



## wwPDB EM Validation Summary Report ⓘ

Oct 20, 2024 – 10:14 AM EDT

PDB ID : 7LG6  
EMDB ID : EMD-23312  
Title : BG505 SOSIP.v5.2 in complex with VRC40.01 and RM19R Fabs  
Authors : Cottrell, C.A.; Torres, J.L.; Wu, N.R.; Ward, A.B.  
Deposited on : 2021-01-19  
Resolution : 3.28 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.39

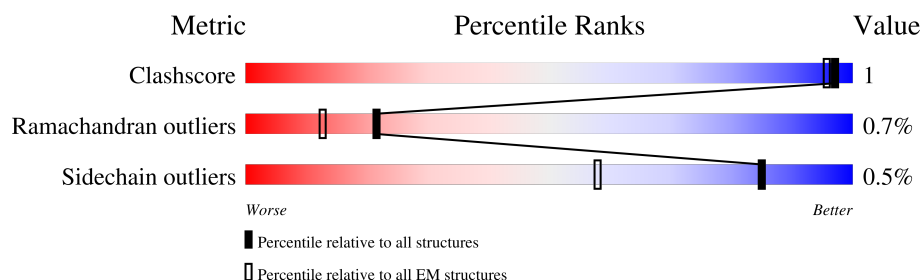
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




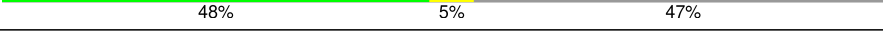
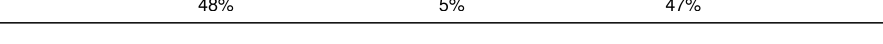
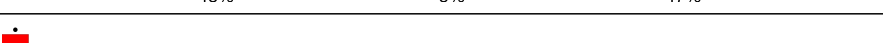


The reported resolution of this entry is 3.28 Å.

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.




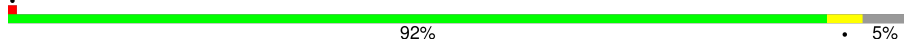
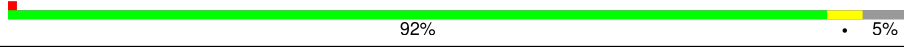
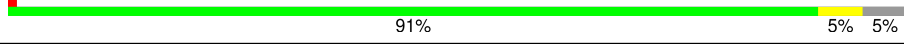



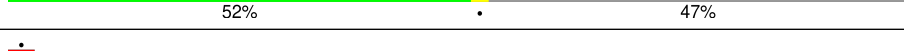
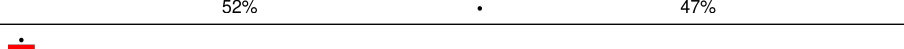
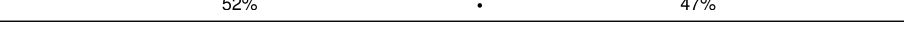
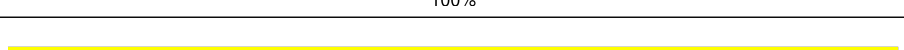
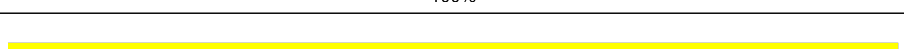

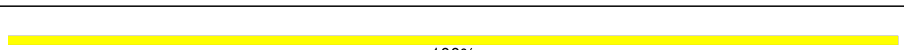
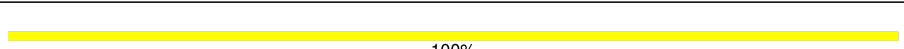
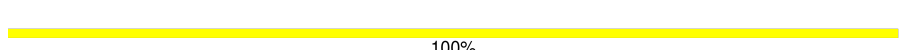
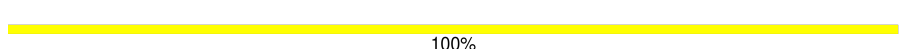


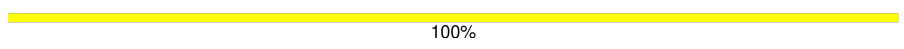
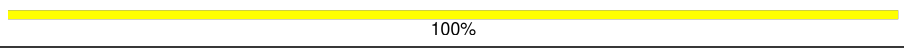
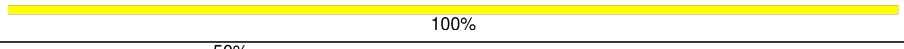
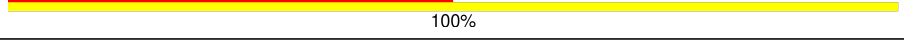
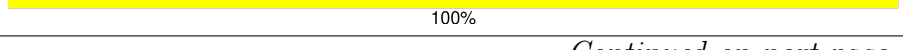

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	475	 89% 5% 5%
1	E	475	 89% 5% 5%
1	F	475	 89% 5% 5%
2	H	231	 48% 5% 47%
2	O	231	 48% 5% 47%
2	P	231	 48% 5% 47%
3	L	214	 47% 50%
3	Q	214	 47% 50%

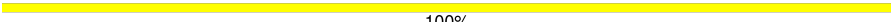
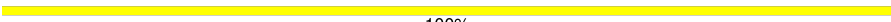
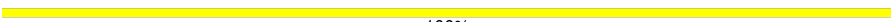

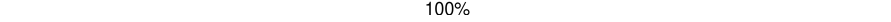

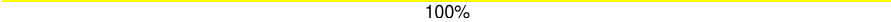
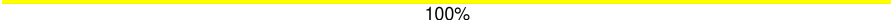
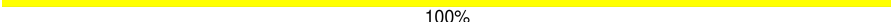
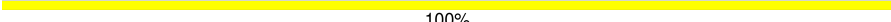
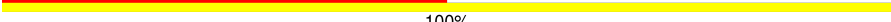
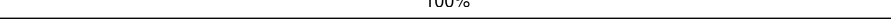
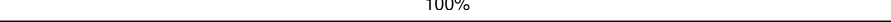
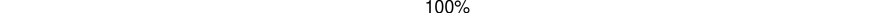
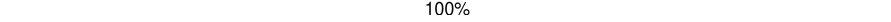
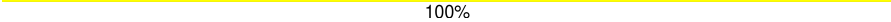
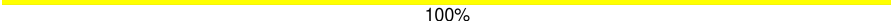

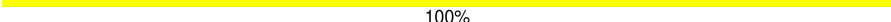
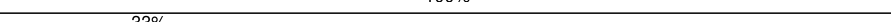
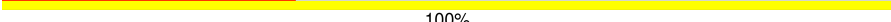
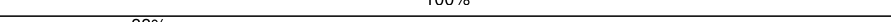
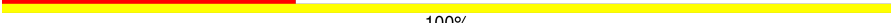
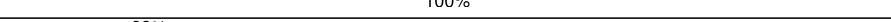
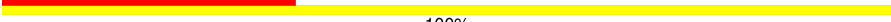
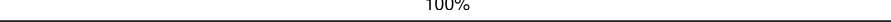













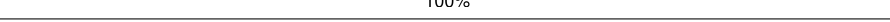
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Mol	Chain	Length	Quality of chain
3	R	214	
4	B	153	
4	G	153	
4	I	153	
5	D	214	
5	M	214	
5	N	214	
6	C	225	
6	J	225	
6	K	225	
7	0	2	
7	1	2	
7	2	2	
7	3	2	
7	4	2	
7	5	2	
7	6	2	
7	S	2	
7	U	2	
7	V	2	
7	Y	2	
7	Z	2	
7	a	2	
7	b	2	
7	c	2	

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Mol	Chain	Length	Quality of chain
7	d	2	 100%
7	e	2	 100%
7	g	2	 100%
7	i	2	 50%  100%
7	j	2	 50%  100%
7	m	2	 100%
7	n	2	 100%
7	o	2	 100%
7	p	2	 50%  100%
7	q	2	 100%
7	r	2	 100%
7	s	2	 100%
7	u	2	 100%
7	w	2	 50%  100%
7	x	2	 50%  100%
8	T	3	 33%  100%
8	h	3	 33%  100%
8	v	3	 33%  100%
9	W	6	 17%  83%
9	k	6	 17%  83%
9	y	6	 17%  83%
10	X	8	 12%  88%
10	l	8	 12%  88%
10	z	8	 12%  88%
11	7	2	 50%  100%

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Mol	Chain	Length	Quality of chain
11	f	2	<div><div>50%</div><div>100%</div></div>
11	t	2	<div><div>50%</div><div>100%</div></div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 26550 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	450	Total	C	N	O	S	0	0
			3552	2235	626	662	29		
1	E	450	Total	C	N	O	S	0	0
			3552	2235	626	662	29		
1	F	450	Total	C	N	O	S	0	0
			3552	2235	626	662	29		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LYS	GLU	engineered mutation	UNP Q2N0S6
A	73	CYS	ALA	engineered mutation	UNP Q2N0S6
A	316	TRP	ALA	engineered mutation	UNP Q2N0S6
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
E	64	LYS	GLU	engineered mutation	UNP Q2N0S6
E	73	CYS	ALA	engineered mutation	UNP Q2N0S6
E	316	TRP	ALA	engineered mutation	UNP Q2N0S6
E	332	ASN	THR	engineered mutation	UNP Q2N0S6
E	501	CYS	ALA	engineered mutation	UNP Q2N0S6
F	64	LYS	GLU	engineered mutation	UNP Q2N0S6
F	73	CYS	ALA	engineered mutation	UNP Q2N0S6
F	316	TRP	ALA	engineered mutation	UNP Q2N0S6
F	332	ASN	THR	engineered mutation	UNP Q2N0S6
F	501	CYS	ALA	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called VRC40.01 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	123	Total	C	N	O	S	0	0
			965	621	171	169	4		
2	O	123	Total	C	N	O	S	0	0
			965	621	171	169	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	123	Total	C	N	O	S	0	0
			965	621	171	169	4		

- Molecule 3 is a protein called VRC40.01 Fab Kappa Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			833	523	146	160	4		
3	Q	107	Total	C	N	O	S	0	0
			833	523	146	160	4		
3	R	107	Total	C	N	O	S	0	0
			833	523	146	160	4		

- Molecule 4 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	146	Total	C	N	O	S	0	0
			1160	733	203	217	7		
4	G	146	Total	C	N	O	S	0	0
			1160	733	203	217	7		
4	I	146	Total	C	N	O	S	0	0
			1160	733	203	217	7		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	561	CYS	ALA	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
G	559	PRO	ILE	engineered mutation	UNP Q2N0S6
G	561	CYS	ALA	engineered mutation	UNP Q2N0S6
G	605	CYS	THR	engineered mutation	UNP Q2N0S6
I	559	PRO	ILE	engineered mutation	UNP Q2N0S6
I	561	CYS	ALA	engineered mutation	UNP Q2N0S6
I	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 5 is a protein called RM19R Fab Kappa Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	105	Total	C	N	O	S	0	0
			817	511	142	161	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	105	Total	C	N	O	S	0	0
			817	511	142	161	3		
5	N	105	Total	C	N	O	S	0	0
			817	511	142	161	3		

- Molecule 6 is a protein called RM19R Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	120	Total	C	N	O	S	0	0
			930	587	160	181	2		
6	J	120	Total	C	N	O	S	0	0
			930	587	160	181	2		
6	K	120	Total	C	N	O	S	0	0
			930	587	160	181	2		

- Molecule 7 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
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	V	2	Total	C	N	O	0	0
			28	16	2	10		
7	Y	2	Total	C	N	O	0	0
			28	16	2	10		
7	Z	2	Total	C	N	O	0	0
			28	16	2	10		
7	a	2	Total	C	N	O	0	0
			28	16	2	10		
7	b	2	Total	C	N	O	0	0
			28	16	2	10		
7	c	2	Total	C	N	O	0	0
			28	16	2	10		
7	d	2	Total	C	N	O	0	0
			28	16	2	10		

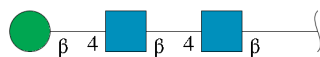
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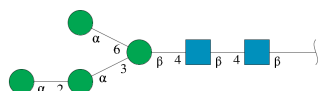
Mol	Chain	Residues	Atoms				AltConf	Trace
7	e	2	Total	C	N	O	0	0
			28	16	2	10		
7	g	2	Total	C	N	O	0	0
			28	16	2	10		
7	i	2	Total	C	N	O	0	0
			28	16	2	10		
7	j	2	Total	C	N	O	0	0
			28	16	2	10		
7	m	2	Total	C	N	O	0	0
			28	16	2	10		
7	n	2	Total	C	N	O	0	0
			28	16	2	10		
7	o	2	Total	C	N	O	0	0
			28	16	2	10		
7	p	2	Total	C	N	O	0	0
			28	16	2	10		
7	q	2	Total	C	N	O	0	0
			28	16	2	10		
7	r	2	Total	C	N	O	0	0
			28	16	2	10		
7	s	2	Total	C	N	O	0	0
			28	16	2	10		
7	u	2	Total	C	N	O	0	0
			28	16	2	10		
7	w	2	Total	C	N	O	0	0
			28	16	2	10		
7	x	2	Total	C	N	O	0	0
			28	16	2	10		
7	0	2	Total	C	N	O	0	0
			28	16	2	10		
7	1	2	Total	C	N	O	0	0
			28	16	2	10		
7	2	2	Total	C	N	O	0	0
			28	16	2	10		
7	3	2	Total	C	N	O	0	0
			28	16	2	10		
7	4	2	Total	C	N	O	0	0
			28	16	2	10		
7	5	2	Total	C	N	O	0	0
			28	16	2	10		
7	6	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 8 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.



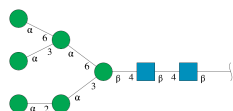
Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	3	Total	C	N	O	0	0
			39	22	2	15		
8	h	3	Total	C	N	O	0	0
			39	22	2	15		
8	v	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 9 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
9	W	6	Total	C	N	O	0	0
			72	40	2	30		
9	k	6	Total	C	N	O	0	0
			72	40	2	30		
9	y	6	Total	C	N	O	0	0
			72	40	2	30		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
10	X	8	Total	C	N	O	0	0
			94	52	2	40		

*Continued on next page...*

Continued from previous page...

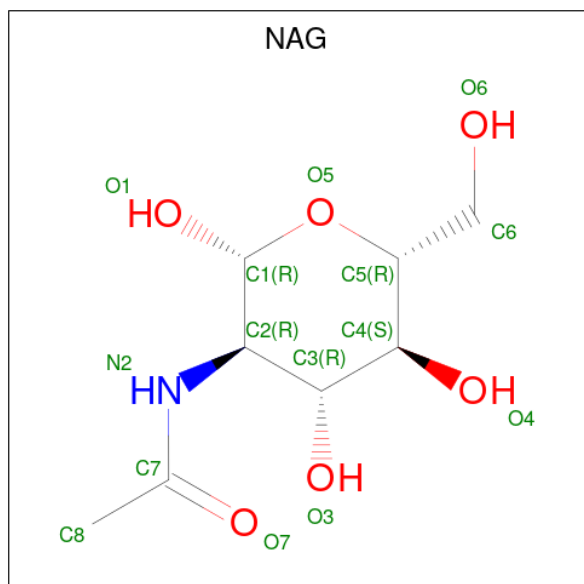
Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	8	Total	C	N	O	0	0
			94	52	2	40		
10	z	8	Total	C	N	O	0	0
			94	52	2	40		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
11	f	2	Total	C	N	O	0	0
			24	14	1	9		
11	t	2	Total	C	N	O	0	0
			24	14	1	9		
11	7	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	N	O	0
			14	8	1	5	

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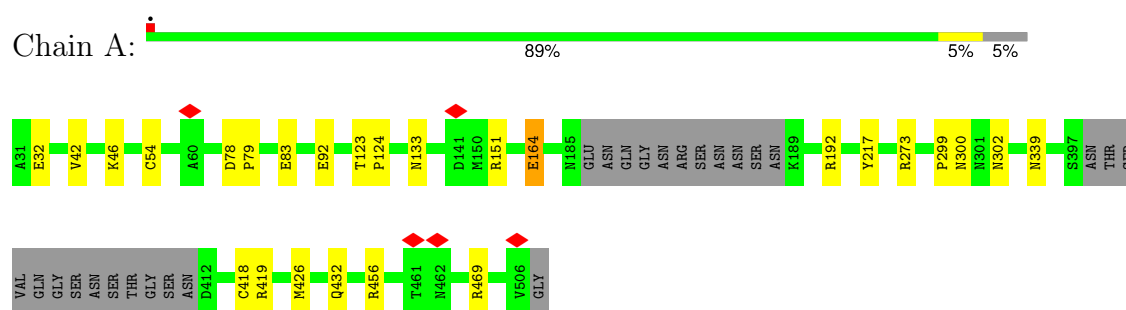
*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	A	1	Total 14	C 8	N 1	O 5	0
12	B	1	Total 14	C 8	N 1	O 5	0
12	B	1	Total 14	C 8	N 1	O 5	0
12	E	1	Total 14	C 8	N 1	O 5	0
12	E	1	Total 14	C 8	N 1	O 5	0
12	E	1	Total 14	C 8	N 1	O 5	0
12	E	1	Total 14	C 8	N 1	O 5	0
12	G	1	Total 14	C 8	N 1	O 5	0
12	G	1	Total 14	C 8	N 1	O 5	0
12	F	1	Total 14	C 8	N 1	O 5	0
12	F	1	Total 14	C 8	N 1	O 5	0
12	F	1	Total 14	C 8	N 1	O 5	0
12	F	1	Total 14	C 8	N 1	O 5	0
12	I	1	Total 14	C 8	N 1	O 5	0
12	I	1	Total 14	C 8	N 1	O 5	0

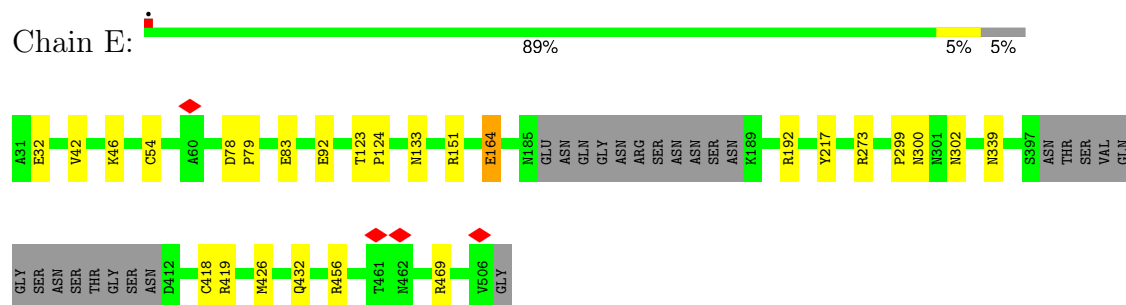
### 3 Residue-property plots [i](#)

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

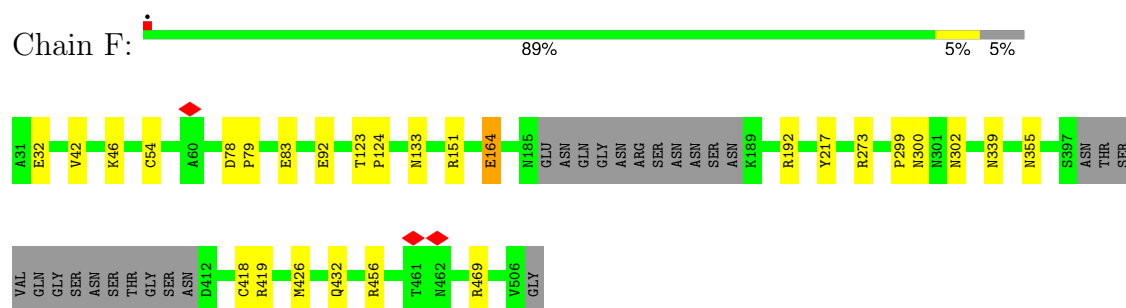
- Molecule 1: Envelope glycoprotein gp120



- Molecule 1: Envelope glycoprotein gp120



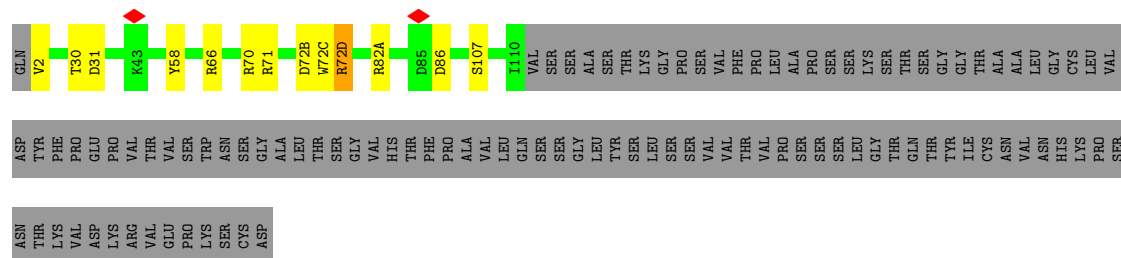
- Molecule 1: Envelope glycoprotein gp120



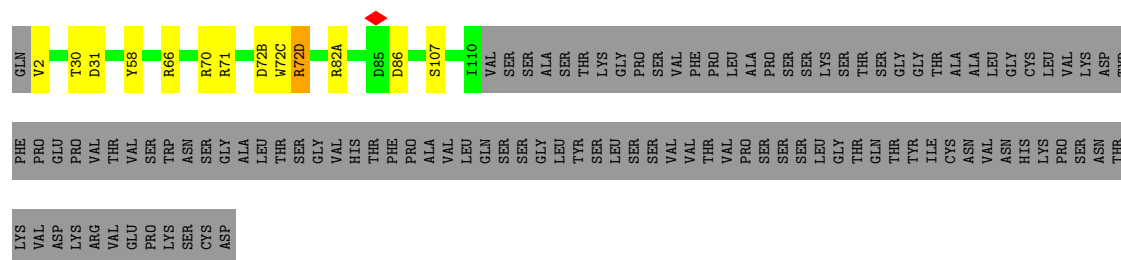
- Molecule 2: VRC40.01 Fab Heavy Chain



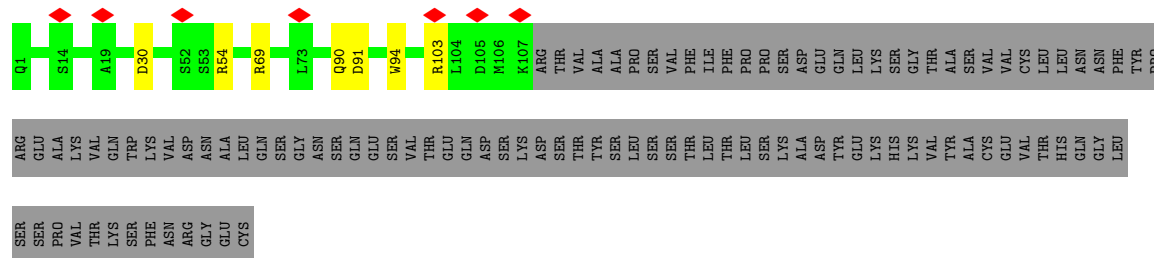
- Molecule 2: VRC40.01 Fab Heavy Chain



- Molecule 2: VRC40.01 Fab Heavy Chain



- Molecule 3: VRC40.01 Fab Kappa Light Chain



- Molecule 3: VRC40.01 Fab Kappa Light Chain





ASP ASN ALA ALA GLN SER GLY ASN ASN GLN GLU SER VAL THR THR TYR SER LEU SER SER SER SER LEU THR LEU THR SER SER SER LYS LYS ASP ASP GLU GLU VAL THR THR HIS HIS LYS VAL THR ALA ALA ASP TYR GLU GLU LYS LYS LYS VAL THR ALA ALA ARG GLY GLU CYS

- Molecule 5: RM19R Fab Kappa Light Chain

Chain M:  46% . 51%

ARG	ASP	ALA
GLY	ASN	ILE
GLU	ALA	R3
CYS	LEU	R24
	GLN	
	SER	
	GLY	R32
	ASN	
	SER	Y36
	GLN	
	GLU	RE4
	SER	
	VAL	D60
	THR	
	GLU	T97
	GLN	
	ASP	K107
	SER	ARG
	LYS	THR
	ASP	VAL
	SER	ALA
	THR	ALA
	TYR	PRO
	SER	SER
	LEU	VAL
	SER	PHE
	SER	ILE
	THR	PHE
	LEU	PRO
	THR	PRO
	LEU	SER
	SER	ASP
	LYS	GLU
	ALA	GLN
	ASP	LEU
	TYR	LYS
	GLU	SER
	LYS	GLY
	HIS	THR
	LYS	ALA
	VAL	SER
	TYR	VAL
	ALA	VAL
	CYS	CYS
	GLU	LEU
	VAL	LEU
	THR	ASN
	HIS	ASN
	GLN	PHE
	GLY	TYR
	LEU	PRO
	SER	ARG
	SER	GLU
	PRO	ALA
	VAL	LYS
	THR	VAL
	LYS	GLN
	SER	THR
	PHE	LYS
	ASN	VAL

- Molecule 5: RM19R Fab Kappa Light Chain

Chain N:  46% . 51%

ARG	ASP	ALA
GLY	ASN	ILE
GLU	ALA	R3
CYS	LEU	R24
	GLN	
	SER	
	GLY	R32
	ASN	
	SER	Y36
	GLN	
	GLU	RE4
	SER	
	VAL	D60
	THR	
	GLU	T97
	GLN	
	ASP	K107
	SER	ARG
	LYS	THR
	ASP	VAL
	SER	ALA
	THR	ALA
	TYR	PRO
	SER	SER
	LEU	VAL
	SER	PHE
	SER	ILE
	THR	PHE
	LEU	PRO
	THR	PRO
	LEU	SER
	SER	ASP
	LYS	GLU
	ALA	GLN
	ASP	LEU
	TYR	LYS
	GLU	SER
	LYS	GLY
	HIS	THR
	LYS	ALA
	VAL	SER
	TYR	VAL
	ALA	VAL
	CYS	CYS
	GLU	LEU
	VAL	LEU
	THR	ASN
	HIS	ASN
	GLN	PHE
	GLY	TYR
	LEU	PRO
	SER	ARG
	SER	GLU
	PRO	ALA
	VAL	LYS
	THR	VAL
	LYS	GLN
	SER	TRP
	PHE	LYS
	ASN	VAL

- Molecule 6: RM19R Fab Heavy Chain

Chain C:  52% 1% 47%

[illegible]

- Molecule 6: RM19R Fab Heavy Chain

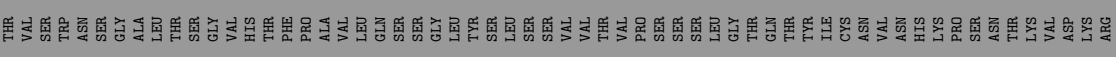
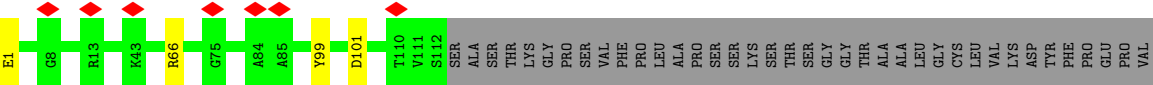
Chain J:  52% . 47%

[illegible]



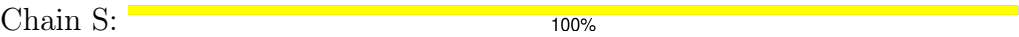
VAL  
GLU  
PRO  
LYS  
SER  
CYS  
ASP

• Molecule 6: RM19R Fab Heavy Chain



VAL  
GLU  
PRO  
LYS  
SER  
CYS  
ASP

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



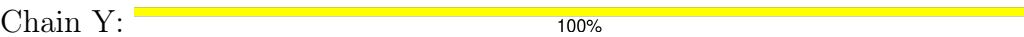
MAG1  
MAG2

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1  
MAG2

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



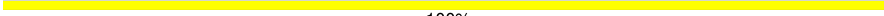
MAG1  
MAG2

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  50% 100%

  
MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%

NAG1  
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1  
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1  
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1  
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1  
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1  
NAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  100%

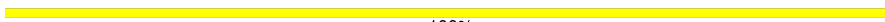


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:  50%  
 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:  50%  
 100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:   50% 100%




- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:  100%

NAG1  
NAG2

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  33%  
100%

NAG1  
NAG2  
BMA3

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  33%  
100%

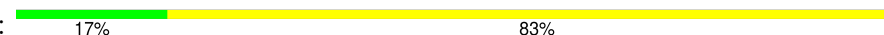
NAG1  
NAG2  
BMA3

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:  33%  
100%

NAG1  
NAG2  
BMA3

- Molecule 9: 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 W:  17%  
83%

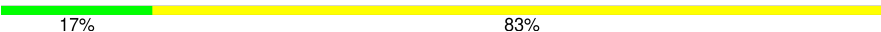
NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 9: 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 k:  17%  
83%

NAG1  
NAG2  
BMA3  
MAN4  
MAN5  
MAN6

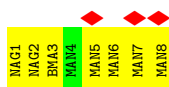
- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y: 



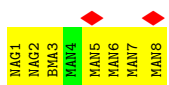
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 



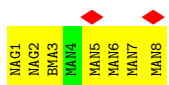
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 



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

Chain z: 



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f: 



- Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: alpha-L-fucopyranose-(1-6)-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	32186	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 ( $e^-/\text{\AA}^2$ )	51.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.001	Depositor
Minimum map value	-1.394	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.097	Depositor
Recommended contour level	0.46	Depositor
Map size (Å)	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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: NAG, MAN, BMA, FUC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.13	6/3628 (0.2%)	0.92	9/4926 (0.2%)
1	E	1.13	6/3628 (0.2%)	0.92	9/4926 (0.2%)
1	F	1.13	6/3628 (0.2%)	0.92	9/4926 (0.2%)
2	H	1.09	1/990 (0.1%)	1.05	7/1344 (0.5%)
2	O	1.09	1/990 (0.1%)	1.05	7/1344 (0.5%)
2	P	1.09	1/990 (0.1%)	1.05	7/1344 (0.5%)
3	L	1.04	2/852 (0.2%)	0.99	3/1156 (0.3%)
3	Q	1.04	2/852 (0.2%)	0.99	3/1156 (0.3%)
3	R	1.04	2/852 (0.2%)	0.99	3/1156 (0.3%)
4	B	1.20	2/1181 (0.2%)	0.87	0/1604
4	G	1.20	2/1181 (0.2%)	0.87	0/1604
4	I	1.20	2/1181 (0.2%)	0.87	1/1604 (0.1%)
5	D	1.10	1/837 (0.1%)	0.99	5/1137 (0.4%)
5	M	1.10	1/837 (0.1%)	0.99	5/1137 (0.4%)
5	N	1.10	1/837 (0.1%)	0.99	5/1137 (0.4%)
6	C	1.12	2/954 (0.2%)	0.98	3/1301 (0.2%)
6	J	1.13	2/954 (0.2%)	0.98	3/1301 (0.2%)
6	K	1.13	2/954 (0.2%)	0.98	3/1301 (0.2%)
All	All	1.12	42/25326 (0.2%)	0.95	82/34404 (0.2%)

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	91	ASP	CB-CG	-6.93	1.37	1.51
3	Q	91	ASP	CB-CG	-6.92	1.37	1.51
3	L	91	ASP	CB-CG	-6.91	1.37	1.51
1	F	418	CYS	CB-SG	-6.43	1.71	1.82
1	A	418	CYS	CB-SG	-6.41	1.71	1.82

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	66	ARG	NE-CZ-NH2	-9.87	115.36	120.30
2	P	66	ARG	NE-CZ-NH2	-9.82	115.39	120.30
2	O	66	ARG	NE-CZ-NH2	-9.77	115.41	120.30
6	K	66	ARG	NE-CZ-NH2	-9.22	115.69	120.30
6	C	66	ARG	NE-CZ-NH2	-9.19	115.71	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3552	0	3493	5	0
1	E	3552	0	3493	5	0
1	F	3552	0	3493	7	0
2	H	965	0	962	2	0
2	O	965	0	962	2	0
2	P	965	0	962	2	0
3	L	833	0	809	0	0
3	Q	833	0	809	0	0
3	R	833	0	809	0	0
4	B	1160	0	1142	2	0
4	G	1160	0	1142	2	0
4	I	1160	0	1142	2	0
5	D	817	0	786	2	0
5	M	817	0	786	2	0
5	N	817	0	786	2	0
6	C	930	0	897	0	0
6	J	930	0	897	0	0
6	K	930	0	897	0	0
7	0	28	0	25	0	0
7	1	28	0	25	0	0
7	2	28	0	25	0	0
7	3	28	0	25	0	0
7	4	28	0	25	0	0
7	5	28	0	25	0	0
7	6	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	S	28	0	25	0	0
7	U	28	0	25	0	0
7	V	28	0	25	0	0
7	Y	28	0	25	0	0
7	Z	28	0	25	0	0
7	a	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
7	d	28	0	25	0	0
7	e	28	0	25	0	0
7	g	28	0	25	0	0
7	i	28	0	25	0	0
7	j	28	0	25	0	0
7	m	28	0	25	0	0
7	n	28	0	25	0	0
7	o	28	0	25	0	0
7	p	28	0	25	0	0
7	q	28	0	25	0	0
7	r	28	0	25	0	0
7	s	28	0	25	0	0
7	u	28	0	25	0	0
7	w	28	0	25	0	0
7	x	28	0	25	0	0
8	T	39	0	34	0	0
8	h	39	0	34	0	0
8	v	39	0	34	0	0
9	W	72	0	61	0	0
9	k	72	0	61	0	0
9	y	72	0	61	0	0
10	X	94	0	79	0	0
10	l	94	0	79	0	0
10	z	94	0	79	0	0
11	7	24	0	22	0	0
11	f	24	0	22	0	0
11	t	24	0	22	0	0
12	A	56	0	52	1	0
12	B	28	0	26	0	0
12	E	56	0	52	1	0
12	F	56	0	52	1	0
12	G	28	0	26	0	0
12	I	28	0	26	0	0
All	All	26550	0	25839	32	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 32 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72(B):ASP:HB3	2:H:72(D):ARG:HG3	1.75	0.69
2:O:72(B):ASP:HB3	2:O:72(D):ARG:HG3	1.75	0.69
2:P:72(B):ASP:HB3	2:P:72(D):ARG:HG3	1.75	0.69
1:F:46:LYS:NZ	4:I:632:ASP:OD2	2.42	0.53
1:E:46:LYS:NZ	4:G:632:ASP:OD2	2.42	0.51

There are no symmetry-related clashes.

