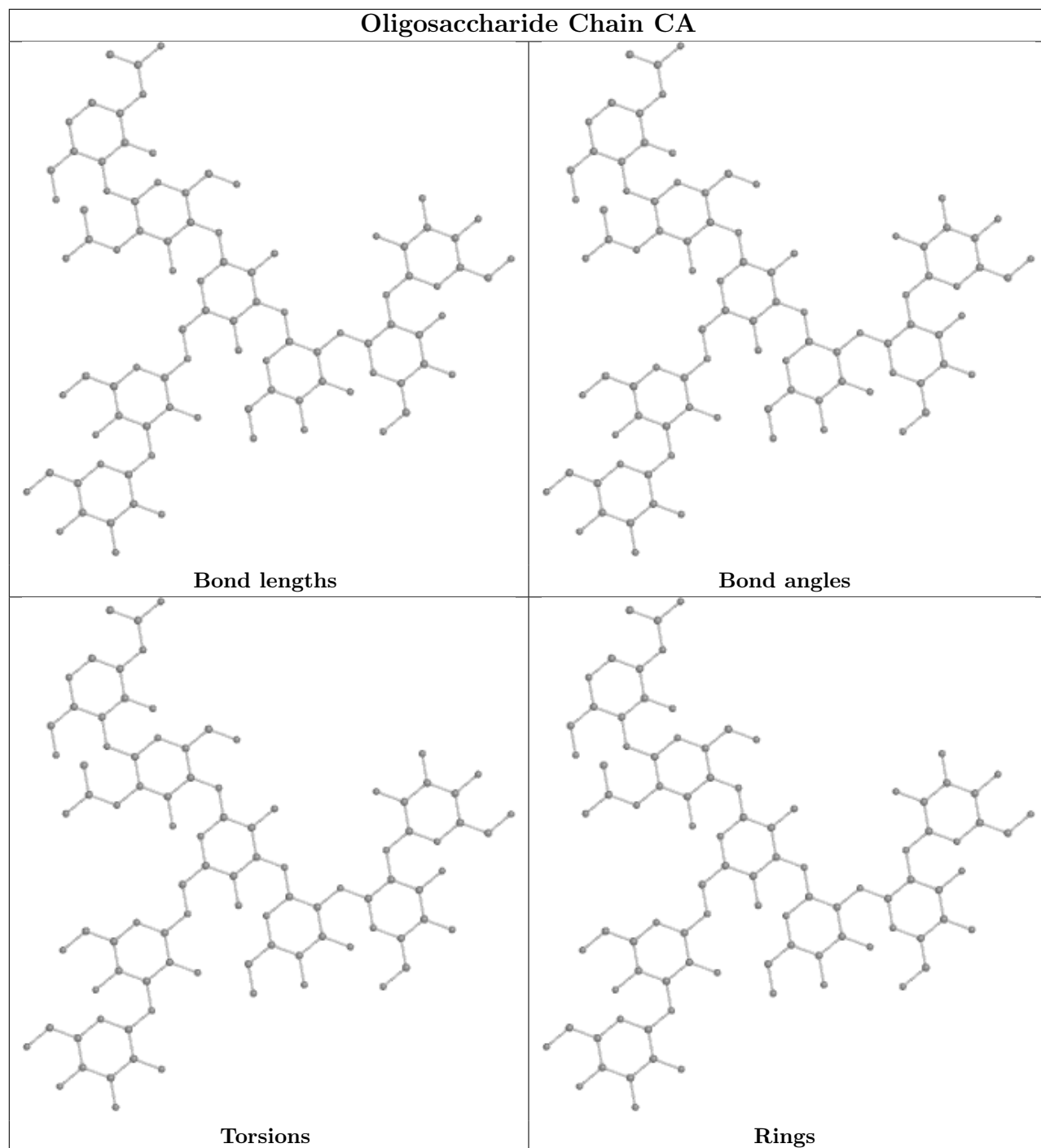


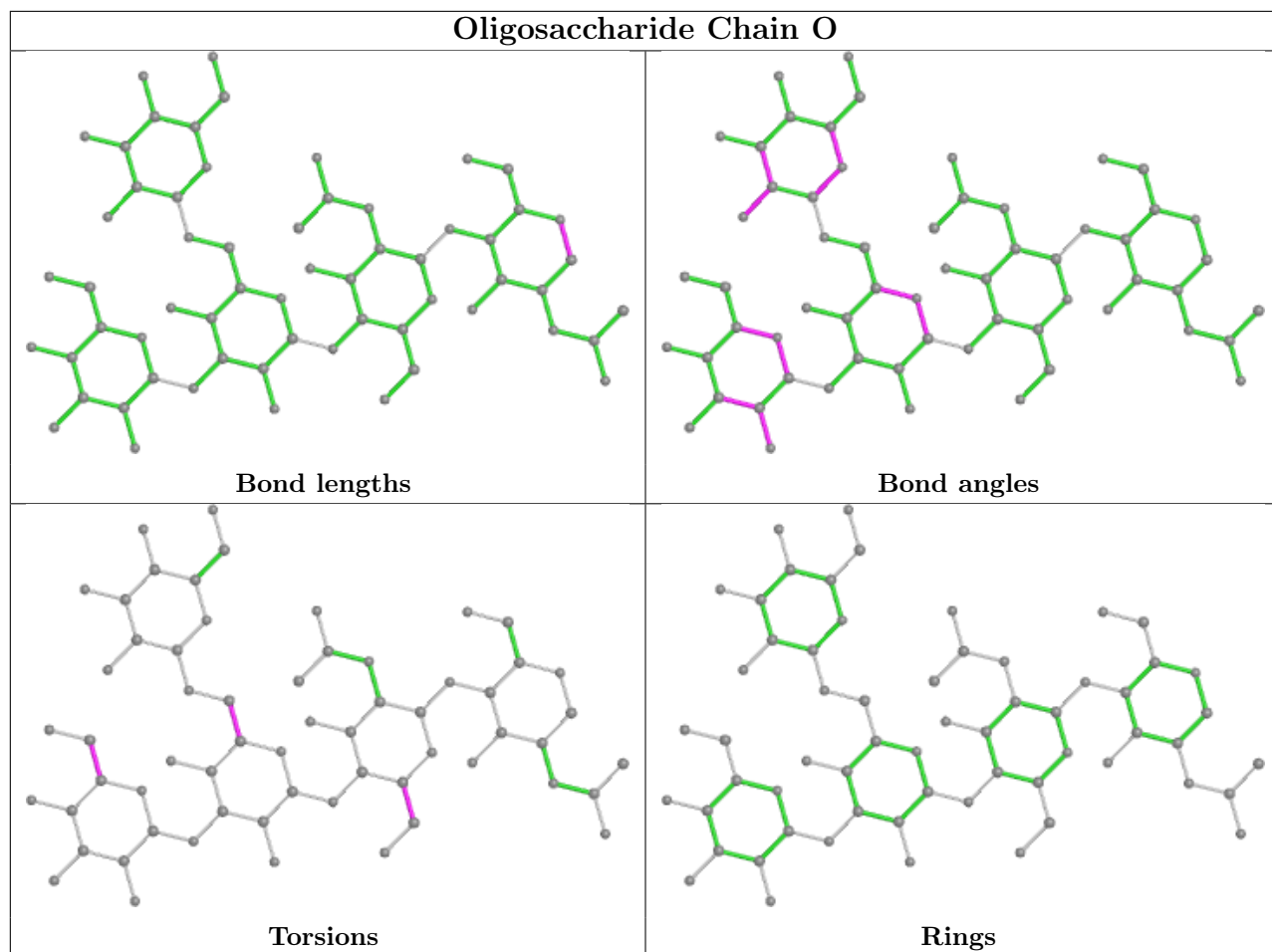


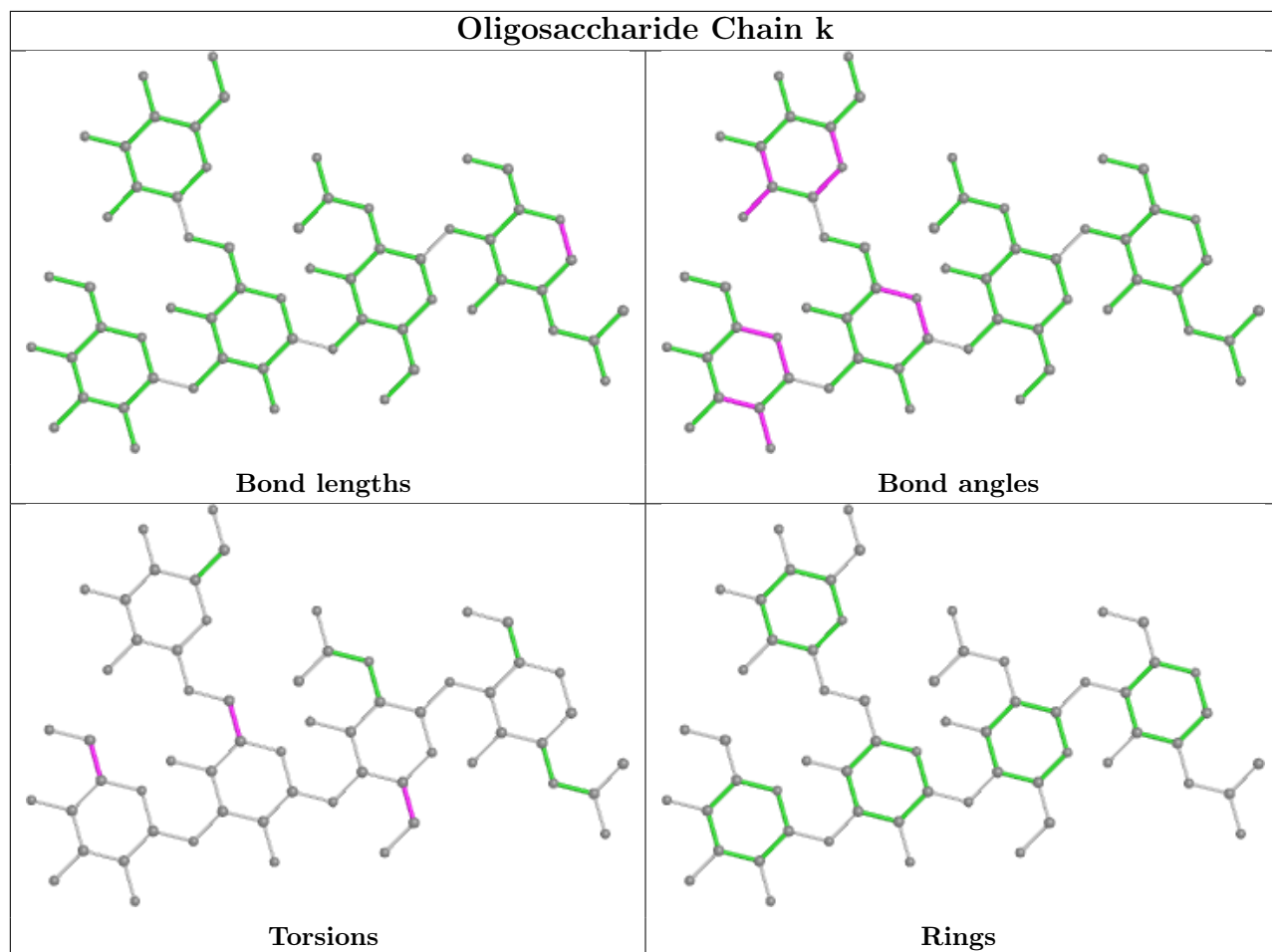