## 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	444/475 (94%)	425 (96%)	14 (3%)	5 (1%)	12	40
1	E	444/475 (94%)	425 (96%)	14 (3%)	5 (1%)	12	40
1	F	444/475 (94%)	425 (96%)	14 (3%)	5 (1%)	12	40
2	H	121/231 (52%)	114 (94%)	6 (5%)	1 (1%)	16	45
2	O	121/231 (52%)	114 (94%)	6 (5%)	1 (1%)	16	45
2	P	121/231 (52%)	114 (94%)	6 (5%)	1 (1%)	16	45
3	L	105/214 (49%)	99 (94%)	5 (5%)	1 (1%)	13	42
3	Q	105/214 (49%)	99 (94%)	5 (5%)	1 (1%)	13	42
3	R	105/214 (49%)	99 (94%)	5 (5%)	1 (1%)	13	42
4	B	144/153 (94%)	136 (94%)	8 (6%)	0	100	100
4	G	144/153 (94%)	136 (94%)	8 (6%)	0	100	100
4	I	144/153 (94%)	136 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D	103/214 (48%)	101 (98%)	2 (2%)	0	100	100
5	M	103/214 (48%)	101 (98%)	2 (2%)	0	100	100
5	N	103/214 (48%)	101 (98%)	2 (2%)	0	100	100
6	C	118/225 (52%)	116 (98%)	2 (2%)	0	100	100
6	J	118/225 (52%)	116 (98%)	2 (2%)	0	100	100
6	K	118/225 (52%)	116 (98%)	2 (2%)	0	100	100
All	All	3105/4536 (68%)	2973 (96%)	111 (4%)	21 (1%)	21	49

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	E	302	ASN
1	F	302	ASN
1	A	54	CYS
1	A	339	ASN

### 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	403/424 (95%)	402 (100%)	1 (0%)	92	96
1	E	403/424 (95%)	402 (100%)	1 (0%)	92	96
1	F	403/424 (95%)	402 (100%)	1 (0%)	92	96
2	H	103/197 (52%)	101 (98%)	2 (2%)	52	72
2	O	103/197 (52%)	101 (98%)	2 (2%)	52	72
2	P	103/197 (52%)	101 (98%)	2 (2%)	52	72
3	L	90/186 (48%)	89 (99%)	1 (1%)	70	82
3	Q	90/186 (48%)	89 (99%)	1 (1%)	70	82
3	R	90/186 (48%)	89 (99%)	1 (1%)	70	82
4	B	126/130 (97%)	125 (99%)	1 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	126/130 (97%)	125 (99%)	1 (1%)	79	87
4	I	126/130 (97%)	125 (99%)	1 (1%)	79	87
5	D	91/188 (48%)	91 (100%)	0	100	100
5	M	91/188 (48%)	91 (100%)	0	100	100
5	N	91/188 (48%)	91 (100%)	0	100	100
6	C	103/194 (53%)	103 (100%)	0	100	100
6	J	103/194 (53%)	103 (100%)	0	100	100
6	K	103/194 (53%)	103 (100%)	0	100	100
All	All	2748/3957 (69%)	2733 (100%)	15 (0%)	85	91

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	72(D)	ARG
3	R	90	GLN
3	Q	90	GLN
4	I	611	ASN
2	P	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	89	GLN
3	Q	89	GLN
3	R	89	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

117 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$
7	NAG	0	1	7,1	14,14,15	1.98	6 (42%)	17,19,21	1.18	2 (11%)
7	NAG	0	2	7	14,14,15	2.05	5 (35%)	17,19,21	0.89	1 (5%)
7	NAG	1	1	7,1	14,14,15	1.91	5 (35%)	17,19,21	1.35	3 (17%)
7	NAG	1	2	7	14,14,15	2.00	5 (35%)	17,19,21	0.85	0
7	NAG	2	1	7,1	14,14,15	1.92	3 (21%)	17,19,21	1.11	1 (5%)
7	NAG	2	2	7	14,14,15	1.93	6 (42%)	17,19,21	1.04	2 (11%)
7	NAG	3	1	7,1	14,14,15	2.10	7 (50%)	17,19,21	1.14	2 (11%)
7	NAG	3	2	7	14,14,15	2.06	6 (42%)	17,19,21	0.86	1 (5%)
7	NAG	4	1	7,1	14,14,15	2.05	6 (42%)	17,19,21	1.13	1 (5%)
7	NAG	4	2	7	14,14,15	1.98	5 (35%)	17,19,21	0.83	1 (5%)
7	NAG	5	1	7,1	14,14,15	2.18	5 (35%)	17,19,21	0.92	0
7	NAG	5	2	7	14,14,15	2.01	6 (42%)	17,19,21	0.89	1 (5%)
7	NAG	6	1	7,1	14,14,15	2.07	6 (42%)	17,19,21	1.18	2 (11%)
7	NAG	6	2	7	14,14,15	1.93	6 (42%)	17,19,21	0.96	1 (5%)
11	NAG	7	1	11,4	14,14,15	2.14	6 (42%)	17,19,21	1.42	3 (17%)
11	FUC	7	2	11	10,10,11	2.08	5 (50%)	14,14,16	0.65	0
7	NAG	S	1	7,1	14,14,15	2.00	5 (35%)	17,19,21	1.20	2 (11%)
7	NAG	S	2	7	14,14,15	2.00	4 (28%)	17,19,21	0.90	1 (5%)
8	NAG	T	1	8,1	14,14,15	1.98	6 (42%)	17,19,21	1.07	1 (5%)
8	NAG	T	2	8	14,14,15	1.98	6 (42%)	17,19,21	0.90	1 (5%)
8	BMA	T	3	8	11,11,12	1.95	6 (54%)	15,15,17	0.66	0
7	NAG	U	1	7,1	14,14,15	2.17	5 (35%)	17,19,21	1.00	0
7	NAG	U	2	7	14,14,15	2.05	6 (42%)	17,19,21	0.88	1 (5%)
7	NAG	V	1	7,1	14,14,15	2.08	4 (28%)	17,19,21	0.96	0
7	NAG	V	2	7	14,14,15	2.01	6 (42%)	17,19,21	0.91	1 (5%)
9	NAG	W	1	9,1	14,14,15	1.92	3 (21%)	17,19,21	1.15	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	W	2	9	14,14,15	1.80	6 (42%)	17,19,21	0.99	1 (5%)
9	BMA	W	3	9	11,11,12	1.34	1 (9%)	15,15,17	0.57	0
9	MAN	W	4	9	11,11,12	0.78	0	15,15,17	0.67	0
9	MAN	W	5	9	11,11,12	1.90	6 (54%)	15,15,17	0.69	0
9	MAN	W	6	9	11,11,12	1.89	4 (36%)	15,15,17	0.67	0
10	NAG	X	1	10,1	14,14,15	1.79	2 (14%)	17,19,21	1.26	2 (11%)
10	NAG	X	2	10	14,14,15	1.79	4 (28%)	17,19,21	1.09	2 (11%)
10	BMA	X	3	10	11,11,12	1.25	1 (9%)	15,15,17	0.61	0
10	MAN	X	4	10	11,11,12	0.72	0	15,15,17	0.65	0
10	MAN	X	5	10	11,11,12	1.93	5 (45%)	15,15,17	0.71	0
10	MAN	X	6	10	11,11,12	1.32	1 (9%)	15,15,17	0.75	0
10	MAN	X	7	10	11,11,12	1.91	4 (36%)	15,15,17	0.66	0
10	MAN	X	8	10	11,11,12	1.90	5 (45%)	15,15,17	0.73	0
7	NAG	Y	1	7,1	14,14,15	1.98	6 (42%)	17,19,21	1.18	2 (11%)
7	NAG	Y	2	7	14,14,15	2.05	5 (35%)	17,19,21	0.89	1 (5%)
7	NAG	Z	1	7,1	14,14,15	1.91	5 (35%)	17,19,21	1.35	3 (17%)
7	NAG	Z	2	7	14,14,15	2.00	5 (35%)	17,19,21	0.86	1 (5%)
7	NAG	a	1	7,1	14,14,15	1.93	3 (21%)	17,19,21	1.11	1 (5%)
7	NAG	a	2	7	14,14,15	1.93	6 (42%)	17,19,21	1.04	2 (11%)
7	NAG	b	1	7,1	14,14,15	2.09	7 (50%)	17,19,21	1.13	2 (11%)
7	NAG	b	2	7	14,14,15	2.06	6 (42%)	17,19,21	0.86	1 (5%)
7	NAG	c	1	7,1	14,14,15	2.05	6 (42%)	17,19,21	1.13	1 (5%)
7	NAG	c	2	7	14,14,15	1.99	5 (35%)	17,19,21	0.83	1 (5%)
7	NAG	d	1	7,1	14,14,15	2.18	5 (35%)	17,19,21	0.92	0
7	NAG	d	2	7	14,14,15	2.01	6 (42%)	17,19,21	0.88	1 (5%)
7	NAG	e	1	7,1	14,14,15	2.07	6 (42%)	17,19,21	1.18	2 (11%)
7	NAG	e	2	7	14,14,15	1.92	6 (42%)	17,19,21	0.95	1 (5%)
11	NAG	f	1	11,4	14,14,15	2.13	6 (42%)	17,19,21	1.42	3 (17%)
11	FUC	f	2	11	10,10,11	2.07	5 (50%)	14,14,16	0.65	0
7	NAG	g	1	7,1	14,14,15	2.00	5 (35%)	17,19,21	1.20	2 (11%)
7	NAG	g	2	7	14,14,15	2.00	4 (28%)	17,19,21	0.90	1 (5%)
8	NAG	h	1	8,1	14,14,15	1.98	6 (42%)	17,19,21	1.07	1 (5%)
8	NAG	h	2	8	14,14,15	1.97	6 (42%)	17,19,21	0.90	1 (5%)
8	BMA	h	3	8	11,11,12	1.94	6 (54%)	15,15,17	0.66	0
7	NAG	i	1	7,1	14,14,15	2.16	5 (35%)	17,19,21	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	i	2	7	14,14,15	2.05	6 (42%)	17,19,21	0.88	1 (5%)
7	NAG	j	1	7,1	14,14,15	2.08	4 (28%)	17,19,21	0.96	0
7	NAG	j	2	7	14,14,15	2.01	6 (42%)	17,19,21	0.91	1 (5%)
9	NAG	k	1	9,1	14,14,15	1.92	3 (21%)	17,19,21	1.15	2 (11%)
9	NAG	k	2	9	14,14,15	1.80	6 (42%)	17,19,21	0.99	1 (5%)
9	BMA	k	3	9	11,11,12	1.34	1 (9%)	15,15,17	0.57	0
9	MAN	k	4	9	11,11,12	0.77	0	15,15,17	0.67	0
9	MAN	k	5	9	11,11,12	1.91	5 (45%)	15,15,17	0.69	0
9	MAN	k	6	9	11,11,12	1.89	4 (36%)	15,15,17	0.66	0
10	NAG	l	1	10,1	14,14,15	1.80	2 (14%)	17,19,21	1.26	2 (11%)
10	NAG	l	2	10	14,14,15	1.78	4 (28%)	17,19,21	1.09	2 (11%)
10	BMA	l	3	10	11,11,12	1.25	1 (9%)	15,15,17	0.61	0
10	MAN	l	4	10	11,11,12	0.71	0	15,15,17	0.65	0
10	MAN	l	5	10	11,11,12	1.93	5 (45%)	15,15,17	0.71	0
10	MAN	l	6	10	11,11,12	1.32	1 (9%)	15,15,17	0.75	0
10	MAN	l	7	10	11,11,12	1.90	5 (45%)	15,15,17	0.66	0
10	MAN	l	8	10	11,11,12	1.90	5 (45%)	15,15,17	0.73	0
7	NAG	m	1	7,1	14,14,15	1.98	6 (42%)	17,19,21	1.17	2 (11%)
7	NAG	m	2	7	14,14,15	2.05	4 (28%)	17,19,21	0.89	1 (5%)
7	NAG	n	1	7,1	14,14,15	1.92	5 (35%)	17,19,21	1.35	3 (17%)
7	NAG	n	2	7	14,14,15	2.00	5 (35%)	17,19,21	0.86	1 (5%)
7	NAG	o	1	7,1	14,14,15	1.92	3 (21%)	17,19,21	1.11	1 (5%)
7	NAG	o	2	7	14,14,15	1.94	6 (42%)	17,19,21	1.04	2 (11%)
7	NAG	p	1	7,1	14,14,15	2.10	7 (50%)	17,19,21	1.13	2 (11%)
7	NAG	p	2	7	14,14,15	2.07	6 (42%)	17,19,21	0.86	1 (5%)
7	NAG	q	1	7,1	14,14,15	2.04	6 (42%)	17,19,21	1.13	1 (5%)
7	NAG	q	2	7	14,14,15	1.99	5 (35%)	17,19,21	0.83	1 (5%)
7	NAG	r	1	7,1	14,14,15	2.18	5 (35%)	17,19,21	0.92	0
7	NAG	r	2	7	14,14,15	2.02	6 (42%)	17,19,21	0.89	1 (5%)
7	NAG	s	1	7,1	14,14,15	2.07	6 (42%)	17,19,21	1.19	2 (11%)
7	NAG	s	2	7	14,14,15	1.93	6 (42%)	17,19,21	0.96	1 (5%)
11	NAG	t	1	11,4	14,14,15	2.13	6 (42%)	17,19,21	1.42	3 (17%)
11	FUC	t	2	11	10,10,11	2.08	5 (50%)	14,14,16	0.65	0
7	NAG	u	1	7,1	14,14,15	2.01	5 (35%)	17,19,21	1.20	2 (11%)
7	NAG	u	2	7	14,14,15	1.99	4 (28%)	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	v	1	8,1	14,14,15	1.98	6 (42%)	17,19,21	1.07	1 (5%)
8	NAG	v	2	8	14,14,15	1.97	6 (42%)	17,19,21	0.90	1 (5%)
8	BMA	v	3	8	11,11,12	1.95	5 (45%)	15,15,17	0.65	0
7	NAG	w	1	7,1	14,14,15	2.16	5 (35%)	17,19,21	1.00	0
7	NAG	w	2	7	14,14,15	2.06	6 (42%)	17,19,21	0.88	1 (5%)
7	NAG	x	1	7,1	14,14,15	2.08	4 (28%)	17,19,21	0.96	0
7	NAG	x	2	7	14,14,15	2.01	6 (42%)	17,19,21	0.91	1 (5%)
9	NAG	y	1	9,1	14,14,15	1.92	3 (21%)	17,19,21	1.15	2 (11%)
9	NAG	y	2	9	14,14,15	1.80	6 (42%)	17,19,21	0.99	1 (5%)
9	BMA	y	3	9	11,11,12	1.34	1 (9%)	15,15,17	0.58	0
9	MAN	y	4	9	11,11,12	0.77	0	15,15,17	0.67	0
9	MAN	y	5	9	11,11,12	1.91	6 (54%)	15,15,17	0.69	0
9	MAN	y	6	9	11,11,12	1.89	4 (36%)	15,15,17	0.67	0
10	NAG	z	1	10,1	14,14,15	1.79	2 (14%)	17,19,21	1.26	2 (11%)
10	NAG	z	2	10	14,14,15	1.78	4 (28%)	17,19,21	1.08	2 (11%)
10	BMA	z	3	10	11,11,12	1.25	1 (9%)	15,15,17	0.61	0
10	MAN	z	4	10	11,11,12	0.71	0	15,15,17	0.65	0
10	MAN	z	5	10	11,11,12	1.93	5 (45%)	15,15,17	0.71	0
10	MAN	z	6	10	11,11,12	1.33	1 (9%)	15,15,17	0.76	0
10	MAN	z	7	10	11,11,12	1.91	6 (54%)	15,15,17	0.66	0
10	MAN	z	8	10	11,11,12	1.90	5 (45%)	15,15,17	0.73	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
7	NAG	0	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	0	2	7	-	0/6/23/26	0/1/1/1
7	NAG	1	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	1	2	7	-	0/6/23/26	0/1/1/1
7	NAG	2	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	2	2	7	-	0/6/23/26	0/1/1/1
7	NAG	3	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	3	2	7	-	0/6/23/26	0/1/1/1
7	NAG	4	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	4	2	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	5	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	5	2	7	-	0/6/23/26	0/1/1/1
7	NAG	6	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	6	2	7	-	0/6/23/26	0/1/1/1
11	NAG	7	1	11,4	-	0/6/23/26	0/1/1/1
11	FUC	7	2	11	-	-	0/1/1/1
7	NAG	S	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
8	NAG	T	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	T	2	8	-	0/6/23/26	0/1/1/1
8	BMA	T	3	8	-	0/2/19/22	0/1/1/1
7	NAG	U	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	U	2	7	-	0/6/23/26	0/1/1/1
7	NAG	V	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	V	2	7	-	0/6/23/26	0/1/1/1
9	NAG	W	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	W	2	9	-	0/6/23/26	0/1/1/1
9	BMA	W	3	9	-	1/2/19/22	0/1/1/1
9	MAN	W	4	9	-	2/2/19/22	0/1/1/1
9	MAN	W	5	9	-	0/2/19/22	0/1/1/1
9	MAN	W	6	9	-	0/2/19/22	0/1/1/1
10	NAG	X	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	X	2	10	-	0/6/23/26	0/1/1/1
10	BMA	X	3	10	-	0/2/19/22	0/1/1/1
10	MAN	X	4	10	-	1/2/19/22	0/1/1/1
10	MAN	X	5	10	-	1/2/19/22	0/1/1/1
10	MAN	X	6	10	-	1/2/19/22	0/1/1/1
10	MAN	X	7	10	-	0/2/19/22	0/1/1/1
10	MAN	X	8	10	-	0/2/19/22	0/1/1/1
7	NAG	Y	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	0/6/23/26	0/1/1/1
7	NAG	Z	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	0/6/23/26	0/1/1/1
7	NAG	a	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	0/6/23/26	0/1/1/1
7	NAG	b	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	0/6/23/26	0/1/1/1
7	NAG	c	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	NAG	d	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
7	NAG	e	1	7,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	e	2	7	-	0/6/23/26	0/1/1/1
11	NAG	f	1	11,4	-	0/6/23/26	0/1/1/1
11	FUC	f	2	11	-	-	0/1/1/1
7	NAG	g	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	g	2	7	-	0/6/23/26	0/1/1/1
8	NAG	h	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	h	2	8	-	0/6/23/26	0/1/1/1
8	BMA	h	3	8	-	0/2/19/22	0/1/1/1
7	NAG	i	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	0/6/23/26	0/1/1/1
7	NAG	j	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	j	2	7	-	0/6/23/26	0/1/1/1
9	NAG	k	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	k	2	9	-	0/6/23/26	0/1/1/1
9	BMA	k	3	9	-	1/2/19/22	0/1/1/1
9	MAN	k	4	9	-	2/2/19/22	0/1/1/1
9	MAN	k	5	9	-	0/2/19/22	0/1/1/1
9	MAN	k	6	9	-	0/2/19/22	0/1/1/1
10	NAG	l	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	l	2	10	-	0/6/23/26	0/1/1/1
10	BMA	l	3	10	-	0/2/19/22	0/1/1/1
10	MAN	l	4	10	-	1/2/19/22	0/1/1/1
10	MAN	l	5	10	-	1/2/19/22	0/1/1/1
10	MAN	l	6	10	-	1/2/19/22	0/1/1/1
10	MAN	l	7	10	-	0/2/19/22	0/1/1/1
10	MAN	l	8	10	-	0/2/19/22	0/1/1/1
7	NAG	m	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	m	2	7	-	0/6/23/26	0/1/1/1
7	NAG	n	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	n	2	7	-	0/6/23/26	0/1/1/1
7	NAG	o	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	o	2	7	-	0/6/23/26	0/1/1/1
7	NAG	p	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	p	2	7	-	0/6/23/26	0/1/1/1
7	NAG	q	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	q	2	7	-	0/6/23/26	0/1/1/1
7	NAG	r	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	r	2	7	-	0/6/23/26	0/1/1/1
7	NAG	s	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	s	2	7	-	0/6/23/26	0/1/1/1
11	NAG	t	1	11,4	-	0/6/23/26	0/1/1/1
11	FUC	t	2	11	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	u	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	u	2	7	-	0/6/23/26	0/1/1/1
8	NAG	v	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	v	2	8	-	0/6/23/26	0/1/1/1
8	BMA	v	3	8	-	0/2/19/22	0/1/1/1
7	NAG	w	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	w	2	7	-	0/6/23/26	0/1/1/1
7	NAG	x	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	x	2	7	-	0/6/23/26	0/1/1/1
9	NAG	y	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	y	2	9	-	0/6/23/26	0/1/1/1
9	BMA	y	3	9	-	1/2/19/22	0/1/1/1
9	MAN	y	4	9	-	2/2/19/22	0/1/1/1
9	MAN	y	5	9	-	0/2/19/22	0/1/1/1
9	MAN	y	6	9	-	0/2/19/22	0/1/1/1
10	NAG	z	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	z	2	10	-	0/6/23/26	0/1/1/1
10	BMA	z	3	10	-	0/2/19/22	0/1/1/1
10	MAN	z	4	10	-	1/2/19/22	0/1/1/1
10	MAN	z	5	10	-	1/2/19/22	0/1/1/1
10	MAN	z	6	10	-	1/2/19/22	0/1/1/1
10	MAN	z	7	10	-	0/2/19/22	0/1/1/1
10	MAN	z	8	10	-	0/2/19/22	0/1/1/1

The worst 5 of 534 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	r	1	NAG	C1-C2	5.92	1.60	1.52
7	d	1	NAG	C1-C2	5.91	1.60	1.52
7	5	1	NAG	C1-C2	5.88	1.60	1.52
7	U	1	NAG	C1-C2	5.70	1.60	1.52
7	w	1	NAG	C1-C2	5.67	1.60	1.52

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	t	1	NAG	C8-C7-N2	3.42	121.79	116.12
11	f	1	NAG	C8-C7-N2	3.42	121.79	116.12
11	7	1	NAG	C8-C7-N2	3.42	121.78	116.12
7	n	1	NAG	C1-C2-N2	-3.16	105.45	110.43
7	Z	1	NAG	C1-C2-N2	-3.15	105.47	110.43

There are no chirality outliers.

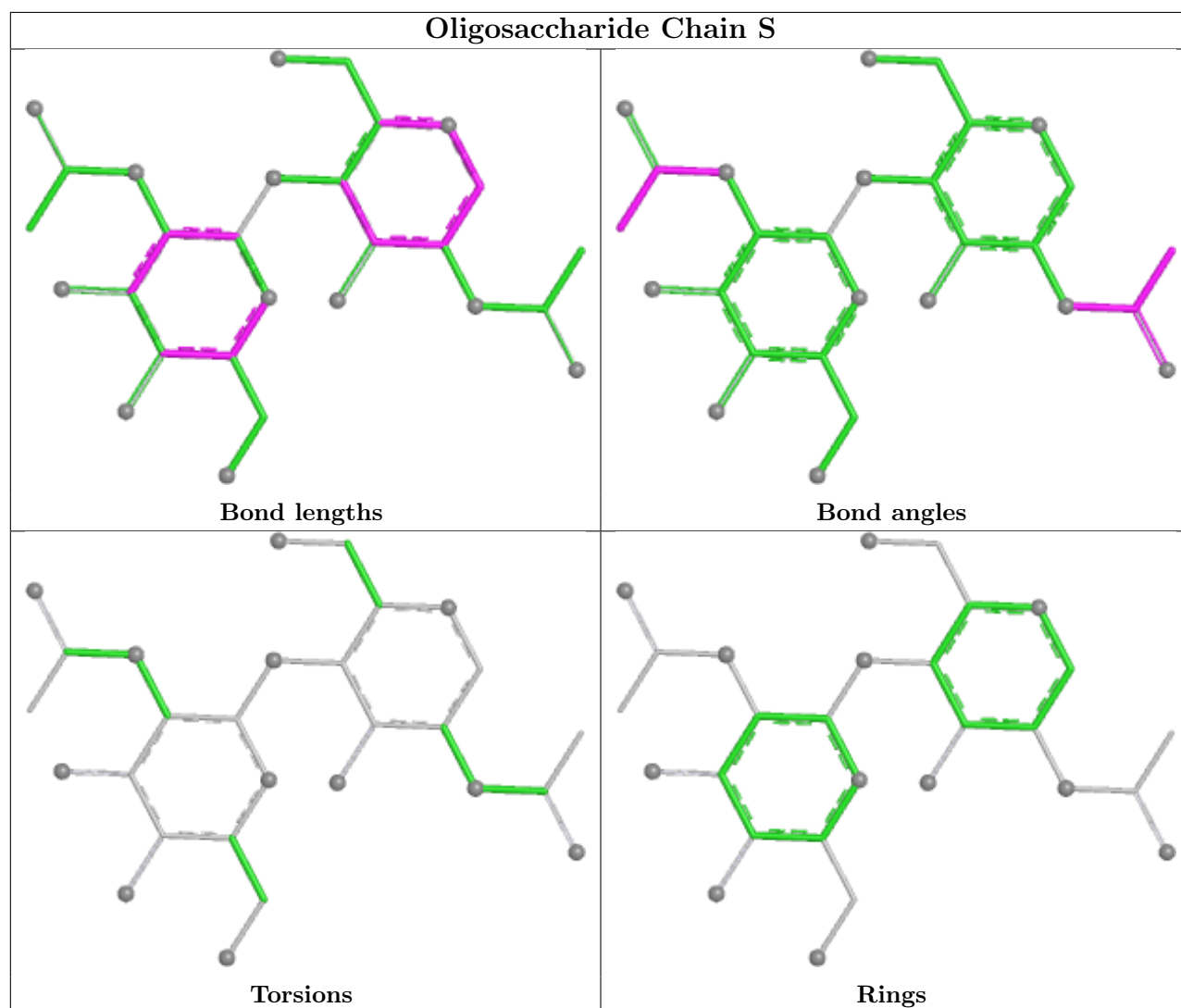
5 of 18 torsion outliers are listed below:

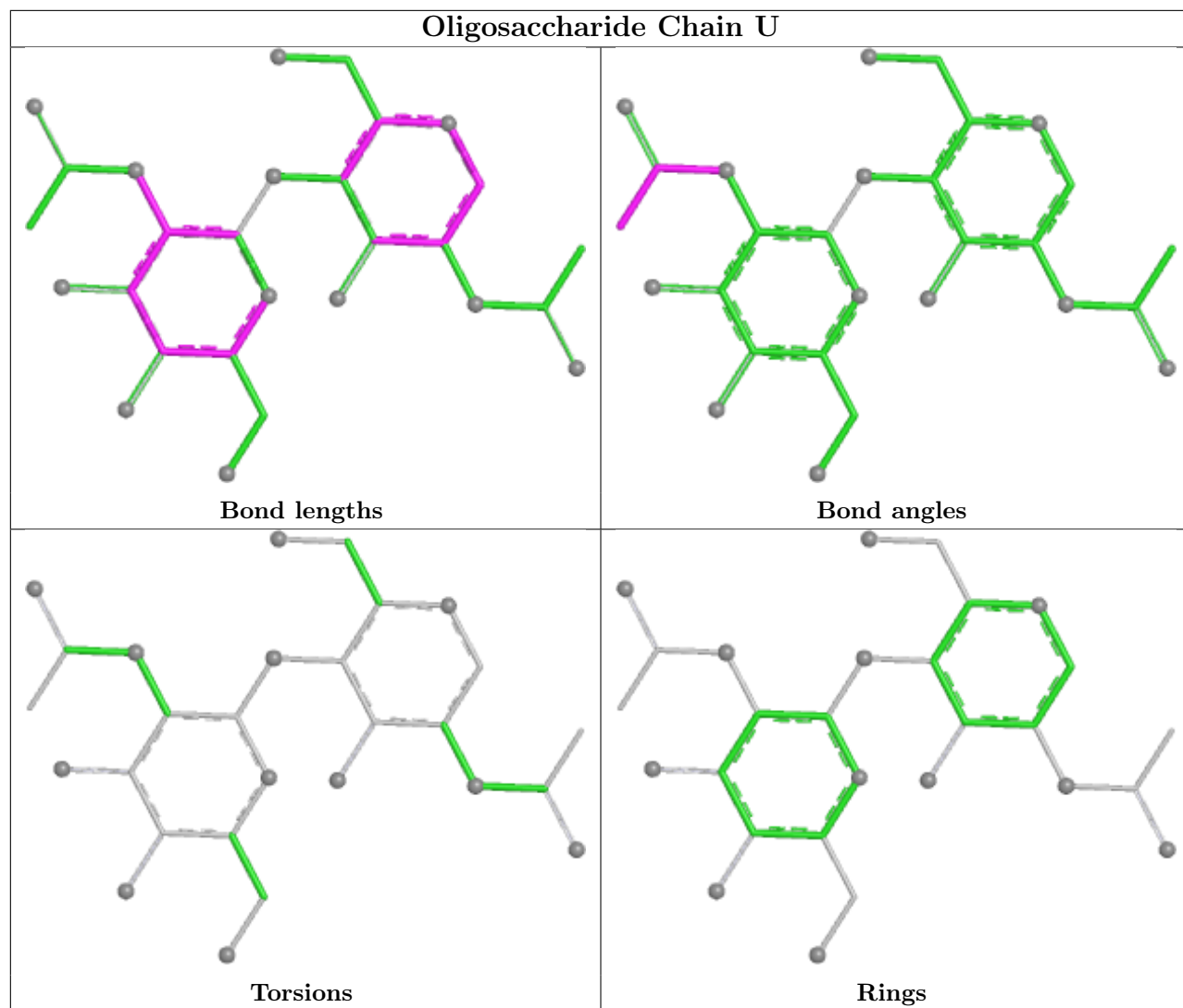
Mol	Chain	Res	Type	Atoms
9	W	4	MAN	O5-C5-C6-O6
9	k	4	MAN	O5-C5-C6-O6
9	y	4	MAN	O5-C5-C6-O6
10	X	5	MAN	O5-C5-C6-O6
10	l	5	MAN	O5-C5-C6-O6

There are no ring outliers.