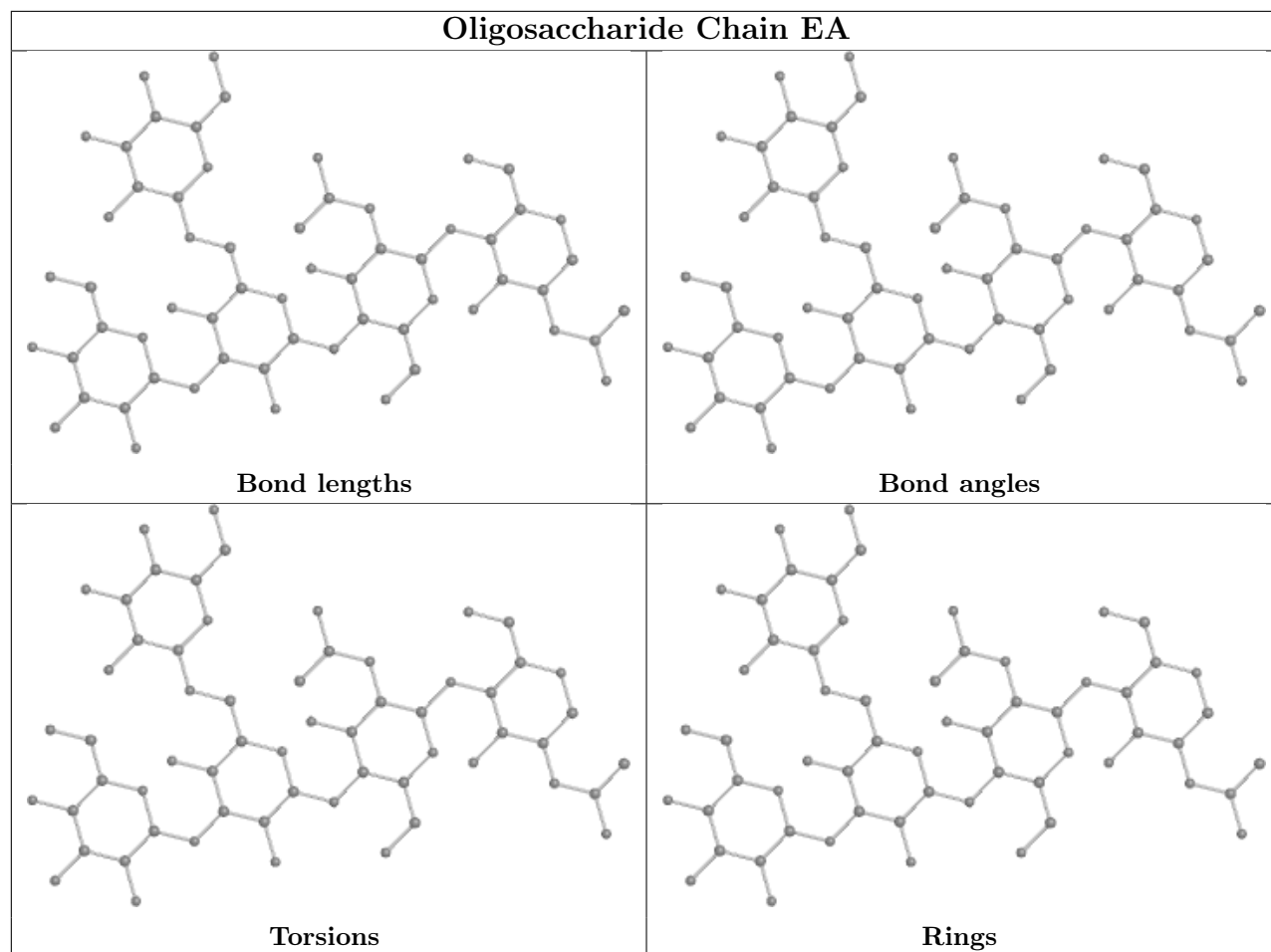


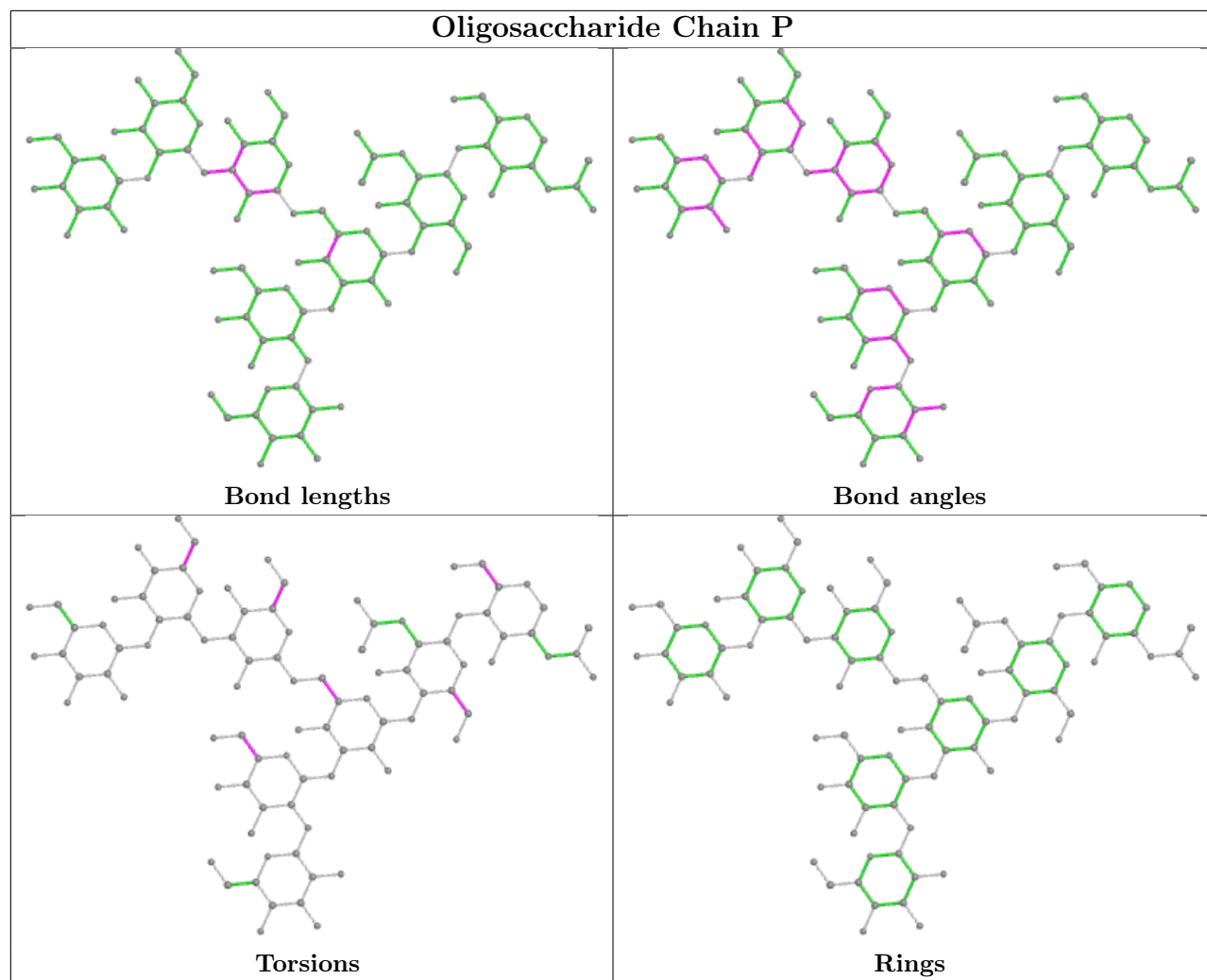


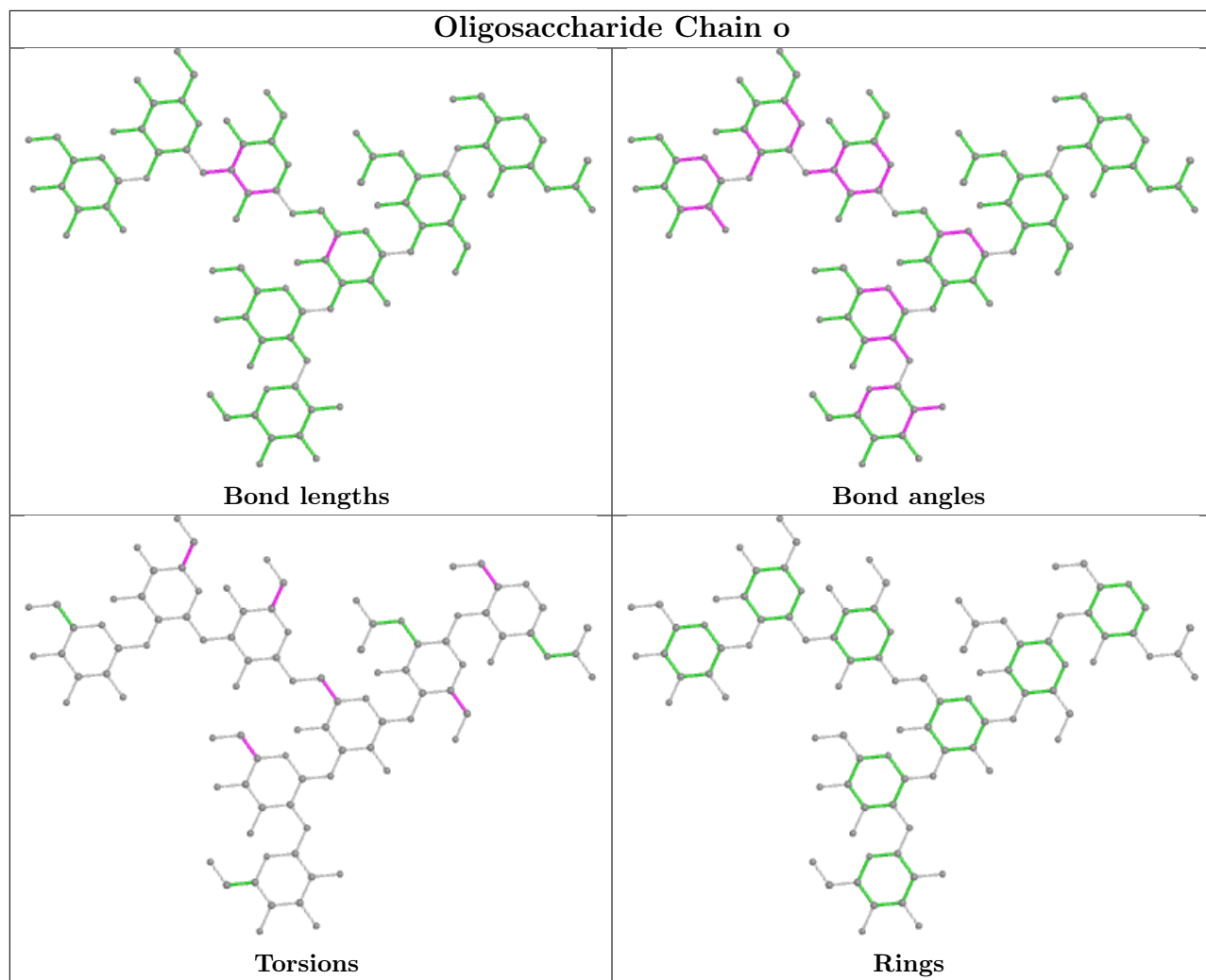