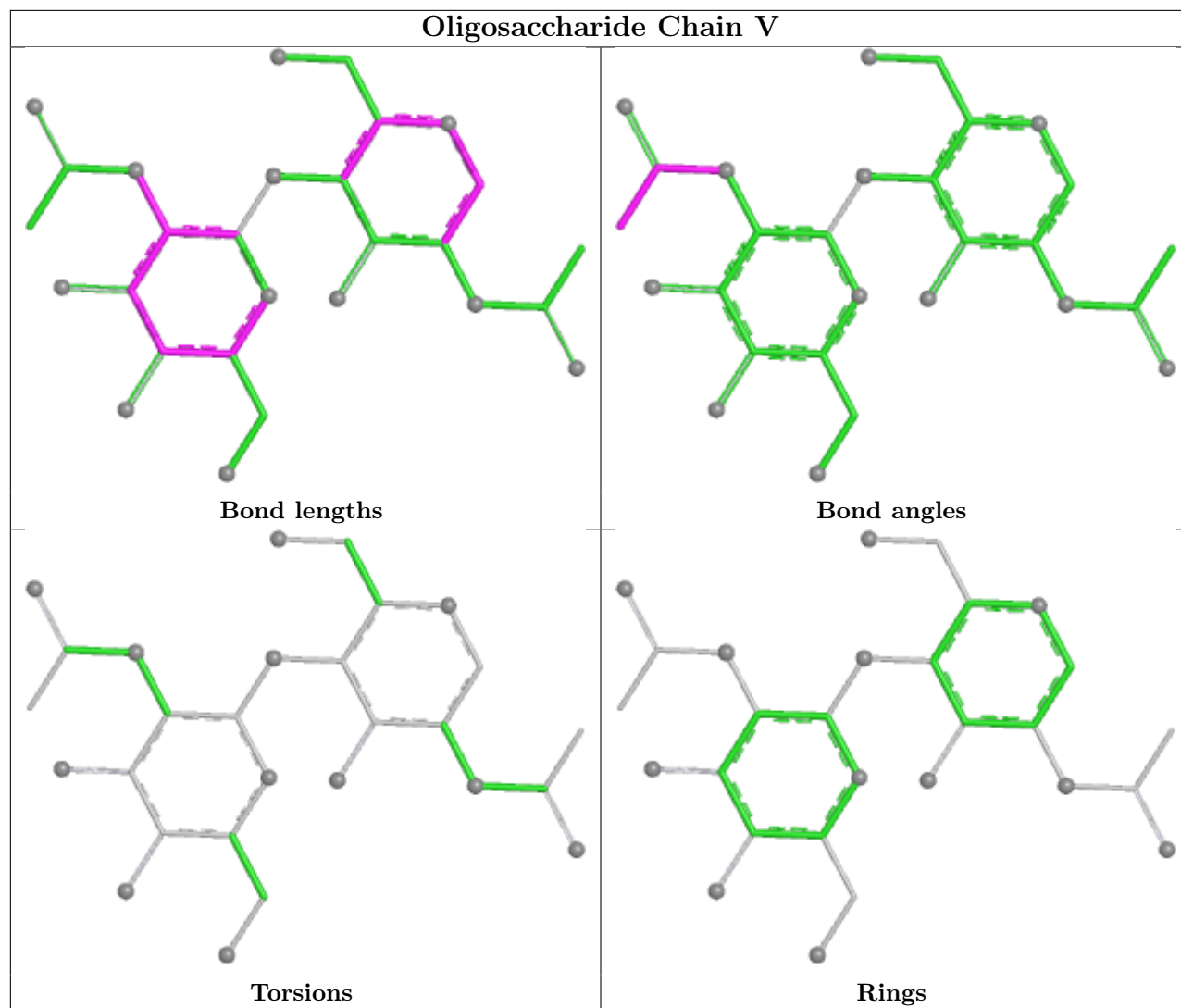
No monomer is involved in short contacts.

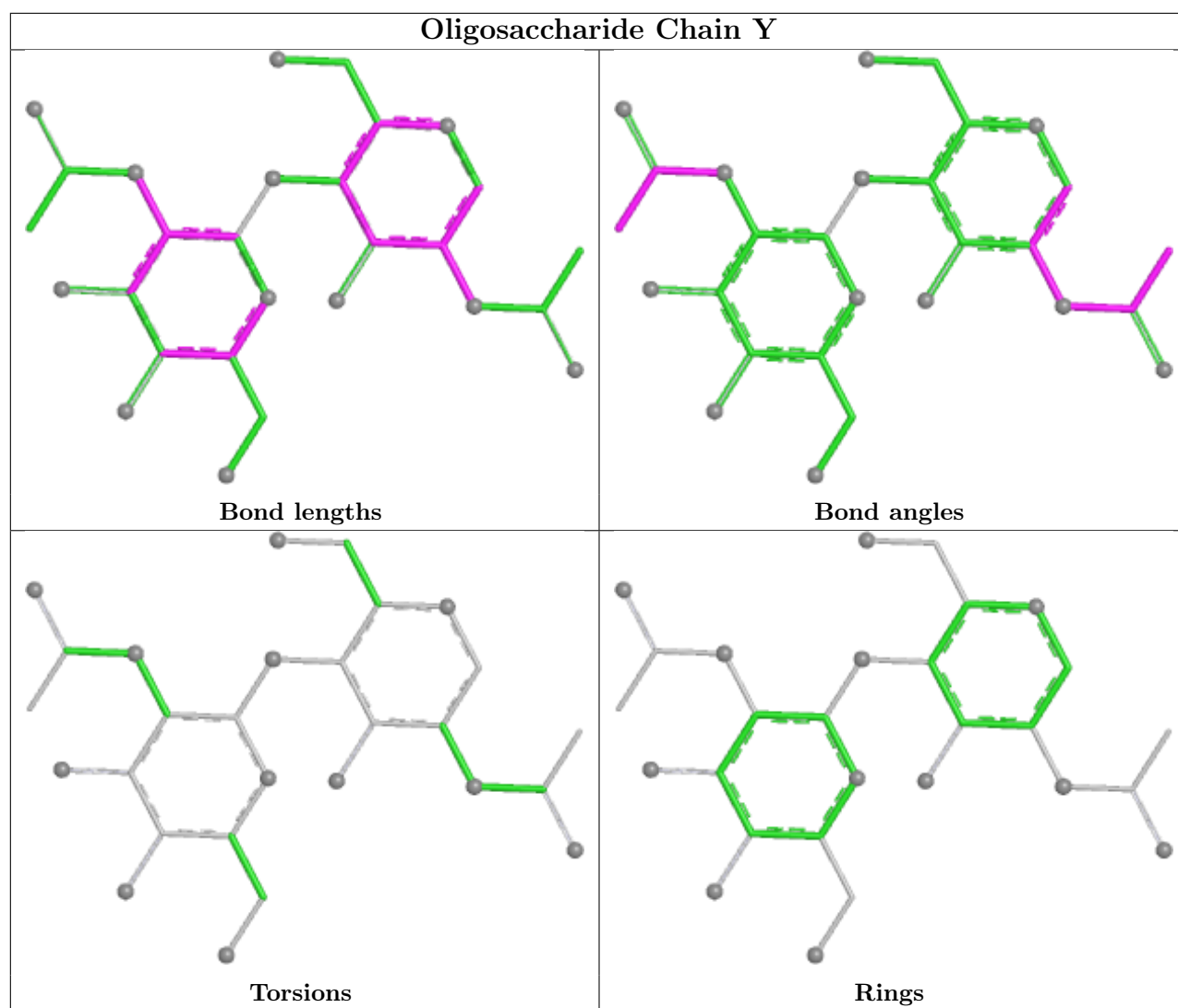
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

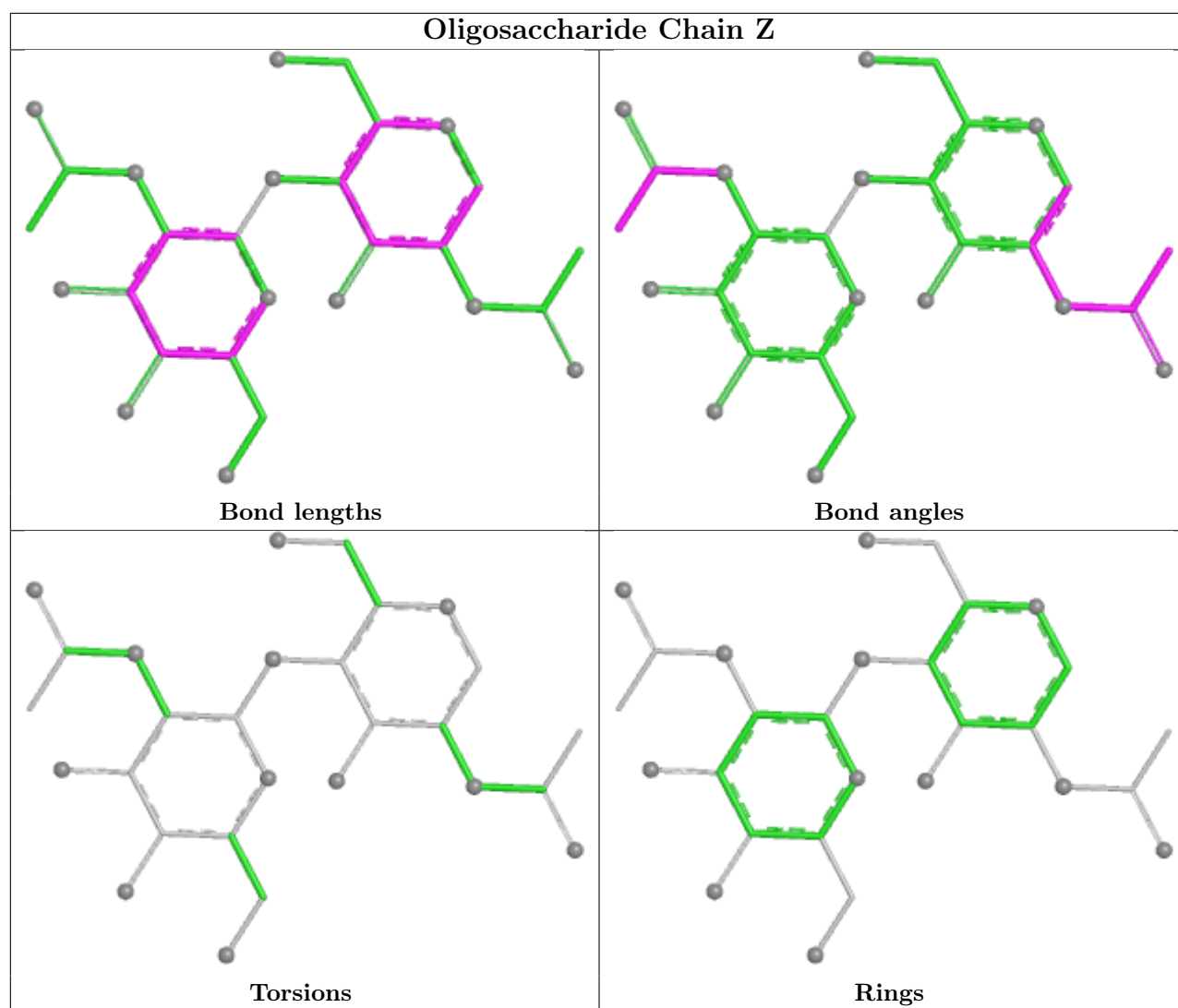


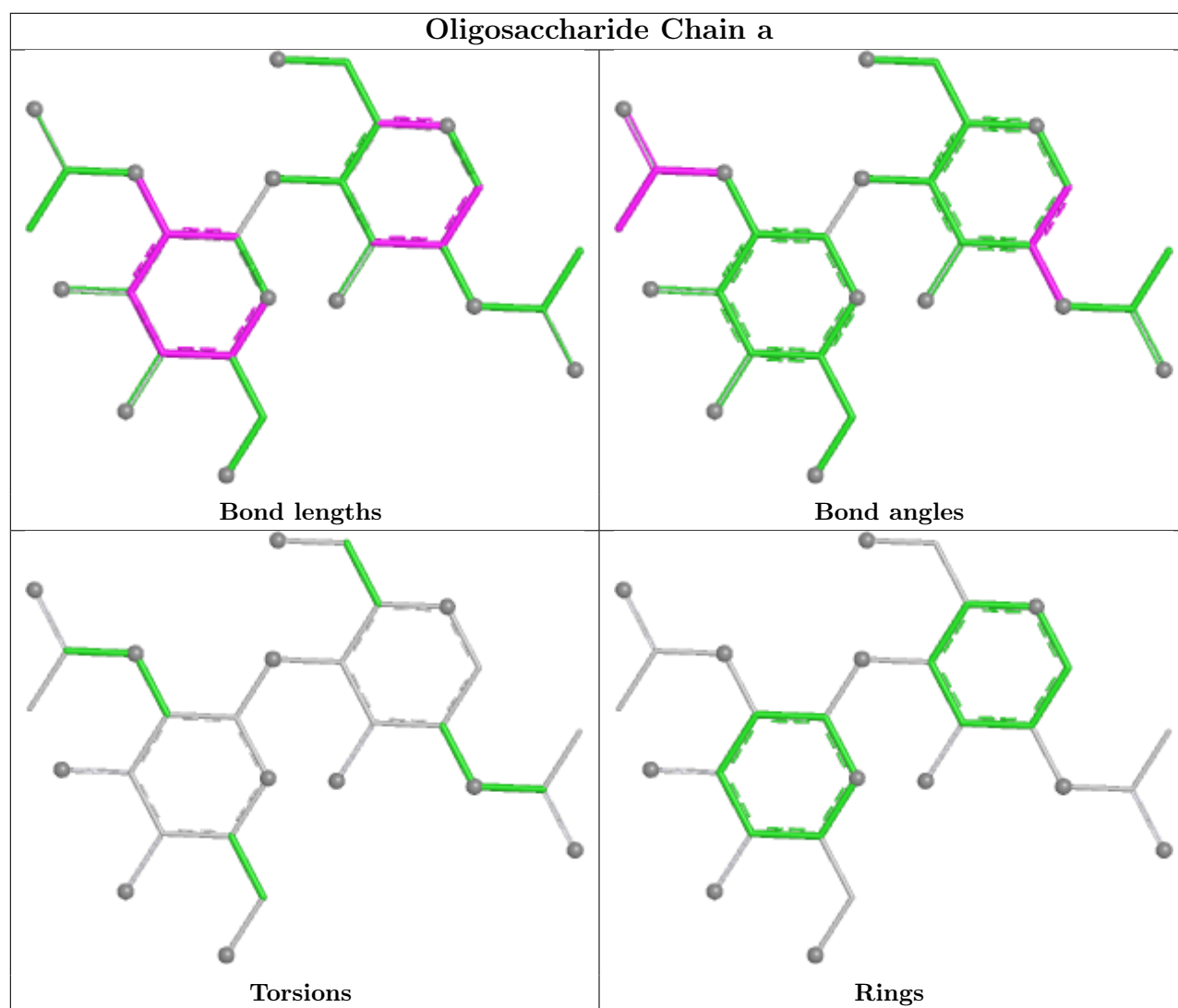


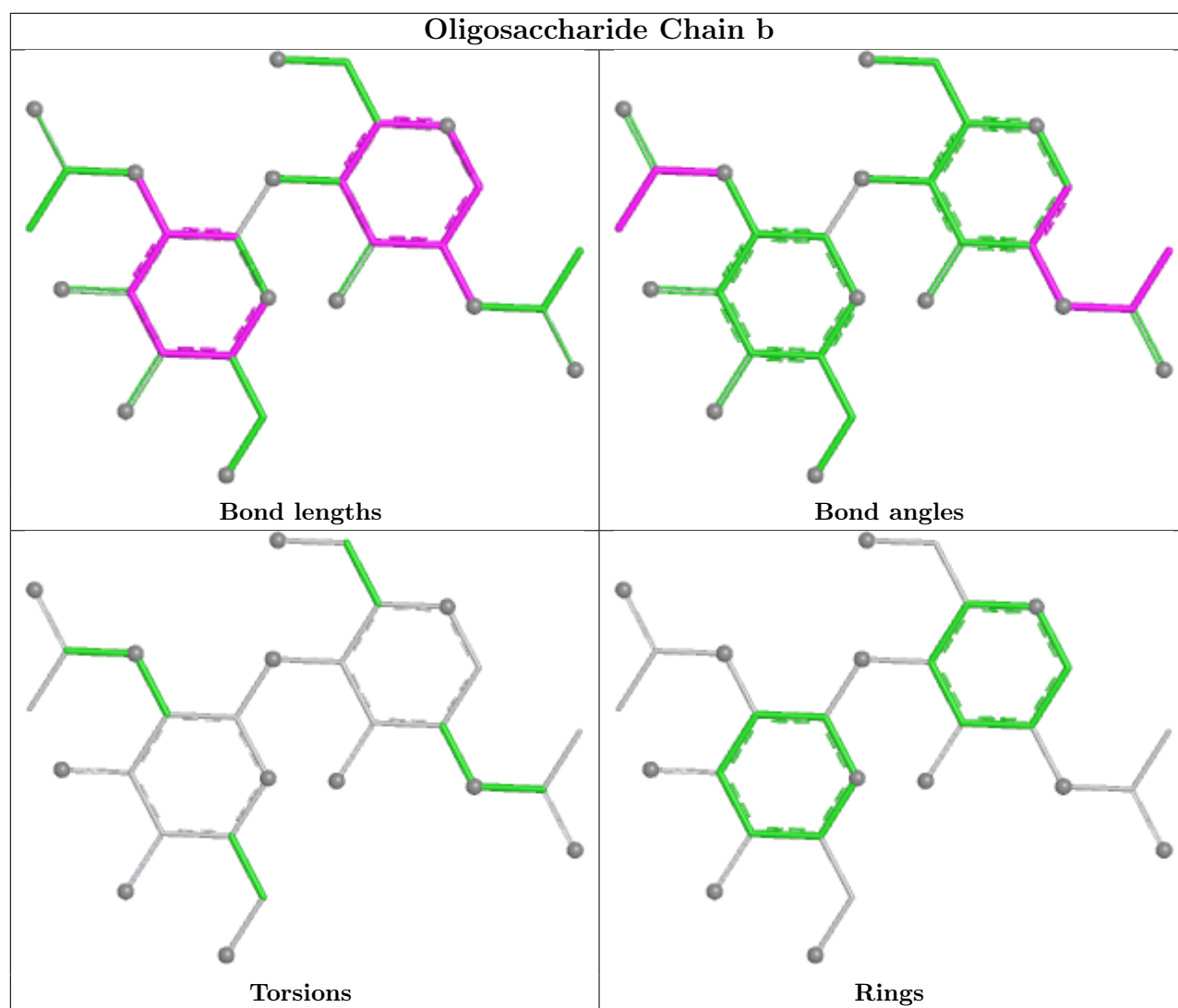


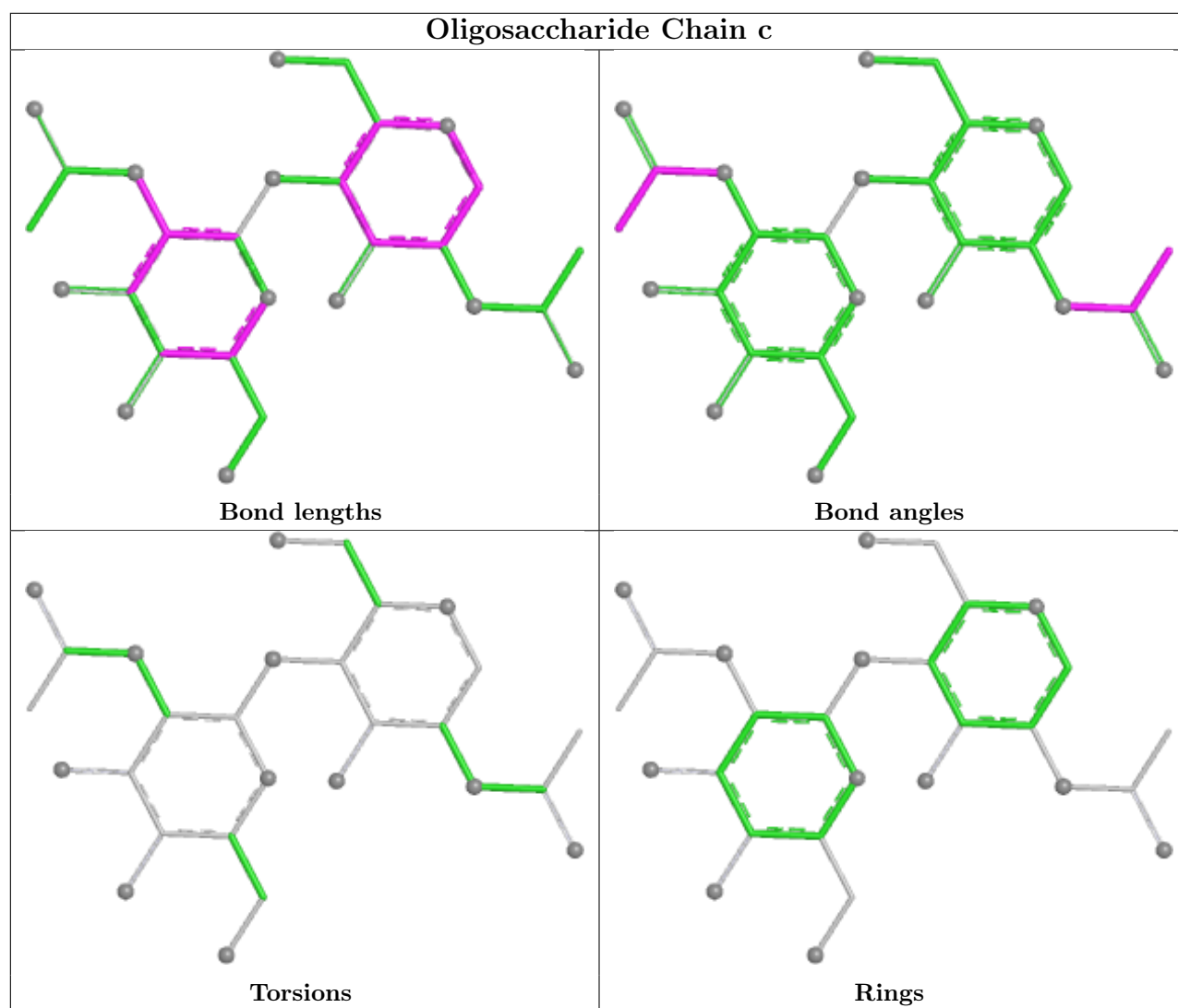


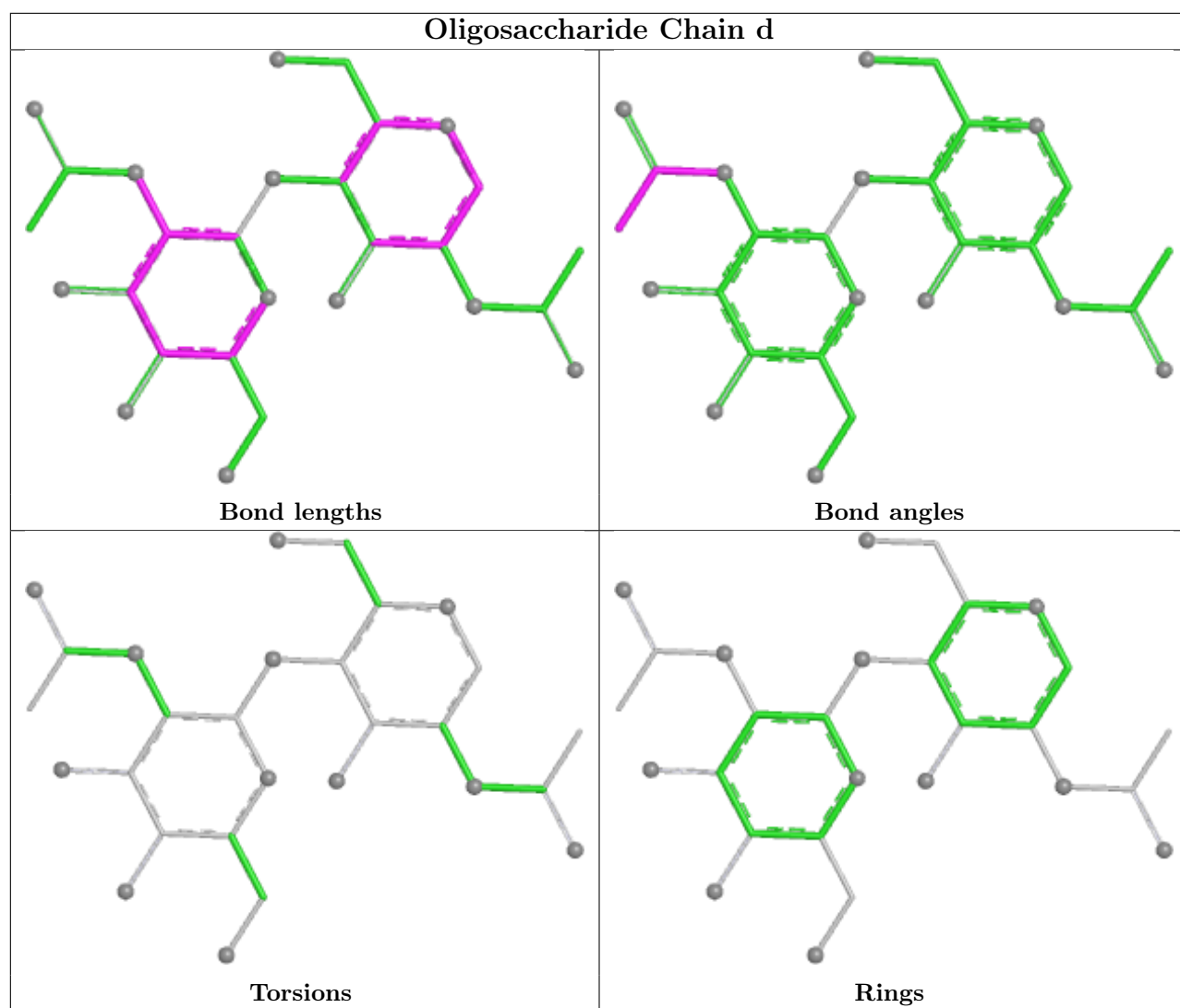


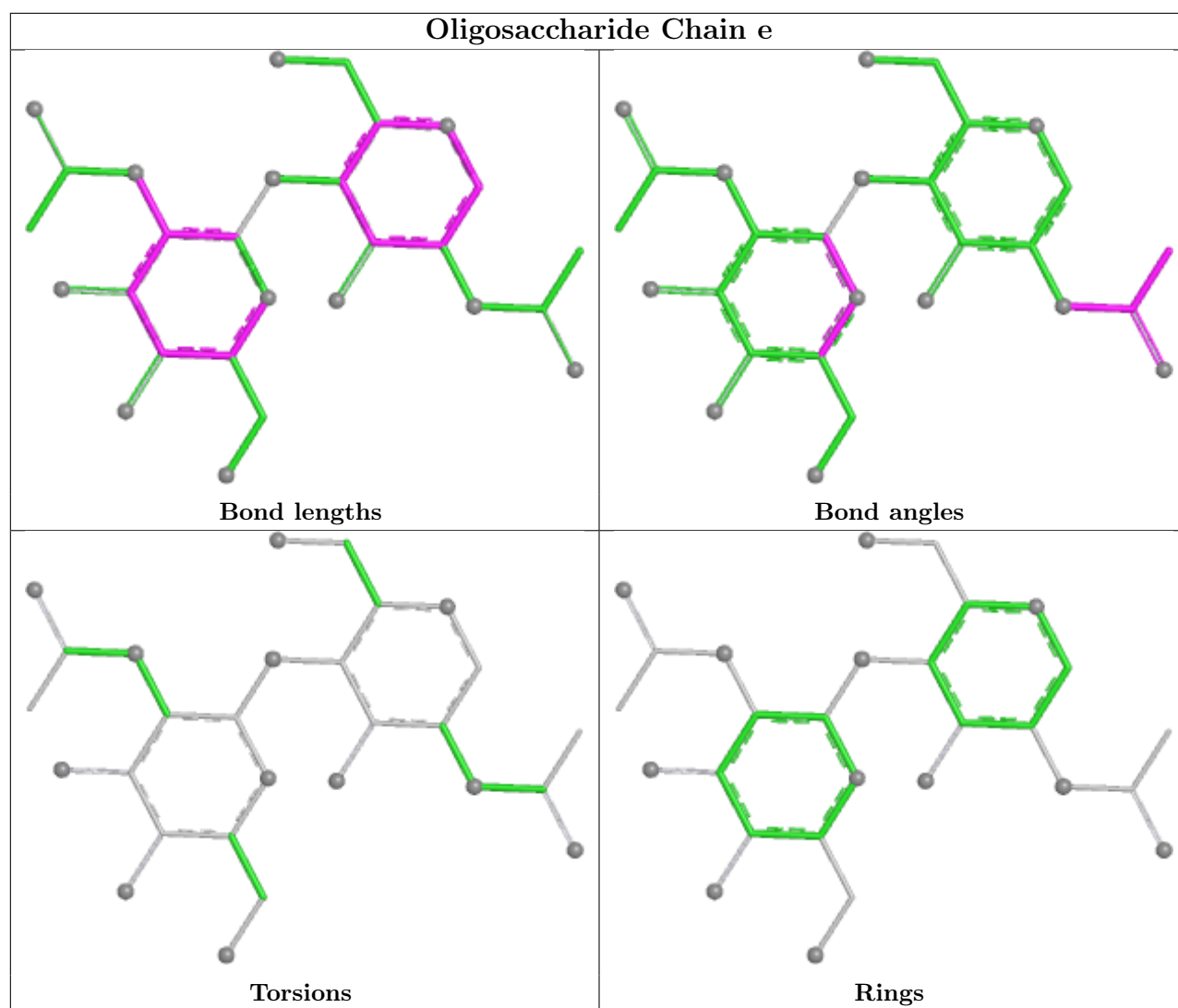




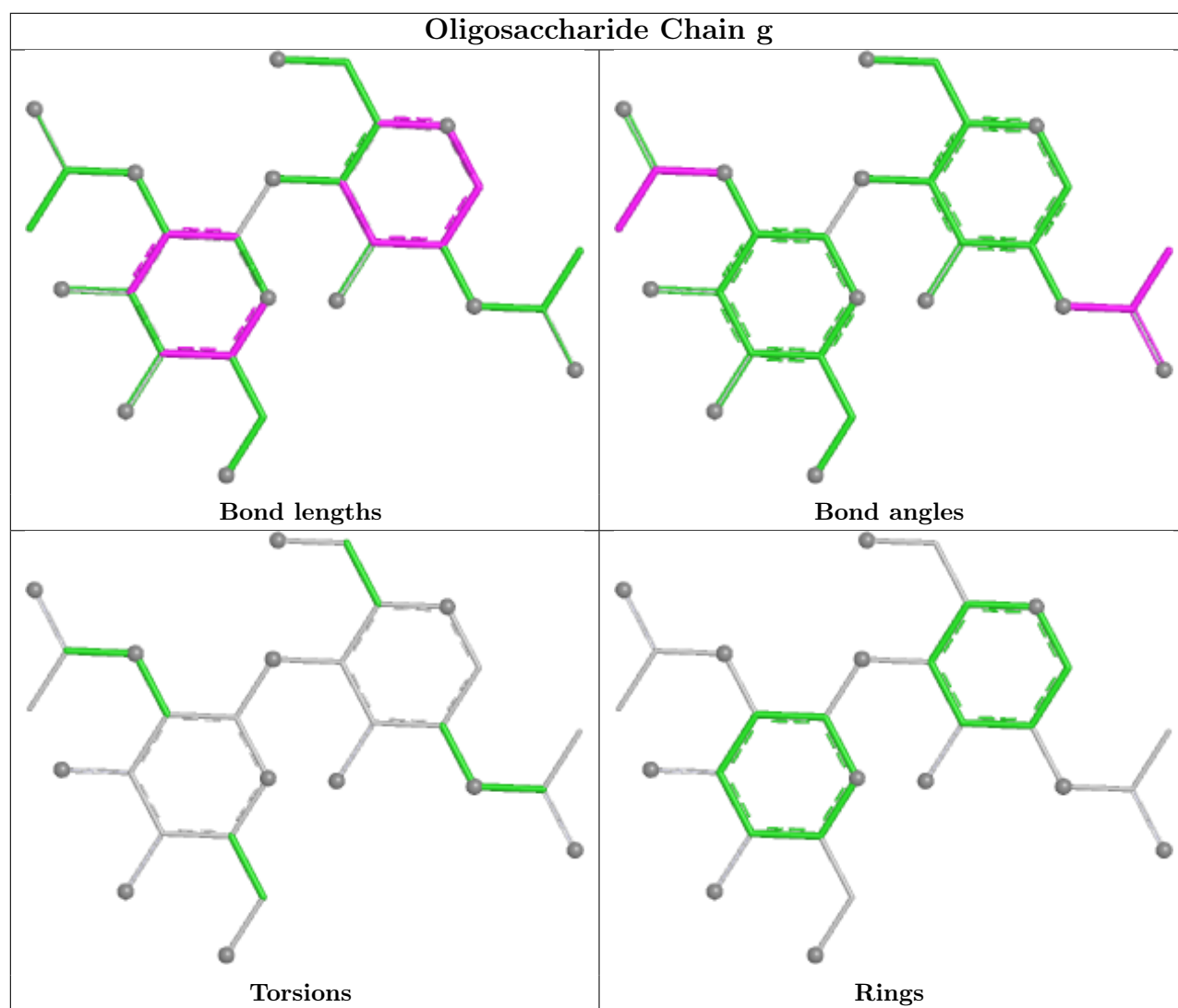


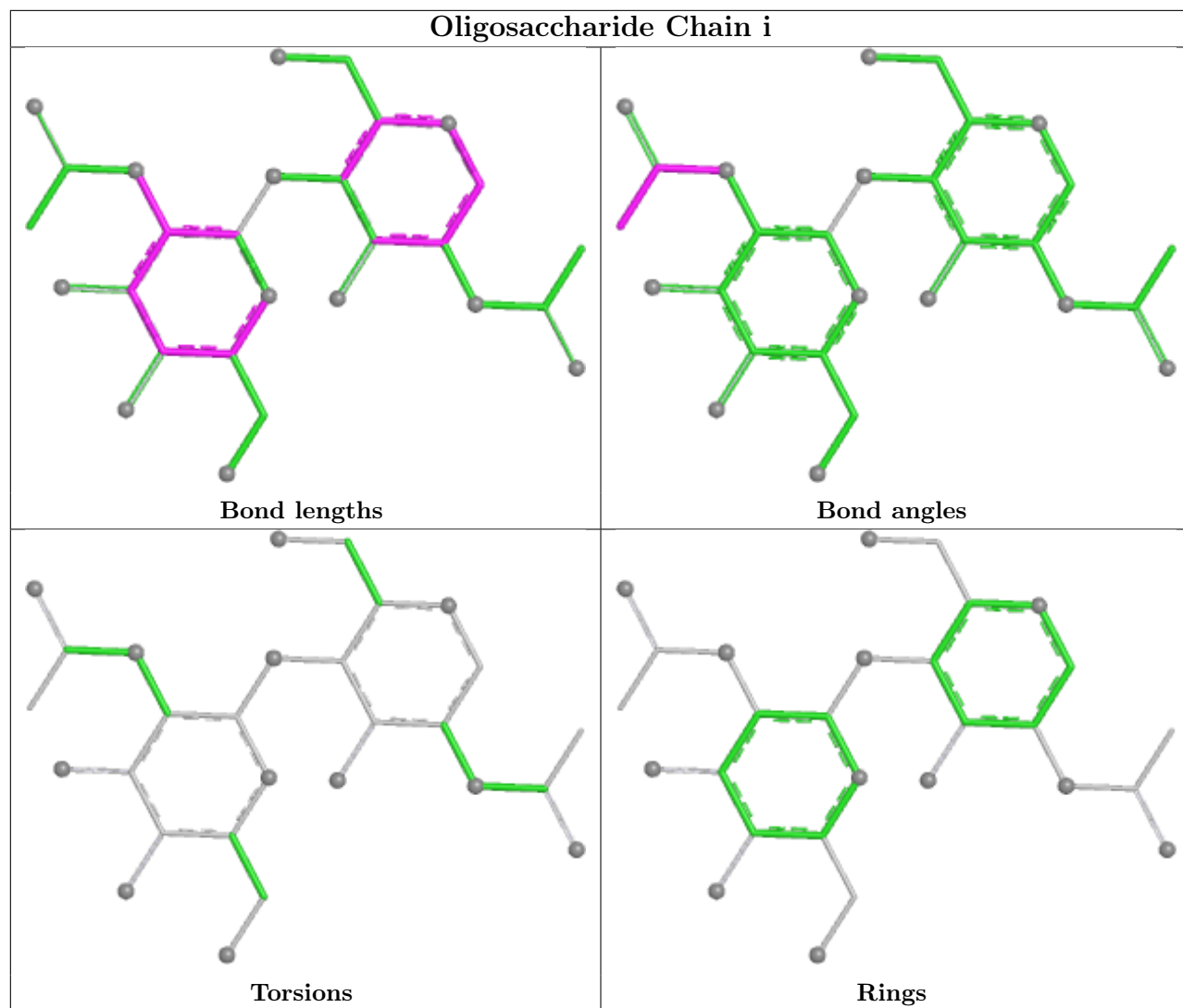


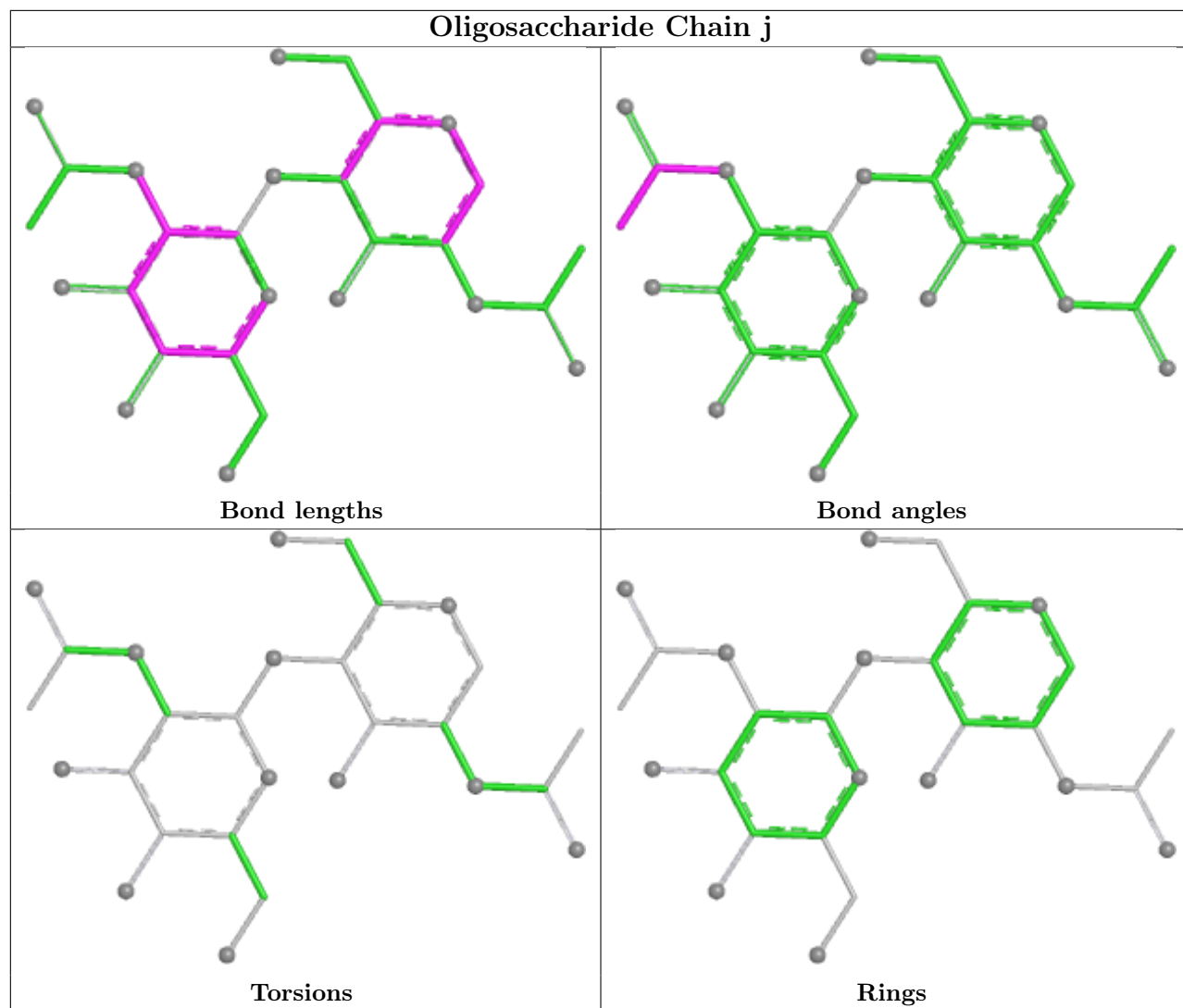