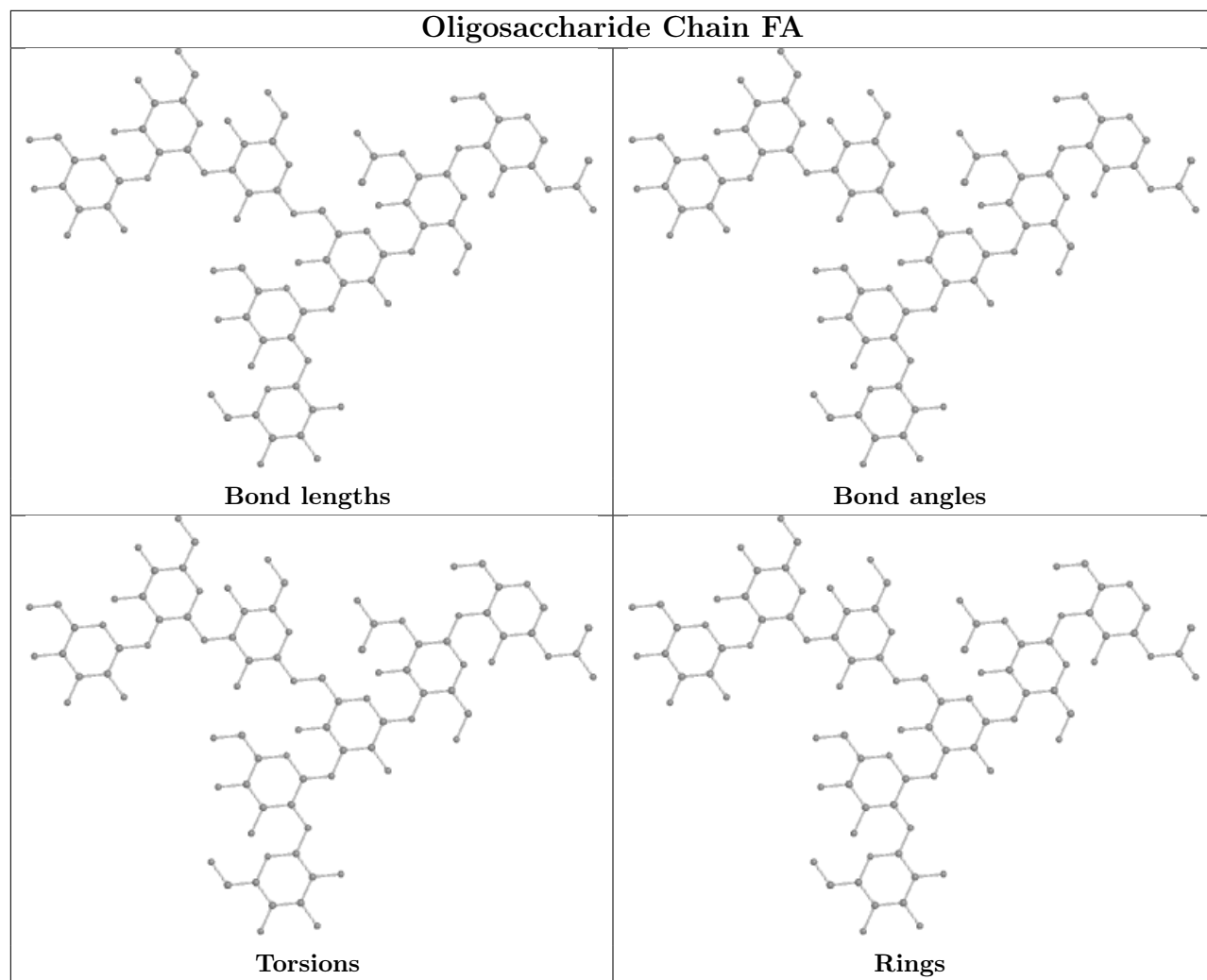


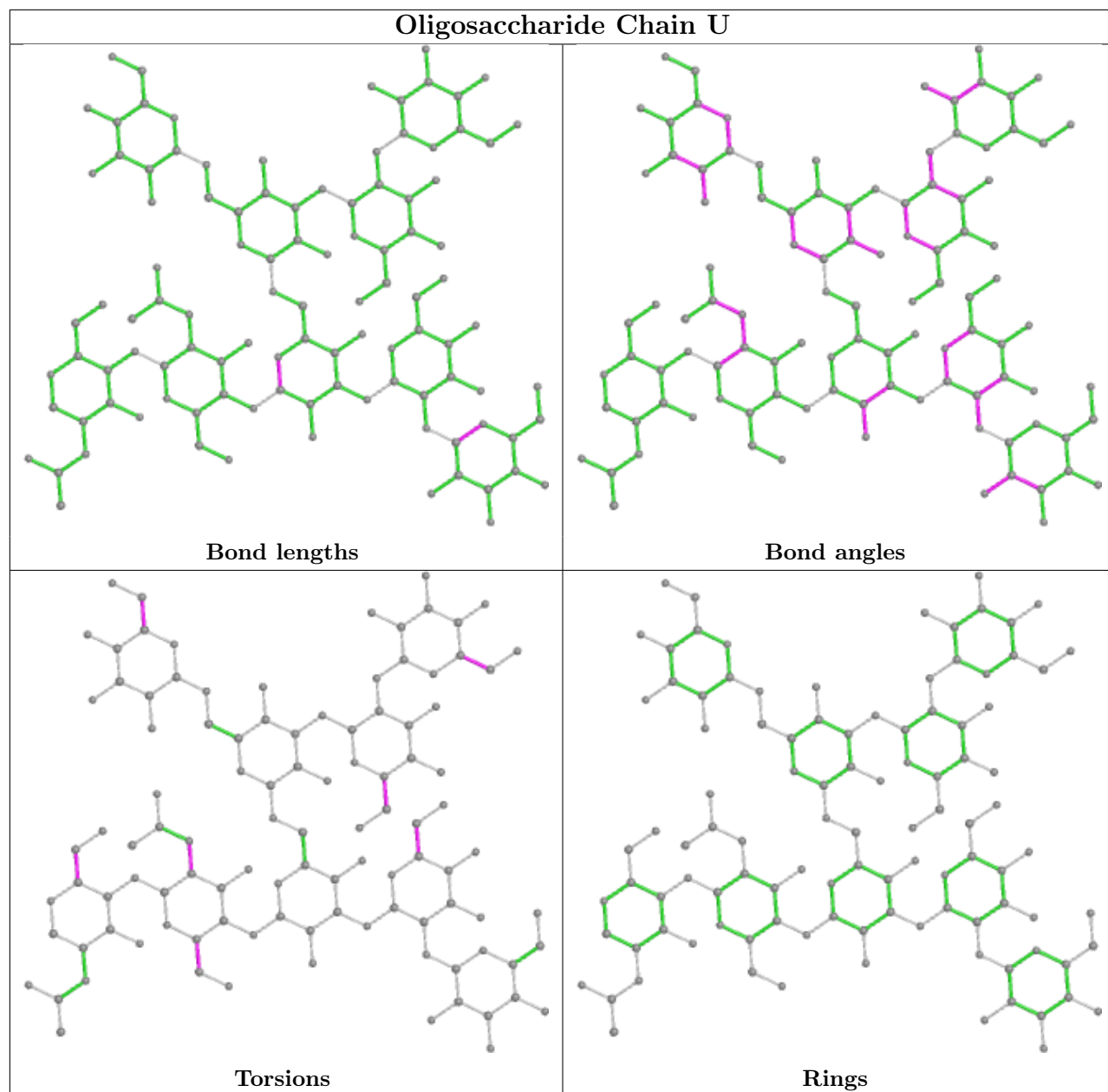


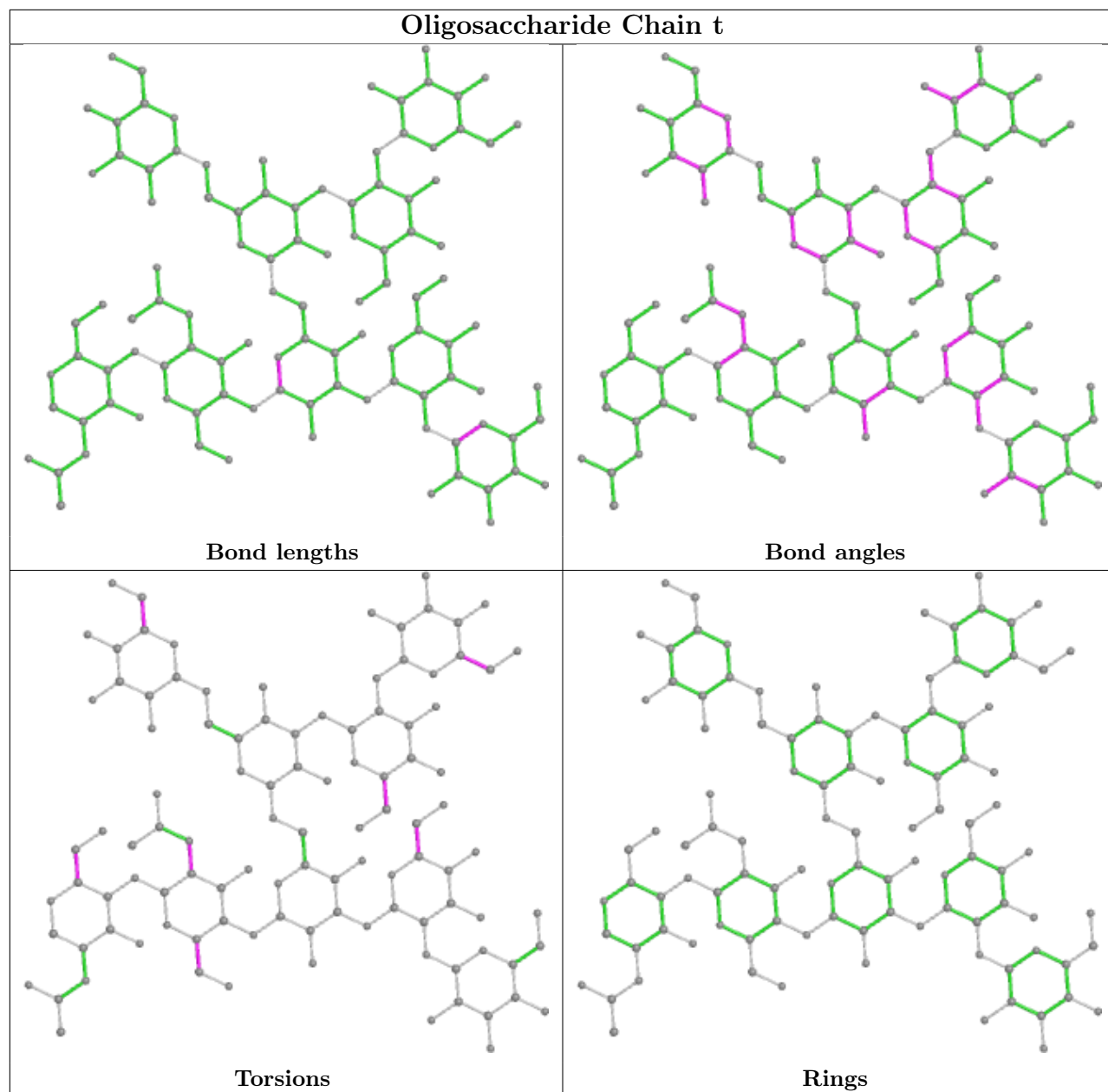