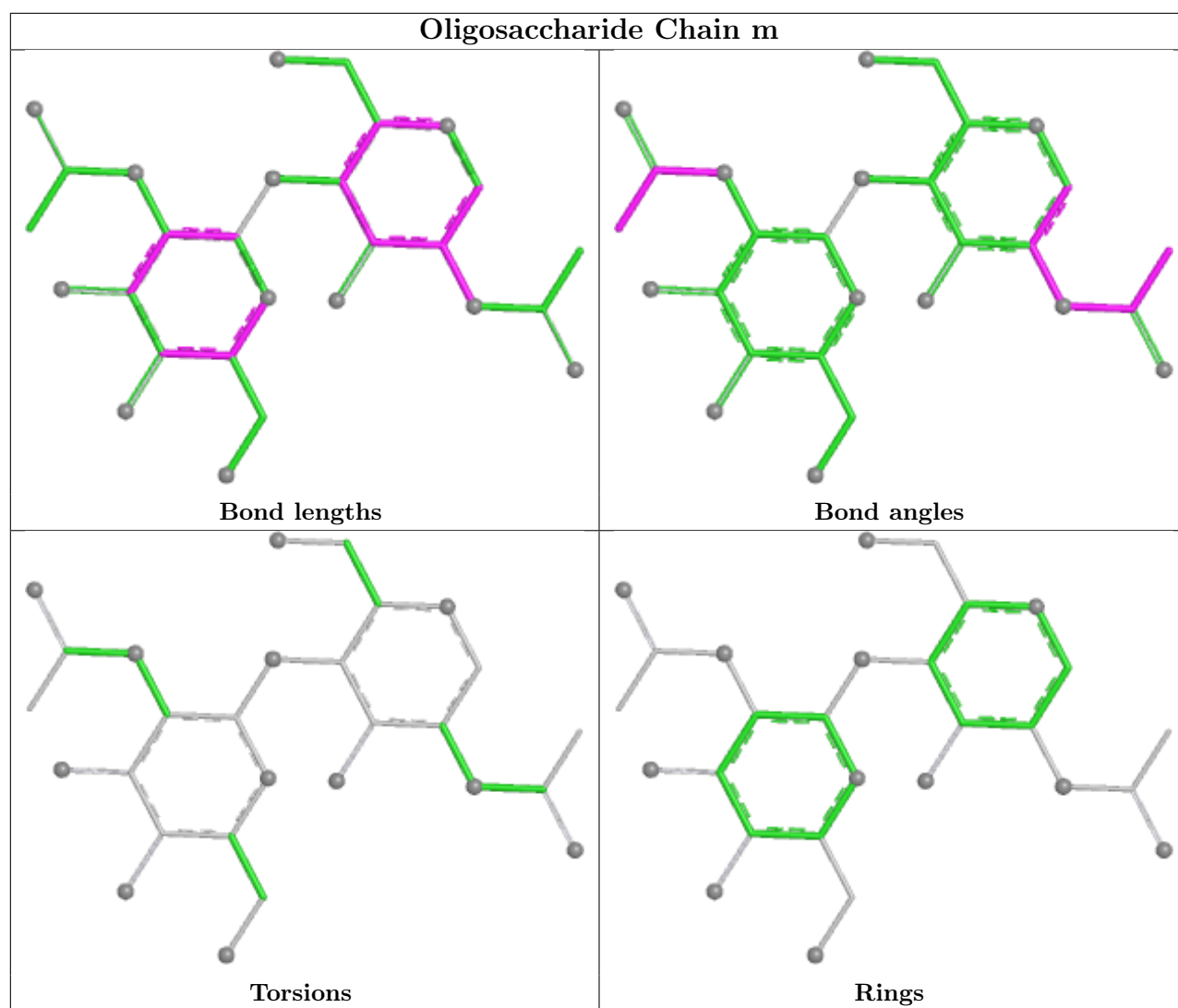


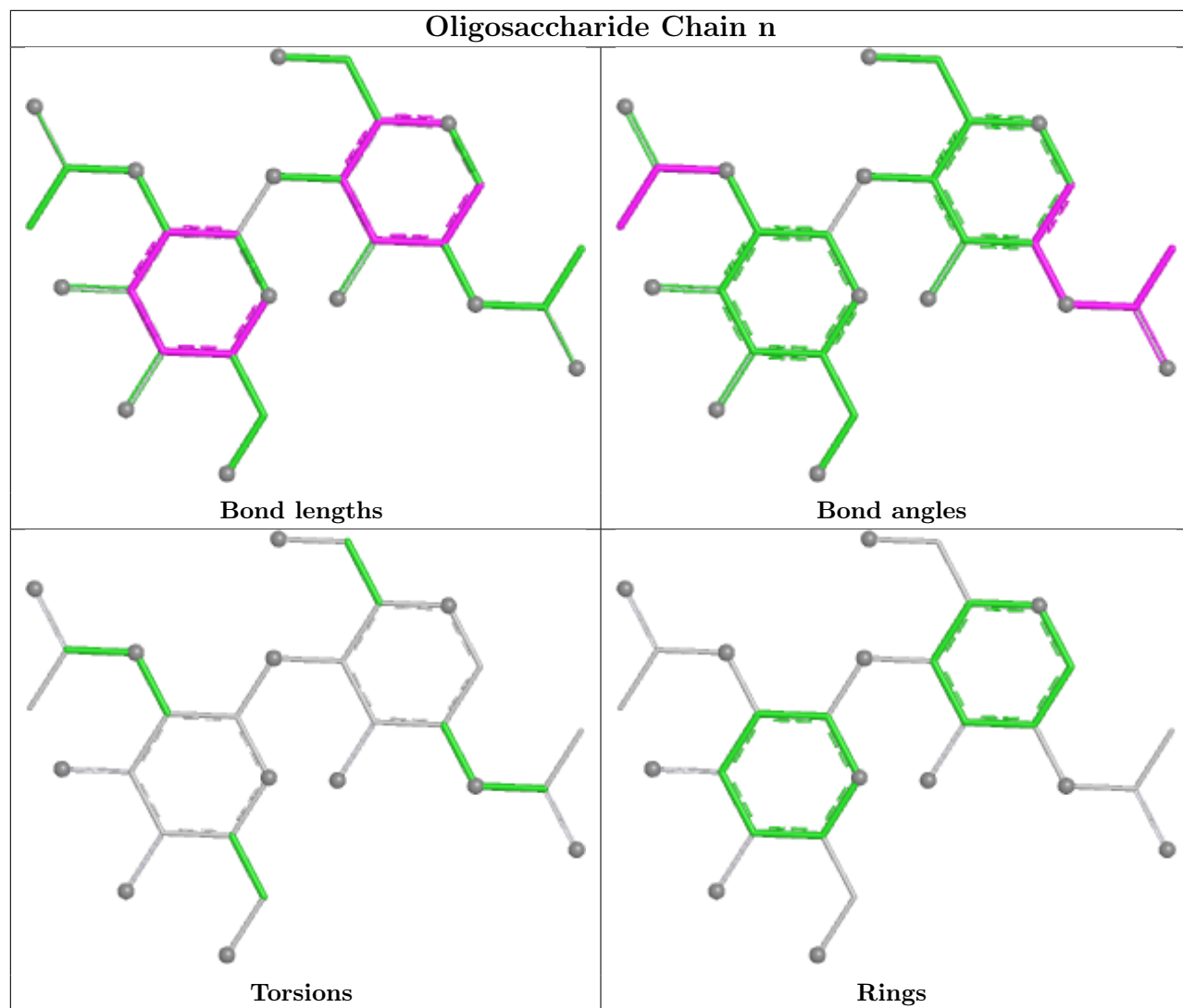


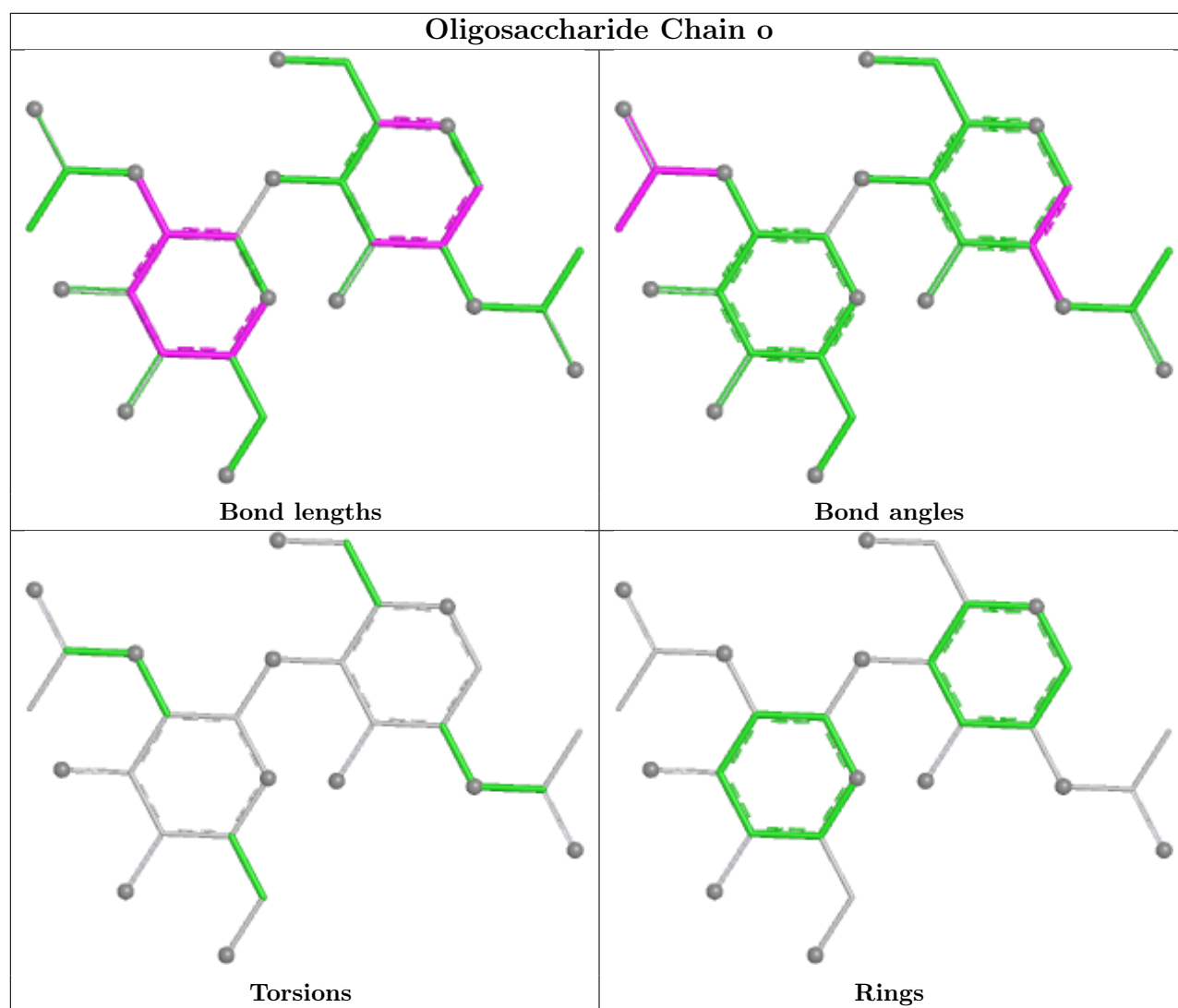


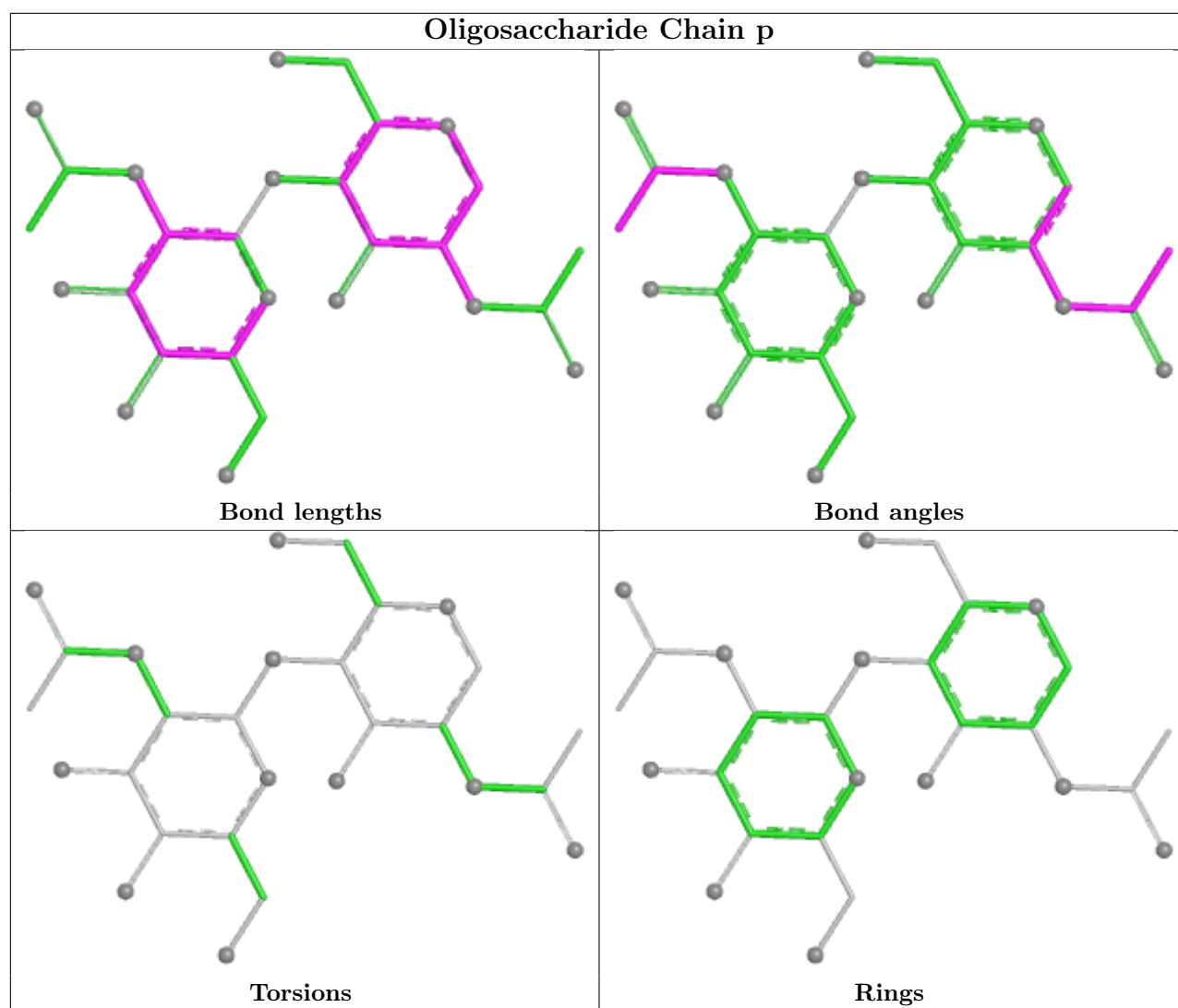


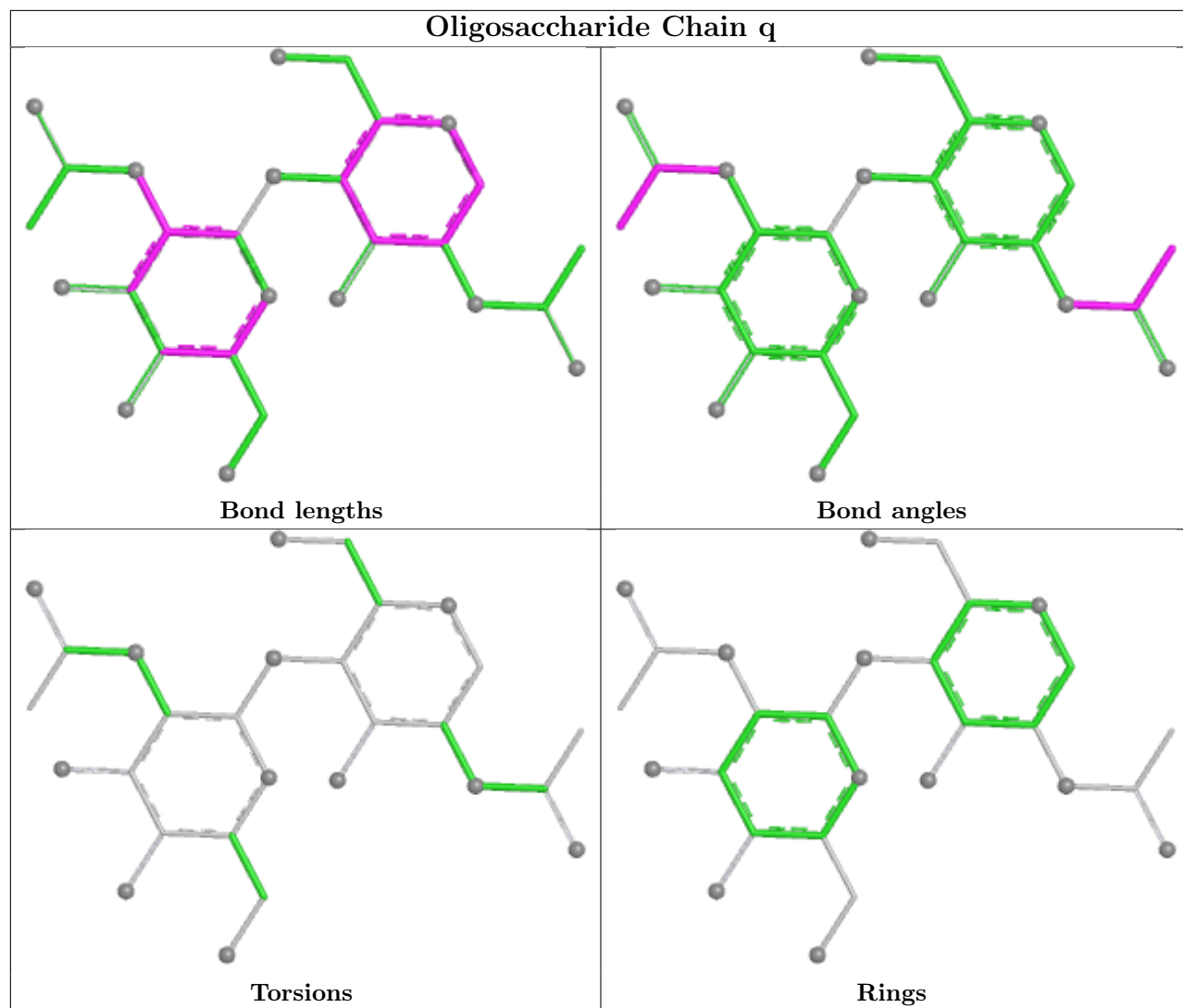




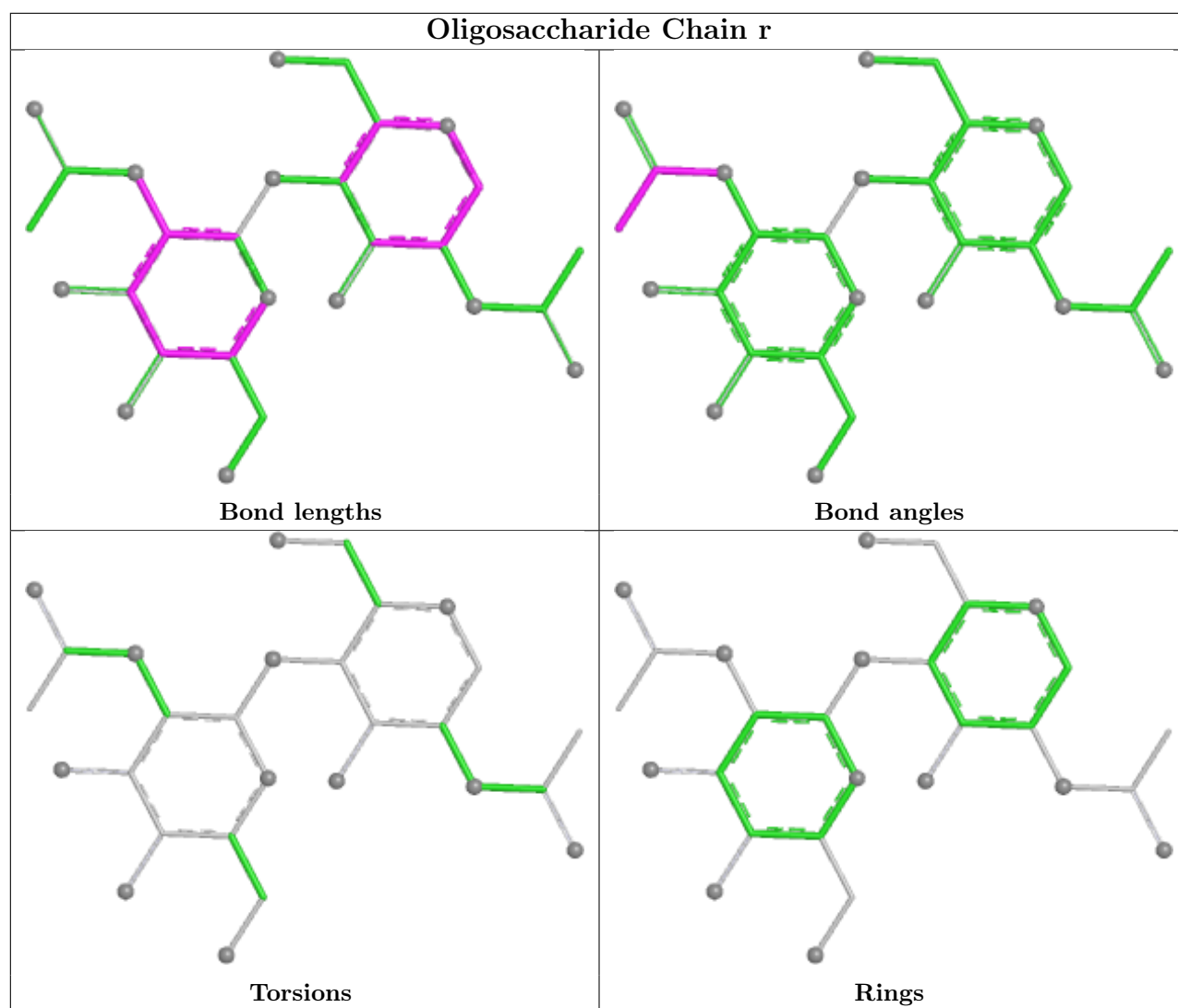


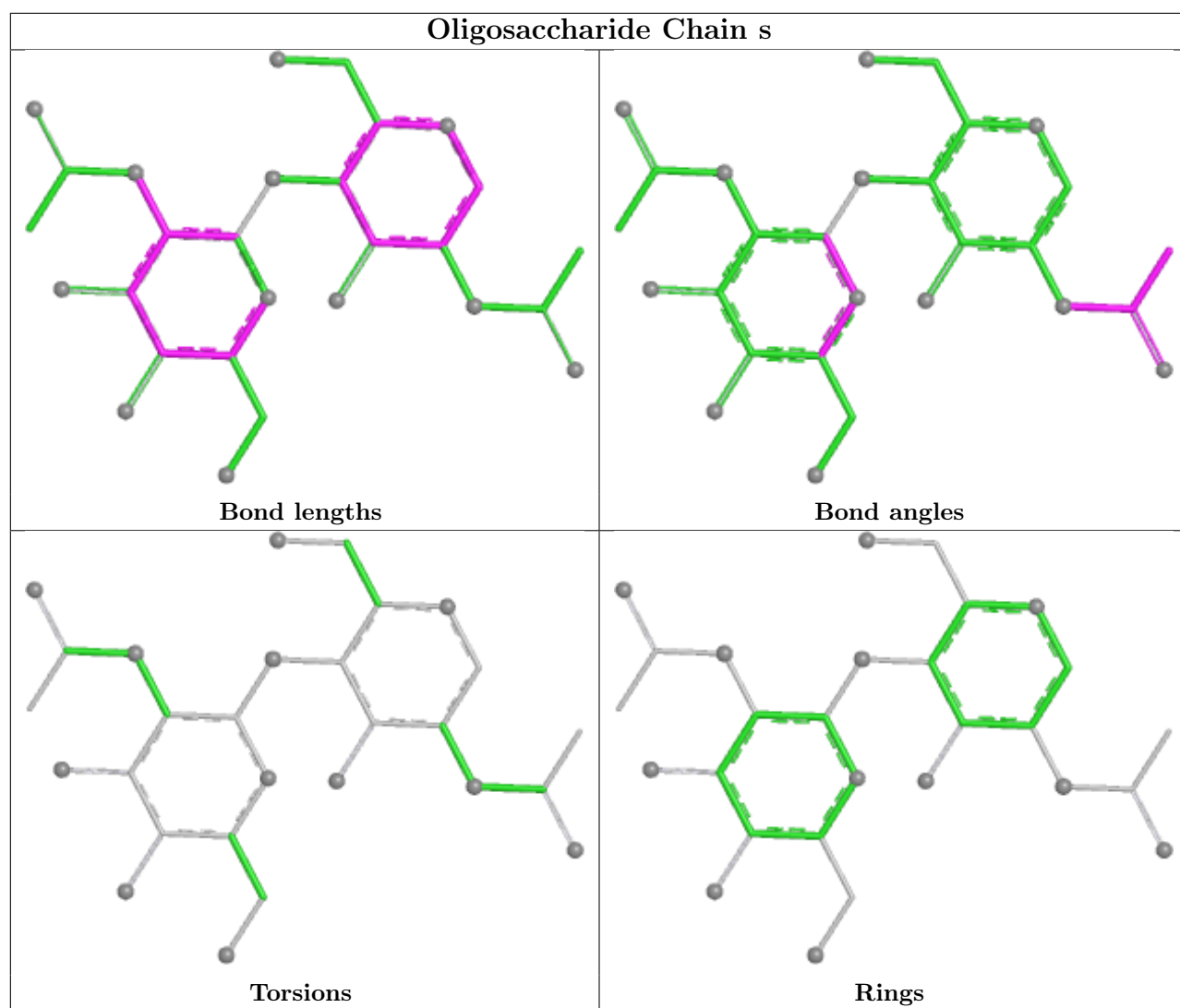


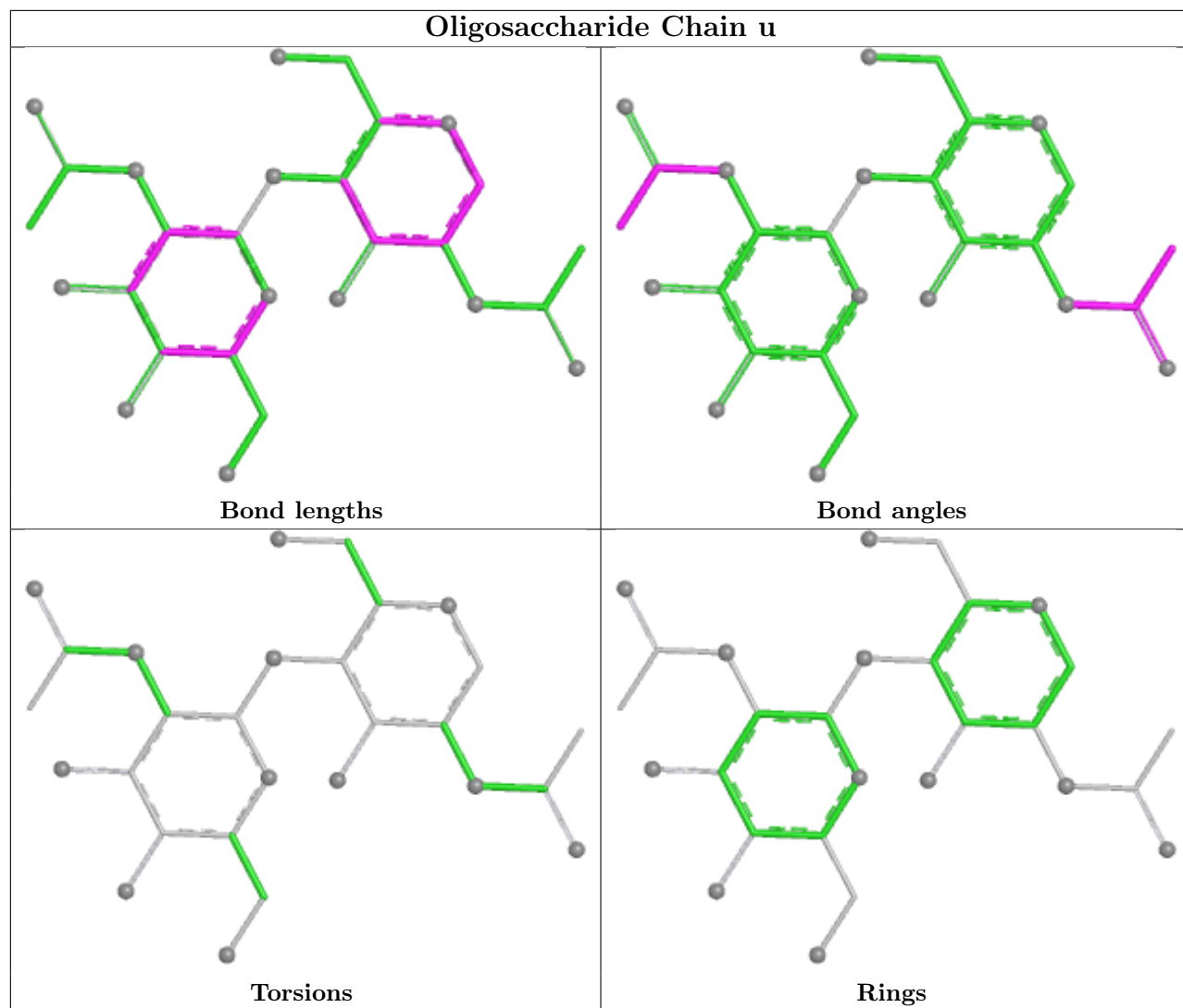


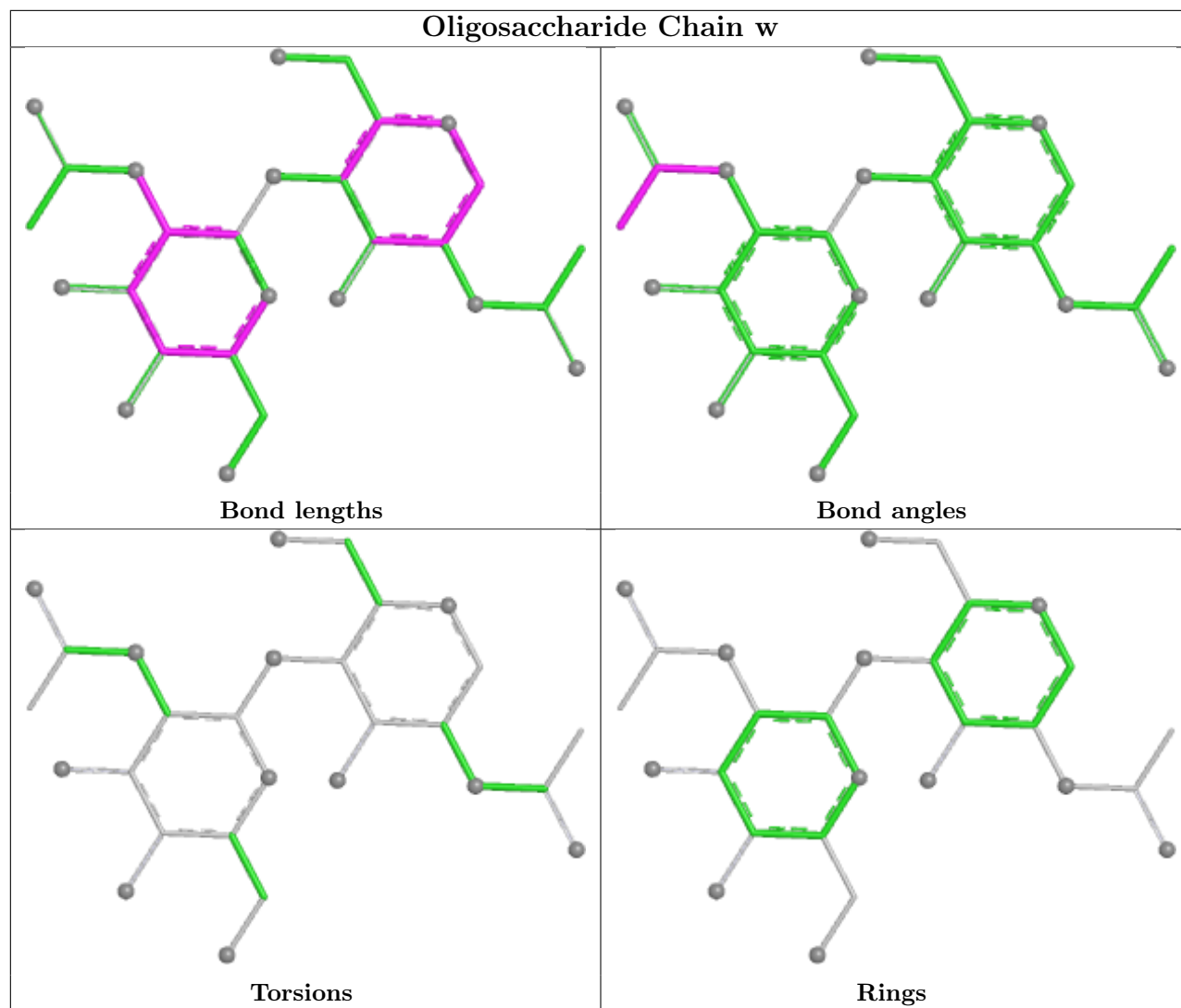


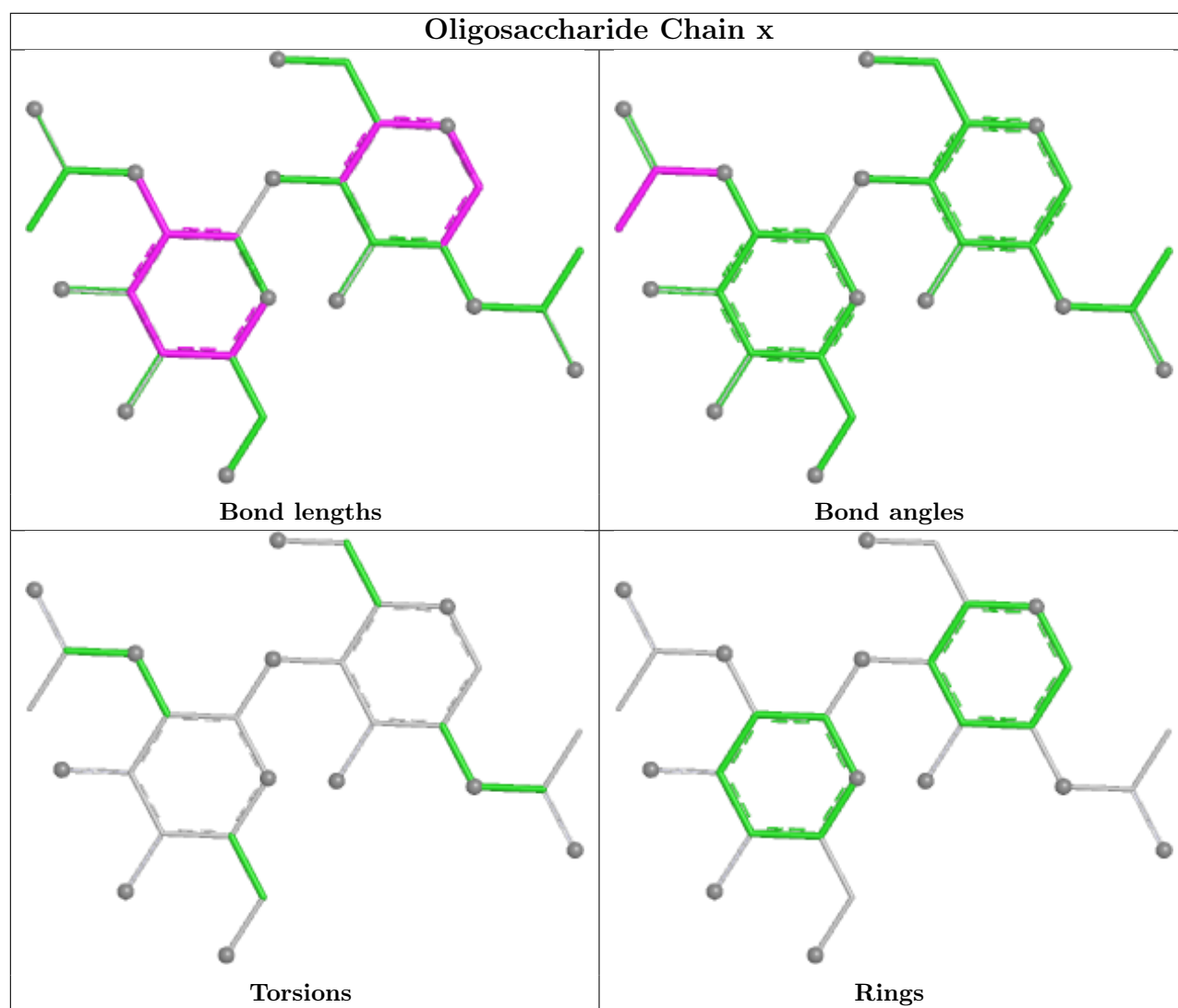


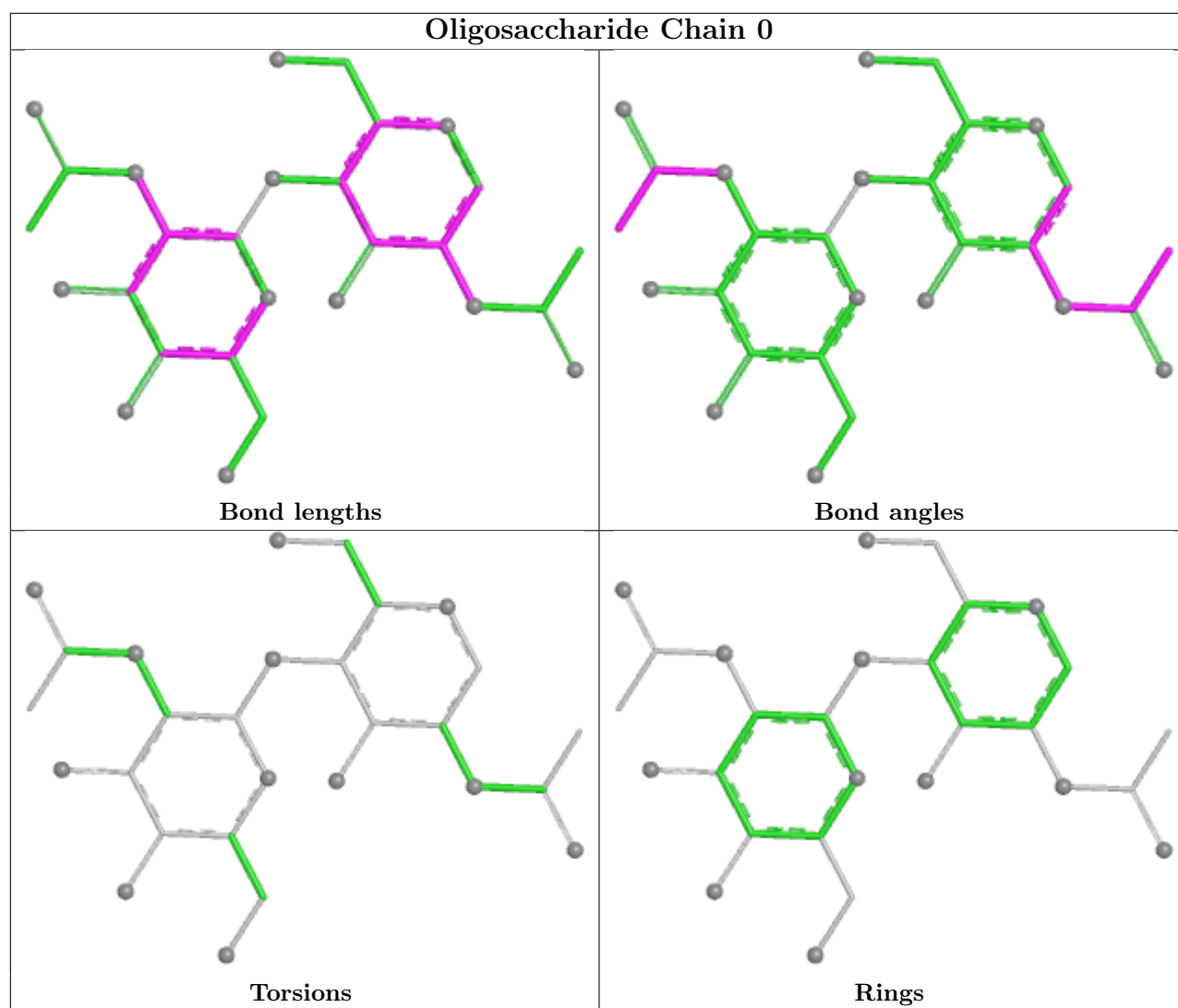


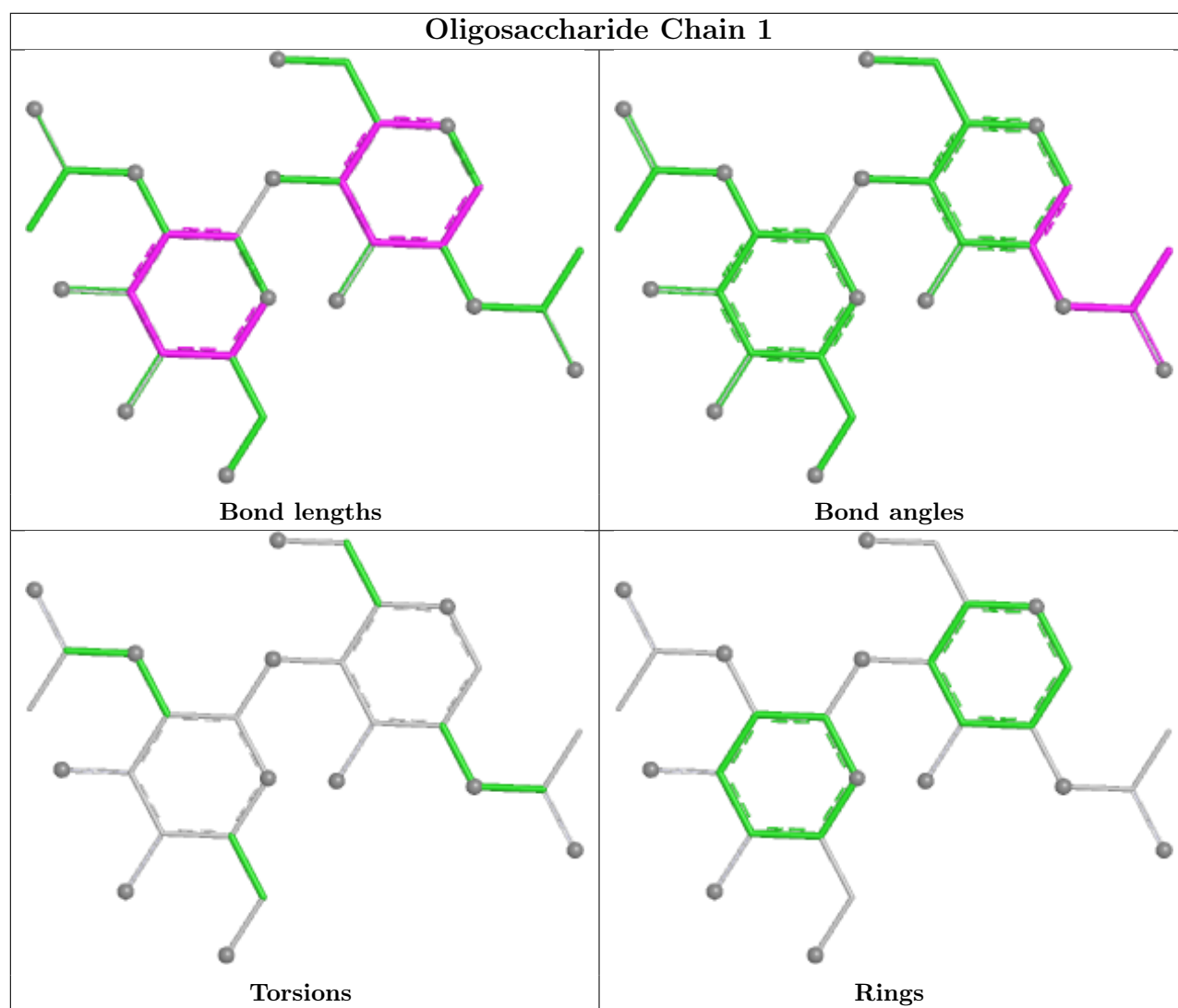


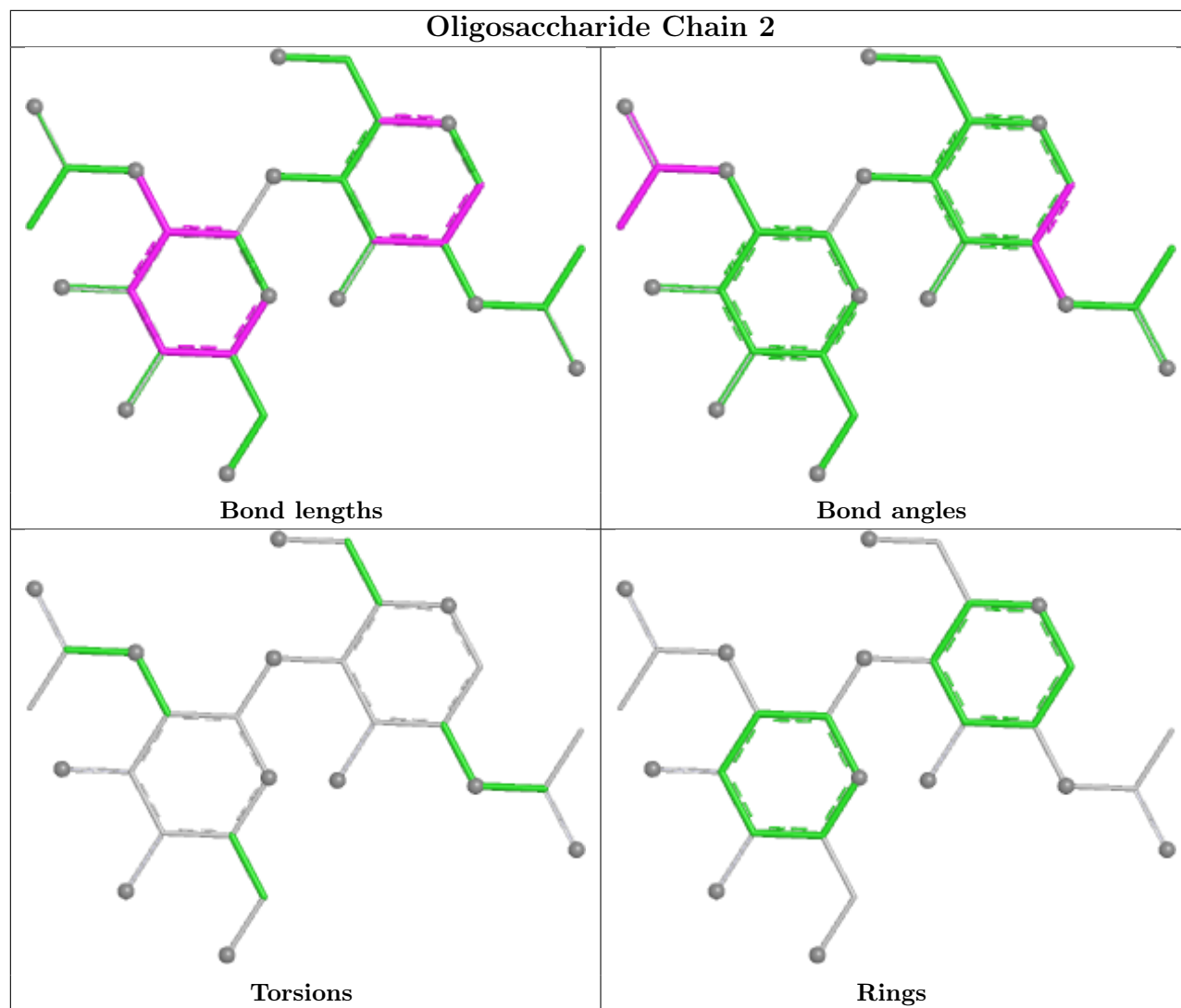




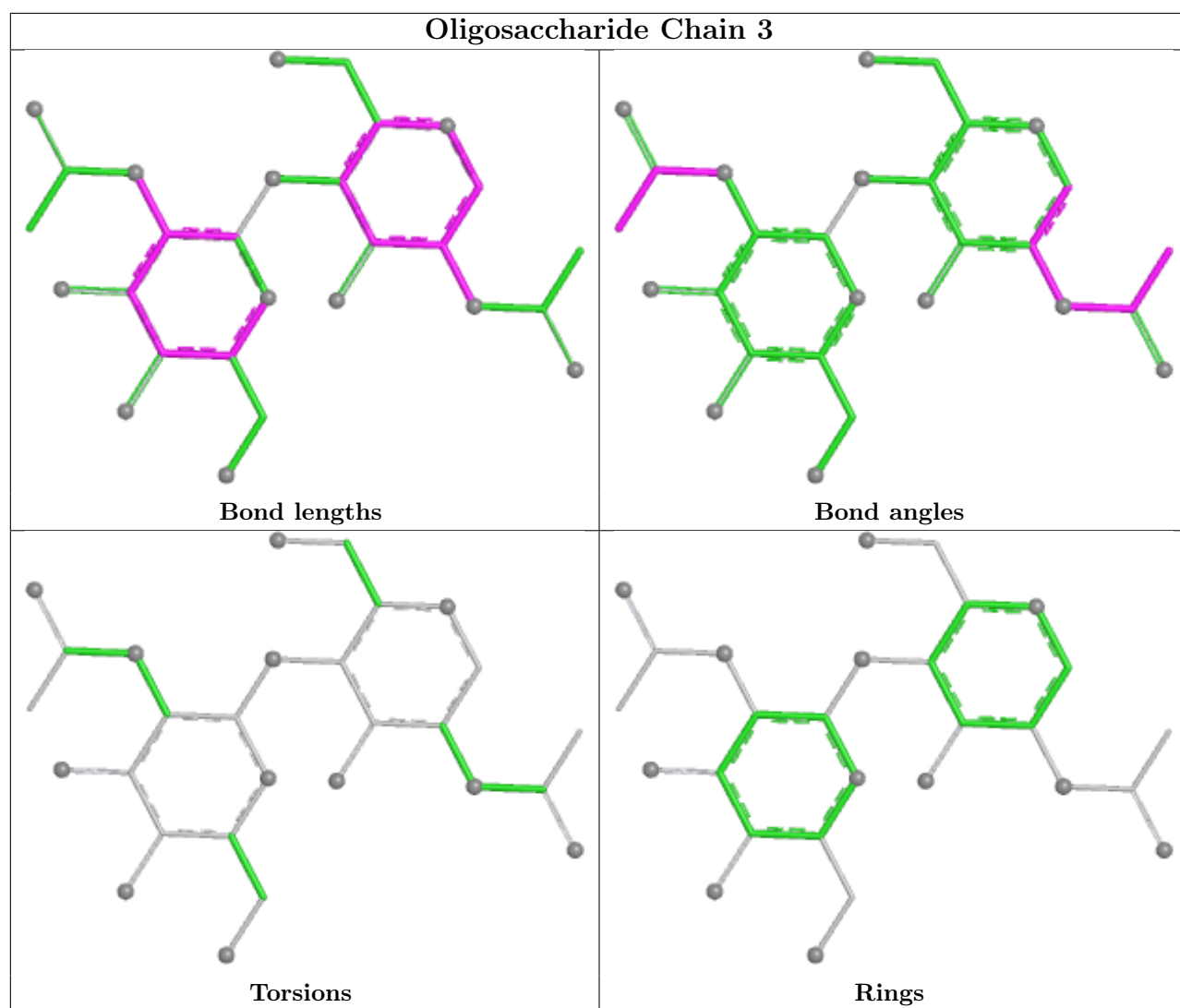


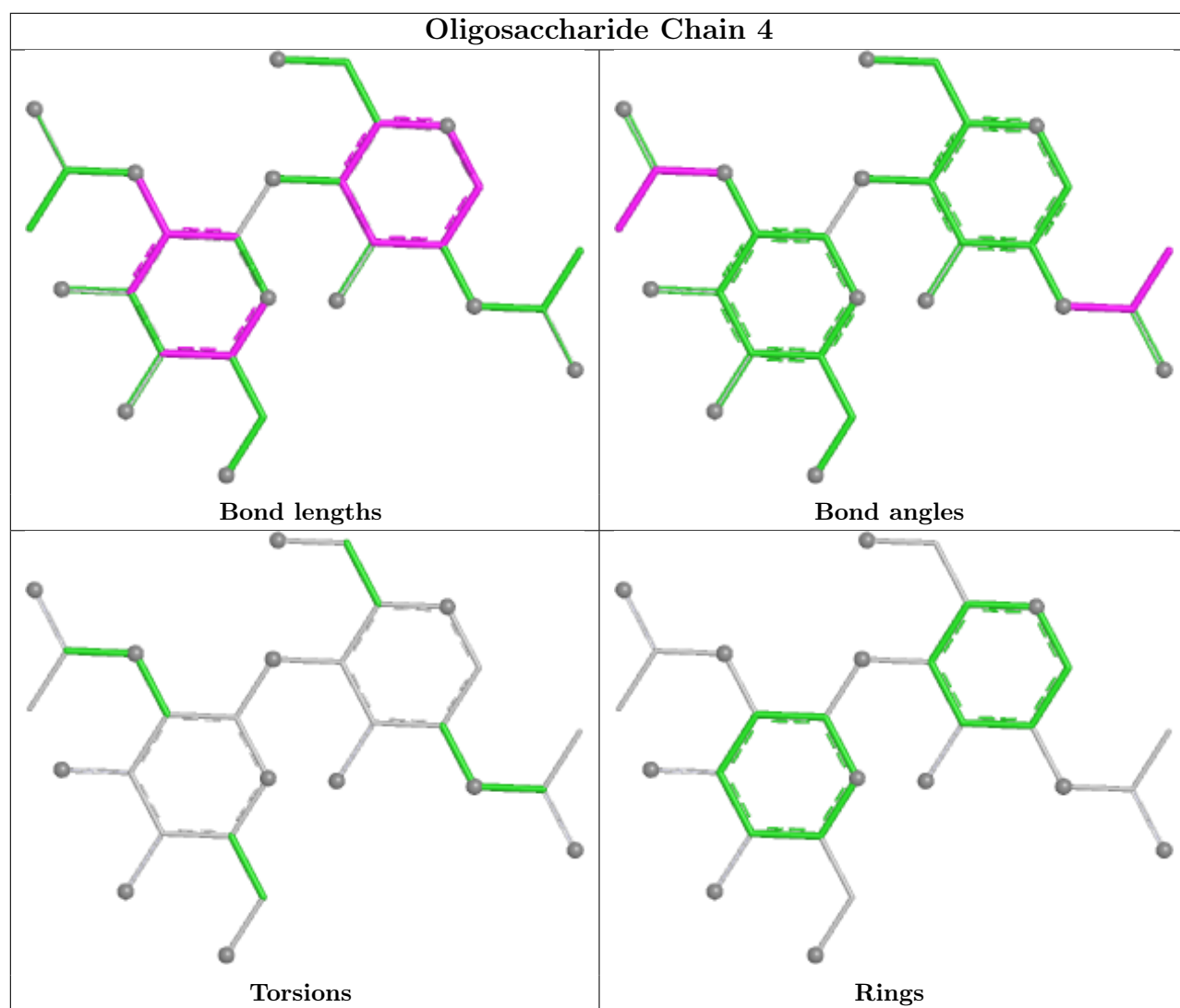


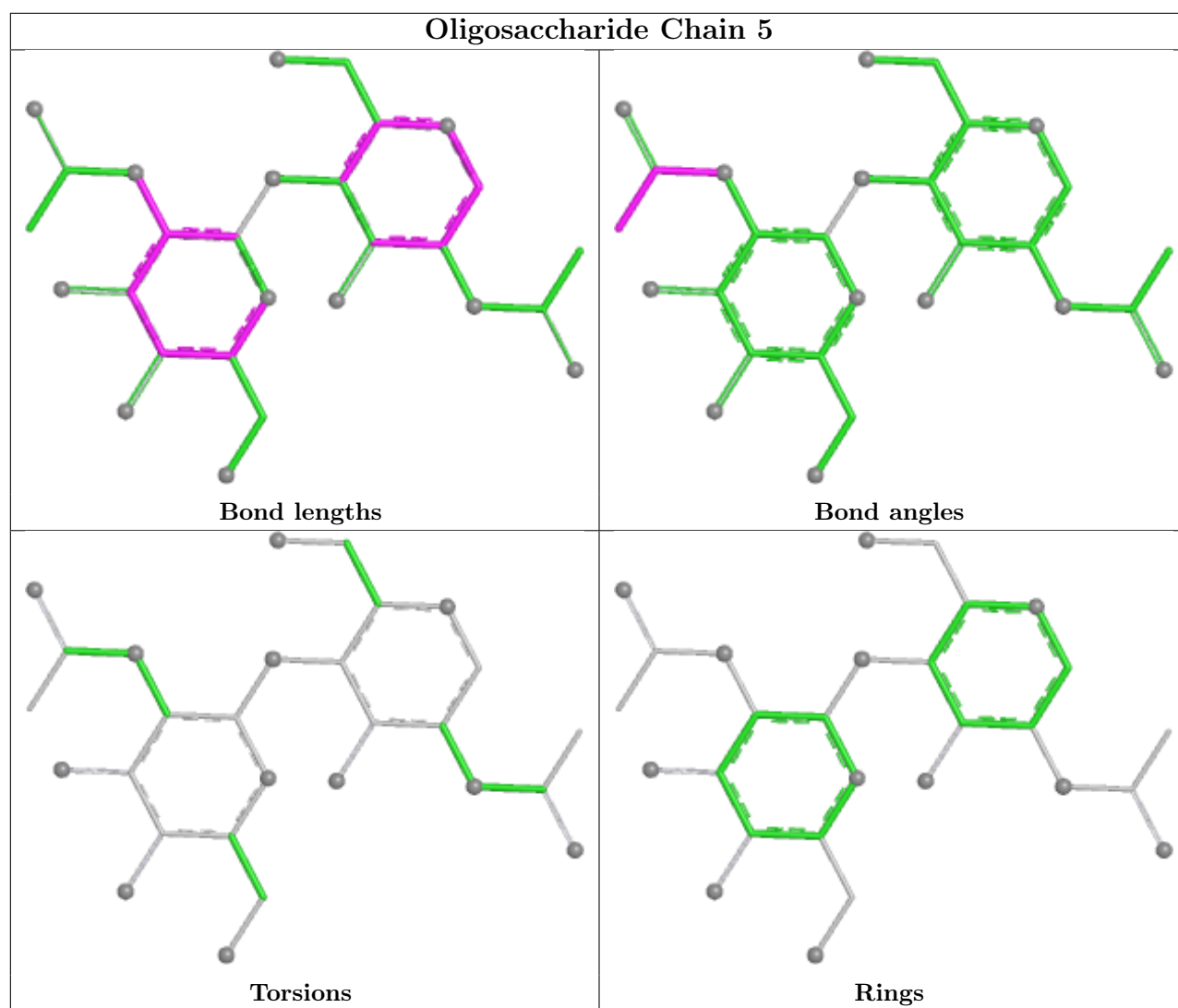


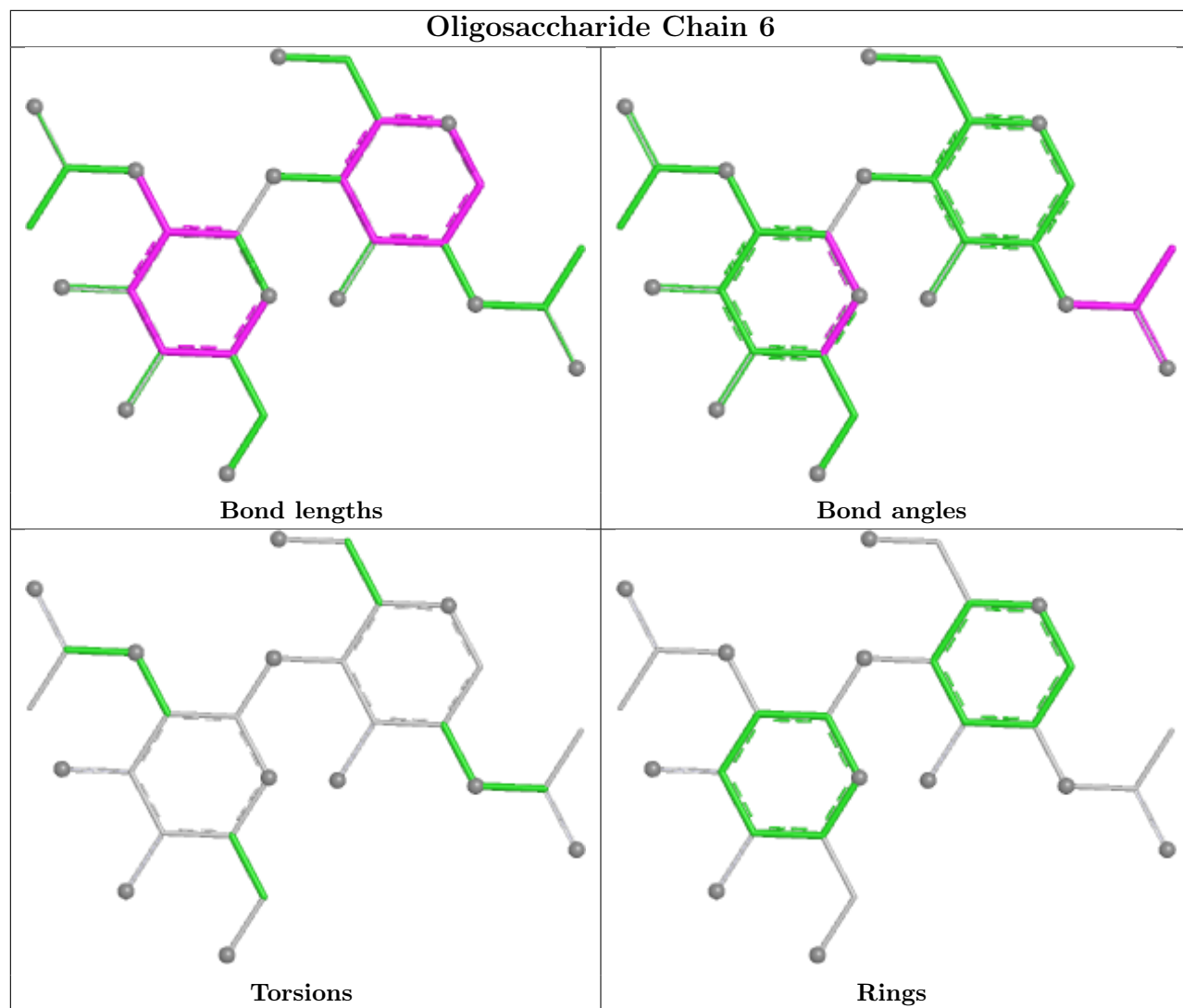


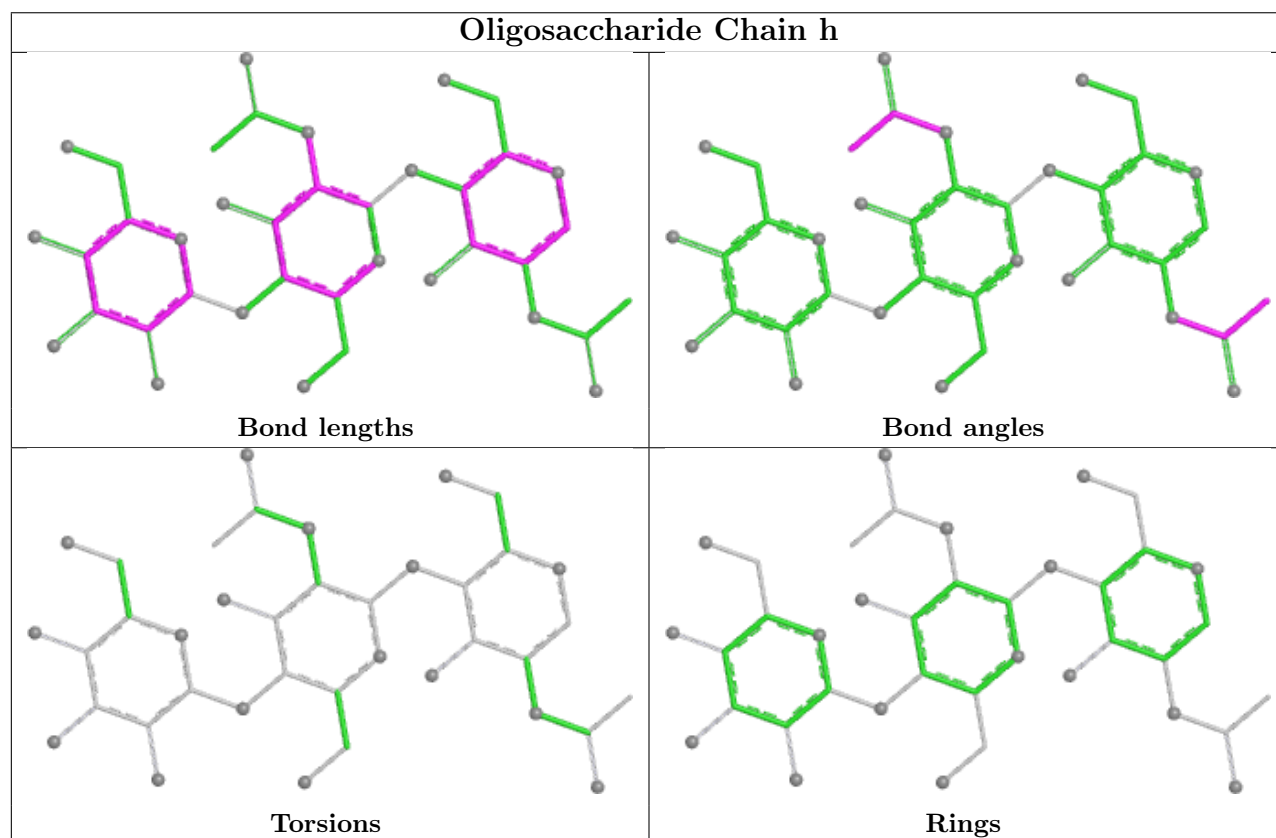
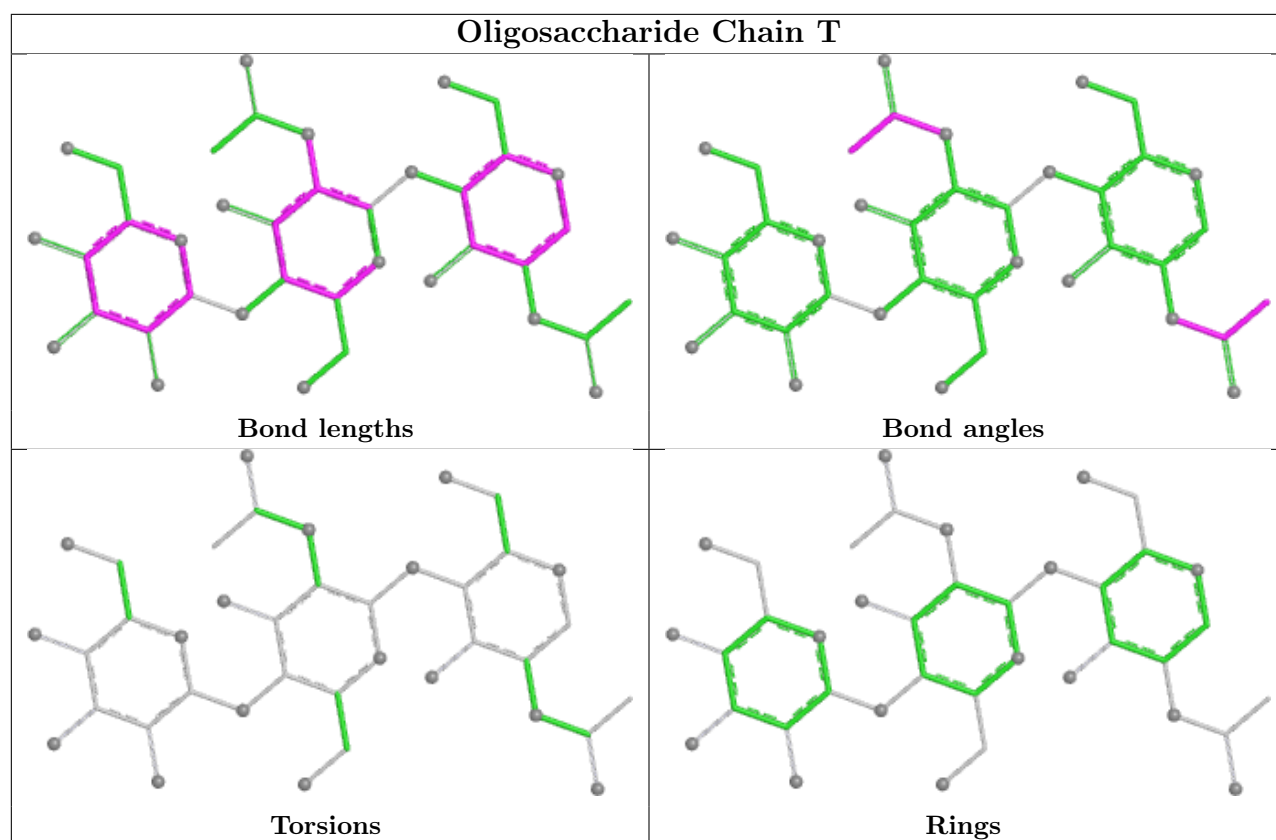