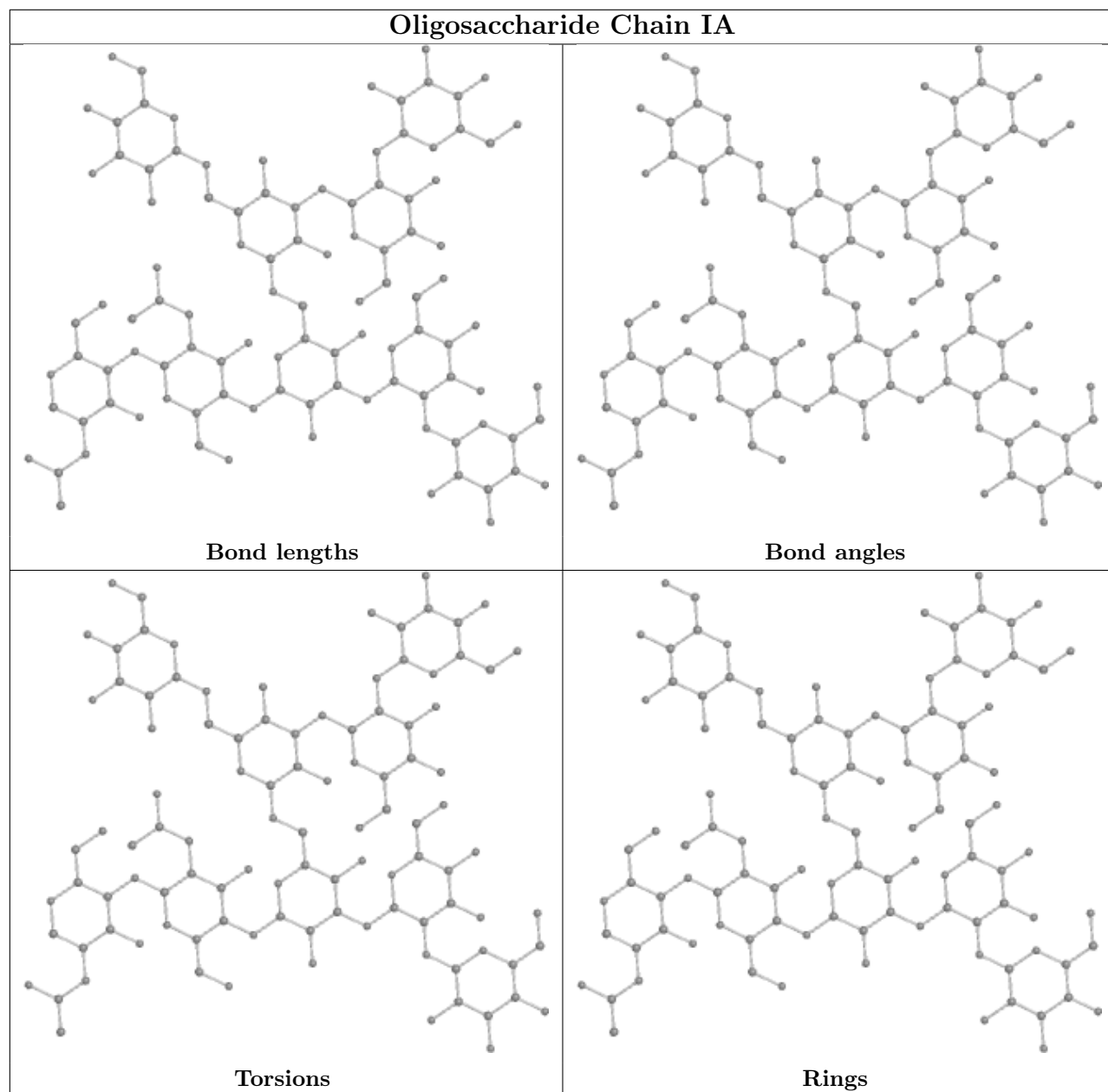


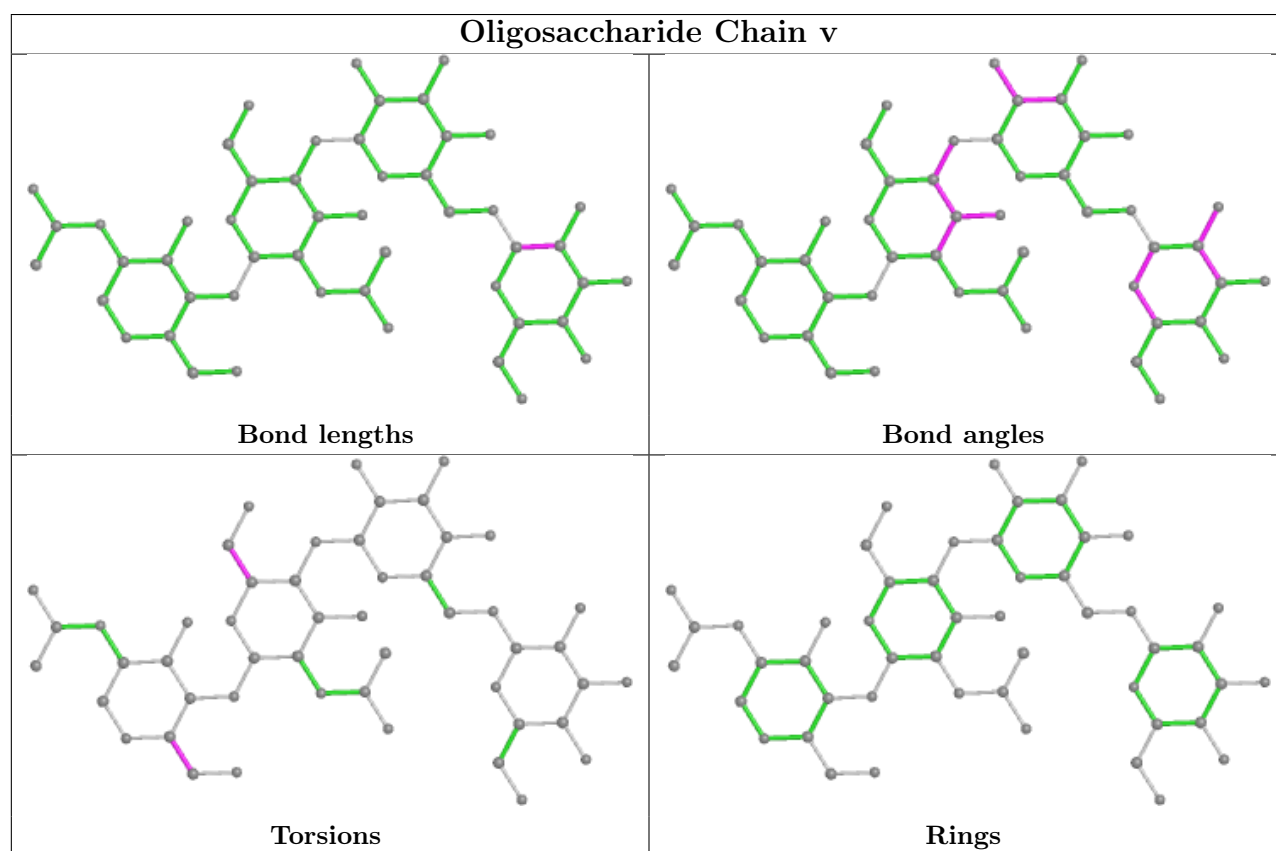
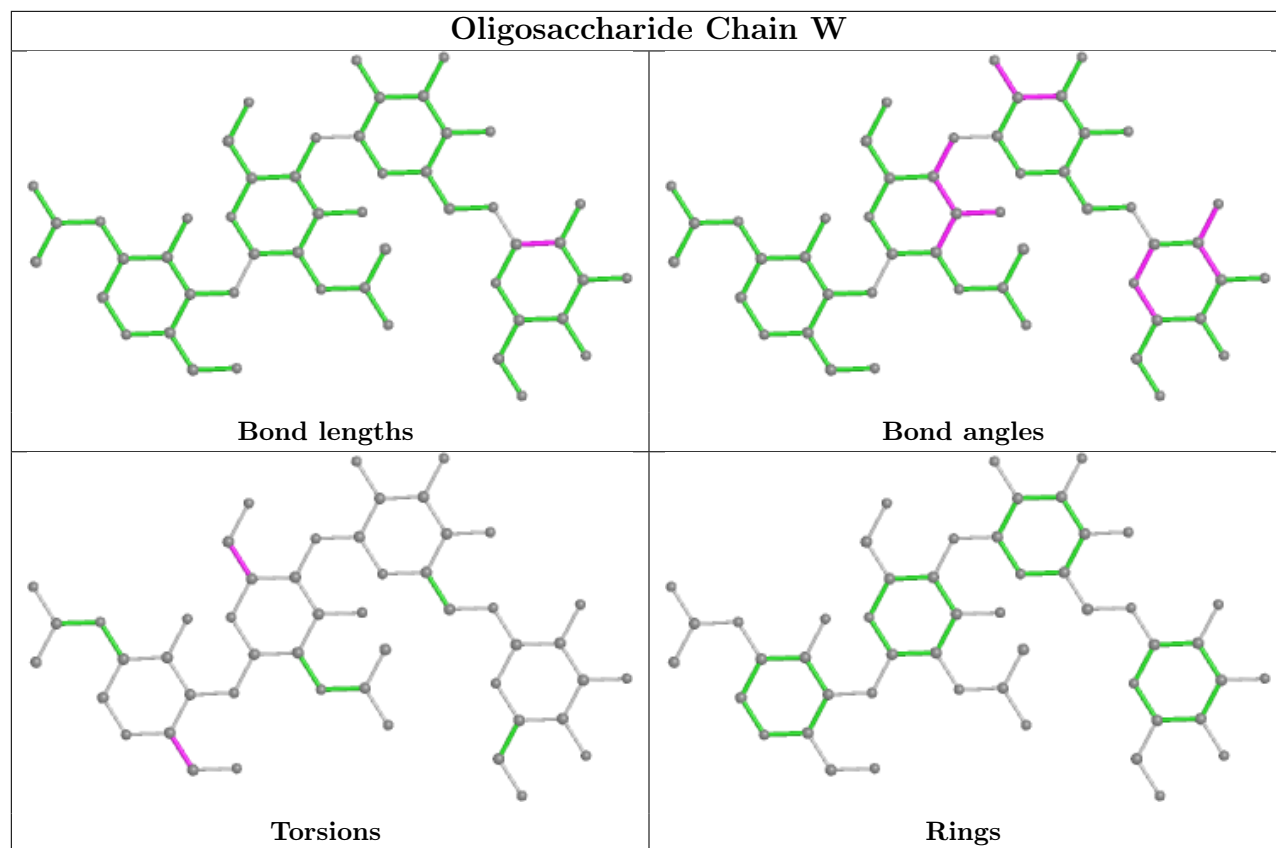