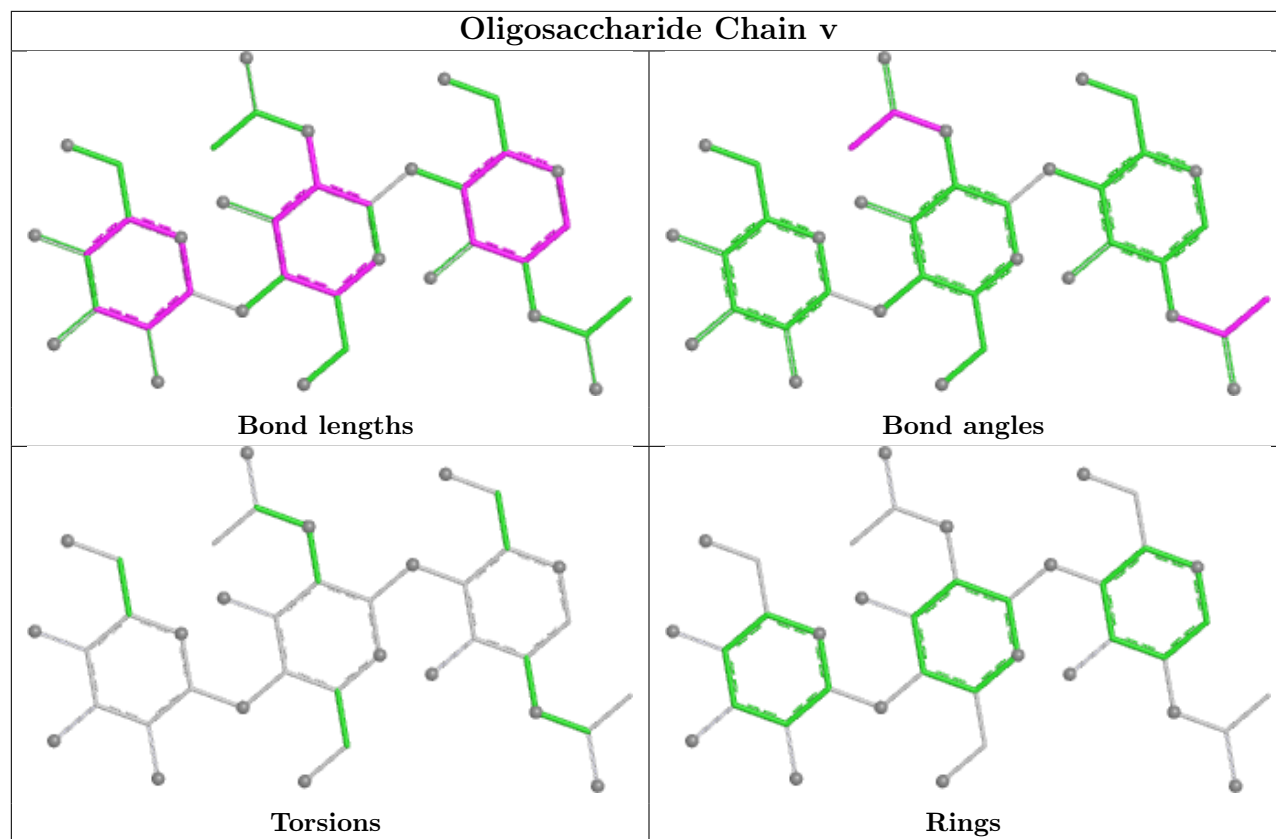


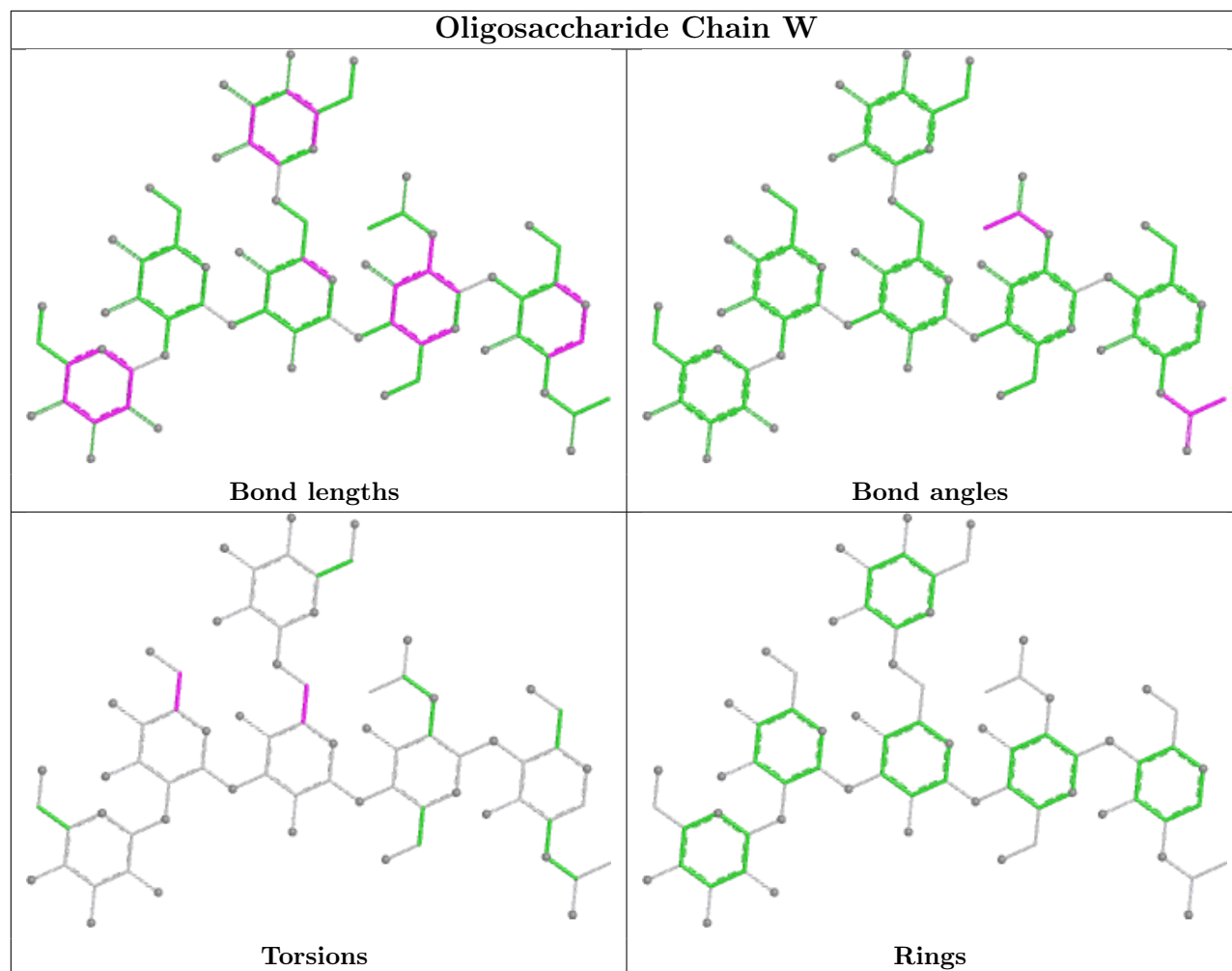


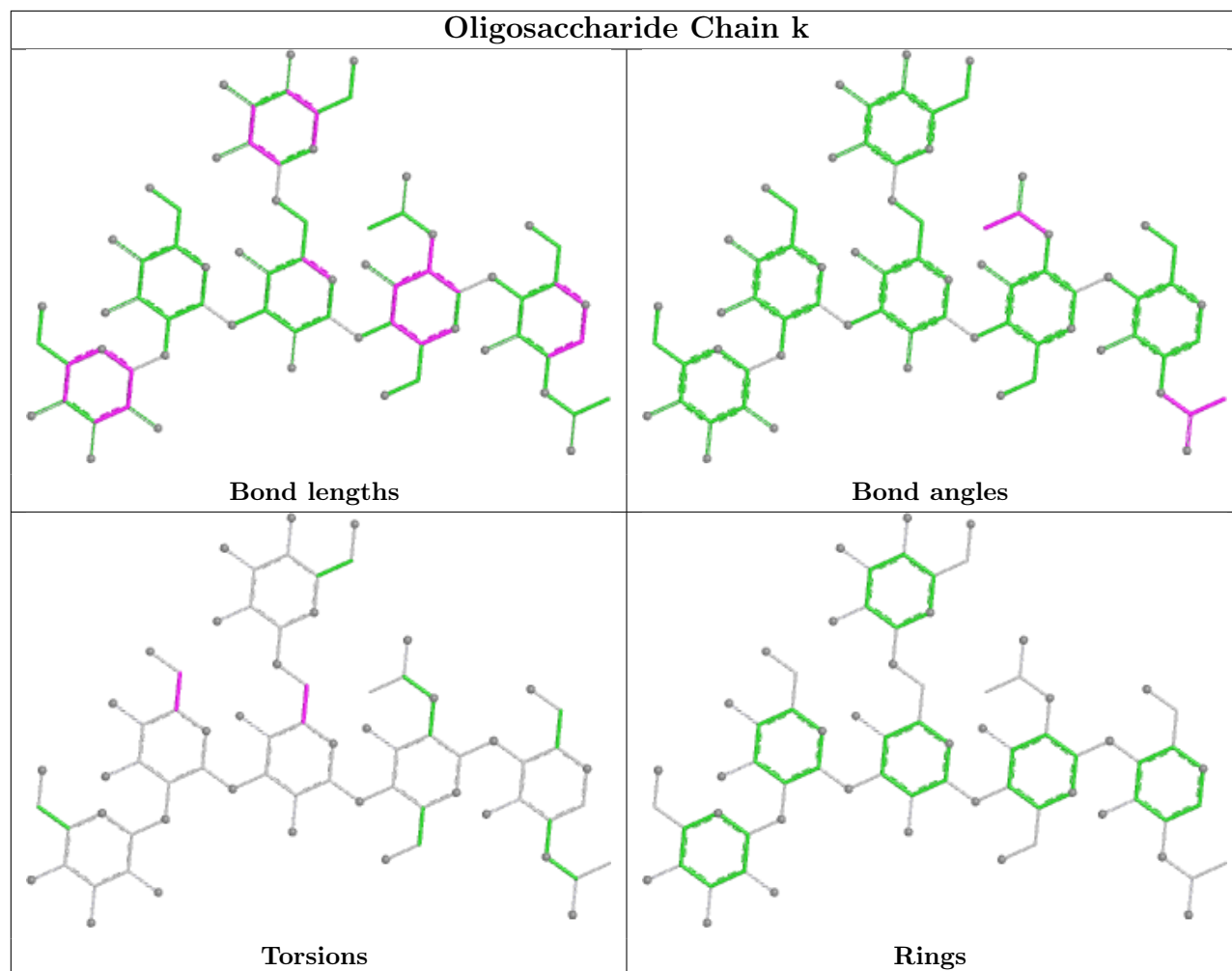




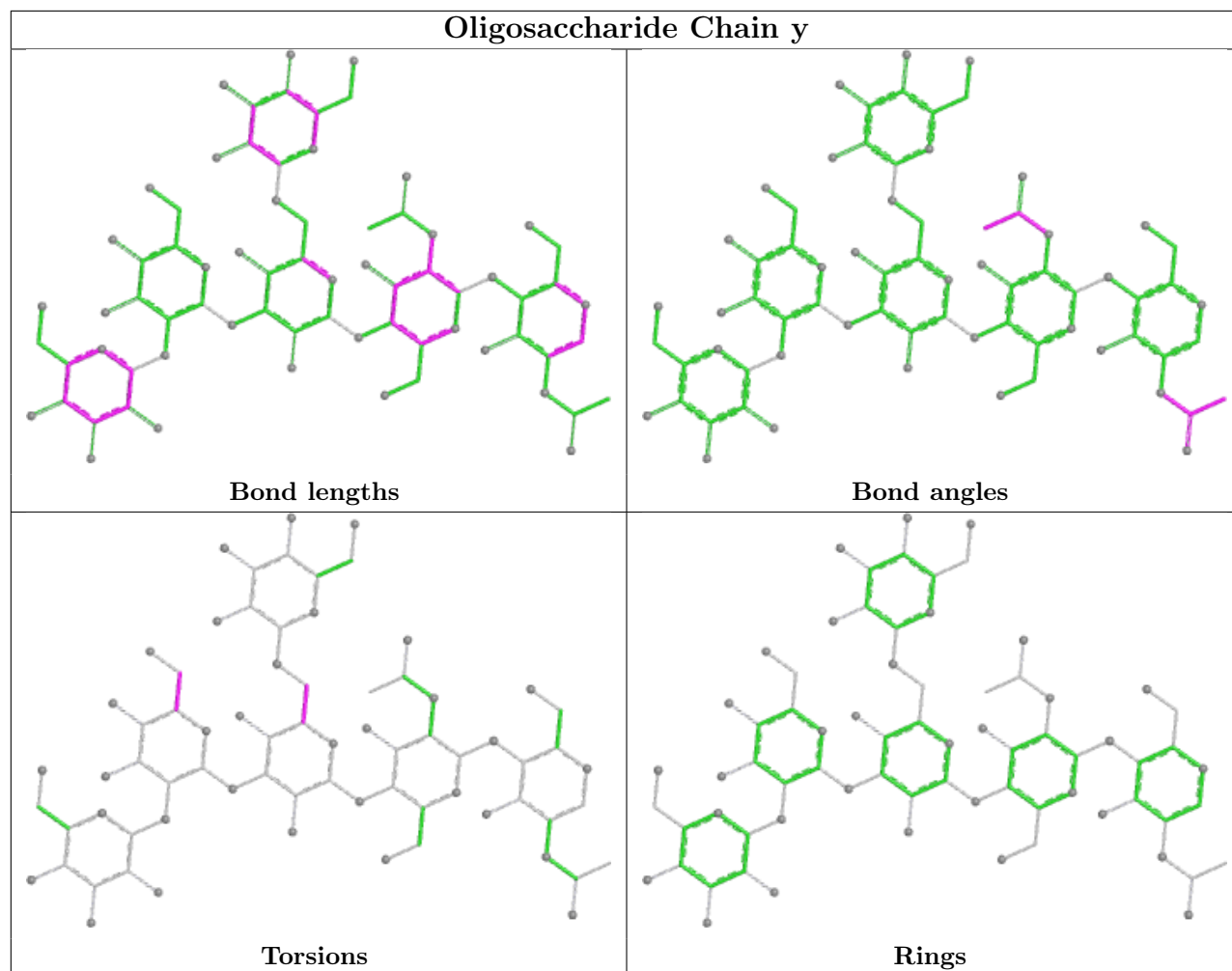


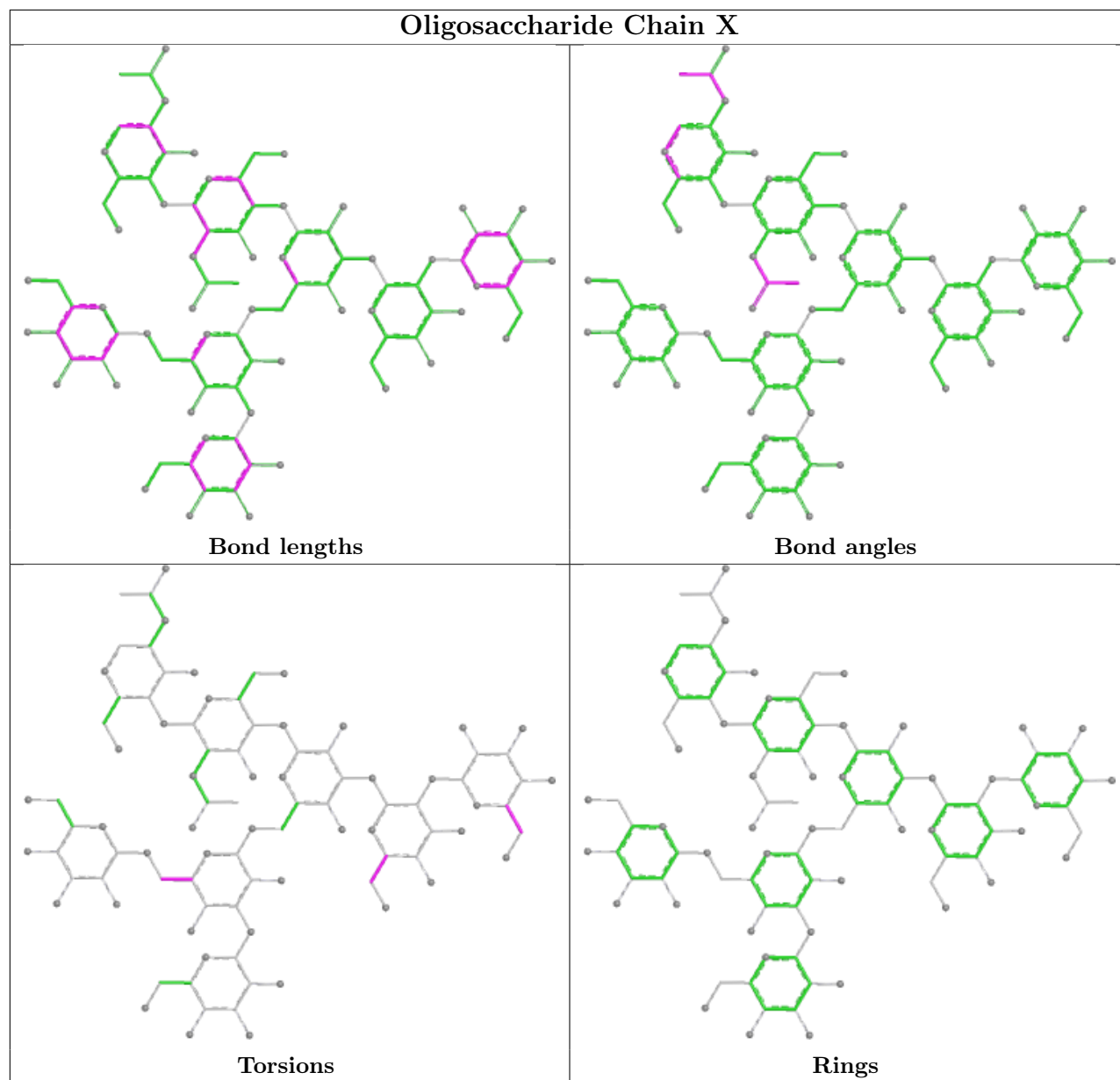


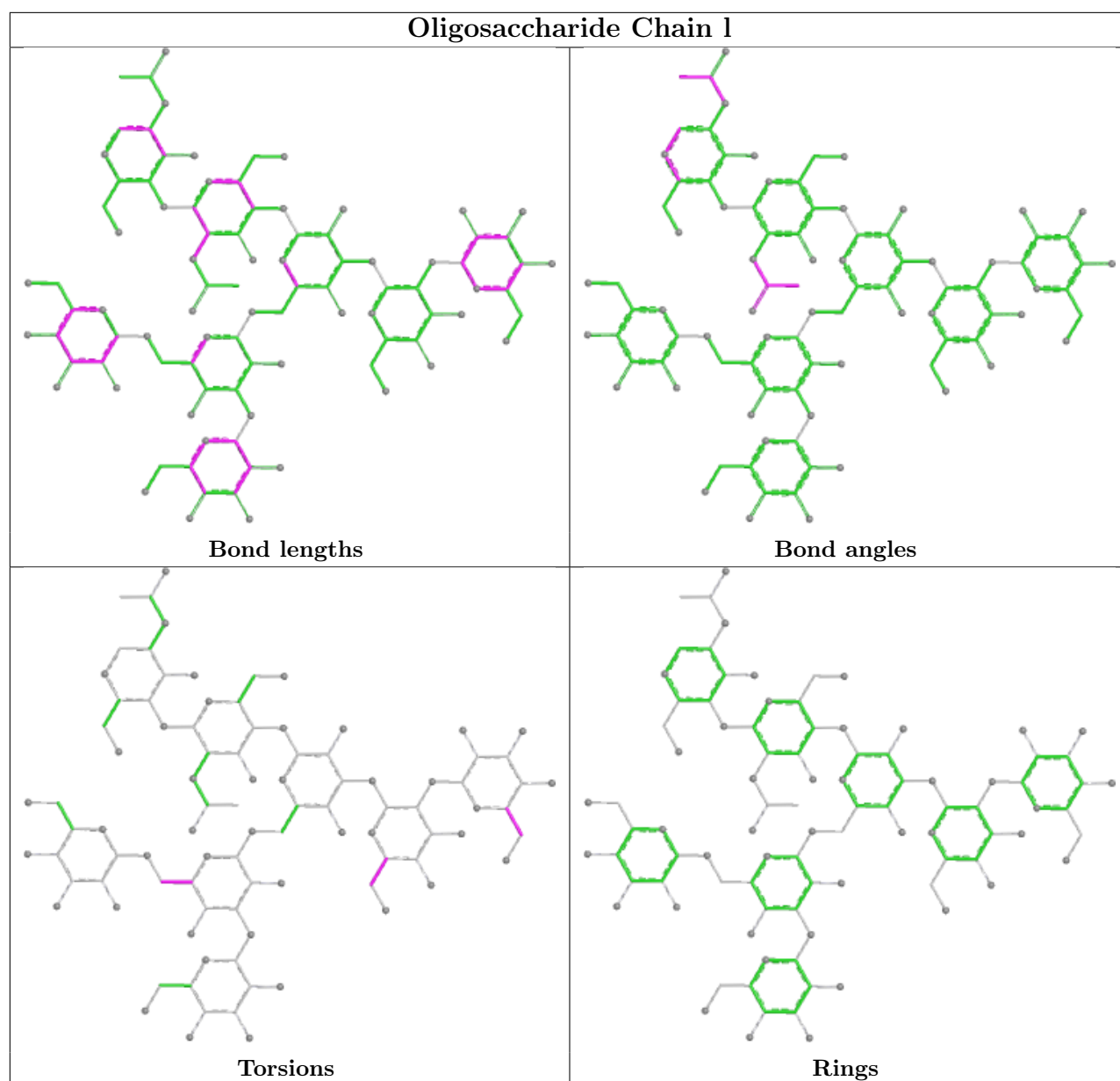


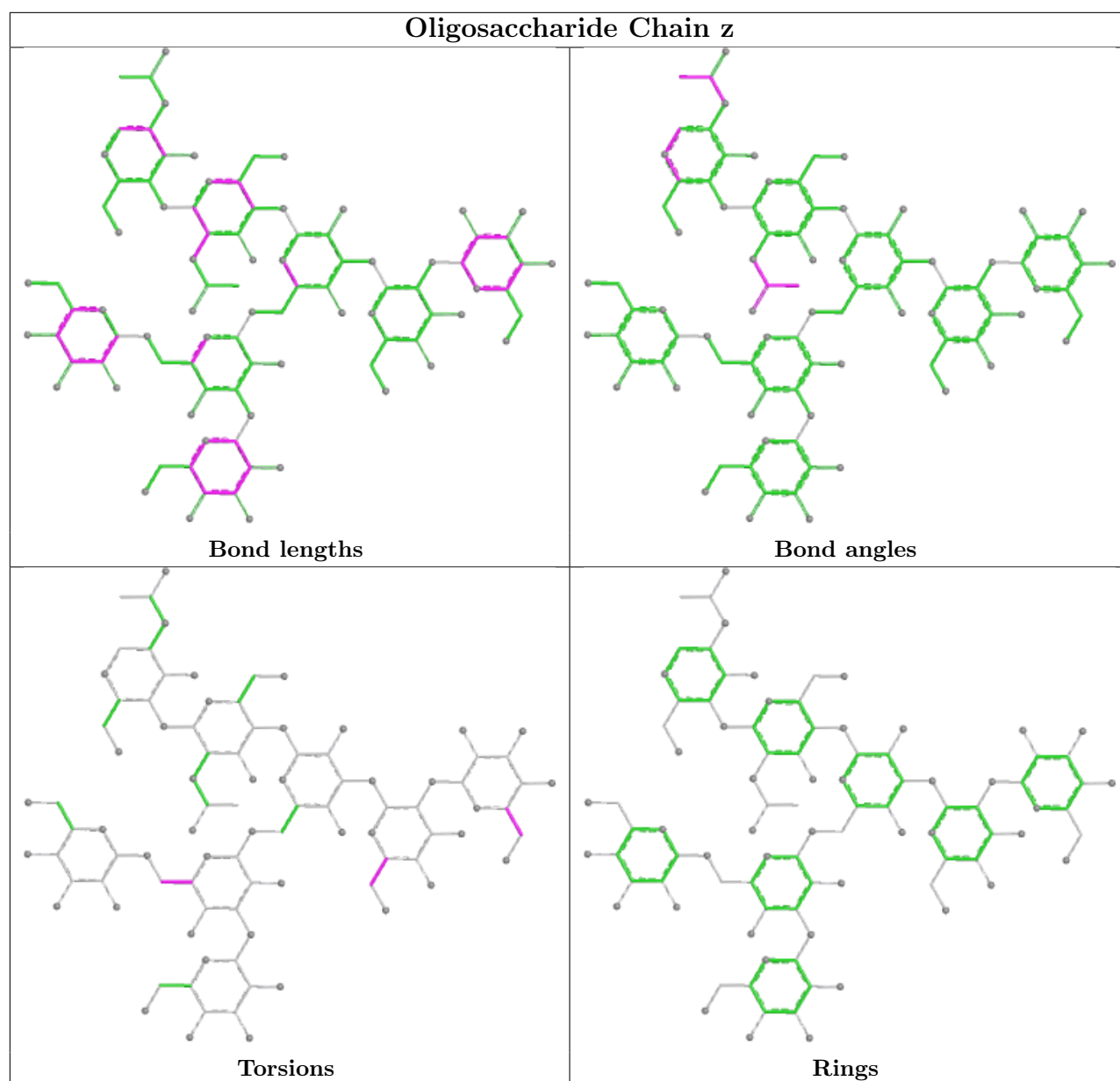


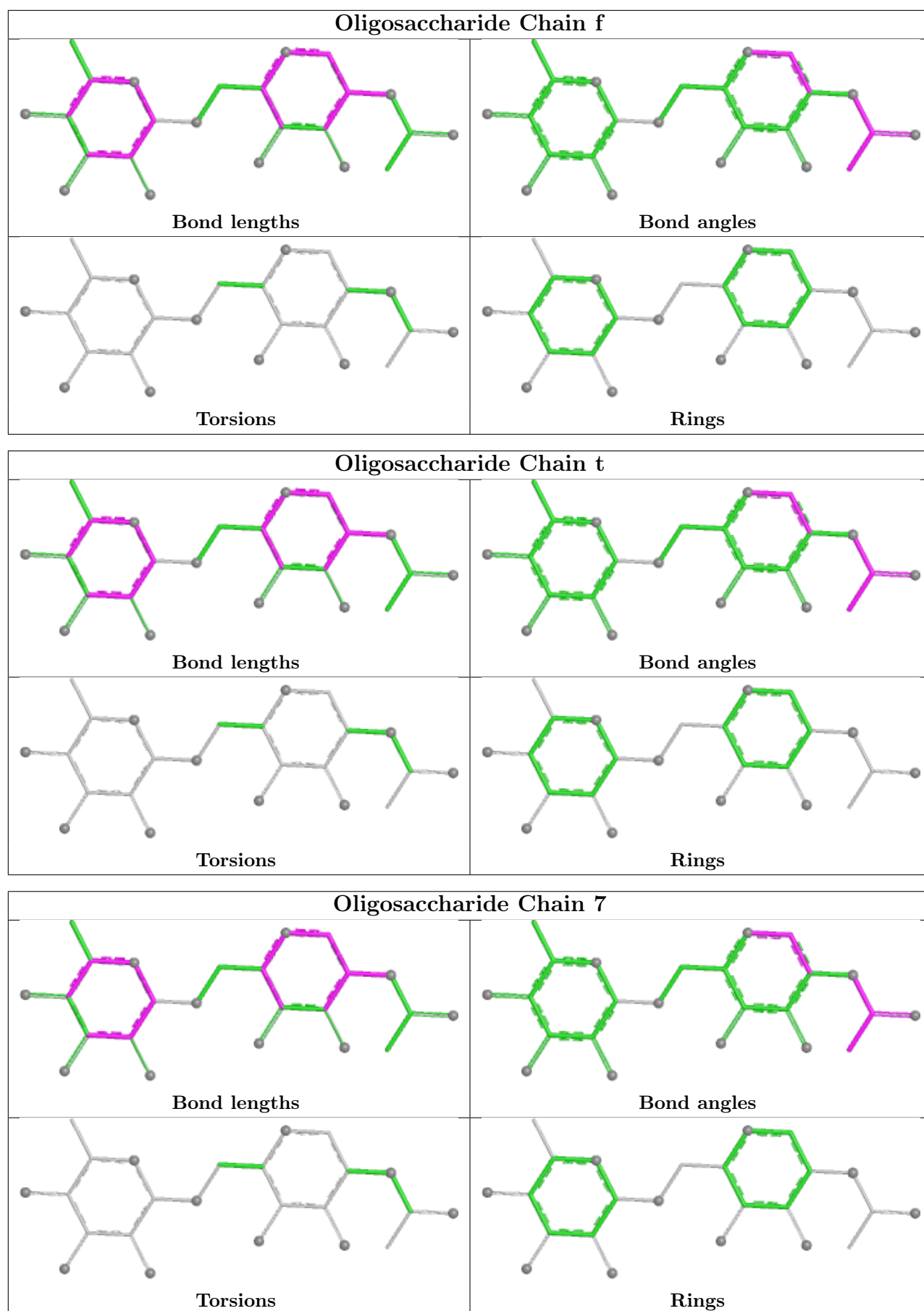












## 5.6 Ligand geometry ⓘ

18 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
12	NAG	I	701	4	14,14,15	2.03	5 (35%)	17,19,21	1.00	1 (5%)
12	NAG	E	603	1	14,14,15	2.16	6 (42%)	17,19,21	1.01	1 (5%)
12	NAG	A	601	1	14,14,15	2.29	6 (42%)	17,19,21	1.00	1 (5%)
12	NAG	F	603	1	14,14,15	2.17	6 (42%)	17,19,21	1.02	1 (5%)
12	NAG	A	602	1	14,14,15	2.23	5 (35%)	17,19,21	1.01	1 (5%)
12	NAG	E	604	1	14,14,15	2.22	7 (50%)	17,19,21	1.09	2 (11%)
12	NAG	A	603	1	14,14,15	2.17	6 (42%)	17,19,21	1.01	1 (5%)
12	NAG	G	701	4	14,14,15	2.03	5 (35%)	17,19,21	1.01	1 (5%)
12	NAG	F	604	1	14,14,15	2.22	7 (50%)	17,19,21	1.09	2 (11%)
12	NAG	I	702	4	14,14,15	2.11	5 (35%)	17,19,21	1.05	1 (5%)
12	NAG	F	601	1	14,14,15	2.29	5 (35%)	17,19,21	1.00	1 (5%)
12	NAG	F	602	1	14,14,15	2.23	5 (35%)	17,19,21	1.00	1 (5%)
12	NAG	E	602	1	14,14,15	2.23	5 (35%)	17,19,21	1.00	1 (5%)
12	NAG	B	701	4	14,14,15	2.04	5 (35%)	17,19,21	1.00	1 (5%)
12	NAG	B	702	4	14,14,15	2.11	5 (35%)	17,19,21	1.05	1 (5%)
12	NAG	E	601	1	14,14,15	2.29	6 (42%)	17,19,21	1.00	1 (5%)
12	NAG	G	702	4	14,14,15	2.11	5 (35%)	17,19,21	1.05	1 (5%)
12	NAG	A	604	1	14,14,15	2.22	7 (50%)	17,19,21	1.09	2 (11%)

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
12	NAG	I	701	4	-	0/6/23/26	0/1/1/1
12	NAG	E	603	1	-	0/6/23/26	0/1/1/1

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	A	601	1	-	0/6/23/26	0/1/1/1
12	NAG	F	603	1	-	0/6/23/26	0/1/1/1
12	NAG	A	602	1	-	1/6/23/26	0/1/1/1
12	NAG	E	604	1	-	0/6/23/26	0/1/1/1
12	NAG	A	603	1	-	0/6/23/26	0/1/1/1
12	NAG	G	701	4	-	0/6/23/26	0/1/1/1
12	NAG	F	604	1	-	0/6/23/26	0/1/1/1
12	NAG	I	702	4	-	2/6/23/26	0/1/1/1
12	NAG	F	601	1	-	0/6/23/26	0/1/1/1
12	NAG	F	602	1	-	1/6/23/26	0/1/1/1
12	NAG	E	602	1	-	1/6/23/26	0/1/1/1
12	NAG	B	701	4	-	0/6/23/26	0/1/1/1
12	NAG	B	702	4	-	2/6/23/26	0/1/1/1
12	NAG	E	601	1	-	0/6/23/26	0/1/1/1
12	NAG	G	702	4	-	2/6/23/26	0/1/1/1
12	NAG	A	604	1	-	0/6/23/26	0/1/1/1

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	601	NAG	C1-C2	5.92	1.60	1.52
12	A	601	NAG	C1-C2	5.92	1.60	1.52
12	F	601	NAG	C1-C2	5.90	1.60	1.52
12	A	602	NAG	C1-C2	5.84	1.60	1.52
12	F	602	NAG	C1-C2	5.83	1.60	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	604	NAG	C8-C7-N2	2.44	120.17	116.12
12	E	601	NAG	C8-C7-N2	2.44	120.16	116.12
12	A	604	NAG	C8-C7-N2	2.43	120.15	116.12
12	E	604	NAG	C8-C7-N2	2.43	120.14	116.12
12	F	601	NAG	C8-C7-N2	2.42	120.13	116.12

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	702	NAG	O5-C5-C6-O6
12	G	702	NAG	O5-C5-C6-O6

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
12	I	702	NAG	O5-C5-C6-O6
12	A	602	NAG	O5-C5-C6-O6
12	E	602	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	601	NAG	1	0
12	F	601	NAG	1	0
12	E	601	NAG	1	0

## 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.



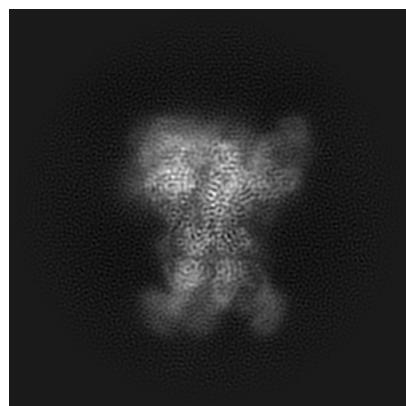
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23312. These allow visual inspection of the internal detail of the map and identification of artifacts.

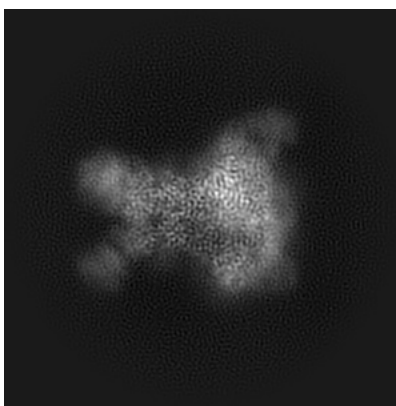
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

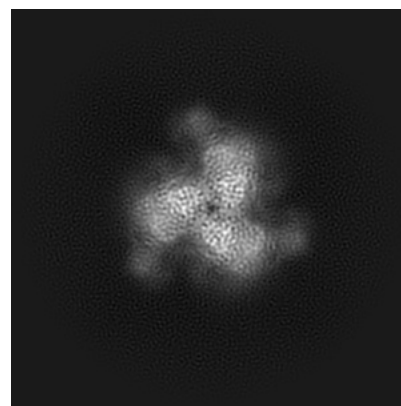
#### 6.1.1 Primary map



X

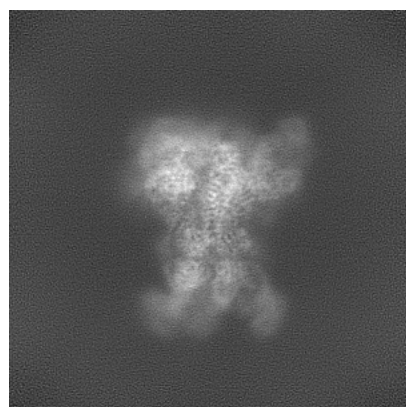


Y

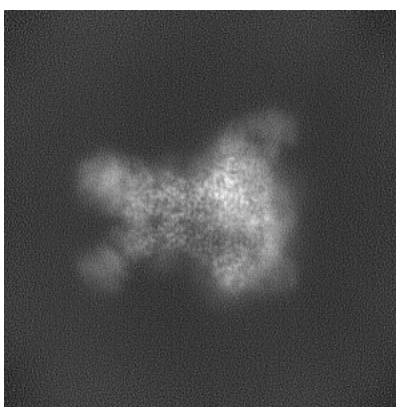


Z

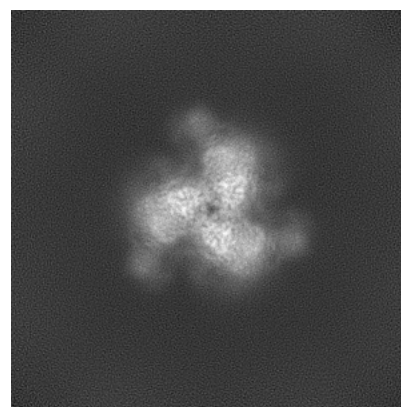
#### 6.1.2 Raw map



X



Y

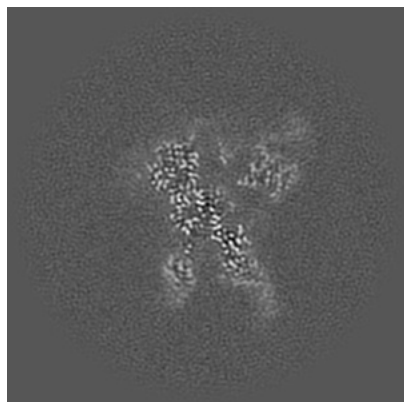


Z

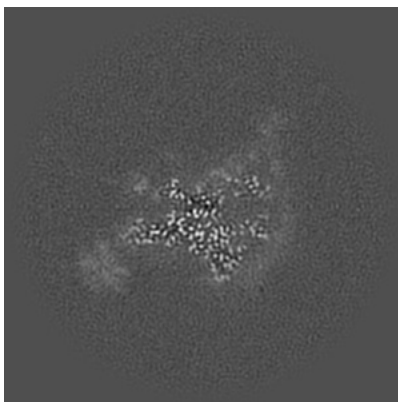
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

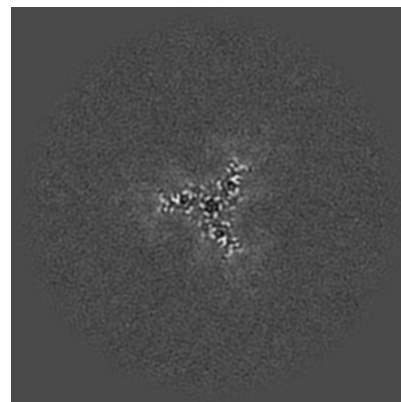
### 6.2.1 Primary map



X Index: 160

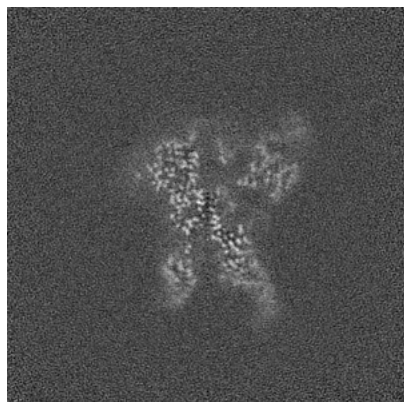


Y Index: 160

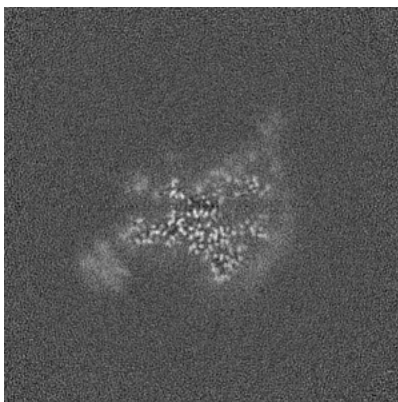


Z Index: 160

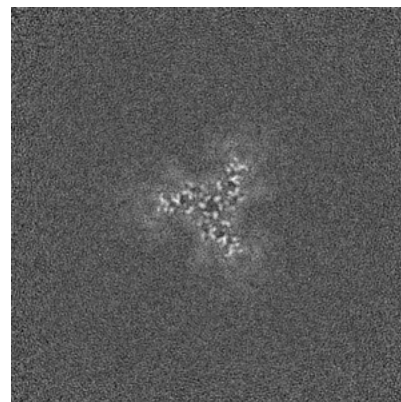
### 6.2.2 Raw map



X Index: 160



Y Index: 160

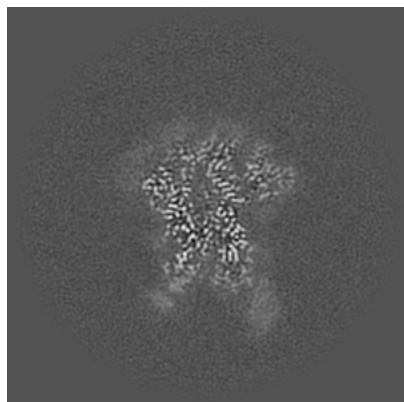


Z Index: 160

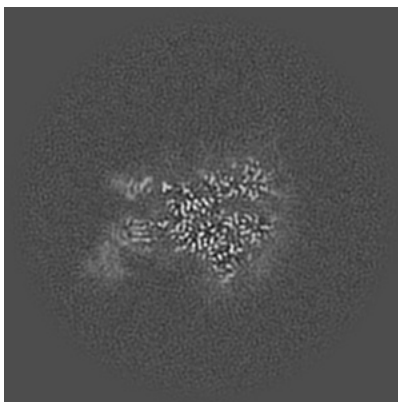
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

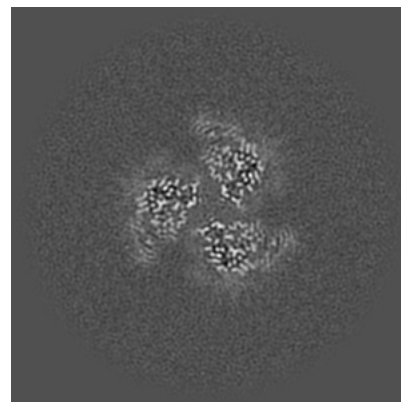
### 6.3.1 Primary map



X Index: 170

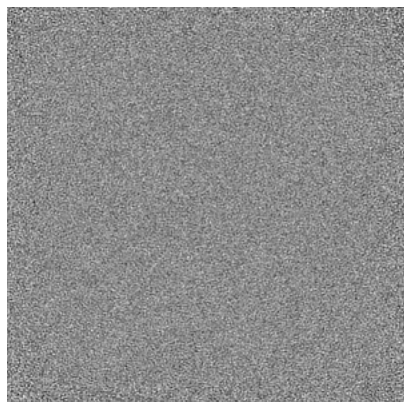


Y Index: 166

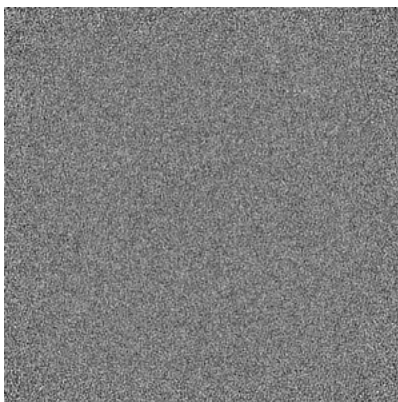


Z Index: 178

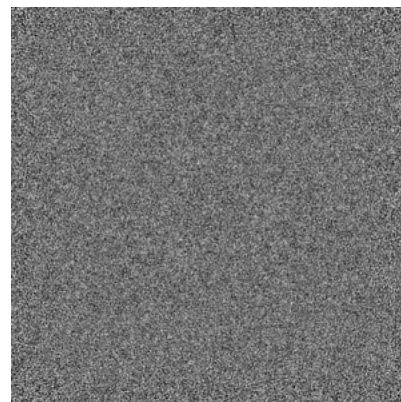
### 6.3.2 Raw map



X Index: 0



Y Index: 0



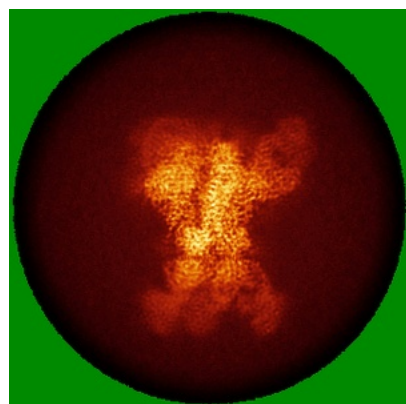
Z Index: 0

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

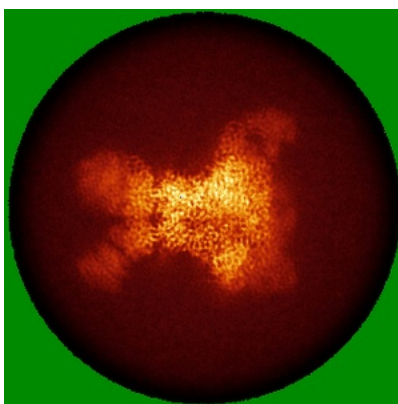


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

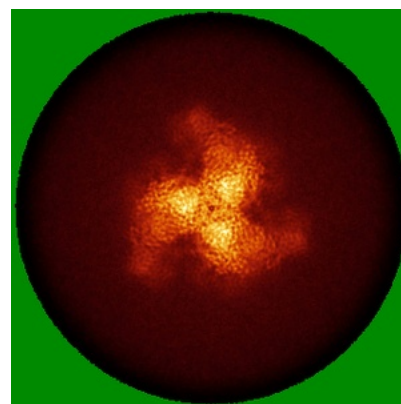
### 6.4.1 Primary map



X

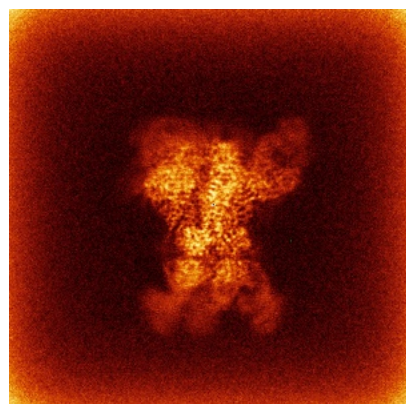


Y

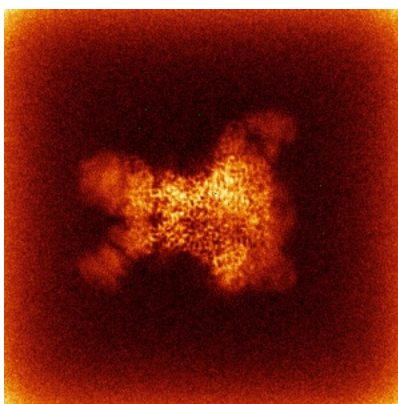


Z

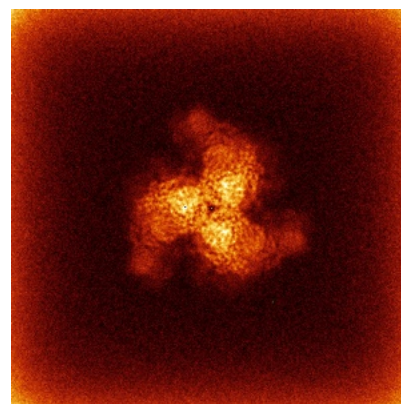
### 6.4.2 Raw map



X



Y



Z

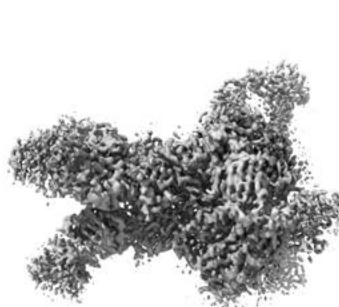
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

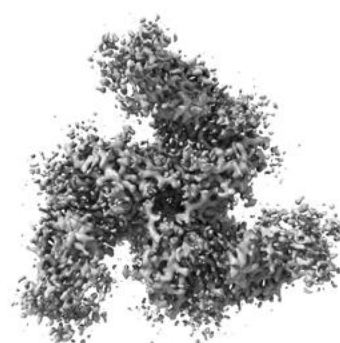
### 6.5.1 Primary map



X



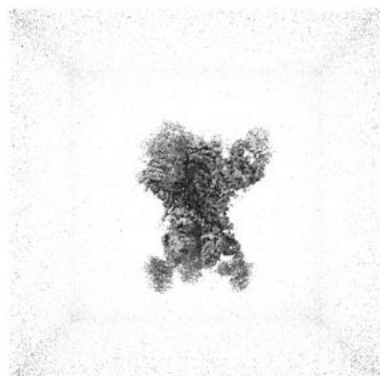
Y



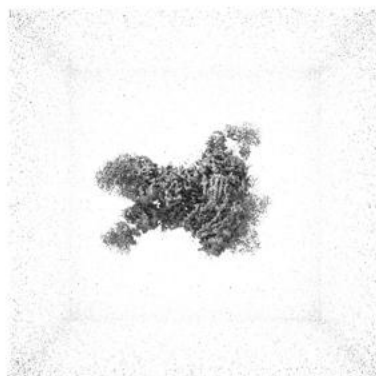
Z

The images above show the 3D surface view of the map at the recommended contour level 0.46. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

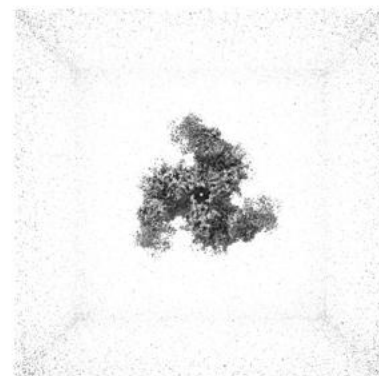
### 6.5.2 Raw map



X



Y



Z

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.