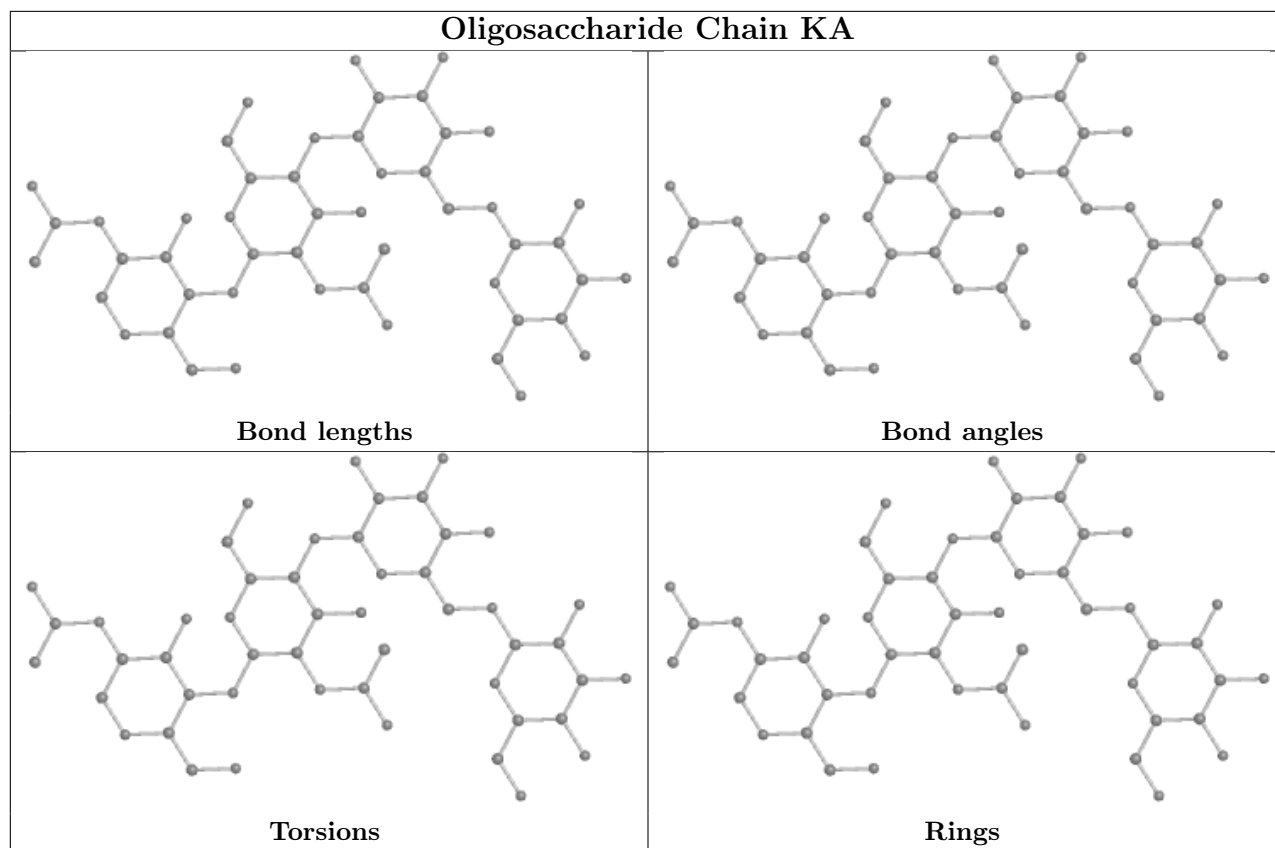












5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
19	MAN	c	615	-	11,11,12	0.84	0	15,15,17	1.19	2 (13%)
18	NAG	D	701	7	14,14,15	0.30	0	17,19,21	0.47	0
18	NAG	C	653	8	14,14,15	0.28	0	17,19,21	0.55	0
18	NAG	2	653	8	14,14,15	0.29	0	17,19,21	0.55	0
18	NAG	c	653	8	14,14,15	0.29	0	17,19,21	0.54	0
18	NAG	c	654	8	14,14,15	0.22	0	17,19,21	0.52	0
18	NAG	d	701	7	14,14,15	0.31	0	17,19,21	0.47	0
18	NAG	2	654	8	14,14,15	0.24	0	17,19,21	0.52	0
19	MAN	C	615	-	11,11,12	0.84	0	15,15,17	1.19	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	NAG	C	654	8	14,14,15	0.23	0	17,19,21	0.51	0
18	NAG	1	701	7	14,14,15	0.30	0	17,19,21	0.47	0
19	MAN	2	615	-	11,11,12	0.84	0	15,15,17	1.18	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	MAN	c	615	-	-	0/2/19/22	0/1/1/1
18	NAG	D	701	7	-	0/6/23/26	0/1/1/1
18	NAG	C	653	8	-	2/6/23/26	0/1/1/1
18	NAG	2	653	8	-	2/6/23/26	0/1/1/1
18	NAG	c	653	8	-	2/6/23/26	0/1/1/1
18	NAG	c	654	8	-	2/6/23/26	0/1/1/1
18	NAG	d	701	7	-	0/6/23/26	0/1/1/1
18	NAG	2	654	8	-	2/6/23/26	0/1/1/1
19	MAN	C	615	-	-	0/2/19/22	0/1/1/1
18	NAG	C	654	8	-	2/6/23/26	0/1/1/1
18	NAG	1	701	7	-	0/6/23/26	0/1/1/1
19	MAN	2	615	-	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	615	MAN	C1-O5-C5	2.78	115.96	112.19
19	2	615	MAN	C1-O5-C5	2.77	115.95	112.19
19	c	615	MAN	C1-O5-C5	2.76	115.94	112.19
19	c	615	MAN	O2-C2-C3	-2.16	105.81	110.14
19	C	615	MAN	O2-C2-C3	-2.16	105.82	110.14

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	653	NAG	C4-C5-C6-O6
18	c	653	NAG	C4-C5-C6-O6
18	2	653	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
18	C	654	NAG	O5-C5-C6-O6
18	c	654	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

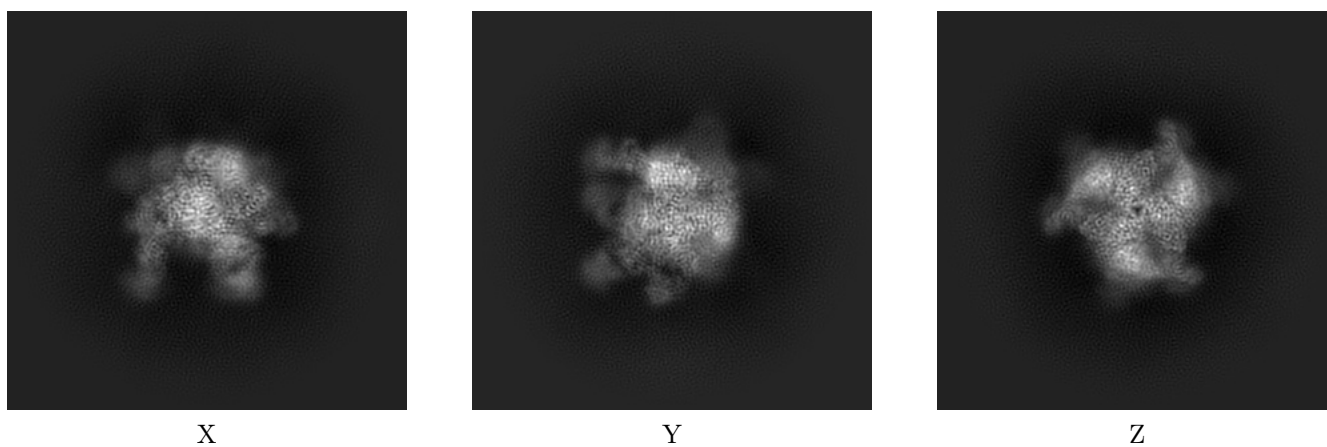
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7459. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

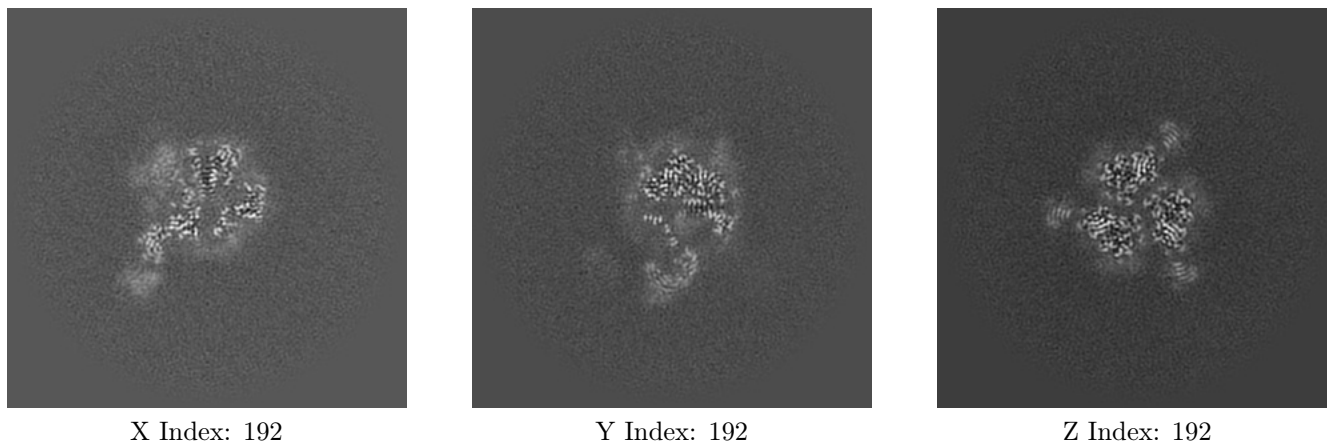
6.1.1 Primary map



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

6.2 Central slices [i](#)

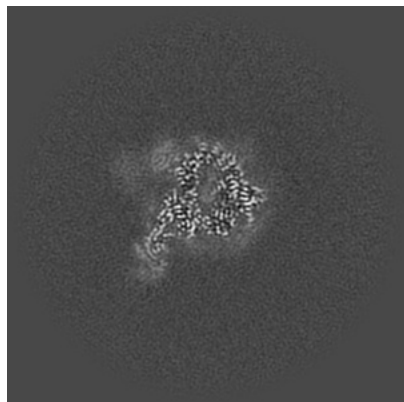
6.2.1 Primary map



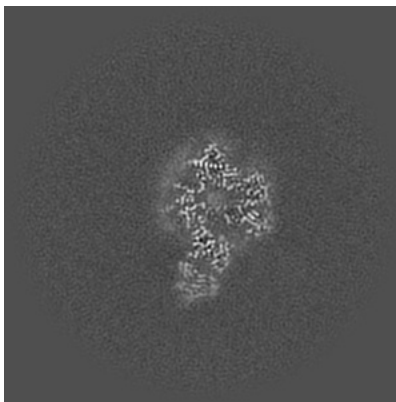
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

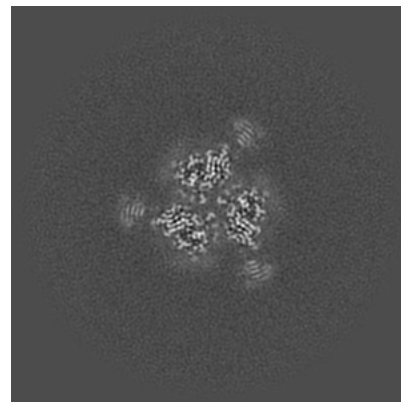
6.3.1 Primary map



X Index: 180



Y Index: 183



Z Index: 191

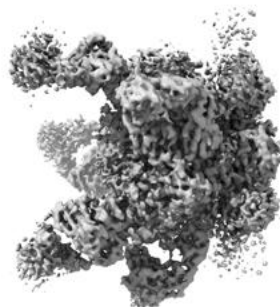
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.544. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

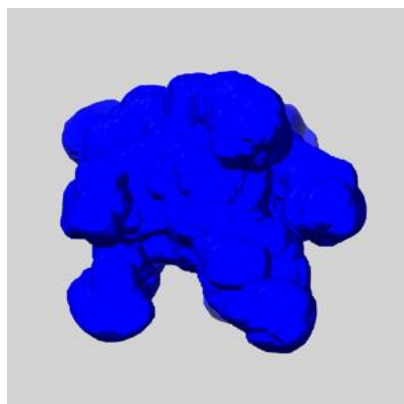
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

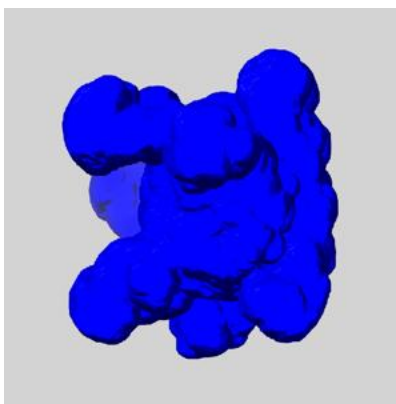
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

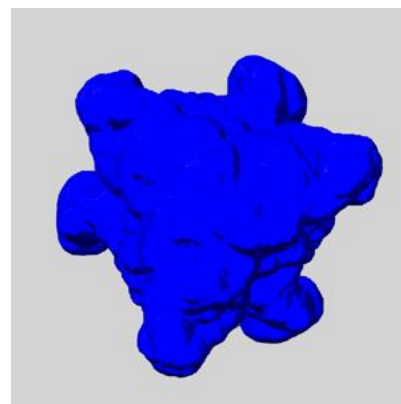
6.5.1 emd_7459_msk_1.map [i](#)



X

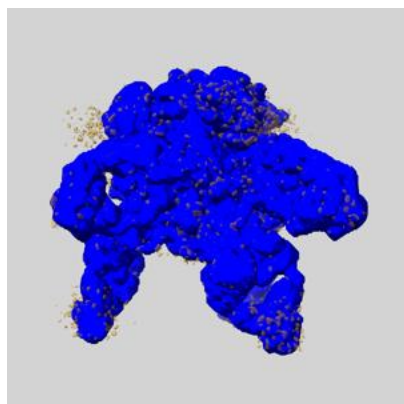


Y

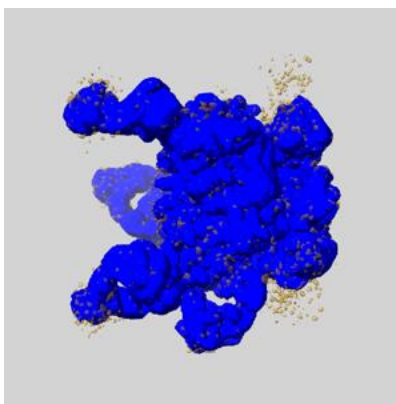


Z

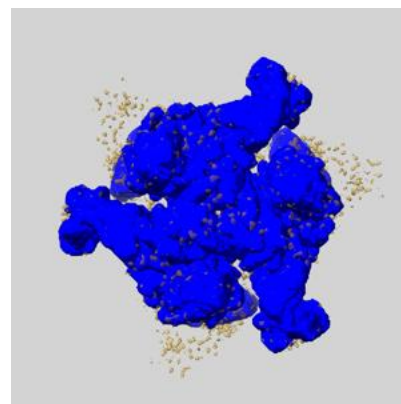
6.5.2 emd_7459_msk_2.map [i](#)