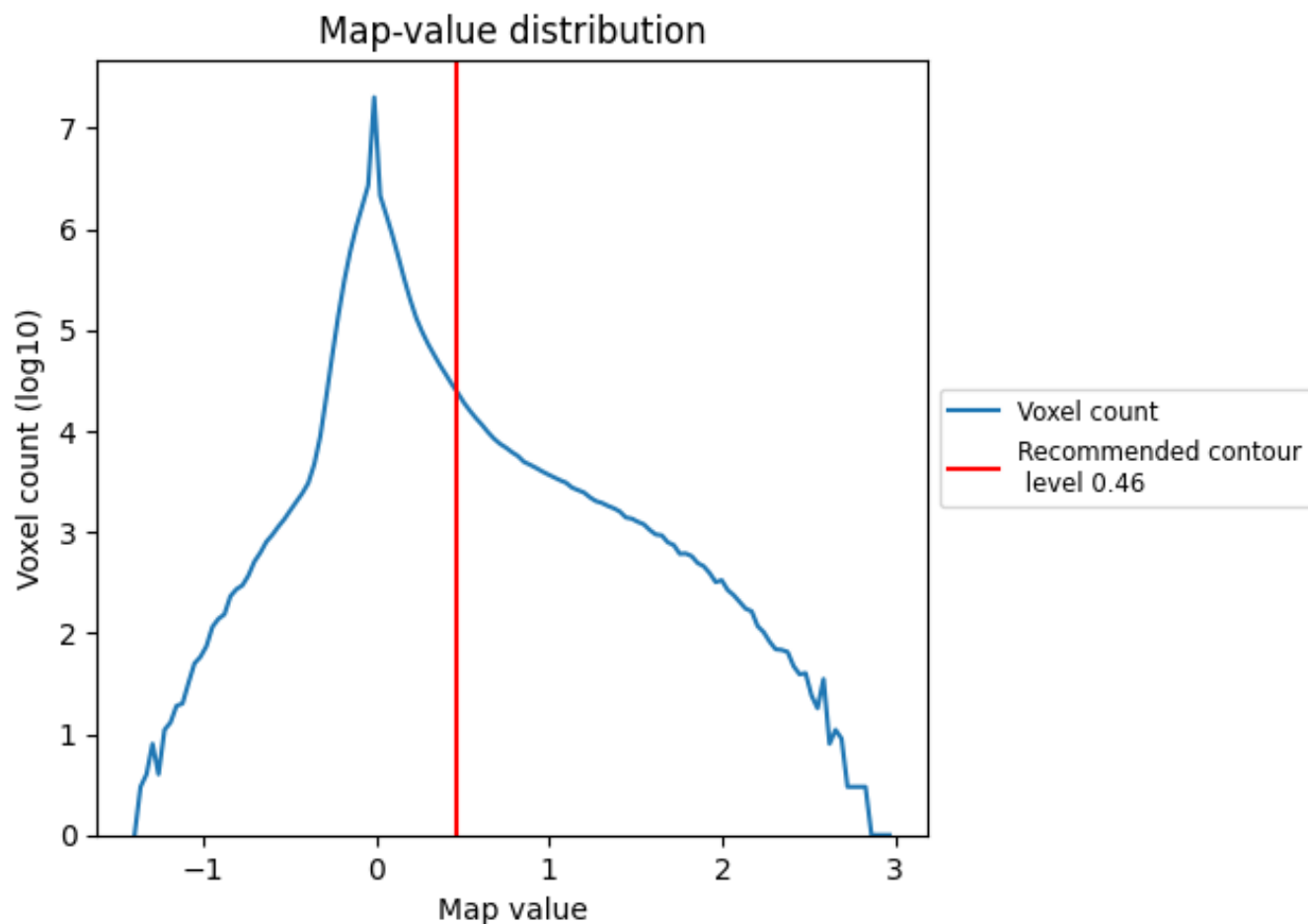
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

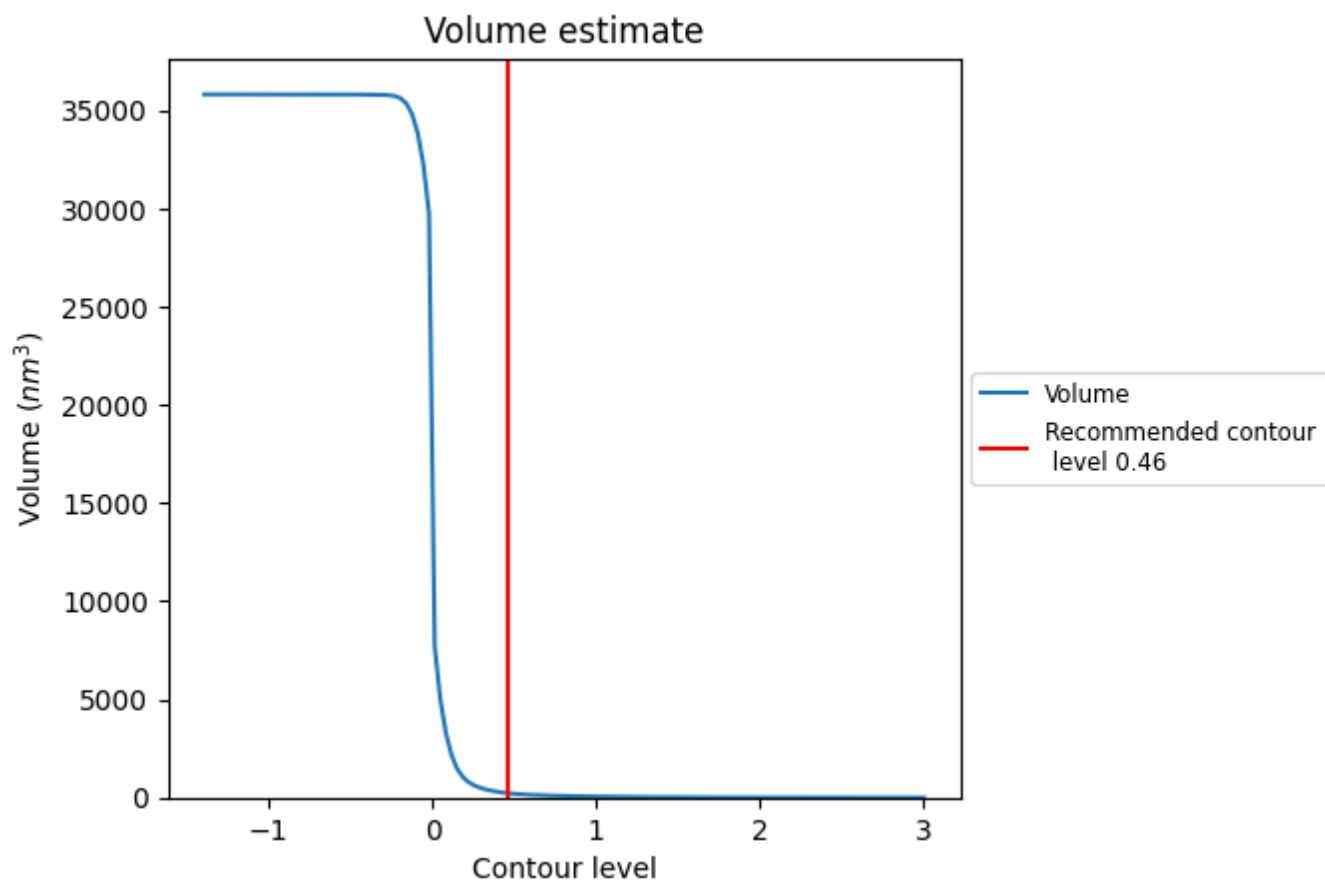
This section contains the results of statistical analysis of the map.

### 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.

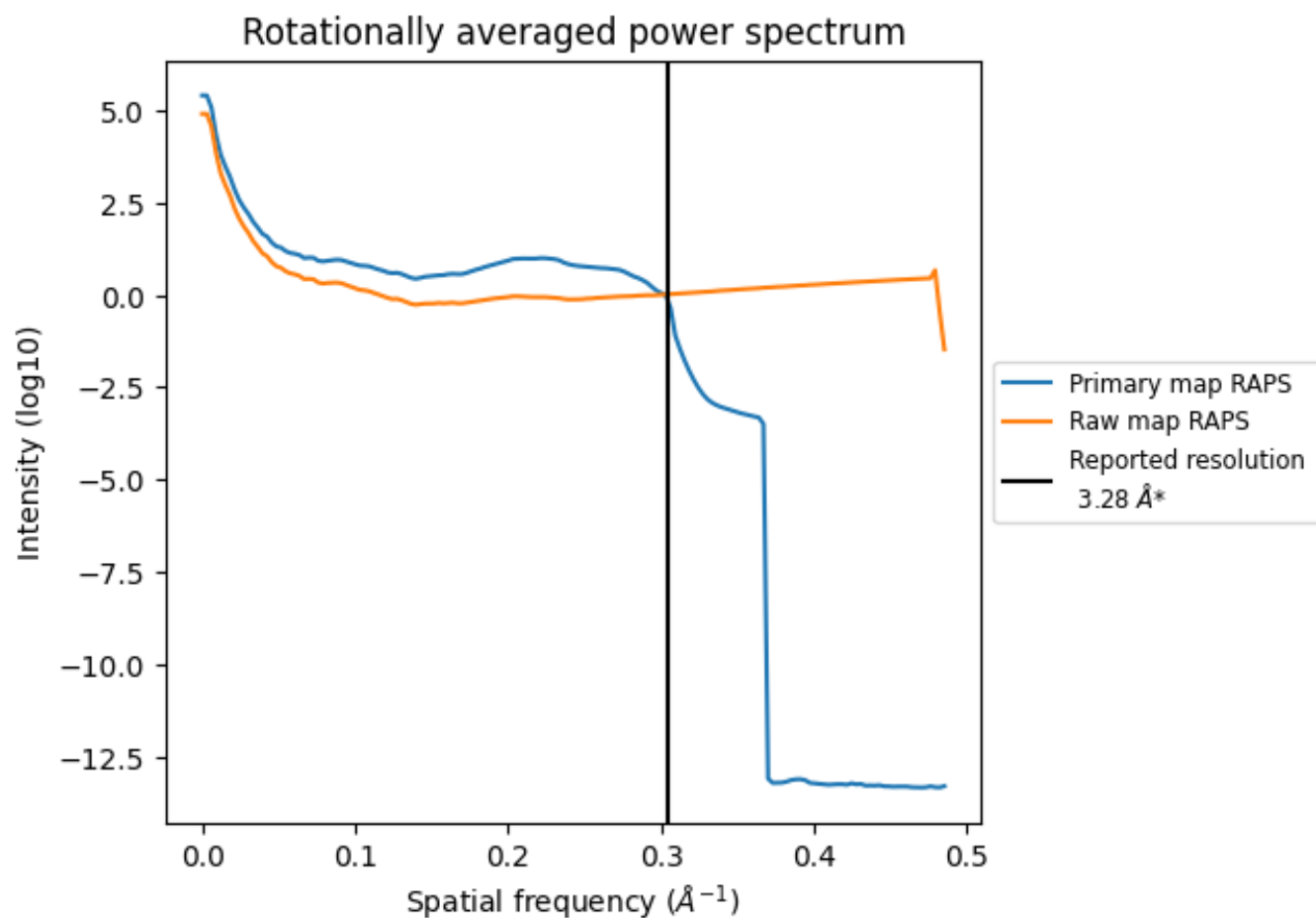
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 224 nm<sup>3</sup>; this corresponds to an approximate mass of 202 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 ⓘ



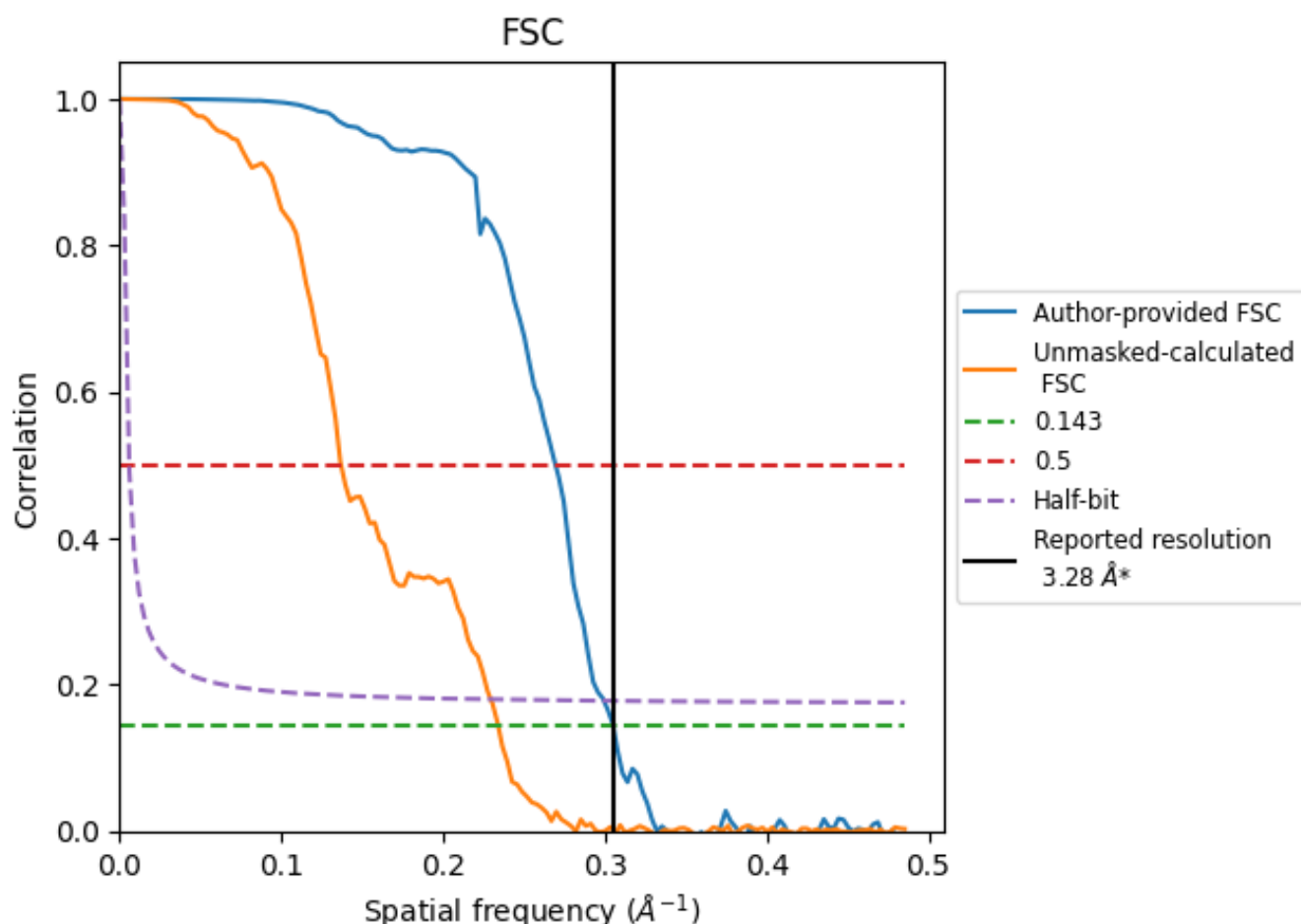
\*Reported resolution corresponds to spatial frequency of 0.305 Å<sup>-1</sup>



## 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 0.305  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

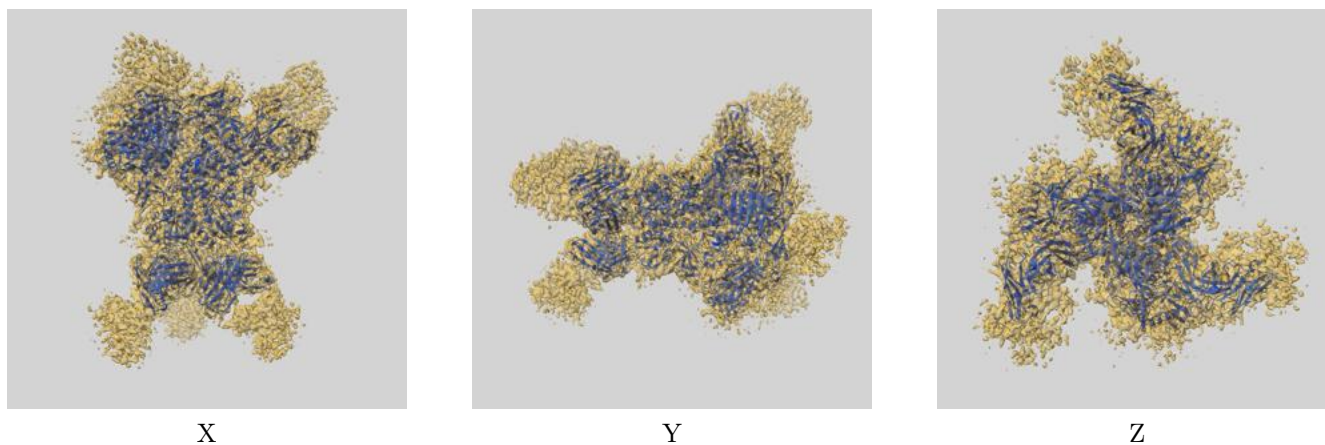
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.28	-	-
Author-provided FSC curve	3.28	3.71	3.34
Unmasked-calculated*	4.27	7.30	4.36

\*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 4.27 differs from the reported value 3.28 by more than 10 %

## 9 Map-model fit [i](#)

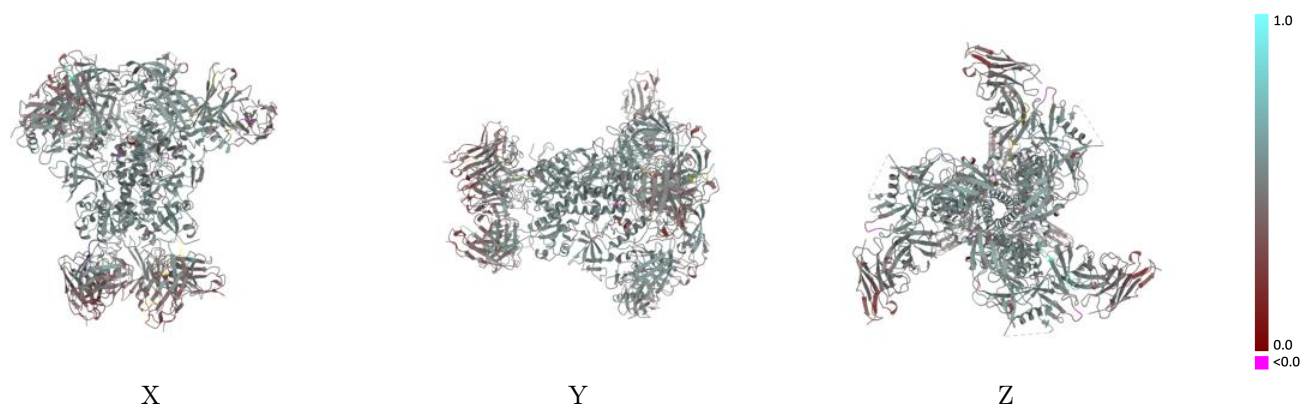
This section contains information regarding the fit between EMDB map EMD-23312 and PDB model 7LG6. Per-residue inclusion information can be found in section [3](#) on page [13](#).

### 9.1 Map-model overlay [i](#)



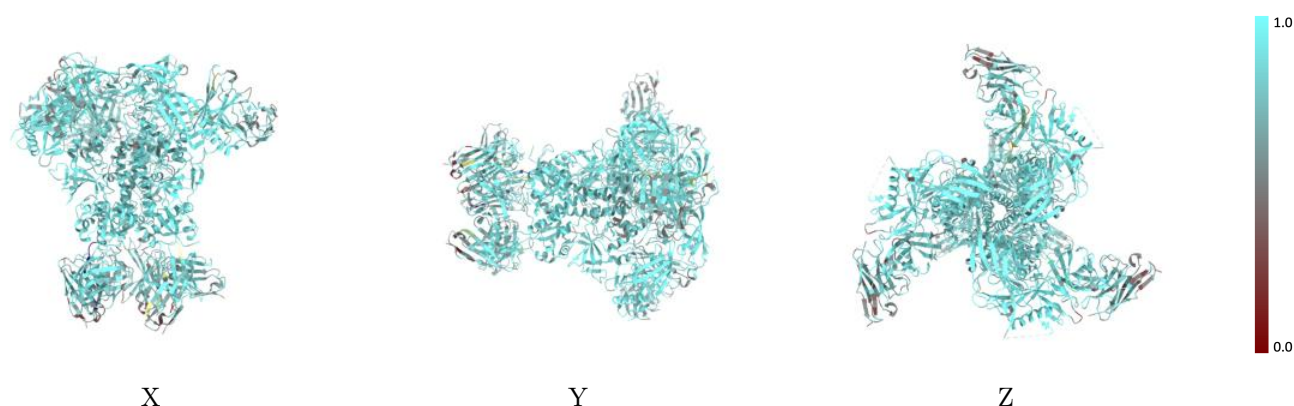
The images above show the 3D surface view of the map at the recommended contour level 0.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



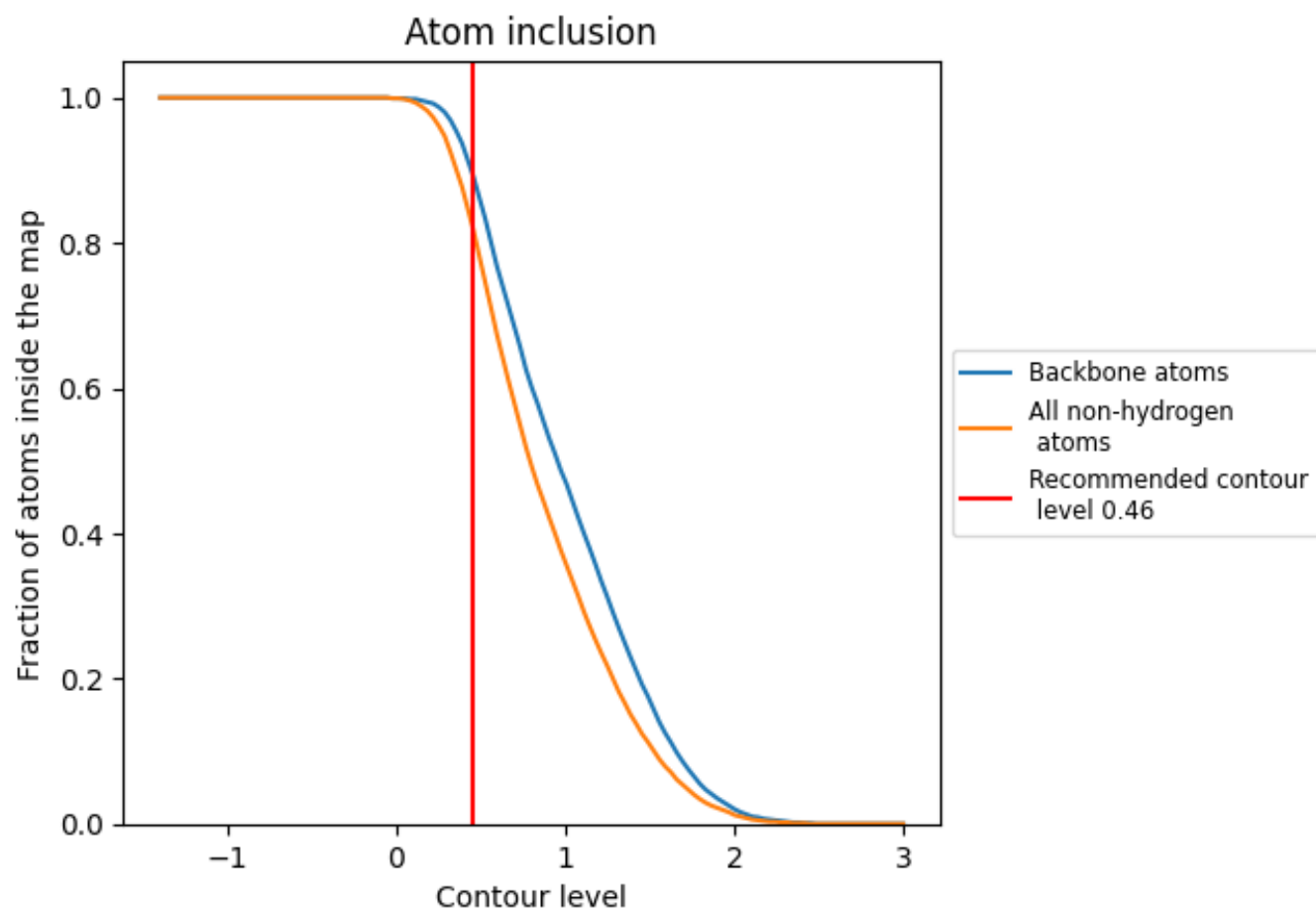
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.46).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% 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 (0.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8160	 0.4840
0	 0.6790	 0.4580
1	 0.7140	 0.3860
2	 0.7500	 0.4130
3	 0.4640	 0.3800
4	 0.6790	 0.3770
5	 0.5710	 0.3440
6	 0.7500	 0.4580
7	 0.4580	 0.4010
A	 0.8670	 0.5160
B	 0.8710	 0.5310
C	 0.7470	 0.4250
D	 0.7920	 0.4280
E	 0.8690	 0.5150
F	 0.8680	 0.5160
G	 0.8710	 0.5290
H	 0.8290	 0.4970
I	 0.8710	 0.5310
J	 0.7470	 0.4230
K	 0.7440	 0.4230
L	 0.7080	 0.4270
M	 0.7890	 0.4280
N	 0.7850	 0.4310
O	 0.8320	 0.4960
P	 0.8350	 0.4970
Q	 0.7040	 0.4290
R	 0.7070	 0.4300
S	 0.7860	 0.4410
T	 0.5380	 0.3540
U	 0.4640	 0.3990
V	 0.5360	 0.3510
W	 0.7220	 0.4460
X	 0.6810	 0.4630
Y	 0.6070	 0.4460
Z	 0.7140	 0.3790



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Chain	Atom inclusion	Q-score
a	 0.7500	 0.4170
b	 0.4640	 0.3810
c	 0.6790	 0.3790
d	 0.5710	 0.3430
e	 0.7500	 0.4740
f	 0.4580	 0.4040
g	 0.7500	 0.4420
h	 0.5380	 0.3510
i	 0.4640	 0.3970
j	 0.5360	 0.3370
k	 0.7500	 0.4450
l	 0.7020	 0.4670
m	 0.6070	 0.4460
n	 0.7140	 0.3760
o	 0.7500	 0.4040
p	 0.4640	 0.3920
q	 0.6790	 0.3620
r	 0.5710	 0.3600
s	 0.7860	 0.4680
t	 0.5420	 0.4050
u	 0.7500	 0.4240
v	 0.4870	 0.3710
w	 0.4640	 0.3910
x	 0.5360	 0.3400
y	 0.7220	 0.4480
z	 0.7020	 0.4660