X



Y

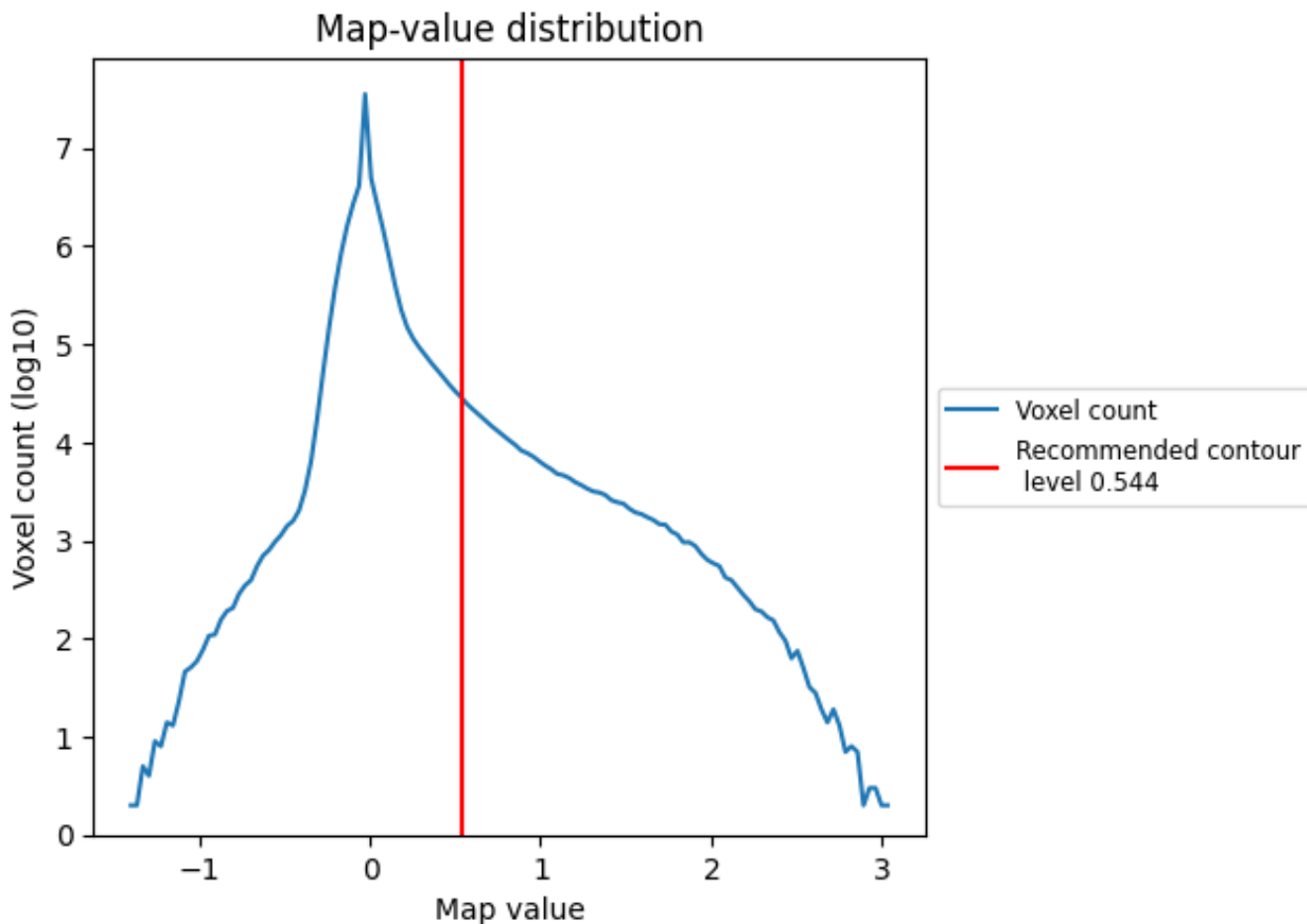


Z

7 Map analysis [i](#)

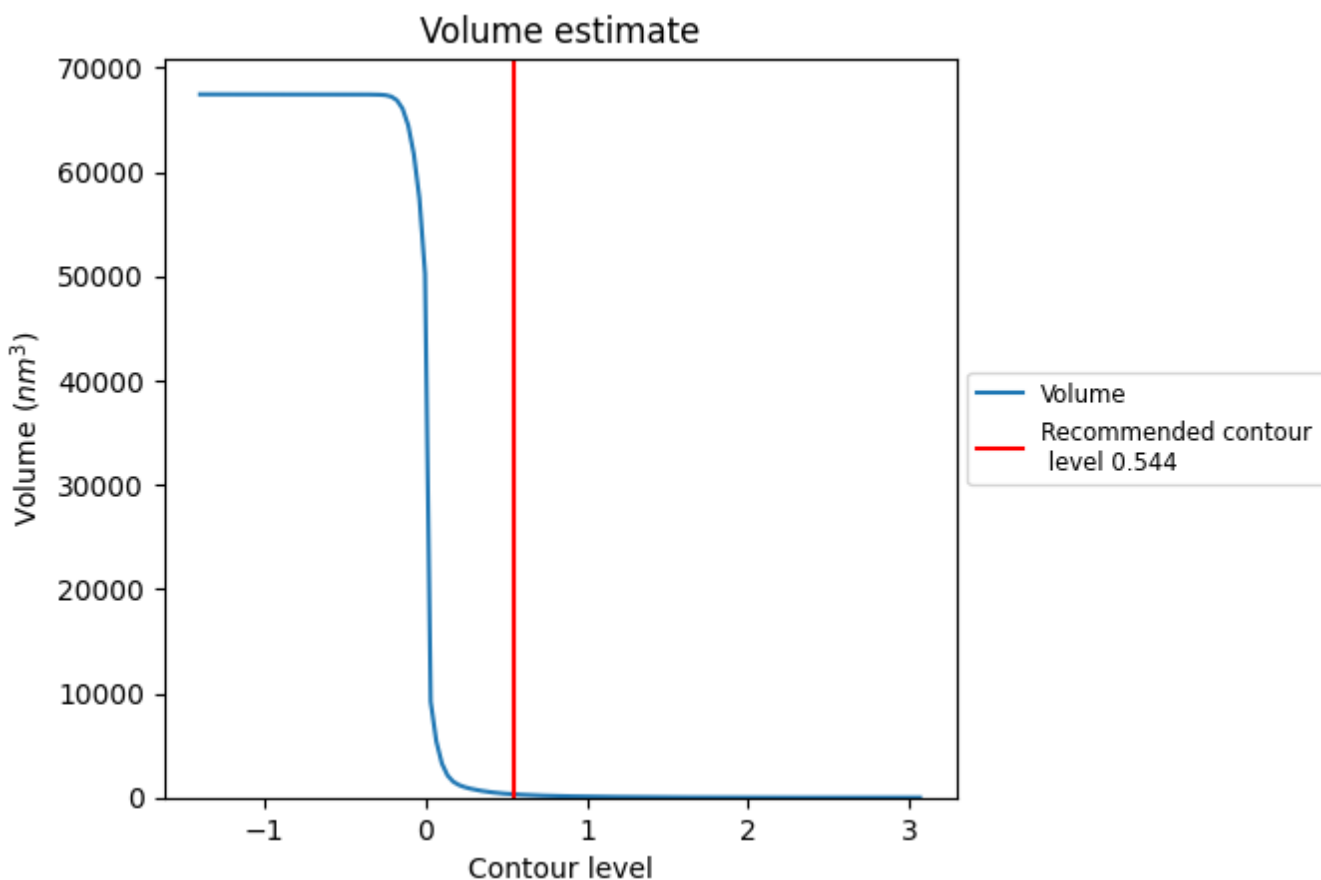
This section contains the results of statistical analysis of the map.

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.

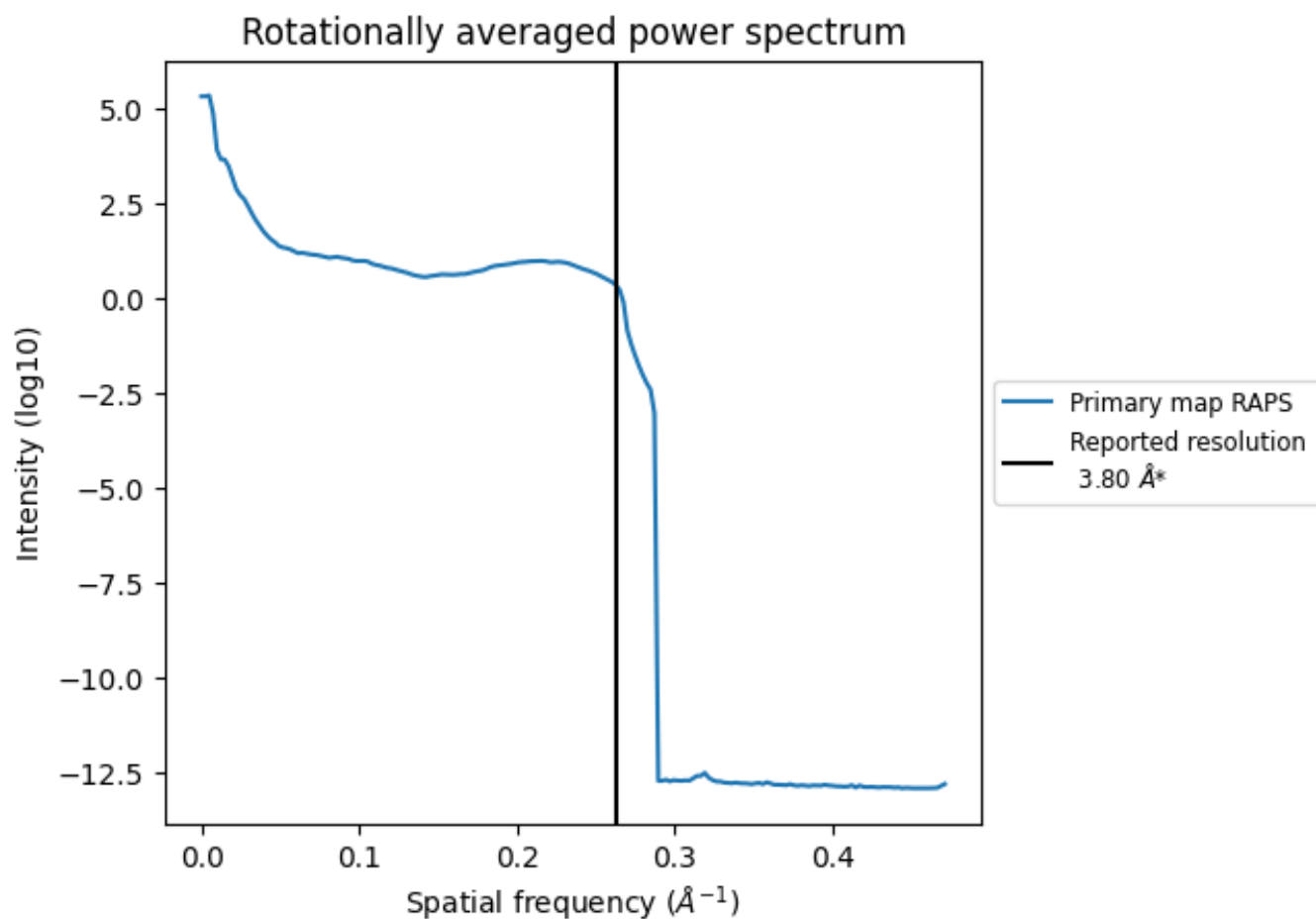
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 319 nm³; this corresponds to an approximate mass of 288 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 [i](#)

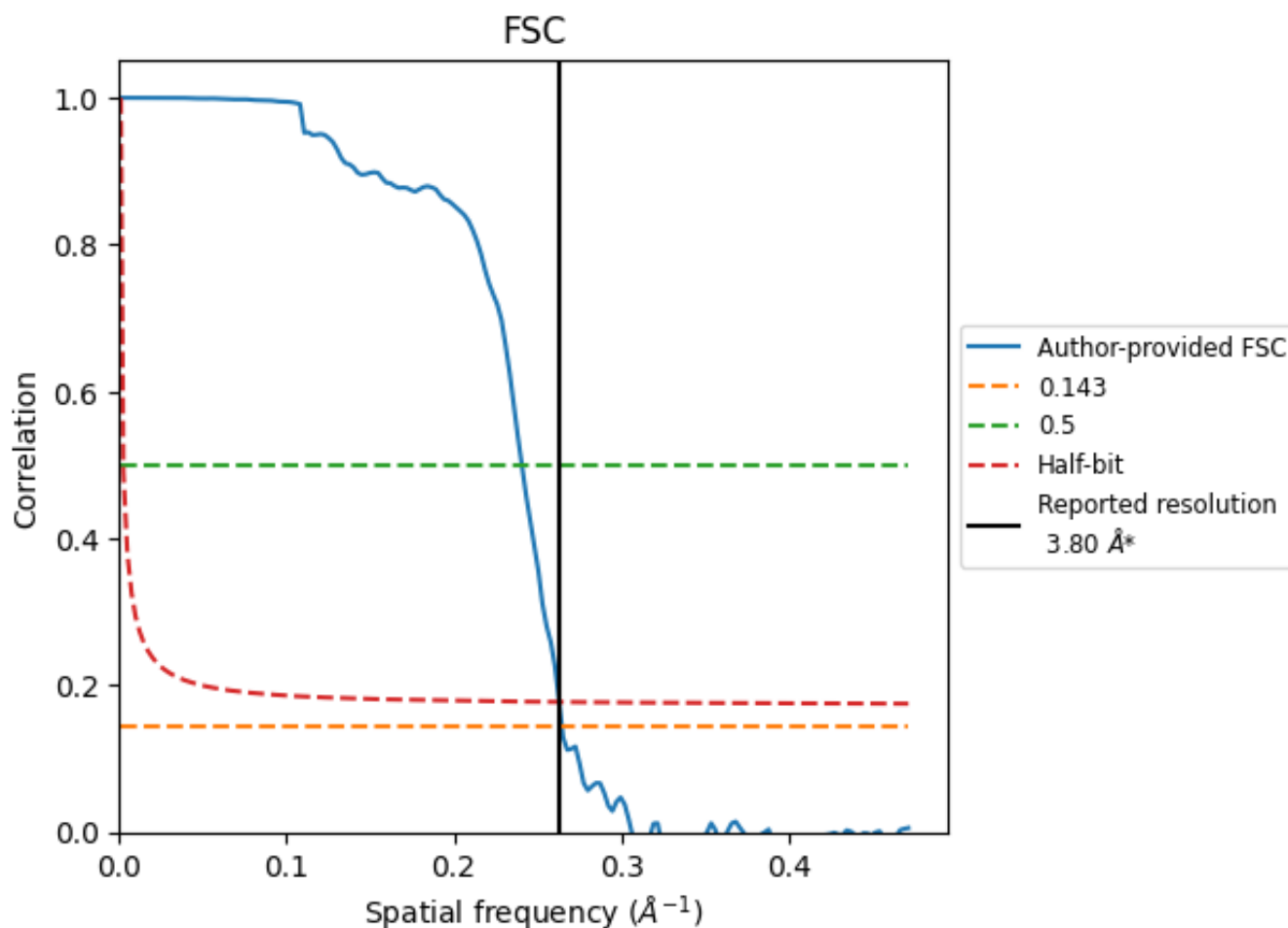


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

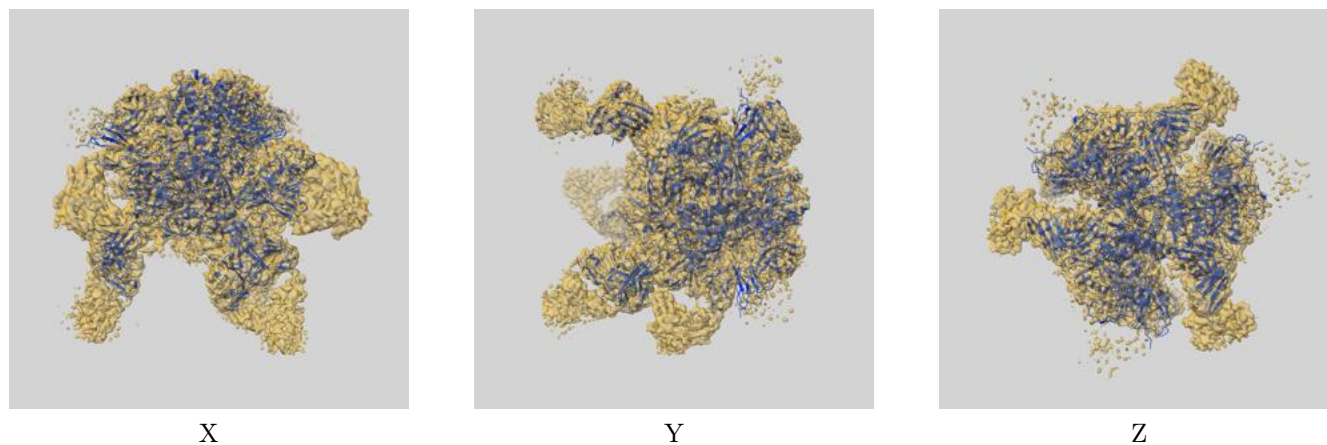
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.16	3.80
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

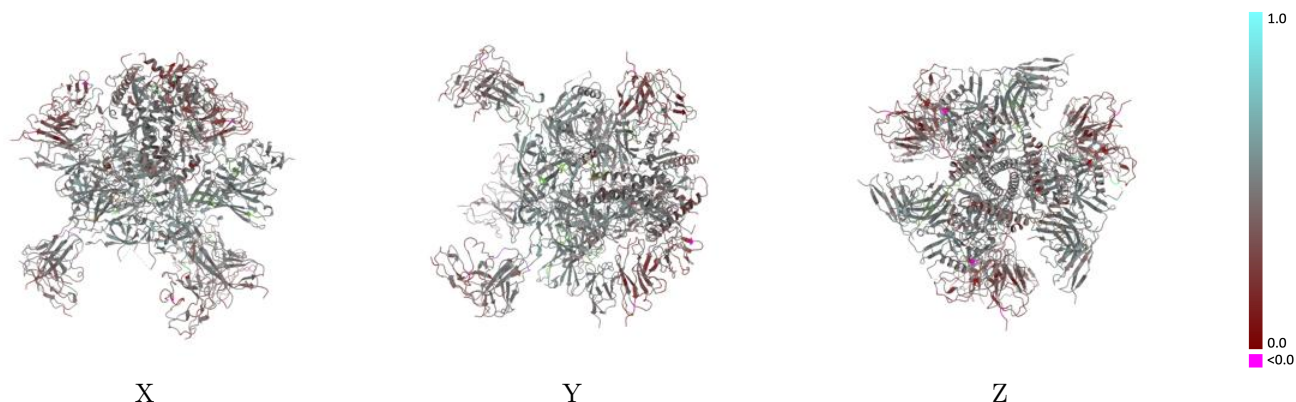
This section contains information regarding the fit between EMDB map EMD-7459 and PDB model 6CDE. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



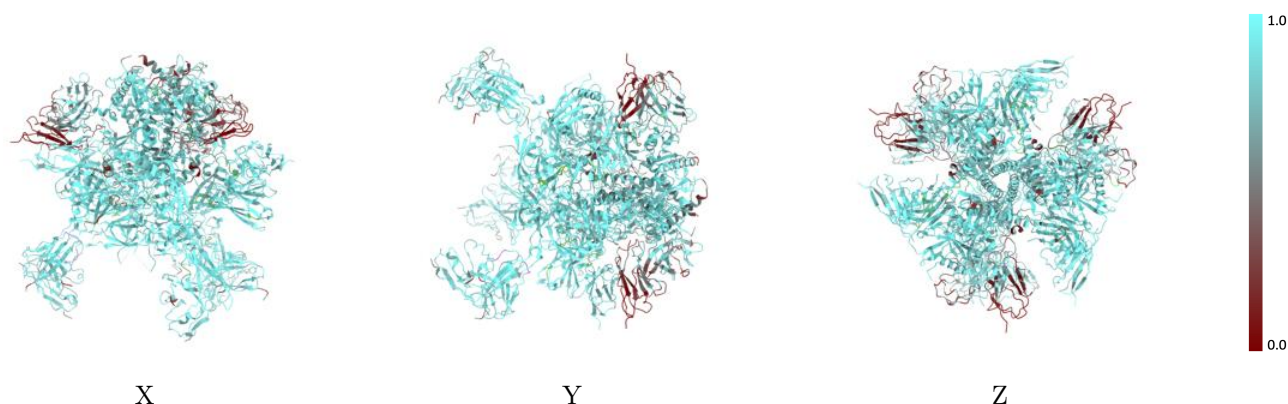
The images above show the 3D surface view of the map at the recommended contour level 0.544 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



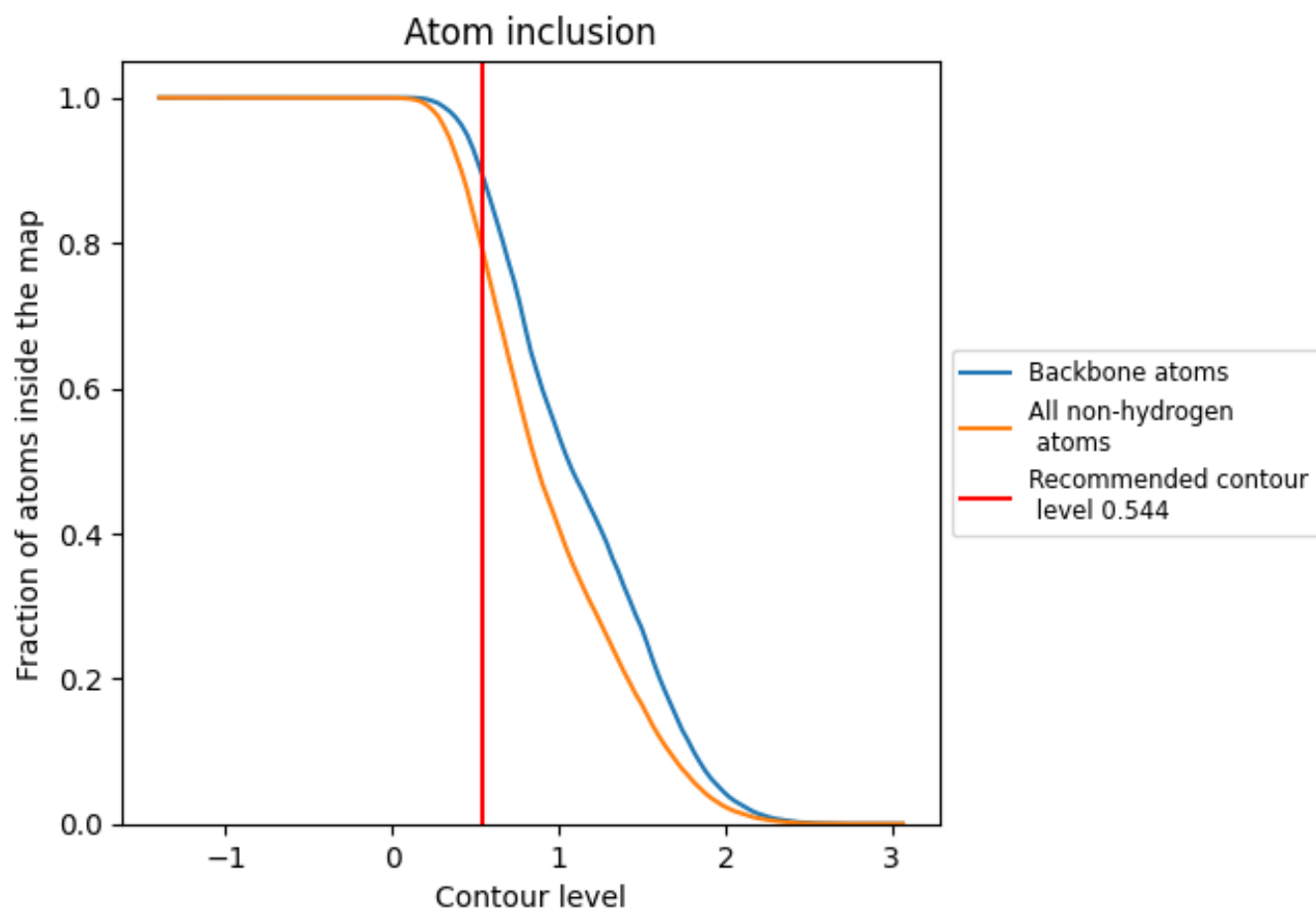
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.544).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 79% 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 (0.544) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7886	 0.4430
0	 0.3929	 0.3870
1	 0.8181	 0.4360
2	 0.8836	 0.4830
3	 0.6439	 0.3620
4	 0.3868	 0.3490
5	 0.9084	 0.5000
6	 0.8851	 0.4860
7	 0.8229	 0.4010
8	 0.8409	 0.4390
9	 0.7857	 0.3480
A	 0.2051	 0.3810
AA	 0.8400	 0.4680
B	 0.1026	 0.1330
BA	 0.7222	 0.4820
C	 0.8825	 0.4850
CA	 0.2766	 0.2950
D	 0.8142	 0.4410
DA	 0.6429	 0.4310
E	 0.3214	 0.3990
EA	 0.6721	 0.4480
F	 0.7857	 0.3590
FA	 0.5745	 0.4190
G	 0.8400	 0.4760
GA	 0.8214	 0.4960
H	 0.6416	 0.3580
HA	 0.6410	 0.4490
I	 0.7083	 0.4870
IA	 0.8857	 0.4860
J	 0.2766	 0.2980
JA	 0.8974	 0.4670
K	 0.6429	 0.4340
KA	 0.8000	 0.4410
L	 0.3902	 0.3510
LA	 0.4615	 0.4140



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Chain	Atom inclusion	Q-score
M	 0.8219	 0.4040
MA	 0.4359	 0.2840
N	 0.8422	 0.4380
O	 0.7049	 0.4360
P	 0.5745	 0.4180
Q	 0.8973	 0.5010
R	 0.8801	 0.4870
S	 0.8214	 0.5010
T	 0.6667	 0.4570
U	 0.8857	 0.4890
V	 0.8974	 0.4760
W	 0.8000	 0.4320
X	 0.4872	 0.4040
Y	 0.4615	 0.2950
Z	 0.2051	 0.3670
a	 0.1026	 0.1080
b	 0.3571	 0.3810
c	 0.8834	 0.4820
d	 0.8161	 0.4390
e	 0.7857	 0.3480
f	 0.8400	 0.4610
g	 0.7222	 0.4860
h	 0.6405	 0.3650
i	 0.2660	 0.2960
j	 0.6429	 0.4260
k	 0.6721	 0.4480
l	 0.3914	 0.3470
m	 0.8268	 0.4040
n	 0.8372	 0.4350
o	 0.5745	 0.4140
p	 0.8214	 0.4910
q	 0.9063	 0.5010
r	 0.8813	 0.4860
s	 0.6667	 0.4440
t	 0.8952	 0.4810
u	 0.8974	 0.4640
v	 0.7800	 0.4430
w	 0.4615	 0.4150
x	 0.4359	 0.2870
y	 0.2051	 0.3660
z	 0.1026	 0.1170